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3.3.2 Number of research papers per teachers in the Journals notified on UGC website during the Academc Year 2017-18

SN	Title of paper	Name of the author/s	Department of the teacher	Name of journal	Year of publication	ISSN number	Link to the recognition in UGC enlistment of the Journal
160	Hand Written Character Recognition System Using Neural Ntework	B.D.Bundele	Electronics	International Advanced Research Jouranal in Sci ,Engg. & Techno	2017-18	23938021	Not listed in present UGC approved list as well as in deleted approved UGC List
161	Use of ANFIS based filter for Reduction of Noise From Biomedical signal	R.J.Gajbe	Electronics	International journal of on recent and innovation Trends in Computing and Communication	2017-18	23218169	Not listed in present UGC approved list as well as in deleted approved UGC List
162	Constructive Dialogue: Dramatic form of Ernest Hemingway's Short Stories	Dr.R.M.Patil	English	Vidya Warta International Multilingual Refereed Research Journal	2017-18	23199318	Not listed in present UGC approved list as well as in deleted approved UGC List
163	Electronic Media, English Language and It's Devaluation	Dr.R.M.Patil	English	LangLit An International Peer-Reviewed Open Access Journal	2017-18	23495189	Not listed in present UGC approved list as well as in deleted approved UGC List
164	Walking for complete health, fitness and wellness	Dr. D. S. Wankhade	Physical Education and Sports	Future Prospective of Physical Education, Sports Science and Yogic Practices	2017-18	23501081	Not listed in present UGC approved list as well as in deleted approved UGC List
165	Role of Nutrition in Sports performance	Dr. D. S. Wankhade	Physical Education and Sports	Education, Physical Education, and Sports Science	2017-18	23501081	Not listed in present UGC approved list as well as in deleted approved UGC List
166	Study the optical properties of solid polymer electrolyte based on polyvinyl alcohol	S. R. Jadhao, R. V. Joat, P. S. Bodkhe	Physics	International Journal of Sciences & Applied Research,	2017-18	2394384X	Not listed in present UGC approved list as well as in deleted approved UGC List
167	Study of DC Conductivity of Polypyrrole doped with SnO2 Nanocomposites	RM Agrawal, TS Wasnik, KB Raulkar, GT Lamdhade	Physics	International Journal of Scientific Research in Science, Engineering and Technology, IJSRSET	2017-18	23944099	Not listed in present UGC approved list as well as in deleted approved UGC List
168	Women Participation in Local Self Government Organizations-A Sociological Study and Perspectives	Dr. Arunsingh D. Chauhan	Sociology	EPRA International Journal of Economic and Business Review	2017-18	23479671	Not listed in present UGC approved list as well as in deleted approved UGC List
169	Sant Gadgebabanche Aarthik Vichar	Dr. D. S. Rangacharya	Economics	Vidyawarta	2017-18	23199318	Not listed in present UGC approved list as well as in deleted approved UGC List
170	Effects of Globalization on Indian Rural Society and Family	Dr. A. D. Chauhan	Sociology	Chronicle of Humanities and Cultural Studies	2017-18	24545503	Not listed in present UGC approved list as well as in deleted approved UGC List

171	Role of Multiculturalism, Professional Ethics and Human values in Current Scenario	Dr. A. D. Chauhan	Sociology	EPRA International Journal of Economic Growth and Environmental Issues	2017-18	23216247	Not listed in present UGC approved list as well as in deleted approved UGC List
172	A herpatofaunal Inventory of Vidarbha Region Maharashtra ,India.	P.S.Joshi V T Tantarpale AP Charjan	Zoology	Bioscience Discovery	2017-18	22293469	Not listed in present UGC approved list as well as in deleted approved UGC List
173	Synthesis and characterization of some new chlorosubstitured Δ2- pyrazoles under microwave irradiation	P.S.Nandurkar,M. M. Rathore, P. R. Rajput	Chemistry	International Journal Of Chemtech Research, 2017	2017-18	9744290	Not listed in present UGC approved list as well as in deleted approved UGC List
174	Microwave Assisted Synthesis Of Some New Chromone And Their Antibacterial Activity	Tejasvini BanteM. M. Rathore	Chemistry	International Journal Of Trend In Scientific Research And Development	2017-18	24566470	Not listed in present UGC approved list as well as in deleted approved UGC List
175	Synthesis charecterization of some bromio and nitro substituted 1-3thiazines	Dr M M Rathod	Chemistry	Aayushi International Interdisciplinary Research Journal (AIIRJ) Special Issue No. 25	2017-18	2349638x	Not listed in present UGC approved list as well as in deleted approved UGC List
176	Study of proton-ligand and metal-ligand stability constants of Cu (II) and Mn (II) complexes with chlorosubstituted pyrazoles and isozoles in 80% DMF-water solvent using pHmeter	P. S. Nandurkar, M. M. Rathore	Chemistry	International Journal of ChemTech Research,Vol.10 No.15, pp 204-212, 2017	2017-18	9744290	Not listed in present UGC approved list as well as in deleted approved UGC List
177	IMPROVED AND SKILLFUL SYNTHESIS OF (±) FENOPROFEN, AN IMPORTANT ANTI-INFLAMMATORY AGENT)	Hemant R.Suryawanshi,M.M.Rathore	Chemistry	INTERNATIONAL JOURNAL OF PURE AND APPLIED RESEARCH IN ENGINEERING AND TECHNOLOGY	2017-18	2319507X	Not listed in present UGC approved list as well as in deleted approved UGC List
178	Synthesis and characterization of some newly synthesized Nitro and Bromo substituted 3, 5-diaryl isoxazolines	Shreya M. Rathore, M.M. Rathore, V.V.Parhate	Chemistry	INTERNATIONAL JOURNAL OF RESEARCHES IN BIOSCIENCES, AGRICULTURE AND	2017-18	2347517X	Not listed in present UGC approved list as well as in deleted approved UGC List
179	Synthesis and biological activities of piperazine derivatives as antimicrobial and antifungal agents	Hemant R.Suryawanshi,M.M.Rathore	Chemistry	ACG publication	2017-18	13076175	Not listed in present UGC approved list as well as in deleted approved UGC List

180	Application a New PyMOL Plugin in Quantitative Structure-Toxicity Relationship Study of Pesticides	VESNA RASTIJA, DEJAN AGIĆ, KRISTIAN BRLAS,	Chemistry	WSEAS TRANSACTIONS on BIOLOGY and BIOMEDICINE, 14, 2017,	2017-18	22242902	Not listed in present UGC approved list as well as in deleted approved UGC List
181	PyDescriptor: A new PyMOL plugin for calculating thousands of easily understandable molecular descriptors	Vijay H. Masand, Vesna Rastija	Chemistry	Chemometrics and Intelligent Laboratory Systems, 169 (2017) 12-18	2017-18	1697439	Not listed in present UGC approved list as well as in deleted approved UGC List
182	Exploration of 3, 6-dihydroimidazo (4, 5-d) pyrrolo (2, 3-b) pyridin-2 (1H)-one derivatives as JAK inhibitors using various in silico techniques	Radhakrishnan S. Jisha, Lilly Aswathy, Vijay H. Masand, Jayant M. Gajbhiye, Indira G. Shibi	Chemistry	In Silico Pharmacology, 2017, 5: 9	2017-18	21939616	Not listed in present UGC approved list as well as in deleted approved UGC List
183	A STUDY OF IMPACT OF DEMONETIZATION ON INVESTMENT PRIORITIES OF INVESTORS"A CASE STUDY OF MBBS DOCTORS OF AMRAVATI CITY, MAHARASHTRA, INDIA	S A Bothra and S S Kavitkar	Management Studies	ISRJ	2017-18	22307850	Not listed in present UGC approved list as well as in deleted approved UGC List
184	An Analytical Study of Cloud Computing: IT Opportunity and Challenges	S A Kazi	Management Studies	IJCRT	2017-18	23202882	Not listed in present UGC approved list as well as in deleted approved UGC List
185	Study of Relation between Big Data & Cloud Computing: Big Data Challenges & Issues	R N Yeotikar	Management Studies	IJCRT	2017-18	23202882	Not listed in present UGC approved list as well as in deleted approved UGC List
186	Discrimination at working place	L.P.Khalid & P.V.Pulate	Botany	New Man Intternattiionall JJournall off Mulltiidiisciiplliinary	2017-18	23481390	Not listed in present UGC approved list as well as in deleted approved UGC List
187	E-Commerce in India: " Role of Online Payment"	Dr. S. B. Kadu	Commerce	"Vidyawarta" International Multilingual Research	2017-18	23199318	Not listed in present UGC approved list as well as in deleted approved UGC List
188	To Measure the Impact of Global Economic Recession on the Financial Performance of Selected Industries in Vidharbha	Dr. S. B. Kadu	Commerce	"Vidyawarta" International Multilingual Research Journal	2017-18	23199318	Not listed in present UGC approved list as well as in deleted approved UGC List
189	An Analytical Study of Government Schemes for Women Empowerment in Amravati District	P.G.Dammani & Dr. S. B. Kadu	Commerce	"Review of Research" International Online Multidisciplinary Journal	2017-18	2249894X	Not listed in present UGC approved list as well as in deleted approved UGC List
190	Gender Inequality in Education Page No.129-131	Dr. S.K.Rodde	Commerce	New man International Multidisciplinary Studies Research Journal	2017-18	23481390	Not listed in present UGC approved list as well as in deleted approved UGC List

191	Biodiversity in Business and Enterprises	Dr. S.K.Rodde	Commerce	"Vidyawarta" International Multilingual Research	2017-18	23199318	Not listed in present UGC approved list as well as in deleted approved UGC List
192	An Empirical Study on CLOUD COMPUTING	Prof. S. B. Bele	Computer Application	International Journal of Computer Science and Mobile Computing Computer Science and Mobile Computing(IJCSMC, Vol.	2017-18	2320088X	Not listed in present UGC approved list as well as in deleted approved UGC List
193	A Comprehensive Study on Cloud Computing	Prof. S. B. Bele	Computer Application	IJIRR,Vol. 05,Issue,03,pp.5310-5313,	2017-18	53105313	Not listed in present UGC approved list as well as in deleted approved UGC List
194	The Concept of Cloud Computing	Prof. S. B. Bele & Dr. V.R. Dhawale	Computer Application	Aayushi International Interdisciplinary Research Journal (AIIRJ) 2018"	2017-18	2349638X	Not listed in present UGC approved list as well as in deleted approved UGC List
195	FIDOOP Algorithm : Data Hierarchy and Parallel Mining of Frequent Itemsets Using MAP REDUCE	Prof. S. K. Totade & Prof. V. N. Mohod	Computer Application	ayushi International Interdisciplinary Research Journal (AIIRJ) Special Issue No. 25	2017-18	2349638X	Not listed in present UGC approved list as well as in deleted approved UGC List
196	How to Raise Kids who will Believe in Gender Equality	Dr. P.S. Yenkar	English	NEWMAN International Interdisciplinary Research Journal Vol.5,Special Issue 4, pg. 113-115,April 2018, ISSN 2348-1390 UGC Approved Journal (Journal	2017-18	23481390	Not listed in present UGC approved list as well as in deleted approved UGC List
197	Changing Language Teaching Methodologies: The Need of the Day	Dr. P.S. Yenkar	English	Vidyavarta International Multilingual Research Journal (VIMRJ) Vol.02 Special Issue(MAH/MUL03051/2012)Feb. 2018 pg. 91-93,	2017-18	23199318	Not listed in present UGC approved list as well as in deleted approved UGC List
198	Axially Symmetric Cosmological Models In Gravity With Time Varying Deceleration Parameter	P. P. Khade	Mathematics	International Journal of Research in Advent Technology	2017-18	23219637	Not listed in present UGC approved list as well as in deleted approved UGC List
199	Dark Matter and Holographic Dark Energy Models In Different Scenarios Of The Universe	P. P. Khade, A. P. Wasnik	Mathematics	International Journal of Science and Research	2017-18	23197064	Not listed in present UGC approved list as well as in deleted approved UGC List
200	Use of Information Technology in Physical Education & Sport	Dr. D. S. Wankhade	Physical Education and Sports	International Conference on Recent Trends in Science & Technology	2017-18	2349638X	Not listed in present UGC approved list as well as in deleted approved UGC List

201	The Role of Technology in the Agricultural Development of India	Dr. D. S. Rangacharya	Economics	Aayushi International Interdisciplinary Research Journal	2017-18	2349638X	Not listed in present UGC approved list as well as in deleted approved UGC List
202	Stiriyanno: Suryodaya Hoat Aahe	Dr. M. M. Kherde	History	NEWMAN International Journal of Interdisiplinary Studies	2017-18	23481390	Not listed in present UGC approved list as well as in deleted approved UGC List
203	Is Social Media Contagion to Emotional States of Collegians offering various study streams	Dr. S. D. Wakode	Psychology	Aayushi International Interdisciplinary Research Journal	2017-18	2349638X	Not listed in present UGC approved list as well as in deleted approved UGC List
204	Revealing Gender Isonomy with Respect to Capacity, Domestic Chores and Domestic Violence	Dr. S. D. Wakode	Psychology	NEWMAN International Journal of Interdisiplinary Studies	2017-18	23481390	Not listed in present UGC approved list as well as in deleted approved UGC List
205	Gender Equality and Women Empowerment of India in Current Scenario	Dr. A. D. Chauhan	Sociology	NEWMAN International Journal of Interdisiplinary Studies	2017-18	23481390	Not listed in present UGC approved list as well as in deleted approved UGC List
206	Basic Knowledge and Attitude Among College Students Towards Snakes in Amravati.(M.S.)	Amjad Hussin and V.T.Tantarpale	Zoology	Review Of Research	2017-18	2249894X	Not listed in present UGC approved list as well as in deleted approved UGC List
207	Anuran Inventory of Vidarbha Region ,Maharashtra	VT Tantarpale SD Puri SP Manekar SS Gijare	Zoology	Aayushi International Interdisciplinary Research Journal Special Issue no 25	2017-18	2349638X	Not listed in present UGC approved list as well as in deleted approved UGC List
208	Vidarbhatil sarwtrik loksabha niwadnuk 2014 yek drushtrishep	Nitin Khobragade	Zoology	Current global reviver	2017-18	23198648	Not listed in present UGC approved list as well as in deleted approved UGC List
209	Gender Inequality In Political System- A Global Problem	Nitin Khobragade	Zoology	New Man International Journal of Multidisciplinary Studies	2017-18	23481390	Not listed in present UGC approved list as well as in deleted approved UGC List
210	QSAR Analysis for Antioxidant Activity of Dipicolinic Acid Derivatives	Vesna Rastija, Maja Molnar, Tena Silađi, Vijay Hariram Masand	Chemistry	Combinatorial Chemistry & High Throughput Screening, 2018, 21, 204-	2017-18	13862073	Not listed in present UGC approved list as well as in deleted approved UGC List
211	AN ANALYTICAL STUDY OF GOVERNMENT SCHEMES FOR WOMEN EMPOWERMENT IN AMRAVATI DISTRICT	P. G. Dammani and Dr. S.B.Kadu	Management Studies	REVIEW OF RESEARCH	2017-18	2249894X	Not listed in present UGC approved list as well as in deleted approved UGC List
212	Digitalization of Ecotourism and Allied Services in Melghat Tiger Reserve of Vidarbha	S B Tripathi	Management Studies	IJETSR	2017-18	23943386	Not listed in present UGC approved list as well as in deleted approved UGC List

213	The Role and Strategy of Women Empowerment of Rural India in Current Scenario	Dr. Arunsingh D. Chauhan	Sociology	EPRA International Journal of Multidisciplinary research	2017-18	24553662	Not listed in present UGC approved list as well as in deleted approved UGC List

IARJSET

ISSN (Online) 2393-8021
ISSN (Print) 2394-1588

International Advanced Research Journal in Science, Engineering and Technology
ISO 3297:2007 Certified
Vol. 4, Issue 11, November 2017

Hand Written Character Recognition System Using Neural Network

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Abstract: In order to recognise the hand written character the system model is developed which is based upon neural network. MATLAB software including neural network toll box is used. The attributes and advantages which ultimately achieve the importance of design model with greatest ability. To interpret the meaning of complex or imprecise data available which is use to recognise the pattern and detect very easily which inherently difficult for human being and to any computer technique .In this technique the neural network is treated as expert which is use to analyse. Study is carried out using artificial neural network (ANN) which is an information processing model that is motivated by biological nervous system works such as human brain processes information. The comparative study to recognise the character is done using multilayer perceptron neural network (MLP), support vector machine (SPM), radial basis function (RBF) After studying it is found that percentage accuracy obtain in support vector machine is 90-100% and main square error (MSE) is least the, percent accuracy obtain in multilayer perceptron neural network is near about 80-90% and MSE is less so SVMNN is the best classifier so far as hand written character recognition system is concerned. MLPNN is slightly inferior in performance as compared to the SVMNN.

Keywords: Neural network: SVM, MLP, RBF, MATLAB, JPG images of 20 person's hand written character

I. INTRODUCTION

In modern world a great deal of activities and researches are going on to solve the complex problems. Among several problems the role of "hand written character recognition system" is significantly important. Neural network works like human brain which is information processing model symmetrical with the nervous system of human being in which neuron is the key element which works by integrating to solve complex problem. In order to recognise and to identify the character with clarity and transparently with full confidence with alphabet a-z or A-Z and numerals 0-9 several neural network like SVM , MLP, RBF, are used in most of the organisation , public sector , LIC, banking , crime investigation , this is the need of modern era

II. OBJECTIVE

To study the architecture of neural network: feed forward network, transfer function, hidden layer ,To study back propagation algorithm for SVMNM , MLPNN , RBFNN use of MATLAB as a software tools for design and analysis , statistics , signal processing and communication , image processing , testing and measurement , financial modelling and analysis to study basic idea of pattern recognition using neural network ,comparative study among SVMNN ,MLPNN,RBFNN then testing tinning and feature extraction ,preparation of JPG image of 20 persons image character ,data collection : name of 20 person and their information

III. METHODOLOGY

1. Preparation of 20 people's hand written characters ," India"
2. Each person will write character, "India" five times in a box (rectangle) provided of specified dimensions
3. Total(100) hand written character ," India " will be scanned and the image file will be stored in JPG format
4. 100 samples of ,"India" characters will be available for 20 different person of varying age and gender there after important features will be extracted from this characters and using this feature neural network will be trained following neural network are used for training and testing SVMNN ,MLPNN, and RBFNN
5. Performance of SVM based classifier on cross validation
6. Performance of SVM based classifier on test on testing
7. Performance of SVM based classifier on test on training
8. Step 5,6,7 are repeated for MLPNN,RBFNN
9. Comparative study is done among these three NN
10. Collection of randomised data and normalised data for this three NN
11. Graphical analysis for sensitivity of these three NN

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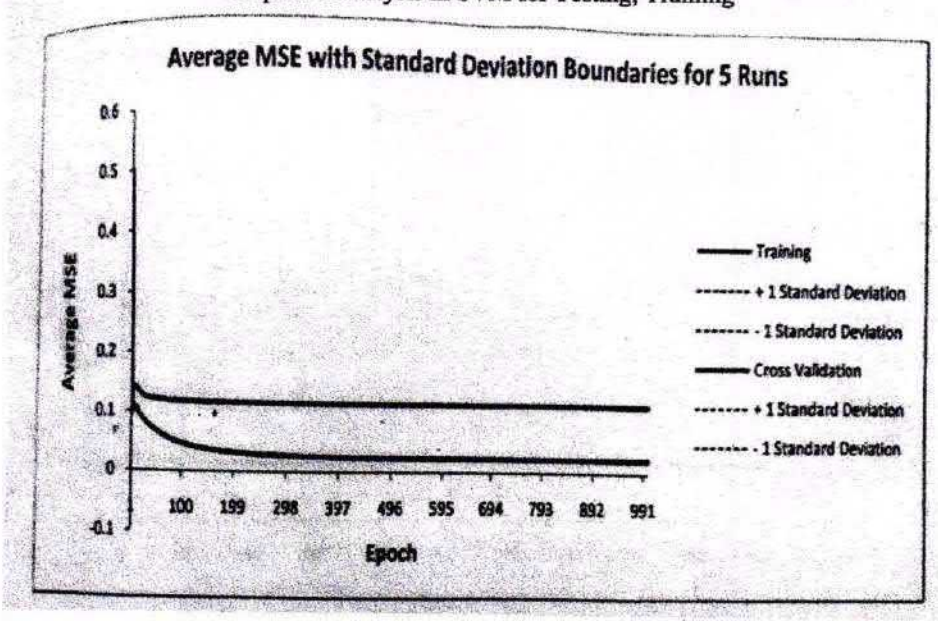
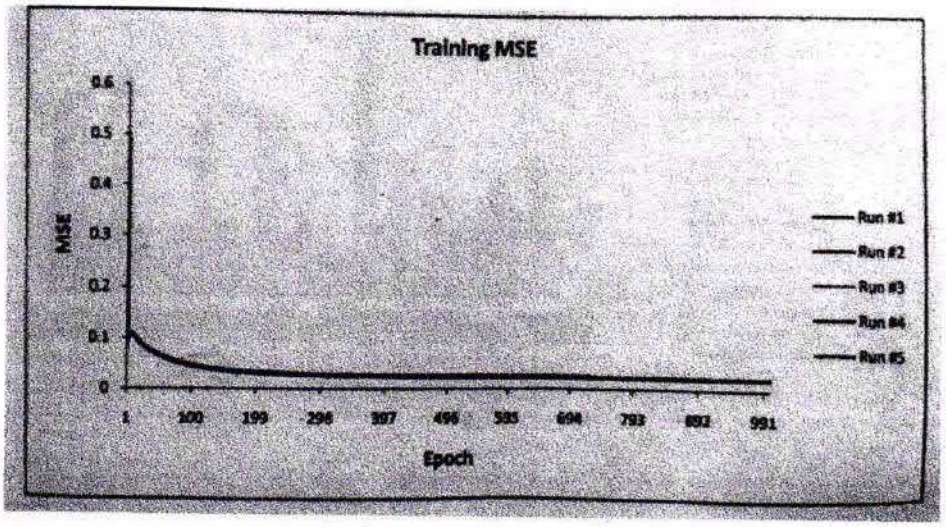
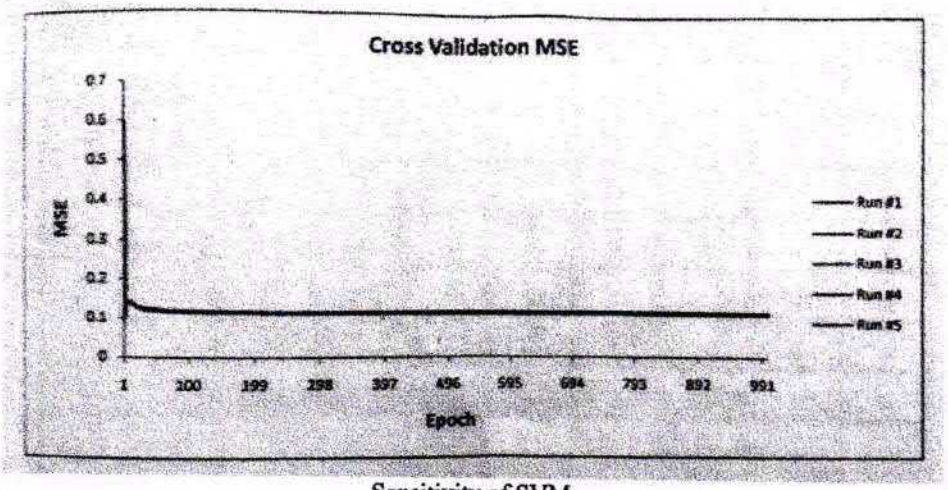
DOI 10.17148/IARJSET.2017.41113

IARJSET
ISSN (Online) 2393-8021
ISSN (Print) 2394-1588
International Advanced Research Journal in Science, Engineering and Technology
ISO 3297:2007 Certified
Vol. 4, Issue 11, November 2017

Graphical Analysis in SVM for Testing, Training







Sensitivity of SVM

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DOI 10.17148/IARJSET.2017.41113

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ISSN (Online) 2393-8021
ISSN (Print) 2394-1588

International Advanced Research Journal in Science, Engineering and Technology
ISO 3297:2007 Certified
Vol. 4, Issue 11, November 2017

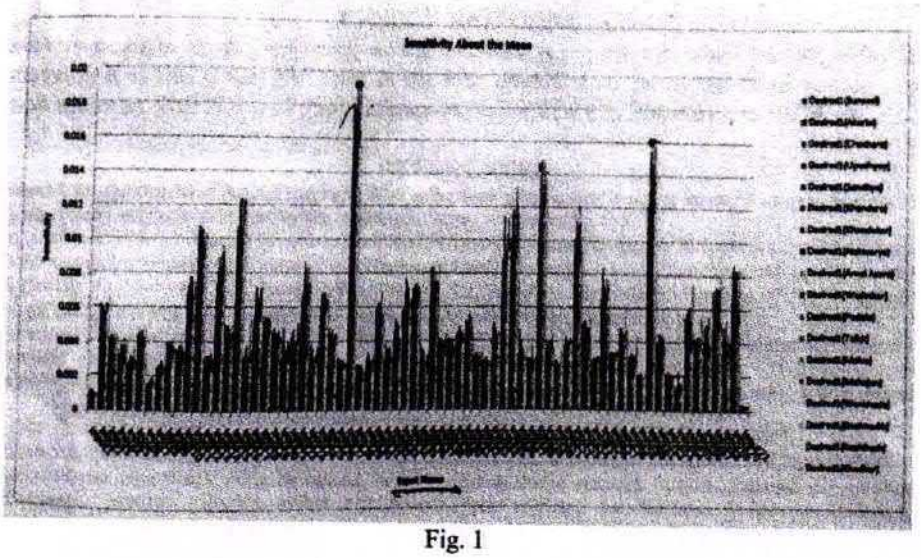

Fig. 1

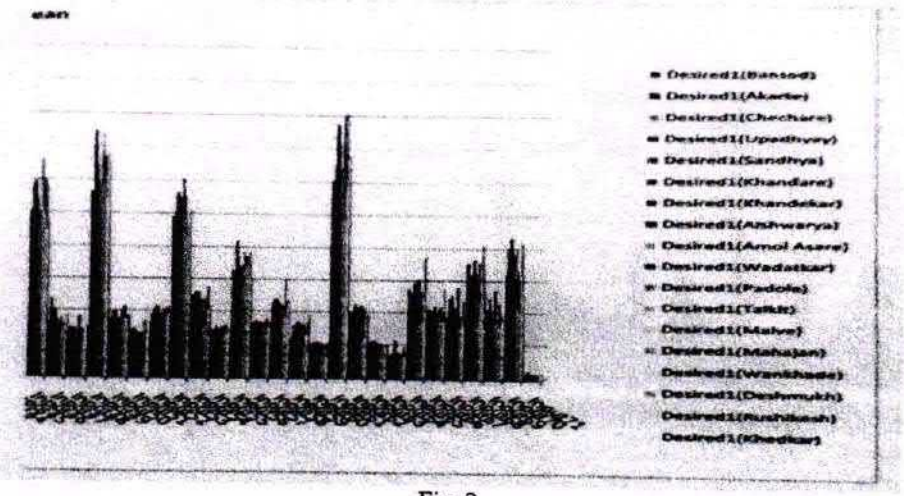

Fig. 2

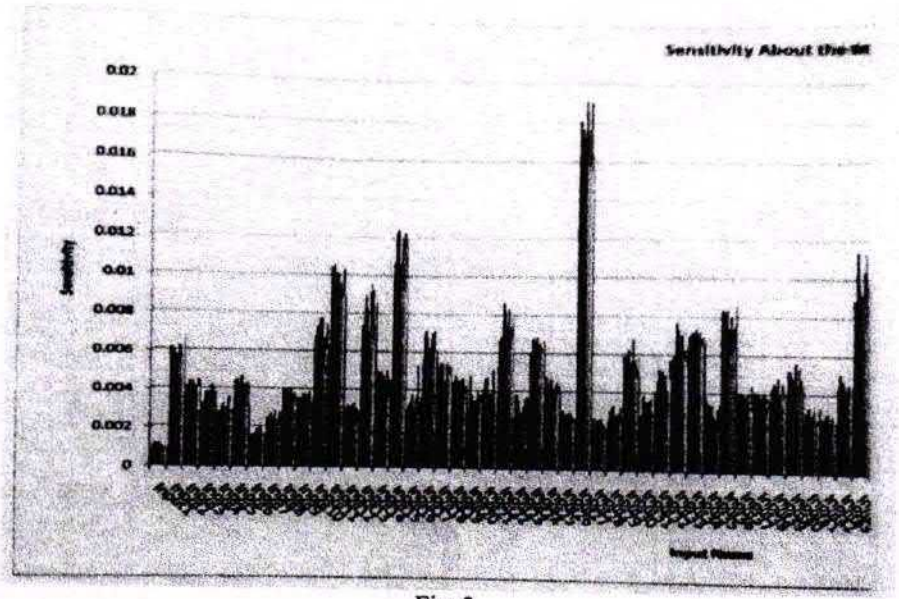

Fig. 3

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ISSN (Online) 2393-8021
ISSN (Print) 2394-1588

International Advanced Research Journal in Science, Engineering and Technology
ISO 3297:2007 Certified
Vol. 4, Issue 11, November 2017

IV. RESULT AND CONCLUSION

Hand written character recognition system using neural network is rigorously studied using SVMNN, MLPNN, and RVFNN. After studying it is found that SVMNN is the best classifier so far as the hand written character recognise system is concerned where as MLPNN is slightly inferior in performance as compared to SVMNN

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[10] visual character recognition artificial neural networks shashcmk araokar* MGM's college of engineering and technology , university of Mumbai, india (shashank.araoksr@iee.org)
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[12] stroke based handwritten Chinese character recognition using neural networks hong-yuan liao jun-shon huang shih-ta huang
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ISSN (Print) 2394-1588

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INTERNATIONAL ADVANCED RESEARCH JOURNAL IN SCIENCE, ENGINEERING AND TECHNOLOGY

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CERTIFICATE OF PUBLICATION

MR. B.D.BUNDELE

Associate professor, Dept. Of Electronic Vidya Bharti Mahavidyalaya Camp Amravati (Maharashtra) India

Published a research paper entitled

Hand Written Character Recognition System Using Neural Network

in IARJSET, Volume 4, Issue 11, November 2017

DOI 10.17148/IARJSET.2017.41113

Certificate Number:10.17148-1/1-A
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INTERNATIONAL JOURNAL
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In recognition of the publication of the paper entitled

Use of ANFIS based Filters For Reduction of Noise From Biomedical Signals

Published in IJRITCC Journal, Volume 5, Issue 9, September 2017

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Use of ANFIS based filters For Reduction of Noise From Biomedical Signals

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Abstract— Biomedical signals are the collection of electrical signals acquired from any organ of human body. These signals acquire noise while traveling through different tissues or blood vessels. Similarly, these signals are affected by electrical noise and some other factors. Electrical noise included inherent noise in Electronic equipments, ambient noise, motion artifacts, power line interference, base line drift, electrosurgical noise and inherent instability of signal. By using conventional methods, it is very difficult to reduce noise from biomedical signal. Therefore different methodologies are used to remove noise and artifacts. This paper describes the adaptive filters and adaptive network based fuzzy inference system (ANFIS) filters which are used to reduce noise from biomedical signals.

Keywords- Adaptive filter, AI, ANFIS, LMS, SLMS, SSLMS, NLMS, NSLMS

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I. INTRODUCTION

Biomedical signal means a collective electrical signal acquired from any organ that represents a physical variable of interest. This signal is normally a function of time and is described in terms of its amplitude, frequency, and phase. The analysis of these signals is very important for researchers and medical practitioners because careful medical diagnosis is very essential for proper treatment. If the signals are not properly diagnosed and analyzed, it will lead to wrong diagnosis and can be dangerous for the lives.

The biomedical signals are noisy as well as artifacts due to electrical noise included inherent noise in Electronic equipments, ambient noise, motion artifacts, power line interference, base line drift, electrosurgical noise and inherent instability of signal. This reduces the performance of desired signal. Therefore for the proper treatment of a patient, it should be removed from the desired signal. Using an amplifier with high gain, high input impedance and differential input with good common mode rejection, various filter circuits could reduce the noise from biomedical signals. But using conventional method, it is difficult to reduce maximum noise from biomedical signal. Therefore there is a need of intelligent solution for this.

In fact, various mathematical techniques and Artificial Intelligence approaches are being used for noise reduction. Literature reviews show that in nonlinear system identification, a mathematical model includes Wavelet Transform, Time Frequency Approaches, Fourier Transforms, Wegner-Villie Distribution, Statistical Measures and Higher Order Statistics. AI includes artificial neural network, dynamic recurrent neural network, Fuzzy logic system and genetic algorithm. Accuracy of biomedical signal also depends on the properties of electrodes and their interaction with skin, amplifier design, the conversion and subsequent storage of the biomedical signal from analog to digital form.

In the recent years, biomedical applications using signal processing techniques are a major area of interest. The lot of bio-engineers and researchers from medical field are keenly interested for design of techniques to obtain noiseless biomedical signals. R. Sehamby and Buta Singh (2016) [14] have designed the adaptive electrocardiogram filter to reduce noise caused by external systems & body artifacts. R. J. George (2015) [12] reveals in his study that the pipelined DLMS adaptive FIR filter is faster than non-pipelined LMS adaptive FIR filter. S. Silarbi, B. Abderrahmane and A. Benyettou (2014) [17] have proposed adaptive network fuzzy inference system for phonemes recognition. H. K. Gupta, R. Vijay and N. Gupta (2013) [5] have observed that the accuracy has been increased by increasing filter order as well as with increased in step size, convergence rate took place fast. B. Chandrakar, O. P. Yadav and V. K. Chandra (2013) [10] have studied Finite Impulse Response (FIR) filter based on various windows and Infinite Impulse Response (IIR) filters for noise removal of ECG signal. The researcher D. C. Dhubkarya and A. Katara [13] have studied the comparison of MATLAB Simulation and DSP Processor implementation of an adaptive filter on Least Mean Squared (LMS) and Normalized Least Mean Squared (NLMS) Algorithms. They suggested NLMS algorithm is superior in hardware implementation.

Jyh-Shing Roger Jang (1993) [18] suggested that the role of neural networks in signal processing have similar applications in Adaptive network based fuzzy inference system (ANFIS). The nonlinear and structured knowledge representation of ANFIS are the primary advantages over classical linear approaches in adaptive filtering and adaptive signal processing such as identification, inverse modeling, predictive coding, adaptive channel equalization, adaptive inference (noise or echo)cancelling, etc.

II. SOFTWARE SPECIFICATION REQUIREMENT AND IMPLEMENTATION DETAILS

In real life situations, the accuracy of the measurement is required. As we know that biomedical signals are error prone due to complicated situations. ANFIS can be used to obtain reasonably good accuracy and intelligently reduce the noise. In this section, we have simulated the

MATLAB codes for the data conversion, adaptive filter algorithm, artificial intelligent [ANFIS] training and its testing.

Database collection:

To design ANFIS Model, a sufficiently large amount of data is required for training and testing. We have collected standard data bases for biomedical signal from the following websites.

https://physionet.org

http://www.emglab.net

https://drive.google.com/file/d/0B3NaVR72FYQcaHAybXVCZ0ViVVk/view.

We have used 500 samples for the training and testing of Adaptive filters and ANFIS based filters.

Software specification:

MATLAB (Matrix Laboratory), 2014b is used for simulation. It is a numerical computing environment and fourth-generation programming language developed by Math-Works. MATLAB allows matrix manipulations, plotting of functions and data, implementation of algorithms, creation of user interfaces, and interfacing with programs written in other languages, including C, C++, Java, and FORTRAN.

Implementation details:

The GUI is constructed by using Matlab codes. Other set of codes have been used to run the various algorithms for noise removal in Matlab simulator.

The main GUI contains four parts-

1] File input and its conversion

2] Adaptive filter algorithm and its Input parameter section

3] Output parameters section

4] Artificial intelligent noise removal section.

File input and its conversion:

Most of the data bases are available in .dat or .xls format. To read this in Matlab, we have designed a code which will convert and save the .dat file or .xls file in .mat file format.

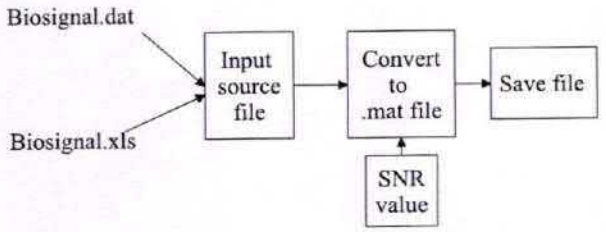

Figure 1: Block diagram of conversion of .dat and .xls files into .m files.

Adaptive filter section and its Input parameter section:

There are numerous Adaptive filter algorithms [22], out of which 5 algorithms were used.

These are

1] Adaptive Least Mean Square (LMS) Algorithm:

If $w(n)$ is the filter coefficient vector at step n (time), then its' updated value $w(n+1)$ is given by

$$w(n+1) = w(n) + 2\mu\, e(n)\, x(n)$$

Where, Filter output $y(n) = w^T(n)\, x(n)$

Error $e(n) = d(n) - x(n)$

Filter taps at time n, $w(n) = [w_0(n)\ w_1(n) \ldots\ldots\ldots\ w_{M-1}(n)]$ and

Input data, $x(n) = [x(n)\ x(n-1)\ \ldots\ldots\ldots\ x(n-(M+1))]^T$

2] Adaptive Normalized LMS Algorithm:

The updated value $w(n+1)$ is given by

$$w(n+1) = w(n) + \frac{1}{x^T(n)\, x(n)}\, e(n)\, x(n)$$

with

$$\mu(n) = \frac{1}{2\, x^T(n)\, x(n)}$$

3] Adaptive Sign LMS Algorithm:

The updated value $w(n+1)$ is given by

$$w(n+1) = w(n) + 2\mu\, e(n)\, Sign(x(n))$$

4] Adaptive Sign Sign LMS Algorithm:

The updated value $w(n+1)$ is given by

$$w(n+1) = w(n) + 2\mu\, Sign(e(n))\, Sign(x(n))$$

5] Adaptive Normalized Sign LMS Algorithm:

The updated value $w(n+1)$ is given by

$$w(n+1) = w(n) + 2\mu\, \frac{Sign(e(n)\, x(n))}{\|x(n)\|^2}$$

Output parameter section:

The performance of ANFIS is assessed on the basis of performance parameters Signal to Noise Ratio (SNR_out). The output SNR (SNR_out), is calculated from the power of input signal x (n) and noise signal e (n) and is given by,

$$SNR_out = 10\ Log_{10}\left[\frac{\text{Signal Power}}{\text{Noise Power}}\right]$$

Or $SNR_out = P_{signal}/P_{noise}$.

Where the power is expressed in decibel.

Artificial intelligent noise removal algorithm:

We have designed an artificial intelligent model for removal of noise from biomedical signal by using Matlab coding. The fig. 2 shows the block diagram of proposed artificial intelligent model of adaptive network based fuzzy inference system (ANFIS).

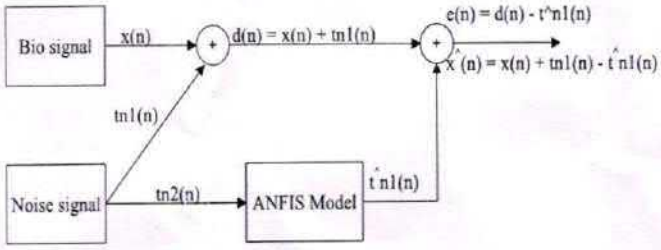

Figure 2: Block diagram of proposed ANFIS Model

ANFIS based Noise Removal Algorithm:

Proposed model have designed on the basis of Sugeno architecture. The basics of Sugeno inference architecture is discussed below.

Sugeno inference architecture [18]:

In TSK or Sugeno architecture, defuzzification block of Mamdani architecture is replaced by a normalization and weighted average. The TSK architecture does not require MAX operators, but a weighted average is applied directly to regions selected by MIN operators. The TSK system is really simple because of the output weights are directly proportional

to the average function values at the selected regions by MIN operators.

Sugeno and Takagi used the following architecture which is graphically represented in Fig. 3.

R1: if x is $A1$ and y is $B1$ then $z1 = p1x + q1y + r1$

R2: if x is $A2$ and y is $B2$ then $z2 = p2x + q2y + r1$

Fact: x is $x0$ and y is $y0$

Consequence: z

The firing levels of the rules are computed by

$w1 = A1(x0) \wedge B1(y0)$, $w2 = A2(x0) \wedge B2(y0)$

Then the crisp control action is expressed as

$$Z_0 = \frac{w_1 z_1 + w_2 z_2}{w_1 + w_2}$$

If we have n rules in our rule-base then the crisp control action is computed as

$$Z_0 = \frac{\sum_{i=1}^{n} w_i z_i}{\sum_{i=1}^{n} w_i}$$

Where wi denotes the firing level of the ith rule, $i = 1, \ldots, n$

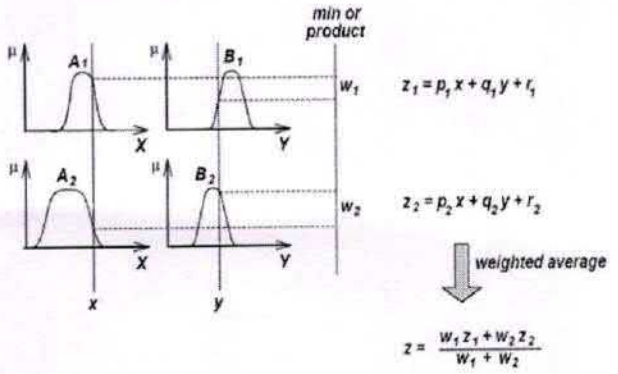

Figure 3 (a): Sugeno Fuzzy Model

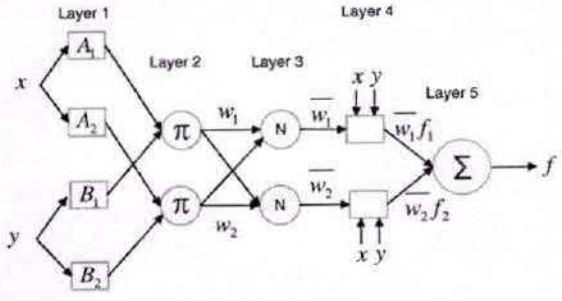

Figure 3 (b): Equivalent ANFIS architecture

For the design of model, we have selected,

Membership Functions per Input = 12

Epoch numbers = 30

No. of taps= 02

However, an epoch corresponds to the entire training set going through the entire network once. It can be useful to limit the over fitting.

In addition to this, generalized Bell Type Membership Function (MF) has been used in the network.

A generalized bell MF is specified by three parameters (a, b, c):

$$f(x; a, b, c) = \frac{1}{1 + \left| \frac{x - c}{a} \right|^{2b}},$$

where the parameter b is usually positive. If b is negative, the shape of this MF becomes an upside-down bell. However, each of these parameters has a physical meaning: c determines the centre of the corresponding membership function; a is the half width; and b (together with a) controls the slopes at the crossover points. Note that this MF is a direct generalization of the Cauchy distribution used in probability theory, so it is also referred to as the Cauchy MF. Because of their smoothness and concise notation, Gaussian and bell MFs are becoming increasingly popular for specifying fuzzy sets [58].

III. SIMULATION RESULTS

The major objective of this study was to investigate a noise removal filters. For this, simulations are carried out on ECG and EMG signals. The results are obtained on output parameter section of Matlab based GUI for removal of noise from biomedical signal. The Table 1 shows the signal to noise ratio of adaptive Filter using algorithms LMS, NLMS, NSLMS, SLMS and SSLMS for various step sizes on ECG signal 1.

Table 1: SNR_out Vs Step size for adaptive filter using various algorithms

No. of taps= 2 and SNR_in= 0

Step Size	SNR_out				
	LMS	NLMS	NSLMS	SLMS	SSLMS
1e-7	-0.19906	26.7339	26.7339	7.97304	26.7338
1e-8	0.21109	26.7339	26.7339	24.324	26.7339
1e-9	1.23573	26.7339	26.7339	26.7018	26.7339
1e-10	10.2783	26.7339	26.7339	26.7336	26.7339
1e-11	24.5255	26.7339	26.7339	26.7339	26.7339
1e-12	26.7039	26.7339	26.7339	26.7339	26.7339
1e-13	26.7336	26.7339	26.7339	26.7339	26.7339
1e-14	26.7339	26.7339	26.7339	26.7339	26.7339
1e-15	26.7339	26.7339	26.7339	26.7339	26.7339

Table 1 shows that Normalized LMS and Normalized Sign LMS algorithm performed better at a small step size also. But overall, all algorithms have good performance on step size 1e-10, which governs the rate of convergence, speed of tracking ability.

However, use of small step size is to ensure a small steady state error. But a small step size decreases the convergence speed of the adaptive filter. However, increase in step size is to improve the convergence speed of the adaptive filter. But a large step size might cause the adaptive filter to become unstable. So we have to select optimum value of step size [57].

For this study, the ANFIS based filters are examined on various biomedical signals (ECG and EMG). The SNR_out of ANFIS based filters are compared with the adaptive filters for the selected parameters; No. of Taps= 02, SNR_in= 0 and Step size= 1e-10. ANFIS based filters have tested on various ECG and EMG signals. For this, we used Generalized Bell Membership Function. The Table 2 shows the comparison of SNR_out of Adaptive and ANFIS based filters.

Table 2: Comparison of SNR_out of Adaptive and ANFIS based filters.

Algorithm	ANFIS based Filter SNR_out			Adaptive Filter SNR_out
	ECG 1	ECG 2	EMG	
LMS	19.5649	35.0811	22.6133	10.2783
NLMS	26.7339	35.1005	35.3044	26.7339
NSLMS	26.7339	35.1005	35.3044	26.7339
SLMS	26.7339	35.1005	35.3044	26.7336
SSLMS	26.7339	35.1005	35.3044	26.7339

From Table 2, it is inferred that SNR_out for all selected algorithms show excellent signal to noise ratio. Thus all algorithms are excellently filtered out the noise signal from the biomedical signal.

IV. DISCUSSION

The amplitude biomedical signals are obtained in mV or in μV ranges. Thus the signals are easily affected by various noise sources result in degrading the signal. Even in the modern world of biomedical instrumentation, all possible filtering arrangements are carried out by the other researchers. But still due to randomness of noise signal, original signal get affected and this process is dynamic. So such problem demands the dynamic solution as well.

Therefore for the dynamic solution, we choose Artificial Intelligent based filtering algorithms. This has only two processes- training and testing. Training process based on subset outcomes of adaptive filtering algorithm in initial stages, which may not require in later time even on change of source input as well, called trained filter / smart filter. Such intelligent filters give the freedom of selection of signal with different SNR values; also not bother about number of parameter settings which lead one more step towards the auto filter concept.

For the simulation, we have used different ECG and EMG signals. The simulation results are carried out by measuring the performance parameters SNR_out and these results are summarized in tabular form in the Tables 1 and 2. The comparison of these two filters reveals that the ANFIS based algorithms give better results than the adaptive filter algorithms.

V. CONCLUSION

The main goal of the current study was to design artificial intelligent filters to reduce noise from the biomedical signals. The implementation of the biomedical signals on various adaptive algorithms (LMS, NLMS, NSLMS, SLMS and SSLMS) is successfully performed. The result of this study indicates that the AI (ANFIS) algorithms give better results than the adaptive filter algorithms. The AI algorithms are excellent systems to filter out the noise signal from the biomedical signal. The proposed algorithm plays an important role in noise reduction from any biomedical signals.

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MAH/MUL/03051/201
ISSN-2319 931

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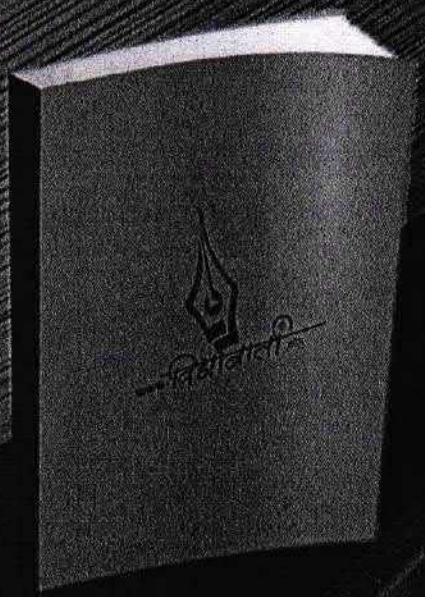

Editor
Dr.Bapu G.Gholap

MAH/MUL/ 03051/2012 ISSN :2319 9318

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विद्यावार्ता

UGC Approved Jr.No.62759

Oct. To Dec. 2017
Issue-20, Vol-16

Editor
Dr. Bapu g. Gholap
(M.A.Mar.& Pol.Sci.,B.Ed.Ph.D.NET.)

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❖ विद्यावार्ता या आंतरविद्याशाखीय बहूभाषिक त्रैमासिकात व्यक्त झालेल्या मतांशी मालक, प्रकाशक, मुद्रक, संपादक सहमत असतीलच असे नाही. न्यायक्षेत्र:बीड

"Printed by: **Harshwardhan Publication Pvt.Ltd.** Published by **Ghodke Archana Rajendra** & Printed & published at Harshwardhan Publication Pvt.Ltd.,At.Post. Limbaganesh Dist,Beed -431122 (Maharashtra) and Editor **Dr. Gholap Bapu Ganpat.**

Reg.No.U74120 MH2013 PTC 251205

Harshwardhan Publication Pvt.Ltd.
At.Post.Limbaganesh,Tq.Dist.Beed
Pin-431126 (Maharashtra) Cell:07588057695,09850203295
harshwardhanpubli@gmail.com, vidyawarta@gmail.com

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Constructive Dialogue: Dramatic form of Ernest Hemingway's Short Stories

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Camp, Amravati.

Ernest Hemingway, the twentieth centu American writer is widely acknowledged for h experiments in English prose. In fact some of th aspects of prose style were so revolutionary that attracted instant negative criticism. It took almo three decades for the critics to assess the value o his experiments in prose style, when he was awarde the NobelPrize in the 1950s. Apart from the ver popular "terse, compact and 'stripped to the bone' aspect of his style, Hemingway's real experiment have remained confined more or less to th knowledge of Hemingway critics and hardcor Hemingway fans and enthusiasts. Omission an concision, repetition and juxtaposition, blending o expressionism and impressionism, differen focalization techniques and constructive dialogue are some of the stylistic aspects that are central to Hemingway's prose-fiction. Most of these stylistic aspects were employed by Hemingway's predecessors like Chekhov, Strandhel, Maupassant, Crane, Kipling, Joyce and others in their own way. Hemingway's contribution was that he made these aspects unique by introducing variations, alterations and changes to suit his beliefs, themes and purpose. It is this aspect of originality that made Hemingway stand tall among the prose stylists of all times.

The paper proposes to demonstrate Hemingway's uniqueness as a prose-stylist, while keeping in mind the prime objective of making the common reader familiar with the writer's not-so-accessible strengths.

Hemingway, in many ways, was a product his age. The typical character of his age—riddled h conflicts, wars, regime change and punctured h socio-political and economical changes—forms basis of the backdrop of the banal and dark ture of his themes. Hemingway himself was a y conscientious reader and liked to keep track whatever remarkable he read. He was a great mirer of the master storytellers, across the guages, already mentioned above. From a very ng age Hemingway started picking the elements effe e storytelling. Though admirer of the sters, he followed them in a limited way: copying ne but picking up something from everybody ore making it his own. Hemingway's description he aftermath of the war in the stories reminds us the ultra-naturalism of Stephen Crane. But he fers from Crane's naturalism by introducing zanne's technique of painting landscapes, layer layer. This technique of using "overlapping planes d underlying geometric shapes" enables mingway to portray the natural landscape by ping in mind the narrator's perspective. (67 illard) Similarly his use of repetitions can be ibuted to the writings of Gertrude Stein. However mingway's repetitions in his best stories are so tle that one is hardly aware of them and still cannot ain u fected by their cumulative impact. Unlike t of Stein the repetitions in Hemingway make their int without overshadowing the prime thematic ncern. Use of dialogue in Hemingway's case is haps his most original contribution to the elopment of English fiction. Till 1920s, it was erally believed that in a short story dialogue can y have illustrative purpose.The constructive ction of dialogue was believed to have meant only dramatic works. This belief was cemented more ause the likes of Henry James already advocated concept of "illustrative function" of the dialoguein stories. Hemingway, for the first time nonstrated that dialogue can have perfectly ural constructive function even in the non-matic writings like short stories.

Short story as an art form differs from drama in many ways. The most significant point of departure though may be that drama is a performing form and that the story is not. However Hemingway's concept of art challenged this very traditional notion that put limitations on the story as an art form. Hemingway believed that every story plays out in the mind of the reader and its success depends on how well he reads between the lines and under the surface of the iceberg! It is due to this belief that Hemingway relied on the dialogue heavily in some of his best stories. In these stories the dialogue is manipulated in such a manner that it altogether removes the narrator's role as an illustrator. The stories like "Hills like White Elephants," "Light of the World," "The Killers," and othershave dialogue constructing the tale with multiple dimensions of meaning without any intrusion of narrative voice. Secondly by means of his constructive dialogue, Hemingway provided voice to those who had been till then kept silent and mute by the other writers. Hemingway while describing the characters from the troubled world, and those considered as social untouchables, successfully captured the difficulties of their world in their own dialect.

Hemingway used dialogue aiming at achieving the things which were thought by others as impossible in short fiction: characterization, emphasizing the theme and taking the story forward. The following analysis here shows that uniquely written dialogue can achieve all these objectives without any help from separatecommentary from the prose-writer.

The specialty of Hemingway's constructive dialogue is that even the crudeness of everyday common conversation has been taken to the level of an exclusive art. In his most famous story for its constructive dialogue, "Hills Like White Elephants," a few sentences of everyday conversation between a man and a woman lays bare the nature of their relationship. The man and the girl, sitting at the outside Café table on the railway station, speak in the manner any engaged couple would do:

'What should we drink?' the girl asked. She had taken off her hat and put it on the table.

'It's pretty hot,' the man said.

'Let's drink beer.' (The Collected Stories 199)

In this casual dialogue both play their role perfectly, waiting for the other to make the decision of ordering the drink first, in spite of their desire to force the individual will. The girl although asks the man to choose the drink does so only after she has taken off her hat and put that on the table. It is her hint for the man to acknowledge that the weather around them is hot. The man on the other hand even after being thus hinted, repeats her action in the words and says "it's hot." It is only after the man has acknowledged her preference; she makes the choice hinted by the man. In reality it is the man who has taken the actual decision. Here the man appears to be the one who wants everything to be controlled by him without being held responsible for anything. On the other hand the girl even though is capable of reading the man correctly, finally submits her will and keeps on playing along with the man on his terms. The dialogue having 28 words spread over one question, one factual piece of information and two statements actually provides a "nutshell-summary" of the whole story. How much more constructive can dialogue become! The story has other well illustrated achievements in dialogue like the use of "repetition and juxtaposition," "objective correlative," and "gender-based miscommunication ." Lamb, in his perceptively done analysis, shows how the use of common pronoun, "it" for ten times in a particular section of verbal exchange between the couple, has been made to refer five different subjects. The fact (which Lamb doesn't mention) that out of nine on six occasions "it" refers to the "abortion" and remaining three times to the "baby," brings out the preference given to the "termination" rather than the "growth" of their relationship. Apart from the objective correlatives of "the labeled bags," and the "landscape," there is one more, which has largely gone unnoticed, appearing as the girl's response to the man when he opens up the topic of abortion:

(1)"It's really an awfully simple operation, Jig,' the man said. 'It's not really an operation at all.'

(2)The girl looked at the ground the table legs rested on.

(3) 'I know you wouldn't mind it, Jig. It's really not anything. It's just to let the air in.'

(4)The girl did not say anything.

(5) 'I'll go with you and I'll stay with you all the time. They just let the air in and then it's all perfectly natural.'

(6) 'Then what will we do afterward?' (Italics mine; The Collected Stories200)

Here the girl looking at the ground on the background to the legs of the table firmly standing on it shows the deep shock she receives as soon as the man hints at the abortion. It is as if she herself goes under the physical procedure of abortion at that instant. The procedure is initiated by the man's words in Line 1. Asshe hears the words the "awfully simple operation" she receives very strong emotional shock so that emotionally she needs something substantial to hold on. It is for this reason that she looks at the table-legs standing on the ground. Here we could see the girl's legs shaking violently. Her emotional response has been captured powerfully only in the singular image. In fact the girl does not say "anything" till she recovers from, "an awfully simple operation." Her response in the Line 6 underlines the fact that, she has now recovered from the "the mental procedure of abortion." Now she can think about the future course— "afterward." Secondly the repetitive use of the word "anything" in Line 3 and Line 4 in place of the usual "nothing" also shows that it means "something" for the girl and the man knows that. It is his autonomous response made to come out as the result of his sudden awareness of the girl's injured state of mind. Further in the story the process of healing of the girl's injury occurs in the unique manner. The man after realizing the girl's shock, tries to justify his thoughts over and over again. The girl is so much irritated by the fake sympathy he is trying to show, that she warns him: "'I"ll Scream.' the girl said" (202)The man gets the message and stops finally his attempts of justifying his decision of abortion. The girl changes the course of conversation by involving the third person—the waitress. It clears the way for her. She smiles at the waitress brightly thanking her. This shows the girl's

acknowledgement of the existence of the world beyond her own problems. She has made peace with the painful decision thrust upon her by the man. We get the hint of her reconciliation when she responds to the man, "All right. Then come back and we'll finish the beer." (202)

The story, "Hills Like White Elephants," successfully fully presents before us the powerful drama of complex human emotions and troubled human souls. With the help of strategically placed words the writer creates all the tension without any ...ward help of extra commentary or any other stagecraft. The story with its uniquely written dialogue plays out on the stage of the minds of the readers. What better way a prose-stylist can prove the dramatic function of the dialogue in a prose story!

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Vidyawarta™ International Multilingual Research Journal

ISSN 2349-5189
Vol. 4 Issue 1 August - 2017

ज्ञान-विज्ञान विमुक्तये
UGC
University Grants Commission
Sr. No. 49124
UGC Approved Journal - Arts & Humanities

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ELECTRONIC MEDIA, ENGLISH LANGUAGE AND IT'S DEVALUATION

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ABSTRACT

Ernest Hemingway the rebel writer had remarked in 1930s that the war had used up the words making them as useless as the used tyres of a motor car. He was referring to the typical vocabulary used excessively to express the abstract notions of bravery, patriotism and honour etc. The excess occurred due to the politics of wars and conflicts in Europe and America in those days. In the contemporary world multiple wars are being waged on many fronts in the name of religion, ethnicity, and identities underlined by other socio-cultural markers. These wars unlike in the olden ages are fought on many fronts—in the newsrooms and the studios of electronic media and on social networking sites. The biggest casualty of these wars is the language used in the increasingly binary narratives. The narrative these days are painted only in vivid blacks or whites. Nobody, no longer seems to have either taste or patience for the subtle shades of grey in the socio-political discussions. In fact these narratives have gained so much of currency these days that the hyperbolic statements shouted in the shrill voice have become the new normal in the electronic media. The nuanced arguments and balanced views with pragmatic approach have given way to simplistic notions clothed in the language of hyperboles and excessive modifiers. So in short the words have been reduced only to the form of sounds without any ideas attached to them. Day by day the words have been losing their values and association of ideas, to become empty and dry rhetoric made in the high pitched voice.The paper here makes a survey of the arguments made on the popular news-channels and TV programs to point out the devaluation of the language. It also attempts to measure the effectiveness of the statements made thereby pointing out the devaluation of the language employed by the speakers.

Language: Tool of miscommunication

The human language is an ingenious way of communicating the thoughts, ideas emotions and feelings. The efficacy of the language and the worth of the speaker are often determined by the kind of values and ideas delivered during a discourse. The understanding of the discourse largely depends on the clarity and simplicity of the diction. Certain words, over the years, due to their judicious use by influential speakers, have gained the status of sublime and noble ideas and symbols. The words like, "Nation," Freedom," "Patriotism," "Sacrifice," are some

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ISSN 2349-5189

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of those words having universal recognition of the great ideas and concepts they represent. As we know, these words themselves do not have any meaning independent of the users. So the value of these words depends on how they are received and reacted to by the users. Sadly these days most of these words, in the eyes of the common users have lost their original values. So when a celebrated news-editor of a popular channel says, "Nation wants to know" people, instead of becoming serious sneer at their TV screens. The phrase often delivered in high-pitched voice and self-righteous tone, is not received the way the speaker intends it to be. When probed into the recent past, Arnab Goswami, the editor in question himself has admitted in his interview[i] that now he is weary of using the famous phrase. The anchor has realized that his famous line has been misinterpreted by the people as comical one while he meant it to be serious one. This is one example of miscommunication that occurs due to random and mindless use of the words. The high profile TV journalist is famous (or infamous?) for his "quarrel-like" panel-discussions. The guests or the co-panelists are often shouted down by the anchor in the rudest manner. Most of the times, the anchor speaks more than his guests. All the time he poses as some authority seated on the high-moral pedestal. His words, though spoken in the highest pitch, often carry nothing more than his empty bravado and fake morality. When he says that, he speaks on the behalf of the whole nation, there is hardly anybody even sitting among the audience who believes him. This disconnect is so great that the serious phrase, "Nation wants to know," just becomes an empty meaningless rhetoric evoking sneers and jibes. The fact that mindless repetition of the words, without putting into them clean commitment and clear unbiased logic, strip the language of their ideas and values. In the first place the values and ideas to the words are given by the users and so in absence of conviction of the speaker they are taken back by them. And the whole exercise otherwise intended to be meaningful becomes a caricature only to be laughed at.

This reminded me another satellite news channel airs the show, ostentatiously titled as "India First," is full of jingoism and hyperbolic rhetoric aimed at the galleries. Every time there is a death of some soldier or some skirmish on the border, clothed in machismo style, the presenter speaks in a thundering voice telling us about the "India First" story where his channel stands first! This rhetoric of "Nation wants to know" or "India First" is found on the arrogant assumption that they are the only representatives of the country and its billion plus people. The show-presenter Gaurav Sawant presentsed the latest news with the intention of putting "the country above all." The whole nation with its vast geographical boundaries along with different cultures, religions and linguistic identities, is reduced to one news item in the program "India First." For that moment, nothing else in the country, with billion lives, is more important than that news item selected by that news-anchor! It is no wonder that the message is miscommunicated. The people don't feel and think that the formidable looking man with his sleeves rolled aggressively is putting their country first. In fact all that he succeeds in communicating is that he is putting his channel first in the competition of TRPs.

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The aggressive stance of this presenter in clothing and presentation can be juxtaposed with that of the quarrelsome tone, offensive language and high pitch of the first presenter discussed. This similarity can also be found on the more subtle level in comparatively balanced and sober shows titled as "Buck Stops Here," and "To The Point." Both these award-winning shows by the respected journalists Barkha Dutt and Karan Thapar respectively used the language in its devaluated form here and there. As opposed to Gosawmi and Sawant, Dutt and Thapar belongs to the other extreme—posing to be the elite and sophisticated westernized thinkers. However the cynicism in their tone blasting everything that is "swadeshi," makes them devaluate the language they speak. So when Barkha says, the Buck stops here, people simply understand that, "buck stops, where it is convenient for her!" Similarly when Thapar declares his intention of being, "to the point," viewers know, that he means, "to the point he has chosen to highlight!"

Post-Truth Era: Age of New Language

The devaluation of the language is a global phenomenon. The language has been constantly stripped of the original values and ideas owing to the round-the-clock technology-driven news-making corporations. Even the most powerful nations of the Western "first world" have not been immune to the effects of this erosion of language. In fact the countries like USA and Great Britain are at the receiving end today. The new term called "Post-Truth age" has been used specifically to describe the events in these two countries. It is not a coincidence that the post-truth era has a new language under its command. In fact "post-truth era" and "the new language" have the child-mother relationship. We have a lot of hard evidence to believe that this "Post-Truth Era" has been born to the "New Language" in the world of social media networks and the 24/7 news networks. Whether it is 9/11 episode or Brexit shock or Trump Election—all are more or less the result of New-Age language. Why in the first place did 9/11 occur? The truth of "Oil-war" was conveniently clothed by the Bush administration under the fabricated "WMD-threat" leading to the attack on Iraq. This one event started it all. The rest of it is history. The world started collapsing in a domino-effect. All these events were created by "alternative reality," or "plastic truth." The plastic truth, we are calling so, as it is moulded in order to suit to the users. The truth becomes a private commodity which can be manipulated in any way just to play the largest number of recipients. Secondly the alternative truth gives a private version the legitimacy of being the truth for the larger audience. The rhetoric put by President Bush, "With us or Against us" falls under this category. The Brexit-phenomenon is the latest example of the new-language taking hold of our minds. The people were systematically fed the "jingoist" and "xenophobic" rhetoric. It created the mass-hysteria born out of the primal instinct of survival. The majority of Britons were made to believe that their jobs and the livelihood were being robbed by the Europeans, Asians and Africans. A very few bothered to check the other version of reality! The Trump election is yet another example of how people are affected by the rhetoric of xenophobia.

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ISSN 2349-5189

An International Peer-Reviewed Open Access Journal

UGC Approved Journal – Arts & Humanities – Sr. No. 49124

Trump, overnight changed the value and idea of the word, "great." His slogan, "let's make America great Again" is a classic example of devaluation of language. For Trump "great" means less-tolerant towards the people of other ethnicity, colour or nationality. It doesn't matter to anybody that such person would originally be termed as, "weak," and "shallow." The majority of the people no longer identify the original values and ideas with the word, "Great." So now with the new meaning the new leader will make the country great again—perhaps he intends to make the America great again—during the time pre-revolution!

Popular Belief means Democratic Edict

The dangers of the devaluation of the language are far more serious than they seem on the face value. The fact that the likes of Arnab Goswamy, Barkha Dutt, Gaurav Savant or Trump or Bush are more popular than those opposing them. According to a report by BARC Goswami commands nearly 76% of English news viewership in his band from 9 to 11 pm. This is a phenomenon that needs serious academic examination.[ii] Similarly Barkha Dutt and Karan Thapar also enjoy a large-scale support among both the elite and common viewers. Even when there are wide spread reports about the biased and highly coloured reporting by many of the channels[iii] the viewership of these news-anchors is on the increase constantly. The critics, thinkers and academicians have been trying to narrow down the factors that make them popular. There are several socio-political and cultural factors that affect the choices of the people when it comes to the newsmakers. But one thing is clear that the Prime Time news shows have become most important for the news channels to survive.[iv] Similarly the politics today cannot survive without the props of social media networks. These so called opinion-makers are in fact the manipulators, creating the realities convenient for the corporations and affiliated political parties and other interest groups. So when the Brexit happens, it becomes the popular will of the people. In the representative democratic societies like England and India and Electoral-college systems like America the popular will of the people is often at odds with the in-depth thinking and policy related views and ideas. This sad reality is reflected in the result of referendum on Brexit. The common people who did not have clearer and subtle understanding of the complex issues like membership of European Union were made to take sides almost blindly. This led to the step that was almost the next moment regretted upon by the whole country! This is a very clear example of degradation of ideas and language: here the popular belief was taken for Democratic edict!

This is the danger looming large owing to the devaluation of language today. The sooner we start identifying the degradation of the language the better as a society we would be able to overcome the dangers of being the inhabitants of world ruled by the alternative reality!

(Which of these is the worst news-show?) (Even among the most reputed and prized anchors we find a "silent hidden" bias as they present and take sides, on news articles.)

(According to a report by BARC Goswami commands nearly 76% of English news viewership in his band from 9 to 11 pm. This is a phenomenon that needs serious academic examination.)

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DOI Prefix: 10.22183
Journal DOI: 10.22183/23501081

UGC Aprroved Journal Sr.No.44476
ISSN 2350-1081

IMPACT FACTOR
5.210

RESEARCH DEMAGOGUE

UGC APRROVED JOURNAL SR.NO.44476
Yaswantrao Chavan Arts & Science Mahavidyalaya, Mangrulpir, Washim, Maharashtra
www.ycjournal.net
SPECIAL ISSUE DECEMBER 2017

INTERNATIONAL CONFERENCE

ON

Future Prospective of Physical Education, Sports Sciences and Yogic Practices

RES ARCH DEMAGO UE

15th December to 16th December 2017

Organized by

Department of Physical Education,
Sant Gadge Baba Amravati University, Amravati,
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DOI Prefix: 10.22183
Journal DOI: 10.22183/23501081

UGC Aprroved Journal Sr.No.44476
ISSN 2350-1081

IMPACT FACTOR
5.210

Research Demagogue

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doi

DR. D. S. WANKHADE
Department of Physical Education, Vidyabharti Mahavidyalaya, Amravati

International Conference on Future Prospective of Physical Education, Sports Sciences and Yogic Practices *(15th to 16th December 2017)*
Department of Physical Education,
S. G. B. Amravati University, Amravati, M.S.

WALKING FOR COMPLETE HEALTH, FITNESS & WELLNESS

ABSTRACT

Hippocrates quoted, "walking is man's best medicine", there is good number of researches show that walking is good for our health & fitness too; major influence has been found to prevent as well as to cure diabetes, heart diseases, cancer high blood pressure, to increase bone density. Walking is a great way to improve or maintain your overall health . walking is low impact, requires minimal equipment, can be done at any time of day & can be performed at your own peace.

Introduction :

Hippocrates quoted, "walking is man's best medicine", there is good number of researches show that walking is good for our health & fitness too; major influence has been found to prevent as well as to cure diabetes, heart diseases, cancer high blood pressure, to increase bone density.

Walking is a great way to improve or maintain your overall health . walking is low impact, requires minimal equipment, can be done at any time of day & can be performed at your own peace.

Health benefits of Walking :

You carry your own body weight when you walk. This is known as weight- bearing exercise some of the benefits include :-

- Reduced risk of cardio vascular events.
- Weight loss/ loss of body fat.
- Improved aerobic fitness (in some people)
- Increased HDL – Cholesterol (i.e. the good cholesterol)
- Improved glucose metabolism.
- Lower blood pressure.
- Improved mood(depression, stress)

Walking has proved its health benefits in numerous studies. You might be surprised to learn that plain old walking, if done regularly, can ward off some really serious diseases.

Prevent type 2 diabetes :-

Type 2 diabetes is a lifelong (Chronic) disease in which there is a high level of sugar in the blood. Studies show that 150 minutes walking per week & losing just 7% of body weight (5.5-12 Kg.) can reduces the risk of having diabetes by 58%.

Reduces Mortality :-

In one study it was found that the retired man who walk more that 3.5 Km per day, in an average they live at least twice as compare to sedentary people who don't walk systematically.

Strengthens Heart :-

In an another study on 72488 women of nurse's healthy study, it was found that women who walk three hours or more per week is lacking the risk of having heart attack or other coronary issues by 35% as compare to them who never exercise of any kind.

Helps to maintain Bone density :-

Research showed that postmenopausal women who walk approximately more than 1 ½ (one & half) Km each day use to have higher whole body bone density than who don't walk in that way.

Reduces the risk of Breast cancer :-

Colon Cancer is cancer of the large intestine (Colon) the lower part of our digestive system. Many studies have shown that exercise like brisk walking can prevent colon cancer & even if an individual person develops colon cancer, regular exercise increases quality of life & reduces mortality.

Reduces the risk of Breast cancer :-

Women who use to perform brisk walking from 1 ¼ hour (One hour & Fifteen minutes) to 2 ½ hours (Two hours & thirty minutes) per week is lacking the risk of having breast cancer by 18% compared with inactive women.

Increases cardiovascular fitness :-

Cardiovascular fitness is the ability of the heart & lungs to supply oxygen rich blood to the working muscle tissues & the ability of the muscles to use oxygen to produce energy for movement walking improves cardiovascular fitness walking just three times a week for 30 minutes can significantly increases cardiovascular fitness.

Improve Blood Circulation :-

Calf muscles are person's second heart on walking these muscles pump the blood to the heart with all force.

Cut Fatigue :-

One daily brisk walking has become a habit you start reaping the benefits soon, the need of any laxatives is controlled & no more low backache or catch is felt while bending above all, body will be in shape & is not easily fatigued Your renewed energy gives you the urge (and ability) to start doing more outdoor activities with you family & friends.

Improve the posture :-

Essential vitamin D can lower cancer rate, risk of osteoporosis in people over 50 year of age walking helps shape & tone your legs & built, slims your waist & helps you sleep better.

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DOI Prefix: 10.22183 | UGC Aprroved Journal Sr.No.44476 | Impact Factor: 1.390
Journal DOI: 10.22183/23501081 | ISSN 2350-1081

RESEARCH DEMAGOGUE

UGC APRROVED JOURNAL SR.NO.44476
Yaswantrao Chavan Arts & Science Mahavidyalaya, Mangrulpir, Washim, Maharashtra
SPECIAL ISSUE JULY 2017

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Education, Physical Education, and Sports Science'

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In Collabration with

UNIVERSITI SAINS MALAYSIA

AND

International Federation of Physical Education, Fitness and Sports Science Associations

DOI Prefix: 10.22183 | UGC Aprroved Journal Sr.No.44476 | Impact Factor: 1.390
Journal DOI: 10.22183/23501081 | ISSN 2350-1081

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DOI Prefix: 10.22183 | UGC Aprroved Journal Sr.No.44476 | Impact Factor: 1.390
Journal DOI: 10.22183/23501081 | ISSN 2350-1081

Research Demagogue | INFOBASE INDEX | MEMBER OF Crossref | OPEN ACCESS | INNO SPACE | doi

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NAAC Re-Accredited Grade 'A' (CGPA 3.17)
2ND INTERNATIONAL CONFERENCE
ON EDUCATION, PHYSICAL EDUCATION & SPORTS SCIENCE
Kuala Lumpur - Malaysia | July 29-31-2017
Collaboration with USM APEX

ROLE OF NUTRITION IN SPORTS PERFORMANCE

ABSTR

This article highlights the Nutrition Ro mance and Fitness. Games Nutrition applies nourishment sta ish with the goal of expanding exhibition. Diets have been endorsed for diverse classifications of games relaying on the form weight and vigor needs. This article outlines the current energy, nutrient, and fluid recommendations for sports person. The performance of athletes and sports person can be enhanced by well-chosen nutrition strategies. It outlines the stance on nutritional factors that have been determined to influence sporting performan trends in the field of sports nutrition.

INTRODUCTION :

Games nourishment gathers basic vitality in light of the fact that long before inadequacy manifestations begin seeming, physical exhibition decays. It might not be reasonable to think regarding least ought to keep the blood levels or chemical levels at ordinary points of confinement. Rather endeavours ought to be made to figure out the level beneath which physical exhibition begins appearing. The level, which allows the jok to attain the greatest conceivable physical exhibition, ought to be the base level pointed in the games nourishment.

An optimal eating methodology may be described as one in which the supply of needed supplements is satisfactory to blanket vigor use, for tissue support, repair and development. The wholesome needs vary from single to single dependent upon age, sex, form measure and arrangement, occupation, physiological condition and so forth. Numerous mentors make dietary suggestions dependent upon their particular "sentiments" and past encounters as opposed to depend on accessible experimental confirmation the way that players frequently have either lacking or erroneous informative content concerning judicious dietary rehearses and the part of particular supplements in the eating regimen.

MEANING OF ENERGY REQUIREMENT :

It is a created certainty that sustenance plays an imperative part in physical exhibition, separated from pl and other identified segments. In India, games sustenance is yet to be distinguished as a paramount part of preparing project, and seems to be passively dismissed.

Sports Author concerning India (SAI) stresses every games nourishment and readiness the diverse games disciplines. As nd requirements are not static. Athletes unde take a periodized program in which preparation for peak performance in targeted events is achieved by integrating different types of workouts in the various cycles of the training calendar. Nutrition plans need to be personalized to the ind vidual athlete to take into account specificity & individueness of the event, performance al challenges, food preferences, responses to various strategies. Energy availability, which considers energy intake in relation to the energy cost of exercise, sets an important foundation for health and the success of sports nutrition strategies. The achievement of the body composition associated with optimal strategies. The achievement of the body composition associated with optimal performance is now recognized as an important but challenging goal that needs to be individualized and periodized. Training and Sports nutrition guidelines should also consider the importance of the timing of nutrient intake and nutritional support over the day and in relation to sport rather than general daily targets. Competition nutrition should target specific

strategies that reduce or delay factors that would otherwise cause fatigue in an event; these are specific to the event, environment / scenario in which it is undertake and the individual athlete. A pragmatic approach to advice regarding the use of supplements and sports foods is needed for high prevalence of interest and use by athletes and the evidence that some products can usefully contribute to a sports nutrition plan and / or directly enhance performance.

ERGOGENIC AID:

An ergogenic aid is any training technique, mechanical device, nutrition practice, pharmacological method, or psychological technique that can improve exercise performance capacity and / or enhance training adaptations. This includes aids that may help to prepare an individual to exercise, improve the efficiency of exercise, and / or enhance recovery from exercise. Ergogenic aids may also allow an individual to tolerate heavy training to a greater degree by helping them recover faster or help them stay injury free and/or healthy during intense training. Some sports nutrition specialists feel that if a supplement helps prepare an athlete to perform or enhances recovery from exercise, it has the potential to improve training adaptations and therefore should be consider ergogenic. Individuals who better adapt to high levels of training usually experience greater gains from training over time which can lead to improved performance. Consequently, employing nutritional practices that help prepare individuals to perform and/or enhance recovery from exercise should also be viewed as ergogenic. One of the most common questions raised by athletes, parents, and professionals regarding dietary supplements relates to how they are manufactured and consumer awareness of supplement quality. In a number of cases, reputable companies who develop dietary supplements have research teams who scour the medical and scientific literature looking for potentially effective nutrients.

GENERAL DIETARY GUIDELINES :

A well-designed diet that meets energy intake needs and incorporates proper timing of nutrients is the foundation upon which a good training program can be developed. Maximum research has clearly shown that not ingesting a sufficient amount of calories and/or enough of the right type of macronutrients may impede an athlete's training adaptations while athletes who consume a balanced diet that meets energy needs can augment physiological training adaptations. Incorporating good dietary practices as part of a training program is one way to help optimize training adaptations and prevent overtraining.

ENERGY INTAKE

To optimize training and performance through nutrition is to ensure the athlete is consuming enough calories to offset energy expenditure. For elite athletes, energy expenditure during heavy training or competition may be enormous. Maintaining energy deficient diet during training often leads to significant weight loss, illness, onset of physical and psychological symptoms of over training, and reductions is performance. Nutritional analyses of athletes' diets have revealed that many are susceptible to maintaining negative energy intakes during training. Female athletes have been reported to have a high incidence of eating disorders. Some athletes do not like to exercise within several hours after eating because of sensations of fullness and predisposition to cause gastrointestinal distress. Care should be taken to plan meal times in concert with training, as well as to make sure athletes have sufficient availability of nutrient dense foods throughout the day for snacking between meals.

CARBOHYDRATE:

Athletes must consume proper amounts of carbohydrate, protein and fat in their diet. However, athletes involved in moderate and high volume training need greater amounts of carbohydrate and protein in their diet to meet macronutrient needs. Many sports nutrition specialist recommend that athletes consume concentrated carbohydrate juices/drinks and consume high carbohydrate supplements to meet carbohydrate needs. Care should be taken to consider the type of carbohydrate to ingest prior to, during, and following intense exercise in order to optimize carbohydrate availability.

PROTEIN :

If insufficient amount of protein is obtained from the diet, an athlete will maintain a negative nitrogen balance, which can increase protein catabolism and slow recovery which way lead to muscle wasting and training intolerance. Care should be taken to ensure that athletes consume a sufficient amount of quality protein in their diet to maintain nitrogen balance. Proteins differ based on the source that the protein was obtained, the amino acid profile of the protein, and the methods of processing or isolating the protein and anabolism.

VITAMINS:

Vitamins are essential organic compounds that serve to regulate metabolic processes, energy synthesis, neurological processes, and prevent destruction of cells. 2 primary classifications of vitamins are fat and water soluble. Some vitamins may help athletes tolerate training to a greater degree by reducing oxidative damage (Vitamin E, C) and help to maintain a healthy immune system during heavy training (Vitamin C). Since dietary analyses of athletes have found deficiencies in caloric and vitamin intake, many sports nutritionists' recommend that athletes consume a low dose daily multivitamin and / or a vitamin enriched post workout carbohydrate / protein supplement during periods of heavy training.

MINERALS

Minerals are essential inorganic elements necessary for a host of metabolic processes. Minerals serve as structure for tissue, important components of enzymes and hormones, and regulators of metabolic and neural control. Some minerals have been found to be deficient in athletes or become deficient in response to training and / or prolonged exercise. When mineral status is inadequate, exercise capacity may be reduced. Dietary supplementation of minerals in deficient athletes has generally been found to improve exercise capacity. Additionally, supplementation of specific minerals in non-deficient athletes has also been reported to affect exercise capacity. Iron supplementation in athletes prone to iron deficiencies and anemia has been reported to improve exercise capacity. Sodium phosphate loading has been reported to increase maximal oxygen uptake, anaerobic threshold, and improve endurance exercise capacity by 8 to 10%. increasing dietary availability of salt (sodium chloride) during the initial days of exercise training in the heat has been reported to help maintain fluid balance and prevent dehydration. There is no benefit of mineral supplementation for athletes and it is unethical for a sports nutrition specialist to recommend that their clients take minerals for health and / or performance benefit is not consistent with current available literature.

WATER :

Most important nutritional ergogenic aid for athletes is water. Exercise performance can be significantly impaired when 2% or more of body weight is lost through sweat. Weight loss of more than 4% of body weight during exercise may lead to heat illness, heat exhaustion, heat stroke, ad possibly death, for this reason, it is critical that athletes consume a sufficient amount of water/sports drinks during exercise in order to maintain hydration status. Athletes should not depend on thirst to prompt them to drink because people do not typically get thirsty until they have lost a significant amount of fluid through sweat, they should weight themselves prior to and during exercise training to ensure that they maintain proper hydration and make sure that they consume more fluid in hotter/humid environments. Sports nutrition specialists can play an important role in educating athletes and coaches about proper hydration methods and supervising fluid intake during training and competition.

DIETARY SUPPLEMENTS :

Dietary supplements can help athletes to consume proper amount of calories carbohydrate, and protein in their diet. However, they should be viewed as supplements to the diet, not replacements for a good diet. Most dietary supplements available for athletes have little scientific date supporting their potential role to enhance training and performance. As, number of nutrients and dietary supplements have shown to help in improving performance and recovery. Supplementation with these nutrients can help to augment normal diets which help to optimize performance. Also, convenience supplements which are meal replacement powders, ready to drink supplements, energy bars, and energy gels currently represent the largest segment of the dietary supplement. They are typically fortified with vitamins and minerals and differ on the amount of carbohydrate, protein, fat they contain. Use of these types of products can be particularly helpful improving carbohydrate, protein, and other nutrients prior to exercise. Care should also be taken to make sure they do not contain any banned or prohibited nutrients.

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International Journal of Sciences & Applied Research

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Study the optical properties of solid polymer electrolyte based on polyvinyl alcohol

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Abstract

Polyvinyl alcohols doped with different percentage of Ammonium fluoride were prepared by solution casting technique. The optical constants such as Absorption coefficient, transmission spectra, refractive index, extinction coefficient, optical band gap were investigated by using UV-Vis Double Beam spectrophotometer in the wavelength range (190-1100) nm. It was found that the energy band gaps are decrease with increase of salt concentration.

Keywords: Polyvinyl alcohol, UV-Vis spectrophotometer, optical band gap, optical properties

Introduction

Solid polymer electrolyte are proficiently significant due to their wide range application in solid state electrochemical devices like batteries, fuel cell, super capacitor, sensors etc. (1-4). In recent year researcher fascinated toward solid proton conductor due to their ease of handling low cost, high environment stability(5). Electrical and optical properties of polymer can be suitability modified by adding of salt. In present study, PVA has been chosen as polymer host due to their mechanical strength, excellent film-forming ability, dopant-depenent electrical and optical properties, low cost and high tensile strength (6-7). PVA is semicrystalline material and it contain hydroxyl group attach to methane carbon which can be source of hydrogen bounding. As per literature survey ammonium salt are very good proton donor (8-10). The polymer electrolyte based on polyvinyl alcohol based with ammonium fluoride has been studied by using UV-Vis Double Beam spectrophotometer.

Materials and methods

Films of Polyvinyl alcohol-Ammonium fluoride were prepared by solution casting method. The suitable amount of Polyvinyl alcohol (PVA) and Ammonium fluoride was dissolved separately in double distill water. These solution was mixed together and stirred well to get homogenous solution. These homogenous solutions were casted on glass plate. The whole assembly was placed in dust free-chamber and allowed to evaporate the solvent slowly in dry atmosphere at room temperature for 4-5 days. The thickness of the films was in the range (0.045-0.021) mm. It was determined

using micrometer at different places in each films and average was taken.

Optical properties

The basic principle behind the UV visible spectroscopic depend on the absorption of photons with energies greater than the band gap energy of carrier which undergoes transition from occupied state in valance band to unoccupied state in conduction band (11-12). The study of optical absorption gives information about band structure of solid. Generally there are two types of optical transition that occur at fundamental edge in solid like insulators/semiconductor such as (a) Direct band gap (b) indirect band gap semiconductor. The top of valance band and the bottom of the conduction band lies at the same zero crystal momentum (zero vector). If the bottom of conduction band does not correspond to zero crystal momentum, then it is called indirect band gap semiconductor. In indirect band gap semiconductor, the transition from valance band to conduction band should always be associated with a phonon of the right magnitude. Davis and Shalliday (13) reported that near fundamental band edge both direct and indirect transition occur can be determine by plotting $\alpha^{1/2}$ and α^2 as function of photon energy hυ.

The Thutupalli and Tomlin gave the relationship based on the analysis for direct and indirect band of semiconductors/insulator respectively

$(h\alpha\upsilon n)^2 = c(h\upsilon - E_{gd})$ ---------- (1)

$(h\alpha\upsilon n)^{1/2} = c(h\upsilon - E_{gi})$ ---------- (2)

Where hυ is the photon energy, E_{gd} is the direct band gap, E_{gi} is the indirect band gap, n is the refractive index, α is absorption coefficient and C_1, C_2 are constants.

The optical studies are carried out to determine optical constant such as absorption coefficient, extingtion coefficient, refractive index, optical band gap. The absorption coefficient was calculated from the absorbance using the relation

$I=I_o\exp(-\alpha x)$

Hence $\alpha = \frac{2.303}{x}\log\left(\frac{I}{I_o}\right) = \left(\frac{2.303}{x}\right)A$

Where x is the thickness of the sample under study. A is the absorbance coefficient.

The extingtion coefficient (K) of the film is calculated using equation

$K=\frac{\alpha\lambda}{4\pi}$

Where λis wavelength of incident light.

Results and discussion

Optical Absorbance Spectra

The optical absorbance spectra as a function of wavelength for prepared polymer composite has been recorded by double beam UV Vis spectrophotometer in the wavelength range (190-1100) nm. The optical absorbance against the wavelength range (190-490) nm of polyvinyl alcohol and polyvinyl alcohol with ammonium salt is shown in fig 1

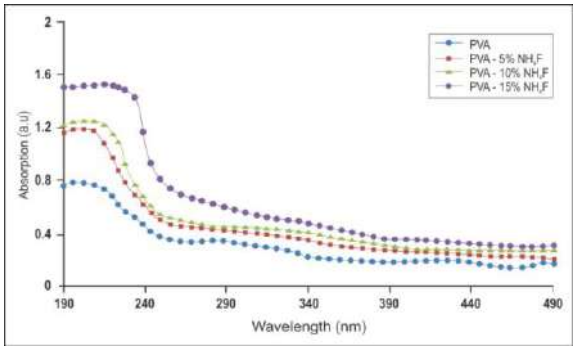

Figure 1

The absorbance shows a sharp increase in absorbance at the wavelength near the absorbance edge of the threshold wavelength. The energy corresponding to this region determine the band gap of the sample(12).

Extinction Coefficient

The Extinction coefficient against wavelength in the wavelength range (190-400) nm is shown in the fig 2.

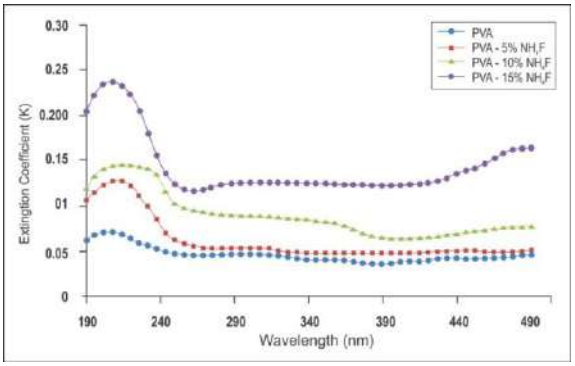

Figure 2

It is observed that composite films dissipate more photon energy than those of pure PVA for higher value of extinction coefficient.

Optical Band Gap

The optical band gap energies were evaluated from $(\alpha h\alpha)^2$ verse photon energy ($h\upsilon$) plot is as shown in fig 3.

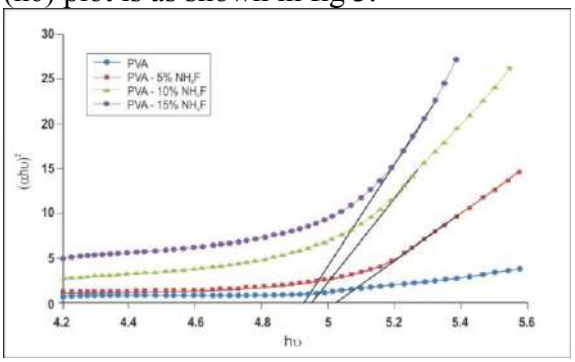

Figure 3

The allowed direct transition energy were determined by extrapolation the linear portion of the curves to zero absorption .The optical band gap decreases from 5.83 eV for pure PVA to 4.98 eV for NH_4F concentration increase up to 15%. The decrease in the optical band gap may be explained on the basis of the fact that the incorporation of small amount of dopant from charge transfer complex in the host matrix (16-17).these charge transfer provides conductivity by providing addition charges this result in decrease of the optical energy gap.

Conclusion

The solid polymer electrolyte based on PVA doped with different concentration of ammonium fluoride has been prepared using solution cast technique. The absorbance coefficient and extingtion coefficient are increasing with increase the concentration of ammonium fluoride. The optical band gap decreases from 5.83 eV for pure PVA to 4.98 eV for NH_4F concentration increase up to 15%. The optical band gap increases due to increase the number of mobile charge carrier into the host polymer.

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Themed Section : Engineering and Technology

Study of DC Conductivity of Polypyrrole doped with SnO_2 Nanocomposites

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ABSTRACT

The nanocomposites of PPy-SnO_2 were prepared by chemical oxidative polymerization technique using an anhydrous ferric chloride ($FeCl_3$) as an oxidizing agent and it was characterized by X-ray diffraction (XRD), field emission scanning electron microscope (FE-SEM), Fourier transform infrared (FTIR). The samples are prepared in the form of thick films by screen printing method. The effect of temperature on DC conductivity of the samples has been measured and the conductivity of sample PS3 (60 % PPy + 40 % SnO_2) was found to be maximum amongst all the prepared samples. Activation energy was found to be 0.1062 eV.

Keywords: PPy-SnO_2 nanocomposites, DC conductivity.

I. INTRODUCTION

Recently, the conducting polymers are important materials emerging with lot of applications in various fields. To improve the quality and applicability the research in the field of such polymers with some modification of existing polymers has been carried out. Some of these modifications involve preparing hybrid materials in which organic materials and inorganic oxides or salts of different metals, viz. SnO_2, ZnO, MgO etc. [1]. The most widely studied conducting polymers are polypyrrole, polyaniline, polythiophene etc. Additionally, PANI can coordinate with metal ions, giving the multi-metallic system and also preparation of nanocomposite materials with other polymers. PPy is one of the most interesting conducting polymers since it is easily deposited from aqueous and non-aqueous media, very adherent to many types of substrates, and is well-conducting and stable. Electrochemical polymerization produces thin films with a thickness of few micrometers on an electrode surface, while a chemical oxidation yields fine-grained materials [2-4]. PPy is known to be capable of storing electrical charges. The stored electrical charges can be recovered upon demand and that is why PPy can be considered as a good candidate for super-capacitor application [5-8].

The present study deals with the synthesis & characterization of PPy/SnO_2 composites and evaluation of dc conductivity for different wt. % of SnO_2 in PPy nanocomposites with an intention to know the effect of SnO_2 doping. The characterization of the composites has been done by SEM analysis techniques.

II. EXPERIMENTAL

A. Synthesis of SnO_2 nanoparticles.

All the chemicals used in this study were of GR grade purchased from Sd-fine, India (purity 99.99%). In preparation of SnO_2, 2g (0.1 M) of stannous chloride dehydrate ($SnCl_2.2H_2O$) is dissolved in 100 ml water. After complete dissolution, about 4 ml ammonia solution is added to above aqueous solution with magnetic stirring. Stirring is continued for 20 minutes. White gel precipitate is immediately formed.

It is allowed to settle for 12 h. Then it is filtered and washed with water 2-3 times by using de-ionized water. The obtained precipitate were mixed with 0.27g carbon black powder (charcoal activated). The obtained mixer is kept in vacuum oven at 70ºC for 24 h to obtain a dried powder. Then this dry product was crushed into a fine powder by grinder. Now the obtained product of fine nanopowder of SnO_2 was calcinated at 700ºC up to 6 h in the auto-controlled muffle furnace (Gayatri Scientific, Mumbai, India.) so that the impurities from products will be completely removed.

B. Synthesis of Polypyrole (PPy)

The Py monomer, anhydrous iron (III) chloride ($FeCl_3$) and methanol were used as received for synthesis of PPy. The solution of 7 ml methanol and 1.892 g $FeCl_3$ was first prepared in round bottom flask. Then 8.4 ml Py monomer was added to ($FeCl_3$ + methanol) solution with constant stirring in absence of light. The amount of Py monomer added to the solution (1/2.33 times of $FeCl_3$) was in such a way to get maximum yield. The resulting black precipitates are filtered and washed with copious amount of distilled water until the washings are clear. PPy so obtained is dried by keeping in oven at 600ºC for 3 h. The synthesized material was characterized by using XRD, SEM.

C. Preparations of films

The thick films were prepared by using screen printing techniques. Initially, for the screen printing the thixotropic paste was formulated by mixing the sintered fine powder of pure and composite nano powder of SnO_2 and PPy in different weight percentage with a solution of ethyl cellulose (as 10% temporary binder) in a mixture of organic solvent such as butyl cellulose, butyl carbitol acetate and turpineol. The ratio of inorganic to organic part was kept as 75:25 in formulating the paste. The paste was then used to prepare thick films of pure and composite materials of SnO_2 and PPy and it was screen printed on a glass substrate. The prepared films were dried at 90-100ºC in oven for 1 h, so that all the organic materials (in the form of binders) and organic impurities can be evaporated from prepared films. For the surface conductance measurement, the electrodes of silver paint were formed on adjacent sides of the films and again, the films were subjected to heating at 70ºC for 15 minutes for drying the silver paint. The series of samples are as shown in table 1.

Table 1

S.N.	Nano composites	Sample Code
1.	Pure Polypyrrole	P
2.	80 % PPy + 20 % SnO_2	PS1
3.	70 % PPy + 30 % SnO_2	PS2
4.	60 % PPy + 40 % SnO_2	PS3
5.	50 % PPy + 50 % SnO_2	PS4
6.	40 % PPy + 60 % SnO_2	PS5
7.	30 % PPy + 70 % SnO_2	PS6
8.	20 % PPy + 80 % SnO_2	PS7
9.	Pure SnO_2	S

III. RESULTS AND DISCUSSION

A. XRD (X-ray Diffraction)

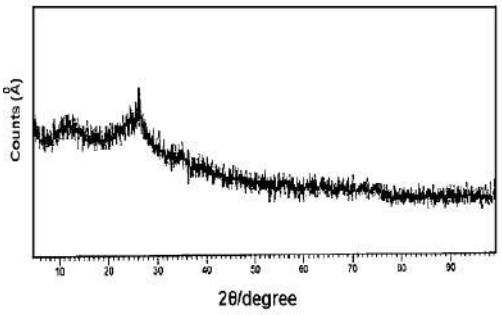

Figure. 1. XRD of pure PPy

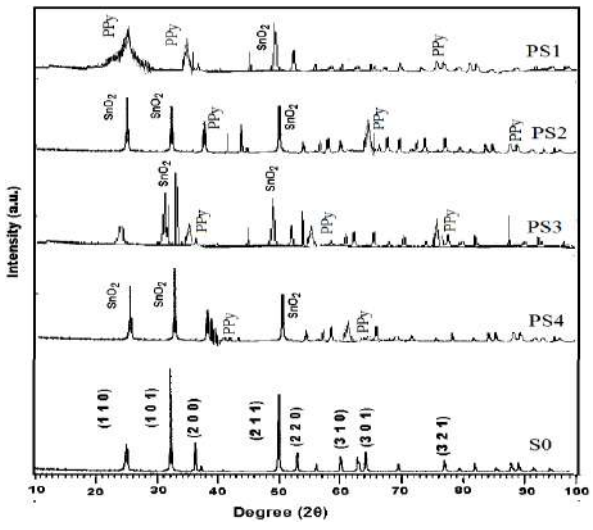

Figure.2. XRD of all composites sample

X-Ray diffraction pattern of pure polypyrrole (PPy) and their composites are as shown in figure (1 and 2). The pure PPy exhibited that, it was amorphous in nature. The broad peak occurred at 24^0 and it is characteristics of amorphous nature of polypyrrole. The broad peak occurs due to the scattering of X-rays from polymer chains at the interplaner spacing. The maximum intensity position of amorphous also depends on monomer to oxidant ratio. The X-ray diffraction patterns of composites of PPy, SnO_2 and pure SnO_2, calcinated at 200°C. Main peak, in case of pure SnO_2, is observed at 26.6° and this peak corresponds to the plane (1 1 0) of SnO_2 in tetragonal structure (JCPDS Card No.3-1114) with 100% intensity and the average crystalline size by using Scherer's formula was found to be 147.31 nm [9,10]. All the peaks are for the composites materials for molar weight percentage of various samples that are perfectly matched.

B. Scanning Electron Microscope (SEM)

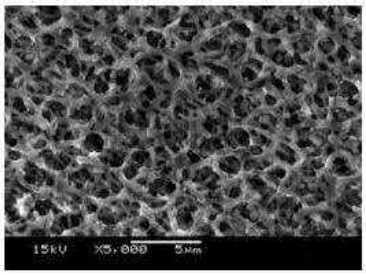

Figure. 3. SEM of Pure PPy

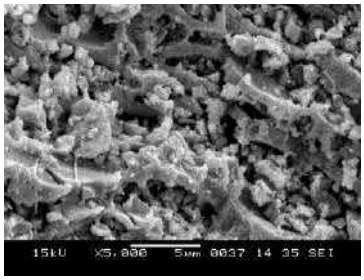

Figure. 4. SEM of PS3

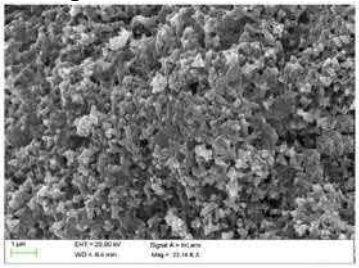

Figure. 5. SEM of Pure SnO_2

From the SEM photos, it is observed that in every inch of the region, number of pores was different and an average number of pores was taken for comparative study. From every photo, porosity was calculated for one inch region and listed in the tabular form. From above figures, it is found that number of porosity of 60PPy:40SnO_2 composition is more among the prepared and pure samples. Due to high porosity, available area for the flow of ions and charges is more and conductivity enhances. High porosity reduces the obstacle to the flow of charges and ions as collisions reduce (relaxation time increases) and charges mobility increases. This tends to high electrical conductivity.

C. DC Conductivity

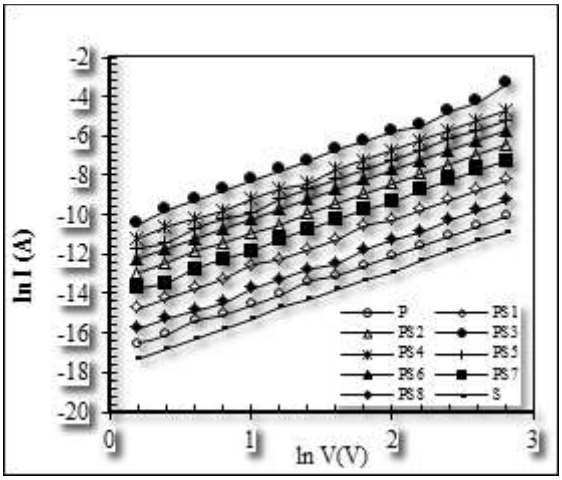

Figure. 6. DC conductivity of samples

The graph is plotted between lnI versus lnV at a constant temperature as shown in figure 6. As the doping percentage of SnO_2 in PPy increases, there is increases current with increase in voltage. It is maximum for PS3 sample (60%PPy + 40 % SnO_2) amongst the prepared samples. It is also manifested that, the nature of all the graphs is nearly straight line with constant slopes i.e. it obeys Ohm's law at temperature range 50°C to 350°C (linear ohmic material) on logarithmic scale [11].

D. Schottky Plots

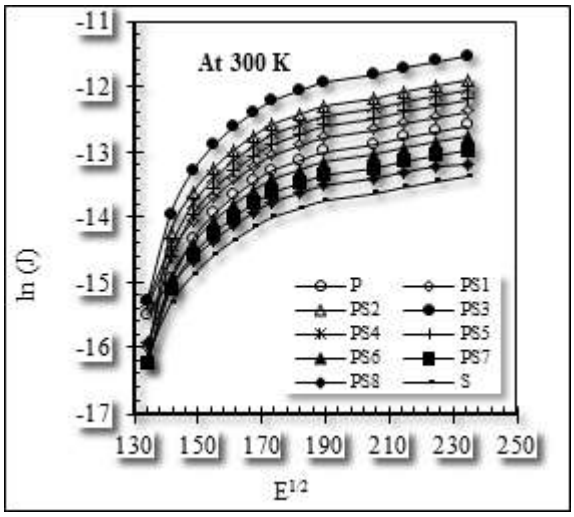

Figure. 7. Graph between Conductivity and $E^{1/2}$ at constant temperature

Then graphs are plotted between ln(J) and $E^{1/2}$ at temperatures 300 K, These graphs are known as Schottky Plots as shown in figure 7. It is observed that as electric field increases, current density increases more in the beginning and then shows saturation. Also ln(J) is maximum for PS3 sample, at constant temperature ln(J) increases. This also shows that with increase in doping of SnO_2 in PPy, ln(J) increases and becomes maximum for PS3. For sample PS3 the current density is $J = 9.8835 \times 10^{-6}$ A/m^2 which is minimum at temperature 300 K (room temperature).

E. Arrhenius Plot

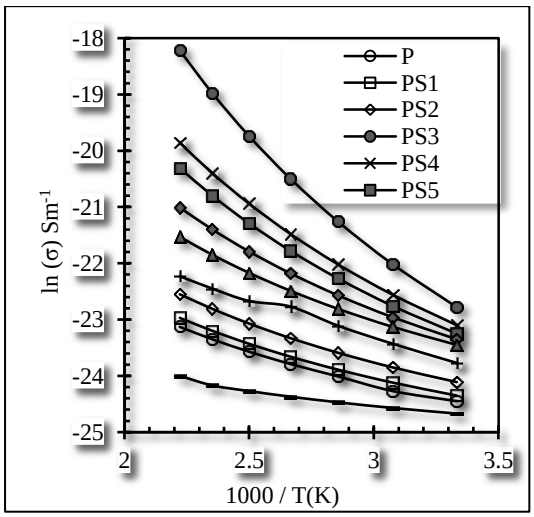

Figure. 8. Variation between ln(σ) and 1000/T(K) of all samples

The graph between ln(σ) and 1000/T(in K) is known as Arrhenius plot as shown in figure 8. It is observed that as temperature increases, ln(σ) increases. This variation is maximum for sample PS3. Due to increase of temperature, more and more charges in samples become free and contribute to the conductivity and electrical conductivity increases. As doping of SnO_2 in PPy increases, electrical conductivity increases and becomes maximum for 60%PPy + 40% SnO_2 sample (PS3 sample) and further increase in doping of SnO_2 in PPy, conductivity decreases. The value of activation energy of sample PS3 was found to be 0.1062 eV which is maximum among all the samples.

IV. CONCLUSION

The X-ray diffraction patterns of composites of PPy, SnO_2 and pure SnO_2, and it shows tetragonal structure and the average crystalline size is found to be 147.31 nm. The current–voltage (I–V) characteristics of the samples and its temperature dependence have been investigated in air at temperature 350°C. The linear nature of plots shows the semiconducting behavior and obeys Ohm's law and it is maximum for sample PS3. The value of activation energy of sample PS3 was found to be 0.1062 eV which is maximum among all the samples.

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SJIF Impact Factor (2016): 6.484
ISI Impact Factor (2013) : 1.259(UAE)
IC Value 2015 : 56.46
Print ISSN : 2349- 0187
Online ISSN : 2347 - 9671

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Volume - 5 Issue - 8 August - 2017

Volume - 5, Issue- 8, August 2017 IC Value : 56.46 e-ISSN : 2347 - 9671| p- ISSN : 2349 - 0187
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Research Paper

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WOMEN PARTICIPATION IN LOCAL SELF GOVERNMENT ORGANIZATIONS-A SOCIOLOGICAL STUDY AND PERSPECTIVES

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ABSTRACT

After British, we got a chance to do the development of our nation. For real development of nation, there is a need to develop rural society. Government of India has framed Balwant Rai Mehta Committee to execute and implement the various schemes and plans through cumulative development program and national welfare extension plan.

This committee has suggested the three tier panchayat raj system i.e. Zilha Parishad, Panchayt Samitee and Gram Panchayat. This committee has suggested the Panchayat Raj system for complete and overall development of rural society. Therefore Balwant Rai committee is known as centralization of power. Through this committee, politicians could get developmental authority and power.

KEYWORDS: *Gram Panchayat, Panchayat samitee, Zilha Parishad*

PANCHAYAT RAJ

Panchayat Raj system is three tier system-

1.Gram panchayat -village level.

2. Panchayat samitee – Block level.

3. Zilha Parishad – District level.

The main aim of this committee is to participate local people in government.

WOMEN RESERVATION

Women Reservation is an important issue in current scenario. Today women got legislative and constitutional authority of equally and freedom. Still, women couldn't get the chance to participate in politics on the basis of fifty percent population. Through conferences, seminars awareness about women empowerment, development spread but the raising voice of women close down by male dominant society.There is a need of active and positive participation of women to get them chance in politics. Due to this effect women got chance of 33% reservation in various field.

PANCHAYAT RAJ SYSTEM AND WOMEN RESERVATION

Women got constitutional authority since independence to 1991 but expected result could not get to women. As per the 13th amendment in 1992, panchyat raj election has been declared after 5 year. On this basis of this decision, women got 30% reservation in three levels. Special posts reserve for women in local self government organizations. This decision is helpful to improve the status of women and to boost their confidence.

Kautilya had propagated the women authority. Women fought in many countries about their rights. Long struggle in England, 1998 women got authority of voting and France got in the year 1928as well as USA in 1944. 'Challenges of women change' book written by Shubhangi Gogate, Ghovtane expressed factual and logical discussion on women problems. Manjusha Gosavi also wrote on quantities and numeric analysis of women.

'Changing status of women' written by Rajiv Kumar covered the overall situation of women from ancient time to modern time. Therefore this research is important for the women participation in Panchayat Raj system of India.

Constitution has awarded many protective and equally rights to women after independence. Awareness about authority, responsibility and use is important in Panchayat Raj. Women's changes become slow in male dominance society. This topic has been selected for research to understanding the role, efforts of women in Panchayat Raj system.

Points need to understand for women development-

1) To take the review of women status in post independence age
2) To understand the secondary place of women in politics due to the dominant attitude of men.
3) To identify the various problems of women in Indian politics.
4) To understand the women empowerment through women movements.
5) To know the causes behind the avoidance of clarence the bills and acts about 33% research of women in politics.
6) To do the study of status of women with respect to current scenario.
7) To understand the perspective of male women through the participation of women in politics.
8) To identity and understand the status of women of Wardha district in Panchayat Raj system.

OVERLOOK OF INDIAN SOCIETY REGARDING PARTICIPATION OF WOMEN IN POLITICS

1) In male dominant society, male appose and restrict to women to take part in politics, therefore the number of women in politics is less.
2) Women have more problem than men therefore women hesitate to take part into politics.
3) Sometimes women is not interested to take part in politics and she prefer the safe life in society.
4) Behind many success women, there are the men.
5) Duo to complexity of Indian society, women cannot freely movable in politics.
6) Men are the main hidden enemies in women reservation bill, therefore this bill yet to be finalized in India.

Overall information about politic has been found at some places on rules and regulations, importance of politics in panchayat raj system, Men were more aware than women about panchayat raj system. The classes should conduct for awareness among the women. After that women can run positive the panchayat raj system i.s. local self government organizations.

To provide the reservation to women in panchayat raj system is the fulfillment of political empowerment with women empowerment in India.

RECOMMENDATIONS AND SUGGESTIONS

1) There is a need of time to provide the training to women regarding panchayat raj system. Therefore government should start the classes for women.
2) Along with political sources, public administration also should teach to students for detail knowledge of local self government organizations.
3) Only reservation is not alternate solution but the gravity of knowledge is always greater to boost the confidence of women for active participation in panchayat raj system.
4) There is a need to aware the women about women power, capacity, ability, and problem solving methods.
5) Women should get the knowledge of women reservation, benefits of reservation, and rules of reservation, delay in reservation, obstacles in the progress of women's authority.
6) Strict application of legal provisions.
7) Role of women empowerment and development.
8) Awareness among the women
9). Curbing quackery, sensitization of doctors, NGOS, govt. machinery, panchayat leaders.

CONCLUSION

Strictly implementation, creation and support of legislative, judiciary will be beneficial to sort out the women related problems in India. Stop the women exploitation, rape sexually harassment, acid throwing, domestic violence, child marriages and female foeticide with proper instruments and control on these problems.

Various issues like women health, education, sports, schemes, equal sex ratio, entertainment, basic facilities, freedom, protection, sanitation arrangement should provide to women. Then definitely we can develop the healthy India. There is a need of time to frame the women empowerment program me at all levels. The great contribution expect from advocacy groups, policymakers ,social researchers, health workers, social thinkers and sociologist for the women empowerment.

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MAH/MUL/03051/2012
ISSN-2319 9318

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समीक्षा

❖ संपादक ❖
प्रा.विराग गावंडे
डॉ.संजय कोठारी
डॉ.दिनेश निचीत

❖ प्रकाशक ❖
संत गाडगे महाराज कला, वाणिज्य व विज्ञान महाविद्यालय, वालेगांव,जि.अमरावती
आणि आधार सामाजिक संशोधन विकास प्रशिक्षण संस्था, अमरावती

अध्यापनाचा वेळ वाया जाऊन अध्यापनावर परिणाम होणार नाही याची काळजी घ्यावी.

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संत गाडगेबाबांचे आर्थिक विचार

डॉ. देवेन्द्र एस. रंगाचार्य

सहाय्यक प्राध्यापक विद्याभारती महाविद्यालय, कॅम्प, अमरावती.

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प्रस्तावना

संत गाडगेबाबा एक लोकोत्तर युगपुरूष! सतत लोकसेवेत रममाण झालेले एक क्रियाशील सत्पुरूष गरीब माणसांच्या सुखासाठी ते रात्रदिवस धडपडत होते. अज्ञान, दारिद्रय, अंधश्रध्दा आणि अनारोग्याच्या अंधारात चाचपडणाऱ्या असंख्य गोरगरीब माणसांच्या हाताला हात धरून ते त्याला ज्ञान, विज्ञान आणि सुसंस्काराच्या प्रकाशाकडे घेवून जात होते. गाडगेबाबा हा लोकजीवनाच्या विकासासाठी सतत क्रियाशील असणारा एक विचार होता. संत गाडगेबाबांनी सामाजिक कार्य करतांना आपल्या अर्थकार्यास महत्त्वाचे स्थान दिले आहे. बाबांनी किर्तनामध्ये गरिबी, लोकसंख्या, वाढणारा खर्च, बेकारी, कर्ज, अन्न, वस्त्र, निवारा, शिक्षण, आरोग्य, पाणी हया मुलभूत गरजा सारख्या आर्थिक समस्या लोकांसमोर मांडल्या त्यातूनच त्यांचे आर्थिक विचार स्पष्ट होतात. श्रमविषयक विचार, गरजा विषयक दृष्टीकोण, उत्पन्न–बचत विषयक विचार गाडगेबाबांच्या ध्यानीमनी रूजला होता. त्रस्थ, पिडीत, तहानलेल्या, भुकेलेल्यांना, उघडया–नागडया, बेघर, बेकार आणि निराधार, लोकांचे आधारस्तंभ होते. समाजात दबलेल्या, दडपलेला, दुर्बल, दुर्मूख आणि दीन माणूस बाबांच्या जीवनकार्याचा केंद्रबिंदू झाला होता. बाबांची किर्तने म्हणजे जनसामान्यांच्या आचाराविचारांमध्ये आमूलाग्र क्रांती घडवून आणणारी तुतारी होती. समाज जीवनाची सांस्कृतिक, आर्थिक शैक्षणिक घडी बसविण्यासाठी सामान्यांच्या काळजाला जाउन भिडणारी ती एक आर्त किंकाळीच होती.

गरीबांना अन्न, वस्त्र आणि निवारा हेच देवाचे

भजन असते अशी व्यापक विचारांची मांडणी करत होते गाडगेबाबा. जीवनभर गरीबी भोगलेले आणि श्रीमंती माहिती नसलेले समाजाला ज्ञान विज्ञानाचे धडे देणारे समाजाला नवी साद घालणारे गाडगेबाबा कर्मयोगी होते.

"प्रपंच करावा नेटका ।
असू नये तो फाटका ।।"

अशा शब्दामधून बाबा माणसांच्या डोक्यावर सदुपदेशाच्या काठीचे फटकारे मारत होते. गाडगेबाबांच्या संदेशातून भुकेलेल्यांना अन्न, तहानलेल्यांना पाणी, उघडया नागडयांना वस्त्र, गरीबांना शिक्षण, गरीबांचे हुंडयविना लग्न, बेघरांना आसरा, निराशांना हिंमत, पशुपक्षांना अभय, रोग्यांना औषध, बेकारांना रोजगार, हाच बाबांचा दहा कलमी संदेश होता. हाच रोकडा धर्म होता. हीच मानवविकासाची गुरूकिल्ली होती, हाच समाज प्रगतीचा ध्येय ध्यास होता. गाडगेबाबांनी कीर्तनाच्या माध्यमातून अज्ञानाच्या अंध:कारात झोपलेल्या महाराष्ट्रातील समाजाला खडबडून जागे केले. कर्जमुक्ती, दारिद्रय मुक्ती, अज्ञानमुक्ती आणि व्यसनमुक्ती या विचारातून समाजाला बाबांनी आदर्शपणे जगण्याचा मार्ग दाखविला. खेडयात यात्रा किंवा उत्सव प्रसंगी सर्वत्र घाण व दुर्गंध निर्माण होत असे त्यामुळे अनेक साथीचे रोग निर्माण होत असत. बाबा यात्रेतील घाण स्वत: स्वच्छ करीत असत. अशाप्रकारे स्वच्छतेला प्रचंड महत्व देवून स्वच्छतेचे फायदे लोकांना पटवून दिले. स्वच्छता असेल तर शरीर निरोगी राहील. रोगराई, बिमारी जवळ येणार नाही. शरीर निरोगी असेल तर कष्टाचे काम करणे कठीण जाणार नाही आणि आपोआपच स्वत:चा घरचा विकास होईल. बिमारीवर पैसा खर्च होणार नाही म्हणजेच आपोआपच बचत सुध्दा होईल. आर्थिक दृष्टया माणुस संपन्न बनेल असे बाबांचे विचार अर्थशास्त्राज्ञ नर्क्सच्या दारिद्रयाच्या दृष्टचक्राच्या आर्थिक विचाराशी मिळते जुळते आहे. विदर्भात आर्थिक दृष्टिकोनातून संत गाडगे महाराजांचे कार्य ग्रामीण विकासाच्या वाटचालीस फार मोलाचे लाभले आहे.

भूकेलेल्यांना अन्न हा गाडगेबाबांचा संदेशाचा पहिला पाठ मनुष्य आणि इतर प्राणी यांच्या अन्न विषयक गरजा सारख्याच असतात. पोटाची भूक भागविणे हा अन्नाचा खास उपभोगाचा भाग होय. अन्नाशिवाय माणसाला जगता येत नाही. सुग्रास अन्नाच्या प्राप्तीसाठी माणसाची अहोरात्र धडपड चाललेली दिसते. गाडगेबाबा म्हणतात, काम करून खाण्यामुळे कामाची प्रतिष्ठा वाढते म्हणजेच गाडगेबाबांनी श्रमाला महत्व दिले. श्रमाचा भरपूर वापर करण्याच्या सल्ला समाजाला दिला. गाडगे बाबा भूकेलेल्यांना अन्न देत होते म्हणजे एक प्रकारे अन्न सुरक्षा देण्याचे काम गाडगेबाबांनी केले. गरीबाची गरीबी दूर झाली पाहिजे, त्यांना अन्न, वस्त्र व निवारा मिळाला पाहिजे. गरीबाला एखादी कला शिकवा म्हणजे त्याच्या पोटापाण्याची सोय होईल यातून हे सिध्द होते की, लोकांची गरीबी दूर करण्यासाठी लोकांना रोजगार दिला पाहिजे असे या विचारातून दिसते.

तहानलेल्यांना पाणी हा गाडगेबाबांचा संदेशाचा दूसरा पाठ पाणी म्हणजे जीवन. जीवन म्हणजे पाणी, पाण्याशिवाय मानव व मानवेत्तर प्राणी तडफडून मरतात इतके महत्व पाण्याचे गाडगेबाबांनी सांगितले. आजच्या पिढीला वाटते की, पुढचे तिसरे युध्द हे पाण्यासाठी होईल हे गाडगेबाबांनी कधीच ओळखले होते.

उघडया नागडयांना वस्त्र देण्यासाठी अवघाची संसार सुखी करण्याचे व्रत बाबांनी सांभाळले ते किर्तनातून सांगायचे. कर्ज काढुन यात्रा करू नका, गाईबैलाची काळजी घ्या, उघडया नागडयांना वस्त्र द्या. गाडगेबाबांनी समाजातील शेवटच्या माणसाची काळजी घेतली, त्यांना पोटभर अन्न मिळावे आणि अंगभर वस्त्र मिळावे यासाठी आयुष्यभर प्रयत्न केले. गाडगेबाबांनी आयुष्यभर गरीबाला दारिद्रियाच्या दृष्टचक्रातून काढण्याचे प्रयत्न केले.

आसरा म्हणजे निवारा घर, उन, वारा, पाउस, हिस्त्र पशूपासुन संरक्षण मिळविण्यासाठी माणसाने घर बांधले. भारतातील बहुसंख्य लोकांना अशाप्रकारचे घर नाही यासाठी गाडगेबाबांनी धर्मशाळा काढल्या. माणसाला माणुस म्हणुन जगण्यासाठी अन्न, वस्त्र आणि निवाऱ्याची गरज आहे हे बाबांनी ओळखले. बाबांनी गोरगरीबांसाठी निवारे उभे केले. हजारो लोकांना आसरा देणारे बाबा खरे दिनबंधू होते.

'बेकाराईले रोजगार द्या' हा बाबांचा महत्वाचा

संदेश होय. जो मनुष्य काम करतो तो सुखाने चार घास खातो. जो मनुष्य काम करत नाही त्याला भीक मागावी लागते. मानव जीवनाचे श्रेष्ठत्व नैपुण्याने केलेल्या कामावर अवलंबुन असते म्हणजे गाडगेबाबांनी श्रम विभाजनाचे महत्व आपल्या संदेशातून सांगीतलेले दिसते.

बाबांनी हजारो माणसांच्या जीवनात नवा विचार दिला, नवे ध्येय दिले, नवी दिशा दिली, नवी गती दिली, नवी जिद्द दिली, नवी हिंमत दिली आणि नवा आनंद दिला म्हणजे बाबा समाजाचे नवप्रवर्तक होते. बाबांनी समाज जोडण्याचे काम केले. बाबा साहसी होते, गाडगेबाबांनी समाजाला आशावाद शिकविला, प्रयत्नवाद शिकविला, नविन गोष्टी शिकण्याची उमेद निर्माण केली. बाबांची व्यक्ती वर्तणूक लोकांचे कल्याण, समाधान, सुख व हिंमत देणारे होते. मुठभर लोक सुखात राहतात तर ढिगभर लोक दु:खात आहे ही विषमता त्यांनी ओळखली. आर्थिक विषमता हीच आपल्या समाजाची खरी कीड, ती कशी नष्ट करता येईल याकडे त्यांनी लक्ष दिले. बाबा कार्लमॉर्क्सच्या विचाराशी ततोतंत जुळणारे होते.

बाबांनी समाजाला आपल्या उत्पन्नाप्रमाणे कसा खर्च करायचा हे शिकविले. शिकलेला माणूस सुखी होईल आणि इतरांना सुखी करण्याचा मनापासुन प्रयत्न करील. समाजातला शोषित माणूस आपल्या शिक्षण विषयक कार्याचा केंद्रबिंदू मानला. शोषित माणसाला शोषणमुक्त करून त्याला सुखाचा मार्ग दाखवत होते बाबा!! ज्ञान हा तिसरा डोळा आहे. सर्वांसाठी शिक्षणाची नितांत गरज आहे, असे बाबा सांगत.

गाडगेबाबांनी ग्रामीण शिक्षणाचा पाया घातला म्हणजे गाडगेबाबा महात्मा गांधीजींच्या विचाराशी मिळते जुळते आहे.

समाजातील दारिद्रयाचे दृष्टचक्र नष्ट करून सृष्टचक्राची निर्मिती करायची असेल तर शिक्षण घ्या, शिक्षणाशिवाय तरणोपाय नाही.

गाडगेबाबांनी समाजाला शास्त्र शिकविली. प्रत्येक गोष्ट शास्त्रीय पध्दतीने करा असा मौलिक विचार समाजाला दिला.

महात्मा गांधीनी 'स्वच्छता म्हणजे परमेश्वर मानले' तर गाडगेबाबांनी तिला 'परमेश्वराची सेवा मानले.' त्यांच्या हातातील खराटा श्रमसंस्कृतीचे प्रतिक आहे. गाडगेबाबा श्रमप्रधान तंत्राला महत्व देणारे होते या सफाई यज्ञामागे त्यांचा शुध्दतेचा, आरोग्याचा तसेच पर्यावरणाचा उदात्त हेतू वा विचार जाणवतो.

निष्कर्ष :—

१. आज दारूबंदीसाठी, पशुहत्या थांबविण्यासाठी भ्रष्टाचाराचे निर्मूलन करण्यासाठी, जातीवाद, भाषावाद, अंधश्रध्दा, स्त्रीभ्रृणहत्या, शेतकऱ्यांची आत्महत्या थांबविण्यासाठी गाडगेबाबांचा विचारच वाचवू शकतो.

२. गाडगेबाबांचे आर्थिक विचार हे कोणत्याही सिध्दांतावर किंवा तत्वावर आधारित नसुन ते प्रत्यक्ष आचरणावर होते. आज प्रत्येक ग्रामीण व गरीब व्यक्तीने त्यांच्या विचारानुसार वर्तणूक केल्यास गरीबी, लोकसंख्यावाढ, कर्जबाजारीपणा, अंधश्रध्दा या सारख्या समस्या समाजात राहणार नाही आणि ग्रामीण समाजाची प्रगती होईल.

३. संत गाडगेबाबांच्या आर्थिक विचारामध्ये महात्मा गांधी, विनोबाजी, कार्लमार्क्स, प्रा. नर्क्स, प्रा. शूम्पीटर, यांच्या विचारांचे साम्य प्रामुख्याने दिसून येते.

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Apr-17-18

ISSN: 2454-5503
IMPACT FACTOR: 3.012(IIJIF)
(UGC Approved Journal No. 63716)

CHRONICLE OF HUMANITIES AND CULTURAL STUDIES

VOL. 3 NO. 6 Nov. 2017

A BIMONTHLY REFEREED INTERNATIONAL JOURNAL

SPECIAL ISSUE

On the Occasion of
UGC Sponsored One Day National Seminar On

IMPACT OF GLOBALIZATION ON RURAL INDIA

21st November, 2017

Guest Editors

Dr. Subhash K. Pawar
Mr. Vikas T. Adlok

ORGANIZED BY

DEPARTMENT OF SOCIOLOGY
LATE DATTATRAYA PUSADKAR ARTS COLLEGE,
NANDGAON PETH, TQ. DIST. AMRAVATI (MS).

ISSN: 2454-5503
Impact Factor: 3.012 (IIJIF)

14.

EFFECTS OF GLOBALIZATION ON INDIAN RURAL SOCIETY AND FAMILY

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&
Dr. Swati Girase
Mahatma Jyotiba Fule Mahavidyalaya, Amravati

Introduction-

Globalization is attaching the transportation, telecommunication, internet, interdependence of world views and activities. Globalization has its own characteristics and values, either positive or negative. Globalization is a vast and deep concept having effects and side effects on society. It has various causes. The main cause of globalization on developing countries is including three parameters like international market, trade, multinational production, and international finance. Every country in the world has accepted the policy of globalization and related concepts in current scenario.

"Globalization can be defined as the ability to produce and good or service anywhere in the world using capital, technology and components from anywhere and to sell the output anywhere. Peter Jay 1996

Globalization has improved the overall economic status of people as well as the Indian nation in current situation. It is one type of motivation process for development of nation.

Industrialization and Globalization are always focus on industrial investment and economic growth process. In 18th century industrial revolution took place first time in United Kingdom. After that the its effects spread on all over the world which was the symbol of globalization.

The effects of science and technology on society shows with number of ways. It has issues like develop the economic growth, global economy, environment, working class structure, class system, changes in values and norms, more importance to money etc. Globalization has its own characteristics and values, either positive or negative. Globalization is a vast and deep concept having effects and side effects on society. It has various causes. The main cause of globalization on developing countries is including three parameters like international market, trade, multinational production, and international finance . Every country in the world has accepted the policy of globalization and related concepts in current scenario.

Globalization shows direct effect on Indian society.

1. Effects on family
2. Effect on marriage institution
3. Effects on status of women
4. Effects on cast and religion
5. Effects on ideology
6. Effects on work culture.
7. Effects on social institutions.
8. Effects on values, norm and social sections.
9. Effects on political system and Administration.
10. Effects on life style and behaviour with creation of social problems.

ISSN: 2454-5503
Impact Factor: 3.012 (IIJIF)

11. Social effects, contact, family, marriages, and divorce-
12. Change in status of women-
13. Economic changes
14. Political changes
15. Changes in cast and religion
16. Educational changes
17. Global and secondary relationship
18. Existence of civilization
19. Different industrial social problems-

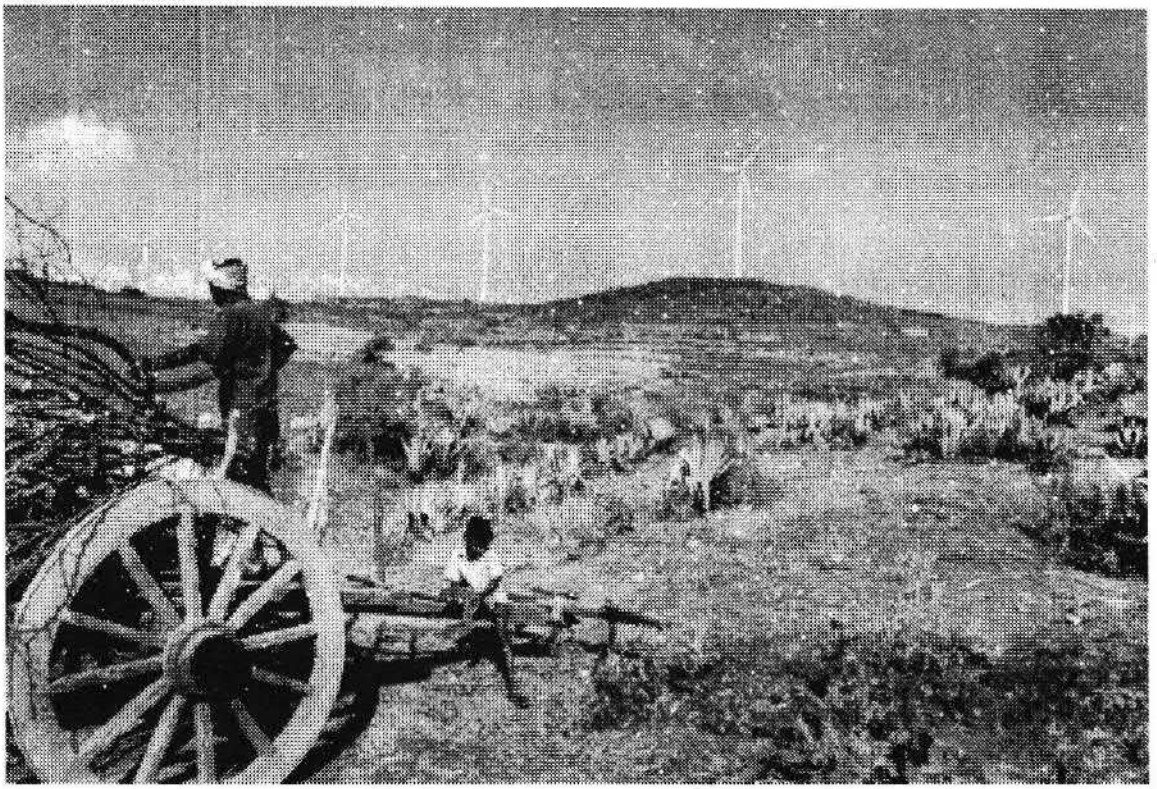
Concept of Family-

Family is a group of people where the socialization of children taking place and all the social, economical, cultural process held up. There are various types of families in society. Family is the main backbone of society. Family is the first school of man. Basic knowledge and information get to man first only by family.

The main function of family is to produce and reproduce persons, biologically and socially.

Family has special history. An ancient time the structure and scope of family were different. With relative the time it has been changing through various stages. Modern family called as a nuclear family which is a gift of modernization, urbanization and globalization. Joint family and nuclear family are the two types of family. Joint family is the characteristics of rural society and nuclear family is the quality of urban society.

Today is a global age in which all things and commodities shows the effects of global phenomenon. All the social, cultural, religious process have been changing by the effects of globalization. In today's global age, man becomes totally global and artificial.



ISSN: 2454-5503
Impact Factor: 3.012 (IIJIF)

Family status in current scenario-

There are various effects and side effects of globalization on family. Mainly raising of the current modern social problems, avoidance of morality, difference among the relatives, anomie social structure and construction etc are the main issues in global age.

Following are the some effects of globalization on family-

1. Social effects-Its truth that by the effects of globalization, joint family is converting into nuclear family .Day by day the population of villages is going to decrees and in cities density of population becoming major problem. Along with migration cultural transmission, complexity of society, secondary relationship etc factors have been affecting in society.

2. Globlization and marginalization-Globalization has given the birth to marginalization. Centralization of wealth, class system, poverty, inequality etc are the different effects of globalization. Marginalization means slightly away from develop issues, ignorance and lack of main facilities which are utilizing by higher groups.

3. Rural Economy of India-Due to global effects and facilities, the growth of Indian rural economy has been increasing with respect to current agriculture productivity. GDP and GNP are affected by the various agriculture implementation programmes and policies.

4. Communication effects-Now a days there is an electronic communication revolution can seen in global society. As per the population the utility of cell phone and other peripheral have been in peak level. Even rural and tribal society also captured by electronic media.

5. Migrant workers-This is a latest and current problem raised in current scenario. For the searching of jobs and survival workers would like to go towards cities. Like Mumbai, Chennai, Delhi, Culcutta etc metropolitan cities are the known examples of migrant workers. They come out from their family, live single or with group in cities and earn the money. In that way most of the joint families transfer into single families.

6. Exitence of fashion and fad in family-With the process of globalization, existence of fashion and fad can seen in society. In spite of culture, civilization raised in society. Each and every stage of life effects of globalization have been noticed in society.

7. Urbanization, industrialization privatilization and modernization are the correlated concepts - Such types of all the concepts are interrelated to each other and frame, develop the particular type of network in society. All the said concepts are closely involved in globalization and affected on social, cultural and economical life of family in modern age.

8. Effects on Education system-In modern world, the effects of globalization directly shows on various contents of social parameters. Boom to the professional and commercial education with the specific development of science and technology, creation and awareness for global education, stress on the human job resources etc are the cognizance issues in globalization process. In this situation the growth and direction of family identify its path.

9. Family structure and scope-Global process affected the family structure and social construction. Small size, heterogeneous groups, money is a center of family, generation gap, secondary relationship etc effects are the gifts of globalization.

10. Divorce and Globalization- In modern, global family the number of divorce cases is increases rapidly. Main causes are global life style and environment at working places. All over India, in

ISSN: 2454-5503
Impact Factor: 3.012 (IIJIF)

various courts the rate of divorce cases is very serious. Even we can say that symbol of degradation of family and society.

Conclusion

Today is a global world. Gloglization is process of nation prosperity and progress as per the current trend. It involves various modern process and concepts. For the development of country, there is no alternative to globalization and related issues.

But while implementation of globalization, we should not ignore our social and familiar construction in society. From all the levels, there should be always taking care and cognizance of global related issues. Identification, sort out and solve the global concerning problems as early as possible and maintain suitable frame of family and society.

Government facilitation plays a key role in this process. At the same time globalization altered available consumption choices, it has also pressured governments to change.

Globalization is close to urbanization, transportation, poverty, industrialization, educational purpose, global issues, social and cultural issues are the components of globalization.

India is a developing country. India needs various things, commodity, science and technology knowledge etc from other develop countries. Developmental countries have to pay revenue as a part of price. That money centralised to the treasury of develop countries. In that way may be we can say that globalization is a one type of side effect to developmental countries

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UGC Approved Journal No: 49229
SJIF Impact Factor(2016) :5.708

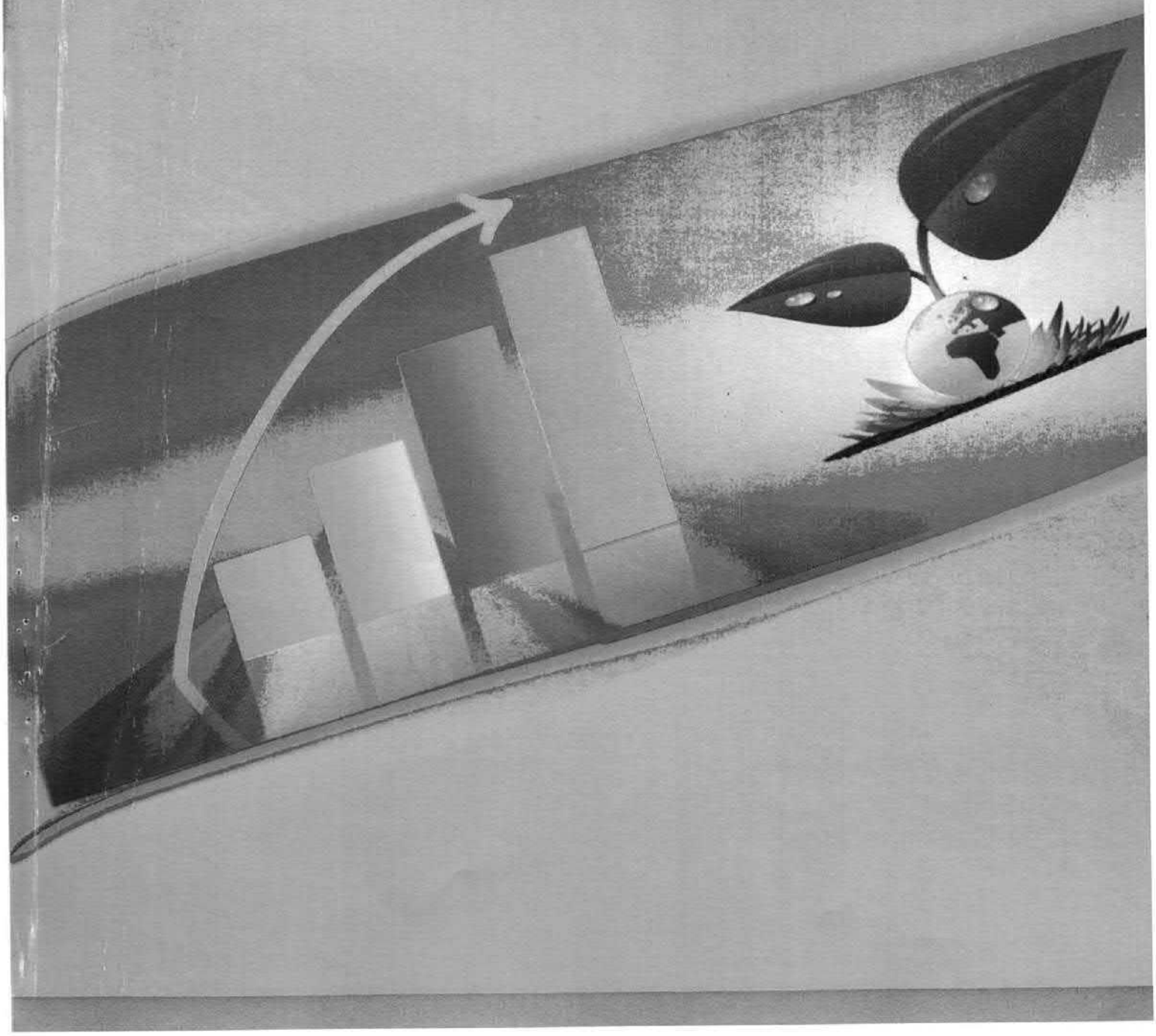
Print ISSN: 2321 - 6247

EPRA International Journal of

ECONOMIC GROWTH AND ENVIRONMENTAL ISSUES

Annual UGC Approved Peer Reviewed & Refereed International Print Journal

volume-5 June - May 2017 - 18



EPRA WISDOM

UGC Approved Journal No: 49229

ISSN: 2321-6247

EPRA International Journal of Economic Growth and Environmental Issues (EGEI)

SJIF Impact Factor:5.708|Volume:5|June-May 2017-18

ROLE OF MULTICULTURALISM, PROFESSIONAL ETHICS AND HUMAN VALUES IN CURRENT SCENARIO

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ABSTRACT

Multiculturalism is a feature of the modern age. Heterogeneous of various types of culture is called as multiculturalism. Macro theory in anthropology is related to the concept multiculturalism. As per the Darwin's theory, the realm of social cultural phenomenon explains the application of technology with environmental aspects for the production and distribution of goods in society. On the Materialism process, Marx and Engel, enlightened with detailed illustration. Multicultural society characterized by cultural pluralism. Basically in the multiculturalism gives the place to cultural variety like linguistic, religious, ethnic diversity of culture which has material and nomadic dimensions.

KEYWORDS: *Multiculturalism, Multicultural society, global culture*

INTRODUCTION

Multiculturalism is a feature of the modern age. Heterogeneous of various types of culture is called as multiculturalism.

Macro theory in anthropology is related to the concept multiculturalism. As per the Darwin's theory, the realm of social cultural phenomenon explains the application of technology with environmental aspects for the production and distribution of goods in society. On the Materialism process, Marx and Engel, enlightened with detailed illustration. Multicultural society characterized by cultural pluralism. Basically in the multiculturalism gives the place to cultural variety like linguistic, religious, ethnic diversity of culture which has material and nomadic dimensions.

Multiculturalism is nature of cultural variation multiculturalism.

Following are the various aspects of multiculturalism

1) Sub culture
2) Caste sub culture.
3) Regional sub culture
4) Occupational sub culture
5) Centro culture.

Marvin Harris has proposed the theory of cultural materialism. In which he has mentioned the various aspects related to race, religion, cast which try to accept the life and frame geographical structure.

India is the well-known example of cultural pluralism and multiculturalism in the world. Multiculturalism is filled towards the cultural diversity.

It is a universal and cultural determination phenomenon in world.

Multiculturalism means place to the civilization. Civilization means coming towards modern process like modernization, urbanization and industrialization. It is a symbol of refinement and progress. Existence of large number of people in cities, specially stratified and governing and ruling by elites in organized political system.

SCOPE OF MULTICULTURALISM

Today, the global culture concept has been raised in society. Migration, development, natural calamities bind to people to move other places. Technology, transportation, communication, connectivity, hypermedia cultural effect etc are responsible for increasing the dimension of global culture. The world coming together and that's why multiculturalism is coming up is current scenario.

Ethnic resurgence and cultural assimilation are the main components of multiculturalism. Multiculturalism is an advance part of cultural pluralism. Pluralistic societies moving towards modern life style are a main cause of multiculturalism.

Definition-

Coping and curbing the divisive pressure in pluralistic or multi- ethnic societies is the adaptation of a public policy based on mutual respect and tolerance for cultural differences called as multiculturalism. It involves the public policy for managing the societal cultural diversity. There is common difference between cultural pluralism and multiculturalism. Globalization is also resulted the multiculturalism phenomenon.

Multiculturalism explains the existence, promotion of multi cultural traditions. It allows people to truly express within society for acceptance of other things for better social issues.

Multiculturalism is formed to the migration of various ethnic groups in one society.

Components of Multiculturalism

1) Religious
2) Linguistic
3) Territory
4) Race

There is need to adopt following points for betterment of multiculturalism-

1) Awareness
2) Empathy
3) Tolerance
4) Compassion
5) Non Discrimination

PROFESSIONAL ETHICS

Morals and values are important to maintain social control and dignity in the society. Moral are standard norms which help to guide our behaviors and accept behavior of value reflect own behavior attitude judgment and self esteem.

Ethic is a philosophical term represents the positive human action in society. Morality, integrity, sincerity and responsibility are the pillars of ethics. It is one type of applied moral science.

Human Values = Morals + Values + Ethics

Human values are integral and core part to maintain the status in society. Human values are form and values of life.

Today is the age of globalization. Many organizations and management provide the job to the job seekers. In organization, work culture promotes the work ethics of particular organization. There is a particular code of conduct. Good work, suitable working method controls the result into the expected productivity. Team work service, attitude, learning, respect to others, courage sharing and caring are important in every organization.

Profession is a self job or occupation and service. After stipulated time, man become perfect in his work and acquires professionalism, expertise and try to maintain quality work in professional ways.

ETHICS

Ethics Means identification of good and rights for society. Every organization expects

professional ethics. Corporate values are common phenomenon and to indulge in today's age. Ethics and virtues, law, facts, rights, environment responsibility etc are the co related terms. Avoidance of professional ethics is dangerous to each organization.

Engineering ethics is inserted in the engineering area. Ethics promote the ethics and values among the engineers. There should be suitable correlations about safely responsibilities and rights. To take risk is harmful work but it is essential in organization to follow the duty and role of management. Today there is most important to professional ethics in engineering.

Professional ethics start from family. Professional ethics carry forward through socialization process. Life in school, college, family and friend are components of ethics. The value education getting in childhood impress on future life. Therefore the most schools and colleges provide value education to the students. Value education is based on universal, rational and harmony pillars.

Professional ethics is cause of nation development through public administration. Transparent and professional administration of organization boosts the quality of work. Ethics and human interface reflect on working culture.

Professional ethics and values are the two sides of same coin.

Socialization is refers to the inculcation of new things and carry forward to others. Human values and directives principle of state policy have some similarity. In chapter 4th of Indian constitution as per the article 14, mentioned the directive principle of state policy.

Emotional intelligence, social competence, social skills, influence on job performance etc are some of the examples of professional ethics.

For promotion or development of professional ethics, following points are essential-

1) Leadership qualities and team work
2) Developing self awareness and mindfulness
3) Efficiency, expertise and equality in own field.
4) Truth
5) Work dedication
6) Honesty
7) Non violence
8) Courage and daring
9) Self discipline
10) Faith and responsibility
11) Impartiality and objectivity.
12) Concentration and mindfulness
13) Emphasis on political professional and personal responsibility.
14) Fallowness of legislation and code of conduct
15) Diligence and respect of law
16) Position of legal, personal, organization values.
17) Quality and excellence
18) Tolerance and openness
19) Creativity and Service
20) Humanity and Neutrality
21) Implementation of code of ethics and conduct

Professional Ethics are effective and useful in following ways-

1. Corruption related issues.
2. Nepotism
3. Administrative lacunas, loopholes, secrecy
4. Leaking of information
5. The imperative related to legality accountability and responsibility.
6. Red tapizem
7. Solution of ethical conflict and negligence
8. Compromise in work due to personal issues.
9. Cases on violations rules and regulation.
10. Dysfunctional system
11. Lack of transparency and poor incentive structure.

Ethics are the principles of right conduct.

Professional ethics help to promote improvement in work culture and quantity of service delivery.

Ethics maintain standard of living, awaking about responsibilities, moral delusions. Ethics is a system of accepted behavior, mores and values. As per the Latin a word, ethics is eticus means morals rule of conduce towards humanity. Ethics is a part of philosophy. Ethics suggested in Ramayana, Mahabharata, Bhagvad Gita, Buddha Charita, Arthashastra, Panchtantra, Kuran , Kadambari and Hitopadesh.

In professional ethics, need of the following factors-

1) Seek to acquire professional code of conduct.
2) Acquired knowledge, skills and duties.
3) Setting target of own work and performance.
4) Positive collaboration between machine and man.
5) Not influence by social economical, political afflation in performance of their duties and role.
6) Positive behaviour with soft skills, dignity and alertness with standard of performance.
7) Pursuit of excellence and expertise in own field with suitable training.
8) Encouragement and recognition about creativity and initiative among subordinate.
9) Maintaining of confidentiality in working organization.
10) Trust full with legitimate confidence about towards work.
11) Update self and maintain the dignity in own organization.
12) Promote the effective, positive control system.
13) Suitable life style, social relation, cultural identity, physical power and social interaction.
14) Prestige and status in society
15) Authority, ability utilization and achievement.
16) Stress management effectively.

Under professional ethics following are the mainly considerable points-

1) Healthy interaction with family member
2) Right code of conduct with higher authority and subordinates.
3) Place to truth, love, peace, tolerance, and non violence, morality, Goodness, understanding, liberal, motivation, and balancing about emotional intelligence
4) Prompt leadership towards conceptual frame work.

Types of Ethics-

1) Metal ethics
2) Normative ethics
3) Applied ethics
4) Descriptive ethics

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Bioscience Discovery, 8(3): 582-587, July - 2017

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Print & Online, Open Access, Research Journal Available on http://jbsd.in
ISSN: 2229-3469 (Print); ISSN: 2231-024X (Online)
Research Article

A Herpetofaunal Inventory of Vidarbha Region, Maharashtra, India

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Article Info

Received: 01-06-2017,
Revised: 26-06-2017,
Accepted: 29-06-2017

Keywords:
Herpetofauna, India, Maharashtra, Vidarbha.

Abstract

The present report provides knowledge about the herpetofauna of Vidarbha region of Indian state Maharashtra. The present inventory of herpetofauna has been compiled primarily from articles and technical reports published in scientific journals. However reports in newsletters, unpublished reports, personal field observations and personal communications with other herpetologists and field workers have also been taken into account. Information on species distribution and taxonomy has been compiled from literature published over past two decades until July 2016. The review cleared the presence of seventy species belongings to four order and seventeen families. There are, in future, chances of more species being reported because few pockets and habitats in the Vidarbha region required extensive exploration.

INTRODUCTION

The diversity of flora and fauna on the earth and its genesis has long been a source of questionable curiosity (Joshi *et al.*, 2015). The study of biodiversity includes both the inherent and anthropocentric principles allied with it. The importance of these incredible biological factors is renowned in relation of the ecosystem services. Biodiversity is the foundation for maintaining the ecosystem and the operative facets of the species that offers many goods and services to for human well being. Examinations of species diversity of a region facilitate the evaluation of potential serviceable role of the species. In any ecosystems, observing the species diversity can be used as a contrivance to minimize the mismanagement and contamination in urbanized, industrial, rural, and managed areas by human (Baumgartner, 2007). Extending this view, the species diversity review in any ecosystems is essential to understand the effect of anthropocentric development on the integrity and sustenance of ecosystem.

The inventories of species diversity are immense resource that provides recent and previous information on their topographic distribution. The elementary species occurrence data have various applications. Species inventories that contain such elementary and collective species-occurrence data, plays a fundamental role in providing information on the status of species transpire in different spatial scales. These inventories have been used for taxonomic and biogeographic studies as well for conservation planning, reserve selection, climate change studies, agriculture, forestry and fishery, and species translocation studies (Chapman, 2005a). The meticulousness of the taxonomic and spatial information is valuable reflection for determination of data quality and validation of the species occurrence data. Hence the significance of the data excellence in the inventory of Indian herpetofauna hardly needs emphasis (Chapman, 2005b). In this perspective, the present communication is part of an effort to verify the validity of herpetofaunal species based on a review of the earlier checklists published over the past two decades.

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Finally, a comprehensive herpetofaunal inventory of Vidarbha region of Maharashtra has been provided along with source literature.

Materials and methods

Study area: Vidarbha is one of the most diversified Regions in Maharashtra State of India, with respect to biodiversity. Its healthy climate, mountainous terrain, rugged configuration and sudden fall in elevation are phenomenal. It is located between 20.9374° north and 77.7796° east. It has a total area of 97,321 square kilometers. The climatic condition of this district is characterized by a hot summer, well-distributed rainfall during the south-west monsoon season and generally dry weather during rest of the year. The cold season is from December to February. The average annual rainfall in the district is 795.7 mm. During summer the mean daily maximum temperature in summer was 44.2° C to minimum as 26.7° C while it decreased toward winter with the mean daily maximum temperature was 27.8° C and minimum 14.9° C.

Primary inventory: The present inventory of herpetofauna has been compiled primarily from articles and technical reports published in scientific journals. However reports in newsletters, unpublished reports, personal field observations and personal communications with other herpetologists and field workers have also been taken into account. Information on species distribution and taxonomy has been compiled from literature published until December 2016.

Taxonomic Treatise: The list provided, is at the species level and the taxonomy follows, Daniel (2002), Das (2003), Whitaker and Captain (2004), Ahmed *et al.* (2009), Khaire (2010) and Venugopal (2010).

Validity of species listed: Based on the distributional records available, the validity of the species listed in the earlier checklists of India, particularly Maharashtra and neighborhood published in the past two decades has been reviewed.

RESULTS/ SPECIES ACCOUNTS

The present comprehensive inventory is based on a review of the earlier checklists of the herpetofauna published over a past decade. The review cleared the presence of following seventy species belongings to four order and seventeen families (Table 1).

Table 1: A Herpetofaunal inventory of Vidarbha region, Maharashtra, India

Sr.	Order	Family	Species	Common name
1.	Anura	Bufonidae	*Duttaphrynus melanostictus* (Schneider,1799)	Asian common toad
2.			*Duttaphrynus stomaticus* (Lutken, 1864)	Indian marbled toad
3.		Dicroglossidae	*Euphlyctis cyanophlyctis* (Schneider, 1799)	Indian skipper frog
4.			*Euphlyctis hexadactylus* (Lesson, 1834)	Indian green frog
5.			*Fejervarya limnocharis* (Gravenhost, 1829)	Asian grass frog
6.			*Hoplobatrachus tigerinus* (Daudin,1803)	Indian bullfrog
7.			*Hoplobatrachus crassus* (Jerdon,1853)	Jerdon's bullfrog
8.			*Sphaerotheca breviceps* (Schneider, 1799)	Indian burrowing frog
9.		Microhylidae	*Microhyla ornata* (Dumeril and Bibron, 1841)	Asian ornate frog
10.			*Kaloula taprobanica* (Parker 1934)	Asian painted frog
11.		Ranidae	*Hylarana malabarica* (Tshudi, 1838)	Fungoid frog
12.		Rhacophoridae	*Polypedatus maculatus* (Gray, 1830)	Indian tree frog
13.	Testudines	Trionychidae	*Lissemys punctata* (Lecepede, 1788)	Indian flapshell turtle
14.	Squamata (Sauria)	Agamidae	*Calotes versicolor* (Daudin, 1802)	Indian garden lizard
15.			*Calotes rouxii* (Dumeril and Bibron, 1837)	Indian forest lizards
16.			*Sitana ponticeriana* (Cuvier, 1829)	Fan throated lizard
17.			*Psammophilus blanfordanus* (Stoliczka, 1871)	Blanford's rock agama
18.		Chamaeleonidae	*Chamaeleon zeylanicus* (Laurenti, 1768)	Indian chamaeleon
19.		Gekkonidae	*Geckoella collegalensis* (Beddome 1870)	Forest spotted gecko
20.			*Geckoella nebulosus* (Agawal and Karanath 2015)	Common spotted gecko

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21.			*Hemidactylus brookii* (Gray, 1845)	Brook's house gecko
22.			*Hemidactylus flaviviridis* (Murray, 1886)	Yellow-green House Gecko
23.			*Hemidactylus frenatus* (Schlegel, 1836)	Asian house gecko
24.			*Hemidactylus giganteus* (Stoliczka, 1871)	Giant Indian gecko
25.			*Hemidactylus hemchandrai* (Dandge and Tiple 2015)	Hemchandrai's gecko
26.			*Hemidactylus leschenaultia* (Dumeril and Bibron, 1836)	Common bark gecko
27.			*Hemidactylus triedrus* (Daudin, 1802)	Termite hill gecko
28.		Scincidae	*Eutropis beddomii* (Jerdon, 1870)	Beddome's skink
29.			*Eutropis carinata* (Schneider, 1799)	Keeled grass skink
30.			*Eutropis macularius* (Blyth, 1853)	Bronze grass skink
31.			*Lygosoma lineate* (Gray, 1839)	lined writhing skink
32.			*Lygosoma punctatus* (Gmelin, 1799)	Spotted supple skink
33.		Varanidae	*Varanus bengalensis* (Daudin, 1803)	Bengal monitor lizard
34.	Squamata (Ophida)	Typhlopidae	*Grypotyphlops acutus* (Dumeril and Bibron, 1844)	Beaked worm snake
35.			*Ramphotyphlops braminus* (Daudin, 1803)	Common worm snake
36.		Pythonidae	*Python molurus molurus* (Linnaeus, 1758)	Indian rock python
37.		Boidae	*Gongylophis conicus* (Schneider, 1801)	Common sand boa
38.			*Eryx johnii* (Russell, 1801)	Red sand boa
39.		Colubridae	*Ahaetulla nasuta* (Lacepede, 1789)	Common vine snake
40.			*Amphiesma stolatum* (Linnaeus, 1758)	Striped keelback
41.			*Argyrogena fasciolata* (Shaw, 1802)	Banded racer
42.			*Atretium schistosum* (Daudin 1803)	Olive kill back
43.			*Boiga forsteni* (Dumeril, 1854)	Forsten's cat snake
44.			*Boiga trigonata* (Bechstein, 1802)	Indian cat snake
45.			*Coelognathus helena helena* (Daudin, 1803)	Common trinket snake
46.			*Coelognathus helena monticollaris* (Schulz, 1992)	Montane trinket snake
47.			*Coronella branchyura* (Gunther, 1866)	Indian smooth snake
48.			*Dendrelaphis tristis* (Daudin, 1803)	Bronzback tree snake
49.			*Elachistodon westermanni* (Reinhardt, 1863)	Indian egg eater
50.			*Lycodon aulicus* (Linnaeus, 1758)	Common wolf snake
51.			*Lycodon flavomaculatus* (Wall, 1907)	Yellow spotted wolf snake
52.			*Lycodon striatus* (Shaw, 1802)	Barred wolf snake
53.			*Macropisthodon plumbicolour* (Cantor, 1839)	Green keelback
54.			*Oligodon arnesis* (Shaw, 1802)	Common kukri snake
55.			*Oligodon taeniolatus* (Jerdon, 1853)	Russell's kukri snake
56.			*Psammophis condanarus* (Merrem, 1820)	Condanarus sand snake
57.			*Psammophis leithii* (Gunther, 1869)	Leith's sand snake
58.			*Psammophis longifrons* (Boulenger, 1897)	Stout sand snake
59.			*Ptyas mucosa* (Linnaeus, 1758)	Indian rat snake
60.			*Sibynophis subpunctatus* (Dumeril, 1854)	Black headed snake
61.			*Xenochrophis piscator* (Schneider, 1799)	Checkered keelback
62.		Elapidae	*Bungarus caeruleus* (Schneider, 1801)	Common krait
63.			*Bungarus fasciatus* (Schneider, 1801)	Banded krait
64.			*Bungarus sindanus walli* (Wall, 1908)	Wall's sind krait
65.			*Calliophis melanurus* (Shaw, 1802)	Slender coral snake
66.			*Naja naja* (Linnaeus, 1758)	Indian spectacle cobra
67.			*Daboia russelii* (Shaw and Nodder, 1797)	Russell's viper
68.			*Echis carinatus* (Schneider, 1801)	Saw-scaled viper
69.			*Trimeresurus gramineus* (Shaw, 1802)	Green pit viper
70.	Crocodilia	Crocodylidae	*Crocodylus palustris* (Lesson, 1831)	Mugger crocodile

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Discussion

Vidarbha is most diversified region with lush green deciduous forests through large protected areas which are home to variety of flora and fauna. It has approximately 37,251 km^2 forest cover. Vidarbha also has many popular wildlife sanctuaries and parks *viz.* Melghat in Amaravti, Amba-barwa and Nalganga in Buldhana, Tadoba-Andhari in Chandrapur, Nagzira and Navegaon Bandh in Gondia, etc. The region is represented with rich herpetofaunal diversity. The utility of herpetofaunal species as indicators of environmental conditions is a basis for preparation of present inventory.

The present inventory of herpetofauna of Vidarbha region is based on available locality records by providing relevant source literature on specimens that would be ensuring its quality. Because, the accurate and precise quality data on species occurrences are imperative for the assessment of conservation status and drawing management considerations hence used for further research purposes such as predictions on species distributions, habitat suitability, and threat assessments etc.

Many researchers from Vidarbha region had given their valuable contribution in development of herpetofaunal studies. The monumental works on Herpetofauna of Vidarbha region mainly includes the Wadatkar (2003), Captain *et al.* (2005), Nande and Deshnukh (2007), Harney *et al.* (2009), Joshi (2009), Sawarkar and Kasambe (2009), Harney (2011), Joshi (2011), Narayanan (2012), Dhande and Khandare (2013), Kumbhar *et al.* (2013), Uke *et al.* (2013), Ingle *et al.* (2014), Joshi *et al.* (2014), Charjan and Joshi (2015), Dandgge and Tiple (2015), Deshmukh *et al.* (2015), Joshi *et al.* (2015), Kakde and Thakur (2015), Khobragade and Pawar (2015), Pandharikar *et al.* (2015 a, b and c), Amjad *et al.* (2016), Joshi *et al.* (2016), Joshi and Tantarpale (2016), Wagh *et al.* (2017) to name a few. These studies explained the herpetofaunal dominance in the terrestrial and aquatic ecosystems and also the provision of ecosystem services (Sirsat *et al.*, 2016).

According to Joshi *et al.* (2015), the herpetofauna is always threatened by anthropogenic and environmental factors. The diverse habitats of the Vidarbha Region are rapidly changing due to new irrigation projects and industrialization. Forest areas are being de-notified for implementing development projects such as mining, industry, communication and tourism. This has resulted in alternating climate as well shrinkage, fragmentation, degradation and destruction of natural habitats. Road accidental killing on highways across wildlife refuges are an intrusion and affect the wildlife and its habitats adversely. Misconceptions and fear about these species especially about snakes are also threatening this important creature of the ecosystem.

In parity with the herpetofaunal species observed in Vidarbha region, Maharashtra, India, it may be assumed that the species carry out diverse functional roles for the sustenance of the ecosystems. The availability of the green space and the heterogeneity of the habitats in terms of the available vegetation and allied factors that render stability to the population and species assemblages in the landscapes are possibly important contributors to the observed variations in the saurian species observed in the present study. The present diversity study is confined to limited area and selected habitats. There are, in future, chance of more species being reported because of few pockets and habitats in the studied area required more extensive exploration.

Acknowledgements

The authors are thankful to Dr K.M. Kulkarni, Former Vice Chancellor (Swami Ramanand Tirtha Marathwada University, Nanded, India) and Former Director (Higher Education, Government of Maharashtra, Pune, India) for erudite guidance during conduct of this study.

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How to Cite this Article:

Joshi PS, Charjan AP and VT Tantarpale, 2017. A Herpetofaunal Inventory of Vidarbha Region, Maharashtra, India. *Bioscience Discovery*, **8**(3):582-587.

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International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.10 No.12, pp 22-26, 2017

Synthesis and characterization of some new chlorosubstitured Δ^2- pyrazoles under microwave irradiation

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Abstract : Heterocyclic system containing pyrazole ring and its derivative have attracted the attention of chemists on account of the significant medicinal properties associated with them. The proposed study deals with the synthesis and characterization of newly synthesized chlorosubstituted Δ^2 -pyrazoles under the microwave irradiation on micro-scale quantity. The short reaction times and expanded reaction range was offered by themicrowave assisted synthesis to the chemists. The reaction of chromones and phenylhydrazine hydrochloride result in the formation of Pyrazoles.
The newly synthesize compounds were characterized on the basis of FTIR, H^1NMR, Uv and Massspectroscopic techniques.
Key Words : Chromanone,chromone,Pyrazole, H^1 NMR, FTIR, Uv and Mass spectra.

Introduction:

Heterocyclic chemistry is the branch of organic chemistry dealing with the synthesis, properties and applications of the heterocycles. Pyrazole is the five membered heterocyclic compound with two nitrogen atoms in the 1, 2-position.

Heterocyclic system containing pyrazolering and its derivative have attracted the attention of chemists on account of the significant medicinal properties associated with them. Pyazoles are reported to have properties such asantibacterial[1],hypoglycamic agent[2], anti-inflammatory[3], antitumour[4]analgesic agent and antipyretic property[5].

Ling[6]*et al* have investigated pyrazoles by the action of 2, 3-dihydropyridine 4, hydrazine hydrate and diethyl maleate. Brone[7]*et al* have synthesized a metal-free continuous flow method for the generation of a variety of N-arylatedpyrazoles.

The proposed study deals with the synthesis and characterization of newly synthesized chlorosubstituted Δ^2-pyrazolesby the reaction of chromones and phenylhydrazinehydrochloride by using the microwave irradiation.

Materials and Methods:-

There are various methods reported for the synthesis of pyrazoles. It is interesting to synthesize and characterized some new chlorosubstitutedΔ^2-pyrazoles from diketone on reactions with aldehydes in ethanolic medium via chromone. The present study deals with the synthesis of pyrazoles through microwave irradiation.The purity of synthesized compounds was tested by TLC. All melting points measured in open glass

capillary tube. All reactions were carried out in laboratory microwave oven (New microwave system model (R-210D, 800w 24L light-up Dial, SHARP TLABMA638). The structures of the newly synthesized compounds were confirmed by using spectroscopic technique via Uv, FTIR, H^1NMR and Mass. The spectral analysis was carried out at SAIF and CIL, Punjab University, Chandigarh, (India).General procedure for the synthesis of pyrazoles:-

(1) Synthesis of 2-hydroxy 3,5-dichloroacetophenone :- (A)

Substitutedphenylacetate (25ml) was mixed with anhydrous aluminiumtrichloride(60g) and heated at 120^0C for 45 minutes on oil bath.The reaction mixture was decomposed by ice cold water containing a little HCl to get the crude product. A greenish white solid of the compound (A) was obtained, yield: 57%,m.p: 59^0C.

Spectral data for compound (A):-

(a) FTIR :- (KBr, cm^{-1}): 3429(OH stretching), 3069 (Ar-CH stretching), 2974 (C-H stretching in CH_3), 1648 (C=O stretching), 643(C-Clstreching).
(b) H^1 NMR: - (400MHz, $CDCl_3$, δ ppm): 2.65 (S, 3H, $COCH_3$), 7.26-7.62 (m, 2H, Ar-H), 12.71 (s, 1H, OH).
(c) UV: - The UV-VIS spectrum of the compound (A) recorded in $CHCl_3$ showed λmax value 250nm corresponding to $n\rightarrow\Pi^*$ transition.
(d) Mass (Ab) **: -** (m/z) = 205.190, 162,134.

(2) Synthesis of 2-aroloxyacetophenone:-(Aband Af)

2-Hydroxy acetophenone(0.04M) and aromatic acid(0.05M) were suspended in dry pyridine (5ml) and to this $POCl_3$ (3 ml) was added dropwise with constant stirring and cooling. The reaction mixture was kept for overnightand then worked up by the dilution andacidification with ice cold HCl (10%) to neutralize pyridine. The solid productthus obtained crystallized from ethanol to get the compound (Af). Yield 71% m.p:76^0C.

2-Hydroxy acetophenone(0.04mol)and aromatic acid(0.05mol) were suspended in 10% NaOH (35 ml). The reaction mixture was shaken for about 25min then product was filtered. The solid productthus obtained crystallized from ethanol to get the compound (Ab). Yield: 67%,m.p: 72^0C.

Spectral data for compound (Af):-

(a) FTIR :-(KBr, cm^{-1}):3070 (Ar-CH stretching), 2974 (C-H stretching in CH_3), 1779, 1740 (C=O stretching), 1021 (C-O stretching), 740 (C-Clstreching).
(b) H^1 NMR: - (400MHz, $CDCl_3$, δ ppm): 2.65 (S, 3H, $COCH_3$), 7.26-7.64 (m, 5H, Ar-H).
(c) UV: - The UV-VIS spectrum of the compound (Af) recorded in $CHCl_3$ showed λmax value nm corresponding to $n\rightarrow\Pi^*$ transition.

Spectral data for compound (Ab):-

(a) FTIR :- (KBr, cm^{-1}): 3082 (Ar-CH stretching), 2925 (C-H stretching in CH_3), 1648, 1776 (C=O stretching), 1608 (benzene), 1114 (C-O stretching), 642 (C-Clstreching).
(b) H^1 NMR: - (400MHz, $CDCl_3$, δ ppm): 2.55 (s, 3H, $COCH_3$), 7.26-7.62 (m, 7H, Ar-H).
(c) UV: - The UV-VIS spectrum of the compound (Ab) recorded in $CHCl_3$ showed λmax value 280nm corresponding to $n\rightarrow\Pi^*$ transition.
(d) Mass: - (m/z) = 309,189, 161, 133.

(3) Synthesis of 1-(2-hydroxyaryl)-3-aryl-1, 3-propanediones :- (B and F)

2-Aroyloxy acetophenone (0.05mol)was dissolved in dry pyridine (40 ml). The solution warmed upto 60^0C and pulverized KOH (0.15 mol)was added slowly with constant stirring. The reaction mixture was kept for overnight and then worked up by the dilution and acidification with ice cold HCl (10%). The solid product thus obtained crystallized from ethanol to get the compounds (B and F). M.p: 99^0C and 120^0C.

Spectral data for compound (B):-

(a) FTIR :- (KBr, cm^{-1}): (B):- 3421 (Ar-OH – stretching), 3074 (Ar-CH-streching), 1768 (C=O stretching), 1680 (C=O stretching), 683 (C-Cl stretching).
(b) H^1 NMR: - (400MHz, $CDCl_3$, δ ppm): 2.22 (s, 2H, $-CH_2-$), 7.52-7.62 (m, 7H, Ar-H), 12.66 (s, 1H, OH).
(c) UV: - The UV-VIS spectrum of the compound (B) recorded in $CHCl_3$ showed λmax value 380nm corresponding to $n\rightarrow\Pi^*$ transition.
(d) Mass: - (m/z) = 309,204,190,162, 133, 132.

Spectral data for compound (F):-

(a) FTIR :- (KBr, cm^{-1}): 3376 (Ar-OH – stretching), 3070 (Ar-CH-streching), 1648 (C=O), 1609 (C=O stretching), 1648 (C=O stretching), 740 (C-Cl stretching).
(b) H^1 NMR: - (400MHz, $CDCl_3$, δ ppm): 2.65 (s, 3H, $COCH_3$), 7.26-7.74 (m, 7H, Ar-H), 12.71 (s, 1H, OH).
(c) UV: - The UV-VIS spectrum of the compound (F) recorded in $CHCl_3$ showed λmax value 320 nm corresponding to $n\rightarrow\Pi^*$ transition.

(4) Synthesis of3-aroylchromanones :(BC1 and FP1)

3-Aroylchromanone was prepared by using microwave irradiation. A mixture (0.01mol) propadiones (Band F), (0.01mol) of aromatic aldehyde dissolved separately in (25ml)ethanol with (0.5 ml)piperidine and irradiated for 2-3 min in microwave. The reaction mixtures on acidification with HCl (10%), followed by washing with water.The solid product thus obtained crystallized from ethanol to get the compounds (BC1 and FP1).

Spectral data for compound (BC1):-

(a) FTIR :- (KBr, cm^{-1}): (BC1):- 3073 (Ar-CH-streching), 2919, 2850 (C-H stretching in CH_3), 1778 (C=O), 1663 (C=O), 1174 (C-O stretching), 697 (C-Cl stretching).
(b) H^1 NMR: - (400MHz, $CDCl_3$, δ ppm): 1.77 (s, 3H,$-CH_3-$), 5.55 (s, 1H, -CH), 6.59-7.91 (m, 14H, Ar-H).
(c) UV: - The UV-VIS spectrum of the compound (BC1) recorded in $CHCl_3$ showed λmax value 350nm corresponding to $n\rightarrow\Pi^*$ transition.
(d) Mass: - (m/z) = 437,422, 320,243,215.

Spectral data for compound (FP1):-

(a) FTIR :- (KBr, cm^{-1}): (FC1): - 3069 (Ar-CH-streching), 1777 (C=O), 1738 (C=O), 1434 (C=N), 1022 (C-O stretching), 644 (C-Cl stretching).
(b) H^1 NMR: - (400MHz, $CDCl_3$, δ ppm): 5.35-6.98 (d, 2H, >C-C<), 6.98-7.64 (m, 8H, Ar-H).
(c) UV: - The UV-VIS spectrum of the compound (FP1) recorded in $CHCl_3$ showed λmax value nm corresponding to $n\rightarrow\Pi^*$ transition.

(5) Synthesis of3-aroychromones :- (BC2 and FP2)

The 3-aroylchromanone (BC1 and FP1)(0.01mol) treated separately with few crystals of iodine and (25ml) DMSO in microwave. After cooling the the reaction mixture was diluted with water. The solid product thus obtained crystallized from petroleum ether to get the compounds (BC2 and FP2).

Spectral data for compound (BC2):-

(a) FTIR :- (KBr, cm^{-1}): (BC2):- 2917 (Ar-CH-streching), 2849 (C-H stretching in CH_3),1632 (C=O), 1551 (C=O), 1088 (C-O stretching), 562 (C-Cl stretching).
(b) H^1 NMR: - (400MHz, $CDCl_3$, δ ppm):1.77 (s, 3H,$-CH_3$), 6.74 (s, 1H, -C=CH-), 7.04-7.82 (m, 12H, Ar-H).
(c) UV: - The UV-VIS spectrum of the compound (BC2) recorded in $CHCl_3$ showed λmax value 400nm corresponding to $n\rightarrow\Pi^*$ transition.
(d) Mass: - (m/z) = 435,420, 318, 213

Spectral data for compound (FP2):-

(a) **FTIR :-** (KBr, cm^{-1}): (FP2): - 3076, 1697 (C=O), 1649 (C=O), 1439 (C=N), 1088 (C-O stretching), 740 (C-Cl stretching).
(b) **H^1 NMR: -** (400MHz, $CDCl_3$, δ ppm): 6.99-7.77 (m, 7H, Ar-H).
(c) **UV: -** The UV-VIS spectrum of the compound (FP2) recorded in $CHCl_3$ showed λmax value nm corresponding to $n\rightarrow\Pi^*$ transition.

Synthesis of pyrazole: - :- (BC3 and FP3)

The 3-aroychromones (BC2 and FP2) (0.01M)separately treated with phenyl hydrazine hydrochloride in (7 ml) DMSO with few drops of piperidine under microwave condition for 4min. The reaction mixture on acidification with HCl (10%), followed by washing with sodium bicarbonate and water gave the compounds. The solid product thus obtained crystallized from ethanol to get the compounds (BC3 and FP3).

Spectral data for compound (BC3):-

(a) **FTIR :-** (KBr, cm^{-1}): (BC3):- 3376 (OH – stretching), 2922 (Ar-CH-stretching),2853 (C-H stretching in CH_3), 1665 (C=O stretching), 1449 (C=N stretching), 758 (C-Clstretching).
(b) **H^1 NMR: -** (400MHz, $CDCl_3$, δ ppm): 1.55 (s, 3H,-CH_3), 5.59 (s, 1H,-CH), 7.20-8.11 (m, 16H, Ar-H), 12.01(s, 1H, OH).
(c) **UV: -** The UV-VIS spectrum of the compound (BC3) recorded in $CHCl_3$ showed λmax value 310nm corresponding to $n\rightarrow\Pi^*$ transition.
(d) **Mass: -** (m/z) = 525,510, 433, 405, 303.

Spectral data for compound (FP3):-

a) **FTIR :-** (KBr, cm^{-1}): (FP3): - 3354 (OH – stretching), 3074 (Ar-CH-stretching), 1666 (C=O stretching), 1495 (C=N stretching), 754 (C-Cl stretching).
b) **(b)UV: -** The UV-VIS spectrum of the compound (FP3) recorded in $CHCl_3$ showed λmax value 390 nm corresponding to $n\rightarrow\Pi^*$ transition.
c) **(c)H^1 NMR: -** (400MHz, $CDCl_3$, δ ppm): 11.97 (s, 1H, OH), 6.96-7.21 (d, 2H, CH_2 in furyl), 7.25-8.26 (m, 14H, Ar-H).

Result and Discussion:-

The present work deals with a new series of (*Z*) - (3-(3, 5-dichloro-2-hydroxyphenyl)-1-phenyl-5-(1-phenylprop-1-en-2-yl)-1*H*-pyrazol-4-yl) (phenyl) methanone (BC3) and (3-(3, 5-dichloro-2-hydroxyphenyl)-1-phenyl-5-(pyridin-2-yl)-1*H*-pyrazol-4-yl)(furan-2-yl) methanone (FP3) were synthesized by phenyl hydrazine hydrochloride and chromones. These reactions were carried out in micro quantity through microwave irradiation. The structures of the newly synthesized compounds were established on the basis of spectroscopic evidences and their synthesis by conventional methods. The title compounds (BC3 and FP3) were prepared according to the following scheme:

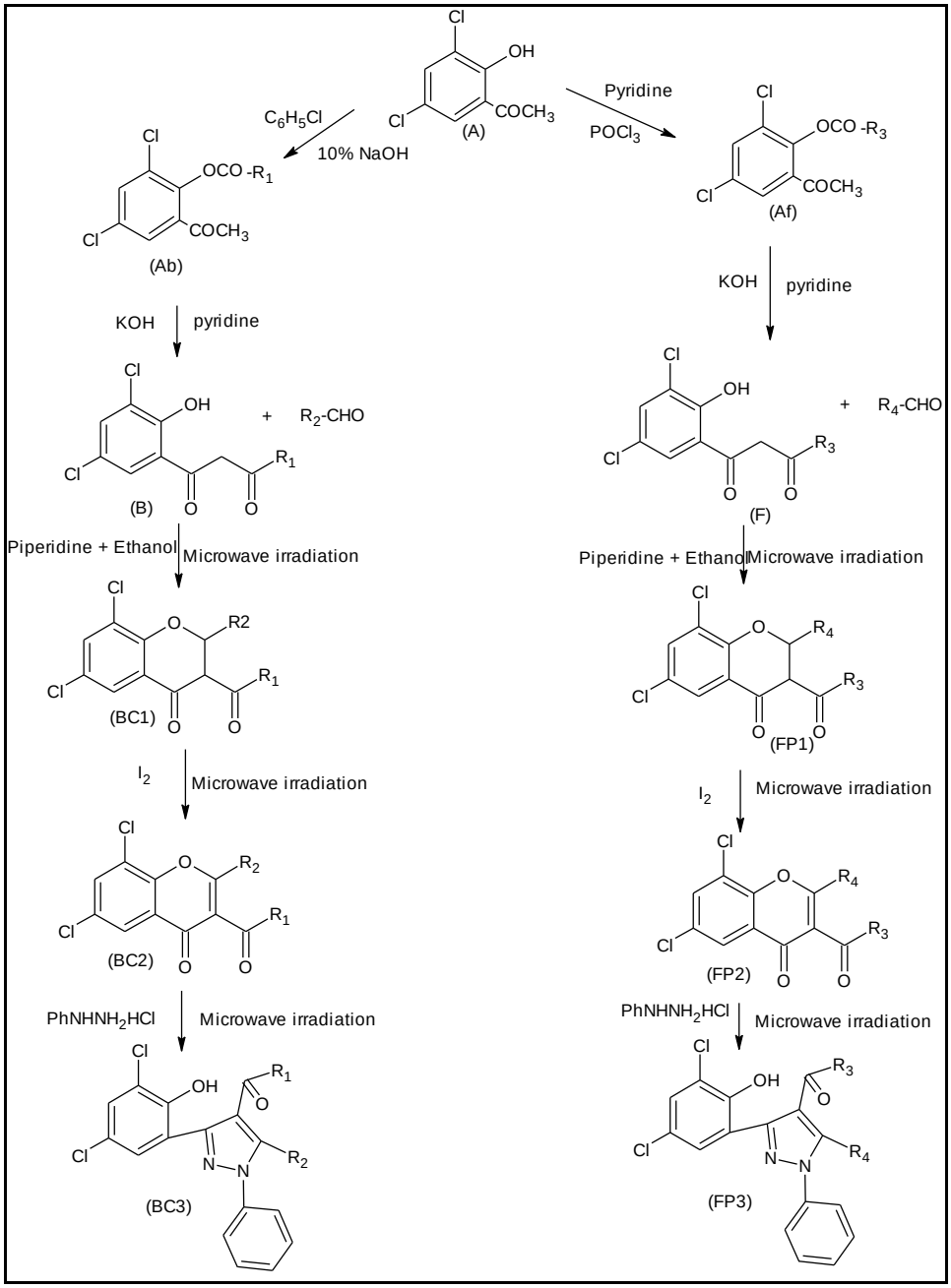
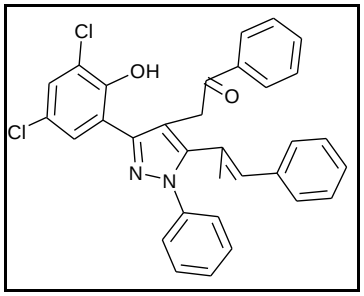
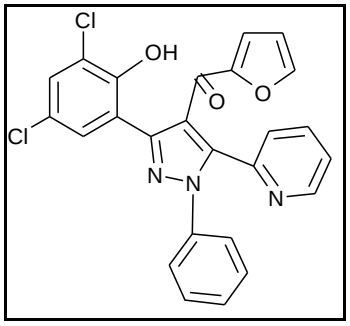


Fig: - The synthetic pathway for synthesis of pyrazole (BC3 and FP3) compound.
(R_3= C_5H_{10}, C_5H_8O. R_1= C_6H_6, C_7H_{14}, R_4= C_5H_8, C_5H_8N. R_2= $C_{10}H_{10}$, C_6H_6,).

The structure of (BC3 and FP3) Pyrazole:



(*Z*)-(3-(3,5-dichloro-2-hydroxyphenyl)-1-phenyl-5-(1-phenylprop-1-en-2-yl)-1*H*-pyrazol-4-yl)(phenyl) methanone (BC3)



(3-(3, 5-Dichloro-2-hydroxyphenyl)-1-phenyl-5-(pyridin-2-yl)-1*H*-pyrazol-4-yl) (furan-2-yl) methanone (FP3)

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International Journal of Trend in Scientific Research and Development (IJTSRD)
International Open Access Journal
ISSN No: 2456 - 6470 | www.ijtsrd.com | Volume - 1 | Issue – 5

Microwave Assisted Synthesis of Some New Chromone and their Antibacterial Activity

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ABSTRACT

Chlorosubstitued3-Aroylchromone were prepared by refluxing of 1-(2-hydroxy-5-chlorophenyl)-3-(2ˈ-furyl)-1, 3-propanedione and glutaraldehyde in ethanol and piperidine..The newly synthesized Chlorosubstitued 3-Aroylchromone were characterized on the basis of elemental analysis and spectroscopic data of IR,NMR. The titled compound were evaluated for their antibacterial activity against species such as Escherichia coli, Staphylococcus aureas, Bacillus subtilis and Pseudomons aeruginosa

Keywords*: Synthesis, Antibacterial Activity, Chromone*

INTRODUCTION

Chromone word is drived from greek word *chroma* meaning "color" which indicates that many chromone derivatives exhibit a broad variation of colors. chromones are the heterocyclic compound with benzopayrone network with substituted keto group on pyrone ring. chromone is an isomer of coumarin. Chromone moity is obtain from number of sourse such as plant marine and synthetic sources. Oxygen containing heterocycles are abundantly found in nature.Flavones, isoflavones, flavones, catechins, anthocynins are some phytoconstitutents collectively grouped as flavanoids and isoflavonoids.[1] Molecules containing the chromone structure (such as flavonoids and chromones) receive considerable attention in the literatures recently, mainly due to their biological and physiological activities including ant mycobacterial, antifungal, anticonvulsant, antimicrobial, mushroom tyrosinase inhibition activities, intermediates to many products of fine chemical industries.[2] The most of chromones are found to be biologically active agents. Some of the biological activities attributed to chromones derivatives include, neuroprotective, HIV-inhibitory, antimicrobial, antibacterial, antitumor, antifungal, antialergic, antiviral, anti-inflammatory, anticancer activities.[3] Many chromone derivatives are also photoactive and can be used easily in various photo induced reactions affording diverse heterocyclic compounds.[4] These derivatives also serve as intermediates to many products of fine chemical industries such as pharmaceuticals, agrochemicals and dyestuffs.[5] In general, chromones are synthesized by the cyclodehydration of 1-(*o*-hydroxyaryl)- 1,3-diketones or equivalent intermediates catalyzed by strong acids or strong bases (Vilsmeier- Haack reaction) .They have been prepared on a large [6] Diels-Alder reactions, Condensation reactions, Dimerization reactions, Colour reactions provide another synthesis of chromone and its derivativ

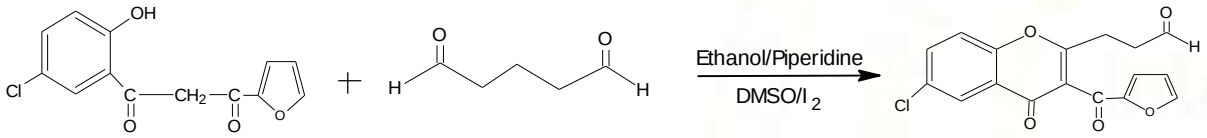
EXPERIMENTAL

The synthesis of 3-furoyl-2-butanal-6-chlorochromone from the mixture of 1-(2-hydroxy-5-chlorophenyl)-3-(2ˈ-furyl)-1,3-propanedione and glutaraldehyde was refluxed in ethanol and piperidine to form chromanone. Again these chromanone was refluxed with crystal of iodine in DMSO to form a chromone. The melting points of these compounds were recorded n 'Tempo' melting point apparatus.

The carbon, hydrogen, oxygen and chlorine analysis was carried out on'Carlo Ebra 1106'analyzer.the IR spectra were recorded on 'Perkin-Elmer Infra Red spectrophotometer. The PMR spectra were recorded on DRX 300 spectrometer in CDCl3. Purity of the compound was tested by TLC. The study were treated for their antibacterial impact against some common pathogenic bacteria viz. *E. Coli, S. aureus, B. Subtilis, P. argenosa.* The solutions of 50 mgof test compounds were prepared in DMSO solvent separately. The discs were soaked, assuming that each disc will contain approximately of the test solution. The culture media was prepared by using following composition for one liter distilled water-

Peptone: 10g
Sodium chloride: 10g
Yeast extract: 10 g
Agar: 20g in 1000ml of distilled water

Initially, the stock cultures of bacteria were revived by inoculating in broth media and grown at 37ºC for 18 hrs. The agar plates of the above media were prepared and wells were made in the plate. Each plate was inoculated with 18 h old cultures (100 µl, 10-4 cfu) and spread evenly on the plate. After 20 min, the wells were filled with compound and antibiotic at different concentrations. All the plates were incubated at 37ºC for 24 h and the diameter of inhibition zone were noted



Compound	Molecular formula	M.P.	Yield	Rf
1	$C_{13}H_9ClO_4$	110^0C	78%	0.76
2	$C_{19}H_{15}ClO_5$	155^0C	80%	0.89

Spectral Interpretation

The important frequencies observed in the IR spectrum recorded in KBr are correlated as Follows-IR **(**υmax**)** cm

(**1a):**748(C-Clstretching); 3432(OHstretching); 1650(C=Cstretching**);** 941(2'Furyl) 1680(C=Ostretching) .The PMR spectrum of the compound was recorded in CDCl3 with TMS as an internal standard. The observed chemical shifts and their correlations are as follows-NMR 12.08(1H, s, Ar-OH); 6.66-7.99(6H, m, Ar-) 9.72(1H,s-CHO)

(2a);1690(C=Ostretching);1653(C=Cstretching);952(furan);2938(-CHOstretching).The observed chemical shifts and their correlations are as follows-NMR;7.39(m,6H,Ar-H); 9.72(s,1H,-CHO-); 2.40(S,2H,-CH2)

RESULT AND DISCUSSION

The Chlorosubstitued3-Aroylchromone were synthesized successfully in moderate to good yield. The newly synthesized compounds were identified melting point, IR, NMR. The chromone were screened in vitro against some commone bacteria (E. coli, S. aureaus, B. subtilis, P. argenosa).It was noticed that most of all these compounds have shown remarkable inhibitory activity. On the newly synthesize chromone were screened for antibacterial activity using Agar diffusion method.

CONCLUSION

In current research It can be concluded that chromone compounds were moderately active against all used bacterial strain. Although the compounds synthesized are not much significant against microbes under investigation but the further purification and

modification of synthesized give scope for further development in the same heterocyclic nucleus. The microwave irradiaton method of reaction activation was in many cases successfully used for increasing the yield as well as to achieve a considerable shorterning of reaction time

Antibacterial activities of test compounds

Test compound	Organism	25 µg	50 µg	100 µg	250 µg	500 µg	MICµg
2a	*E. coli*	26	29	32	34	38	25
	B. subtilis	20	24	27	30	36	25
	P.aeruginosa	30	32	34	35	38	25
	S. aures	25	28	31	34	36	25

ACKNOWLEDGEMENTS

The authors are thankful to V.B.M.V. Amravati for providing all the facilities to carry out the work.

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International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.10 No.15, pp 204-212, 2017

Study of proton-ligand and metal-ligand stability constants of Cu (II) and Mn (II) complexes with chlorosubstituted pyrazoles and isozoles in 80% DMF-water solvent using pH-meter

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Abstract : The hydrogen-ion activity in water-based solutions, its acidity or alkalinity expressed as pH scientifically is measured on the pH meter. pH meter instrument is also used to find out stability of complexes through titrations. Stability constant is equilibrium constant for the formation of a complex in solution. It is a measure of the strength of the interaction between the reagents that come together to from the complex. The proposed study deals with the proton-ligand stability constant and metal-ligand stability constant of chlorosubstituted pyrazoles and isoxazoles by Calvin Bjerrum titration on pH meter.
Key Words : pH- meter, chlorosubstituted pyrazole, chlorosubstituted isoxazole, Calvin Bjerrum titration.

Introduction:

The determination pH of a solution, we can employ number of methods like potentiometric, conductometric, cryscopic but for the purpose of titrations, we can directly use the pH meter. The pH-metric is an automatic instrument of measuring the pH of a solution. There are number of pH- meters, involving different principles, but most of the chemists use only the direct reading type pH meter. The hydrogen-ion activity in water-based solutions, its acidity or alkalinity expressed as pH scientifically is measured on the pH meter. The combined glass electrode is used in the pH meter. The glass electrode is the most widely used hydrogen ion responsive electrode and its use depends on the fact that when a glass membrane is immersed in a solution, a potential is developed which is a linear function of the solution[1].

pH meter instrument is also used to find out stability of complexes through titrations. Stability constant is equilibrium constant for the formation of a complex in solution. It is a measure of the strength of the interaction between the reagents that come together to from the complex. Ramteke[2] *et al* determined stability constants of 4-(2-chlorophenyl)-3-(3-furanoyl-5-(2-hydroxyphenyl)pyrazole with Cu(II), Ni(II), Co(II) and Nd(III) metal ions in 70% dioxane-water mixture. Pethe[3] *et al* reported the interaction of 3-(4'-bromophenyl)-4-benzoyl-5-(2-hydroxyphenyl)pyrazole and 3-(4'-chlorophenyl)-4-benzoyl-5-(2-hydroxyphenyl)pyrazole with Co(II) and Ni(II) by pH metrically.

The proposed study deals with the proton-ligand stability constant and metal-ligand stability constant of chlorosubstituted pyrazoles and isoxazoles by Calvin Bjerrum titration on pH meter.

Materials and Methods:

Proton-ligand stability constants and metal-ligand stability constants studied on three ligands which are:

1. (3-(3,5-Dichloro-2-hydroxyphenyl)-1-phenyl-5-(1-phenylprop-1-en-2-yl)-1*H*-pyrazol-4 yl)(phenyl)methanone. (**ligand BC3**)

2. (3-(3, 5-Dichloro-2-hydroxyphenyl)-5-(1-phenylprop-1-en-2-yl) isoxazole-4-yl)(phenyl) methanone. (**ligand BC4**)

The ligands (BC3, FP3 and BC4) were completely dissolved in 80% DMF-water mixture. This is useful in pH metric titrations because all equilibrium processes that take place in water containing solvent-mixtures sensitively. The two metals selected for metal-ligand stability constants were: Cu (II) and Mn (II).

The Calvin-Bjerrum titration method was used to calculate proton-ligand stability constant and metal-ligand stability constant. The titration data were used to draw the graphs. Three kinds of titrations were performed against volume of NaOH. The ligands (BC3 and BC4) were separately titrated with metal complexes. These titrations were:

(a) Acid titration.
(b) Acid + Ligand titration.
(c) Acid + Ligand + Metal titration.

The titration procedures are:

(a) Acid titration: 5 ml HNO_3 (0.1M) + 5 ml KNO_3 (0.1M) + 35ml DMF + 5 ml water.
(b) Acid + Ligand titration: 5 ml HNO_3 (0.1M) + 5 ml KNO_3 (0.1M) + 10 ml ligand (in DMF-water 80%) + 25ml DMF + 5 ml water.
(c) Acid + Ligand + metal titration: 5 ml HNO_3 (0.1M) + 5 ml KNO_3 (0.1M) + 10 ml ligand (in DMF-water 80%) + 25ml DMF + 2 ml metal ion solution + 3 ml water.

Here 0.1 M HNO_3 acids were used for the preparation of a stock solution. The exact normality was calculated by titrating against standard sodium hydroxide solution. 0.1 M KNO_3 solution which was prepared from carbonates free double distilled water. Ionic strength of sodium hydroxide is kept constant as 0.1 M by addition of potassium nitrate solution.

The titration curves were prepared by plotting pH of solution and volume of NaOH added as shown in tables 1 to 4 and in graphs 1 to 4.The dissociation of OH^- is clearly indicated by the titration (acid + ligand) curves deviated from acid curves at pH 4.86 and continued up to pH 12.67 (Graphs 1 to 4).

Calculation of proton-ligand formation number ($\bar{n}_A$):

The proton-ligand formation numbers $\bar{n}_A$ were calculated from acid titration. The $\bar{n}_A$ values (proton-ligand formation numbers) were calculated by Irving Rossoti's expression curve (A) acid and acid + ligand titration curves (A+L).

The difference ($V_2 - V_1$) between the volumes (A+L) and (A) was measured accurately. The values of V_1 and ($V_2 - V_1$) were used in the calculations which are represented in tables 3.7 to 3.9.

$$\bar{n}_A = \gamma - \frac{(V_2 - V_1)(N + \varepsilon_0)}{(V_0 + V_1)T^0_L}$$

Where, γ = Number of replaceable hydrogen atoms per ligand molecule,
V_0 = Total initial volume of the solution
V_1 and V_2 are the volumes of alkali required during the acid and ligand titration at the given pH.
N = Normality of NaOH used for titration

ε_0 and T^0_L are the initial concentrations of free acids and the ligands

pH Metric Titration Data:

3.3.2.1 Titration data of ligand (BC3) with Cu (II):

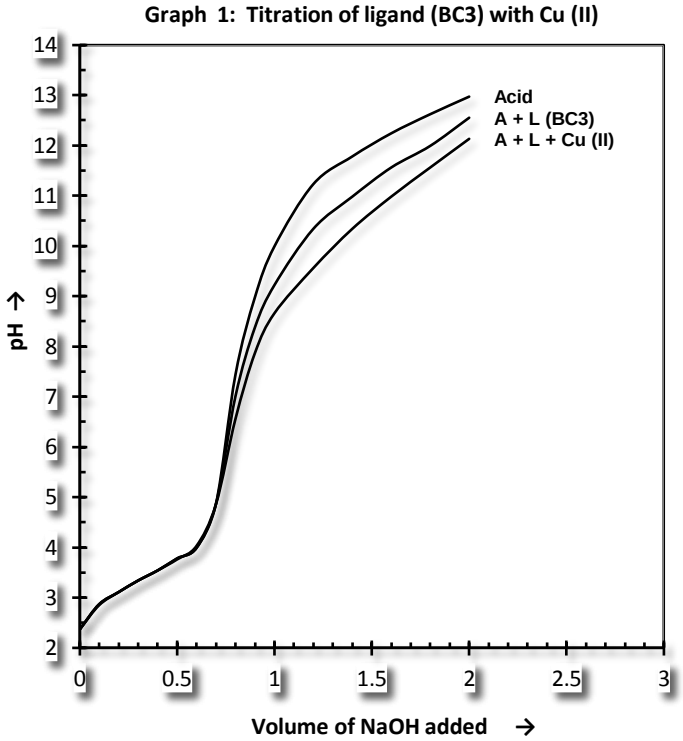
System: Ligand (BC3) with Cu (II), Medium: 80% (DMF: water), N = 0.2 N (NaOH)
Temperature = 25^0C, Ionic strength (μ) = 0.1 M KNO_3, ε_0 = 0.002 M HNO_3
T^0_m = 0.0004 M

Table 1: Titration data of ligand (BC3) with Cu (II)

Vol. of NaOH added	Acid	A+L(BC3)	A+ L+ Cu (II)
0	2.37	2.37	2.37
0.1	2.87	2.87	2.85
0.2	3.11	3.11	3.11
0.3	3.34	3.34	3.34
0.4	3.54	3.54	3.54
0.5	3.78	3.78	3.76
0.6	3.99	3.99	4.03
0.7	4.87	4.87	4.86
0.8	7.44	7.01	6.56
0.9	8.98	8.38	7.87
1.0	9.99	9.22	8.66
1.2	11.23	10.34	9.56
1.4	11.78	10.98	10.34
1.6	12.24	11.56	10.98
1.8	12.62	11.99	11.56
2.0	12.97	12.55	12.13

Table No. 2 Titration data of ligand (BC3) with Mn (II)

Vol. of NaOH added	Acid	(A+L+BC3)	A+L+Mn(II)
0	2.37	2.37	2.37
0.1	2.87	2.87	2.86
0.2	3.11	3.11	3.1
0.3	3.34	3.34	3.34
0.4	3.54	3.54	3.54
0.5	3.78	3.78	3.75
0.6	3.99	3.99	3.98
0.7	4.87	4.87	4.89
0.8	7.44	7.01	6.45
0.9	8.98	8.38	7.56
1.0	9.99	9.22	8.45
1.2	11.23	10.34	10.01
1.4	11.78	10.98	10.56
1.6	12.24	11.56	10.98
1.8	12.62	11.99	11.34
2.0	12.97	12.55	12.08



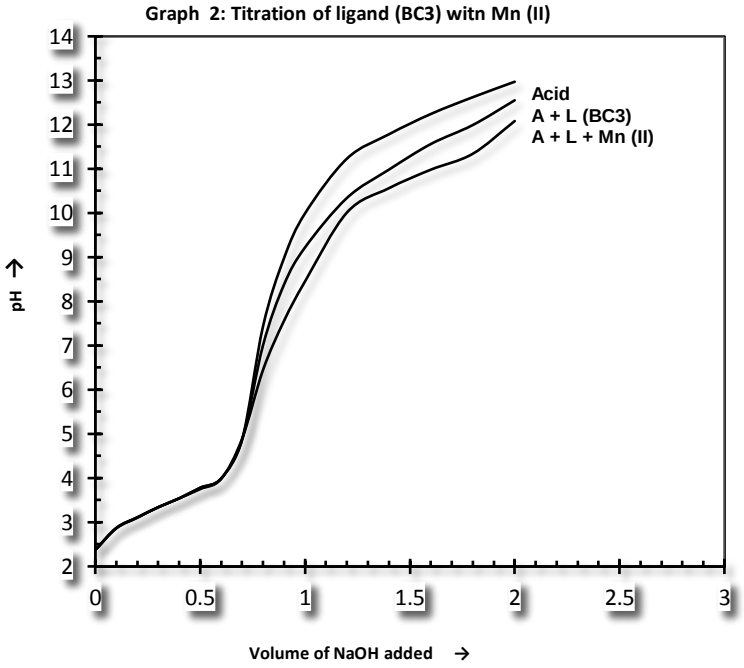


Table 3: Titration data of ligand BC4 with Cu (II)

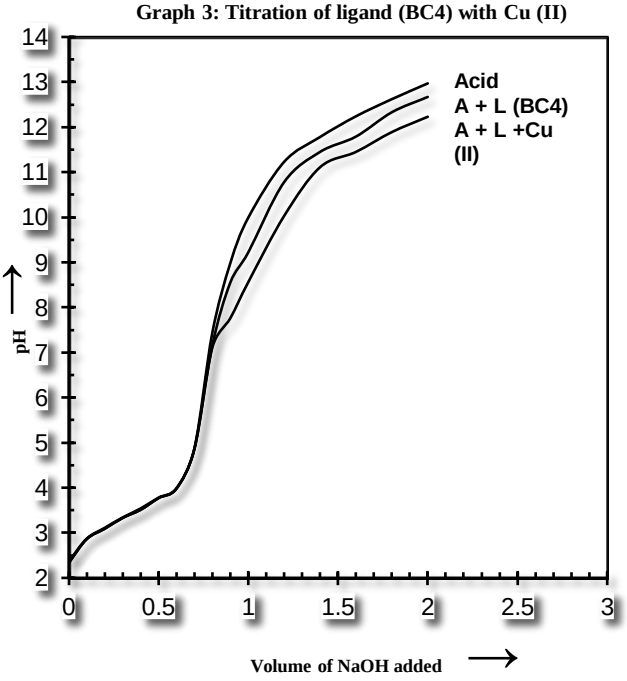
Vol. of NaOH added	Acid	A+L(BC3)	A+ L+ Cu (II)
0	2.37	2.34	2.34
0.1	2.87	2.86	2.86
0.2	3.11	3.09	3.09
0.3	3.34	3.33	3.33
0.4	3.54	3.51	3.51
0.5	3.78	3.77	3.77

0.6	3.99	3.98	3.98
0.7	4.87	4.86	4.86
0.8	7.44	7.16	7.11
0.9	8.98	8.55	7.76
1.0	9.99	9.22	8.56
1.2	11.23	10.78	10.03
1.4	11.78	11.45	11.11
1.6	12.24	11.79	11.45
1.8	12.62	12.33	11.89
2.0	12.97	12.67	12.23

Table 4: Titration data of ligand BC4 with Mn (II)

Vol. of NaOH added	Acid	A+ L (BC4)	A+ L+ Mn (II)
0	2.37	2.34	2.33
0.1	2.87	2.86	2.87
0.2	3.11	3.09	3.08
0.3	3.34	3.33	3.32
0.4	3.54	3.51	3.5
0.5	3.78	3.77	3.76
0.6	3.99	3.98	3.97
0.7	4.87	4.86	4.84
0.8	7.44	7.16	6.87
0.9	8.98	8.55	7.67
1.0	9.99	9.22	8.67
1.2	11.23	10.78	10.21
1.4	11.78	11.45	11.11
1.6	12.24	11.79	11.32
1.8	12.62	12.33	11.67
2.0	12.97	12.67	12.07

Graph 3: Titration of ligand (BC4) with Cu (II)



Graph 4: Titration of ligand (BC4) with Mn (II)

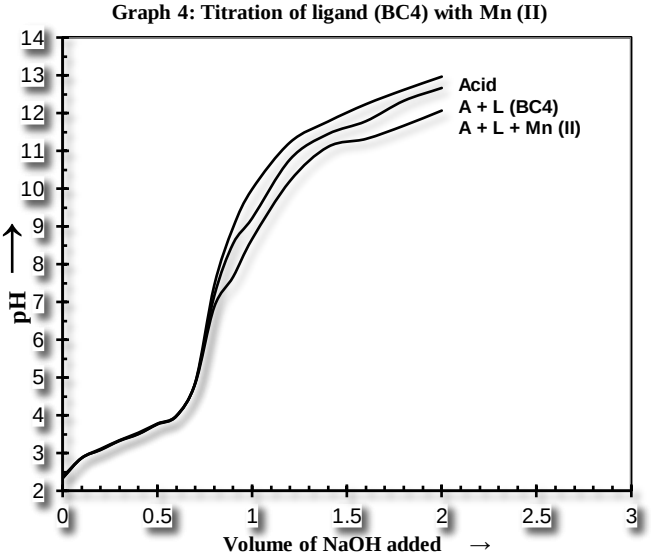


Table 1.1: Metal Complex Titration data:

Ligands	Metal ions	pH at Commencement of Hydrolysis (deviation of A + L curve from A acid curve)	pH at Commencement of Hydrolysis (deviation of A + L + M curve from A + L curve)
BC3	Cu (II)	7.01	6.56
	Mn (II)	7.01	6.45
BC4	Cu (II)	7.16	7.11
	Mn (II)	7.16	6.87

The departure of metal complex titration curve from reagent titration curve is seen at around pH 7. The pH of hydrolysis for all the metal ions under investigation was around pH = **7 to 7.6.**

The Pattern of Titration Curves:

The acids + ligand titration curves (A+L) are deviated from acid titration curves (A) for all systems at pH (4.87 for BC3), (4.86 for BC4) and continuously increased deviation up to pH (12.55 in BC3) and (12.67 in BC4). These kinds of deviations show the dissociation of -OH group of ligands. The present investigation consider the ligand (BC3 and BC4) having only one dissociable H^+ ion from -OH group.

$$HL \rightarrow H^+ + L^-$$

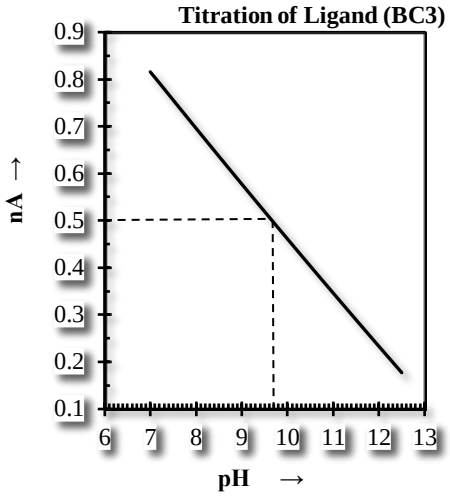
H = Acids, L = Ligand.

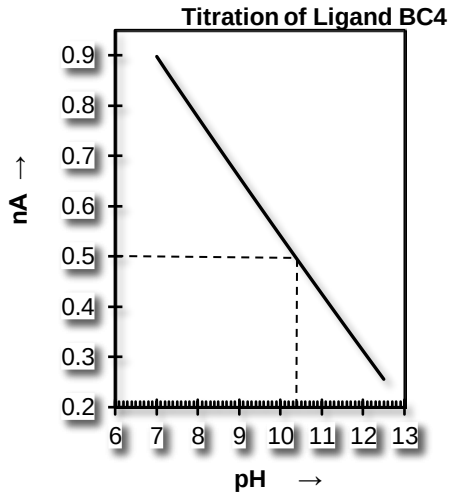
The (0.2 N) NaOH is used in the pH metric titration. The difference (V_2 and V_1) is estimated from the plot between the volume of NaOH and pH of the solution.

Calculation of proton-ligand formation number ($\bar{n}_A$):

$$\bar{n}_A = \gamma - \frac{(V_2 - V_1)(N + \varepsilon_0)}{(V_0 + V_1)T^0_L}$$

The values of $\bar{n}_A$ (average number of protons) were calculated along with the values of (V_2 - V_1) at various pH are presented in following graphs:





Graph 1. Titration of ligand (BC3) **Graph 2. Titration of ligand (BC3)**

Proton-ligand stability constant:

There are many methods for calculating pK_1 and pK_2 values. Here we have used the half integral method for determination of pK_1 values. Naik[14] *et al* and Patil[38] used half integral method and calculated pK_1 and pK_2 values. The pK values were initially calculated from formation curves $\bar{n}_A$ versus pH. The values of pH were $\bar{n}_A = 0.5$ correspond to the value of pK_1 for one dissociable group.

Table 1.1.1 Proton-ligand stability constant of BC3, and BC4 systems

Systems	proton-ligand stability constant (pK) by half integral method
BC3	9.7
BC4	10.4

Determination of metal-ligand stability constants:

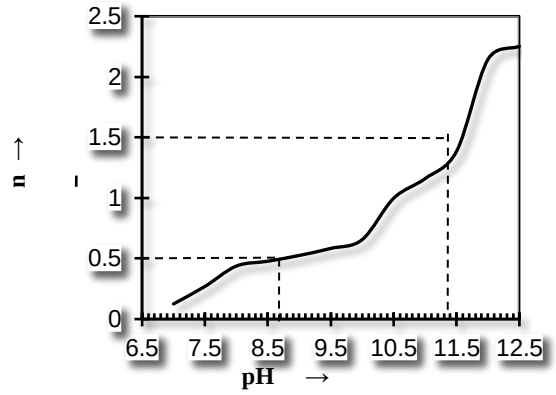
The stability constant of metal complex can be calculated by following $\bar{n}$ equation. $\bar{n}$ is defined as the average number of ligands bounds per metal atom and it can be calculated from the formula,

$$\bar{n} = \frac{(V_3 - V_2)(N + \varepsilon_0)}{(V_0 + V_2)\,\bar{n}_A\,T^0_M}$$

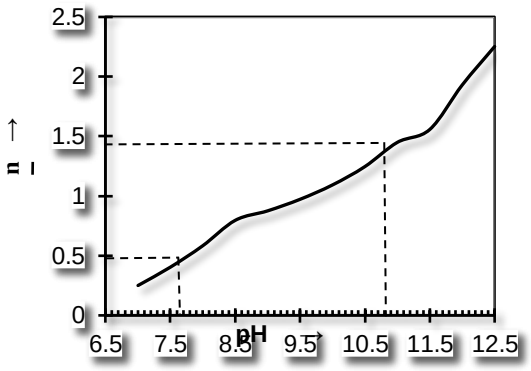
The value of $\bar{n}$ is corresponding pH value.

$$pL = \log\left[\frac{\left[H^+\right]}{K_L\left(T^0_L - T^0_M\left(\bar{n}\right)\right)}\right]$$

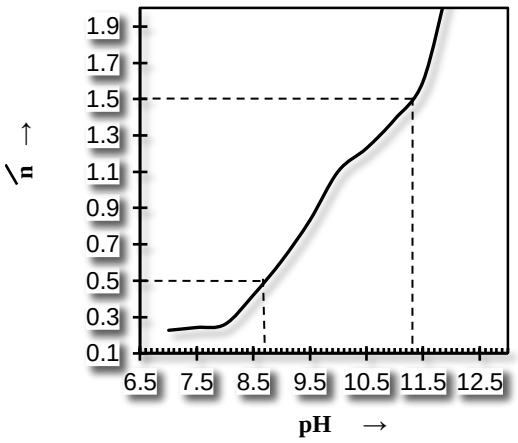
The plots of variation of $\bar{n}$ with pH that is metal-ligand formation curves are given in the graphs 3 to 6.



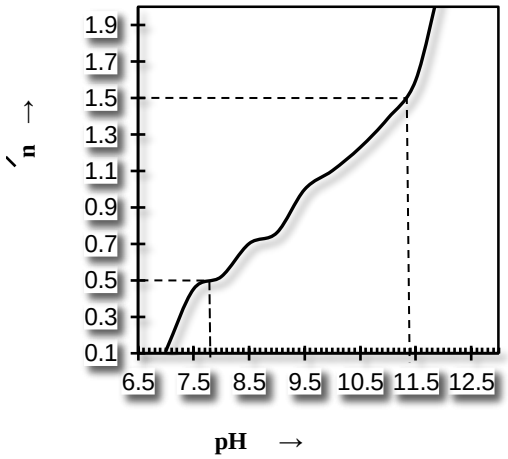
Graph 3. Ligand (BC3) with Cu (II)



Graph 4. Ligand (BC3) with Mn (II)



Graph 5. Ligand (BC4) with Cu (II)



Graph 6. Ligand (BC4) with Mn (II)

The pK values were calculated from formation curves of $\bar{n}$ versus pH. The value of pH was $\bar{n}$ = 0.5 which corresponds to the value of $\log K_1$ and the value of pH was $\bar{n}$ = 1.5 which corresponds to the value of $\log K_2$. The values of $\log K_1$ and $\log K_2$ of the complexes with metal ions were calculated by using half integral method:

Table 1.2 Metal-ligand stability constant $\log K_1$ and $\log K_2$ by half integral method

System	$\log K_1$	$\log K_2$	$\log K_1 / \log K_2$
Ligand (BC3) with Cu (II)	3.644	0.9546	2.689
Ligand (BC3) with Mn (II)	4.644	1.154	3.49
Ligand (BC4) with Cu (II)	4.443	1.953	2.49
Ligand (BC4) with Mn (II)	5.343	1.853	3.49

Result and discussion:

The proton-ligand stability constants (pK_1values) for substituted ligands were found to be 9.7 and 10.4 in BC3 and BC4 systems respectively. This is due to phenolic –OH group dissociating at 9.5 and above it in aqueous medium. The metal ligand stability constants log K1 and log K2 shows low stability at higher pH for 1:2 complexes as compare to 1:1 complex. Half cell configurations have more stability. From this tabulated data, it is observed that large difference between $\log K_1$ and $\log K_2$ values exhibits stepwise complex formation.

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International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.10 No.15, pp 204-212, 2017

Study of proton-ligand and metal-ligand stability constants of Cu (II) and Mn (II) complexes with chlorosubstituted pyrazoles and isozoles in 80% DMF-water solvent using pH-meter

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Abstract : The hydrogen-ion activity in water-based solutions, its acidity or alkalinity expressed as pH scientifically is measured on the pH meter. pH meter instrument is also used to find out stability of complexes through titrations. Stability constant is equilibrium constant for the formation of a complex in solution. It is a measure of the strength of the interaction between the reagents that come together to from the complex. The proposed study deals with the proton-ligand stability constant and metal-ligand stability constant of chlorosubstituted pyrazoles and isoxazoles by Calvin Bjerrum titration on pH meter.
Key Words : pH- meter, chlorosubstituted pyrazole, chlorosubstituted isoxazole, Calvin Bjerrum titration.

Introduction:

The determination pH of a solution, we can employ number of methods like potentiometric, conductometric, cryscopic but for the purpose of titrations, we can directly use the pH meter. The pH-metric is an automatic instrument of measuring the pH of a solution. There are number of pH- meters, involving different principles, but most of the chemists use only the direct reading type pH meter. The hydrogen-ion activity in water-based solutions, its acidity or alkalinity expressed as pH scientifically is measured on the pH meter. The combined glass electrode is used in the pH meter. The glass electrode is the most widely used hydrogen ion responsive electrode and its use depends on the fact that when a glass membrane is immersed in a solution, a potential is developed which is a linear function of the solution[1].

pH meter instrument is also used to find out stability of complexes through titrations. Stability constant is equilibrium constant for the formation of a complex in solution. It is a measure of the strength of the interaction between the reagents that come together to from the complex. Ramteke[2] *et al* determined stability constants of 4-(2-chlorophenyl)-3-(3-furanoyl-5-(2-hydroxyphenyl)pyrazole with Cu(II), Ni(II), Co(II) and Nd(III) metal ions in 70% dioxane-water mixture. Pethe[3] *et al* reported the interaction of 3-(4'-bromophenyl)-4-benzoyl-5-(2-hydroxyphenyl)pyrazole and 3-(4'-chlorophenyl)-4-benzoyl-5-(2-hydroxyphenyl)pyrazole with Co(II) and Ni(II) by pH metrically.

The proposed study deals with the proton-ligand stability constant and metal-ligand stability constant of chlorosubstituted pyrazoles and isoxazoles by Calvin Bjerrum titration on pH meter.

Materials and Methods:

Proton-ligand stability constants and metal-ligand stability constants studied on three ligands which are:

1. (3-(3,5-Dichloro-2-hydroxyphenyl)-1-phenyl-5-(1-phenylprop-1-en-2-yl)-1*H*-pyrazol-4 yl)(phenyl)methanone. (**ligand BC3**)

2. (3-(3, 5-Dichloro-2-hydroxyphenyl)-5-(1-phenylprop-1-en-2-yl) isoxazole-4-yl)(phenyl) methanone. (**ligand BC4**)

The ligands (BC3, FP3 and BC4) were completely dissolved in 80% DMF-water mixture. This is useful in pH metric titrations because all equilibrium processes that take place in water containing solvent-mixtures sensitively. The two metals selected for metal-ligand stability constants were: Cu (II) and Mn (II).

The Calvin-Bjerrum titration method was used to calculate proton-ligand stability constant and metal-ligand stability constant. The titration data were used to draw the graphs. Three kinds of titrations were performed against volume of NaOH. The ligands (BC3 and BC4) were separately titrated with metal complexes. These titrations were:

(a) Acid titration.
(b) Acid + Ligand titration.
(c) Acid + Ligand + Metal titration.

The titration procedures are:

(a) Acid titration: 5 ml HNO_3 (0.1M) + 5 ml KNO_3 (0.1M) + 35ml DMF + 5 ml water.
(b) Acid + Ligand titration: 5 ml HNO_3 (0.1M) + 5 ml KNO_3 (0.1M) + 10 ml ligand (in DMF-water 80%) + 25ml DMF + 5 ml water.
(c) Acid + Ligand + metal titration: 5 ml HNO_3 (0.1M) + 5 ml KNO_3 (0.1M) + 10 ml ligand (in DMF-water 80%) + 25ml DMF + 2 ml metal ion solution + 3 ml water.

Here 0.1 M HNO_3 acids were used for the preparation of a stock solution. The exact normality was calculated by titrating against standard sodium hydroxide solution. 0.1 M KNO_3 solution which was prepared from carbonates free double distilled water. Ionic strength of sodium hydroxide is kept constant as 0.1 M by addition of potassium nitrate solution.

The titration curves were prepared by plotting pH of solution and volume of NaOH added as shown in tables 1 to 4 and in graphs 1 to 4.The dissociation of OH^- is clearly indicated by the titration (acid + ligand) curves deviated from acid curves at pH 4.86 and continued up to pH 12.67 (Graphs 1 to 4).

Calculation of proton-ligand formation number ($\bar{n}_A$):

The proton-ligand formation numbers $\bar{n}_A$ were calculated from acid titration. The $\bar{n}_A$ values (proton-ligand formation numbers) were calculated by Irving Rossoti's expression curve (A) acid and acid + ligand titration curves (A+L).

The difference ($V_2 - V_1$) between the volumes (A+L) and (A) was measured accurately. The values of V_1 and ($V_2 - V_1$) were used in the calculations which are represented in tables 3.7 to 3.9.

$$\bar{n}_A = \gamma - \frac{(V_2 - V_1)(N + \varepsilon_0)}{(V_0 + V_1)T^0_L}$$

Where, γ = Number of replaceable hydrogen atoms per ligand molecule,
V_0 = Total initial volume of the solution
V_1 and V_2 are the volumes of alkali required during the acid and ligand titration at the given pH.
N = Normality of NaOH used for titration

ε_0 and T^0_L are the initial concentrations of free acids and the ligands

pH Metric Titration Data:

3.3.2.1 Titration data of ligand (BC3) with Cu (II):

System: Ligand (BC3) with Cu (II), Medium: 80% (DMF: water), N = 0.2 N (NaOH)
Temperature = 25^0C, Ionic strength (μ) = 0.1 M KNO_3, ε_0 = 0.002 M HNO_3
T^0_m = 0.0004 M

Table 1: Titration data of ligand (BC3) with Cu (II)

Vol. of NaOH added	Acid	A+L(BC3)	A+ L+ Cu (II)
0	2.37	2.37	2.37
0.1	2.87	2.87	2.85
0.2	3.11	3.11	3.11
0.3	3.34	3.34	3.34
0.4	3.54	3.54	3.54
0.5	3.78	3.78	3.76
0.6	3.99	3.99	4.03
0.7	4.87	4.87	4.86
0.8	7.44	7.01	6.56
0.9	8.98	8.38	7.87
1.0	9.99	9.22	8.66
1.2	11.23	10.34	9.56
1.4	11.78	10.98	10.34
1.6	12.24	11.56	10.98
1.8	12.62	11.99	11.56
2.0	12.97	12.55	12.13

Table No. 2 Titration data of ligand (BC3) with Mn (II)

Vol. of NaOH added	Acid	(A+L+BC3)	A+L+Mn(II)
0	2.37	2.37	2.37
0.1	2.87	2.87	2.86
0.2	3.11	3.11	3.1
0.3	3.34	3.34	3.34
0.4	3.54	3.54	3.54
0.5	3.78	3.78	3.75
0.6	3.99	3.99	3.98
0.7	4.87	4.87	4.89
0.8	7.44	7.01	6.45
0.9	8.98	8.38	7.56
1.0	9.99	9.22	8.45
1.2	11.23	10.34	10.01
1.4	11.78	10.98	10.56
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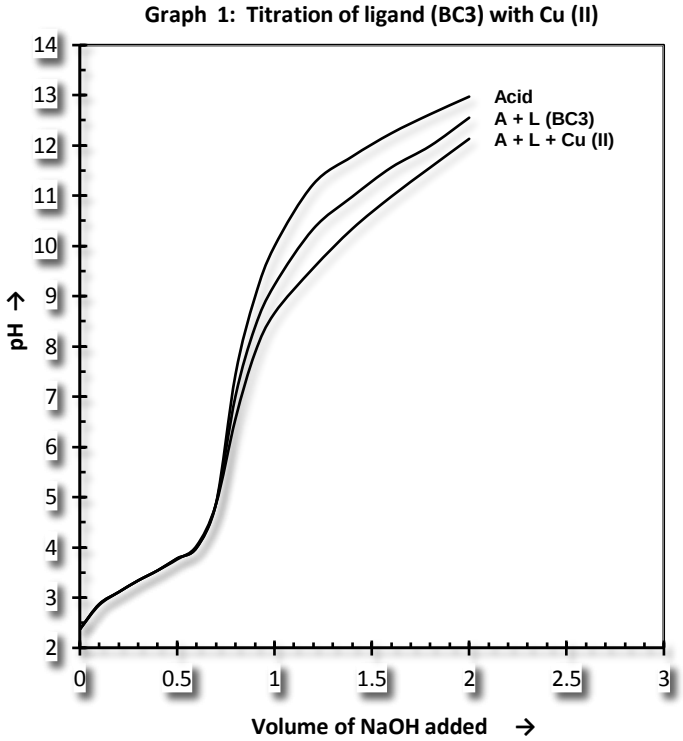
1.8	12.62	11.99	11.34
2.0	12.97	12.55	12.08



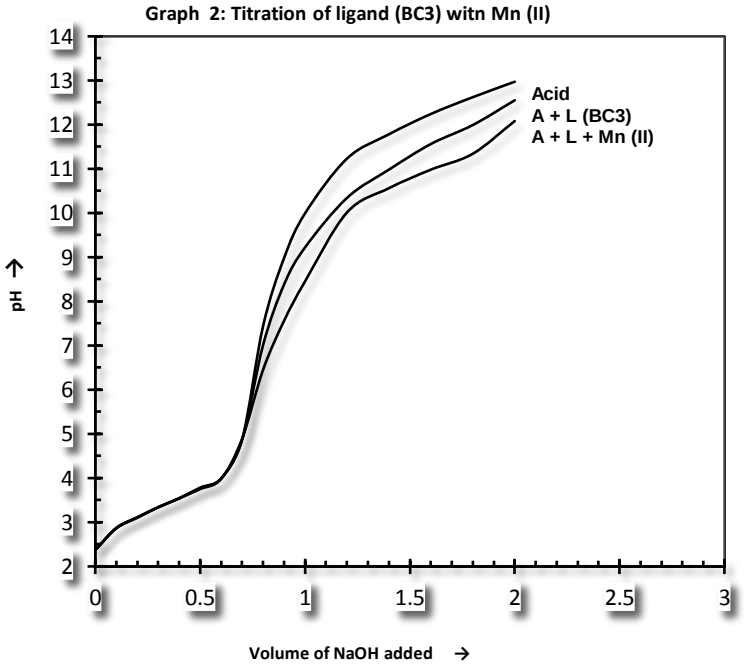


Table 3: Titration data of ligand BC4 with Cu (II)

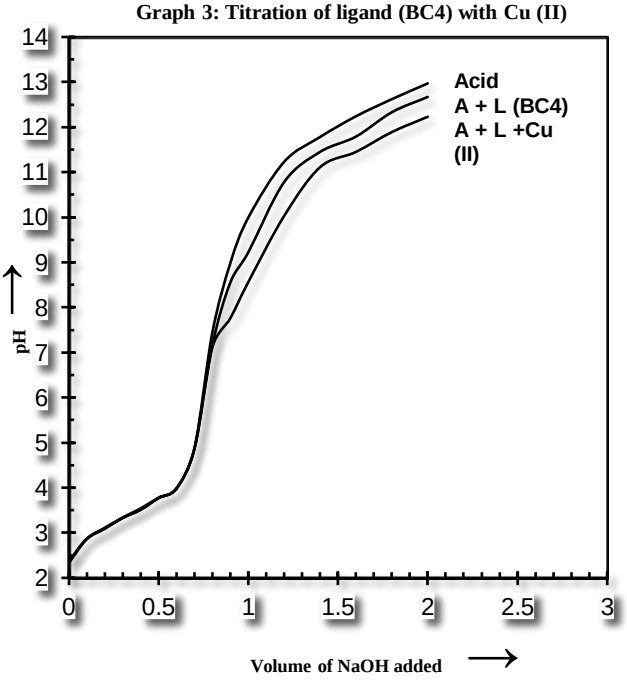
Vol. of NaOH added	Acid	A+L(BC3)	A+ L+ Cu (II)
0	2.37	2.34	2.34
0.1	2.87	2.86	2.86
0.2	3.11	3.09	3.09
0.3	3.34	3.33	3.33
0.4	3.54	3.51	3.51
0.5	3.78	3.77	3.77

0.6	3.99	3.98	3.98
0.7	4.87	4.86	4.86
0.8	7.44	7.16	7.11
0.9	8.98	8.55	7.76
1.0	9.99	9.22	8.56
1.2	11.23	10.78	10.03
1.4	11.78	11.45	11.11
1.6	12.24	11.79	11.45
1.8	12.62	12.33	11.89
2.0	12.97	12.67	12.23

Table 4: Titration data of ligand BC4 with Mn (II)

Vol. of NaOH added	Acid	A+ L (BC4)	A+ L+ Mn (II)
0	2.37	2.34	2.33
0.1	2.87	2.86	2.87
0.2	3.11	3.09	3.08
0.3	3.34	3.33	3.32
0.4	3.54	3.51	3.5
0.5	3.78	3.77	3.76
0.6	3.99	3.98	3.97
0.7	4.87	4.86	4.84
0.8	7.44	7.16	6.87
0.9	8.98	8.55	7.67
1.0	9.99	9.22	8.67
1.2	11.23	10.78	10.21
1.4	11.78	11.45	11.11
1.6	12.24	11.79	11.32
1.8	12.62	12.33	11.67
2.0	12.97	12.67	12.07

Graph 3: Titration of ligand (BC4) with Cu (II)



Graph 4: Titration of ligand (BC4) with Mn (II)

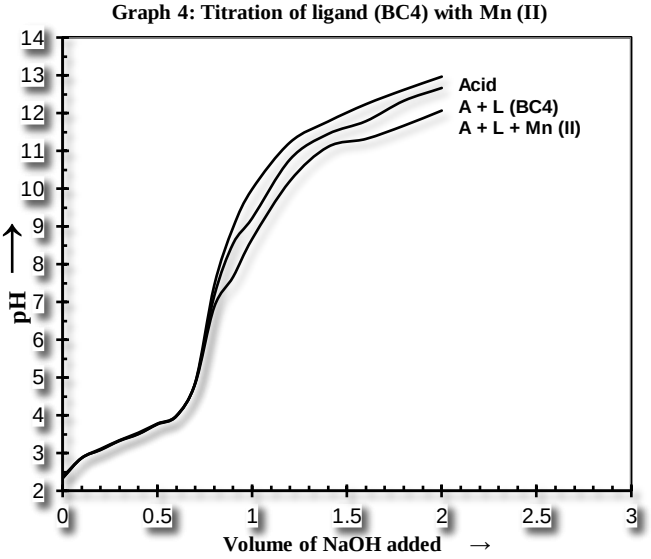


Table 1.1: Metal Complex Titration data:

Ligands	Metal ions	pH at Commencement of Hydrolysis (deviation of A + L curve from A acid curve)	pH at Commencement of Hydrolysis (deviation of A + L + M curve from A + L curve)
BC3	Cu (II)	7.01	6.56
	Mn (II)	7.01	6.45
BC4	Cu (II)	7.16	7.11
	Mn (II)	7.16	6.87

The departure of metal complex titration curve from reagent titration curve is seen at around pH 7. The pH of hydrolysis for all the metal ions under investigation was around pH = **7 to 7.6.**

The Pattern of Titration Curves:

The acids + ligand titration curves (A+L) are deviated from acid titration curves (A) for all systems at pH (4.87 for BC3), (4.86 for BC4) and continuously increased deviation up to pH (12.55 in BC3) and (12.67 in BC4). These kinds of deviations show the dissociation of -OH group of ligands. The present investigation consider the ligand (BC3 and BC4) having only one dissociable H^+ ion from -OH group.

$$HL \rightarrow H^+ + L^-$$

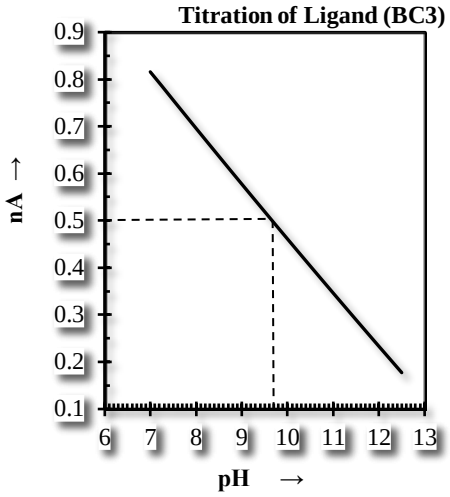
H = Acids, L = Ligand.

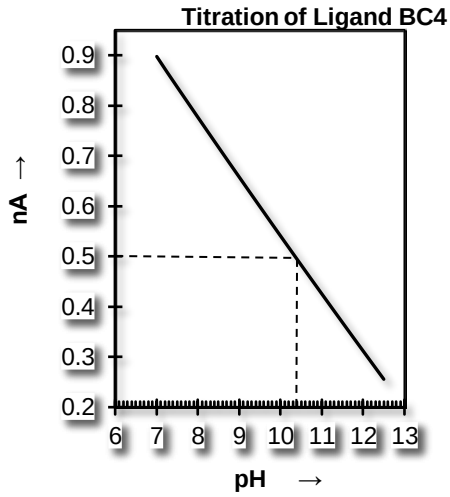
The (0.2 N) NaOH is used in the pH metric titration. The difference (V_2 and V_1) is estimated from the plot between the volume of NaOH and pH of the solution.

Calculation of proton-ligand formation number ($\bar{n}_A$):

$$\bar{n}_A = \gamma - \frac{(V_2 - V_1)(N + \varepsilon_0)}{(V_0 + V_1)T^0_L}$$

The values of $\bar{n}_A$ (average number of protons) were calculated along with the values of (V_2 - V_1) at various pH are presented in following graphs:





Graph 1. Titration of ligand (BC3) **Graph 2. Titration of ligand (BC3)**

Proton-ligand stability constant:

There are many methods for calculating pK_1 and pK_2 values. Here we have used the half integral method for determination of pK_1 values. Naik[14] *et al* and Patil[38] used half integral method and calculated pK_1 and pK_2 values. The pK values were initially calculated from formation curves $\bar{n}_A$ versus pH. The values of pH were $\bar{n}_A = 0.5$ correspond to the value of pK_1 for one dissociable group.

Table 1.1.1 Proton-ligand stability constant of BC3, and BC4 systems

Systems	proton-ligand stability constant (pK) by half integral method
BC3	9.7
BC4	10.4

Determination of metal-ligand stability constants:

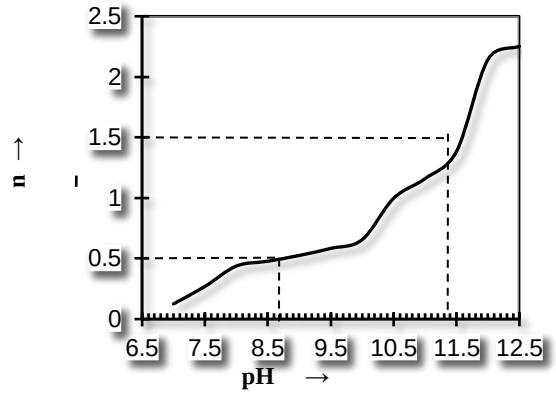
The stability constant of metal complex can be calculated by following $\bar{n}$ equation. $\bar{n}$ is defined as the average number of ligands bounds per metal atom and it can be calculated from the formula,

$$\bar{n} = \frac{(V_3 - V_2)(N + \varepsilon_0)}{(V_0 + V_2)\,\bar{n}_A\,T^0_M}$$

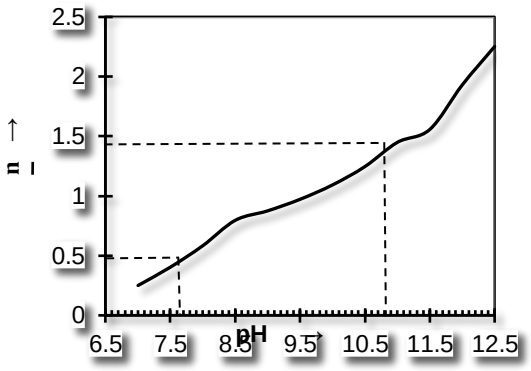
The value of $\bar{n}$ is corresponding pH value.

$$pL = \log\left[\frac{\left[H^+\right]}{K_L\left(T^0_L - T^0_M\left(\bar{n}\right)\right)}\right]$$

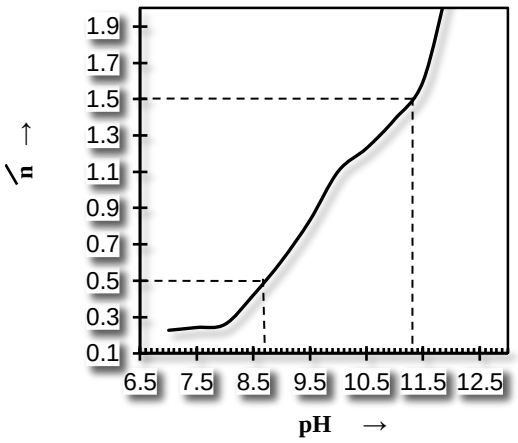
The plots of variation of $\bar{n}$ with pH that is metal-ligand formation curves are given in the graphs 3 to 6.



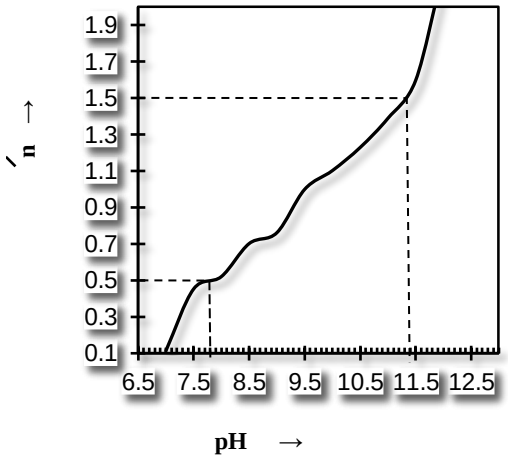
Graph 3. Ligand (BC3) with Cu (II)



Graph 4. Ligand (BC3) with Mn (II)



Graph 5. Ligand (BC4) with Cu (II)



Graph 6. Ligand (BC4) with Mn (II)

The pK values were calculated from formation curves of $\bar{n}$ versus pH. The value of pH was $\bar{n}$ = 0.5 which corresponds to the value of $\log K_1$ and the value of pH was $\bar{n}$ = 1.5 which corresponds to the value of $\log K_2$. The values of $\log K_1$ and $\log K_2$ of the complexes with metal ions were calculated by using half integral method:

Table 1.2 Metal-ligand stability constant $\log K_1$ and $\log K_2$ by half integral method

System	$\log K_1$	$\log K_2$	$\log K_1 / \log K_2$
Ligand (BC3) with Cu (II)	3.644	0.9546	2.689
Ligand (BC3) with Mn (II)	4.644	1.154	3.49
Ligand (BC4) with Cu (II)	4.443	1.953	2.49
Ligand (BC4) with Mn (II)	5.343	1.853	3.49

Result and discussion:

The proton-ligand stability constants (pK_1values) for substituted ligands were found to be 9.7 and 10.4 in BC3 and BC4 systems respectively. This is due to phenolic –OH group dissociating at 9.5 and above it in aqueous medium. The metal ligand stability constants log K1 and log K2 shows low stability at higher pH for 1:2 complexes as compare to 1:1 complex. Half cell configurations have more stability. From this tabulated data, it is observed that large difference between $\log K_1$ and $\log K_2$ values exhibits stepwise complex formation.

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SPECIAL ISSUE FOR INTERNATIONAL LEVEL CONFERENCE "ADVANCES IN SCIENCE, TECHNOLOGY & MANAGEMENT" (IC-ASTM)

IMPROVED AND SKILLFUL SYNTHESIS OF (±) FENOPROFEN, AN IMPORTANT ANTI-INFLAMMATORY AGENT

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Accepted Date: 05/09/2017; Published Date: 10/10/2017

Abstract: Several of the alpha-aryl-propionic acids are used as critical pharmaceutical agents much similar to how ibuprofen, ketoprofen, and flurbiprofen are used as non-steroidal anti-inflammatory agents. Many synthetic routes for producing arylpropionic acids have been proposed over the few years. Several of the present studies are focused on preparing pharmaceutically useful alpha-aryl-propionic acids. . The healing efficacy of this class of medicine is properly attested through the introduction and massive use of more than a dozen of compounds exemplified by ibuprofen, ketoprofen, flurbiprofen, and fenoprofen. It has been proven that appropriate alpha halo ketone can be easily transformed to ester, which on further hydrolysis yields alpha-aryl-propionic acid. A new and convenient synthesis of ether linkage utilizing Ullmann reaction has been suggested as an important step in the synthesis of Fenoprofen. In this paper, we report the total synthesis of Fenoprofen.

Keywords: Fenoprofen, Ullmann reaction, alpha halo ketone, alpha-aryl-propionic acid.

PAPER-QR CODE

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Access Online On:

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How to Cite This Article:

Hemant R. Suryavanshi, IJPRET, 2017; Volume 6 (2): 200-209

INTRODUCTION

Several 2-arylpropionic acids have been described as non-steroidal anti-inflammatory agents (NSAIs), which are useful in the treatment of osteoarthritis and rheumatoid arthritis.[1] Some NSAIs also are used to treat several long term health problems. There are three general classes of drugs commonly used in the treatment of rheumatic arthritis: (a) non-steroidal anti-inflammatory agents (NSAIs) [2] such as celecoxib, diclofenac sodium, ibuprofen, etc., (b) glucocorticoids[3] such as betamethasone, prednisone etc., and (c) disease modifying anti-rheumatic drugs[4] (DMARs) such as hydroxychloroquine, leflunomide, methotrexate, sulfasalazine, etc. The key objective of these drugs is to reduce inflammation leading to a subsequent reduction in pain intensity and improved function. In addition to anti-inflammatory effects, these agents are also known to have mild to moderate analgesic properties. Examples of some non-steroidal anti-inflammatory drugs (NSAIDs) include ibuprofen, indomethacin, nabumetone, naproxen, and others. These drugs are helpful in the treatment of mild to moderate pain, fever, and inflammation. They are effective in reducing the levels of prostaglandins, chemicals that are responsible for causing these ailments. [6] Fenoprofen, a NSAID, functions by blocking the activity of cyclooxygenases, which in turn lowers the level of prostaglandins. As a result, inflammation, swelling, pain, and fever are reduced.

Aspirin is one of the NSAIs agents which has largely been replaced by the other NSAIDs as the initial drug of choice for the management of inflammation due to its higher dosage requirement and high rate of gastrointestinal toxicity[7]. There are a large number of NSAIs available which are equally efficacious at full dosages. Fenoprofen is commercially available non-steroidal anti-inflammatory and analgesic drug used for the treatment of pain and inflammation caused due to rheumatoid arthritis and osteoarthritis. There are several synthetic routes available for the manufacture of Fenoprofen . One of the processes involves the reaction of 3-phenoxy chlorobenzene with sodium cyanoacetate followed by methylation and latter hydrolysis of cyano group.[8] Some other processes include the electrochemical synthesis of 2-aryl propionic acids by carbonyl group insertion by reaction of alpha methyl benzyl chlorides and carbon dioxide by [Co(Salen)].[9] The key step in the construction of diaryl ether unit during the synthesis of fenoprofen is by means of Ullmann reaction. This has been proved to be useful in a variety of transformation in organic synthesis.

The preparation of 3-bromoacetophenone was done using bromine and aluminium chloride.[10] Previously, the preparation of 3-bromo propiophenone was reported by reaction using 3-bromobenzonitrile and ethyl magnesium bromide. We optimized the synthesis of 3-bromopropiophenone from propiophenone, bromine, and aluminum chloride. It must be noted that the reaction using meta bromination with the commercially available propiophenone (**2)** is an important step in the synthesis of fenoprofen. Again, temperature plays a crucial role in this reaction.

The formation of C-O bond using 3,4,7,8-tetramethyl-1,10-phenanthroline (Me4Phen) or 1,10-phenanthroline as a ligand improves the Cu-catalyzed cross-coupling reactions of aryl halides with primary and secondary aliphatic, benzylic, allylic, and propargylic alcohols under mild reaction conditions.[11] Ullmann ether synthesis is an efficient method for the synthesis of diaryl ethers and is performed at 90°C using either aryl iodides or aryl bromides as the substrates under the assistance of amino acids.[12] Another general method involves developing a mild, palladium-free synthetic protocol for the cross-coupling reaction of aryl iodides and thiols using Cu catalyzed reaction and neocuproine ligand at high temperatures.[13]

Another efficient method for the synthesis of diaryl ethers under inexpensive ligand and mild conditions is the Ullmann-type coupling of aryl bromides or iodides with phenols. A number of diaryl ethers are obtained with excellent yields in acetonitrile in the presence of Cs_2CO_3 and catalytic copper(I) oxide.[14]The arylation of ethyl acetoacetate, ethyl benzoyl acetate, and dialkyl malonate under the catalysis of CuI and L-proline in DMSO proceed smoothly at lower temperatures in good yields. Both aryl iodides and aryl bromides are compatible with these reaction conditions.[15] The efficacy of copper-mediated cross-coupling reactions can be fairly increased with the initiation of mild reaction conditions and ability to employ catalytic amounts of copper. Again, the utilization of diamine-based ligands are of high importance in the synthesis of pharmaceuticals and designed materials.[16] By employing (2-pyridyl) acetone as a new supporting ligand, the copper-catalyzed coupling reactions of aryl halides with various phenolic moieties gives good yields under mild conditions. This reaction displays great functional groups compatibility and excellent reactive selectivity.[17] In this study, we have developed an effective new strategy for the synthesis of fenoprofen in good yield from propiophenone.

2. EXPERIMENTAL

2.1. General method

All manipulations were performed using standard Schlenk techniques under a dry nitrogen atmosphere. All the experiments were performed in flame-dried Schott Duran® bottles. Analytical thin layer chromatography (TLC) was performed on silica gel 60 F254 plates (Merck; 0.25 mm thickness) and visualized under UV light followed by spraying with 5% solution of phosphomolybdic acid (PMA) in ethanol, subsequently followed by charring with a heat gun. Column chromatography was performed on 60 silica gel (Merck; 230-400 mesh). All other reagents of analytic grade were used without any further purification. ^{1}H-NMR (hydrogen-1 NMR) and ^{13}C (carbon-13 NMR) were recorded using Varian NMR 500 instrument (NMR Laboratory, Urbana, IL) at 500 MHz. The chemical shifts were reported in parts per million (ppm) relative to tetramethylsilane (TMS), which was used as internal and external standards for ^{1}H-NMR. Mass spectra were recorded on a Shimadzu 2010s mass spectrometer (Shimadzu Biotech, Manchester, UK). The IR spectra were recorded on a Spectrum 100 spectrometer (Waltham, MA, USA).

2.2. Procedure for the synthesis of (±) fenoprofen (1)

3-Bromopropiophenone (3):

Aluminium chloride ($AlCl_3$) (67.0 g, 502 mmol) was taken in 500 mL RBF. Propiophenone, **2** (27.0 g, 201 mmol) was added drop wise (highly exothermic) over the period of 10-15 min (temperature reaches ~ 80°C), a molten mass formed. Stir it at same temperature for 10 min. Bromine (12.46 mL, 241 mmol) was added drop wise over a period of 20 min. Continue the stirring at room temperature for 1.5 hrs. Reaction mass was poured over Concentrated HCl and ice mixture under vigorous stirring. Slowly the solid was precipitated out. Washed the solid with ice water for 3 times. Filter the solid and air dried to afford **2** (27.0 g, 63%). (mp 39°C); IR: 1691, 1567, 1458, 1417, 1211 Cm^{-1}. ^{1}H NMR (DMSO d_6): 8.08 (s, 1H); 7.97-7.94(m, 1H); 7.85-7.83(m, 1H); 7.51-7.48(m, 1H); 3.08(q, *J* = 7.2 Hz, 2H); 1.05(t, *J* = 7.2 Hz, 3H). MS$[M+H]^+$ Calculated for $C_9H_{10}BrO$:m/z 214.08, found 214.70.

General procedure for the Ullmann coupling of 3-bromopropiophenone with phenol:

A pressure tube equipped with Teflon cap was charged with magnetic stir bar, [Cu] catalyst (5-10 mol%), Base (2 eq.), 3-bromopropiophenone (1 eq.), and phenol (1.2 eq.) in a suitable solvent (mentioned in Table 2). The

tube was evacuated and purged with argon for 20 min. Under a counter flow of argon ligand (Lig 1- Lig 8) was added. The tube was refilled with argon and sealed. The reaction mixture was heated to the indicated temperature (80-120°C) for the required time. After cooling to the room temperature, reaction mixture was diluted with ethyl acetate (25 mL), and then passed through a bed of celite to remove inorganic salts and the solvent was evaporated under vacuum. The residue was purified by column chromatography on silica gel and the product was dried under high vacuum.

1-(3-phenoxyphenyl) propan-1-one (4):

To a solution of Cs_2CO_3 (29.97 g, 92 mmol), 3-bromopropiophenone, **2** (10.0 g, 46 mmol), Phenol (6.62 g, 70 mmol), in dry DMF (100 mL) was added 1-(pyridin-2-yl) propan-2-one (1.24 g, 9.2 mmol). Contents were degassed for 30 min under vacuum, and then added Cu(I)Br (0.659 g, 4.6 mmol), again degassed for 10 min. under vacuum. Contents were heated at 120°C for 16 hrs. Reaction was monitored by TLC, water was added and extracted with ethyl acetate, and brine washing was given to organic layer, dried and evaporated. Crude compound was purified by column chromatography to afford **4** (7.34 g, 69.18%). IR: 1687, 1581, 1489, 1435, 1247 Cm^{-1}. ^{1}H-NMR: DMSO-d6: 7.75-7.05(m, 9H), 2.98(q, *J* = 7.2 Hz, 2H), 1.06(t, *J* = 7.2 Hz, 3H). MS[M+H]$^+$ Calculated for $C_{15}H_{15}O_2$:m/z 227.11, found 227.15.

α- Chloro-3-phenoxypropiophenone (5):

To a solution of 1-(3-phenoxyphenyl) propan-1-one, **4** (5.0 g, 22.22 mmol) in DMF (25 mL) was added Copper chloride. $2H_2O$ (7.50 g, 44.44mmol), followed by LiCl (0.932 g, 22.22mmol) and heated at 80-90°C for 15 h with constant stirring. The reaction mixture was cooled and poured over 0.5 N HCl (50 mL) and extracted with diethyl ether (30 mL X 3). The combined extract was successively washed by 0.5N HCl, aq. NaHCO3 solution, water and brine. The organic layer was dried over anhydrous sodium sulfate, filters and evaporated. The residue was purified by column chromatography on SiO_2 (100-200 mesh) using hexane as eluent to afford **5**(3.75 g, 65.10%). IR: 1691, 1580, 1488, 1436, 1258 Cm^{-1}. ^{1}H-NMR (DMSO d_6): 7.82-7.05(m, 9H), 5.73(q, *J* = 6.8 Hz, 1H), 1.58(t, *J* = 6.8 Hz, 3H). MS[M+Na]$^+$ Calculated for $C_{15}H_{13}ClO_2$m/z 260.06, found 283.85

α -Hydroxy-3-phenoxy propiophenone dimethyl acetal (6):

To a freshly prepared sodium methoxide, compound α- Chloro-3-phenoxy propiophenone, **5** (2.0 g, 7.67 mmol) in methanol (10 mL) was added drop wise under nitrogen atmosphere over 30 min. Reaction was monitored by TLC. Water was added and extracted with diethyl ether (20 mL X 3). Water washing was given to ether layer. Organic layer was dried over anhydrous sodium sulfate, filters and evaporated to afford **6** (1.6 g, 72.72%). ^{1}H-NMR: DMSO-d6: 7.45-7.35(m, 3H), 7.20-7.08(m, 2H), 7.04-6.95(m, 4H), 4.68(d, *J* = 4.4 Hz, 1H), 3.93(m, 1H), 3.18(s, 3H), 3.10(s, 3H), 0.78(d, *J* = 6.5 Hz, 3H).

Methyl α - (3-phenoxy phenyl propionate) (7):

To a solution of dimethylacetal, **6** (1.2 g, 3.9 mmol) and triethyl amine (1.05 mL, 7.5 mmol) was taken in dry DCM (12 mL) was cooled to -5^{0}C and sulfuryl chloride (0.835 g, 6.2 mmol) in dry DCM (12 mL) was added drop-wise by maintaining the reaction temperature -5°C under dry conditions under constant stirring. After complete addition of sulfuryl chloride, the reaction mixture was allowed to attain room temperature and stirred at same temperature for overnight, sat. aq. $NaHCO_3$ was added to it. The aqueous layer was extracted with DCM. The combined organic

layer was washed with water and brine, dried the organic layer, evaporated. The crude compound was purified by column chromatography over silica (100-200 mesh) using 10% Ethyl acetate in hexane to afford **7 (**0.65 g, 64.35%). IR: 1736, 1583, 1486, 1443, 1241 $cm^{-1.}$ ^{1}H-NMR (DMSO-d_6): 7.45-6.85(m, 9H), 3.78(q, *J* = 7.2 Hz, 1H), 3.58(s, 3H), 1.37(d, *J* = 7.2 Hz, 3H). MS[M]$^+$ Calculated for $C_{16}H_{16}O_3$**:**m/z 256.11, found 256.5.

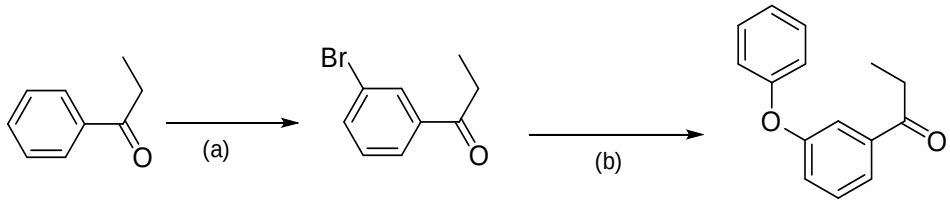
α -(3-phenoxy phenyl) propionic acid (1):

To a solution of ester, **7** (0.5 g, 0.0019 moles) in methanol (5 mL) was added 10 % aq. NaOH for alkaline hydrolysis. Contents were stirred at room temperature for 2h at room temperature. After completion of reaction acidified with 1 N HCl and extracted with ethyl acetate, dried and evaporated to afford, α-(3-phenoxy phenyl) propionic acid, **1 (**0.41 g, 86.86%). bp 169°C. **IR:** 1709, 1583, 1487, 1244 cm^{-1}**.** ^{1}H-NMR (500 MHz, DMSO-d_6): δ 12.35(s, 1H) 7.45-6.85(m, 9H), 3.67(q, *J* = 7.2 Hz, 1H), 1.30(d, *J* = 7.2 Hz, 3H). ^{13}C-NMR (125 MHz, DMSO-d_6): δ 175.10, 156.75, 156.50, 143.48, 130.04, 129.97, 123.51, 122.49, 118.70, 117.66, 116.75, 44.54, 18.47. MS[M-H]$^-$: Calculated for $C_{15}H_{13}O_3$ m/z 241.09, found 240.90.

3. RESULT AND DISCUSSION

At first, we synthesized 3-bromopropiophenone (**3**) from propiophenone using bromine and aluminum chloride. The diaryl ether was (**4**) synthesized by Ullmann reaction using 3-bromopropiophenone and phenol. For the optimization of the Ullmann reaction, screening of various ligands (Lig 1- Lig 8) was done using different copper-catalyzed coupling reactions as shown in scheme 1**.**

I. Scheme 1:



2 **3** **4**

Reagents and conditions: (a) $AlCl_3$, Br_2, r.t., 1.5 h, 63%; (b) Phenol, **3**, 5-10 mol% [Cu], 10 mol% Lig 1-Lig 8, Base, Solvent, Ar, 80-110°C, 12-24h; 69%

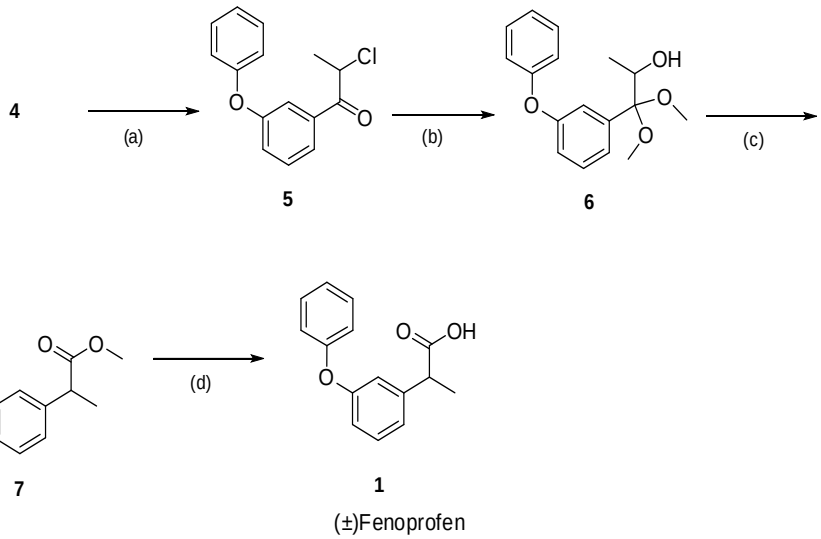
A variety of ligands such as 1,10-phenanthroline (Lig 1), 3,4,7,8-tetramethyl-1,10- phenanthroline (Lig 2), N, N-dimethylglycine.HCl (Lig 3), neocuproine (Lig 4), salicylaldoxime (Lig 5), L-proline (Lig 6), N-N-dimethylcyclohexane-1,2-diamine (Lig 7), and 1-pyridin-2-yl-propan-2-one (Lig 8) were screened in the reaction of phenol with 3-bromopropiophenone using the following catalyst system: 5-10 mol % CuI, 10 mol % ligand including the base in suitable solvent from 80°C-120°C from 12-24h (Table 1). Employing 1-(pyridin-2-yl) propan-2-one as a new supporting ligand, the copper-catalyzed coupling reactions of aryl bromide (3-bromopropiophenone) with phenol successfully proceeded in good yields. In this study, a new facile approach towards the synthesis of 1-(3-phenoxyphenyl) propan-1-one via Ullmann coupling, catalyzed by Cu(I)Br for the construction of diaryl ether fragment is described (**Entry 8 - Table 1**). Structures of ligands **Lig 1- Lig 8** were shown in **Figure 1**.

After optimizing the ligand (1-pyridin-2-ylpropan-2-one) via the Ullmann coupling condition, we were required to improve the yield of the reaction. For that purpose, screening of variety of catalysts and bases were carried out. We found that using copper bromide (CuBr), Lig 8, Cs_2CO_3 as a base in dimethyl sulfoxide solvent gives better yield (**Entry 3 - Table 2**).

After optimized Ullmann coupling condition, we used compound **4**, for the synthesis of fenoprofen. Earlier, fenoprofen could be readily prepared via cyanation reaction (NaCN, KCN, K_3FeCN_6). However, to avoid the usage of these hazardous cyanating reagents, we have proposed a better method for the synthesis of (±) fenoprofen. Our proposed method can prove to be more effective facilitating easy accessibility of raw materials as well as the use of special techniques for bulk synthesis. This is the safest route to synthesize fenoprofen. To summarize, we propose a simple and convenient method for the synthesis of Fenoprofen (**Figure 2**).

The synthesis of alpha halo ketone **(5)** from 3-phenoxy propiophenone **(4)** using copper chloride and lithium chloride in *N*,*N*-dimethyl formamide (DMF) was optimized.[18] Earlier the conversion of alpha halo ketone to aryl propionic acid was reported by photochemical transformation using propylene oxide and aqueous acetone.[19] This alpha haloketone was converted to alpha hydroxyl acetal intermediate (**6**) using sodium methoxide.[18, 20] The intermediate (**6**) converts into its chlorosulfonyl ester in situ and it rearranges to its methyl ester **(7)** in high yields.[21] The final fenoprofen (**1**) was isolated in excellent (87%) yields by basic hydrolysis of methyl ester with high purity. The sequence of reaction employed is depicted in below scheme **2**. The structure was confirmed by IR, mass, ^{1}H-NMR and ^{13}C-NMR.

Scheme 2:



Reagents and conditions: (a) $CuCl_2$, LiCl, DMF, 90°C, 15 h; 65% (b) NaOMe, MeOH; 72% (c) Et_3N, SO_2Cl_2, r.t., 16 h; 64% (d) aq. NaOH, MeOH, r.t., 2h, 87%.

4. CONCLUSION

Here, an efficient copper-catalyzed synthesis of diaryl ethers from phenol and 3-bromopropiophenone was developed after screening of different ligands (Lig 1- Lig 8). Out of legends screened, 1-(pyridin-2-yl) propan-2-one

was found to give a better yield. The CuBr-Lig 8 catalytic system showed an excellent yield at higher temperature. Our report provides an attractive addition to the existing strategies implemented for the synthesis of diaryl ethers via Ullmann coupling. We developed a concise and convenient new strategy for the synthesis of (±) fenoprofen in good yield from propiophenone with several prominent advantages of easy operation, convergence, and broad scope of applicability.

ACKNOWLEDGMENT

The authors are thankful to Head of Chemistry Department and Principal of Vidya Bharati Mahavidyalaya, Amravati for providing the necessary facilities to facilitate this study.

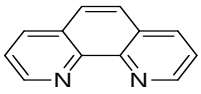
5. REFERENCES

Table 1 Standardization of Ullmann reaction using different ligands.

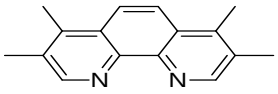
Entry	Ligand	Base	Solvent	Temp.(°C)	Time (h)	Yield (%)
1	Lig 1	Cs_2CO_3	Toluene	80	12	26
2	Lig 2	Cs_2CO_3	Toluene	110	24	12
3	Lig 3	Cs_2CO_3	1,4-dioxne	90	24	38
4	Lig 4	^tBuONa	Toluene	110	16	--
5	Lig 5	Cs_2CO_3	DMF	110	24	13
6	Lig 6	Cs_2CO_3	DMSO	90	22	18
7	Lig 7	K_3PO_4	DMSO	80	24	16
8	Lig 8	Cs_2CO_3	DMSO	120	24	45

Table 2 Improvement of the yield of Ullmann reaction using different catalyst and bases.

Entry	Catalyst	Base	Solvent	Temp.(°C)	Time (h)	Yield (%)
1	CuCl	Cs_2CO_3	NMP	130	12	12
2	CuBr	K_3PO_4	Toluene	100	24	28
3	CuBr	Cs_2CO_3	DMSO	120	16	69
4	CuI	Cs_2CO_3	Dioxane	90	24	41
5	CuI	K_2CO_3	DMA	120	7	18
6	CuI	K_3PO_4	Toluene	110	18	36
7	CuI	Cs_2CO_3	Toluene	110	24	16
8	CuI	Cs_2CO_3	Dioxane	100	24	12



Lig 1



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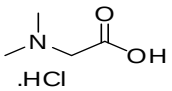

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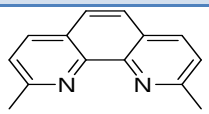
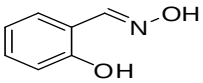
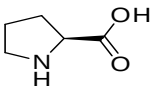


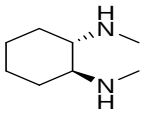
Lig 4



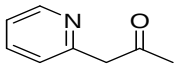
Lig 5



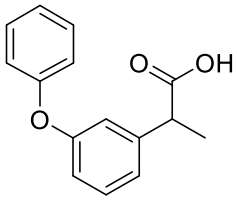
Lig 6



Lig 7



Lig 8



(±) Fenoprofen (**1**)

Figure 1 Structures of ligands **Lig 1- Lig 8**.

Figure 2 Chemical structure of (±) Fenoprofen.

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Synthesis and characterization of some newly synthesized Nitro and Bromo substituted 3, 5-diaryl isoxazolines

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ABSTRACTS
Five membered heterocycles like isoxazolines have found wide application as pharmaceutical and agrochemical agents. The present work deals with the synthesis of bromo and nitro substituted 3, 5-diarylisoxazolines from bromo and nitro substituted chalcone and hydroxylamine hydrochloride in the presence of ethanol solvent by refluxing for 2 hours.

INTRODUCTION:

The azole containing one oxygen and one nitrogen atom at 1, 2-position are designated as isoxazoles.

The dihydroderivative of isoxazole are known isoxazolines. A heterocyclic compound is one which possesses a cyclic structure with at least two different kinds of atoms in the ring. Compound incorporating heterocyclic ring systems continue to attract considerable interest due to the wide range of biological activities. Amonst them five membered heterocyclic compounds occupy a unique place in the realm of natural and synthetic organic chemistry. Five membered heterocycles like isoxazolines have found wide application as pharmaceutical and agrochemical agents.

The synthesized 3,3-diaryl-4-aroyl isozolines from 3-aroy flavnones and 3-aroyl chomones by the action of hydroxylamine hydrochloride in ethanol[1] also the synthesis of 3-(2'-hydroxy-3'-bromo-5'-5'-ethylchalcone and hydroxylamine hydrochloride in ethanol[2] and the preparation of substituted fluro isoxazolines from flurochalcones in DMF[3].also the preparation of of some chlorosubstituted nitrogen and oygen containing heterocycles and their use in controlling horticulture crops pathogens.[4]The Clean and effeIcient synthesis of isoxazalose derivative in aquaes media Synthesis of biocyclic isoxazoles isozaxoliness via intra molecular nitrile oxidecycloaddition[5-6]. The Synthesis and characteraisation of some novel isoxazoles via chalcone intramediates and The novel isoxazolines ectoparasiticide furalaner selective inhibition of orthopad aminobutyric acid and l-glutamate gated chloride and chanels and insteticidals acaricidal activity.[7-8] Expeditious preparation of isoxazole from isoxazoline and advanced intermediate for functional materials and Synthesis of some 3,5-diary-2-isoxazolines derivatives in ionic media[9-10]

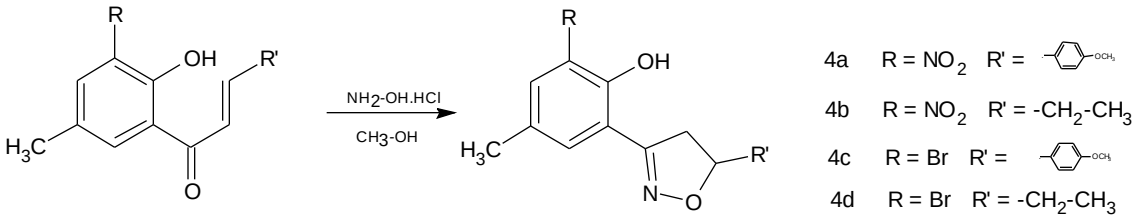
EXPERIMENTAL WORK:

The interaction of hydroxyl amine hydrochloride and chalcones has the most convenient method for the synthesis of isoxazolines.

The synthesis of isoxazoline from 1-(2-hydroxy-3-nitro-5-chlorophenyl)-3-(4-chloro phenyl) chalcone (0.01mole) treated with ortho-chlorobenzaldehyde in presence of KOH. The melting points of these compounds were recorded on 'Tempo' melting point apparatus and are uncorrected. The carbon nitrogen hydrogen and oxygen analysis was carried out on 'Carlo Ebra 1106' analyzer. The IR spectra were recorded on 'Perkin-Elmer' Infra Red spectrophotometer. The PMR spectra recorded on DRX300 spectometer in $CDCl_3$. Purity of this compound tested by TLC.

A) preparation of 3-(2-hydroxy-3-bromo/nitro-5-chlorophenyl)-5-(4 methoxychloro-phenyl)-isoxazoline (IIa/b)

A mixture of 1-(2-hydroxy-3-bromo/nitro-5-chlorophenyl)-3-(4-chloro phenyl)- chalcone(0.01 mole) and hydroxyl amine hydrochloride (0.02 mole)was refluxed for 2.5 hr.in methanol (25ml).The reaction mixture was decomposed crystalline solid product thus separate was filtered and crystallized from ethanol.



3 (a-d) 4 (a-d)

SPECTRAL INTERPRETATION:

Compound (4b): $C_{12}H_{14}N_2O_4$; **IR (cm^{-1}):** 3398.57 (-OH bonding), 3072.60 (Aro. stret.), 2927.94 (sp^3 C-H stret.), 1448.54 (-CH_2 bend.), 1365.60 (-CH_3 bend.), 1537.27 (NO_2 stret.), 1200 (C-O stret.), **NMR (δ ppm):** 12.86 (s, 1H, Ar-OH), 7.5-7.6 (m, 2H, Ar-H), 2.5 (d, 2H, Hetero –CH_2), 6.7 (m, 1H, Hetero –CH), 2.24 (m, 2H, -CH_2), 2.2 (t, 3H, -CH_3).

Compound (4d): $C_{12}H_{14}BrNO_2$; **IR (cm^{-1}):** 3435 (-OH bonding), 3055.24 (Aro. stret.), 2995.45 (sp^3 C-H stret.), 1319.31 (-CH_3 bend.), 578.64 (C-Br stret.), 1400.32 (-CH_2 bend.), 1319 (C-O stret.), **NMR (δ ppm):** 11.8 (s, 1H, Ar-OH), 6.8 (m, 2H, Ar-H), 2.27 (s, 3H, Ar-CH_3), 2.5 (d, 2H, Hetero –CH_2), 6.7 (m, 1H, Hetero –CH), 2.24 (m, 2H, -CH_2), 2.2 (t, 3H, -CH_3).

RESULT AND DISCUSSION

Synthesis of some Nitro and Bromo analogues of 3, 5-Diaryl Isoxazolines were achieved and their structures were confirmed on the basis of UV, IR and NMR spectral analysis.

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ORIGINAL ARTICLE

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Synthesis and biological activities of piperazine derivatives as antimicrobial and antifungal agents

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(Received May 31, 2017; Revised August 20, 2017; Accepted August 21, 2017)

Abstract: Apart from thiazole, benzimidazole, and tetrazole family, some of the piperazine analogs also show significant pharmacophoric activities. The synthesis of piperazine through intermediate **3** occurred via coupling of substituted benzenethiol with chloro-nitrobenzene. The nitro group of the isolated intermediate was reduced via an iron-acetic acid system. The aniline intermediate was cyclized with bis(2-chloroethyl)amine hydrochloride to obtain piperazine moiety. The synthesized substituted piperazine derivatives were screened for antibacterial and antifungal activities. The antibacterial activity was tested against *Staphylococcus aureus, Streptomyces epidermidis, Pseudomonas aeruginosa* and *Escherichia coli*, and antifungal activity was tested against *Candida albicans, Aspergillus niger, Aspergillus flavus* and *Aspergillus fumigatus*. As a result, many of the synthesized compounds showed significant antimicrobial and antifungal properties.

Keywords: Antibacterial activity; antifungal activity; piperazine derivatives. ©2017 ACG Publications. All rights reserved.

1. Introduction

Antibiotics are a class of drug that covers a wide range of pathogenic infections. Without causing any harm to the human organs or tissues, antibiotics interfere with the natural life cycle of bacteria, thus creating evolutionary pressure on them. Recently, many antibiotics-related researches have been conducted aiming at curing bacterial infections in humans. Antibiotics are now commonly used for medicinal purpose and during pre- and post-operation conditions. In critical operations involving use of oncology-based drugs, to prevent any infections, prompt antibiotic therapy is instituted.[1]

Penicillin was the first antibiotic to be discovered in 1928, followed by clinically efficient sulfonamide. After regular use of penicillin, the microbes developed resistance towards the antibiotic. Breeding of a host of penicillin-fast organisms was reported, which were transferred to other individuals leading to pneumonic conditions, because of which penicillin became ineffective.[2] Periodic supervision of these drugs has been conducted to prevent transmission of infections; however, these parameters have often been considered as a reactionary tool rather than a piece of any strategic planning and vision.[3] Hence, there is a need for a wide scope of research in finding new antibiotic molecules to overcome the bacterial infections. As the bacterium changes its nature regularly from one phase to another, studies with updated possible solutions are needed.

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The article was published by ACG Publications
www.acgpubs.org/OC/index.htm © Published online 08/25/2017 EISSN:1307-6175
DOI:http://doi.org/10.25135/acg.oc.23.17.05.026

To address the absence of development in the field of new anti-toxins, initially the purposes behind the hindered improvement should be comprehended. Although antibacterial and antifungal illnesses exist for long time, their clinical analysis is still difficult. Since previous two decades, various classes of antibacterial[4-10] and antifungal agents[11-17] have been found. Cotrimoxazole, Trimethoprim, sulfasalazine are few manufactured and semi-engineered antibacterial sulfa drugs. Penicillin drugs, such as Amoxicillin, Ampicillin, Penicillin G, and Cephalosporins have also been used for their bactericidal effects. Cephalosporins are known to eliminate microbes and work comparatively to penicillin. Antifungal drugs, such as Clotrimazole, Fluconazole and Amphotericin B, have been used to treat fungal infections. The most successive contagious pathogens are *Candida*, *Histoplasma*, *Stachybotrys*, *Aspergillus*, *Pneumocystis* and *Cryptococcus*, causing more than 1 million deaths globally every year. To restrict death rate, fast diagnosis and rapid execution of proper therapeutics need to be followed.[18] Due to nosocomial bloodstream infections, many deaths are reported. Majority of cases (2/3) are due to gram positive organisms and remaining due to gram negative organisms and fungi.[19]

The most common microbial infections in the hematopoietic stem cell transplant (HSCT) recipients are ~~is~~ caused by *Aspergillus*.[20] Currently, almost half of the patients suffer from invasive *aspergillosis*die, and the mortality rate for *candidemia* also remains high at approximately 50%.[21] Four classes of antifungal drugs, i.e. triazoles, polyenes, pyrimidine analogs and echinocandins, are available to treat fungal infections.[22] Increasing incidence of vancomycin-resistant *Enterococcus faecalis* and methicillin-resistant *Staphylococcus aureus* have been marked as a serious menace. However, limitation to infusion-related reactions and nephrotoxicity has been exhibited by amphotericin B, an antifungal drug used to treat serious fungal illnesses.[23, 24]

Piperazines and substituted piperazines constitute an important class of pharmacophores. One of the well-known piperazine category is indinavir (trade name: Crixivan), which functions as an HIV protease inhibitor. Piperazinyl cross-linked ciprofloxacin dimers, when used against resistant bacteria strain, exhibited low antibacterial activity.[25] When piperazine derivatives were linked to benzimidazole and benzotriazole molecules, they showed antifungal activity. Similarly, piperazine derivatives, containing tetrazole nucleus, have been reported as antifungal agents.[26] The details of the scaffold synthesis included coupling reaction, which was followed by reduction of nitro group and then cyclization.[27-28] In the present study, synthesis of a series of *N*-alkyl piperazine derivatives as a new class of synthetic antimicrobial and antifungal agents is disclosed.

2. Experimental

Analytical thin-layer chromatography (TLC) was performed on Merck 60 F254 silica gel plate (0.25 mm thickness) and visualized under UV light, and/or by spraying with 5% solution of phosphomolybdic acid (PMA) in ethanol, followed by charring with a heat gun. Following this, column chromatography was performed on Merck 60 silica gel (230-400 mesh). ^{1}H-NMR was recorded on Varian NMR 500 instrument at 500 MHz. Chemical shifts were reported in parts per million (ppm) relative to tetramethylsilane (TMS), which was used as internal and external standards for ^{1}H-NMR. Mass spectra were recorded on Shimadzu 2010s mass spectrometer.

2.1. Chemistry

*2.1.1. Procedure for Synthesis of **1-3***

*(2,4-Dimethylphenyl)(2-nitrophenyl)sulfane (**1**) :* To a solution of 1-chloro-2-nitrobenzene (**b**) (10.00 g, 63.47 mmol) in dry DMF (30 mL), K_2CO_3 (10.51 g, 76.16 mmol) and 2,4-dimethylbenzenethiol (9.03 mL, 66.64 mmol) were added, and the resulting reaction mixture was stirred at 25 °C for 18 h. Water (60 mL) was added and obtained mixture was stirred at 25 °C for 30 min. Yellow precipitate was then filtered off, washed with water (2 x 50 mL) and dried to afford the title compound **1** as yellow solid. Yield: 16.30 g, 99.08 %. ^{1}H NMR: ($CDCI_3$, 500 MHz) δ 8.25 (dd, *J* = 1.4, 8.2 Hz, 1 H), 7.46 (d, *J* = 7.8 Hz, 1 H), 7.32 (m, 1 H), 7.22-7.18 (m, 2H), 7.11 (m, 1H), 6.71 (dd, *J* = 1.2, 8.2 Hz, 1H), 2.40 (s, 3H), 2.30 (s, 3H).

*2-((2,4-Dimethylphenyl)thio)aniline (**2**):* To a mixture of (2,4-dimethylphenyl)(2-nitrophenyl)-sulfane **(1)** (10.0 g, 38.6 mmol) and AcOH (100 mL), Fe (8.61 g, 154.4 mmol) was added, and the resulting reaction mixture was stirred at 30 °C for 16 h. The reaction mixture was then filtered through a bed of Celite, and the filtrate was concentrated. To the residue, 300 mL saturated $NaHCO_3$ and 100 mL EtOAc were added. Organic layer was separated, water layer was re-extracted with EtOAc (100 mL), the combined organic layers were dried over Na_2SO_4, and the solvent was evaporated to afford **2** as an orange oil. Yield: 8.85 g, 99%. ^{1}H NMR: ($CDCI_3$, 500 MHz) δ 7.38 (dd, *J* = 1.5, 7.6 Hz, 1 H), 7.23 (m, 1H), 7.02 (m, 1H), 6.87 (m, 1H), 6.75-6.81 (m, 2H), 6.71 (d, *J* = 8.0 Hz, 1H), 4.24 (br s, 2H), 2.40 (s, 3H), 2.28 (s, 3H).

*1-(2-(2,4-Dimethylphenylthio)phenyl)piperazine (**3**):* A mixture of 2-((2,4-dimethylphenyl)thio)-aniline **(2)** (5.0 g, 21.8 mmol), bis(2-chloroethyl)amine hydrochloride (3.89 g, 21.8 mmol) and *N*, *N*-dimethylformamide (10 mL) was stirred at 110 °C for 48h. The reaction mixture was then cooled to 25 °C, the solvent was evaporated completely. Water (25 mL) and 25 mL ethyl acetate was added, and the mixture then further cooled to ~ 5°C while stirring. The formed white solid was filtered and washed with cold ethyl acetate (10 mL), and dried to afford **3** as a white powder as a HCl salt. ^{1}H NMR: ($CDCI_3$, 500 MHz) δ 7.39 (d, *J* = 7.8 Hz, 1H), 7.16 (m, 1H), 7.06-7.10 (m, 2H), 7.04 (m, 1H), 6.87 (m, 1H), 6.52 (m, 1H), 3.02-3.09 (m, 8H), 2.37 (s, 3H), 2.33 (s, 3H), 1.63 (br s, 1H, NH).

*2.1.2. Procedure for Synthesis of **4a-4p***

*2-(2-(4-(2-(2,4-Dimethylphenylthio)phenyl)piperazin-1-yl)ethoxy)ethanol (**HS-4a**):* To a solution of 1-(2-(2,4-dimethylphenylthio)phenyl)piperazine (0.5 g, 1.67 mmol) in DMF (5 mL) was added di-isopropyl ethyl amine (0.6 mL, 3.35 mmol) and 2-(2-chloroethoxy)ethanol (0.31 g, 2.51 mmol), which was followed by addition of potassium iodide (0.069 g, 0.41 mmol). The contents were stirred at 100 °C for 16 h. It was cooled to room temperature, water was added and extracted with ethyl acetate. Brine washing was performed with the organic layer, which was dried over anhydrous sodium sulfate, filtered and the solvent was evaporated. The crude product was purified by column chromatography to afford **HS-4a**, 0.23 g, 35%. IR: 3537, 3240, 3192, 3180, 3080, 3051, 3007, 2978, 2941, 2914, 2891, 2875, 2864, 2833, 2816, 2785, 2750, 2706, 2684, 25511934, 1913, 1897, 1643, 1600, 1577, 1556, 1514, 1348, 1307, 1269, 1138, 1114, 1074, 1060, 1043, 954, 923, 885, 819, 779, 761, 752, 729 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.37 (d, *J* = 9.5 Hz, 1H), 7.22 (s, 1H), 7.11-7.07 (m, 3H), 6.90-6.86 (m, 1H), 6.37 (d, *J* = 10 Hz, 1H), 4.62 (m, 1H), 3.56-3.49 (m, 4H), 3.43-3.41 (m, 2H), 2.97 (br s, 4H), 2.59-2.56 (m, 4H), 2.51 (t, *J* = 10 Hz, 2H), 2.32 (s, 3H), 2.23 (s, 3H). MS $[M+H]^+$ Calculated for $C_{22}H_{30}N_2O_2S$: *m/z* 387.21, found 387.20

*1-(4-(2-(2,4-Dimethylphenylthio)phenyl)piperazin-1-yl)-2-methylpropan-2-ol (**HS-4b**):* To a solution of 1-(2-(2,4-dimethylphenylthio)phenyl)piperazine (0.5 g, 1.67 mmol) in ethanol (10 mL) was added triethyl amine (0.7 mL, 5.01 mmol), which was followed by addition of 2,2-dimethyloxirane (0.31 g, 4.36 mmol) in a sealed tube. The contents were stirred at 90 °C for 6 h. The mixture was cooled to room temperature, the solvent was evaporated, water was added and extracted with ethyl acetate. Brine washing was performed with the organic layer, which was dried over anhydrous sodium sulfate, filtered and the solvent was evaporated. The crude product was purified by column chromatography to afford **HS-4b**, 0.4 g, 64%. IR: 3045, 2981, 2966, 1579, 1471, 1440, 1402, 1228, 1176, 1039, 960, 921, 804, 763, 754, 732 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.32 (d, *J* = 9.0 Hz, 1H), 7.15-7.02(m, 4H), 6.91 (t, *J* = 9.0 Hz, 1H), 6.49 (d, *J* = 9.5 Hz, 1H), 5.20-4.80 (br s, 1H, OH), 3.84-3.78 (m, 4H), 3.36-3.09 (m, 6H), 2.35 (s, 3H), 2.28 (s, 3H), 1.48 (s, 6H). MS $[M+H]^+$ Calculated for $C_{22}H_{30}N_2OS$: *m/z* 371.22, found 371.15.

*1-(Cyclopropylmethyl)-4-(2-(2,4-dimethylphenylthio)phenyl)piperazine (**HS-4c**):* To a solution of 1-(2-(2,4-dimethylphenylthio)phenyl)piperazine (0.5 g, 1.67 mmol) in DMF (5 mL) was added di-isopropyl ethyl amine (0.6 mL,3.35 mmol) and (bromomethyl) cyclopropane (0.31 g, 2.51 mmol), which was followed by addition of potassium iodide (0.069 g, 0.41 mmol). The contents were stirred at 100 °C for 12 h. It was cooled to room temperature, water was added and extracted with ethyl acetate. Brine washing was performed with the organic layer, which was dried over anhydrous sodium

sulfate, filtered and the solvent was evaporated. The crude product was purified by column chromatography to afford **HS-4c**, 0.15 g, 26%. IR: 2941, 2916, 2816, 1577, 1471, 1452, 1440, 1373, 1296, 1224, 1143, 1043, 1016, 813, 761, 750, 729 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.38 (d, *J* = 10.0 Hz, 1H), 7.14 (s, 1H), 7.10-7.01 (m, 3H), 6.85 (t, *J* = 8.5 Hz, 1H), 6.49 (d, *J* = 9.5 Hz, 1H), 3.14 (br s, 4H), 2.75 (br s, 4H), 2.36-2.32 (m, 8H), 0.98-0.88 (m, 1H), 0.55-0.53 (m, 2H), 0.15-0.14 (m, 2H). MS $[M+H]^+$ Calculated for $C_{22}H_{28}N_2S$: *m/z* 353.21, found 353.15

*1-(Cyclopentylmethyl)-4-(2-(2,4-dimethylphenylthio)phenyl)piperazine (**HS-4d**):* To a solution of 1-(2-(2,4-dimethylphenylthio)phenyl)piperazine (0.5 g, 1.67 mmol) in DMF (5 mL) was added di-isopropyl ethyl amine (0.6 mL,3.35 mmol) and bromomethylcyclopentane (0.41 g, 2.51 mmol), which was followed by addition of potassium iodide (0.069 g, 0.41 mmol). The contents were stirred at 100 °C for 16 h. It was cooled to room temperature, water was added and extracted with ethyl acetate. Brine washing was performed with the organic layer, which was dried over anhydrous sodium sulfate, filtered and the solvent was evaporated. The crude product was purified by column chromatography to afford **HS-4d**, 0.12 g, 19%. IR: 3047, 2939, 2812, 1577, 1450, 1373, 1222, 1139, 1124, 1043, 1001, 931,812, 765, 731 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.38 (d, *J* = 9.5 Hz, 1H), 7.14 (s, 1H), 7.10-7.01 (m, 3H), 6.84 (t, *J* = 8.0 Hz, 1H), 6.49 (d, *J* = 10 Hz, 1H), 3.10 (br s, 4H), 2.65 (br s, 4H), 2.36-2.32 (m, 8H), 2.15-2.07 (m, 1H), 1.85-1.75 (m, 2H), 1.68-1.49 (m, 4H), 1.28-1.18 (m, 2H). MS $[M+H]^+$ Calculated for $C_{24}H_{32}N_2S$**: m/z** 381.24, found 381.30

*2.1.3. General procedure for the synthesis of **4e,4f,4g,4k, 4l, 4m, 4n, 4o,4p***

To a solution of 1-(2-(2,4-Dimethylphenylthio)phenyl)piperazine (1 eq) in dry THF (10 mL) was added sodium hydride (2 eq) at 0 °C. The reaction mixture was stirred at the same temperature for 20 min, and then alkyl halide (1.5 eq) was added. The contents were stirred at room temperature for 4 h. The reaction was quenched using ice-water and extracted with ethyl acetate. Brine washing was performed with the organic layer, which was dried over anhydrous sodium sulfate, filtered and the solvent was evaporated. The crude product was purified by column chromatography.

*1-(2-(2,4-Dimethylphenylthio)phenyl)-4-methylpiperazine (**HS-4e**):* Yield: 0.03 g, 19%. IR: 2933, 2829, 2787, 1579, 1471, 1440, 1369, 1288, 1230, 1145, 1008, 923, 813, 763, 734 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.40 (d, *J* = 9.5 Hz, 1H), 7.15 (s, 1H), 7.10-7.01 (m, 3H), 6.84 (m, 1H), 6.51 (d, *J* = 10.0 Hz, 1H), 3.12 (br s, 4H), 2.65 (br s, 4H), 2.39 (s, 3H), 2.36 (s, 3H), 2.32 (s, 3H). MS $[M+H]^+$ Calculated for $C_{19}H_{24}N_2S$: *m/z* 313.17, found 313.19

*1-(2-(2,4-Dimethylphenylthio)phenyl)-4-ethylpiperazine (**HS-4f**):* Yield: 0.2 g, 46%. IR: 2970, 2954, 2810, 2762, 1577, 1471, 1448, 1436, 1375, 1303, 1224, 1147, 1126, 1043, 1029, 952, 813, 752, 731 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.39 (d, *J* = 7.0 Hz, 1H), 7.16 (s, 1H), 7.09-7.03 (m, 3H), 6.86-6.87 (m, 1H), 6.51(d, *J* = 7.5 Hz, 1H), 3.14 (br s, 4H), 2.68 (br s, 4H), 2.52 (q, *J* = 6.0 Hz, 2H), 2.37 (s, 3H), 2.33 (s, 3H), 1.16 (t, *J* = 6.0 Hz, 3H). MS $[M+H]^+$ Calculated for $C_{20}H_{26}N_2S$: *m/z* 327.19, found 327.10

*1-(2-(2,4-Dimethylphenylthio)phenyl)-4-isopropylpiperazine (**HS-4g**):* Yield: 0.16 g, 35%. IR: 2960, 2918, 2816, 1577, 1448, 1438, 1377, 1328, 1224, 1145, 1043, 979, 765, 754, 731 Cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.39 (d, *J* = 10.0 Hz, 1H), 7.16 (s, 1H), 7.11-7.03 (m, 3H), 6.88-6.85(m, 1H), 6.51 (d, *J* = 9.0 Hz, 1H), 3.16 (br s, 4H), 2.82-2.73 (m, 5H), 2.37 (s, 3H), 2.33 (s, 3H), 1.13 (d, *J* = 8.5 Hz, 6H). MS $[M+H]^+$ Calculated for $C_{21}H_{28}N_2S$: *m/z* 341.21, found 341.20

*1-(2-(2,4-Dimethylphenylthio)phenyl)-4-(2-(trifluoromethyl)benzyl)piperazine (**HS-4k**):* Yield: 0.38 g, 62%. IR: 2951, 2808, 1577, 1469, 1456, 1373, 1355, 1311, 1220, 1170, 1111, 1058, 1010, 929, 817, 763, 748, 729 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.83 (d, *J* = 9.0 Hz, 1H), 7.61 (d, *J* = 9.5 Hz, 1H), 7.52-7.49 (m, 1H), 7.36-7.29 (m, 2H), 7.12 (s, 1H), 7.05-6.99 (m, 3H), 6.82-6.81 (m, 1H), 6.48 (d, *J* = 10.0 Hz, 1H), 3.73 (s, 2H), 3.09 (br s, 4H), 2.67 (br s, 4H), 2.33 (s, 3H), 2.28 (s, 3H). MS $[M+H]^+$ Calculated for $C_{26}H_{27}F_3N_2S$: *m/z* 457.19, found 457.36

*1-(2-(2,4-Dimethylphenylthio)phenyl)-4-(2-fluorobenzyl)piperazine (**HS-4l**):* Yield: 0.31 g, 57%. IR: 2956, 2812, 1579, 1489, 1471, 1454, 1442, 1348, 1271, 1224, 1139, 1120, 1043, 1002, 941, 931, 815, 729.cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.44-7.36 (m, 2H), 7.25-7.24 (m, 1H), 7.14-7.01 (m, 6H), 6.87-6.83 (m, 1H), 6.50 (d, *J* = 10.0 Hz, 1H), 3.69 (s, 2H), 3.11 (br s, 4H), 2.71 (br s, 4H), 2.36 (s, 3H), 2.31 (s, 3H). MS $[M+H]^+$ Calculated for $C_{25}H_{27}FN_2S$: *m/z* 407.20, found 407.25

*1-(2-(2,4-Dimethylphenylthio)phenyl)-4-(4-nitrobenzyl)piperazine (**HS-4m**):* Yield: 0.21 g, 36%. IR: 2933, 2816, 1595, 1579, 1514, 1344, 1222, 1138, 1043, 1010, 943, 921, 850, 835, 763, 736 Cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 8.19 (d, *J* = 11.0 Hz, 2H), 7.56 (d, *J* = 10.5 Hz, 2H), 7.37 (d, *J* = 10.0 Hz, 1H), 7.14 (s, 1H), 7.07-7.01 (m, 3H), 6.87-6.83 (m, 1H), 6.49 (d, *J* = 9.5 Hz, 1H), 3.68 (s, 2H), 3.11 (br s, 4H), 2.67 (br s, 4H), 2.35 (s, 3H), 2.30 (s, 3H). MS $[M+H]^+$ Calculated for $C_{25}H_{27}N_3O_2S$: *m/z* 434.19, found 434.26.

*1-(2-(2,4-Dimethylphenylthio)phenyl)-4-(4-methylbenzyl)piperazine (**HS-4n**):* Yield: 0.32 g, 59%. IR: 2953, 2814, 1579, 1469, 1450, 1438, 1224, 1139, 1124, 1043, 1043, 1008, 815, 750 Cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.37 (d, *J* = 9.0 Hz, 1H), 7.25-7.23 (d, *J* = 9.5 Hz, 2H), 7.14-7.13 (m, 3H), 7.05-7.00 (m, 3H), 6.84-6.81(m, 1H), 6.48 (d, *J* = 9.5 Hz, 1H), 3.55 (s, 2H), 3.09 (br s, 4H), 2.64 (br s, 4H), 2.35 (s, 3H), 2.34 (s, 3H), 2.30 (s, 3H). MS $[M+H]^+$ Calculated for $C_{26}H_{30}N_2S$: *m/z* 403.22, found 403.29.

*1-(2-(2,4-Dimethylphenylthio)phenyl)-4-(3-methylbenzyl)piperazine (**HS-4o**):* Yield: 0.38 g, 70%. IR: 2943, 2814, 1579, 1471, 1452, 1373, 1338, 1222, 1139, 1124, 1043, 1010, 929, 813, 761, 752, 729 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.39 (d, *J* = 9.5 Hz, 1H), 7.25-7.15 (m, 4H), 7.10-7.02 (m, 4H), 6.87-6.83 (m, 1H), 6.50 (d, *J* = 10.0 Hz, 1H), 3.57 (s, 2H), 3.12 (br s, 4H), 2.68 (br s, 4H), 2.37 (s, 6H), 2.32 (s, 3H). MS $[M+H]^+$ Calculated for $C_{26}H_{30}N_2S$: *m/z* 403.22, found 403.35.

*1-(4-Chlorobenzyl)-4-(2-(2,4-dimethylphenylthio)phenyl)piperazine (**HS-4p**):* Yield: 0.32 g, 56%. IR: 3066, 2926, 2821, 1575, 1469, 1220, 1138, 1043, 1008, 817, 798, 763, 729, 688 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.39 (d, *J* = 10.0 Hz, 1H), 7.33-7.31 (m, 4H), 7.16-7.14 (m, 1H), 7.07 (d, *J* = 5.0 Hz, 2H), 7.05-7.02 (m, 1H), 6.89-6.84 (m, 1H), 6.51 (d, *J* = 9.5 Hz, 1H), 3.57 (s, 2H), 3.11 (br s, 4H), 2.66 (br s, 4H), 2.37 (s, 3H), 2.32 (s, 3H). MS $[M+H]^+$ Calculated for $C_{25}H_{27}ClN_2S$: *m/z* 423.17, found 423.27.

*1-(2-Chloroethyl)-4-(2-(2,4-dimethylphenylthio)phenyl)piperazine (**HS-4h**):* To a solution of 1-(2-(2,4-dimethylphenylthio)phenyl)piperazine (0.4 g, 1.34 mmol) in dry DMF (10 mL) was added potassium carbonate (K_2CO_3) (0.54 g, 4.02 mmol) and 1-bromo-2-chloroethane (0.22 g, 1.60 mmol). The reaction mixture was stirred at the same temperature for 16 h and the reaction was quenched using water and extracted with ethyl acetate. Brine washing was performed with the organic layer, which was dried over anhydrous sodium sulfate, filtered and the solvent was evaporated. The crude product was purified by column chromatography. Yield: 0.048 g, 10%. IR: 2943, 2816, 1579, 1454, 1373, 1224, 1139, 1124, 1043, 1006, 929, 813, 758, 729 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.39 (d, *J* = 9.5 Hz, 1H), 7.16 (s, 1H), 7.08-7.02 (m, 3H), 6.90-6.82 (m, 1H), 6.51 (d, *J* = 7.5 Hz, 1H), 3.66 (m, 2H), 3.13 (br s, 4H), 2.84 (m, 2H), 2.75 (br s, 4H), 2.37 (s, 3H), 2.33 (s, 3H). MS $[M+H]^+$ Calculated for $C_{20}H_{25}ClN_2S$: *m/z* 361.15, found 361.15.

*2-(4-(2-(2,4-Dimethylphenylthio)phenyl)piperazin-1-yl)ethanol (**HS-4i**):* To a solution of 1-(2-(2,4-dimethylphenylthio)phenyl)piperazine (0.35 g, 1.17 mmol) in dry acetone(10 mL) was added triethyl amine (0.23 mL, 1.17 mmol), which was followed by addition of 2-iodoethanol (0.09 mL, 1.17 mmol). The contents were stirred at room temperature for 6 h. The solvent was evaporated, water was added and extracted with ethyl acetate. Brine washing was performed with the organic layer, which was dried over anhydrous sodium sulfate, filtered and the solvent was evaporated. The crude product was purified by column chromatography to afford **HS-4I.** Yield: 0.05g, 12%. IR: 2914, 2818, 1579, 1469, 1454, 1438, 1311, 1224, 1126, 1043, 952, 813, 761, 750, 729 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.37(d, *J* = 7.0 Hz, 1H), 7.17(s, 1H), 7.11-7.03 (m, 3H), 6.92-6.88 (m, 1H), 6.52 (d, *J* = 9.5

Hz, 1H), 3.88 (t, *J* = 6.0 Hz, 2H), 3.33-3.31 (m, 4H), 3.06 (m, 5H), 2.91 (t, *J* = 6.5 Hz, 2H), 2.37 (s, 3H), 2.32 (s, 3H). MS $[M+H]^+$ Calculated for $C_{20}H_{26}N_2OS$: *m/z* 343.18, found 343.20.

*1-(2-(2,4-Dimethylphenylthio)phenyl)-4-propylpiperazine (**HS-4j**):* To a solution of 1-(2-(2,4-dimethylphenylthio)phenyl)piperazine (0.4 g, 1.34 mmol) in dry acetone (10 mL) was added triethyl amine (0.19 mL, 1.34 mmol) followed by addition of 1-bromopropane (0.16g, 1.34 mmol). The contents were stirred at room temperature for 6 h. The solvent was evaporated, water was added and extracted with ethyl acetate. Brine washing was performed with the organic layer, which was dried over anhydrous sodium sulfate, filtered and the solvent was evaporated. The crude product was purified by column chromatography to afford **HS-4j.** Yield: 0.26 g, 65%. IR: 2956, 2812, 1579, 1471, 1373, 1224, 1147, 1122, 1043, 1008, 931, 813, 761, 750, 729 cm^{-1}. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.38 (d, *J* = 9.5 Hz, 1H), 7.14 (s, 1H), 7.07-7.01 (m, 3H), 6.86-6.82 (m, 1H), 6.49 (d, *J* = 10.0 Hz, 1H), 3.11 (br s, 4H), 2.66 (br s, 4H), 2.41-2.35 (m, 5H), 2.31 (s, 3H), 1.61-1.52 (m, 2H), 0.93 (t, *J* = 9.0 Hz, 3H). MS $[M+H]^+$ Calculated for $C_{21}H_{28}N_2S$: *m/z* 341.21, found 341.25.

2.2. Biologigal Assay to Determine Antibacterial Activity

The final compounds (**4a-4p**) were tested for antibacterial and antifungal activities. The antibacterial activity was screened against Gram-positive bacteria, such as *Staphylococcus aureus and Streptomyces epidermidis*, and the Gram-negative bacteria, such as *Pseudomonas aeruginosa* and *Escherichiacoli*, in the agar disc diffusion method. The sample preparation was conducted by dissolving 1 mg of each sample in 1 ml of dimethyl sulphoxide (DMSO). For diffusion test against microbes, the agar plates were prepared by using agar solid medium. The media was poured into sterilized Petri dishes. The Petri dishes were then cooled for solidification. Then, a uniform mixture of inoculate was introduced to every Petri dish. The sterilized paper discs were loaded with samples of 1 mg/ml concentration and incubated at 37 °C. In successful reactions, clear zones of inhibition appeared around the discs. Ampicillin (19-21 mm, zone of inhibition) was used as a standard.

2.3. Biological Assay to Determine Antifungal Activity

Stock culture was prepared by transferring a loopful of fungal strain into the sterilized solid lipid micro-particles (SLM) with 25 ± 1°C incubation period for 48 h and 7 days for *Candida albicans*and *Aspergillus* species (*A. Niger, A. Fumigatus* and *A. flavus*), respectively. The stock was further sub-cultured by repeating the process mentioned above. *C. albicans* culture was harvested and diluted with the sterilized saline solution to obtain the spore count of about 1×10^7 CFU/mL. In the same manner, *Aspergillus* species cultures were harvested and the spore count was adjusted to about 1×10^7 CFU/mL with a sterilized saline solution. For inoculation of the culture, 0.1 mL of this saline solution consisting of fungal strain was used.[29-31]

2.3.1. Determination of the MIC range

A set of seven sterilized culture tubes were taken, and 1.0 mL of sterilized double strength Sabouraud liquid medium (DSSLM) was transferred aseptically to Tube I and 1.0 mL of sterilized nutrient broth was transferred aseptically to the remaining six tubes. Different concentrations of all the compounds to be tested, including the standard drug, were prepared by serial dilution method to obtain the drug concentration of 5.0 μg/mL, 2.5 μg/mL, … 0.078125 (0.08) μg/mL in Tube I to Tube VII, respectively. A control tube was also prepared by aseptically transferring 0.5 mL of sterilized DSSLM and 0.5 mL of solvent (DMSO). The culture tubes were inoculated with0.1 mL of fungal culture in a sterilized saline solution having microbial count of about 1 × 107 CFU/mL, so that the final microbial count in each culture tube would be about 1 × 106 CFU/mL. The tubes were incubated for 48 h at 25 ± 1°C. To check the turbidity, tubes were monitored under the microscope. The lower and higher concentrations gave the MIC range for the compound.[32,33]

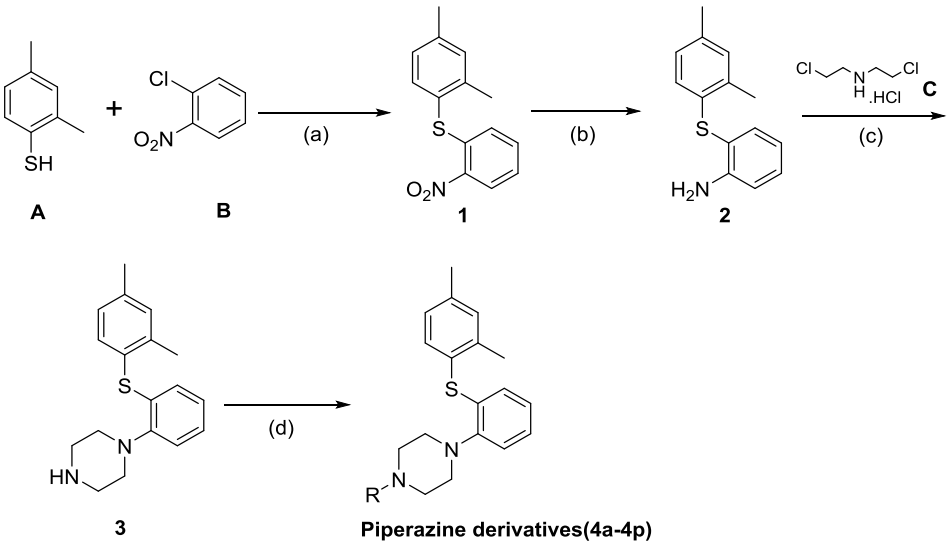
3. Results and Discussion

3.1. Chemistry

Earlier, the antimicrobial ativities of piperazine dithiocarbonate derivatives were investigated.[33] The synthesized compounds had more potency to inhibit gram-negative bacteria than gram positive ones. Among the bacterial strains, *E. faecalis* (ATCC 51922) and *P. aeruginosa* (ATCC 27853) were found to be the most susceptible ones. Few final compounds (**6a-d**) including alkyl groups in their structure displayed the same potency like that of Chloramphenicol against *E. faecalis* (ATCC 51922).

1-Chloro-2-nitrobenzene and 2,4-dimethylbenzenethiol were used as starting materials for the synthesis of piperazine derivatives. Addition[23] of 1.1 eq. of 2,4-dimethylbenzenethiol (**A**) to 1-chloro-2-nitrobenzene (**B**) in the presence of potassium carbonate (K_2CO_3) in *N*,*N*-dimethylformamide for 18 h afforded (2,4-Dimethylphenyl)(2-nitrophenyl)sulfane (**1**) in good yield (99%). The nitro group of compound (**1**) was reduced in the presence of iron in acetic acid for 16 h at room temperature to give 2-((2,4-Dimethylphenyl)thio)aniline (**2**), which was cyclized using bis(2-chloroethyl)amine hydrochloride in *N*, *N*-dimethylformamide at 110 ℃ for 48 h. Structures of the compounds were explained on the basis of spectral data and comparison with their authentic samples (**3**).

The reaction of compound (**3**) with alcohol, oxirane, cyclic alkyl halide, alkyl halides and various substituted benzyl halides yielded piperazine analogs (**4a-4p**) (Scheme 1).



Scheme 1. Synthesis of compounds **4a-4p.** a) A, B, K_2CO_3, DMF, 25°C, 18h b) Fe, AcOH, 30°C, 16h c) bis(2-chloroethyl)amine hydrochloride, DMF, 110°C, 48h d) Base, RX, solvent, 0-100°C, 4-16h.

Coupling reaction of (**3**) with different alkylating agents in the presence of base, such as sodium hydride, triethyl amine, di-isopropyl ethylamine, potassium carbonate, etc. also yielded the piperazine analogs. The products were separated on a silica gel column chromatography eluting with hexane/ethyl acetate. After the separation, structures of the compounds were determined by nuclear magnetic resonance (NMR), infrared (IR) and liquid chromatography/mass spectrometry (LCMS) studies. It was observed ~~seen~~ that the isolated products had high purity. Disappearance of a broad singlet at 1.63 ppm (piperazine NH) confirmed the coupling reaction yielding the desired products. The piperazine proton abstraction by base and nitrogen attak to the halide produced the final compounds. In piperazine, four CH_2 (8 protons) ranging from 3.02-3.09 confirmed the new product formation. Moreover, IR and LCMS data also confirmed the formation of the new compounds **4a-4p**.

3.2. Biological assay

3.2.1. In vitro Antibacterial Activity

All the isolated compounds were tested for their antibacterial activities against *Staphylococcus aureus, Streptomyces epidermidis, Pseudomonas aeruginosa* and *Escherichia coli* by agar disc diffusion method. For testing, the bacteria were obtained from agar slants. Loopful samples were grown in sterile nutrient broth medium, autoclaved at 121 °C at 15 atm for 15 min and left to grow for 48 h at 37 °C in an incubator. Ampicillin was used as reference drug for bacteria. The compound was tested at the concentration of 1 mg/mL, using DMSO as a solvent. From screening result, it was observed that most of the compounds were highly active against bacterial pathogens as well as fungus. The zone of inhibition (mm) of the final compounds against pathogenic bacterial strains is shown in Table 1.

Table 1. Antibacterial activity of newly synthesized piperazine derivatives

Compounds	***S.aureus***	***S.epidermidis***	***P.aeruginosa***	***E. Coli***
HS-4a	20	19	15	16
HS-4b	17	17	20	18
HS-4c	21	18	14	20
HS-4d	15	20	18	19
HS-4e	20	17	18	20
HS-4f	20	19	15	16
HS-4g	20	17	07	18
HS-4h	21	18	14	20
HS-4i	15	20	18	19
HS-4j	20	17	18	20
HS-4k	20	19	15	16
HS-4l	17	17	20	18
HS-4m	04	18	14	18
HS-4n	15	20	13	19
HS-4o	20	17	18	20
HS-4p	15	17	18	20
Ampicillin*	21	20	19	20

*Positive control

In general, while most of the final compounds showed better antibacterial activities, the compounds **4g** and **4m** showed moderate antibacterial activities against *P. aeruginosa and S. aureus,* respectively. 1-(2-(2,4-dimethylphenylthio)phenyl)-4-methylpiperazine (**4e)**, 1-(2-(2,4-dimethylphenylthio)phenyl)-4-propylpiperazine **(4j)**, and 1-(2-(2,4-dimethylphenylthio) phenyl)-4-(3-methylbenzyl)piperazine (**4o)** had the best antibacterial activity against pathogenic bacterial strains with a zone of inhibition in the range of 17-20 mm. The other compounds also showed good activities, except **4g** and **4m**.

3.2.2. In vitro Antifungal Activity

Antifungal activities of the newly derived piperazine derivatives were screened against pathogenic fungal strains, such as *Candida albicans, Aspergillus niger, Aspergillus flavus* and *Aspergillus fumigates* where Clotrimazol was used as the standard drug. Antifungal activities of the final compounds were conducted by using two-fold serial dilution methods. Stock solutions of the final compounds and the standard drug having the concentration 10 μg/mL were prepared in dimethyl sulfoxide (DMSO). The required dilutions were made from these stock solutions. The MIC (μg/mL) of the screened compounds by pathogenic fungi is shown in Table 2.

Table 2. Antifungal activity of newly synthesized piperazine derivatives*

Compounds	*C. albicans*	*A. niger*	*A. flavus*	*A.Fumigatus*
HS-4a	0.60	0.50	0.45	0.60
HS-4b	0.55	0.60	0.50	0.60
HS-4c	0.50	0.60	0.60	0.50
HS-4d	0.60	0.50	0.50	0.60
HS-4e	0.50	0.35	0.60	0.40
HS-4f	0.50	0.50	0.45	0.60
HS-4g	0.55	0.60	0.50	0.55
HS-4h	-	0.40	0.60	0.50
HS-4i	0.60	0.50	0.50	0.60
HS-4j	0.30	0.50	0.45	0.60
HS-4k	0.55	0.60	-	-
HS-4l	-	0.30	0.60	0.50
HS-4m	0.60	0.50	0.45	0.60
HS-4n	0.55	0.60	0.50	0.60
HS-4o	0.50	0.30	0.60	0.40
HS-4p	0.30	-	0.45	0.60
Clotrimazole$^{\phi}$	0.10	0.30	0.30	0.30

*MIC values are given as μg/mL; $^{\phi}$Positive control.

While most of the synthesized compounds showed significant antifungal activities, the compounds **4h, 4k, 4l, and 4p** showed moderate antifungal activities. The compounds **4a, 4b, 4c, 4d, 4e, 4f, 4g, 4i, 4j, 4m,** and **4n** showed better activities against *C. albicans* and *Aspergillus*. All the compounds having better activities had MIC values ranging between 0.35-0.6 μg/mL. The activities of piperazine derivatives were observed due to the alkylation of piperazine derivatives. So, Considering overall activities of the compounds **4a**, **4b**, **4e**, **4j** and **4o**, they had good antibacterial and antifungal activities.

4. Conclusion

Novel 1-(2-(2,4-Dimethylphenylthio)phenyl)-4-piperazine derivatives (**4a-4p**) were obtained through the reaction of 1-(2-(2,4-dimethylphenylthio)phenyl)piperazine (**3**) with alcohols, alkyl halides and substituted aromatic benzyl halides in presence of suitable base. The structures of the obtained compounds were characterized using conventional spectroscopic methods (NMR, IR, LCMS). The compounds (**4a-4p**) were tested for their antibacterial and antifungal activities, which showed both antibacterial as well as antifungal activities. From the screening results, it was observed that the compounds **4a, 4b, 4c, 4d, 4f, 4i, 4j** and **4o** were found to have high activity against both Gram-positive and Gram-negative bacteria and fungi, while the other compounds possessed week to modern activities. Compounds **4a, 4b, 4e, 4j** and **4o** showed maximum zone of inhibition. Thus, the compounds **4a**, **4b**, **4e**, **4j** and **4o** could be used for the antibacterial and antifungal appliations.

Acknowledgements

Authors are thankful to the Head of Chemistry Department and Principal of Vidya Bharati Mahavidyalaya, Amravati for providing the necessary facilities.

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Application a New PyMOL Plugin in Quantitative Structure-Toxicity Relationship Study of Pesticides

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Abstract: - Pesticides are toxic chemicals aimed for the destroying pest on crops. Since pesticides with similar properties tend to have similar biological activities, toxicity may be predicted from structure. Their structure feature and properties are encoded my means of molecular descriptors. Molecular descriptors can capture quite simple two-dimensional (2D) chemical structures to highly complex three-dimensional (3D) chemical structures. Quantitative structure-toxicity relationship (QSTR) method uses linear regression analyses for correlation toxicity of chemical with their structural feature using molecular descriptors. Molecular descriptors were calculated using open source software PaDEL and in-house built PyMOL plugin (PyDescriptor). *PyDescriptor* is a new script implemented with the commonly used visualization software PyMOL for calculation of a large and diverse set of easily interpretable molecular descriptors encoding pharmacophoric patterns and atomic fragments. *PyDescriptor* has several advantages like free and open source, can work on all major platforms (Windows, Linux, MacOS). QSTR method allows prediction of toxicity of pesticides without experimental assay. In the present work, QSTR analysis for toxicity of a dataset of mixtures of 5 classes of pesticides comprising has been performed. A good number of molecular descriptors were calculated followed by extensive objective and subjective feature selection to avoid redundant descriptors. For model building, the dataset was divided into training (80%) and test (20%) sets. A QSAR model built using three easily interpretable descriptors was subjected to extensive internal and external validation. The QSAR model is statistically robust with R^2 = 0.872, Q^2 = 0.844, CCC_{ex} = 0.845. The analysis revealed that lipophilicity, frequency of occurrence of hydrogen within 3 Å from phosphorus, and the presence of two benzene rings with $–CH_2–$ group as linker have good correlation with the toxicity of the pesticides.

Key-Words: - pesticides, toxicity, molecular descriptors, free software, plugin, regression analyses, lipophilicity.

1 Introduction

Pesticides are used extensively to control agricultural pest and to improve crop yields. However, small fraction of the pesticides is moving up from surface into stream, rivers and lakes and cause of considerable environmental concern as a result from application drift, rainfall runoff, or residue leaching through the soil into groundwater [1]. The contamination of water by pesticides increasing around the world, so the knowledge of eco-toxicological effects for aquatic organisms for the environmental risk assessment is essential.

Before pesticides are registered they must undergo laboratory testing on animals for short-term (acute) and long-term (chronic) health effects. Laboratory animals are purposely fed doses high enough to cause toxic effects. Small planktonic crustaceans *Daphnia*, fish, and algae are the most common organisms tested for the evaluation of toxic effects of pesticides. In order to reduce expensive and time-consuming experiments and reduce animal testing quantitative structure-toxicity relationship (QSTR) method is valuable [2]. Molecular descriptors, which are used to represent the structural features in terms of numbers, encode valuable information about structure or patterns in the molecular structures. Molecular descriptors are mostly classified as one-dimensional (1D), two-dimensional (2D) and three-dimensional (3D) descriptors. The 1D molecular descriptors represent bulk properties of compounds, such as the number of particular atoms, molecular weight, etc., and can be computed using molecular formula. 2D-molecular descriptors characterize structural information that can be calculated from 2D-structure of a molecule, such as the number of rings,

the number of hydrogen bond acceptors, etc. 3D-molecular descriptors stand for structural information that has to be obtained from 3D-structure of a molecule, such as solvent accessible surface area with negative partial charge in the structure. 2D and 3D molecular structure considerable influence on properties of pesticides, such as absorption, distribution, metabolism, and excretion (ADME). QSTR method allows prediction of environmental toxicity derived from the molecular structure and fills an important gap in risk assessment studies (REACH) [4]. QSTR method involves representations of molecules or molecular patterns in the form of numerical descriptors that capture the structural features and properties of molecules, generally known as molecular descriptors. Molecular descriptors describe: chemical properties (electrophilicity, hydrogen bonding), physical-chemical properties (lipophilicity, polar surface area), 2D structure (topological, information, connectivity, information indices, 2D frequency fingerprints), 3D structure (RDF, WHIM, GETAWEY, geometrical descriptors). Correlation of toxicity of molecule and molecular descriptors is most often expressed by linear equation calculated by multiple linear regression (MLR), or partial least squares (PLS) [5]. Computational neural networks (CNN) are usually performed if there is an assumption about a nonlinear and a highly complex relationship between the structure and the observed toxicity [6].

There are many commercial and free academic packages developed for calculation of molecular descriptors. Most of the molecular descriptors can be calculated by using commercial software packages such as CODESSA [7] and DRAGON [8]. Limitations of most of those packages are high price and hardly interpretable calculated molecular descriptors in terms of structural features. To overcome this, we have developed, *PyDescriptor*, a new script implemented with the commonly used visualization software PyMOL for calculation of a large and diverse set of easily interpretable 1D- to 3D- descriptors. They are also easy interpreting in terms of structural moieties, applicable for representing local environment or structure, simple to understand, independent of experimental properties, sensitive to changes in conformation molecule. PyMOL is free open source molecular graphics tool for 3D visualization of proteins, small molecules, density, surfaces, and trajectories [9]. *PyDescriptor* is a useful addition to the currently existing molecular descriptor calculation software. It has several advantages like free and open source and it is able to works on all major platforms (Windows, Linux, MacOS). It is a new chem-informatics tool which transforms a variety of structural features and local environment of a molecule to understandable 1D- to 3D- descriptors, which include encoding pharmacophoric patterns, atom-centred descriptors and a variety of fingerprints. These descriptors are either available in costly commercial softwares or in operating system dependent free softwares, thereby restricting their wide use. The script is freely available for academic use [10].

In the present paper we have generated QSTR models using molecular descriptors calculated by *PyDescriptors* for estimation of toxicity of 43 pesticides obtained on aquatic vertebrates bluegill sunfish (*Lepomis macrochirus*) [1].

2 Methods

2.1 Toxicity data

Toxicity data for aquatic vertebrates bluegill sunfish (*Lepomis macrochirus*) were retrieved from literature. Toxicity of 43 pesticides is expressed as LC_{50} (lethal concentration that kills 50 % of the animals in a test population / $molL^{-1}$). LC_{50} were converted in the form of a logarithm (log LC_{50}) (Table 1).

2.2 Calculation of molecular descriptors

Molecular descriptors were calculated using open source software PaDEL [11] and a new in-house built PyMOL plugin (PyDescriptor) [9] followed by extensive objective and subjective feature selection to avoid redundant descriptors.

2.3 Regression analysis and validation of models

For model building, the dataset was divided into training (80%) and test (20%) sets. The best QSAR models were obtained using a Genetic Algorithm using QSARINS v 2.2 [12].

The models have been assessed by: fitting criteria; internal cross-validation using leave-one out (LOO) method and Y-scrambling; and external validation. Fitting criteria included: the coefficient of determination (R^2), adjusted (R^2_{adj}), cross-validate R^2 using leave-one-out method (Q^2_{LOO}), global correlation among descriptors (*Kxx*), difference between global correlation between molecular descriptors and *y* the response variable, and global correlation among descriptors (ΔK), standard deviation of regression (*s*), and Fisher ratio (*F*).

Internal and external validations also included the following parameters: root-mean-square error of the training set ($RMSE_{tr}$); root-mean-square error of the training set determined through cross validated LOO method ($RMSE_{cv}$), root-mean-square error of the external validation set ($RMSE_{ex}$), concordance correlation coefficient of the training set (CCC_{tr}), test set using LOO cross validation (CCC_{cv}), and of the external validation set (CCC_{ex}), mean absolute error of the training set (MAE_{tr}), mean absolute error of the internal validation set (MAE_{cv}) and mean absolute error of the external validation set (MAE_{ex}), predictive residual sum of squares determined through cross-validated LOO method ($PRESS_{cv}$) in the training set and in the external prediction set ($PRESS_{ex}$). The analysed external validation parameters also include the coefficient of determination (R^2_{ex}). Robustness of QSAR models was tested by Y-randomisation test. New parallel models were developed based on fit to randomly reordered Y-data (Y scrambling), and the process was repeated several times (2000 iterations) [13-15]. Investigation of the applicability domain of a prediction model was performed by leverage plot or Williams plot (plotting residuals vs. leverage of training compounds). Detection of outliers was carried out for compounds that have values of standardized residuals greater than two standard deviation units using QSARINS. The leverage *h* of a compound is the measure of its influence on the model.

3 Result and discussion

The best three-descriptor based QSTR model for prediction of toxicity for the *Lepomis acrochirus* is:

$$\log LC_{50} = 1.948 - 0.588\ ALogP + 1.223\ FP747 - 0.375\ fPH3A \quad (1)$$

$N_{\text{training set}} = 34 \quad N_{\text{prediction set}} = 9$

The statistical results of the obtained QSTR model are presented in Table 2. Satisfaction of fitting criteria implies the following: the closer R^2 values are to unity, the more similar calculated values are to the experimental ones, that is, $R^2 \geq 0.60$. Also, larger *F* statistic and lower standard deviation means that the model is more significant. In order to avoid overfitting, inter-correlation between the descriptors included in the equation is detected based on *Kxx* and ΔK.

Table 1. Experimentally obtained toxicity endpoint and estimated values by eq. (1) of pesticides for *Lepomis acrochirus*

	Chemical	Exp. endpoint	Prediction fitting
		$\log LC_{50}$ mol/L	$\log LC_{50}$ mol/L
1	bensulfuron	2.43	-0.26
2	chlorimuron	0.59	1.39
3	chlorsulfuron*	0.92	0.86
4	flumetsulam	2.97	-0.36
5	halosulfuron	2.22	0.01
6	imazapyr*	3.19	-0.03
7	imazaquin	3.13	0.11
8	imazethapyr	3.17	-0.14
9	metsulfuron*	2.61	-0.35
10	nicosulfuron	3.39	0.36
11	primisulfuron*	2.34	-0.99
12	prosulfuron	2.57	-0.96
13	sulfometuron	2.22	-0.48
14	triasulfuron	2.40	-0.49
15	atrazine*	2.22	-0.19
16	cyanazine	1.97	-0.28
17	metribuzin	2.65	-0.33
18	prometon	2.12	0.29
19	prometryn	1.62	0.36
20	simazine	2.53	-0.68
21	acetochlor	0.74	0.25
22	alachlor*	1.31	0.03
23	metolachlor	1.64	-0.51
24	propachlor	0.86	0.55
25	azinphos-methyl	-1.19	0.40
26	chlorpyrifos	-1.25	0.26
27	diazinon	-0.13	-0.53
28	disulfoton	-0.34	-0.24
29	ethoprophos	1.19	-0.16
30	fonofos	-1.35	-0.22
31	malathion	-0.45	0.49
32	parathion	-0.24	-0.47
33	parathion methyl	0.86	0.51
34	phorate*	-1.82	1.25
35	terbufos	-1.89	0.92
36	butylate*	1.39	-0.62
37	carbaryl	1.69	0.25
38	carbofuran	0.45	0.85
39	EPTC	2.13	-0.40
40	molinate	1.87	0.25
41	pebulate*	1.54	0.35
42	thiobencarb	0.84	-0.52
43	tri-allate	0.74	-0.21
* member of the test set			

Low *Kxx* and $\Delta K \geq$ 0.05 implies no chance correlation between descriptors. The minimum acceptable statistical parameters for internal and

external predictivity include the following conditions: $R^2_{ext} \geq 0.60$; $CCC_{ext} \geq 0.85$; $RMSE_{cv}$ and MAE_{cv} close to zero; and $RMSE_{tr} < RMSE_{cv}$. Robust QSAR models should have low R^2_yscr and low Q^2_yscr values and R^2_yscr > Q^2_yscr. In order to investigate the applicability of a prediction model and detect possible outliers, the applicability domain of the selected model was evaluated by a leverage analysis expressed as Williams plot, in which residuals and the leverage values were plotted. Williams plot is given in Figure 1. A scatter plot of experimentally obtained toxicity calculated by QSTR model versus values calculated by Eq. (1) is presented in Figure 2.

Table 2. Statistical parameters of the obtained QSAR models.

	Statistical parameters	Value
Fitting criteria	R^2	0.87
	R^2_{adj}	0.86
	F	68.24
	Kxx	0.35
	ΔK	0.19
	$RMSE_{tr}$	0.51
	MAE_{tr}	0.43
	CCC_{tr}	0.93
Internal cross-validation	Q^2_{loo}	0.84
	$RMSE_{cv}$	0.56
	MAE_{cv}	0.48
	$PRESS_{cv}$	0.92
	CCC_{cv}	0.92
Y-scrambling	R^2_yscr	8.67
	Q^2_yscr	-19.05
External validation	R^2_{ext}	0.79
	$RMSE_{ext}$	0.66
	MAE_{ext}	0.52
	$PRESS_{ext}$	3.95
	CCC_{ext}	0.85

Obtained model has satisfactory results of fitting parameters and internal validation and low collinearity between the three descriptors. The results of Y-scrambling demonstrated that model wasnot obtained by chance correlation. Model 1 may be considered as predictive due to the high values of R^2_{ext} and CCC_{ext}, as well as small difference between $RMSE_{tr}$ and $RMSE_{ex}$, and between MAE_{tr} and MAE_{ex}. As can be seen from the Williams plot (Figure 1), toxicity of pesticides **30** (fonofos) predicted my model (1) must be used with reserve, because its leverage value is greater than the warning leverage (h^* = 0.353). Also, the same model has generated one outliers, pesticides **2** (chlorimuron) because its standardized residual is greater than ± 2.5.The best QSTR model obtained include the following descriptors: lipophilicity (ALog*P*), PaDEL fingerprint descriptor *FP747* and PyMOL descriptor *fPH3A*.Considering the negative coefficient of ALog*P* in Eq. (1) highly toxic compounds have a high lipophilicity. High lipophilic compounds my easily pass lipidous membranes and accumulate in fat tissue, therefore cause enhanced toxic effect [16]. Negative coefficient of PyDescriptor *fPH3A* implies that frequency of occurrence of hydrogen within 3 Å from phosphorus positively influence on increased toxicity of pesticides. QSAR study of toxicity of phoshorhydrazide (PHA) derivates revealed that the NH–P(X) moiety has a much higher inhibitory activity than the NH–C(X) moiety. The presence of the electron acceptor substituent around the P=X group increases the inhibitory potential of the PHA derivatives [17].

Obtained results are in accordance with previous findings of QSTR modeling of toxicity of organic molecules to *Daphnia magna* [4]. Obtained PLS a model suggests that higher lipophilicity and electrophilicity, and hydrogen bond donor groups are responsible for greater toxicity.

Figure 3a presents a chemical structure of the most toxic compound (**35**), an aliphatic organothiophosphate insecticide, terbufos. Thiophosphates are a very toxic class of organophosphorus compounds, especially if possess reactive functional groups such as: methyl, phosphate ester (P=O type) and unsubstituted phenyl group [18].

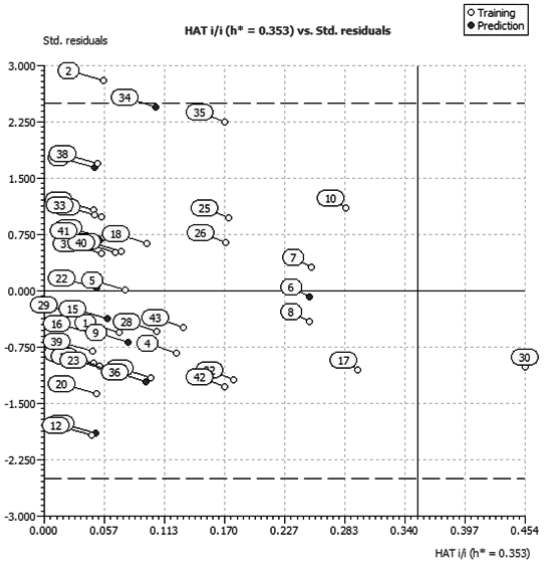


Fig. 1. Applicability domain of the QSAR model for log1/C_{50} expresses by eq. (1).

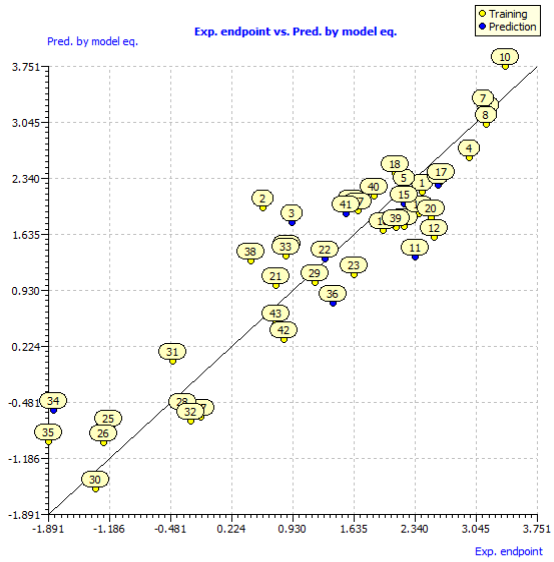
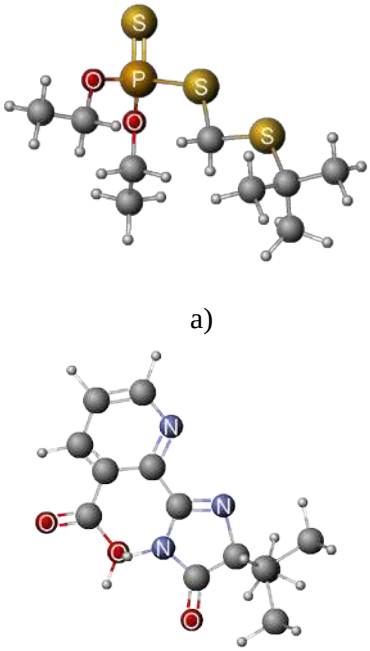


Fig. 2. A scatter plot of experimentally obtained toxicity calculated by QSTR model versus values calculated by eq. (1).

QSTR study of some organophosphorus compounds performed by using the quantum chemical and topological descriptors relieved that the sulphur atoms instead of oxygen atoms improved toxicity [19].

Figure 3b shows a structure of minimum toxic compound (**6**) imazapyr, an imidazolinone herbicide. Imazapyr does not contain phosphorus atom. According a positive coefficient of fingerprint descriptor *FP747* in eq. (1) imply that higher values of this descriptor mean lower toxicity.

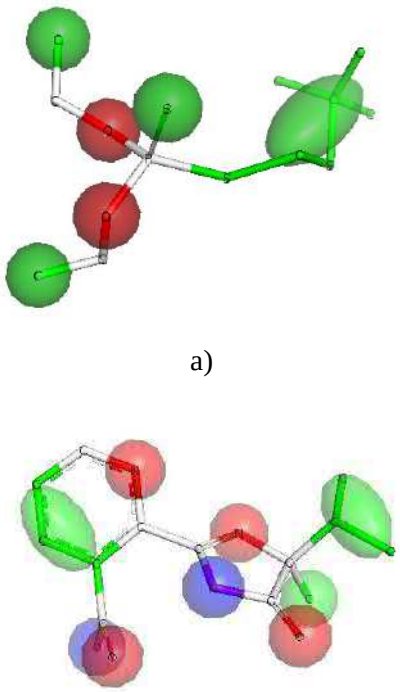
Plugin *PyDescriptor* allows visualization software PyMOL to encode a pharmacophoric patterns for lipophilicity, donors and acceptors of hydrogen atom. By means of new plugin, PyMOL can display a lipophilic area of molecule. In Figure 4 shows lipophilic area (green) of most toxic compound (**35**) and at least toxic compound (**6**). As can be see, terbufos (**35**), the most toxic analyzed pesticide has greater lipophilic area than imazapyr (**6**). Lipophilic areas in terbufos (**35**) are located on the aliphatic carbon atoms at the two ethoxy groups and *tert*-butyl group. Imazapyr (**6**) possess smaller lipophilic area located at the aromatic carbon atoms, methyl and isopropyl radical. Since we confirmed that toxicity increase with lipophilicity, as a consequence of the enhanced ability of toxicants to enter the organism (narcosis), this method allows prevision of possible locations in molecule for contact with lipid bilayer of cell membranes.



a)

b)

Fig. 3. Structure of: a) the most toxic pesticide, terbufos (**35**); b) the least toxic pesticide imazapyr (**6**).



a)

b)

Fig. 4. Lipophilic area (green) of: a) the most toxic pesticide, terbufos (**35**); b) the least toxic pesticide imazapyr (**6**).

4 Conclusion

In the present work, we have used an open source molecular descriptor calculation PyMOL plugin *PyDescriptor* for calculation easily interpretable and informative molecular descriptors. Robust QSTR models with good external predictive ability have been developed for the toxicity of pesticides for the fish, bluegill sunfish. The developed models, since, satisfy the threshold values for many statistical parameters could be useful for the prediction of experimentally undermined toxicity of known pesticides, as well as new pesticides. The model can also be employed to better understand the mechanism of toxicity of the various families of pesticides on the aquatic organisms, as well as the identification of potential aquatic pollutant.

Our results indicates that future QSTR analysis of pesticides should apply a specific group of descriptors relates with lipohilicity and structure fragment involved in electron transfer.

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Chemometrics and Intelligent Laboratory Systems 169 (2017) 12–18

Contents lists available at ScienceDirect

Chemometrics and Intelligent Laboratory Systems

journal homepage: www.elsevier.com/locate/chemometrics

PyDescriptor: A new PyMOL plugin for calculating thousands of easily understandable molecular descriptors

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ARTICLE INFO

Keywords:
Molecular descriptors
PyMOL
PyDescriptor
QSAR
Interpretation

ABSTRACT

The field of Quantitative Structure-Activity Relationship (QSAR) relies heavily on molecular descriptors. Among various guidelines suggested by Organisation for Economic Co-operation and Development (OECD), a very important guideline demands the mechanistic interpretation of a QSAR model. For this, a very attractive idea is to build a QSAR model using easily understandable molecular descriptors. To address this important issue, in the present work, we present an innovative chem-informatics tool, *PyDescriptor*. It can calculate a diverse pool of 11,145 molecular descriptors comprising easily understandable 1D- to 3D- descriptors encoding pharmacophoric patterns, atomic fragments and a variety of fingerprints. It is a new Python based plugin implemented within the commonly used visualization software PyMOL. *PyDescriptor* has several advantages like easy to install, open source, works on all major platforms (Windows, Linux, MacOS), easy to use through graphical user interface (GUI) and command-line, and output is saved in comma separated values (CSV) file format for further QSAR procedure. The plugin is freely available for academia.

1. Introduction

Computer Aided Drug Designing (CADD) has advanced with innovations in its thriving branches viz. Quantitative Structure-Activity Relationship (QSAR), molecular docking, pharmacophore modelling. The field of QSAR is among the oldest branches of CADD with its emphasis on prediction of activity/property (quantitative QSAR) and determination of pharmacophoric features or mechanistic interpretation (qualitative QSAR) [1–4].

Structure drawing and optimization, molecular descriptor calculations, model building and model validation are four basic steps of a typical QSAR analysis [5–8]. Molecular descriptors, which are used to represent the structural features in terms of numbers, encode valuable information about structure or patterns in the molecular structures [9–16].

Molecular descriptors have occupied unique place in chemistry, pharmaceutical sciences, quality control, etc. to provide valuable representation of molecular features in numerical and computational form for further evaluations [9–18]. With the progress of QSAR field, the types of descriptors have changed from simple and easily interpretative like number of carbon atoms, number of nitrogen atoms, log*P*, etc. to very complex descriptors like WHIM, BCUT, 3D-MoRSE, RDF, GETAWAY, and others [17,18]. These molecular descriptors are mostly classified as 1D-, 2D- and 3D- descriptors. The 1D- molecular descriptors represent bulk properties of compounds, such as the number of particular atoms, molecular weight, etc., and can be computed using molecular formula. 2D-molecular descriptors characterize structural information that can be calculated from 2D- structure of a molecule, such as the number of rings, the number of hydrogen bond acceptors, etc. 3D- molecular descriptors stand for structural information that has to be obtained from 3D- structure of a molecule, such as solvent accessible surface area with negative partial charge in the structure [17,18].

Manual calculation of descriptors like 3D-MoRSE, WHIM, BCUT, and similar complex (or esoteric [5]) descriptors was a very time consuming and laborious process [1,9–12,15,16]. To overcome this difficulty, computer programs were developed for computing descriptors either as independent software or as a part of QSAR software. The rapid developments in the field of computers and algorithms have made exact and

Abbreviations: OECD, Organisation for Economic Co-operation and Development; WHO, World health organisation; ADMET, Absorption, Distribution, Metabolism, Excretion and Toxicity; OLS, Ordinary Least Square; QSARINS-Chem, QSAR Insubria-Chemistry; GA, Genetic algorithm; MLR, Multiple linear Regression; OFS, Objective Feature Selection; SFS, Subjective Feature Selection; MMFF94, Molecular Mechanics Force Field 94; MAE, mean Absolute Error; CCC, Concordance Correlation Coefficient.

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http://dx.doi.org/10.1016/j.chemolab.2017.08.003
Received 11 May 2017; Received in revised form 15 July 2017; Accepted 10 August 2017
Available online 13 August 2017
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precise calculations of theoretical molecular descriptors possible in shorter time and cost-effective [1,9–12,15,16]. At present, there are many free and commercial softwares like Dragon (Talete) [17,18], PaDEL [19], MOE [20], Schrodinger [21], ChemDes [22], etc. which can calculate a variety of molecular descriptors viz. 1D- to 3D-, constitutional, topological, fingerprints. Some of these have been developed exclusively for the calculation of molecular descriptors only such as PaDEL-Descriptor [19], ChemDes [22], etc. while others are QSAR softwares which have descriptor calculation as one of their features (e.g., CODESSA Pro [23], Accelrys Discovery Studio [24], Sybyl-x [25], MOE [20]). Also, there are some open source libraries, such as JOELib [26,27], Chemistry Development Kit [28], and Chemical Descriptors Library [29], to name a few, which have molecular descriptor calculation functionality. It is reasonable that a good descriptor calculation software should have following features [19]:

1. Free or low-priced so that it is easy to purchase it.
2. Open source so that researchers could introduce their specific molecular descriptor calculations.
3. Has an easy to use graphical user interface (GUI).
4. Independent of operating system.
5. Possibly processes different molecular file formats like mol2, mol, sdf, etc.
6. Ability to compute numerous types of molecular descriptors.

A careful analysis of various currently available molecular descriptor calculating softwares reveals that many softwares lack one or more above mentioned features, besides, having its own advantages and limitations. An important area of research in the field of molecular descriptors is introduction of new descriptors or improvements in existing descriptors with easy correlation in terms of structural and pharmacophoric patterns [1,10–16,22,28,29]. Therefore, the field of molecular descriptors is dynamic and open for future developments like introduction of new softwares with ease of use and better user control functionalities, new descriptors with enhanced abilities to capture structural features [1,10–16,22,28,29].

Among various guidelines suggested by Organisation for Economic Co-operation and Development (OECD), a very important guideline demands the mechanistic interpretation of a QSAR model. For this, a very attractive idea is to build a QSAR model using easily understandable molecular descriptors. Unfortunately, the physical correlation of esoteric descriptors like WHIM, GETAWAY, RDF, etc. with one or more structural features/patterns is very complicated and an active area of qualitative and quantitative QSAR [5]. Therefore, there is need for introduction of easily understandable molecular descriptors. In the present work, we present a new PyMOL plugin, *PyDescriptor*, which has capacity to calculate 11,145 easily understandable molecular descriptors. It is a new chem-informatics tool which transforms a variety of structural features and local environment of a molecule to understandable 1D- to 3D- descriptors, which include encoding pharmacophoric patterns, atom-centred descriptors and a variety of fingerprints. These descriptors are either available in costly commercial softwares or in operating system dependent free softwares, thereby restricting their wide use. *PyDescriptor* possesses many advantageous features and plethora molecular descriptors, which justify its usefulness and wide acceptance in the field of QSAR and allied areas.

2. Experimental details

2.1. Plugin design and availability

PyDescriptor has been written in the object-orientated programming language Python 2.7.10 (64 bit) as a plugin for the three-dimensional molecular viewer PyMOL 1.8.2 and higher versions (Schrödinger, LLC. http://www.pymol.org/). Therefore, the advantages and limitations of Python 2.7.10 and PyMOL are associated with this plugin also. PyMOL is a widely-used software proficient in rendering and ray-tracing high resolution molecular representations in publication quality [30]. Due to availability of an open-source version of PyMOL, it is an attractive choice for academic and educational use [30]. Apart from visualizations of molecular structures, PyMOL has emerged as a calculation software due to availability of different open source plugins for a variety of purposes for example APBS for electrostatic map calculation, CAVER for calculation and visualization of tunnels, MIPTOOL for LogP calculation, DYNAMICS for molecular dynamic simulations with Gromacs, a few to mention [30]. In addition, LIQUID is an open source plugin for PyMOL, which is capable of generating pharmacophore model for a molecule. The output of LIQUID is available in the form of spheres and ellipsoids in the 3D- viewer of PyMOL [31]. Though, *PyDescriptor* uses the framework of PyMOL, it has been fully coded by our group. Practical information, such as a user guide/manual and application notes, along with the plugin '*PyDescriptor*', are available free of charge from authors.

2.2. System requirements and installation

In order to use *PyDescriptor*, a working installation of PyMOL version ≥1.8.2 on a standard Linux or Windows or MacOS installations with Python 2.7.10 is essential. *PyDescriptor* can be used without any dependencies i.e. there is no need to install any other module or software. At present, the plugin has been built to use MOL2 file format containing single molecule only. MOL2 format has the benefit of storing all the essential information for atom type, position, partial charges, and connectivity. In addition, it is also a well-known standardized format that many programs can read. It is one of the few public formats capable of supporting both a chemically-accurate description of small organic molecules as well as protein or nucleic acid also. Other formats for representing molecular structure have to be converted to an MOL2 file format for use in *PyDescriptor*. For this purpose, users can use open-source programs (e.g. Open babel, Avogadro) to convert other file formats into MOL2 format. While using MOL2 file format, all atom-typing and atomic partial charges assignments need to be performed correctly with all hydrogen atoms added. After successful completion of the descriptor calculations, the molecular descriptor values are automatically saved in CSV file format.

2.3. Parsing and calculations

PyDescriptor performs the main task of reading the MOL2 files and calculating the molecular descriptor value for all the MOL2 files located in the folder (for windows users, C:\PyDescriptor). As shown in Fig. 1, when the user clicks 'Compute descriptors', the plugin executes the calculation of molecular descriptors. The values for all the molecular descriptors are entered and automatically saved iteratively into the CSV columns along with the name of MOL2 file in the first column.

The following set of codes is used to read MOL2 files:

```
import os, glob, csv, pymol
os.chdir('C:\PyDescriptor')
from pymol import cmd, stored, util
path = os.path.dirname(pymol.__script__)
cmd.delete('all')
mol_files = glob.glob(os.path.join(path, '*.mol2'))
```

***PyDescriptor* Protocol:**

- Read all the MOL2 files from a particular folder (for windows users, C:\PyDescriptor)
- Calculate the molecular descriptors for all the molecules in the given folder
- Read the name of the files and enter in the CSV file together with their corresponding descriptor values

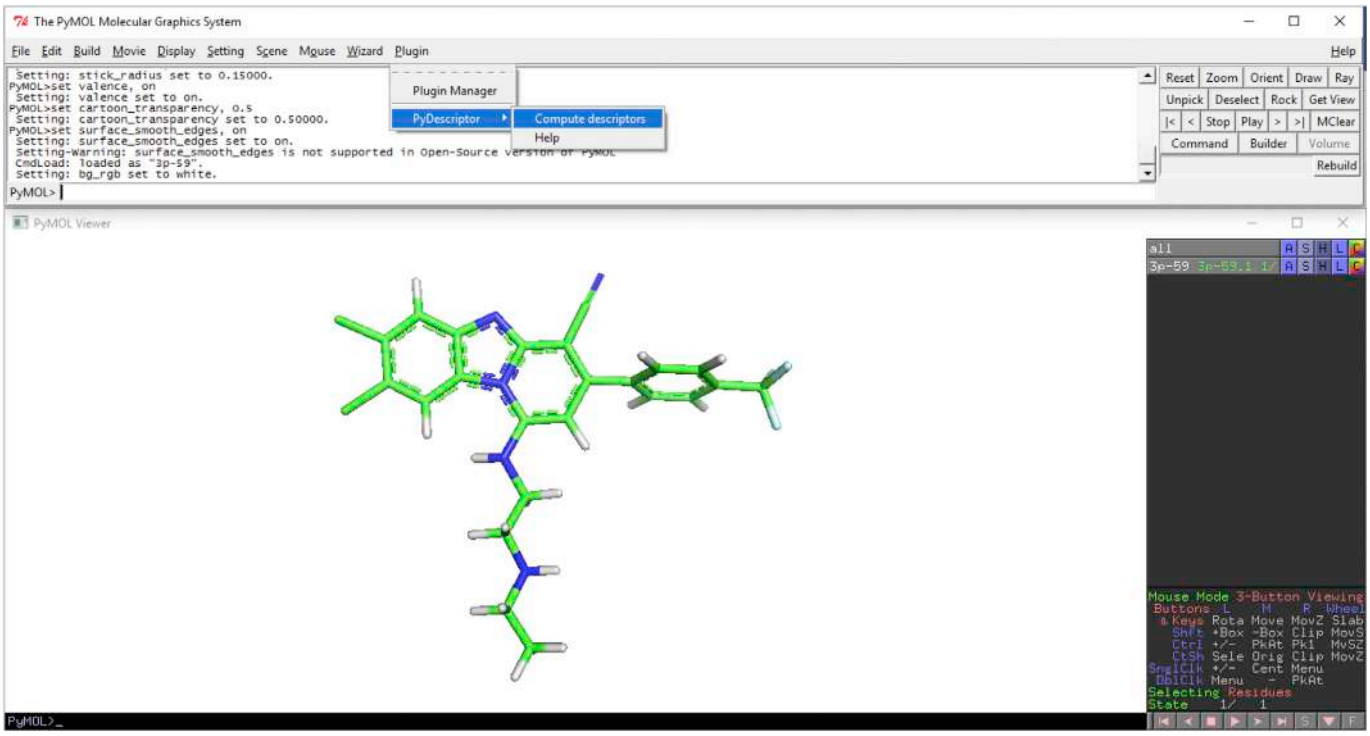

Fig. 1. GUI for *PyDescriptor* plugin loaded with a 3D molecule.

2.3.1. Descriptors calculation speed experiments

A straightforward comparison of the descriptor calculation speed of different softwares in a strict way is hard as the number and types of descriptors calculated by each software are different [19]. Therefore, all experiments for calculating the speed of descriptor calculations were accomplished only for *PyDescriptor* using Windows 7 (64 bit) on two different computers with varying architectures. Each experiment was repeated five times and the average of the total time needed to complete the calculation has been reported. Python's "timeit" module was employed for the measurement of calculation time. The details of computers and data set are as following:

1. Computer-1: Windows 7 (64 bit) operating system installed on a Lenovo G560 system with Intel® Pentium® P6100 2.00 GHz processor with 3 GB RAM.

2. Computer-2: Windows 7 (64 bit) operating system installed on a Dell system with Intel i7 2.00 GHz processor with 8 GB RAM.

Data set: The data set contains a diverse set of 1290 molecules as reported by Xu et al. [32]. The data set was converted from the SMILES flat file representation to individual MOL2 file using OpenBabel 2.4.0 using MMFF94 for structure optimization.

2.3.2. Derivation of interpretable QSAR

As the present plugin calculates 11,145 molecular descriptors, a very logical question can arise about the possibility of using these descriptors for developing scientifically interesting new, better and interpretable models as well as about the diversity of pool of descriptors calculated by *PyDescriptor*.

In majority of situations, a small dataset is available to a QSAR researcher for building the models. Hence, to address these issues, new QSAR models were built and statistically compared for two datasets of small size using the molecular descriptors calculated by *PyDescriptor*.

Dataset 1. It comprises a small dataset of sixty phosphoramidate and phosphorothioamidate analogues of amiprophos methyl reported as antimalarial [33].

Dataset 2. This dataset encompasses ninety-seven substituted phenyl 4-(2-oxoimidazolidin-1-yl) benzenesulfonates exhibiting antiproliferative activity [4].

2.3.3. Procedure for QSAR model development

For QSAR model development, OECD guidelines were followed to ensure internal and external predictive ability with mechanistic interpretation. The procedure mentioned in development of QSAR model for dataset 1 and 2 has been followed to assure reproducibility of results and fair comparison [4,33]. That is, the training and prediction sets were kept identical with the training and prediction sets as in the respective original publication [4,33]. In addition, statistically robust multiple QSAR models were also developed by changing the composition of training and prediction sets. These multiple models are available in supporting information. In general, the structures were drawn and optimized using MMFF94, followed by calculation of molecular descriptors using PaDEL, e-Dragon and *PyDescriptor*. The next step comprises elimination of highly correlated ($|R| > 0.90$) and constant variables (>95%). Subjective feature selection was used to build the statistically robust OLS QSAR models using genetic algorithm (GA) in QSARINS-Chem 2.2.1 [34,35] using Q^2_{LOO} as the fitness function. The exhaustive search of optimum number and set of descriptors was performed till there was improvement in the value of Q^2_{LOO}. Th e GA module of QSARINS-Chem 2.2.1 does not require a prior knowledge of important descriptors, that is, an important descriptor may or may not be in the final QSAR model [34,35]. Exhaustive internal as well as external validation along with Y-scrambling and analysis of Applicability Domain (AD) by Williams plot [34,35] for all the developed models were performed using QSARINS-Chem 2.2.1 to reject over-fitting and spurious models. Various parameters for internal and external validation includes: determination coefficient R^2, leave-one-out (LOO) cross-validation Q^2, leave-many-out (LMO) Q^2_{LMO}, coefficient of determination for Y-scrambling R^2_{Yscr}, root mean squared error (RMSE), $RMSE_{ex}$, MAE_{ex}, R^2_{ex}, Q^2_{F1}, Q^2_{F2}, Q^2_{F3}, and CCC_{ex}. The mean value of Q^2_{LMO} has been reported.

3. Results and discussion

Molecular descriptors occupy a unique place in QSAR. The success of

QSAR models not only lies on accurate set and number of descriptors with proper validation but on correct correlation and interpretation of molecular descriptors in terms of structural features also [5]. Many a time, the QSAR models are derived using a set of esoteric descriptors only [5,7,33,36,37]. This substantially limits the use of a properly validated QSAR model by synthetic chemists, to whom the descriptor calculating software is not available, or he/she is unable to correlate structural feature with a specific descriptor, or has little knowledge of QSAR field [5,7,33,36,37]. Therefore, the molecular descriptors involved in an appropriately validated QSAR model must be understandable in terms of structural features and the descriptor calculating software must be available either free or at very low cost. To address this crucial issue, we have developed *PyDescriptor*. The sole purpose of *PyDescriptor* is to facilitate calculation of easily understandable molecular descriptors.

This PyMOL plugin possesses following merits: easy to operate, reproducible results, calculates thousands of molecular descriptors (11,145 descriptors), calculates unique molecular descriptors which are either available in commercial or operating system dependent free softwares, the results are directly saved in a CSV file, and free for academia. In addition, molecular descriptors are easily and rapidly calculated with no missing values, a common difficulty with many existing commercial systems.

3.1. PyDescriptor descriptors

PyDescriptor computes 11,145 easily understandable molecular descriptors using conventions and idioms used in PyMOL. The molecular descriptors that are calculated using this plugin possess a value that is independent of the particular characteristics of the molecular representation, such as atom numbering or labelling, spatial reference frame, translational invariance and rotational invariance, etc. The descriptors possess following additional advantages: easy interpretation in terms of structural moieties, applicable for representing local environment or structure, simple to understand, independent of experimental properties, efficient construction possible, use of familiar structural concepts, conformation dependent, and change according to continuing modification in structures. A majority of descriptors calculated by the present plugin are information-based descriptors i.e. encode the information stored in molecular structures. It can calculate 1D- descriptors like molecular weight, number of atoms, etc., 2D- descriptors like charge descriptors, H-bond donor acceptors, 2D- fingerprint, etc. and 3D-descriptors like charged partial surface area, three-dimensional autocorrelation (3DA) descriptors, etc. A majority of 2D- and 3D- descriptors calculated by *PyDescriptor* represent the relative position of atoms or atom properties by calculating the separation between atom pairs in terms of number of bonds (2DA) or Euclidean distance (3DA) [38].

A very important feature of *PyDescriptor* is its ability to calculate a good number of circular fingerprints (CFP) [39], extended connectivity fingerprints (ECFP) [40], and their variants. These fingerprints are extensively used in high-throughput screening (HTS), similarity searching, including chemical clustering and compound library analysis, etc. [39] [40] These fingerprints can capture rich local structural information available in a molecule. For example, *O_N_5A* is a circular fingerprint descriptor calculated by *PyDescriptor*. *O_N_5A*, which stands for the presence of N atoms within a spatial distance of 5 Å from O atom, looks for the N atom(s) within the radius of 5 Å whose center is O atom. *PyDescriptor* not only counts ECFP/FCFP/CFP but it can calculate several ECFP/PFP/Circular fingerprints inspired 'specific' descriptors containing additional features such as partial charges, frequency of connected or non-connected atoms or functional groups, etc. For example, *O_N_5Ac* stands for sum of partial charges on N atoms which are within 5 Å from O atom. Another example is *O_N_7Bc* which corresponds to sum of partial charges on N atoms which are within seven bonds from O atom.

As *PyDescriptor* is a software plugin dedicated for molecular descriptor calculations only, henceforth its comparisons shall only be made with other similar dedicated software instead of comparing it with general QSAR software. For comparison purpose, molecular weight, average molecular weight and number of atoms for simple organic molecules calculated by PaDEL, e-Dragon and *PyDescriptor* have been tabulated in Table 1. From Table 1, it is clear that the values of molecular descriptors calculated by *PyDescriptor* are in good agreement with the values for same descriptors calculated by PaDEL and e-Dragon.

PyDescriptor has numerous benefits that are generally associated with existing open and free dedicated molecular descriptor calculation software. Being free will broaden the easy availability of the software to a good number of users and open source will permit users to easily check the code and amend it to suit their requirements. This could possibly help in the recognition of errors/bugs and increase the number of molecular descriptor calculation abilities. Since *PyDescriptor* is a plugin built within the framework of PyMOL, the users of *PyDescriptor* must also agree with the respective licenses of PyMOL and Python. Another important advantage of *PyDescriptor* is that it can work on any platform on which PyMOL 1.8.2 and Python 2.7 have been installed. This allows it to run on the three major platforms, Windows, Linux, and MacOS.

In addition, *PyDescriptor* can be used not only through GUI but using command line (via PyMOL) also. Having both GUI and command line options for running *PyDescriptor* is important, as the GUI will cater the need of a large number of users while the command line is useful for those who need to run *PyDescriptor* in computer clusters for big databases.

At present, a major caveat of *PyDescriptor* is its inefficiency to calculate graph-based topological descriptors; work is in progress to overcome this limitation. However, to our knowledge, no simple, freely available Python and PyMOL tool is available that can easily perform molecular descriptor calculation using PyMOL (see Table 2).

3.2. Descriptor calculating speed

For a data set of 1290 molecules, computer-1 and computer-2 took 19406.00 (15.04 s per molecule) and 8845.56 (6.86 s per molecule) seconds, respectively. Thus, it is clear that *PyDescriptor* works well on a computer with high computational abilities. We clarify that *PyDescriptor* has not been optimized for speed. As *PyDescriptor* is open source, users can modify it for speed and their specific use.

3.3. Developing new QSAR models

According to OECD guideline, “mechanistic interpretations of (Q) SARs begin with the number and the nature of the molecular descriptors used in the model”. According to Johnson [41,42], a QSAR modeler must always keep in mind that mechanistically interpretable models are more likely to define causative relationships and are less liable to be the result of chance correlations. Therefore, understanding of the meaning of descriptors is very important during QSAR interpretation step. The mechanistic interpretation of a QSAR model helps to develop “action plan” by a decision maker, for example a medicinal chemist [43]. Since, many easily understandable descriptors calculated by *PyDescriptors* are able to provide useful information about local environment in the molecule and capture specific pharmacophoric patterns, deriving new QSAR models using descriptors calculated by *PyDescriptors* will be beneficial in mechanistic interpretation of QSAR model and in decision making.

1. **QSAR modelling for anti-malarial activity of phosphoramidate and phosphorothioamidate analogues of amiprophos methyl** [33]

Recently, our group published [33] multiple properly validated QSAR models for anti-malarial activity of phosphoramidate and phosphorothioamidate analogues of amiprophos methyl using understandable molecular descriptors for the best model (termed as Old Model 1 in the present work).

Table 1
Comparison of different molecular descriptors calculated by PaDEL, e-Dragon and *PyDescriptor*.

S.N.	Molecule	Molecular Weight			Number of rings			Number of Atoms		
		PaDEL	e-Dragon	*PyDescriptor*	PaDEL	e-Dragon	*PyDescriptor*	PaDEL	e-Dragon	*PyDescriptor*
1	Acetylene	26.01565	26.04	26.03728	0	0	0	4	4	4
2	Aniline	93.05785	93.14	93.12648	1	1	1	14	14	14
3	Benzene	78.04695	78.12	78.11184	1	1	1	12	12	12
4	Benzimidazole	117.04530	118.15	118.13590	2	2	2	14	15	15
5	Cyclohexane	84.09390	84.18	84.15948	1	1	1	18	18	18
6	Cyclopropane	42.04695	42.09	42.07974	1	1	1	9	9	9
7	Ethane	30.04695	30.08	30.06904	0	0	0	8	8	8
8	Ethene	28.03130	28.06	28.05316	0	0	0	6	6	6
9	Naphthalene	128.06260	128.18	128.1705	2	2	2	18	18	18
10	Phenol	94.04186	94.12	94.11124	1	1	1	13	13	13
11	Propane	44.06260	44.11	44.09562	0	0	0	11	11	11
12	Pyridine	80.05002	79.11	79.09990	1	1	1	12	11	11

Table 2
A representative list of different types of molecular descriptors calculated by *PyDescriptor* (see supporting information for complete list).

S.N.	Type of Molecular Descriptor	Some examples of Molecular Descriptor	Total Number
1	Constitutional • Functional groups • Molecular weight • Simple Atom counts • Ratio of various types of atoms	Molecular weight, Average Molecular weight, -OH, 3° Amine, number of atoms, total number of bonds, total number of rings, etc.	235
2	Geometric • Molecular surface area (MSA) • Solvent accessible molecular surface area (SASA) • Ratio of MSA and SASA of various types of atoms	Molecular Surface area and Solvent accessible molecular surface area of molecule, positively/negatively/neutral atoms, etc. Absolute Surface Area, MSA of C atoms, MSA of N atoms, SASA of C atoms, SASA of F atoms, etc.	212
3	Circular fingerprint • Presence/Absence of different types of atom pairs at specific spatial distance	Number of C atoms within 5 Å from ring atoms, etc.	2650
4	Quantum chemical • Charges	Sum of partial charges of C atoms within 4 bonds from O atoms, Sum of partial charges of C atoms within 4 Å from O atoms, etc.	3548
5	Topological • Atom-pairs	Number of C atoms within 9 bonds from O atoms, Number of N atoms within 5 bonds from Cl atoms, etc.	4500

Old Model-1: pIC_{50} = 2.3367 (±0.7641) + 1.5695 (±1.7697) *R6p* − 0.0306 (±0.0254) *nBT* + 0.4084 (±0.1941) *nN* + 0.6338 (±0.1605) ALogP
R^2_{tr} = 0.79, Q^2 = 0.72, MAE_{cv} = 0.27, R^2_{ex} = 0.81 and CCC_{ex} = 0.89

In the present work, the same dataset (Keto form) was used for developing new QSAR model using the molecular descriptors calculated by *PyDescriptor*, e-dragon and PaDEL with identical training and prediction sets as mentioned in our previous publication. The newly derived best four parametric QSAR model built for anti-malarial activity of phosphoramidate and phosphorothioamidate analogues of amiprophos methyl is as following:

New Model-1: pIC_{50} = +2.682 (±0.411) − 0.104 (±0.071) * *N_O_3A* − 13.310 (±9.785) * *all_O_8Ac* + 0.422 (±0.168) * *plus_N_2A* + 0.434 (±0.091) * *ALOGP*
R^2_{tr} = 0.83, $RMSE_{tr}$ = 0.25, MAE_{tr} = 0.19, CCC_{tr} = 0.91, Q^2_{loo} = 0.79, $RMSE_{cv}$ = 0.28, MAE_{cv} = 0.21, CCC_{cv} = 0.89, $RMSE_{ex}$ = 0.32, MAE_{ex} = 0.28, Q^2_{F1} = 0.75, Q^2_{F2} = 0.73, Q^2_{F3} = 0.72, CCC_{ex} = 0.89, R^2_{ex} = 0.81

The symbols used for various statistical parameters have their usual meaning and available in supporting information [34,35]. The descriptor ALOGP represents lipophilicity of the molecule. The descriptors *N_O_3A* stands for the presence of oxygen atom within a spatial distance of 3 Å from nitrogen atom. The descriptor *all_O_8Ac* corresponds to sum of partial charges of all atoms within 8 Å from oxygen atom. The descriptor *plus_N_2A* corresponds to the number of nitrogen atom present within 2 Å from positively charged atoms. The descriptors *N_O_3A*, *all_O_8Ac* and *plus_N_2A* have been calculated by *PyDescriptor* and represent local environment inside the molecule, while *ALOGP* is a property of whole molecule.

A simple comparison of statistical parameters of model-1 and old model-1 reveals that the new model has improved performance not only with respect to fitting but for cross-validation parameters like Q^2, MAE_{cv}, etc. also.

In addition, another adequately validated QSAR model was built using molecular descriptors calculated by *PyDescriptor* only (neither PaDEL nor e-Dragon descriptors were used) with identical training and prediction sets as stated in our previous publication. The newly derived best four parametric QSAR model is as following:

New Model-2: pIC_{50} = +3.333 (±0.356) + 5.159 (±1.351) * *H_S_4Ac* − 0.123 (±0.046) * *byring all_S_4A* + 0.096 (±0.062) * *fHS6B* + 0.099 (±0.038) * *C_don_6A*
R^2_{tr} = 0.82, $RMSE_{tr}$ = 0.26, MAE_{tr} = 0.22, CCC_{tr} = 0.90, Q^2_{loo} = 0.75, $RMSE_{cv}$ = 0.30, MAE_{cv} = 0.26, CCC_{cv} = 0.86, $RMSE_{ex}$ = 0.33, MAE_{ex} = 0.27, Q^2_{F1} = 0.74, Q^2_{F2} = 0.72, Q^2_{F3} = 0.71, CCC_{ex} = 0.88, R^2_{ex} = 0.81

The symbols used for various statistical parameters have their usual meaning and available in supporting information also [34,35]. The descriptor *H_S_4Ac* indicates sum of partial charges of sulphur atoms which are at a spatial distance of 4 Å from hydrogen atom. The descriptor *byring all_S_4A* stands for the presence of sulphur atoms which are at a spatial distance of 4 Å from ring atoms. The descriptor *fHS6B* corresponds to frequency of occurrence of hydrogen and sulphur atoms separated by six bonds. The descriptor *C_don_6A* resembles the number of

presence of donor atom or group at a distance of 6 Å from carbon atom.

A comparison of statistical measures of model-2 with old model-1 indicates that the model-2 has outperformed the previously reported model. From model-2, it is clear that the model, derived using molecular descriptors calculated by *PyDescriptor* only, has better statistical performance and high degree of correlation of molecular descriptors with structure feature than the old model-1. This indicates that the molecular descriptors calculated by *PyDescriptor* could result in useful augmentation of statistical performance of the model and increase in mechanistic interpretation as well. It also indicates that scientifically interesting new and improved models could be built using descriptors calculated by *PyDescriptor*. In addition, the diversity of pool of descriptors calculated by *PyDescriptor* is also reflected.

A comparison of statistical parameters of model-1 and 2, derived in the present work, reveals that model-1 has better statistical performance than model-2. This indicates that a combination of molecular descriptors calculated by *PyDescriptor* with different types of descriptors generates a thriving QSAR model with easy interpretation and statistical robustness. Therefore, it is logical to use molecular descriptors calculated by *PyDescriptor* with different types of descriptors calculated by other softwares.

2. **QSAR modelling for anti-proliferative activity of substituted phenyl 4-(2-oxoimidazolidin-1-yl) benzenesulfonates** [4]

An appropriately validated QSAR model for undivided dataset of ninety-seven substituted phenyl 4-(2-oxoimidazolidin-1-yl) benzenesulfonates for anti-proliferative activity using three molecular descriptors was published by our group [24].

Old model-1b: $\log IC_{50} = -8.5590\ (\pm 4.0430) + 55.8097\ (\pm 23.1356)$ * Xt – 71.0572 (±18.4287) * VEA2 + 0.7420 (±0.2572) * nHDon.
$R^2_{tr} = 0.87$, $Q^2 = 0.85$, $RMSE_{tr} = 0.50$, $RMSE_{cv} = 0.52$, $F = 205.12$, $CCC_{tr} = 0.93$, $CCC_{cv} = 0.92$

In the present work, the same dataset was used for developing new QSAR model using the molecular descriptors calculated by *PyDescriptor*, e-dragon and PaDEL. The newly constructed best three parametric QSAR model built for anti-proliferative activity of substituted phenyl 4-(2-oxoimidazolidin-1-yl) benzenesulfonates is as following:

New Model-1b: $\log IC_{50} = -29.646\ (\pm 3.549) + 1.043\ (\pm 0.135)$ * *lipo_N_2B* + 0.649 (±0.206) * *all_N_6Ac* + 115.995 (±19.541) * *X3A*
$R^2_{tr} = 0.93$, $Q^2 = 0.92$, $RMSE_{tr} = 0.36$, $RMSE_{cv} = 0.38$, $F = 409.17$, $CCC_{tr} = 0.96$ and $CCC_{cv} = 0.96$

The descriptor *X3A* accounts for the multiplicity of the bond and for the presence of hetero atoms in the molecule, especially the hydrogen bond donor/acceptor atoms. The descriptor *lipo_N_2B* stands for number of lipophilic atoms separated by two bonds from nitrogen atoms. The third descriptor *all_N_6Ac* corresponds to sum of partial charges of all atoms present within a spatial distance of 6 Å from nitrogen atom. The descriptors *lipo_N_2B* and *all_N_6Ac* have been calculated by *PyDescriptor* and represent local environment of the molecule, whereas *X3A* is a property of whole molecule.

It is evident from the statistical parameters of **old model-1b** and **new model-1b** that the new model has superior statistical robustness not only with respect to fitting but also for cross-validation parameters like R^2, $RMSE_{cv}$, etc. Additionally, a different statistically validated QSAR model was built using molecular descriptors calculated by *PyDescriptor* only (neither PaDEL nor e-Dragon descriptors were used) with identical training set as specified in our previous publication. The newly derived best three parametric QSAR model is as following:

Model-2: $\log IC_{50} = -3.471\ (\pm 0.852) - 1.223\ (\pm 0.265)$ * *N_lipo_3Bc* – 5.082 (±2.065) * *S_all_8Bc* − 0.250 (±0.049) * *S_byring all_9B*
$R^2_{tr} = 0.90$, $Q^2 = 0.89$, $RMSE_{tr} = 0.43$, $RMSE_{cv} = 0.45$, $F = 285.36$, $CCC_{tr} = 0.95$ and $CCC_{cv} = 0.94$

The descriptor *N_lipo_3Bc* corresponds to sum of partial charges of all lipophilic atoms which are separated from nitrogen atoms by three bonds. The descriptor *S_all_8Bc* represents sum of partial charges of all atoms separated from sulphur atom by eight bonds. The third descriptor *S_byring all_9B* stands for number of ring atoms which are separated from sulphur atom by nine bonds.

It is clear from the statistical measures of **model-2** that it has better statistical performance when compared with **old model 1b**. Thus, this again confirms that the molecular descriptors calculated by *PyDescriptor* are advantageous for increasing the statistical robustness of the model and mechanistic interpretation of the model in terms of structural features.

3.4. General comparison of newly developed models with old models

A comparison of newly developed models with the old models points out that the new QSAR models have better statistical performance and greater number of easily understandable molecular descriptors. The molecular descriptors used in the present models not only represent the local environment of the molecule but complete molecule also. This would have been difficult without the incorporation of new descriptors calculated by *PyDescriptor*. It appears that the use of esoteric descriptors along with the descriptors calculated by *PyDescriptor* significantly augment the statistical performance and mechanistic interpretation of the QSAR model. Therefore, a combination of e-Dragon, PaDEL and descriptors from *PyDescriptor* is useful for deriving quantitative and qualitative QSAR models with high statistical performance and mechanistic interpretation. A statistically best QSAR equation may have only complex descriptors which cannot be easily interpretable at the level of substructures of the molecules. In our opinion, a QSAR model should be selected which should be statistically sound and easier to relate to the structural features of the molecules under study.

4. Conclusions

The use of esoteric descriptors along with easily understandable descriptors provided models with better accuracy, fidelity and easy physical clarification in a biological perspective which, in turn, could yield perceptions of a causal mechanism of action, ways of decreasing a drug's toxicity or increasing its efficacy. In the present work, a PyMOL plugin *PyDescriptor* molecular descriptor calculator has been reported which possesses a good number of advantages. The plugin can be used on all the popular platforms (Windows, Linux, MacOS). The 11,145 *PyDescriptor* descriptors calculated here consists of 1D- to 3D- molecular descriptor. For QSAR community, it provides a zero-cost option for calculating a good number of easily understandable and informative molecular descriptors with broad applicability to various types of problems. To summarize, *PyDescriptor* is a useful addition to the currently existing molecular descriptor calculation software.

Acknowledgements

Authors are thankful to Josip Juraj Strossmayer University of Osijek, Osijek, Croatia for financial support to the project INGI-2015-20 to complete the present work. The authors are also thankful to anonymous reviewers of this manuscript for constructive observations and suggestions.

Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.chemolab.2017.08.003.

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In Silico Pharmacol. (2017) 5:9
https://doi.org/10.1007/s40203-017-0029-x

ORIGINAL RESEARCH

Exploration of 3,6-dihydroimidazo(4,5-d)pyrrolo(2,3-b) pyridin-2(1H)-one derivatives as JAK inhibitors using various in silico techniques

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Received: 28 July 2017 / Accepted: 26 September 2017 / Published online: 12 October 2017
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Abstract This study focuses on understanding the structural features of 3,6-dihydroimidazo(4,5-d)pyrrolo(2,3-b) pyridin-2(1H)-one (dpp) derivatives to computationally identify new JAK inhibiting compounds. For the purpose, a novel virtual screening strategy, with 2D and 3D-QSAR (CoMFA and CoMSIA), data mining, pharmacophore modeling, ADMET prediction, multi-targeted protein-based docking and inverse QSAR, was employed. The 2D-QSAR equations developed for the JAK3, JAK2 and JAK1 involved five physicochemical descriptors. These descriptors correlate with the anti-RA activity with R^2 values for JAK3, JAK2 and JAK1 are 0.9811, 0.8620 and 0.9740, respectively. The 3D-QSAR studies such as CoMFA and CoMSIA carried out through PLS analysis of the training set of JAK3, JAK2 and JAK1, gave Q^2 values as 0.369, 0.476 and 0.490; R^2_{nev} values as 0.863, 0.684 and 0.724 and, F values as 23.098, 28.139 and 31.438, respectively. The contour maps produced by the CoMFA and CoMSIA models were used to understand the importance of hydrogen bond donor, acceptor, hydrophobic, steric and electrostatic interactions. The molecular docking studies of these selected compounds with various JAK proteins were carried out and the protein–ligand interactions were also studied. The study concluded that dpp15(s) is a highly potent JAK inhibitor with a very good predicted IC_{50} value.

Keywords Rheumatoid arthritis · Janus kinase · 2D and 3D QSAR · Weka · Molecular docking

Introduction

Rheumatoid arthritis (RA) causes inflammation of the membrane around the joints and muscles and it leads to pain and stiffness, and results in deformities and loss of function of synovial joints. Associated severe inflammation, secondary to RA, often leads to changes in bone metabolism and high risk of cardiovascular disease. Around 1% of the adult population in the developed countries is reported to be affected by RA and most of them have self-limited diseases, joint-destructions, severe physical disability, etc. (Riise et al. 2000; Jacobsson et al. 1994; Plenge 2009). The disease commonly appears among the age group of 25–50 and affects women three times more than it affects men (Smith and Haynes 2002). The diagnosis of RA is very difficult because of the difference of symptoms in different patients (Kroot et al. 2000). RA increases the mortality rate of patients who are suffering from other diseases (Gonzalez et al. 2007). Pulmonary disease is a major cause of death in RA and patients carrying the epitope of two HLA-DRB1*04 clusters run a higher risk (Toyoshima et al. 1993; Smolen et al. 2007; Weyand et al. 1992). There are also reports that among almost 50% of the RA patients some kind of respiratory problems develop.(Fujii et al. 1993; Gabbay et al. 1997).

Studies have revealed that pro-inflammatory cytokines TNF-α and IL-6; IL-1 and IL-17 and effector cells (T cells

Electronic supplementary material The online version of this article (doi:10.1007/s40203-017-0029-x) contains supplementary material, which is available to authorized users.

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and B cells) are the different immune modulators, and the corresponding signaling pathways play an important role in the pathophysiology of RA (Smolen et al. 2007; Smolen and Steiner 2003). The joint damage begins at the synovial membrane mainly due to the complex interaction of these immune modulators (Smolen and Steiner 2003). An enhanced knowledge of the disease pathology has made the treatment strategies better now. But many medications, when used for a long-term, create side effects and so are dangerous. Many medicines used for the treatment for RA lead to progressive toxicity and thus necessitate the urge for developing new drugs for RA treatment (Boers et al. 1997; Orbach et al. 2002).

Janus Kinases (JAKs) are regarded as potential targets for the treatment of autoimmune disease RA because of their unique role in the immune system. JAKs are cytoplasmic protein tyrosine kinases containing four different groups such as JAK1, JAK2, JAK3 and TYK2, which play vital roles in several forms of cytokine-mediated signal transduction (Imada and Leonard 2000). Adopting kinase inhibition methods for the treatment of RA has now become very common (Fridman et al. 2010). Therefore in this study, we selected the JAKs targets, compounds and the corresponding inhibitory values, in order to probe the structural features of the compounds with a view to developing structure–activity relationships. Recently, Yamagishi et al. (2015) prepared some derivatives of 3,6-dihydroimidazo(4,5-d)pyrrolo(2,3-b)pyridin-2(1H)-one and conducted in vitro studies to correlate structure and activity to explore the inhibitory activities (IC50) against JAK3, JAK2 and JAK1. We selected these datasets and focused on in silico analyses to understand the structural features of the scaffold of 3,6-dihydroimidazo(4,5-d)pyrrolo(2,3-b)pyridin-2(1H)-one (dpp) and their derivatives, with a view to finding new lead compounds. Another advantage is that these compounds have the 1H-pyrrolo(2,3-b)pyridine ring which matches well with the pyrrolopyrimidine scaffold of the widely used tofacitinib, which is a prominent JAK inhibiting drug.

In the study, Yamagishi et al. have concluded that (±)-cis-3-(4-Methyl-3-(2-oxo-3,6-dihydroimidazo(4,5-d)pyrrolo(2,3-b)pyridin-1(2H)-yl)piperidin-1-yl)-3-oxopropanenitrile is an attractive lead with potent JAK inhibitory nature. For the design of the molecule, the approach adopted was to reduce the lipophilicity by substituting the cyclohexane ring with heterocycles of the parent scaffold. Their experimental results fulfilled their intention to find novel tricyclic JAK inhibitors. To design a better analogue, the present study attempts to develop a new strategy for lead optimization by employing Computer Aided Drug Design (CADD) (Kapetanovic 2008). In the present work, a combined approach, whereby ligand-based drug design techniques, viz. QSAR (2D- and 3D-), data mining through machine learning, molecular docking and pharmacophore modeling, has been made to determine the structural features of the molecules in the experimental dataset so as to develop a significant correlation with the JAK activity profile of 3,6-dihydroimidazo(4,5-d)pyrrolo(2,3-b)pyridin-2(1H)-one derivatives.

CADD is a better method than the conventional 'trial and error' methods of drug discovery process because its associated methods evidently unravel the intricate structural patterns that mainly contribute towards the inhibitory activity, pharmacokinetics, and toxicity profiles of a drug candidate. The in silico techniques are faster, more economical and obviously more successful than the conventional methods. However, 2D-QSAR studies alone are insufficient to draw reliable conclusions, especially for comparatively small datasets. A right blend of different ideas, algorithms, tools and techniques thus become essential to comprehend the reasons behind the definite interactions of various molecules. A judicious combination of the well-known CADD methods like 3D-QSAR, molecular docking, pharmacophore modeling, ADMET prediction and data mining is employed to deliver important information, which are vital for lead/drug optimization. These methods developed valid models, leading to the identification of the unique structural patterns that govern the specific activity, and better perception regarding the mechanism of the molecular inhibitory actions of the drug candidates. These studies further explored the structure-based design methods so as to incorporate a better understanding of the ligand drug characters and drug–target interactions.

The usual approach for developing a QSAR model involves the generation of some valuable descriptors representing various molecular properties of the ligand. These may be physicochemical properties or topological indices that encrypt features like the properties of individual atoms and bonds. The present study used an in-house built new Pymol plug-in, of which 40% are new descriptors that are easily interpretable and can capture the local environment of the molecules (Masand and Rastija 2017). Based on the inputs from 2D QSAR, molecular docking, data mining using Weka, ADMET and pharmacophore studies, novel chemical entities (NCEs) were designed so as to satisfy the JAK inhibitory nature in a better way. The final QSAR model developed was utilized further to test these NCEs to know whether they possess a better inhibitory effect. The present study was thus able to successfully design several virtual molecules, and predict their corresponding inhibitory activities, using the selected descriptors present in the built model and thereby suggest a lead molecule.

Materials and methods

Dataset

The present study is based on datasets consisting of 19, 19 and 17 derivatives of 3,6-dihydroimidazo(4,5-d)pyrrolo(2,3-b)pyridin-2(1H)-one (dpp) and their corresponding IC_{50} values related to the inhibition of JAK3, JAK2 and JAK1, respectively (Yamagishi et al. 2015). Though each of the datasets is small, it comprises substituted rings as substituents, thus covering a broad chemical space. The chemical structures of dpp derivatives were drawn and optimized by using the software, molecular operating environment (MOE). Merck molecular force field was used for the energy minimization and optimization of the compounds (Halgren 1996). The anti-inflammatory activities reported for various JAK inhibitors expressed in IC50 and the structures of the corresponding dpp derivatives are given in Table 1.

Toxicity and drug likeness

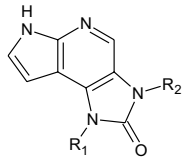
A Java-based application called Toxtree v1.60 which functions on the basis of quantitative structure–toxicity relationships was used for toxicity prediction. In Toxtree (toxic hazard estimation by decision tree approach) (Patlewicz et al. 2008) the carcinogenicity and mutagenicity of the compound were analyzed using Benigni–Bossa rule base (Benigni and Bossa 2008). The drug-likeness of the compounds was carried out using MayaChemTools.

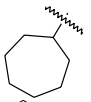
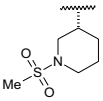
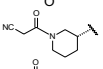
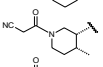
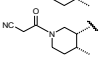
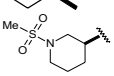
Calculation and selection of descriptors

Using MOE, PaDEL-descriptor and an in house built new Pymol plugin program, a total of 19737 descriptors, which included 2D-, 3D- molecular descriptors and fingerprints were generated for each of the energy-minimized molecules. The main key descriptor filtration algorithms, "General" and "CORCHOP" in the PHAKISO software were used for descriptor pruning. The descriptors which have the same values and missing values were removed using the "General". The inter-correlated, correlated and the repeated descriptors were removed using the "CORCHOP" and thus the number of necessary descriptors was reduced to 180, 180 and 164, for the sets of JAK3, JAK2 and JAK1, respectively.

Many of the descriptors thus generated have wide ranging diverse numerical values. If no scaling is done, it becomes very difficult to understand and estimate the comparative contribution of those descriptors to the QSAR. Most often those descriptors with higher numerical values govern and influence the model, and essentially limit the statistical validity of the developed models. Hence scaling of descriptors is carried out in the present study using the software, PHAKISO. The nearly constant and highly correlated descriptors were eliminated through subjective selection and the descriptors were further reduced to 12, 17 and 12, for JAK3, JAK2 and JAK1, respectively.

Table 1 Molecular structures of dpp derivatives and their activity values



Compound	R1	R2	IC_{50} (nM)		
			JAK3	JAK2	JAK1
dpp1		H	54	43	79
dpp2		H	180	97	110
*dpp3		H	22	23	30
dpp4		H	60	88	1000
dpp5		H	3.0	4.4	14
dpp6		H	21	23	430
dpp7		H	42	23	24
dpp8		H	69	85	90
dpp9		H	3.0	3.6	18
dpp10		H	270	500	520
*dpp11		H	1200	1300	-
dpp12		H	710	140	140
*dpp13		H	63	82	230
dpp14		H	28	17	20
*dpp15		H	1.1	2.6	1.5
dpp16		Me	5.0	7.3	29
dpp17		H	27	17	28
dpp18		H	460	850	-
dpp19	H	H	0.8	3.1	3.7

*Test Set Compounds

2D-QSAR

2D-QSAR studies were performed by means of the software, BuildQSAR using multiple linear regression (MLR) models for finding out the optimum number and the sets of necessary descriptors. For 2D-QSAR analysis, pIC_{50} ($-\log IC_{50}$) values were obtained by converting the corresponding IC_{50} (nM) values. This is used as dependent variable in the 2D-QSAR analysis. The selected descriptors were considered as independent variables and pIC_{50} values were considered as the dependent variable in all the three cases. The subjective feature selection was performed using Genetic Algorithm (GA) method, and the multiple linear regression (MLR) analysis method was used to construct the 2D-QSAR model of the 19 derivatives of 3,6-dihydroimidazo(4,5-d) pyrrolo(2,3-b)pyridin-2(1H)-one. The correlation coefficient (R), standard deviation (s), Fischer's test (F), level of confidence (p), squared cross correlation coefficient (Q^2), standard deviation error in prediction (S_{DEP}) and predicted residual sums of squares standard deviation (S_{PRESS}) were calculated for validating the QSAR-model.

3D-QSAR

Three-dimensional quantitative structure–activity relationship (3D-QSAR) methods such as comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) were performed for all the derivatives using the molecular modeling package SYBYL-X 1.3 (Tripos International, Missouri, USA). This helps to associate the bioactivity of compounds with structural descriptors and has been proved to be a very suitable method for accelerating the drug design process (Zhao et al. 2011).

3D-QSAR dataset preparation

For the development of thriving 3D-QSAR models, the whole set of 19 molecules was grouped randomly into a training set and a test set containing 15 and 4 molecules, respectively, in JAK3 and JAK2. The models were generated using the training set and the test set in turn was used to validate the models. Compounds 3, 11, 13 and 15 were used as the test set and the remaining were considered as the training set. But in the case of JAK1 for the development of 3D-QSAR models, only 17 molecules were grouped randomly into a training set and a test set containing 14 and 3 molecules, respectively, since the IC_{50} values of the compounds dpp11 and dpp18 were not reported.

Molecular alignment

Molecular alignment of compounds, which is a crucial step in the process of creating 3D-QSAR models, was performed using a common scaffold. A molecule with relatively high biological activity is usually adopted as the template molecule. In this work, compound 19 was used as the template molecule. Using ALLIGN DATAQBASE function available in SYBYL, the ligand-based alignment of the molecules was carried out on the basis of an atom-by-atom superimposition principle. The alignment of 19 compounds is shown in Fig. 1. These alignments were used subsequently in calculating the CoMFA/CoMSIA probe interaction energy-values.

The initial optimization was carried out using the standard TRIPOS force field (Clark et al. 1989) with 1000 iterations, with a distance-dependent dielectric and the Powell conjugate gradient algorithm with a convergence criterion of 0.01 kcal mol^{-1} Å. Gasteiger-Hückel method was used to assign the partial atomic charges of the compounds (Gasteiger and Marsili 1980).

CoMFA and CoMSIA studies

For the CoMFA analysis, steric (Lennard-Jones potentials) and electrostatic field (Coulombic potentials) energies were calculated using a sp^3 carbon with a van der Waals' radius of 1.52 Å as the steric probe; and a single positive charge (+ 1) as the electrostatic probe in 3D cubic lattice with a grid spacing of 2.0 Å in x, y and z directions, using Tripos module in SYBYL. The electrostatic and steric influences

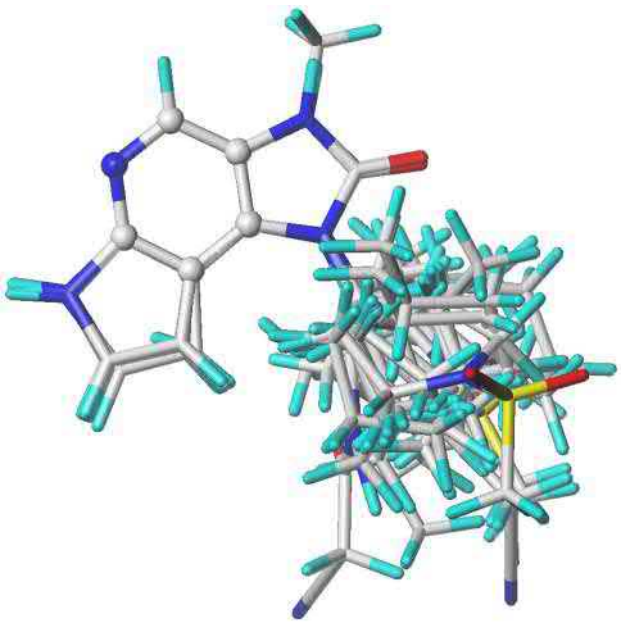


Fig. 1 Alignment of 19 compounds

were reduced to + 30.0 kcal/mol. The electrostatic contributions were excluded at the lattice intersections with maximal steric interactions. For obtaining suitable results, the "StDev*coeff" (the standard deviation and the coefficient) values were utilized as various weighing factors, apart from the grid spacing. Crammer et al. suggested the impact of various parameter settings on CoMFA, electrostatic and steric cutoffs and grid spacing (Cramer et al. 1988).

It is reported that the CoMSIA method is based on the molecular similarity indices within the same lattice box (Klebe et al. 1994). In the present study, standard settings of CoMSIA, sp^3 carbon atom as a probe with charge + 1, radius 1 Å and hydrophobicity + 1, hydrogen-bond donor + 1, hydrogen-bond acceptor + 1, attenuation factor of 0.3 were used for each lattice with a grid of 2 Å. Mainly five similarity indices including that of steric (S), electrostatic (E), hydrophobic (H), hydrogen bond donor (D) and hydrogen bond acceptor (A) fields were computed.

3D-QSAR statistical results

Partial least square (PLS) analysis

Partial least-squares (PLS) (Bush and Nachbar 1993; Wold et al. 2001) method is regarded as an extension of the multiple regression analysis for deriving the 3D-QSAR models. Here the CoMFA and CoMSIA descriptors were taken as independent variables and pIC_{50} values were considered as dependent variables. The statistical importance of the models was analyzed by the cross-validation analysis performed by the leave-one-out (LOO) method to find the optimum number of components (N), which was later used to generate the final QSAR model. A column filter value of 2.0 kcal/mol was used to accelerate the regression analysis and to reduce the noise for all the cross-validated PLS analyses. To validate a QSAR model, different statistical parameters such as cross-validated correlation coefficient (Q^2), non-cross-validated correlation coefficient (R^2_{nev}), predicted correlation coefficient (R^2_{pred}), and standard error of estimate (SEE) were found out. The optimum number of components (OPN) was found out by considering the number of components that gave the smallest SEE and F values.

In CoMSIA, five different descriptor fields available are not totally independent of each other. This could decrease the statistical significance of the models (Bringmann and Rummey 2003) considered. We have generated 25 different models in order to build the optimal 3D-QSAR models with the highest Q^2 values and good statistical results for each class (Shibi et al. 2015). A model is said to be strong and predictive only when the statistical parameters $R^2_{nev} > 0.6$, $R^2_{pred} > 0.5$, and $Q^2 > 0.6$ (Afantitis et al. 2009; Golbraikh and Tropsha 2002).

Predictive correlation coefficient (R^2_{pred})

Biological activities of the test set molecules were predicted for the further validation of the model using the models derived from the training set. The Predictive Correlation Coefficient (R^2_{pred}) value was computed using the following equation:

$$R^2_{pred} = 1 - \frac{\sum(Y_{predicted} - Y_{observed})^2}{\sum(Y_{observed} - Y_{mean})^2}, \quad (1)$$

where $Y_{predicted}$, $Y_{observed}$ and Y_{mean} are the predicted, the actual and the mean values of the activity, respectively. $\sum \left(Y_{predicted} - Y_{observed}\right)^2$ is the predictive sum of squares (PRESS).

The predictive ability of the models developed was further confirmed by the Eq. 2 given below (Rannar et al. 1994):

$$R^2_{m\ (overall)} = R^2 \times (1 - \sqrt{R^2 - R^2_0}) \quad (2)$$

where R^2 is the squared correlation coefficient between observed and predicted pEC_{50} values and R^2_0 is the squared correlation coefficient with intercept set to zero. The parameter determines whether the range of predicted activity values for the whole dataset is close to the observed activity or not. The value of $R^2_{m(overall)}$ should be greater than 0.5 for a satisfactory model.

Data mining using WEKA

Using a software called WEKA 3.7.3, an artificial intelligence technique was used for developing the model and for screening compounds to understand the anti-rheumatoid action of the derivatives. Anti-inflammatory Bioassays AID 1852 and AID 2001 were retrieved from PubChem BioAssay Database. The bioassay AID 1852 contains 2481 tested compounds, of which 1149 are reported to be active and the remaining 1332, inactive. Similarly, in AID set 2001, out of the 545 tested compounds, 263 are active and 282 are inactive.

Using PowerMV software, 155 descriptors, which included 147 pharmacophore finger prints and 8 various properties such as XLogP, PSA, number of rotatable bonds, H-bond acceptors, H-bond dinners, molecular weight, Blood–Brain Barrier and Bad Group, were generated for the active and inactive compounds of both AIDs and were saved as CSV files (Liu et al. 2005). For creating binary classifiers for the molecules based on their bio-activity viz.,

actives and inactives, a Machine Learning (ML) method Weka (Waikato Environment for Knowledge Analysis) was used (Jamal et al. 2013; Gaba et al. 2014; Aswathy et al. 2016; Shibi et al. 2016).

Weka introduces base model through a confusion matrix. True Positives (TP) are the actives which are correctly classified as actives; False Positives (FP) represent inactives classified incorrectly as actives. Similarly True Negatives (TN) represents the inactives which are classified correctly as inactives and False Negatives (FN) are active compounds which are classified incorrectly as inactive (Vinita et al. 2011). The classification process involves building a classifier (model), which is a mathematical function that assigns class (e.g., active/inactive) labels to instances defined by a set of attributes (e.g. descriptors) (Frank et al. 2004).

Protein–ligand Molecular docking

In order to reduce the experimental costs of large-scale inhibitor screening and to increase the success rate, we designed a multi-target molecular docking system capable of predicting JAK inhibitor interactions. So we have selected a total of four protein molecules for each protein JAK1, JAK2 and JAK3 and subsequently performed molecular docking to calculate the binding affinities of JAK inhibitor pairs. The molecular docking studies of the selected 9 compounds with various JAK proteins viz. 3LXK, 3PJC 4HVG and 4RIO (JAK3); 3IO7, 3TJD, 4F08 and 4FVP (JAK2); 3EYH, 4E4N, 4EI4 and 4K77 (JAK1) were carried out using MOE 2014.0901. The default 'Site Finder' tool was used to identify the active site of the proteins.

ADME properties prediction

Adsorption, distribution, metabolism and excretion (ADME) were predicted using the online software PreADMET (http://preadmet.bmdrc.org/).

Pharmacophore elucidation

3D-pharmacophore model was developed by Pharmacophore Elucidation Query module of MOE. We have constructed the pharmacophore of the whole dataset and that of the three most active compounds 15, 19 and 5. Then it was compared with the drug molecule, Tofacitinib which has a similar scaffold.

Results and discussion

In silico toxicity studies and Lipinski's rule of five (Ro5) filters

One of the most important reasons for the late stage failure in drug development is the possible toxicity of any active molecule. The dpp derivatives selected for the present study were, therefore, screened using in silico tools for predicting the most relevant toxicity endpoints. By a Toxtree scan using Benigni/Bossa rule, we obtained 49 distinctive structural alerts (SAs). It was found that all the dpp derivatives are non-carcinogenic and non-mutagenic. The drug-likeness of the derivatives was then analyzed using Lipinski's Ro5 which indicated that all the molecules followed Lipinski's Ro5.

Prediction of metabolic behavior

The prediction of metabolic behavior also helps to understand the toxicity risks of the compounds. Vital ADMET properties such as maximal achievable drug concentration and drug toxicity have a great influence on the metabolic stability (Trunzer et al. 2009; Vasanthanathan et al. 2009). Like other ADMET properties, metabolism plays an important role in the failure of drugs to perform their proposed action in the human body (Guner and Bowen 2013). Sheridan et al. have also reported a QSAR based metabolic site prediction approach (Sheridan et al. 2007).

The liver is the main organ for human drug clearance. Cytochrome (CYP) enzymes contribute to the phase I metabolism of 70–80% of the drugs used currently (Pang 2009). Drugs entering the body generally undergo oxidation reactions catalyzed by CYP P450 enzymes. The most important isoforms of CYP enzymes are CYP3A4 (45%), CYP2C9 and CYP2C19 (25%), CYP2D6 (15%) and CYP1A2 (5% of current drugs) (Williams et al. 2004a, b). These CYP isoforms demonstrate typical inhibitor profiles and overlapping substrate specificities (Miners and Birkett 1998). The metabolite prediction of CYP3A4 substrates by MetaSite with 78% accuracy was reported by Zhou et al. (2006). Cytochrome CYP3A4 is the most abundant hepatic P450 isoform of the complex heme-containing enzyme responsible for the metabolism of more than 50% of the marketed drugs, in humans (Schlichting 2000). An enhanced knowledge regarding the molecular interactions between drugs and CYP3A4 are valuable perceptions for developing new medications. The shape and size of the active site cavity of the CYP3A4 structures are remarkable and the cavity is much larger near the heme iron (Scott and Halpert 2005). The large binding site cavities, reported in the literature allow this enzyme to accommodate substrates of various size (Williams et al. 2004a, b; Yano et al. 2004). And such large size would also indicate the capacity of the enzyme that can bind more than one substrate simultaneously (Kapelyukh et al. 2008; Korzekwa et al. 1998; Shou et al. 1994).

We used the molecular docking method to understand the metabolic behavior of the 19 compounds and analyzed the binding modes of compounds towards the cavity of the enzyme CYP3A4. The human microsomal cytochrome P450 3A4 protein structures, with PDB ID: 1TQN and 1WOE

were downloaded from Protein Data Bank and all the 19 dpp derivatives were successfully docked into the active site of these proteins. The relatively high docking score revealed that almost all the compounds bind tightly to CYP3A4 and thus can undergo metabolism easily. The high docking score is the representation of high metabolic behavior and represents the proximity of the substrate molecule to the iron atom in the heme (Prusis and Afzelius 2009).

2D-QSAR

A 2D-QSAR model is a mathematical equation that correlates the biological activity of a molecular system to its molecular descriptors. The 2D QSAR equations developed for the JAK3, JAK2 and JAK1 are, respectively as follows,

$$\begin{aligned} pIC_{50} = &+0.0983(\pm 0.0171)\ \text{lipoplus_AbSA} \\ &-0.8984(\pm 0.2198)\ \text{ExtFP264} \\ &-2.7992(\pm 0.8027)\ \text{PM3_LUMO} \\ &-1.2468(\pm 0.3202)\ \text{MACCSFP91} \\ &-0.2697(\pm 0.1024)\ \text{com_H_3A} \\ &+7.3986(\pm 0.0699), \end{aligned} \tag{3}$$

$$\begin{aligned} pIC_{50} = &+2.9878(\pm 1.2465)\ \text{O_lipo_3Ac} \\ &+2.7150(\pm 0.9546)\ \text{Wnu1.polar} \\ &+1.6867(\pm 0.9677)\ \text{KRFPC232} \\ &+0.0195(\pm 0.0090)\ \text{SlogP_VSA9} \\ &+7.5542(\pm 0.1702), \end{aligned} \tag{4}$$

$$\begin{aligned} pIC_{50} = &+4.8195(\pm 1.2571)\ \text{byring all_H_2Ac} \\ &+2.7439(\pm 1.1214)\ \text{vsurf_EWmin2} \\ &+0.2863(\pm 0.0525)\ \text{vsurf_W6} \\ &-3.8536(\pm 1.6767)\ \text{byring allplus_sumpc} \\ &+1.7154(\pm 0.5880)\ \text{O_lipo_3Ac} \\ &+0.2760(\pm 0.1128)\ \text{KRFPC3662} \\ &+0.1811(\pm 0.1651)\ \text{da_H_3A} \\ &+7.2962(\pm 0.0884). \end{aligned} \tag{5}$$

The physicochemical descriptors such as lipoplus_AbSA, ExtFP264, PM3_LUMO, MACCSFP91and com_H_3A are included in Eq. 3. O_lipo_3Ac, Wnu1.polar, KRFPC232 and SlogP_VSA9 in Eq. 4 and byring all_H_2Ac, vsurf_EWmin2, vsurf_W6, byring allplus_sumpc, O_lipo_3Ac, KRFPC3662 and da_H_3A are included in Eq. 5.

The meaning of descriptors are as follows:

a. lipoplus_AbSA: absolute surface area of positively charged lipophilic atoms.
b. ExtFP264: extended fingerprints with additional bits describing ring features.
c. PM3_LUMO: the energy (eV) of the lowest unoccupied molecular orbital calculated using the PM3 Hamiltonian (Stewart 1993).
d. MACCSFP91: is a molecular access system key fingerprint.
e. com_H_3A: presence of H within 3 Å from center of mass of the molecule.
f. O_lipo_3Ac: sum of charges of lipophilic atoms present within 3 Å from oxygen atom.
g. Wnu1.polar: is a 3D directional WHIM descriptor, weighted by atomic polarizabilities. Todeschini and Gramatica (1998) described that WHIM are Holistic descriptors, which belongs to a class of hybrid descriptors.
h. KRFPC232 (padel): SlogP_VSA9: Sum of νi such that Li > 0.40. Is a subdivided surface area descriptor based on an approximate accessible van der Waals surface area (in Å2) calculation for each atom. Here Li denotes the contribution to logP(o/w) for atom I (Wildman and Crippen 1999).
i. byring all_H_2Ac: sum of charges of H atoms present within 2 Angstrom from ring atoms.
j. vsurf_EWmin2: Cruciani et al. (2000) reported that the vsurf_ descriptors are similar to the VolSurf descriptors, for the pharmacokinetic property prediction and these descriptors to be very useful. vsurf_EWmin is one of the Lowest hydrophilic energy descriptors.
k. vsurf_W6: hydrophilic volume descriptor.
l. byring allplus_sumpc: sum of charges of positively charged atoms present in the ring.
m O_lipo_3Ac: sum of charges of oxygen atoms present within 3 Å from lipophilic atoms.
n. KRFPC3662: Klekota–Roth fingerprint count which represents the count of chemical substructures (Klekota and Roth 2008).
o. da_H_3A: presence of donor or acceptor within 3 Å from H atom.

Ponce et al. (2004) reported that the consistency of a 2D-QSAR model depends on both Q^2 and R^2 values and it should be high. More often, a value of $Q^2 > 0.5$ is considered satisfactory (Strazielle and Ghersi-Egea 2005).

As per the generated model, mainly three descriptors influence the pIC_{50} of 3,6-dihydroimidazo(4,5-d) pyrrolo(2,3-b)pyridin-2(1H)-one derivatives. For JAK3, JAK2, and JAK1, the model possesses high correlation coefficient values $R^2 = 0.981$, 0.862 and 0.974, respectively and

low standard deviation values such as s = 0.117, 0.320 and 0.161, respectively. This indicates the good capacity of the models to explain the observed values of biological activity. The low values of S_{PRESS} and S_{DEP} confirm the accurateness of the model. Further, evaluation of the degree of statistical significance was accomplished by the level of confidence (p = 0) and Fischer test (F). The validation parameters (Q^2 and S_{PRESS}), reflect the good predictive power of the generated model. Observed and predicted inhibitory activities and residual values of the statistically significant model obtained are shown in Table 2.

The correlation between experimental and calculated activity values graphically establishes the predictive capability of the developed QSAR models with R^2 values of 0.988, 0.862 and 0.974, respectively for JAK3, JAK2 and JAK1 (Fig. 2).

Table 2 Statistical parameters of 2D-QSAR

Statistical output	JAK3	JAK2	JAK1
n	15	17	17
k	5	4	7
R^2	0.988	0.862	0.974
R^2-Adj	0.981	0.816	0.954
s	0.117	0.320	0.161
F	146.322	18.744	48.124
p	0	0	0
Q^2	0.967	− 0.048	0.896
S_{Press}	0.192	0.882	0.322
S_{DEP}	0.154	0.764	0.242

Y-randomization test

The Y-randomization test was performed using MLR YRandomization 1.2 software to validate and analyze the robustness of the developed 2D-QSAR models. The test identifies the chance of correlation between dependent and independent variables. Here the biological activity is randomized while keeping the other descriptors as constant, and fifty models were thus developed. A QSAR model is acceptable when the average correlation coefficient (R_r) of randomized models is less than the correlation coefficient (R) of the non-randomized model. Milano (2010) proposed that for succeeding Y-randomization test the value of $^cR_p^2$ should be more than 0.5 and reported that the magnitude of difference in the mean squared correlation coefficient values of the randomized (R_r^2) and non-randomized (R^2) models are reflected in the value of $^cR_p^2$ parameter.

$$^cR_p^2 = R \times \sqrt{R^2 \times R_r^2} \quad (6)$$

All the fifty models developed for the three sets of biological activity have low R^2 and Q^2 values which signify the strength of the 2D-QSAR models built. The model parameters obtained in the present study are shown in Table 3. The $^cR_p^2$ values obtained are 0.747, 0.704 and 0.722 for JAK3, JAK2 and JAK1, respectively, during the Y-randomization test and indicate the success of the generated models.

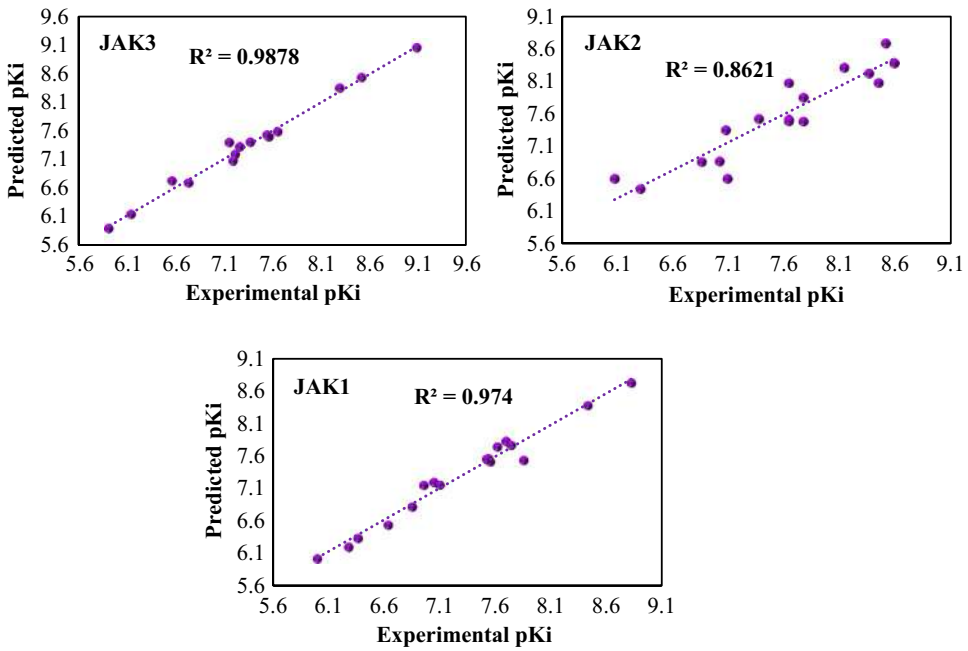


Fig. 2 Predicted inhibitory activities with experimental values

Applicability domain (AD)

The developed QSAR model is useful when it can be successfully employed to predict the activity of newly designed molecules. The estimation of a modeled response using QSAR is usable and valid when the compounds being predicted falls within the AD of the model. AD is a theoretical region in chemical space covering the model descriptors and modeled response. The uncertainty in the estimation of the activity of a compound can be thus eliminated.

The AD of the developed QSAR model was analyzed using AD Using Std Approach 1.0 software based on the basic theory of standardization approach. The methodology and algorithm suggested by Roy et al. (2015) were used to define the outliers in the case of the training set and to understand the compounds which are residing outside the AD. No outliers were identified in the training and the test set, which indicates that there are no chances of uncertainty in the prediction of QSAR models. This also demonstrates that the training set compounds are not dissimilar and the modelled 3D descriptors and the modelled response exist within the AD.

3D-QSAR

Statistical evaluation of CoMFA

The summary of the results from CoMFA models using LOO-CV constructed for dpp derivatives with steric and electrostatic fields are given in Table 4. PLS analyses of the training sets of JAK3, JAK2 and JAK1 show the Q^2 values 0.369, 0.476 and 0.490 using three, one, one as principal components, respectively. Böhm et al. (1999) reported that in CoMFA and CoMSIA studies, a Q^2 value of 0.3 is considered to be statistically significant while a Q^2 value of 0.4 is generally considered to be better. The non-cross-validated PLS analyses of these give high conventional R^2_{nev} values such as 0.863, 0.684 and 0.724 and low standard error of estimate (0.356, 0.434 and 0.374) respectively. The F values like 23.098, 28.139 and 31.438 indicate the high statistical significance of the model. The steric and electrostatic field contributions calculated by the CoMFA models of JAK3 were 44.7 and 55.3%, for JAK2 56.3 and 43.7% and for JAK1 33.6 and 21.8%, respectively suggesting that the steric and electrostatic fields were found to be almost equally important to the binding affinities of the ligands to the target.

Table 3 R^2 and Q^2 values after 50 Y-randomizations

Random models parameters	JAK3	JAK2	JAK1
Average R_r	0.515	0.451	0.663
Average R^2_r	0.287	0.221	0.456
Average Q^2_r	− 0.951	− 0.475	− 1.437
$^cR^2_p$	0.747	0.704	0.722

The CoMFA model of JAK3, JAK2 and JAK1 showed R^2_{pred} and $R^2_{m(overall)}$ values of 0.731 and 0.650, 0.757 and 0.404 and 0.465 and 0.327, respectively. The correlation between experimental and predicted pIC_{50} values by CoMFA models are represented in Fig. 3. It shows an R^2 value of 0.863 for the training set and 0.787 for the test molecules in JAK3. For JAK2, the training and test set value of R^2 is 0.712 and 0.939, respectively and for JAK1 the R^2 value is found to be 0.798 and 0.875, respectively. The experimental and predicted pIC_{50} values and the residual values of the dataset by CoMFA model are listed in Table 5.

CoMFA contour map analysis

The CoMFA contour maps of JAK1, JAK2 and JAK3 are shown in Fig. 4. The steric contributions were represented by green and yellow contours. The green contour represents the preferred steric bulk, which on adding a group near this region will improve the inhibitory activity. The yellow contour represents the disfavored steric bulk, adding a group near this region will decrease the inhibitory activity. The electrostatic contributions were represented by blue and red contours. Here the blue services the positive charge and disservices the negative charge, that is, by adding a positively charged group near this region may improve the inhibitory activity and on adding a negatively charged group may weaken the activity. Similarly, the red areas in the electrostatic contours represent the negative charge favor and positive charge disfavor.

The electrostatic contribution of JAK3 is represented in Fig. 4a. The contour map shows a large blue contour near R1 group. This can be explained by considering the molecules dpp9 and dpp17, where insertion of ethyl group in dpp9 increased the inhibitory activity from a value of 7.658 (of compound dpp17) to 8.523. Comparing the molecules dpp1 and dpp8, it can be seen that the introduction of two methyl groups in dpp 8 increased the electrostatic factor resulting in an increase in inhibitory activity from 5.921 to 7.553.

The steric contributions of JAK3 are shown in Fig. 4b. The contour map shows a large green contour and two small yellow contours near the R1 group. The green contour can be explained by considering the molecules dpp9 and dpp5. Introduction of an ethyl group in the molecule dpp9 instead of the methyl group in dpp5 has increased the activity from 6.745 to 8.523. The molecule dpp9 shows an activity value of 8.523 when compared to the molecule dpp1 with an activity value of 5.921. This is because dpp9 has

Table 4 Statistical results of CoMFA and the best CoMSIA models

	CoMFA			CoMSIA	
	JAK3	JAK2	JAK1	JAK3 (ADES)	JAK2 (ADH)
[a]Q^2/ONC	0.369/3	0.476/1	0.490/1	0.462/3	0.512/2
[b]R^2_{nev}	0.863	0.684	0.724	0.871	0.815
[c]SEP	0.765	0.559	0.509	0.706	0.561
[d]SEE	0.356	0.434	0.374	0.346	0.346
[e]R^2_{pred}	0.731	0.757	0.465	0.757	0.768
$R^2_{m(overall)}$	0.650	0.404	0.327	0.668	0.641
F value	23.098	28.139	31.438	24.772	26.349
Field contribution					
Steric	44.7	56.3	55.2	13.7	–
Electrostatic	55.3	43.7	44.8	27.7	–
Hydrophobic	–			–	16.2
H-bond donor	–			38.4	42.2
H-bond acceptor				20.2	41.6

[a] Cross-validated correlation coefficient

[b] Non cross-validated correlation coefficient

[c] Standard error of prediction

[d] Standard errors of estimate

[e] Predicted correlation coefficient for the test set

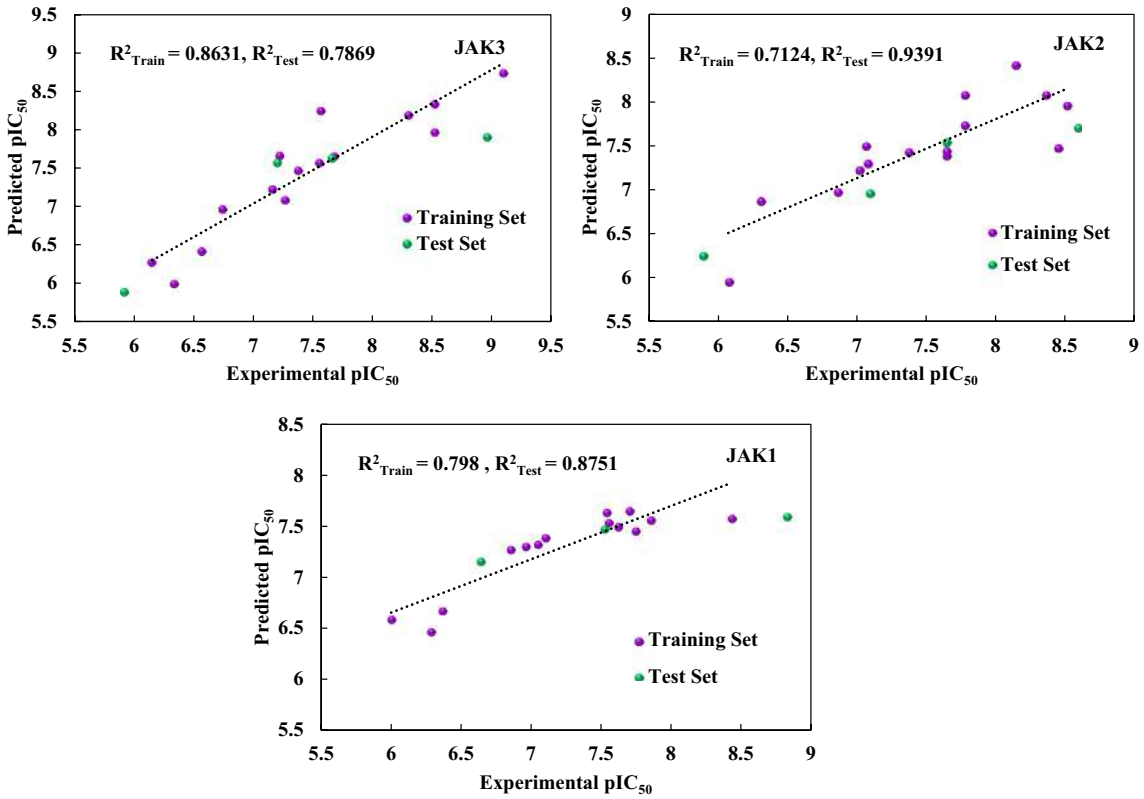


Fig. 3 Plot of actual versus predicted pIC_{50} values for the CoMFA model

Table 5 Experimental and predicted activities (pIC_{50}) with residual values of CoMFA models

Compound ID	JAK3			JAK2			JAK1		
	Actual pIC_{50}	Predicted	Residual	Actual pIC_{50}	Predicted	Residual	Actual pIC_{50}	Predicted	Residual
dpp1	7.268	7.078	0.190	7.367	7.419	− 0.053	7.102	7.398	− 0.296
dpp2	6.745	6.957	− 0.212	7.013	7.215	− 0.202	6.959	7.313	− 0.354
dpp3[a]	7.658	7.620	0.038	7.638	7.533	0.105	7.523	7.481	0.042
dpp4	7.222	7.655	− 0.433	7.056	7.491	− 0.436	6.000	6.597	− 0.597
dpp5	8.523	8.330	0.193	8.357	8.068	0.289	7.854	7.569	0.285
dpp6	7.678	7.647	0.031	7.638	7.379	0.259	6.367	6.684	− 0.318
dpp7	7.377	7.464	− 0.087	7.638	7.434	0.204	7.620	7.506	0.114
dpp8	7.161	7.222	− 0.061	7.071	7.288	− 0.217	7.046	7.329	− 0.283
dpp9	8.523	7.959	0.564	8.444	7.468	0.976	7.745	7.462	0.283
dpp10	6.569	6.412	0.157	6.301	6.865	− 0.564	6.284	6.477	− 0.193
dpp11[a]	5.921	5.884	0.037	5.886	6.246	− 0.360	–	–	–
dpp12	6.149	6.268	− 0.119	6.854	6.969	− 0.115	6.854	7.282	− 0.428
dpp13[a]	7.201	7.566	− 0.365	7.086	6.949	0.137	6.638	7.163	− 0.525
dpp14	7.553	7.561	− 0.008	7.770	7.726	0.044	7.699	7.661	0.038
dpp15[a]	8.959	7.893	1.066	8.585	7.697	0.888	8.824	7.603	1.221
dpp16	8.301	8.178	0.123	8.137	8.408	− 0.271	7.538	7.645	− 0.108
dpp17	7.569	8.235	− 0.666	7.770	8.068	− 0.298	7.553	7.543	0.010
dpp18	6.337	5.990	0.347	6.071	5.949	0.122	–	–	–
dpp19	9.097	8.726	0.371	8.509	7.946	0.563	8.432	7.585	0.847

[a] Test set compounds

an ethyl as an additional group in R1, so it increases the bulkiness of the R1 group. This can also be explained by illustrating the activity of the molecules dpp8 and dpp1, where dpp8 has two methyl groups, and dpp1 has no methyl group (7.553 > 5.921). The relative contributions of steric and electrostatic fields in this model are 44.7 and 55.3%, respectively.

Figure 4c represents the steric contribution of JAK2. The contour map for steric shows two small green contours near R1 group. This can be explained by considering the molecules dpp16 and dpp17. The introduction of the bulky R1 group in dpp16 has increased the activity of the molecule when compared with the dpp17 molecule (8.608 > 8.068). Same is the case with the molecules dpp16 and dpp14. Introduction of a methyl group has increased the activity of the molecule dpp16 to 8.608 from an activity of 7.726. Comparing the molecules dpp 9 and dpp1, it can be seen that, insertion of an ethyl group has increased the activity from 7.419 to 7.468 for dpp9.

The electrostatic contribution of JAK2 is shown in Fig. 4d. The electrostatic contour map shows a large blue contour near R1 group. This means that increasing the positively charged group as R1 helps to increase the activity of the molecules. Molecule dpp8 shows increased activity when compared with dpp13. The molecule dpp8 has two methyl groups in the R1 position as compared to an electron withdrawing bulky group in the R1 position of the molecule dpp13. Due to the introduction of ethyl group in dpp 9, there is an increase in the activity of the molecule dpp9 compared to that of dpp1. The relative contributions of steric and electrostatic fields in this model were 56.3 and 43.7%, respectively. In JAK1, the relative contributions of steric and electrostatic fields were 55.2 and 44.8%, respectively.

The electrostatic contour map of JAK1 shows a large blue contour near R1 group (Fig. 4e). Increasing the positive charge of the R1 group will increase the activity of the molecules. Molecule dpp1 shows increased activity when compared with dpp10, as dpp10 has a lone pair of electrons in groups in the R1 position.

The steric contribution of JAK1 is shown in Fig. 4f. The contour map for steric shows two small green contours near R1 group. This can be explained by considering the molecules dpp15 and dpp5. By the introduction of the bulky R1 group in dpp15 the activity of the molecule has increased (5.824), compared with that of dpp5 molecule (5.432). Same is the case with the molecules dpp8 and dpp6. Introduction of a methyl group has increased the activity of the molecule dpp8 from 3.366 to 4.045. Insertion of an ethyl group has increased the activity of dpp9 from 4.102 to 4.744 of dpp1.

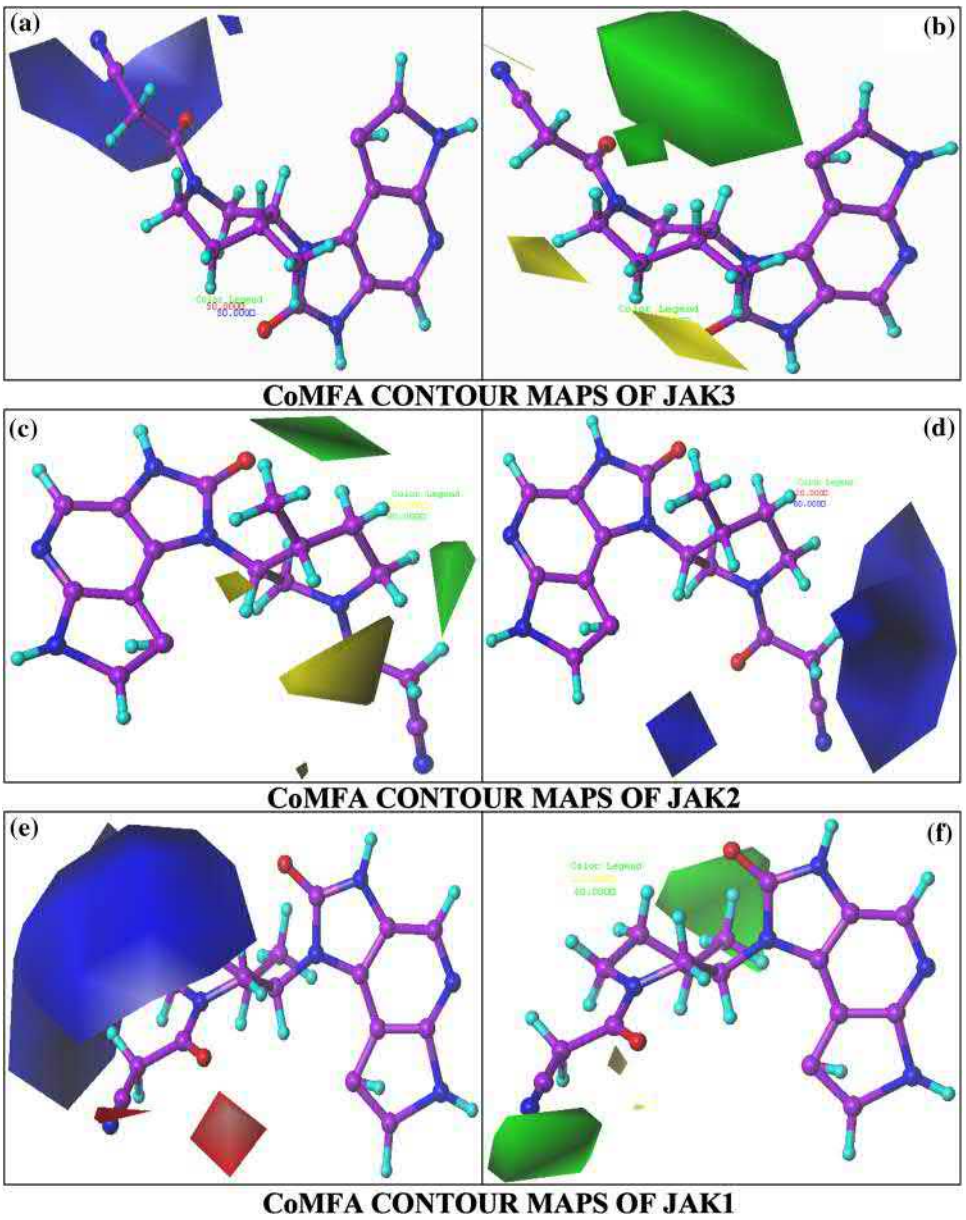


Fig. 4 CoMFA contour maps of three different activity. Green fields represents the preferred steric bulk, yellow field represents the disfavored steric bulk, Blue fields indicate favored electropositive groups and red fields indicate favored electronegative groups

Statistical evaluation of CoMSIA

Both the hydrophobic and hydrogen bond donor descriptors, in addition to the steric and electrostatic fields in CoMFA, were defined using CoMSIA method that is not usually available with standard CoMFA. The field combinations were changed systematically to select the best result. Twenty-five different combinations for each set were generated in this study. Table 4 shows the summary of the statistical analysis of CoMSIA. The CoMSIA model with all the combination fields yielded a LOO cross-validated Q^2 value > 0.3 with different components, and the non-cross-validated $R^2 > 0.5$ and F value > 10.

On comparing the statistical parameters of various models it is found that ADES i.e., hydrogen bond acceptor (A), hydrogen bond donor (D), electrostatic (E) and steric (S) is comparatively good. In the JAK3 set a cross-validated Q^2 value 0.469, non-cross-validated R^2 0.872 with SEE 0.344 and F-value 25.066 are obtained. This model gives an overall R^2_m 0.668 and R^2_{pred} 0.757. Comparison of JAK2 models gives ADH, i.e., hydrogen bond acceptor (A), hydrogen bond donor (D) and hydrophobic (H) as a good model, which gives 0.512 and 0.815 as the cross-validated Q^2 and non-cross-validated R^2 values, respectively. The model gives an F value of 26.349, $R^2_{m(overall)}$ value of 0.687 and R^2_{pred} value of 0.711. Since the statistical parameters of JAK1 model are not good, the CoMSIA contour analysis was carried out only for JAK2 and JAK3.

The plot of actual vs predicted activities for the training and test set molecules of both models are shown in Fig. 5. It shows an R^2value of 0.872 for the training set and 0.813 for the test molecules for ADES, and an R^2 value of 0.815 for the training set and 0.773 for the test molecules for ADH. The experimental and predicted pIC_{50} values and the residual values of these dataset by both CoMSIA models are listed in Table 6.

CoMSIA contour map analysis

In the CoMSIA contour map of JAK3, the preferred steric contributions are represented by yellow, which on adding a group near this region will improve the inhibitory activity. The violet contour represents the disfavored steric, which on adding a group near this region will decrease the inhibitory activity. The contour map of this model is shown in the Fig. 6a.

The electrostatic contributions are represented by blue and green contours in Fig. 6b. Here the blue services the positive charge and disservices the negative charge. Similarly, the green areas in the electrostatic contours represent the negative charge favor and positive charge disfavor. The electrostatic contour map shows a large blue contour near R1 group. This means that increasing the positively charged group as R^2 will help to increase the activity of the molecules. Molecule dpp9 shows increased activity when compared with dpp13, as dpp9 has ethyl and methyl groups in the R1 group instead of –N–CO–CH_2–CN group which is an electron rich group in the R1 group of the molecule dpp13. This can be explained by considering the molecules dpp5 and dpp1. The introduction of one more methyl group in dpp5 has increased the activity of the molecule to 6.745.

In Fig. 6c, the cyan contour indicates the hydrogen bond donor contour maps. The substituents in this region will increase the activity. The hydrogen bond donor substituents in this region leads to a decrease in activity as indicated by the purple coloured contour. The hydrogen bond donor contour map can be explained by comparing the molecules dpp11 and dpp15, where dpp11 has a –NH group and hence shows a decrease in activity.

Table 6 Experimental and predicted activities (pIC_{50}) with residual values of CoMSIA Models

Compound ID	JAK3		JAK2	
	Predicted	Residual	Predicted	Residual
dpp1	7.515	− 0.247	7.561	− 0.195
dpp2	6.952	− 0.207	7.283	− 0.270
dpp3[a]	7.640	0.018	7.619	0.019
dpp4	7.543	− 0.321	7.384	− 0.329
dpp5	8.104	0.419	7.876	0.481
dpp6	7.648	0.030	7.580	0.058
dpp7	7.506	− 0.129	7.618	0.020
dpp8	7.361	− 0.200	7.350	− 0.279
dpp9	7.763	0.760	7.663	0.781
dpp10	6.392	0.177	6.302	− 0.001
dpp11[a]	5.850	0.071	5.804	0.082
dpp12	6.186	− 0.037	6.916	− 0.062
dpp13[a]	7.516	− 0.315	7.930	− 0.844
dpp14	7.587	− 0.034	7.994	− 0.224
dpp15[a]	7.937	1.022	8.150	0.435
dpp16	8.177	0.124	8.488	− 0.351
dpp17	8.023	− 0.454	7.843	− 0.073
dpp18	6.177	0.160	5.935	0.136
dpp19	9.137	− 0.040	8.201	0.308

[a] Test set compounds

The magenta contour represents the favored H-bond acceptor contour map, which is shown in Fig. 6d. Here the hydrogen bond acceptor contour map can be explained by considering the molecules dpp18 and dpp11. Molecule dpp18 has a hydrogen bond acceptor group and thus it showed an increase in anti-inflammatory activity of 9.097, while molecule dpp11 showed a decreased inhibitory activity due to the presence of a methyl group. Same is the case with molecules dpp11 and dpp16.

In the CoMSIA contour map of JAK2, magenta contour represents the favored hydrogen bond acceptor contributions, suggesting that more bulky groups are favorable. The contour map of this model is shown in the Fig. 7a. The hydrogen bond acceptor contour map can be explained by considering the molecules dpp16 and dpp5. Molecule dpp16

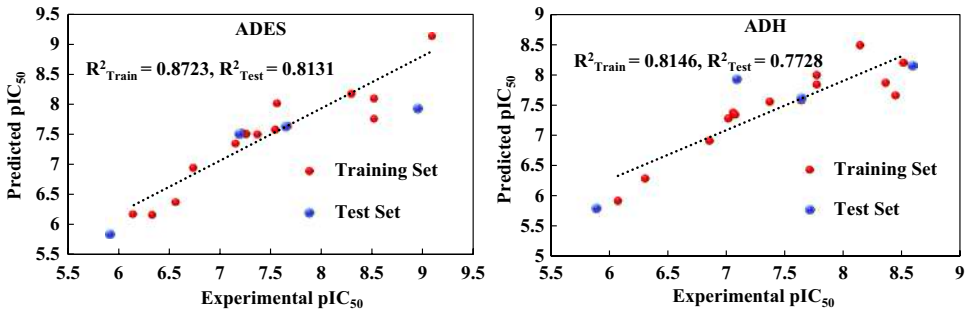


Fig. 5 Plot of actual versus predicted pIC_{50} values for the CoMSIA model

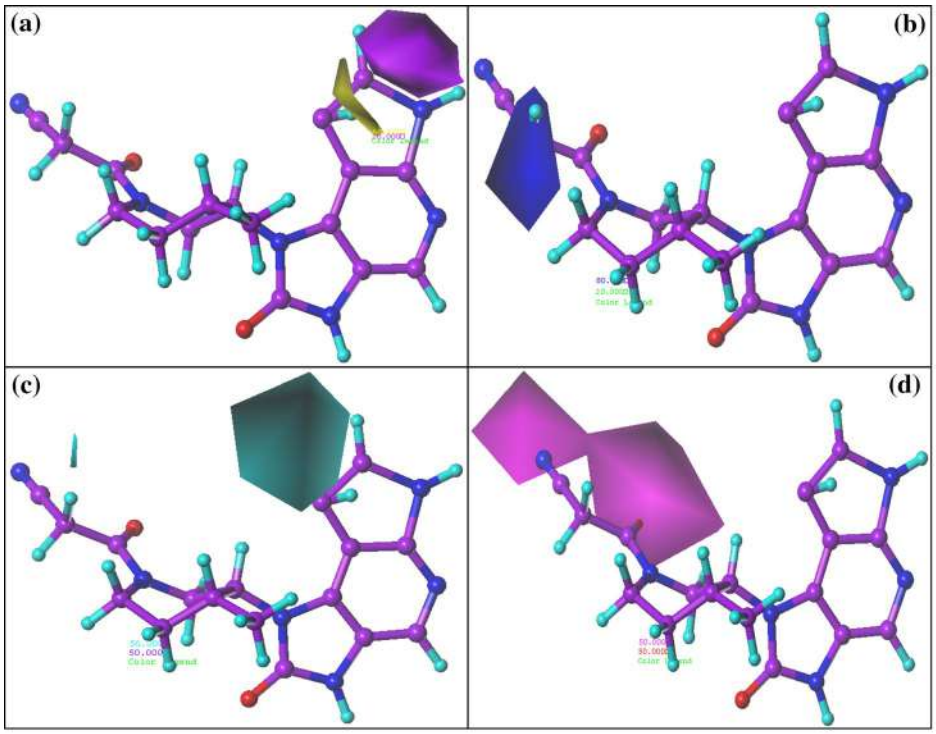


Fig. 6 CoMSIA contour maps of JAK3 model. **a** Violet and yellow contour represents the favored and disfavored steric contributions; **b** the electropositive contributions were represented by blue contours; **c** cyan contour indicates the favored H-bond donor contributions; **d** magenta contour represents the favored H-bond acceptor contributions

has a hydrogen bond acceptor group and thus it showed an increase in anti-inflammatory activity of 8.608, while molecule dpp5 showed a decreased inhibitory activity. Same is the case with molecules dpp14 and dpp1 where the molecule dpp14 with a hydrogen bond acceptor group showed an increase in anti-inflammatory activity (7.726) when compared with the molecule dpp1 which has no hydrogen bond acceptor group (7.419).

In Fig. 7b the cyan contour indicates that hydrogen bond donor substituents in this region will improve the activity. The yellow region of the CoMSIA hydrophobic contour plot in Fig. 7c, reveals that the hydrophobic substituents in this region could enhance the inhibitory activity. The relative contributions of hydrogen bond acceptor (A), hydrogen bond donor (D), and hydrophobic (H), of this model were 42.2, 41.5 and 16.1%, respectively.

Data mining

The random forest (RF) algorithm gives high accuracy and time efficiency for predictive data modelling. Sajeev et al. (2013), Seal et al. (2012) and Periwal et al. (2011) had also reported that random forest provided the best classifier. Therefore in the present study, we tested the activity of the dpp derivatives using the classifier based on RF. Using the tenfold cross validation (CV), the RF classifier was evaluated.

In this study RF model corresponding to the AID 1852 gives accuracy and precision values of 61.7 and 0.616%, respectively and with Kappa value 0.219, TP rate 0.617, FP rate 0.401, F measure value 0.611, and ROC area 0.657. Similarly, for the AID 2001 accuracy and precision values of 60.7 and 0.613%, respectively were obtained with Kappa value 0.219, TP rate 0.607, FP rate 0.387, F measure value 0.605, and ROC area 0.647.

With RF, 19 derivatives were screened using both AIDs and from the confusion matrix obtained, 9 molecules (dpp 1, 2, 4, 5, 6, 7, 17, 15 and 19) from the AID 1852 and 18 (except dpp 16) from AID 2001 were predicted as active by the model. On comparing these two results altogether, 9 molecules were found common to both sets. So these molecules (dpp 1, 2, 4, 5, 6, 7, 17, 15 and 19) were taken for further studies in the present work and the statistical parameters of the RF predictive model are shown in Table 7.

Molecular docking

The selected protein targets were validated by the primary structure and secondary structure analyses. The quality of each of the proteins was evaluated using Ramachandran plot obtained from MOE 2014.0901 (Supplementary material S1). On comparing the docking results with respect to a various set of JAK target proteins, 3LXK exhibited good E score for all the compounds in the JAK3 set; 3EYH showed the good docking score values for all the compounds in JAK1 set. But in the case of JAK2 the good docking score was obtained from the various proteins. That is, except dpp19, dpp17 and dpp15 all other compounds give a good result

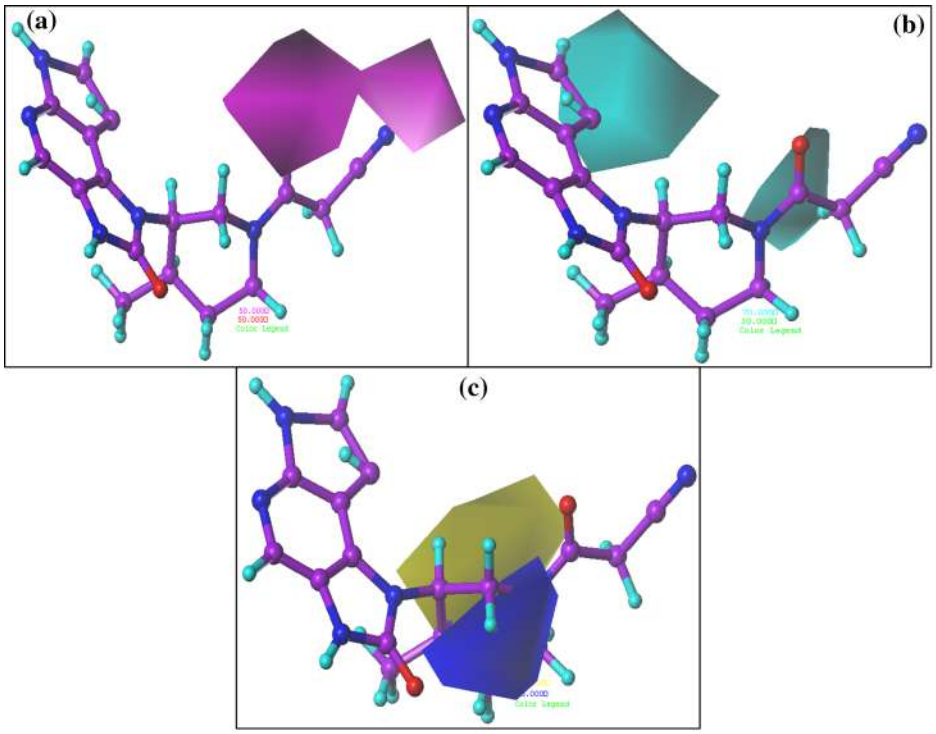


Fig. 7 CoMSIA contour maps of JAK2 model. **a** magenta contour represents the favored H-bond acceptor contributions; **b** cyan contour indicates the H-bond donor contributions; **c** yellow region represents the favored hydrophobic contributions

Table 7 Statistics of random forest predictive model

AID SET	TP rate	FP rate	F measure	Kappa value	Precision	Accuracy	ROC area
AID 2001	0.607	0.387	0.605	0.219	0.613	60.73%	0.647
AID 1852	0.628	0.371	0.629	0.257	0.613	62.84%	0.684

TP rate true positive, *FP rate* false positive, *TN rate* true negative, *FN rate* false negative, *ROC area* receiver operating characteristic, *BCR* balanced classification rate

with 4F08; dpp19 and dpp15 give good score with the protein 4FVP; and dpp17 gives good E score value with the target protein 3IO7. The molecular docking results are shown in the Table 8. 2D interaction and docking pose of the active compounds with good docking score in the binding pocket of the proteins are shown in Fig. 8. Binding interaction studies of the compounds having comparatively good docking score with respective proteins are analyzed using LigPlot analysis.

Molecular docking and interaction of the selected compounds with 3LXK

The molecular docking studies of dpp15, dpp7 and dpp6 gave results with comparatively good docking score with 3LXK. Maximum docking score obtained is for the compound dpp15 and is − 15.104 kcal/mol. This may be due to the large number of indirect hydrogen bonding interactions between the oxobutanenitrile group with various amino acid residues such as Arg953 and Lys830. The solvent exposure of this group is also very high. But there are no prominent interactions detected for the dpp15.

No prominent interactions are seen in the compound dpp7, but it shows an indirect hydrogen bonding interaction only with a basic amino acid residue Arg953. The carboxyl group is highly exposed to the solvent. The docking score of dpp7 is − 12.937 kcal/mol.

The binding mode for the compound dpp6 indicates that the pyridine ring gives a backbone donor bonding interaction with an acidic residue Glu903 (2.78 Å, 20%). The unbroken dotted outline surrounding the ligand indicates the closeness of the ligand to the active site. If the ligand is close to the receptor, the line will be drawn very tightly around the ligand (Wallace et al. 1995). Here the side which contains the pyridine ring is very close to the active site. The docking score is found to be − 13.659 kcal/mol.

Molecular docking and interaction of the selected compounds with JAK2 proteins

The molecular docking studies of dpp17, dpp15 and dpp5 gave results with comparatively good docking score with 4FVP. Compound dpp17 gave a comparatively good

Table 8 Molecular docking result with respect to the selected proteins

Compound	JAK3 E score, kcal/mol				JAK2 E score, kcal/mol				JAK1 E score, kcal/mol			
	3LXK	3PJC	4HVG	4RIO	3IO7	3TJD	4F08	4FVP	3EYH	4E4N	4EI4	4K77
dpp1	− 12.630	− 8.893	− 9.330	− 9.586	− 10.225	− 9.607	− 11.182	− 9.954	− 12.529	− 11.443	− 10.209	− 11.118
dpp2	− 12.174	− 9.646	− 9.270	− 10.341	− 10.515	− 10.096	− 10.822	− 9.599	− 12.489	− 11.012	− 10.317	− 10.287
dpp4	− 11.859	− 9.231	− 9.913	− 9.869	− 11.173	− 9.727	− 11.495	− 10.295	− 13.055	− 12.207	− 9.998	− 10.419
dpp5	− 12.767	− 9.159	− 9.431	− 9.925	− 10.513	− 9.635	− 12.659	− 10.317	− 12.304	− 11.479	− 10.441	− 10.660
dpp6	− 13.659	− 9.233	− 9.513	− 9.537	− 9.931	− 9.770	− 10.889	− 10.129	− 13.194	− 11.480	− 10.594	− 10.721
dpp7	− 12.937	− 10.734	− 9.965	− 10.215	− 10.164	− 9.603	− 11.139	− 10.349	− 13.257	− 11.917	− 10.188	− 11.088
dpp15	− 15.104	− 12.223	− 10.423	− 10.797	− 11.758	− 12.010	− 12.451	− 13.435	− 14.542	− 13.056	− 11.557	− 12.973
dpp17	− 12.787	− 9.871	− 9.828	− 8.998	− 12.411	− 9.690	− 12.256	− 11.081	− 12.816	− 12.114	− 10.655	− 10.484
dpp19	− 10.159	− 8.667	− 8.821	− 8.740	− 9.430	− 8.379	− 9.652	− 10.012	− 10.442	− 10.118	− 8.7632	− 10.861

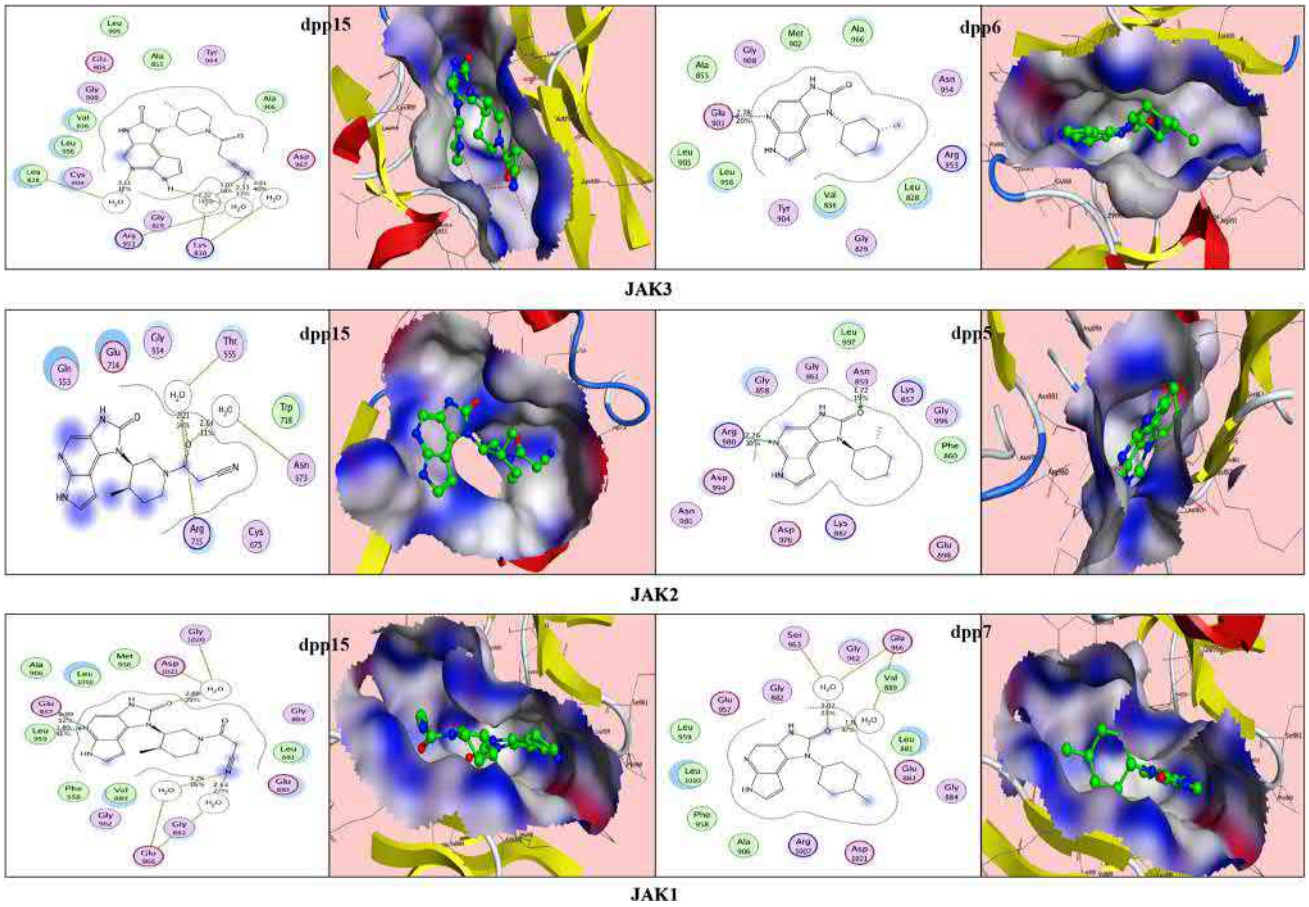


Fig. 8 2D interaction and docking pose of the active compounds with good docking score in the binding pocket of the proteins

molecular docking score − 12.411 kcal/mol with the protein 3IO7 and shows an arene–cation interaction between both the pyrrole and pyridine ring and a basic amino acid residue Arg980. The solvent exposure of dpp 17 is comparatively very good.

Molecular docking of dpp15 with docking score − 13.435 kcal/mol did not show any prominent interactions. But the carbonyl group present in the oxobutanenitrile side chain displays an indirect hydrogen bonding interaction with a polar amino acid residue Thr555 and with a basic residue Arg715. Here also the blue smudges appeared behind most

of the atoms indicate that the compound is highly exposed to the solvent.

The binding mode observed for dpp5 shows that the N atom of the pyridine ring shows a side chain acceptor bonding interaction with a basic amino acid residue Arg980 (2.26 Å, 10%). The carbonyl group present in the compound also shows a side chain acceptor interaction with a polar amino acid residue Asn895 (1.72 Å, 19%). The proximity contour shows the closeness of the compound in the active site. The molecular docking score is − 12.659 kcal/mol.

Molecular docking and interaction of the selected compounds with 3EYH

Compound dpp15 shows both prominent and indirect bonding interactions. The N atom of the pyridine ring shows both side chain and backbone acceptor bonding interaction with greasy and acidic amino acid residues Leu959 and Glu957 respectively at a distance of 1.89 Å (41%) and 2.99 Å (12%) with a docking score of − 14.542 kcal/mol. The carbonyl group present in the imidazolone ring shows indirect hydrogen bonding interactions with polar and acidic amino acid residues Gly1020 and Asp1021, respectively. Similarly the –CN group present in the oxobutanenitrile link of the compound gives an indirect bridging interaction with polar Gly882 and acidic Glu966 residues. The blue smudge around this –CN group clearly represents the good exposure to the solvent. The proximity contour shows the closeness of the dihydroimidazo(pyrrolo-pyridin-one) part of the compound in the active site.

No prominent interactions were observed for the compounds dpp7 and dpp6. In dpp7, the carbonyl group present in the imidazolone ring shows indirect hydrogen bonding interactions with polar Ser963 and acidic Glu966 amino acid residues. Similarly, the same carbonyl group present in dpp6 gives an indirect hydrogen bonding interaction with an acidic amino acid residue Glu966. The docking scores are − 13.257 and − 13.194 kcal/mol for dpp7 and dpp6, respectively.

The results show that our multi-target docking system accurately predicts the interactions between the molecules and JAKs and that the calculated binding affinities are highly correlated with the experimental values.

Prediction of ADME properties

ADME prediction of the finally selected three compounds was done using the preADMET tool. The relative ADME outlines of the selected three molecules are shown in Table 9. The in vivo blood–brain barrier penetration (C_{brain}/C_{blood}), in vitro Caco-2 cell permeability (nm/s), in vitro MDCK cell permeability (nm/s), CYP 3A4 inhibition, human intestinal absorption (%) and in vitro plasma protein binding (%) details were obtained from this ADME calculation.

The Blood–Brain Barrier (BBB) penetration values help to know whether the compounds are able to pass across the BBB or not. A compound having BBB value > 2.0 is considered to have high absorption to CNS (Central Nervous System); with BBBvalue 2.0 ~ 0.1 are considered as middle absorption to CNS and with BBB value < 0.1 are to be considered as low absorption to CNS (Ma et al. 2005).The result shows that the compounds dpp5 and dpp17 have middle absorption to CNS and the compound dpp15 has very low absorption to CNS.

For evaluating the intestinal absorption of drug candidates, several in vitro methods have been used. Among them, for the prediction of oral drug absorption, Caco-2 cell permeability and MDCK cell model have been suggested as dependable in vitro models (Yamashita et al. 2000). A compound having Caco-2 less than 4 is considered as low permeable and the value between 4 and 70 is considered as middle permeable and which has more than 70 is considered as highly permeable compound (Irvine et al. 1999). Through in silico analysis, it is seen that all the compounds have moderate cellular permeability against Caco-2 cells. The Mandin Darby canine kidney (MDCK) cell permeability value of dpp5 and dpp17 are high among the selected compounds. The sum of absorption evaluated from the ratio of cumulative excretion and bioavailability are called human intestinal absorption (HIA) data. The HIA value for poorly absorbed compounds is between 0 and 20%. For a moderately absorbed compound, the HIA value is 20–70%, and for the well-absorbed compounds, the HIA value ranges from 70 to 100% (Yee 1997). In this study we obtained very good HIA values for all the three compounds. The plasma protein binding PPB of a drug influences the drug's action and disposition, and the efficacy of a drug candidate. For a strongly bound chemical, the PPB value will be > 90% and

Table 9 ADME properties obtained from PreADMET server

Properties	dpp5	dpp15	dpp17
BBB[a]	1.565	0.026	1.565
Caco2[b]	15.411	6.433	15.411
CYP_3A4_inhibition	Inhibitor	Inhibitor	Inhibitor
HIA[c]	90.223	89.870	90.223
MDCK[d]	47.935	1.277	47.935
Plasma_protein_binding	83.875	43.439	83.875

[a] Blood–brain barrier

[b] Caco-2 cell permeability

[c] Human intestinal absorption

[d] Madin–Darby canine kidney cells

in the present study we obtained PPB value < 90% for all the three compounds, which means they are weakly bound.

Comparative study of molecular docking score with IC_{50}

In the case of JAK3 and JAK1 sets except dpp19, all other compounds have comparatively good and high docking score. The IC_{50} values were also good for the compounds except dpp1, dpp2, dpp4 and dpp7 in JAK3. In JAK1, the IC_{50} values of dpp1, dpp2, dpp4 and dpp6 are comparatively high. In JAK2, only dpp17, dpp15 and dpp5 show good docking score values. The IC_{50} values of these three compounds are also good (Table 10). Further comparison of the docking score and IC_{50} values among the three sets of JAK proteins, shows that dpp17, dpp15 and dpp5 are comparatively good. Therefore, the three compounds, dpp17, dpp15 and dpp5 are considered as the lead compounds for the development of new anti-RA drugs.

Pharmacophore elucidation

The 3D pharmacophore designing methods take into account both the three-dimensional structures and binding modes of receptors and inhibitors. This is to understand whether the regions are favorable or not for a specific receptor–inhibitor interaction. The pharmacophore model generated for the dataset showed two aromatic, two H-bond donor, two H-bond acceptor and one pi ring centers features, which are shown in Fig. 9. The pharmacophore developed for the drug molecule Tofacitinib also showed similar pharmacophoric features such as two aromatic, four H-bond acceptors, one H-bond donor, and one hydrophobic center. This reveals that the compounds can be used as excellent lead compounds for the treatment of RA.

Design of novel chemical entities

The models obtained through the various studies could be effectively used as basic strategy to modify the most preferable scaffold with a view to design some novel potent JAK

Table 10 Comparison of Molecular docking score with IC50 values of the active compounds

Compounds	IC_{50}			E score (kcal/mol)		
	JAK3	JAK2	JAK1	JAK3	JAK2	JAK1
dpp1	54	43	79	− 12.630	− 11.182	− 12.529
dpp2	180	97	110	− 12.174	− 10.822	− 12.489
dpp4	60	88	1000	− 11.859	− 11.495	− 13.055
dpp5	3	4.4	14	− 12.767	− 12.659	− 12.304
dpp6	21	23	430	− 13.659	− 10.889	− 13.194
dpp7	42	23	24	− 12.937	− 11.140	− 13.257
dpp15	1.1	2.6	1.5	− 15.104	− 13.435	− 14.542
dpp17	27	17	28	− 12.787	− 12.411	− 12.816
dpp19	0.8	3.1	3.7	− 10.159	− 10.012	− 10.442

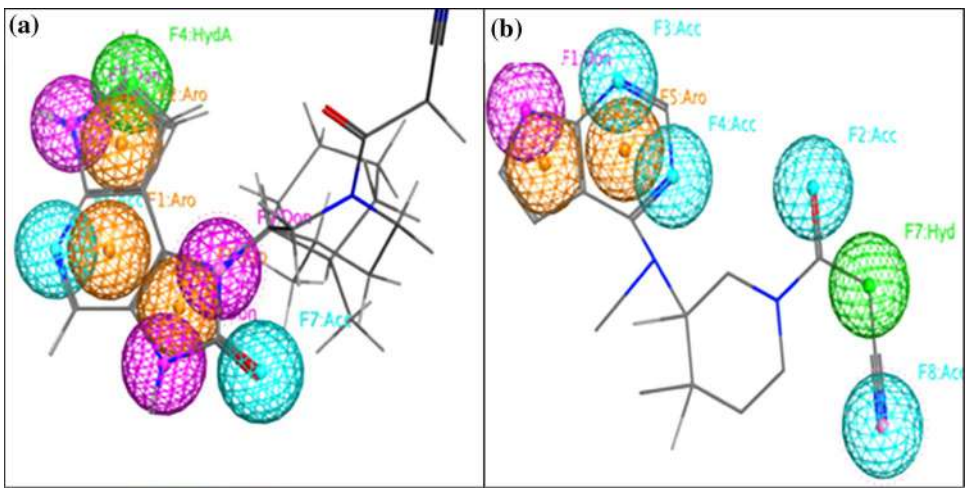


Fig. 9 Pharmacophore mapping for the dataset (cyan: H-bond acceptor, magenta: H-bond donor, orange: Pi ring center). **a** Pharmacophore mapping of the most active compounds dpp19, dpp15 and dpp5; **b** pharmacophore mapping of the drug molecule Tofacitinib

inhibiting compounds. Building a QSAR model and validating the same makes it useful for predicting the activity of newly designed chemical entities whose activities depend on their molecular properties represented by the descriptors. Following the chemical information gathered through the in silico studies performed, the most dependable compound dpp 15 was further modified in order to improve its activity. By doing so, the underlying principles which form the basis for enhancing the biological activities obtained through various QSAR studies and docking-based scoring were utilized. CoMFA and CoMSIA contour maps derived from dpp derivatives provide valuable information regarding how to design novel molecules with improved anti-RA activity.

In CoMFA and CoMSIA contour maps, the existence of a blue contour near R1 position indicates that bulky electropositive groups are favorable for increasing the anti-RA activity. In designing novel chemical entities of the selected scaffold of dpp15, we have incorporated the structural features of the compound dpp15 since the compound has been concluded as to have exhibited potent JAK3, JAK2 and JAK1 inhibitory activities. Based on this, we introduced bulky electropositive groups at the R1 position of dpp 15 and created 20 virtual molecules, which are shown in Supplementary Material Fig. S2.

For evaluating and screening the new virtual molecules with respect to the anti-RA action, the descriptors were generated using PowerMV software and virtual screening was performed using WEKA. The developed RF model predicted that all the 20 newly modified compounds are anti-RA active. The toxicity predictions of these compounds performed using Toxtree, also suggested that all the generated compounds are non-carcinogenic and non-mutagenic in nature. The drug-likeness of these compounds was checked using Lipinski's rule of five; the result showed that all the molecules obeyed Ro5.

The ADME properties of these compounds were evaluated, and were found to be very good and are included in Table 11. Molecular docking with respect to the human microsomal cytochrome P450 3A4 proteins 1TQN, 1W0E, 1W0G, 4I4H and 4NY4 were performed to understand the metabolic capability of these compounds. The relatively high molecular docking score (Table 12) of these compounds revealed that all the compounds were well docked into the active site of these proteins, which means these compounds are easily metabolized.

Using SMARTCyp, the CYP3A4 sites of metabolism of these compounds were predicted. The results obtained are shown in Table 13, which indicates that all the compounds show three common CYP3A4 sites of metabolism.

To find out the activity of the modified molecules, the molecular descriptors of these 20 active virtual molecules were calculated using MOE and PaDEL-Descriptor software. Using the developed 2D-QSAR equations and the respective descriptors involved in the equations, we generated the pIC_{50} value of these molecules. The descriptors used to find out the anti-RA activity and the resulted pIC_{50} values of these compounds are listed in Table 14. The predicted molecular parameters of the modified compounds are listed in this Table. Seven novel chemical entities showed greater JAK inhibition when compared to the parent dpp derivatives. The modified compounds such as dpp15(d), dpp15(m), dpp15(p), dpp15(q) and dpp15(r) showed greater inhibition with respect to JAK3. Compounds dpp15(e) and dpp15(i) showed better inhibition of both JAK3 and JAK2 compared to the activity of any of the parent molecules. The compound dpp15(m) showed higher inhibitory activity for JAK2. Thus it is seen that the molecule, dpp15(s) has much better inhibitory activity values when compared to other novel chemical entities with JAK3 and JAK1. The results of the present study thus confirm the predictive ability of the structure–activity relationships and docking studies. The designed molecules testified by us impart leads for forthcoming research.

Table 11 ADME properties obtained for modified compounds

Compounds	BBB[a]	Caco2[b]	HIA[c]	MDCK[d]	Plasma_protein_binding
dpp15(a)	0.049	10.451	91.171	8.818	69.772
dpp15(b)	0.095	12.536	91.775	7.750	81.633
dpp15(c)	0.120	13.635	92.056	0.977	83.238
dpp15(d)	0.249	14.892	92.610	0.092	86.571
dpp15(e)	0.232	19.211	92.878	0.062	87.216
dpp15(f)	0.044	16.261	91.170	5.269	65.733
dpp15(g)	0.050	14.806	91.489	8.720	74.012
dpp15(h)	0.064	12.542	91.490	13.056	76.498
dpp15(i)	0.189	16.349	92.607	0.061	85.481
dpp15(j)	0.166	14.743	92.334	0.134	84.916
dpp15(k)	0.049	9.764	90.880	14.011	66.925
dpp15(l)	0.072	9.894	91.180	10.931	75.091
dpp15(m)	0.096	11.058	91.471	1.092	78.345
dpp15(n)	0.057	10.091	91.179	10.196	73.578
dpp15(o)	0.049	13.596	91.178	10.955	70.603
dpp15(p)	0.736	17.023	93.146	0.052	88.537
dpp15(q)	0.440	18.810	93.145	0.058	88.177
dpp15(r)	0.046	8.102	90.880	9.583	66.850
dpp15(s)	0.031	4.989	90.234	1.868	47.312
dpp15(t)	0.035	6.222	90.566	2.818	52.490

[a] Blood–brain barrier

[b] Caco-2 cell permeability

[c] Human intestinal absorption

[d] Madin–Darby canine kidney cells

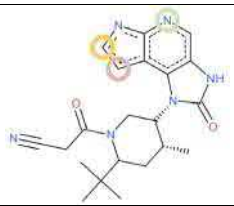
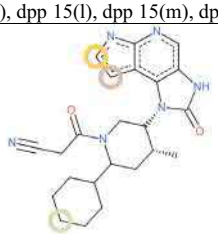
Table 12 Molecular docking result of modified compounds with respect to CYP3A4 Proteins

Compounds	E score (kcal/mol)				
	1TQN	1W0E	1W0G	4I4H	4NY4
dpp15(a)	− 14.795	− 12.792	− 11.624	− 11.356	− 11.263
dpp15(b)	− 13.848	− 12.538	− 11.398	− 11.450	− 11.128
dpp15(c)	− 12.555	− 12.275	− 11.300	− 10.628	− 11.222
dpp15(d)	− 12.612	− 12.993	− 12.119	− 11.138	− 10.581
dpp15(e)	− 12.938	− 13.037	− 12.284	− 12.936	− 11.540
dpp15(f)	− 12.944	− 11.593	− 10.881	− 10.108	− 10.762
dpp15(g)	− 13.180	− 12.492	− 10.842	− 10.949	− 11.713
dpp15(h)	− 12.561	− 11.752	− 11.119	− 10.391	− 12.617
dpp15(i)	− 13.570	− 12.444	− 11.151	− 12.933	− 11.278
dpp 15(j)	− 12.719	− 11.129	− 11.378	− 11.746	− 10.502
dpp15(k)	− 14.045	− 11.982	− 11.390	− 10.344	− 11.127
dpp 15(l)	− 13.272	− 12.674	− 10.481	− 10.045	− 11.878
dpp15(m)	− 12.408	− 11.805	− 10.191	− 10.965	− 10.073
dpp15(n)	− 12.365	− 11.326	− 10.507	− 10.834	− 10.863
dpp15(o)	− 12.522	− 12.149	− 10.455	− 10.506	− 10.742
dpp15(p)	− 11.991	− 11.951	− 11.871	− 11.494	− 11.353
dpp15(q)	− 13.868	− 11.739	− 11.700	− 11.222	− 11.949
dpp15(r)	− 13.235	− 11.939	− 10.290	− 10.081	− 10.377
dpp15(s)	− 15.416	− 11.803	− 11.292	− 10.511	− 10.382
dpp15(t)	− 13.415	− 11.767	− 10.626	− 11.793	− 10.873

Conclusion

During the first stage of this study, the toxicity analysis showed that all the derivatives selected are non-carcinogenic and mutagenic in nature. All the compounds obey Lipinski rule of five. The relatively high docking score with respect to the enzyme CYP3A4 revealed that most of the derivatives metabolize easily. Genetic algorithm and MLR analysis method were used to construct the 2D-QSAR model of the 19 derivatives and the model was validated by the Y-randomization method. 3D-QSAR studies such as CoMFA and CoMSIA analysis revealed various structural features affecting the anti-RA activity of the compounds. Form the CoMFA and CoMSIA field contributions we confirmed the importance of hydrogen bond donor, acceptor, hydrophobic, steric and electrostatic interactions. A machine learning technique was able to successfully filter out the active compounds computationally using the Random forest classifier in the Weka. The molecular docking studies of these selected compounds with various JAK proteins such as 3LXK, 3PJC 4HVG and 4RIO (JAK3); 3IO7, 3TJD, 4F08 and 4FVP (JAK2); 3EYH, 4E4N, 4EI4 and 4K77 (JAK1) indicated that all the compounds in the JAK3 set exhibited good E score for 3LXK, and all the compounds in JAK2 set showed good docking score values for 3EYH. The various binding interactions between the proteins and the corresponding

Table 13 SMARTcyp result of the modified compounds

	Atom	Score	Energy	*2DSASA
	C.8	43.41	52.9	37.15
	C9	60.94	69.4	29.64
	N.3	66.84	75.6	18.99
This is common for dpp 15(a), dpp 15(c), dpp 15(d), dpp 15(e), dpp 15(f), dpp 15(g), dpp 15(i), dpp 15(j), dpp 15(k), dpp 15(l), dpp 15(m), dpp 15(n), dpp 15(o), dpp 15(p), dpp 15(q), dpp 15(r), dpp 15(s), dpp 15(t)				
	C.8	43.41	52.9	37.15
	C.9	60.94	69.4	29.64
	C31	66.39	75.9	37.72
dpp 15(b)				
	C.8	69.4	52.9	37.15
	C.9	60.94	69.4	29.64
	C.29	66.34	75.9	38.92
dpp 15(h)				

*Solvent Accessible Surface Area

Table 14 Predicted anti-RA activity of modified compounds with respect to the 2D-QSAR equations

Modified compounds	Predicted pIC50 values		
	JAK3	JAK2	JAK1
dpp15(a)	8.482	8.338	8.091
dpp15(b)	8.955	7.621	6.971
dpp15 (c)	8.836	8.448	7.547
dpp15(d)	9.115	7.883	7.369
dpp15(e)	9.136	8.806	6.879
dpp15(f)	6.901	8.334	8.187
dpp15 (g)	7.379	6.916	6.381
dpp15(h)	7.914	8.030	7.146
dpp15(i)	9.016	9.178	7.298
dpp15 (j)	8.779	7.990	7.408
dpp15(k)	7.275	8.304	7.816
dpp15 (l)	8.340	8.389	8.129
dpp15(m)	7.967	8.668	8.550
dpp15 (n)	8.654	8.188	8.285
dpp15(o)	7.228	8.051	7.734
dpp15(p)	10.588	7.642	6.999
dpp15(q)	9.795	7.775	6.683
dpp15(r)	9.056	7.960	7.479
dpp15(s)	15.444	8.518	9.018
dpp15(t)	7.936	8.225	8.134

ligands were also understood in detail. Further comparison of the docking score and IC_{50} values among the three sets of JAK proteins, and pharmacological properties showed that dpp15 is the best among the molecules studied. So this compound was selected as the basic scaffold for the design of novel chemical entities. The biological activities of all the 20 new molecules were found out using the already developed 2D-QSAR equation. Compound dpp15(s), 3-((3S,4R)-2,4-dimethyl-3-(2-oxo-3,6-dihydroimidazo(4,5-d)pyrrolo(2,3-b)pyridin-1(2H)-yl)piperidin-1-yl)-3-oxopropanenitrile showed maximum inhibitory activity potential against Janus kinase and is selected as the lead molecule.

Acknowledgements Jisha, R.S. is thankful to the University of Kerala, Thiruvananthapuram for providing financial assistance in the form of University Junior Research Fellowship for this work. Aswathy L. is thankful to CSIR, New Delhi for the financial assistance in the form of Senior Research Fellowship.

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Vol 7 Issue 5 June 2017

ISSN No : 2230-7850

International Multidisciplinary Research Journal

Indian Streams Research Journal

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RNI MAHMUL/2011/38595 **ISSN No.2230-7850**

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ISSN: 2230-7850 IMPACT FACTOR : 5.1651(UIF)

INDIAN STREAMS RESEARCH JOURNAL

VOLUME - 7 | ISSUE - 5 | JUNE - 2017

"A STUDY OF IMPACT OF DEMONETIZATION ON INVESTMENT PRIORITIES OF INVESTORS" A CASE STUDY OF MBBS DOCTORS OF AMRAVATI CITY, MAHARASHTRA, INDIA

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ABSTRACT

Demonetization means the process of taking back or withdrawal of a specific currency notes from the circulation in the financial market. It is the act of stripping a currency unit of its status as a legal tendor. The act of demonetization affects the investment decisions of investors hence researcher decided to study the impact of demonetization on investment priorities of investors in which a case study of MBBS doctors of Amravati city is taken into consideration. The said study is based on primary and secondary data as well. With the help of survey method Primary data has been collected from 60 respondents by using structured questionnaire which distributed among MBBS Doctors of Amravati city with the help of simple random sampling technique. By using chi-square test, it is concluded that there is a significant impact of demonetization on the investment priority of MBBS Doctors of Amravati city. Finally from the outcomes/findings of the said study it is further concluded that the economical and financial policies of the country impacts a lot on the investment decisions of investors as compare to other demographic factors.

KEYWORDS: *Demonetization, Investment options, Investment Priorities, MBBS Doctors.*

INTRODUCTION :

Demonetization is the process of taking back or withdrawal of a specific currency notes from the circulation in the financial market. It is the act of stripping a currency unit of its status as a legal tender. Due to this old units of currency must be replaced by new currency units. This measure/step has been taken by the Indian Prime Minister Hon'ble Narendra Modi to resolve the corruption, black money and counterfeit notes from the market. With this move it is expected to cleanse the formal economic system and eliminate black money from the market.

The main reasons behind demonetization in India are as follows:-

1. To eliminate black money
2. To eradicate corruption
3. To control inflation
4. To eradicate counterfeit/ fake currency
5. To promote cashless economy.

Due to the above stated reasons of demonetization we can say that the act of demonetization affects the investment decisions of investors as well and henceforth we have decided to study the impact of demonetization on investment priorities of investors in which a case study of MBBS doctors of Amravati city is taken into consideration.

Impact of Demonetization on Investment Options:-

1. Shares/Equity: After demonetization, if sluggish phase passes away then huge amount of liquidity will be available in the market due to which bank lending interest rates goes down. It positively affects the corporate sector in raising the share prices. Banking, Infrastructure and Manufacturing sector positively benefitted and on the contrary IT and Pharma sector negatively performing after demonetization and due to change in government of USA as well. The risk averse investors should not directly invest in equities/shares without consulting financial expert or they can invest through Equity mutual funds.

2.Equity Mutual Funds: It is expected that after demonetization stock market will be the biggest beneficiary due to which equity mutual funds may also gets positive approach from investors. Hence the investor must continue to invest through SIPs according to their goals with long term horizon. This is also one of the better investment option for the investor after demonetization.

3.Debt Mutual Funds: After demonetization, government of India has enough liquidity so it will not borrow funds from the market. This brings the rate of government bonds down due to which prices of already issued bonds will raise and hence debt mutual funds may give very good returns in long term. Accordingly this investment option may the better choice for the investors.

4.Real Estate: The real estate sector facing a lot of problems due to demonetization as the transactions involved maximum black money and it will not be available for builders and developers in the current phase. They are facing lots of pressure to sell already developed projects and it leads towards 20 to 30% reduction in their prices depending upon their nature and location. Again for new investor with long term horizon it is also better option to invest.

5. Gold : The impact of demonetization on gold /precious metals is of mixed character i.e. neutral. The investors who have lots of black money with him they invested in such option immediately after demonetization to convert their black into white. If inflation increases a bit in short term period then gold prices will also increases which will be more beneficial to the gold investors in future. So it is also the better choice among investors to further invest.

6. Fixed Deposits: After demonetization banks have huge liquidity available with them so that banking institutions reduced their deposit rates and lending rates around 3% since last year. The companies FDs have also followed a similar trend as they will get cheap lending from banks. This time is difficult for those investors who want fixed and secured returns especially retirees. Investors are advisable to shift their investments to Bond Funds from Mutual Funds.

REVIEW OF LITERATURES:-

1. Bothra S. A. & Kawitkar Dr. S. S. (2016) carried out a study of impact of savings on investment preferences of investors, a case study of BHMS Doctors of Amravati city, Maharashtra, India. They found that most of the respondents believe in savings which leads towards their further investments. They also stated that there is a significant relationship between age and saving objectives of investors and there is significant impact of saving objectives of investors on their preferred investment avenues.

2. Pandey Priyanka (2014) carried out a study of saving and investment pattern of investors of Haridwar District. She revealed that the awareness of investment knowledge and investment opportunities among investors of Haridwar District was quite high. Even having sound knowledge of financial market, investors need an assistance of financial planners. Most of the investors rely on fixed deposit and PPF as a best investment avenue. It also revealed that preference to invest in a specific investment avenue is strongly affected by objective of saving.

3. Chaturvedi Meenakshi & Khare Shruti (2012) carried out study on the Saving Pattern and Investment Preferences of Individual Household in India. They found that most investors give the preference to Bank Deposit as the first choice of investment and next to bank deposits they prefer small saving schemes constituting the second choice of investment.

4. Syed Tabassum Sultana (2010) concluded that individual investor still prefer to invest in financial products which give risk free returns. The study confirmed that Indian investors even if they are of high income, well-educated, salaried, and independent are conservative investors who prefer to play safe in the market.
5. Gupta Sunil (2008), studied the investment pattern among different groups in Shimla had revealed a clear as well as a complex picture. The complex picture means that the people are not aware about the different investment avenues and they did not respond positively, probably it was difficult for them to understand the different avenues. The study showed that the more investors in the city prefer to deposit their surplus in banks, post offices, fixed deposits, saving accounts and different UTI schemes, etc.

NEED/ IMPORTANCE OF THE STUDY:

Doctors are among those professionals who have a sound source of income and they belong to a better earner group of the society. Hence in this regard, researcher has tried to study the impact of demonetization on investment priorities of MBBS doctors in Amravati city. It is helpful to study and understand the investment diversification made by them after demonetization. This research paper will become an effective tool to the research scholars and students for their related studies in the respective field.

RESEARCH PROBLEM DEFINITION:

To study the impact of demonetization on the investment priorities of MBBS Doctors of Amravati City
To know the relationship between income and other demographics of investors and their investment priorities among various investment options

OBJECTIVES OF THE STUDY:

1. To study the priorities given by MBBS Doctors towards investment in various investment options.
2. To know the best investment priority among MBBS Doctors after demonetization.
3. To know objectives of MBBS Doctors towards making investments in various investment options.
4. To study the impact of demonetization on the priorities of investment options of MBBS Doctors in Amravati city.
5. To find out the risk bearing capacity of MBBS Doctors

HYPOTHESIS OF THE STUDY:

1. There is no significant impact of demonetization on the best investment priority of MBBS Doctors.
2. There is no significant relationship between age and the best investment priority of MBBS Doctors after demonetization.
3. There is no significant impact of income on the best investment priority of MBBS Doctors after demonetization.

RESEARCH METHODOLOGY:

The said study is based on primary and secondary data as well. With the help of survey method Primary data has been collected from 60 respondents by using structured questionnaire which distributed among MBBS Doctors of Amravati city with the help of simple random sampling technique.

Secondary data has been collected from various books, journals, review of literatures, relevant articles, reports and related websites.

Statistical tools:

Following statistical tools are used for representing and analyzing the collected data:

1. Table
2. Percentage
3. Charts/graphs

The collected data was analyzed by using the chi-square technique.

Limitations of the study:-

1. Sample size is of only 60 respondents.

2. It is assumed that the information provided by respondents is true and fair.
3. This study is restricted to MBBS Doctors of Amravati city only.

DATA ANALYSIS AND INTERPRETATION:

After collection of data, it has been arranged in a tabular form for its suitable analysis and interpretation so that the true and fair results may be drawn towards the stated study.

Table 1: Gender wise distribution of MBBS doctors:-

Sr. No.	Gender	No. of Respondents	Percentage (%)
1	Male	42	70%
2	Female	18	30%
	TOTAL	**60**	**100%**

Analysis:

From the above table, it is revealed that majorities i.e. 70% of the respondents are male and the balance 30% are female.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 70% of the respondents are male.

Table 2: Age wise distribution of MBBS doctors:-

Sr. No.	Age Groups	No. Of Respondents	Percentage (%)
1	Up to 30 years	17	28.33%
2	30 to 40 years	23	38.33%
3	40 to 50 years	14	23.33%
4	Above 50 years	06	10.00%
	Total	**60**	**100%**

Analysis:

From the above table, it is revealed that majority i.e. 38.33% of the respondents belongs to the age group of 30 to 40 years, 28.33% respondents belongs to the age group of up to 30 years, 23.33% respondents belongs to the age group of 40 to 50 years and the least 10% respondents belongs to the age group of above 50 years.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 38.33% of the respondents belongs to the age group of 30 to 40 years and the least 10% respondents belongs to the age group of above 50 years.

Table 3: Income wise distribution of MBBS doctors:-

Sr. No.	Income Group	No. Of Respondents	Percentage (%)
1	Below Rs. 2,50,000	12	20%
2	Rs. 2,50,000 to Rs. 5,00,000	30	50%
3	Rs. 5,00,000 to Rs. 7,50,000	12	20%
4	Above Rs. 7,50,000	06	10%
	TOTAL	**60**	**100%**

Analysis:

From the above table, it is revealed that majority of the respondents i.e. 50% are from the income group of Rs.2,50,000 to Rs.5,00,000, 20% respondents are from the income group of below Rs.2,50,000, 20% respondents are from the income group of Rs.5,00,000 to Rs.7,50,000 and the least 10% respondents are from the income group of above Rs.7,50,000.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 50% of the respondents belongs to the income group of Rs. 2,50,000 to Rs. 5,00,000 and the least 10% respondents belongs to the income group of above Rs.7,50,000.

Table 4: Believe of MBBS Doctors, whether demonetization brings positive changes in investment sector / Indian financial market:-

Sr. No.	Particulars	No. Of Respondents	Percentage (%)
1	YES	45	75%
2	NO	15	25%
	TOTAL	60	100%

Analysis:

From the above table, it is revealed that majority i.e. 75% of the respondents believe that demonetization brings positive changes in investment sector/ Indian financial market and only 25% of the respondents are not believe that demonetization brings positive changes in investment sector/ Indian financial market.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 75% of the respondents believe that demonetization brings positive changes in investment sector/ Indian financial market.

Table 5: Whether demonetization affects investment priorities of MBBS Doctors:-

Sr. No.	Particulars	No. Of Respondents	Percentage (%)
1	YES	45	75%
2	NO	15	25%
	TOTAL	60	100%

Analysis:

From the above table, it is revealed that majority i.e. 75% of the respondents believe that demonetization affects their investment priorities and only 25% of the respondents are not believe that demonetization affects their investment priorities.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 75% of the respondents believe that demonetization affects their investment priorities.

Table 6: After demonetization which investment option is the best priority of investors to invest in the Indian Financial Market:- (Single Choice)

Sr. No.	Investment Avenues	No. Of Respondents	Percentage (%)
1	Insurance policy	09	15.00%
2	Bank fixed deposits	03	05.00%
3	Equities / shares	10	16.67%
4	Real estate	06	10.00%
5	Mutual funds	15	25.00%
6	Gold / Precious metal	10	16.67%
7	PPF	04	06.67%
8	Government securities/ Bonds	03	05.00%
	TOTAL	60	100%

Analysis:

From the above table, it is revealed that majority i.e. 25% respondents believe that mutual funds are the best investment option after demonetization in the Indian Financial Market, 16.67% respondents believe that equities/ shares are the best investment option, 16.67% respondents believe that gold/ precious metals are the best investment option,15% respondents believe that insurance policy is the best investment option, 10% respondents believe that real estate is best investment option, 6.67% respondents believe that PPF is best investment option, least 5% respondents believe that bank fixed deposit is the best investment option and also 5% respondents believe that government securities/bonds are the best investment option after demonetization in the Indian Financial Market.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 25% respondents believe that mutual funds are the best investment option after demonetization in the Indian Financial Market and the least 5% respondents believe that bank fixed deposit is the best investment option and also 5% respondents believe that government securities/bonds are the best investment option after demonetization in the Indian Financial Market.

Table 7: Objectives MBBS Doctors towards investment in various investment options:-

Sr. No.	Objectives towards investment	No. Of Respondents	Percentage (%)
1	For Future Safety of family	09	15%
2	For Tax Savings/Benefits	24	40%
3	For Children education & welfare	21	35%
4	For meeting contingencies	03	05%
5	For wealth creation	03	05%
	TOTAL	60	100%

Analysis:

From the above table it is revealed that majority i.e. 40% respondent's objective towards investment is tax savings/ benefits, 35% respondent's objective towards investment is for children education & welfare, 15% respondent's objective towards investment is for future safety of their family, the least 5% respondent's objective towards investment is for wealth creation and for meeting contingencies respectively.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 40% respondents objective towards investment is tax savings/benefits and the least i.e. 5% respondents investment objective is wealth creation and meeting contingencies respectively.

Table 8: Factors taken into consideration before making any investment :- (Multiple Choice)

Sr. No.	Factors considered before making any investment	No. Of Respondents	Percentage (%)
1	Rate of Return	42	19.81%
2	Safety of Principal Amount	47	22.17%
3	Hedge against inflation	15	07.07%
4	Liquidity	31	14.62%
5	Diversification of Funds	52	24.53%
6	Risk involved in investment option	25	11.79%
	TOTAL	212	100%

Note:- Most of the respondents mentioned more than one response so that responses are outnumbered the respondents.

Analysis:

From the above table it is revealed that majority i.e. 24.53% respondents considered diversification of funds as a factor before making any investment, 22.17% respondents considered safety of principal amount as a factor, 19.81% respondents considered rate of return as a factor, 14.62% respondents considered liquidity as a factor, 11.79% respondents considered risk involved in investment option as a factor and the least 7.07% respondents considered hedge against inflation as a factor before making any investment.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 24.53% respondents considered diversification of funds as a factor before making any investment and the least 7.07% respondents considered hedge against inflation as a factor before making any investment.

Table 9: Priorities of investment options given by MBBS Doctors:- (Multiple Choice)

Sr. No.	Investment Avenues	No. Of Respondents	Percentage (%)
1	Insurance policy	39	14.66%
2	Bank fixed deposits	23	08.65%
3	Equities / shares	40	15.04%
4	Real estate	37	13.90%
5	Mutual funds	50	18.80%
6	Gold / Precious metal	42	15.79%
7	PPF	20	07.52%
8	Government securities/ Bonds	15	05.64%
	TOTAL	**266**	**100%**

Note:- Most of the respondents mentioned more than one response so that responses are outnumbered the respondents.

Analysis:

From the above table, it is revealed that majority i.e. 18.80% respondents first investment priority is mutual funds, 15.79% respondents investment priority is gold/ precious metals, 15.04% respondents investment priority is equities/ shares, 14.66% respondents investment priority is insurance policy, 13.90% respondents investment priority is real estate, 8.65% respondents investment priority is bank fixed deposits, 7.52% respondents investment priority is PPF and the i.e. 5.64% respondents investment priority is government securities/bonds.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 18.80% respondents first investment priority is mutual funds and the least i.e. 5.64% respondents investment priority is government securities/bonds.

Table 10: Risk bearing capacity of MBBS Doctors:-

Sr. No.	Kind Of Risk bearing capacity	No. Of Respondents	Percentage (%)
1	**Low Risk -Low Return**	**20**	**33.33%**
2	**Moderate Risk- Moderate Return**	**25**	**41.67%**
3	**High Risk- High Return**	**15**	**25.00%**
	TOTAL	**60**	**100%**

Analysis:

From the above table it is analyzed that majority i.e. 41.67% of the respondents prefer to take a moderate risk to earn moderate return, 33.33% of the respondents prefer to take a lower risk for earning low returns and the

least 25% of the respondents prefer to take a higher risk for earning high returns.

Interpretation:

From the above analysis, it is interpreted that majority i.e. 41.67% of the respondents prefer to take moderate risk to earn moderate return and the least i.e. 25% of the respondents prefer to take a higher risk for earning high returns.

Testing Of Hypotheses:

1. There is no significant impact of demonetization on the best investment priority of MBBS Doctors.

To test this null hypothesis the researcher has used chi-square test:-

Observed Frequency and expected frequency showing relationship between impact of demonetization and the best investment priority of MBBS Doctors (Primary Data):-

Sr. No.	Investment Options	Demonetization affects	Demonetization not affects	Total
1.	Insurance policy	07 (6.75)	02 (2.25)	**09**
2.	Bank fixed deposits	01 (2.25)	02 (0.75)	**03**
3.	Equities / shares	09 (7.50)	01 (2.50)	**10**
4.	Real estate	06 (4.50)	00 (1.50)	**06**
5.	Mutual funds	12 (11.25)	03 (3.75)	**15**
6.	Gold / Precious metal	08 (7.50)	02 (2.50)	**10**
7.	PPF	01 (3.00)	03 (1.10)	**04**
8.	Govt. securities/ Bonds	01 (2.25)	02 (0.75)	**03**
	TOTAL	**45**	**15**	**60**

Conclusion: The table value of chi-square at 5% significance level with 7 degree of freedom is 14.067 which is less than 14.4591 the calculated value of chi-square. Hence the stated null hypothesis is rejected due to which we can conclude that there is a significant impact of demonetization on the investment priority of MBBS Doctors of Amravati city.

2. There is no significant relationship between age and the best investment priority of MBBS Doctors after demonetization.

To test this null hypothesis the researcher has used chi-square test:-

Observed Frequency and expected frequency showing relationship between age of respondents and their best investment priority after demonetization (Primary Data):-

SR. No.	Age Group/ Investment Priority	Up to 30 years	30 to 40 years	40 to 50 years	Above 50 years	Total
1.	Insurance policy	04 (2.55)	03 (3.45)	02 (2.10)	00 (0.90)	**09**
2.	Bank fixed deposits	00 (0.85)	01 (1.15)	02 (0.70)	00 (0.30)	**03**
3.	Equities / shares	03 (2.83)	04 (3.83)	02 (2.33)	01 (1.00)	**10**
4.	Real estate	01 (1.70)	03 (2.30)	01 (1.40)	01 (0.60)	**06**
5.	Mutual funds	03 (4.25)	06 (5.75)	05 (3.50)	01 (1.50)	**15**
6.	Gold / Precious metal	03 (2.83)	03 (3.83)	01 (2.33)	03 (1.00)	**10**
7.	PPF	02 (1.13)	02 (1.53)	00 (0.93)	00 (0.40)	**04**
8.	Govt. securities/ Bonds	01 (0.85)	01 (1.15)	01 (0.70)	00 (0.30)	**03**
	TOTAL	**17**	**23**	**14**	**06**	**60**

Conclusion: The table value of chi-square at 5% significance level with 21 degrees of freedom is 32.671 which is greater than 15.0747 the calculated value of chi-square. Hence the stated null hypothesis is accepted due to which we can conclude that there is no significant relationship between age and the best investment priority of MBBS Doctors of Amravati city.

3. There is no significant impact of income on the best investment priority of MBBS doctors after demonetization.

To test this null hypothesis the researcher has used chi-square test:-

Observed Frequency and expected frequency showing relationship between income of respondents and their best investment priority after demonetization (Primary Data):-

SR. No.	Income Group/ Investment Priority	Below Rs.2,50,000	Rs.2,50,000 to Rs. 5,00,000	Rs.5,00,000 to Rs. 7,50,000	Above Rs.7,50,000	Total
1.	Insurance policy	03 (1.8)	04 (4.5)	02 (1.8)	00 (0.9)	**09**
2.	Bank fixed deposits	02 (0.6)	01 (1.5)	00 (0.6)	00 (0.3)	**03**
3.	Equities / shares	03 (2.0)	05 (5.0)	02 (2.0)	00 (1.0)	**10**
4.	Real estate	01 (1.2)	01 (3.0)	01 (1.2)	03 (0.6)	**06**
5.	Mutual funds	02 (3.0)	08 (7.5)	04 (3.0)	01 (1.5)	**15**
6.	Gold / Precious metal	01 (2.0)	06 (5.0)	01 (2.0)	02 (1.0)	**10**
7.	PPF	00 (0.8)	02 (2.0)	02 (0.8)	00 (0.4)	**04**
8.	Govt. securities/ Bonds	00 (0.6)	03 (1.5)	00 (0.6)	00 (0.3)	**03**
	TOTAL	**12**	**30**	**12**	**06**	**60**

Conclusion: The table value of chi-square at 5% significance level with 21 degrees of freedom is 32.671 which is greater than 27.6777 the calculated value of chi-square. Hence the stated null hypothesis is accepted due to which we can conclude that there is no significant impact of income on the best investment priority of MBBS Doctors after demonetization.

FINDINGS, CONCLUSIONS AND SUGGESTIONS:-

Findings:-

1. It is interpreted that majority i.e.70% respondents are male and 30% respondents are female.
2. It is interpreted that majority i.e. 38.33% of the respondents belongs to the age group of 30 to 40 years and the least 10% respondents belong to the age group of above 50 years.
3. It is interpreted that majority i.e. 50% of the respondents belongs to the income group of Rs. 2,50,000 to Rs. 5,00,000 and the least 10% respondents belongs to the income group of above Rs.7,50,000.
4. It is interpreted that majority i.e. 75% of the respondents believe that demonetization brings positive changes in investment sector/ Indian financial market.
5. It is interpreted that majority i.e. 75% of the respondents believe that demonetization affects their investment priorities.
6. It is interpreted that majority i.e. 25% respondents believe that mutual funds are the best investment option after demonetization in the Indian Financial Market and the least 5% respondents believe that bank fixed deposit is the best investment option and also 5% respondents believe that government securities/bonds are the best investment option after demonetization in the Indian Financial Market.
7. It is interpreted that majority i.e. 40% respondents objective towards investment is tax savings/benefits and the

least i.e. 5% respondents investment objective is wealth creation and meeting contingencies respectively.
8. It is interpreted that majority i.e. 24.53% respondents considered diversification of funds as a factor before making any investment and the least 7.07% respondents considered hedge against inflation as a factor before making any investment.
9. It is interpreted that majority i.e. 18.80% respondents first investment priority is mutual funds and the least i.e. 5.64% respondents investment priority is government securities/bonds.
10. It is interpreted that majority i.e. 41.67% of the respondents prefer to take moderate risk to earn moderate return and the least i.e. 25% of the respondents prefer to take a higher risk for earning high returns.

CONCLUSIONS:-

1.By using chi-square test, it is concluded that:-
A.There is a significant impact of demonetization on the best investment priority of MBBS Doctors of Amravati city.
B.There is no significant relationship between age and the best investment priority of MBBS Doctors after demonetization.
C.There is no significant impact of income on the best investment priority of MBBS Doctors after demonetization.

Finally from the outcomes/findings of the said study it is further concluded that the economical and financial policies of the country impacts a lot on the investment decisions/priorities of investors as compare to other demographic factors.

SUGGESTIONS:-

1.In the current scenario in India, investors are suggested to shift their investments to bond funds from mutual funds as per their risk taking ability.
2.For retail investors it is suggested that mutual funds will be the best way to invest through SIPs.
3.In general, the diversified portfolio will be suggested to the investors of India by keeping in mind the long term horizon in all the investment options.
4.The regular and positive changes in the economical and financial policies of the country may bring positive changes in the investment sector i.e. in capital and stock market specially because even at lesser financial literacy, investors gets attracted towards investment in mutual funds and shares in the current phase after demonetization in India. Hence it is suggestive to do the regular and positive changes in the economical and financial policies of India as and when necessary for the country.

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IJCRT Publish Paper record is available at DOI: http://doi.one/10.1727/IJCRT.17196

An Analytical Study of Cloud Computing: IT Opportunity and Challenges

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Abstract---**Cloud Computing is a new technology that provides us all the services and resources for retrieving our data globally. Now a days IT industry is standing at the threshold of a new era in the technological field. Cloud computing is everything that could answer the problems of IT companies. Cloud computing has the ability to make IT resources more cost-effective and it gives businesses a great flexibility to expand.**

There are several fields including business, e-governance, utility computing, military, and healthcare where computer system play a vital role. All the fields include the sharing of data among each other's. So if we want a channel through which we will have easy way to communicate and share the data then cloud computing provides us a very seamless way to communicate. But as the time is growing cloud computing should also have to enhance its performance. Many big companies are not adopting this technology till now because of many challenges. The different types of challenges are:

1. Performance
2. Security and privacy
3. Bandwidth cost

In this paper we have tried to summarize the uses ,opportunity and challenges of cloud computing and we also have tried to explain how the cloud computing can help in business in today's scenario.

Keywords—**Cloud computing, Utility computing, E-Governance, Internet, Security.**

I. INTRODUCTION

Cloud computing is the use of computing resources both hardware as well as software that are delivered as a service over a network typically the Internet. As the name suggests clouds means that the network is of the cloud type as the clouds spreads in the sky as a network. In cloud computing we may access our data globally via the use of internet. Internet plays a vital role while sharing of data in between various networks. We run many applications via the use of a cloud and Cloud providers manage the infrastructure and platforms that run the applications.

Day by day, big companies spend millions of dollars on their IT infrastructure that consist of hardware, system software, applications, networks, people, and other organizational assets. Now a day's computing is becoming as import part of our life as the importance of water in human life. So we will also have to change our mind as per the technology is changing. The cloud is simply a service where all the data saves but when it combines with computing then it became very complex and fuzzy. Here different services- such as servers, storage and applications are delivered to an organization's computers and devices through the Internet.

II. HOW CLOUD WORKS

The main goal of cloud computing is to apply supercomputing or high-performance computing power to the organizations such as military, healthcare, utility computing and all to perform trillions of computations per second to provide a very large data storage.

IJCRT Publish Paper record is available at DOI: http://doi.one/10.1727/IJCRT.17196

Suppose we have an organization. In that organization we will also have to provide all the facilities to all of the employees of that organization like right hardware and software they need to do their jobs. We will buy the computers for each and every employee of the organization but that is not enough we will also have to provide the software and tools required for the job. Whenever we have a new hire, we have to buy more software or make sure our current software license allows another user. That is a very long lasting process so the solution of the problem is cloud computing. In which we will have a centralize server which will provide all the services to the employees as well as to the customers.

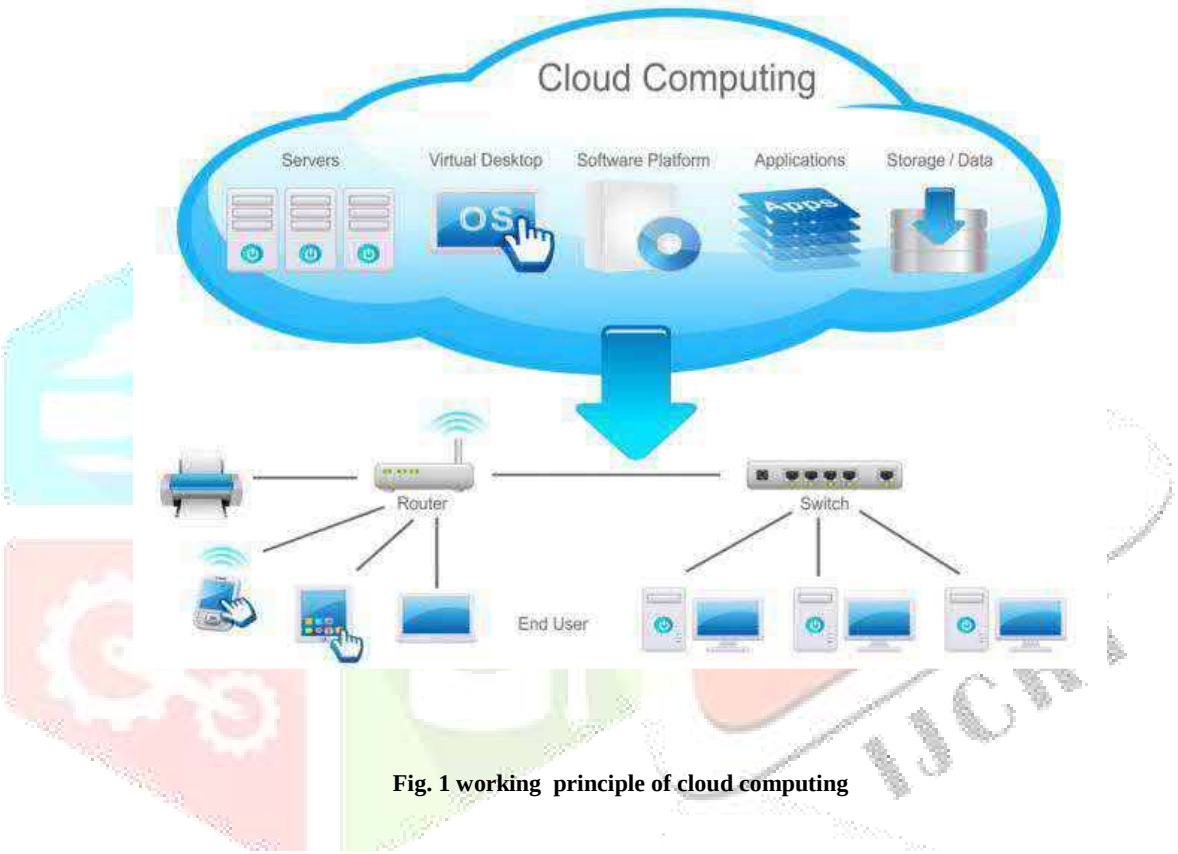

Fig. 1 working principle of cloud computing

The total workload of the local computers shifted to server computers by using cloud computing technology. Local computers no longer have to do all the heavy lifting of data and all when it comes to running applications. The network of computers that make up the "cloud" handles them. We have a very good example of cloud computing that is the E-mail which most of us have used many times but we did not notice that where our data actually saved, that is in the cloud and we access our data whenever we want to access.

III. SECURITY ISSUES AND CHALLAGES

Everywhere you turn these days "the cloud" is being talked about. This ambiguous term seems to encompass almost everything about us. While "the cloud" is just a metaphor for the internet, cloud computing is what people are really talking about these days. Cloud computing is the delivery of hosted services over the internet, through a network of remote servers. These remote servers are busy storing, managing, and processing data.

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Cloud computing comes into focus when you think about IT. If we are using this technique in our business applications then we will also have to make our business more secure. There are mainly three models of cloud computing IaaS (Infrastructure as a Service), PaaS (Platform as a Service), SaaS (Software as a Service) and Utility Computing.. These three models have different impact on different types of applications. Two main questions arise while using these models that are: –
-How secure is the Data?
-How secure is the Code?

The capabilities and breadth of cloud computing are enormous. The IT industry broke it into three categories to help better define use cases.

A. Software as a Service (SaaS) – Software is owned, delivered and managed remotely by one or more providers. To start, Software-as-a-Service, or SaaS, is a popular way of accessing and paying for software. Instead of installing software on your own servers, SaaS companies enable you to rent software that's hosted, this is typically the case for a monthly or yearly subscription fee. More and more CRM, marketing, finance, and business intelligence and even Adobe's Creative Suite has adopted the model.

B. Infrastructure as a Service (IaaS) – Compute resources, complemented by storage and networking capabilities are owned and hosted by providers and available to customers on-demand.

C. Platform as a Service (Paas) – The broad collection of application infrastructure (middleware) services. These services include application platform, integration, business process management and database services.

D. Utility computing- Utility computing is mainly a business model which provides services as per the demand. As the name suggest "utility computing" which generally means that any service which is mostly needed by any customer? Better economic is the main benefit of utility computing.

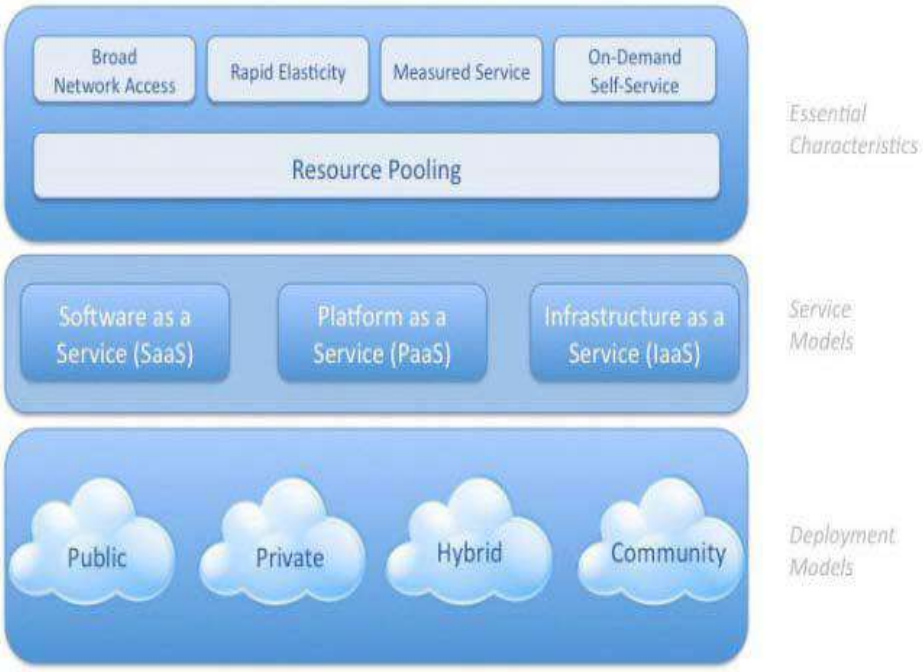

Fig. 2 Visual model of cloud computing definition

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All of this is a deviation from traditional on-premise computing which is done via a local server or personal computer. These traditional methods are increasingly being left behind. In fact, IDG's recently published Enterprise Cloud Computing Survey (2016) found that by 2018 the typical IT department will have the majority of their apps and platforms (60%) residing in the cloud.

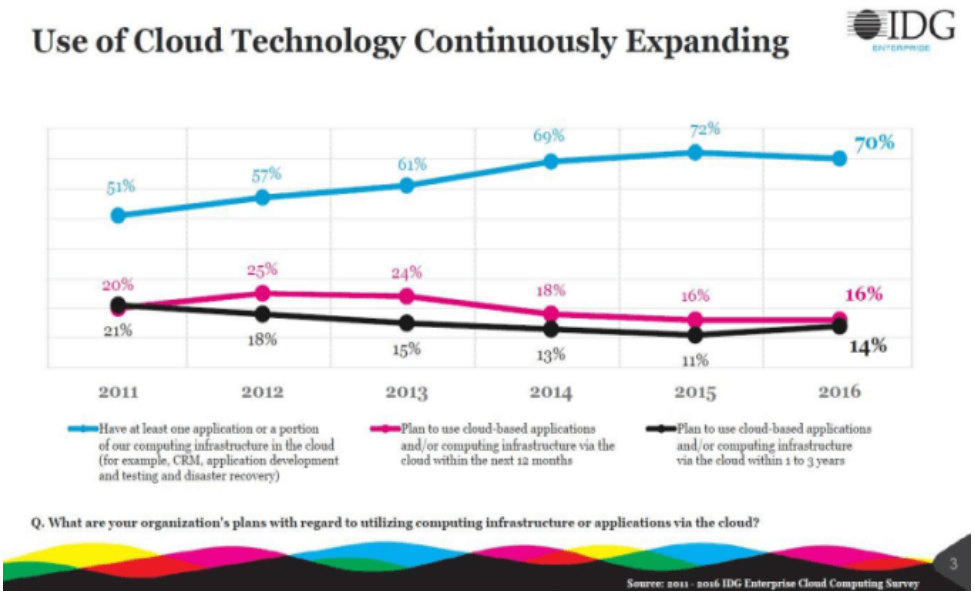

Fig. 3 Graphical Representation: Growth Of Cloud Computing Technology

In an effort to do everything from offer better in-store customer service to fully leverage advances in manufacturing, companies from even most traditional and change-resistant sectors are seeing the writing on the wall: Cloud technology strategies cut cost and risk.

Though the opportunities are great, the cloud computing explosion hasn't come without challenges. Now let's go over more of those challenges organizations are facing, and how they are being addressed.

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IV. CURRENT CLOUD COMPUTING CHALLENGES

Below, we have expanded upon some of additional cloud computing problems that businesses may need to address.

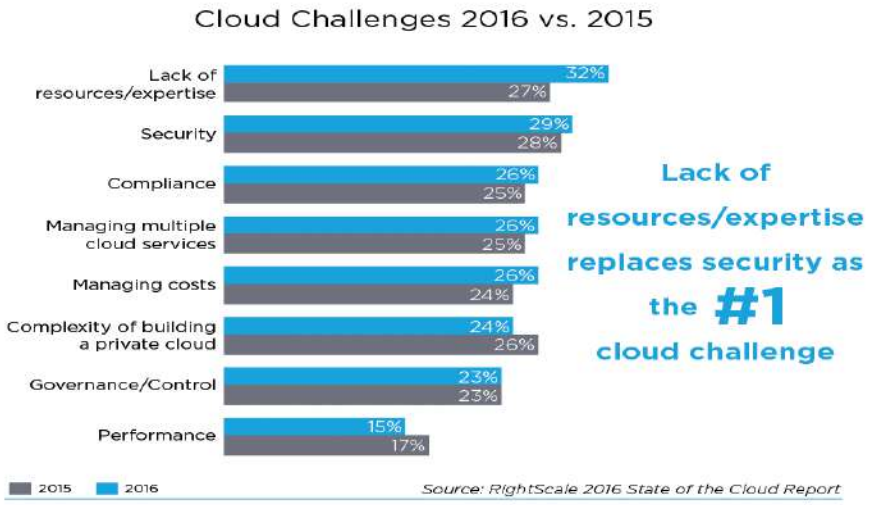

Fig. 4 Comparison Of Challenges For The Year 2015-16

A. Lack of resources/expertise

For the longest time, security was the number one voiced cloud challenge. In 2016 however, lack of resources/expertise inched ahead. Organizations are increasingly placing more workloads in the cloud while cloud technologies continue to rapidly advance. Due to these factors organizations are having a hard time keeping up with the tools. Also, the need for expertise continues to grow. These challenges can be minimized through additional training of IT and development staff.

B. Security issues

Resource/expertise concerns slightly passed security cloud computing problems in 2016. Security has indeed been a primary, and valid, concern from the start of cloud computing technology: you are unable to see the exact location where your data is stored or being processed. Headlines highlighting data breaches, compromised credentials and broken authentication, hacked interfaces and APIs, account hijacking haven't helped alleviate concerns. All of this makes trusting sensitive and proprietary data to a third party hard to stomach for some. Luckily as cloud providers and users, mature security capabilities are constantly improving. To ensure your organization's privacy and security is intact, verify the SaaS provider has secure user identity management, authentication and access control mechanisms in place

While you are auditing a provider's security and privacy laws, make sure to also confirm the third biggest issue is taken care of compliance. Your organization needs to be able to comply with regulations and standards, no matter where your data is stored. Speaking of storage, also ensure the provider has strict data recovery policies in place.

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C. Cost management and containment

For the most part cloud computing can save businesses money. In the cloud, an organization can easily ramp up its processing capabilities without making large investments in new hardware. Businesses can instead access extra processing through pay-as-you go models from public cloud providers. However, the on-demand and scalable nature of cloud computing services makes it some times difficult to define and project quantities and costs.

D. Governance/Control

Proper IT governance should ensure IT assets are implemented and used according to agreed-upon policies and procedures; ensure that these assets are properly controlled and maintained; and ensure that these assets are supporting your organization's strategy and business goals. In today's cloud based world, IT does not always have full control over the provisioning, de-provisioning and operations of infrastructure. This has increased the difficulty for IT to provide the governance, compliance and risk management required. To mitigate the various risks and uncertainties in transitioning to the cloud, IT must adapt its traditional IT governance and control processes to include the cloud. To this effect the role of central IT teams in cloud has been evolving over the last few years. Along with business units, central IT is increasingly playing a role in selecting, brokering, and governing cloud services. On top of this third party cloud computing/management providers are progressively providing governance support and best practices.

E.. *Performance*

When a business moves to the cloud it becomes dependent on the service providers. This partnership often provides businesses with innovative technologies they wouldn't otherwise be able to access. On the other hand the performance of the organization's BI and other cloud based systems is also tied to the performance of the cloud provider when it falters. When your provider is down, you are also down.

This isn't uncommon, over the past couple of years all the big cloud players have experienced outages. Make sure your provider has the right processes in place and that they will alert you if there is ever an issue.

For the data driven organization real time data is imperative. With an inherent lack of control that comes with cloud computing, companies may run into real time monitoring issues. Make sure your SaaS provider has real time monitoring policies in place to help mitigate these issues.

F. Segmented usage and adoption

Most organizations did not have a robust cloud adoption strategy in place when they started to move to the cloud. Instead, ad-hoc strategies sprouted, fueled by several components. One of them was the speed of cloud adoption. Another one was the staggered expiration of data centre contracts/equipment, which led to intermittent cloud migration. Finally, there also were individual development teams using public cloud for specific applications or projects. These bootstrap environments have fostered full integration and maturation issues including:

1) *Isolated cloud projects lacking shared standards*
2) *Ad hoc security configurations*
3) *Lack of cross-team shared resources and learnings*

V. CONCLUSION

In an emerging discipline of cloud computing, security is the main issue that should have to be provided by big companies who are providing the service of clouds. So we may say that cloud computing brings both opportunities as well as challenges for us. In this paper we mainly focus on the services provided by cloud and new opportunities and challenges in the IT industries by using cloud computing. We have three models of cloud computing that are IaaS, PaaS and SaaS and utility computing. All the three models are important because all have different impact on implementation of the services.

While cloud computing challenges do exist, if properly addressed these 6 issues don't mean your IT roadmap has to remain anchored on-premise. Business intelligence (BI) and cloud computing are an ideal match, as the first one provides the right information to the right people while the latter is an agile way to access BI applications

So we may say that cloud computing is a leading technology worldwide. If security, authentication and authorization will be provided effectively then this will be one of the most promising technologies

ACKNOWLEDGMENT

The making of this paper needed co-operation and guidance of a number of people. We therefore consider it our prime duty to thank all those who had helped me through their venture. It's my immense pleasure to express our gratitude to teachers of VidyaBharati Mahavidylaya.

I am also thankful to our college for providing Internet Service and Library facility during the preparation of this paper.

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IJCRT Publish Paper record is available at DOI: http://doi.one/10.1727/IJCRT.17197

Study of Relation between Big Data & Cloud Computing: Big Data Challenges & Issues

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Abstract

The amount of data in world is growing day by day. Data is growing because of use of internet, smart phone and social network. Big data is a collection of data sets which is very large in size as well as complex. Now a days, Big data is one of the most talked topic in IT industry. It is going to play important role in future. Big data changes the way that data is managed and used. Communicating by using information technology in various ways produces big amounts of data. Such data requires processing and storage. The cloud is an online storage model where data is stored on multiple virtual servers. Big data processing represents a new challenge in computing, especially in cloud computing. Data processing involves data acquisition, storage and analysis. In this respect, there are many questions including, what is the relationship between big data and cloud computing? The answer to this question will be discussed in this paper, where the big data and cloud computing will be studied, in addition to getting acquainted with the relationship between them in terms of safety and challenges. I have suggested a term for big data, and a model that illustrates the relationship between big data and cloud computing.

Keywords: **Big Data; security; systematic mapping study, cloud, resources, 'five Vs'.**

I. INTRODUCTION

Data is the raw material for information before sorting, arranging and processing. It cannot be used in its primary form prior to processing. Information represents data after processing and analysis. The technology has been developed and used in all aspects of life, increasing the demand for storing and processing more data. As a result, several systems have been developed including cloud computing that support big data. While big data is responsible for data storage and processing, the cloud provides a reliable, accessible, and scalable environment for big data systems to function. Big data is defined as the quantity of digital data produced from different sources of technology for example, sensors, digitizers, scanners, numerical modeling, mobile phones, Internet, videos, e-mails and social networks. The data types include texts, geometries, images, videos, sounds and combinations of each. Such data can be directly or indirectly related to geospatial information.

Cloud computing refers to on-demand computer resources and systems available across the network that can provide a number of integrated computing services without local resources to facilitate user access. These resources include data storage capacity, backup and self-synchronization. Most IT Infrastructure computing consists of services that are provided and delivered through public centers and servers based on them. Here, clouds appear as individual access points for the computing needs of the consumer. They are an online storage model where data are stored on multiple virtual servers, rather than being hosted on a specific server, and are usually provided by a third party. The hosting companies, which have advanced data centers, rent spaces that are stored in a cloud to their customers in line with their needs.

The relationship between big data and the cloud computing is based on integration in that the cloud represents the storehouse and the big data represents the product that will be stored in the storehouse, since it is not possible to create storehouses without storing any product in them. The traditional databases known as 'relational' are no longer sufficient to process multiple-source data. For example, how can these traditional methods deal with data such as record of transactions, customer behavior, mobile phone and GPS navigation, and others. Here comes the role of cloud computing. At this

point, a relationship between big data and the cloud will arise. In this paper, the relationship between them will be discussed, in addition to the challenges and issues that Big Data may encounter.

II. BIG DATA

Big data comes and is composed through electronics operations from multiple sources. It requires proper processing power and high capabilities for analysis. The importance of big data lies in the analytical use which can help generate an informed decision to provide better and faster services.

The term big data is called on the huge amount of high-speed big data of different types; this data cannot be processed and stored in regular computers. The main characteristics of big data known as 'five Vs', are as follows:

1. Volume: It represents the amount of data produced from multiple sources which show the huge data in numbers by zeta bytes. The volume is most evident dimension in what concerns to big data.
2. Variety: It represents data types, with, increasing the number of Internet users everywhere, smart phones and social networks users, the familiar form of data has changed from structured data in databases to unstructured data that includes a large number of formats such as images, audio and video clips, SMS, and GPS data.
3. Velocity: It represents the speed of data frequency from different sources, that is, the speed of data production such as Twitter and Facebook. The huge increase in data volume and their frequency dictates the need for a system that ensures super-speed data analysis.
4. Veracity: It represents the quality of the data, it shows the accuracy of the data and the confidence in the data content. The quality of the data captured can vary greatly, which affects the accuracy of analysis. Although there is wide agreement on the potential value of big data, the data is almost worthless if it is not accurate.
5. Value: It represents the value of big data, i.e. it shows the importance of data after analysis. This is due to the fact that the data on its own is almost worthless. The value lies in careful analysis of the exact data, the information and ideas it provides. The value is the final stage that comes after processing volume, velocity, variety, contrast, validity and visualization .

III. CLOUD COMPUTING

It is a term that refers to on-demand computer resources and systems that can provide a number of integrated computer services without being bound by local resources to facilitate user access. These resources include data storage, backup and self-synchronization, as well as software processing and scheduling tasks. Cloud computing is a shared resource system that can offer a variety of online services such as virtual server storage, and applications and licensing for desktop applications. By leveraging common resources, cloud computing is able to achieve expansion and provide volume.

A. *Characteristics of cloud computing*

That cloud computing is one of the distributed systems that represents a sophisticated model. NIST has identified important aspects of the cloud, as it shortened the concept of cloud computing in five characteristics as follows:

1) *On-demand self-service*: Cloud services provide computer resources such as storage and processing as needed and without any human intervention.

2) Broad network access: cloud computing resources are accessible over the network , mobile and smart devices even sensors can access computing resources on the cloud.

3) Resource Pooling: Cloud platform users share a vast array of computing resources; users can determine the nature of resources and the geographic location they prefer but cannot determine the exact physical location of these resources.

4) Rapid Elasticity: Resources from storage media, network, processing units and applications are always available and can be increased or decreased in an almost instantaneous fashion, allowing for high scalability to ensure optimal use of resources.

5) Measured service: Cloud systems can measure the processes and consumption of resources as well as surveillance, control and reporting in a completely transparent manner.

B. Cloud computing service models.

Cloud computing types are classified on the basis of following models:

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1) *Software as a service (SAAS)*: Cloud service providers provide various software applications to users who can use them without installing them on their computer. The user is not responsible for anything other than adjusting the settings and customizing the service as appropriate to his needs. SAAS helps big-data clients to perform data.
2) *Platform as a service (PAAS)*: Cloud service providers provide platforms, tools and other services to users, where the cloud service provider manages everything else, including the operating system and middleware., with resources that enable you to deliver everything from simple cloud-based apps to sophisticated.
3) *Infrastructure as a service (IAAS)*: Cloud service providers provide infrastructure such as storage, computing capacity, etc. is a form of cloud computing that provides virtualized computing resources over the Internet , In an IaaS model, a third-party provider hosts hardware, software, servers, storage and other infrastructure components on behalf of its users.
4) *DaaS* : It is the alternative cloud computing model, as it differs from traditional models like (SAAS, IAAS, PAAS) in providing data to users through the network, as data is considered the value of this model in conjunction with cloud computing based on solving some of the challenges in managing a huge amount of data. For these reasons, DaaS is closely related to big data whose technologies must be utilized. DaaS provides highly efficient methods of data distribution and processing. DaaS is closely related to SaaS (storage as a service) and SaaS (software as a service) which can be combined with one of these models or both of them.

IV. THE RELATIONSHIP BETWEEN THE CLOUD AND BIG DATA

Cloud computing is a trend in the development of technology, as the development of technology has led to the rapid development of electronic information society. This leads to the phenomenon of big data and the rapid increase in big data is a problem that may face the development of electronic information society. Cloud computing and big data go together, as big data is concerned with storage capacity in the cloud system, cloud computing uses huge computing and storage resources. Thus, by providing big data application with computing capability, big data stimulate and accelerate the development of cloud computing. The distributed storage technology in environmental computing helps to manage big data.

Cloud computing and big data are complementary to each other. Rapid growth in big data is regarded a problem. Clouds are evolving and providing solutions for the appropriate environment of big data while traditional storage cannot meet the requirements for dealing with big data, in addition to the need for data exchange between various distributed storage locations. Cloud computing provides solutions and addresses problems with big data. The cloud computing environment is expanding to be able to absorb big amounts of data as it follows the policy of data splitting, that is, to store data in more than one location or availability area. Cloud computing environments are built for general purpose workloads and resource pooling is used to provide flexibility on demand. Therefore, the cloud computing environment seems to be well suited for big data.

Big data processing and storage require expansion as the cloud provides expansion through virtual machines and helps big data evolve and become accessible. This is a consistent relationship between them. Google, IBM, Amazon and Microsoft are examples of the success in using big data in the cloud environment. In order for the cloud environment to fit with big data the cloud computing environment must be modified to suit data and cloud work together. Many changes are needed to be made on the cloud: CPUs to handle big data and others.

V. CHALLENGES IN BIG DATA AND CLOUD COMPUTING

The security challenges in cloud computing environments fall under several levels: the network level which includes dealing with network protocols and network security such as distributed nodes, distributed data, and communications between the nodes; authentication level where the user handles encryption / decryption techniques, authentication methods such as contract administrative rights, authentication of applications and nodes, and logging entry; the data level which is concerned with data integrity and availability as well as data protection and data distribution. Cloud computing follows the policy of shared resources, where the privacy of data is very important because it faces some challenges like integrity, authorized access, and availability of (backup / replication). Data integrity ensures that data is not corrupted or tampered with during communication. Authorized access prevents data from infiltration attacks while backups and replicas allow access to data efficiently even in case of technical error or disaster in some cloud location .

Big data face some challenges as they can be classified into groups: data sets, processing and management challenges. When dealing with big amounts of data we face challenges such as volume, variety, velocity and verification which are also known as 5V of big data . Also, in the field of computer networks the

cost of communications is a major concern compared to the cost of processing the same data, as the challenge is to reduce the cost of communications to the minimum while meeting the requirements of storage and additional data from the general cloud to handle big data . Among the factors and challenges that affect the processing of big data in a timely manner is The bandwidth and latency . Where several challenges can be summarized in the relationship between big data and cloud computing.

i) Data Storage: The storage of big data through traditional storage is problematic because hard drives often fail, data protection mechanisms are not effective, and the speed of big data requires storage systems in order to expand rapidly, which is difficult to achieve with conventional storage systems. Cloud storage services offer almost unlimited storage with a great deal of error tolerance, which offers potential solutions to address the challenges of big data storage.

ii) Variety of data: Big data naturally grow, increase and vary, which is the result of the growth of almost unlimited sources of data. This growth leads to the heterogeneous nature of big data. Generally speaking, data from multiple sources of different types and representations are highly interrelated. They have incompatible shapes and are inconsistent. A user can store data in structured, semi-structured, or unstructured formats. Structured data format is suitable for today's database systems, while semi- structured data formats are only fairly suitable. Unstructured data is inappropriate because it contains a complex format that is difficult to represent in rows and columns.

iii) Data transfer: The data goes through several stages: data collection, input, processing, and output. Big data transfer is a challenge, so data compression techniques need to be reduced to reduce the volume, where data volume is a hindrance to transfer speed. It also affects the cost, while cloud computing provides distributed storage resources and data transfer on high-speed lines, reducing costs through virtual resources and resource use at user's request.

iv) Privacy and data ownership: The cloud environment is an open environment and the user's role in monitoring is limited. Privacy and security are an important challenge for big data. Big data and cloud computing come together in practice. According to (IDC) estimates, by 2020, around 40% of global data will be accessed by cloud computing. Cloud computing provides strong storage, calculation and distribution capability to support big data processing. As such, there is a strong demand to investigate the privacy of information and security challenges in both cloud computing and big data.

VI. BIG DATA TECHNICAL ISSUES AND CHALLENGES

A. *Fault Tolerance*: With the advent of technologies like cloud computing the aim must remain such that whenever failure occurs the damage done must occur within acceptable threshold rather than the entire work requiring to be redone. Fault-tolerant computing is tedious and requires extremely complex algorithms. A foolproof, cent percent reliable fault tolerant machine or software is simply a far-fetched idea. To reduce the probability of failure to an acceptable level we can do.

B. *Divide the entire computation to be done into tasks* and assign these tasks to different nodes for computation.

C. *Keep a node as a supervising node* and look over all the other assigned nodes as to whether they are working properly or not. If a glitch occurs the particular task is restarted. There are however certain scenario where the entire computation can't be divided into separate tasks as a task can be recursive in nature and requires the output of the previous computation to find the present result. These tasks can't be restated in case of an error. Here checkpoints are applied to keep the state of the system at certain intervals of time so that computation can restart from the last checkpoint so recorded.

D. *Data Heterogeneity***:** 80% of data in today's world are unstructured data. It encompassed almost every kind of data we produce on a daily basis like social media interaction, document sharing, fax transfers, emails, messages and a lot more. Working with unstructured data is inconvenient and expensive too. Converting these to structured data is unfeasible as well.

E. *Data Quality***:** As has been mentioned earlier, storage of big data is very expensive and there is always a tiff between business leaders and IT professionals regarding the amount of data the company or the organization is storing. The quality of data is an important factor to be looked into here. There is no point in storing very large data sets that are irrelevant as better result and conclusions can't be drawn from them. Ensuring whether the amount of data is enough for a particular conclusion to be drawn or whether the data is relevant at all are further queries.

F. *Scalability***:** The challenge in scalability of big data has led to cloud computing. It is capable of aggregating multiple different workloads with different performance goals into very large clusters. This needs high level of sharing of resources that is quite expensive and brings along with it various challenges like executing various jobs so that the goal of every workload is met successfully. It also has to deal with system failures in an efficient manner as it is quite common when working with large clusters. Hard disk drives being replaced by solid state drives and phase change technology do not have the same performance between sequential and random data transfer. The kind of storage device to be used is thus a large question looming around big data storage issue.

VII. BIG DATA PROCESSING ISSUES AND CHALLENGES

Effective processing of big data requires immense parallel processing and new analytics algorithms so as to provide rapid information. Often it may be unknown how to deal with a very large and varied volume of data and whether all of it needs to be analyzed. Challenges also include finding out data points that are really of importance and how to utilize the data to extract maximum benefit from it.

VIII. BIG DATA PRIVACY AND SECURITY ISSUES AND CHALLENGES

Often in big data analysis, the personal information of people from a database or from social networking sites need to be combined with external large data sets. Thus facts about anyone which might have been confidential become open to the world. Often it leads to taking insights in people's lives of which they are unaware of. Often it happens that a more educated person having better knowledge and concepts about big data analysis takes advantage of predictive analysis over a person who is less educated than him.

IX. CONCLUSION

Big data and cloud computing have been studied from several important aspects, and we have concluded that the relationship between them is complementary. Big data and cloud computing constitute an integrated model in the world of distributed network technology. The development of big data and their requirements is a factor that motivates service providers in the cloud for continuous development.

Cloud computing represents an environment of flexible distributed resources that uses high techniques in the processing and management of data and yet reduces the cost. All these characteristics show that cloud computing has an integrated relationship with big data. Both are moving towards rapid progress to keep pace with progress in technology requirements and users.

To handle big data and to work with it and obtaining benefits from it a branch of science has come up and is evolving, called Data Science. Data Science is the branch of science that deals with discovering knowledge from huge sets of data, mostly unstructured and semi structured, by virtue of data inference and exploration. It's a revolution that's changing the world and finds application across various industries like finance, retail, healthcare, manufacturing, sports and communication. As far as security is concerned the existing technologies are promising to evolve as newer vulnerabilities to big data arise and the need for securing them increases.

ACKNOWLEDGEMENT

I would like to thank Vidya Bharati Mahavidyalaya for providing full time internet service to do this research and development, for providing library facility also. I thank with high gratitude to my beloved colleagues for providing guidance to prepare this paper.

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New Man International Journal of Multidisciplinary Studies
(UGC Approved Journal No. 45886)
ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

Discrimination at working place

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What is Discrimination?

"Treating one or more members of a specified group unfairly as compared with other people. Discrimination may be illegal on the ground of sex, sexual orientation, race, religion, disability, or nationality." The term *discriminate* appeared in the early 17th century in the English language. "Discrimination" derives from Latin, where the verb *discrimire* means "to separate, to distinguish, to make a distinction". Discriminatory traditions, policies, ideas, practices and laws exist in many countries and institutions in every part of the world, including in territories where discrimination is generally looked down upon.

What is sex or gender discrimination?

Sex or gender discrimination is treating individuals differently in their employment specifically because an individual is a woman or a man. If you have been rejected for employment, fired, or otherwise harmed in employment because of your sex or gender, then you may have suffered sex or gender discrimination.

Discrimination in working places can be in different form. According to a survey made by TEAMLEASE, 48% of Indian has faced same kind of discrimination or the other discrimination at workplace. Most of the biases are based on Gender (25%), Age (22%) and Cast and Religion (18%).Amongst the cities employees in Delhi, Pune and Chennai faced the highest rate of discrimination, while employees in Ahmadabad faced the lowest amount of discrimination. While certain type of discrimination are illegal in India like equal remuneration, sexual harassment, discrimination due to pregnancy and disability.

Legal Protections: The Constitution of India has several provisions which grant certain fundamental rights to its citizen, which includes right to equality.

Article 14 guarantees Equality before Law.

Article 15 prohibits state from discrimination on the grounds of religion, race, caste, sex and place of birth.

Article 16 empowers the state to make reservations with respect to appointment for posts in favour of backward classes of citizens if in the opinion of state such classes are under-privileged.

However, these protections can only be opted when the discrimination has been made by the State or any Governmental bodies, including Government offices of both Central and State Governments. In case of discrimination on any of the grounds mentioned in Article 15, i.e., religion, race, caste, sex and place of birth by the Government through its policies, or regulations, or otherwise, including recruitment, promotions, transfers, demotions and removals, the affected person can file a writ before the concerned High Court of the State or the Supreme Court.

The Constitution further lays down certain fundamental duties, which though cannot be challenged before a Court of law; the duties should ideally be implemented by the Government. **Article 39** in part IV of the constitution urges state to ensure that citizens ,men and women equally have the right to an adequate means of livelihood, right to shelter ,food, education and work.

Below is a list of federal laws that prohibit discrimination based on gender in a number of settings.

- **Civil Rights Act of 1964: Title VII (Equal Employment Opportunities)** the Civil Rights Act of 1964 protects individuals against discrimination in many different areas. Title VII prohibits employee discrimination or harassment based on sex, race, color, religion, and national origin (including limited English proficiency).
- **The Equal Credit Opportunity Act** (ECOA) ECOA guarantees an equal opportunity to obtain credit and prohibits creditors from discriminating against credit applicants on the basis of sex, familial status, race, color, religion, national origin, age, or because an applicant receives income from a public assistance program.
- **Fair Housing Act** (FHA) The FHA prohibits discrimination in the sale, rental, and financing of housing based on sex, familial status, race, color, national origin, religion, and disability.
- **Equal Pay Act of 1963** (EPA) The EPA requires that employers pay all employees equally for equal work, regardless of whether the employees are male or female.
- **Family and Medical Leave Act** (FMLA) The FMLA gives employees the right to take time off

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ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

from work in order to care for a newborn (or recently adopted) child, or to look after an ill family member.

- **Pregnancy Discrimination Act** The Pregnancy Discrimination Act prohibits employment discrimination against female workers who are (or intend to become) pregnant - including discrimination in hiring, failure to promote, and wrongful termination.
- **Title IX of the Education Amendments of 1972** Title IX prohibits sex discrimination in education programs that receive federal funds, to increase educational and athletic opportunities for females in schools and colleges nationwide.
- **U.S. Code Title 42, Chapter 21 - Civil Rights** Title 42, Chapter 21 of the U.S. Code prohibits discrimination against persons based on gender, age, disability, race, national origin, and religion (among other things) in a number of settings including: education, employment, access to businesses and buildings, federal services, and more. Chapter 21 is where a number of federal acts related to civil rights have been codified including: the Civil Rights Act of 1866, Civil Rights Act of 1964, and the Civil Rights of Institutionalized Persons Act.

Conclusion: If we considering gender equality in all fields it is necessary to create work environment that discourage discrimination and encourage employees to treat each other with respect. There are many benefits to employers for creating a work environment free of discrimination and harassment such as a harmonious work environment, increased productivity, reduced absenteeism, decreased turnover, an environment of trust, collaboration and cooperation between employees and increased employee and customer/client satisfaction.

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MAH/MUL/03051/2012
ISSN-2319 9318

International Multilingual Research Journal

Vidyawarta®

Special Issue February-2018.

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श्री व्यंकटेश कला, वाणिज्य व विज्ञान महाविद्यालय

देऊळगाव राजा, जि.बुलडाणा. पिन-४४३ २०४.

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ISSN: 2319 9318

06

E-Commerce In India: "Role Of Online Payment System"

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Introduction:

In many respects, online payment is the foundation of systems for e-commerce. The ability to take payment distinguishes an e-commerce system. Must be sufficient to protect the system. From one that provides only advertising or other communications capabilities. Incorporating payment abilities, however, adds considerable complexity to a system first, the security of both the payment mechanism and the overall system must be sufficient to protect the system. Second, the system must provide a high degree of integrity for transactions the system must not lose or inadvertently change a payment transaction.

Online payment system is a back bone of e-commerce in India. All transaction depends on e-commerce in online payment system. Increasingly business potential timely and accurately captured and efficiently e-business data. Interchange, is the key to any business success.

In e-commerce, every transaction is done electronically due to this system is important in online payment system in India. Many types are available in e-commerce for online payment system and some models are available depend on e-commerce

1) Business to Business
2) Business to consumer.
3) Consumer to consumer
4) Business to Government

5) Government to Business

6) Government to Citizen.

This model depend on 92% and Government sector depend on 90% on online payment system. The Impact of e-commerce all sector due to consumer social and economical status up-lifment and consumer improve has living standard.

E-Commerce:

The word "Commerce" is the concept for electronic commerce or e-commerce, pertaining to the buying and selling of goods. While commercial "denotes business practice and activities intended to make profit E-commerce like any other business, deals, with the exchange of money for soft or hard goods and services.

In other words substantial commerce is a process of distribution of goods form the place where they are produced and found in plenty to a place where the goods are short supply or scarce and hence in demand. The concept of commerce is a very comprehensive and complex organism and includes all the necessary functions involved in buying and selling. It consists of all persons. Organizations and institutions engaged in the distribution of goods. They include railways, road transport, shipping, merchants, Bank, Insurance, Companies, brokers whole sellers, retailers, stock market, distributors, agents, service, providers etc.

E-commerce is a selling and transfer process requiring several institutes. It is a systematic and organized network for the exchange of goods between producers and consumer directly and in this the net embraces all those related activities which are indispensable for maintaining a continuous, free and uninterrupted distribution and transfer of goods.

Role of Electronic Payment System:

Electronic payment system is essential part of between consumer and Business. Traditional Commerce's in use cash but not use cash in e-commerce. Nevertheless now in India 65% transaction is depend on online payment system. The payment mechanism which constitutes the core of e-commerce process has become on important business strategy. It is simply because the payment mechanism has the potential to change the very essence of commercial transaction, business and industry models throughout the world. Payment processing system play a critical role in e-business and any company considering launching its business must have chalked out plans well in advance. It is strategic business needs.

There are a number of payment options available. They are broadly classified as offline payment option and online payment system.

1: Offline Payment System.

These systems mostly related to the conventional payment methods. Under this method An individual may use.

1)A phone

2. Drop a cheque in to the postal head box

3. Earn and we discounts

4. Bills

5. Drafts

6. Money order

7. Cash on delivery.

2. Online Payment System.

Doing business online is an innovative strategy and the payback or payment through the e-shop is one of the most critical and challenging issues for any such business. Haw to make payment for online buying is a frequently asked question.

Electronic Payment via the web is catching up gradually. Even today, many customers prefer using the traditional payment methods such as cash on delivery. This system divided in to three stages.

A) Bank and financial organization Payment:

1. Large scale on payment: Bank to Bank transfer

2. Small and medium scale on payment: Automated trailer machine (ATM) or by cash Payment.

B) Retail Payment:

1) Credit card

VOL-07

Special Issue March 2018

Vidyawarta®

International Multilingual Research Journal

MAH/MUL/03051/2012
ISSN-2319 9318

Jr.No.62759

Chief Editor
Prof. Virag Gawande

Published By
Aadhar Social Research Development Training Institute, Amravati.

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TO MEASURE THE IMPACT OF GLOBAL ECONOMIC RECESSION ON THE FINANCIAL PERFORMANCE OF SELECTED INDUSTRIES IN VIDARBHA

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ABSTRACT

The purpose of this research was to evaluate the changing dynamics during recession and recovery with reference to its effect on industry in Vidarbha.

The focus of empirical study has been on recession and to a lesser extent on recovery, and its impact on industry. Hardly any in-depth research on the critical evaluation of the changing dynamics during recession and recovery with reference to its effect on industry has been conducted in the Vidarbha context. A few of the doctoral studies have been completed on changing dynamics during recession and recovery in Vidarbha and even fewer have focused particularly on the changing dynamics during recession and recovery with reference to its effect on industry in Vidarbha.

INTRODUCTION

Due to substantial increase in financial globalization the recessionary cycles not only made deeper impact on the real economies of advanced countries, but doomed emerging market economies as well. As this crisis unfolded, credit markets appeared to be drying up in the developing economies along with the developed world. The Keynesian economics substantiates that demand-driven theories were at the root of recession as once panic and deflation set in, many people avoided further losses by keeping clear of the markets, resulting in falling investment & aggregate demand. On the other hand the monetarists believe that the recession started due to significant policy mistakes by monetary authorities especially the Federal Reserve's expansionary monetary policy and the Community Reinvestment Act. Along with it Government's inability to evaluate counter-party risk due to opaque financial statements and the unpredictable nature of government's response germinated the present crisis. The end result was internal as well as external instability in the economies of the world, that needs an appropriate use of Monetary and Fiscal Policy' to combat such situations. MUNDELL Model explains that 'internal balance in an economy is achieved by reducing inflation and unemployment to zero whereas external balance is achieved by reducing balance of payments deficits and surpluses to zero' through expansionary monetary policy and expansionary fiscal policy. Expansionary fiscal and monetary policies constitute expenditure increasing policy measures, whereas contractionary monetary and fiscal policies constitute expenditure reducing policy measures. To maintain internal balance as well as external balance during recession a mixed package of various fiscal & monetary measures used by the Government of India has been studied through this model in this study.

OVERVIEW OF ECONOMIC SITUATION

Theoretical work in earlier chapters is much in needed to calculate with current data enabling to understand the current situation of the World, nation, markets leading to the analysis of situation of the organisation and industry sectors.

Table no. 1

Effects of recession on loss of sales volume

Effect on Sales Volume	No.of Respondents	Percentage of Respondents
Least	18	11%
Somewhat	0	0%
Moderate	93	56%
Much	18	11%
More	37	22%
Total	166	100%

56% of the respondents reported a moderate loss of sales volumes,

11% reported some loss of sales and

11%of the respondents reported much loss of sales

22% reported more sales volume loss.

Table 2:

Effects of recession on loss of Customer / market share

Effect on market share	No.of Respondents	Percentage of Respondents
Least	73	44%
Somewhat	18	11%
Moderate	55	33%
Much	20	12%
More	0	0%
Total	166	100%

Some 44% of the interviewed respondents reported least loss of customer share or market share.

11% reported some loss of customer share.

11% of the respondents reported much loss of market share.

33% reported moderate market share loss.

None lost most or total market share.

Table 3 :

Effects of recession on other factors .-like Reduction in customer orders, extended Business Cycle, Market Competition, Price Competition, Extent of Sales Cost

Effect on other factors	No.of Respondents	Percentage of Respondents (out of 166)
Reduction in customer orders	73	44%
extended Business Cycle	18	11%
Market Competition	129	78%
Price Competition	166	100%
Extent of Sales Cost	73	44%

Only 44% of the respondents' companies lost the least number of customers or market share,

11% of the respondents reported to have been faced with the challenge extended Business Cycle

All 100% of the respondents reported to have been faced with the challenge of fierce price competition.

44% of the respondents reported to have been faced with the challenge of market competition.

78% of the respondents reported to have been faced with the challenge of extent of sales cost.

Table 4:

Strategies adopted for recovery purpose

Effect on other factors	No. of Respondents	Percentage of Respondents (out of 166)
Adjust company goals	166	100%
Asking support from Government	97	60%
Kept regular contact with Market	133	80%
Smart Management Techniques	166	100%
Used loyalty Programmes	116	70%

All of the representatives interviewed reported that their companies had adjusted their sales volumes down in response to the phenomenon.

60% devoted their efforts to ask support from government

80% reported that it was good to keep regular contact with market situation.

100% of the respondent reported to have improvised on use of their smart management

techniques.

In their endeavors to keep the customer base and market share, loyal customers, employees, supplies were rewarded, overall 70% of respondents claim to have used this strategy.

CONCLUSION

Many of the companies have had to make large scale organisational changes to deal with the impact of recession and have had to make changes (sometimes substantial) to their existing business strategies. They recognise that in the 'good times' prior to recession there was some degree of loss of focus on certain aspects of management and financial management but remedial action has been taken to alleviate these problems.

India has been hit by the global meltdown, it is clearly due to India's integration into the global economy. The strategy to counter these effects of the global crisis on the Indian economy. The strategy to counter these effects of the global crisis on the Indian economy and prevent the latter from any further collapse would require an effective departure from the dominant economic philosophy of the neo-liberalism.

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"AN ANALYTICAL STUDY OF GOVERNMENT SCHEMES FOR WOMEN EMPOWERMENT IN AMRAVATI DISTRICT"

Awarded to

P. G. Dammani and Dr. S.B.Kadu

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International Recognition Multidisciplinary Research Journal

Associated & Indexed by EBSCO, USA

ISSN 2249-894X

Impact Factor : 5.2331(UIF)

Review of Research

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Laxmi Book Publication

258/34, Raviwar Peth, Solapur-413005 Maharashtra India

Contact Detail: +91-0217-2372010 / 9595-359-435

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Website: www.lbp.world

Authorised Signature

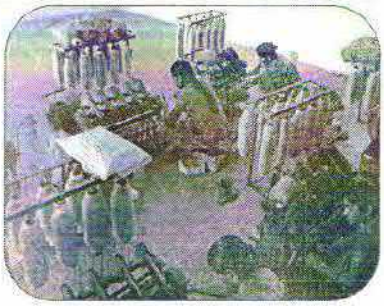
Ashok Yakkaldevi

Editor-in-Chief

IMPACT FACTOR : 5.2331(UIF) REVIEW OF RESEARCH UGC APPROVED JOURNAL NO. 48514 ISSN: 2249-894X

VOLUME - 7 | ISSUE - 7 | APRIL - 2018

"AN ANALYTICAL STUDY OF GOVERNMENT SCHEMES FOR WOMEN EMPOWERMENT IN AMRAVATI DISTRICT"



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ABSTRACT:

In the process of poverty eradication and reducing gender discrimination, the governments have been implementing various schemes and programmes providing ways and means towards women development and empowerment, SHG movement, one among such programmes which has been proved successful in fulfilling its objectives. However, it is felt that the other schemes and programmes do have their prominent part in the process of women development and empowerment and which are being successfully implemented. The present proposal is an attempt to develop conceptual clarity of the term empowerment delineating it with several other overlapping concepts of gender equality, social inclusion, powerful etc. and suggest and advocate an inclusive approach of policy measures whereby the Government working towards an empowerment approach develop ways enabling women themselves to critically review their own situation and participate in creating and shaping the society as agents of change and economically empowering themselves.

The participation of women is important to make a significant impact on their empowerment both in social and economical aspects therefore this study addresses impacts and problems of Economic empowerment of women through Government schemes in Amravati District of Maharashtra. The information required for the study has been collected from primary sources through structured questionnaire and personal interview and secondary sources. The research will be based on various statistical tools, techniques and methods such as collection, classification, tabulation, graphic presentation, percentages, averages, correlation and regression analysis etc. The researcher has also applied, wherever necessary and possible, tests of significance such as Chi-square Test for drawing inference and testing of hypothesis. Women participation through various government schemes have obviously created tremendous impact upon the life pattern and style of poor women and have empowered them at various levels not only as individuals but also as members of the family members of the community and the society as whole. The results of the study revealed that the Government schemes have had positive impact on both economic and social aspects of the beneficiaries.

KEYWORDS : *Government Schemes, Economic Empowerment, Empowerment of Women.*

1. INTRODUCTION:

Women are the part of our society but they have less authority. Society cannot be created without women contribution. Empowerment has many elements which depend upon and relate to each other i.e. economic, social, political and personal. Economic empowerment means to give woman her rights in the economy. Social empowerment means status of woman in the society should be equal to man by eliminating injustice and inequity. Women should have respectable value in the society. Political empowerment means

women should have seats in provincial and national assemblies and giving one woman right of one vote. Personal empowerment means women should have freedom in their personal matters. Women can change their status in the economy, and also of the societies and countries. Often contributions of women in the economy are ignored, and their work is underestimated.

Economic empowerment is thought to allow poor people to think beyond immediate daily survival and to exercise greater control over both their resources and life choices. For example, it enables households to make their own decisions around making investments in health and education, and taking risks in order to increase their income. There is also some evidence that economic empowerment can strengthen vulnerable groups' participation in the decision-making. For example, microfinance programmes have been shown to bolster women's influence within the household and marketplace. The evidence also suggests that economic power is often easily 'converted' into increased social status or decision-making power.

The literature on economic empowerment is vast, and a large part of this focuses on the economic empowerment of women - a key strategy in addressing gender inequality. More generally, the discourse on economic empowerment centers around four broad areas: a) the promotion of the assets of poor people; b) transformative forms of social protection; c) microfinance; and d) skills training.

In the words of ex. President Dr. A.P. J. Abdul Kalam, "Empowering women is a prerequisite for creating a good nation, when women are empowered, society with stability is assured". Empowerment of women is essential because their thoughts and value systems leads to the development of a good family, good society and ultimately a good nation.

In India women development has carved out a prominent figure in the development planning right from the dawn of independence. But the concept of women development has been changing. The welfare-oriented approach adopted in the First Plan continued till the end of the Fourth-Five Year Plan. During the Fifth Plan there was a shift from welfare to development approach. However, during the 6th plan (1980-85) a multi-disciplinary development approach emphasizing on women's health, education and employment was adopted. During the 7th plan, there was a paradigm shift of development approach to empowerment.

But despite all these constitutional safeguards and colossal investment on women development in India, women are lagging much behind than men, which can be visualized from the following analysis. It exhibits the role of women in different social activities. Thus, the researcher has therefore attempted to study the Analysis of government schemes in economic empowerment of women during the 10th and 11th Five Year plan with reference to Amravati district, Maharashtra.

2. IMPORTANCE & NEED OF STUDY:

Despite impressive contributions to the society, women in India have only secondary status in the society. They are generally under employed due to limited command over resources. Their position can be improved only by providing employment opportunities. The successful functioning of these enterprises provides economic independence to women.

Women are generally under employed due to their limited command over resources. Hence several programmes have been introduced by the central and state governments by recognizing that women empowerment is the best strategy for poverty alleviation and for ensuring gender equality.

Entrepreneurial development is also one of the important area majority countries has been focus upon as a part of over all Human Resource Development. It is well ascertained by policy makers across the countries that strategic development of an economy required equal participation and equal opportunities to all sectors and genders. Entrepreneurial development is one the significant factor for sustainable socio-economic development. Especially, development of women is inviting special significance because many small and medium firms are well operated through women and though it is less recognized. In order to ensure better support from various levels, it is necessary to understand, what are the motivational factors which influence women to become entrepreneurs? Contemporarily less research has been conducted in

rural and semi urban areas that give specific focus on women entrepreneurs' motivational factors and awareness regarding different employment schemes.

Hence it is necessary to explore what are the factors which influences the motivation of women and to what extend it influence their entrepreneurial aspirations? How rural women looks on entrepreneurial opportunities and what are their concerns to enter into such ventures? Are they conducive that the schemes provided by government for their empowerment will help economic growth & self-reliance? This particular research tries to understand the motivational factors, effectiveness of various government schemes for women which influence on entrepreneurial factors, and how it facilitate the educators and educational institutions to develop infrastructure, design programs and course ware, ensure training and development activities that in tune with the requirement of entrepreneurial education in rural and semi urban areas where small and medium scale industries are more located. Hence there is need to increase awareness about government schemes for self-employment and economic empowerment among women.

3. RESEARCH PROBLEM

Most of the Government schemes are executed effectively, as the statistics revealed. But it is noted that still major portion of the population, especially women are unaware about these policies and programmes. Hence the present study was conducted to look into the awareness and knowledge of women on these women empowerment schemes.

4. HYPOTHESIS OF THE STUDY

1. The role of government schemes in economic empowerment of women during 10^{th} and 11^{th} Five Year Plan is positive.
2. There is a positive impact of government schemes in economic empowerment of women with reference to their occupational activity during 10^{th} and 11^{th} Five Year Plan.
3. There is a positive impact of government schemes in economic empowerment of women with reference to their Expenditure Pattern during 10^{th} and 11^{th} Five Year Plan.
4. There is a positive impact of government schemes in economic empowerment of women with reference to their Educational Expenditure during 10^{th} and 11^{th} Five Year Plan.
5. The implementation of government schemes for economic empowerment of women during the 10^{th} and 11^{th} plan faces a number of problems and there is an urgent need of training the government officials as well as the women folk with a view to change their approaches and mindsets.

5. PROBABLE IMPLICATIONS:

1 When women's participation in the labor force grew fastest, the economy experienced the largest reduction in poverty rates.
2 When women farmers can access the resources they need, their production increases, making it less likely that their families are hungry and malnourished.
3 When women own property and earn money from it, they may have more bargaining power at home. This in turn can help reduce their vulnerability to domestic.
4. When women have access to time-saving technologies & Skill training programmes they increase their productivity as well as launch income-generating pursuits and entrepreneurial ventures. Those kinds of outcomes empower women to become stronger leaders and to more effectively contribute financially to their families, communities and countries.
5. Investing in women helps speed up the development of local economies and creates more equitable societies.
6. Increased income controlled by women gives them self confidence, which helps them obtain a voice and vote in for empowerment

7. Household decisions such as domestic well-being decisions as women tend to use income clout for more equitable decisions about sons and daughters' diet, education and health.
8. Economic empowerment makes conducive the Economic decisions of acquiring, allocating, and selling assets.
9. Increasing the role of women in the economy is part of the solution to the financial and economic crises and critical for economic resilience and growth.

6 REVIEW OF LITERATURE

According to Roy and Niranjan (2004), Empowerment is associated with indirect indicators like Education and work participation of women, and direct indicators of female autonomy (empowerment) such as decision-making, mobility and access to economic resources that can be viewed both as an outcome and a process.

According to Malhotra, Schuler & Boender 2002, Empowerment is a dynamic process. Separating the process into components (such as enabling factors, agency and outcomes)

According to Prahlad Kumar and Tinku Paul, Empowerment cannot be defined in terms of specific activities or end results because it involves a process whereby women can freely analyze, develop and voice their needs and interests, without them being pre-defined, or imposed from above.

According to Naila Kabeer, empowerment is "the expansion in people's ability to make strategic life choices in a context where this ability was previously denied to them." Empowerment cannot be reduced to a single aspect of process or outcome. Moreover, impacts on empowerment perceived by outsiders might not necessarily be those most valued by women themselves.

Dr.vasanthakumari (2012) in his study he recognized that by organizing poor women into groups, they not only expand options available to them for their development but also provide them with opportunities to develop their confidence and skills to improve their status and to bring about a change in the attitude of the society towards women.

According to Golla, A. M., Malhotra, A., Nanda, P. and Mehra, R., 2011 their paper provided an Understanding and Measuring of Women's Economic Empowerment with a framework to guide the design, implementation and evaluation of economic advancement programmes, schemes and various policies.

According to Kabeer, N., Mahmud, S. and Tasneem, S. 2011, in his paper 'Does Paid Work Provide a Pathway to Women's Empowerment?, describes combination of survey data and qualitative interviews to explore the impact of paid work on various indicators of women's empowerment, ranging from shifts in intra-household decision-making processes to women's participation in public life. It finds that forms of work that offer regular and relatively independent incomes hold the greatest transformative potential.

According to Reena , Rajdeep Kaur , Nikita who studies a Comparative Analysis of Women's Economic Empowerment through Self Help Groups to evaluate the level of Women's economic empowerment through SHG i.e. income, expenditure and saving of the member after joining SHG.

7 OBJECTIVES OF STUDY:

1. To present an overview of role, Functioning and Performance of government schemes in economic empowerment of women in India particularly with reference to Amravati District of Maharashtra State.
2. To study the awareness & effectiveness of Government schemes for economic empowerment of women
3. To study the socio-economic impact of economic empowerment of women through government schemes during the 10^{th} and 11^{th} Five Year Plan with special reference to Amravati district of Maharashtra.

4. To study the performance and impact of various government schemes with reference to economic empowerment of women during the 10th and 11th Five Year Plan with special reference to Amravati district of Maharashtra.
5. To study the problems of economic empowerment of women during the 10th and 11th Five Year Plan with special reference to Amravati district of Maharashtra.

8. RESEARCH METHODOLOGY:

The said study is based on primary as well as secondary data. Primary Data has been collected through well structured questionnaire and survey method wherein the questionnaire was distributed among 50 members of different Women Beneficiaries of various state and central Government schemes in Amravati district with the help of Stratified Random sampling technique as the selection of the sampler requires the separation of defined target population into different groups based on some strata like income groups (Low, Middle, high), rural & urban area, age, profile of beneficiaries, kind of employment etc., which represents the entire population. The secondary data is collected from various published sources such as published data of various government agencies, Research journals and periodicals, Newspapers; other sources etc. also will be used to support the conclusions. The major source of secondary data is the published annual reports of the sample banks under study.

9. LIMITATIONS OF STUDY:

1. The study will be limited to Amravati city. As such the finding of the study may not be totally applicable to other cities.
2. The study will be limited for empowerment of Women Beneficiaries of various Central and state Government schemes run in Amravati District.
3. Conclusions and suggestions are drawn on the basis of information provided by women beneficiaries only.
4. Sample size is of 50 only

10. DATA ANALYSIS AND INTERPRETATION:

The data after collection has been analyzed, arranged in tabular form followed by Analysis and Interpretation of data in a general way involves a number of closely related operations, which are performed with the purpose of summarizing the data that fulfill the research objective.

Table No. 1 Education-Wise Details of Women Beneficiaries:-

Sr. No.	Particulars	Responses	%
A	Upto SSC	21	46.6%
B	Under Graduate	18	36%
C	Graduate and Above	7	14%
D	Illiterate	4	08%
Total		50	100%

Table No.2 Age-wise Distribution of Women Beneficiaries

Sr.No.	Particulars	Responses	%
A	Below 30 years	15	30%
B	30-40 Years	24	48%
C	Above 40 years	11	22%
Total		50	100%

Table No.3 Income Group wise Classification of the Sample

Sr.No.	Particulars	Responses	%
1	Low Income Group	16	32.00
2	Medium Income Group	28	56.00
3	High Income Group	6	12.00
Total		50	100%

Table No .4 Utilization of Income wise Classification of the Sample

Sr.No.	Particulars	Responses	%
1	Household Expenses	23	46.00
2	Child's Education	12	24.00
3	Saving & Investment	7	14.00
4	Repayment of Loans	4	8.00
5	Medicinal Expenses.	4	8.00
Total		50	100%

Table No.5 Reasons of Working of Sample Respondents

Sr.No.	Particulars	Responses	%
1	Economic Empowerment	33	66.00
2	Use of Skills	12	24.00
3	Self-Identity	4	8.00
4	Other	1	2.00
Total		50	100%

Table No.6 Treatment Given by the Family of the Sample Respondents

Sr.No.	Particulars	Responses	%
1	Normal	10	20.00
2	Good	8	16.00
3	Force for Earning	20	40.00
4	Always Helping	7	14.00
5	Cruel	5	10.00
Total		50	100%

Table No.7 Sources of Capital of the Sample Respondents

Sr.No.	Particulars	Responses	%
1	Personal Savings	13	26.00
2	Friends & Relatives	18	36.00
3	Financial Institutions	37	74.00
4	Government Schemes	43	86.00
5	Sale of Personal Property	28	56.00
6	Money Lenders	23	46.00
Total		50	100%

Table No. 8 Financial Security Status of the Sample Respondents

Sr.No.	Particulars	Responses	%
1	Partly Secured	12	24.00
2	Fully Secured	28	56.00
3	Not Secured	10	20.00
Total		50	100%

Table No.9 Awareness of Government Schemes to the Sample Respondents

Sr.No.	Particulars	Responses	%
1	Partly Aware	9	18.00
2	Fully Aware	30	60.00
3	Not Aware	11	22.00
Total		50	100%

Table No.10 Participation in the Scheme by the Sample Respondents

Sr.No.	Particulars	Responses	%
1	MNREGA	13	26.00
2	NRLM-SGSY-SHG's Initiative	14	28.00
3	MAVIM-CAIM, Tejaswini	32	64.00
4	PMKVY	22	44.00
5	DDU-GKV Yojana	6	12.00
6	MSRLM-UMED	14	28.00
7	EDTP	14	28.00
8	DIC Loan Scheme	9	18.00
9	PMEGP/PMKY	12	24.00
10	Seed Money Scheme	12	24.00
11	Any Other	19	38.00
	Total	50	100.00

11. MAJOR FINDINGS

Following Are the Conclusions of the Present Study

1. It is concluded that, majority of the respondents are form low income group.
2. It is concluded that, Majority of the respondents are utilizing their income for household expenses
3. It is concluded that, majority of the respondents are working for Economic Empowerment.
4. It is concluded that, majority of the respondents have reported that the treatment given by their family is Force for Earning.
5. It is concluded that, majority of the respondents have reported that the source of capital is Government Schemes, whereas very few have reported that the source of capital is Personal Savings.
6. It is concluded that, majority of the respondents have reported that the financial security is fully secured.
7. It is concluded that, majority of the respondents have reported that they are fully aware of the government schemes.
8. It is concluded that, majority of the respondents have reported that they are participated in MAVIM-CAIM, TEJASWINI Scheme
9. It is concluded that, there is significant difference between the opinions of sample respondents before and after Government Schemes for Economic Empowerment of Women about
   i. The impact of Government Schemes for Economic Empowerment of Women on occupational activity.

ii. The impact of Government Schemes for Economic Empowerment of Women on expenditure pattern.
iii. The impact of Government Schemes for Economic Empowerment of Women on Health Care Expenditure.
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vi. The impact of Government Schemes for Economic Empowerment of Women on Social Status Expenses.
vii. The impact of Government Schemes for Economic Empowerment of Women on Expenses on Consumer Durables.

10. It is concluded that, out of the total 50 sample respondent majority of women beneficiaries have reported the problem of Following aspects:

i. Security Aspects
ii. Lack of training and Communication Skills
iii. Lack of Marketing Skills
iv. Negative social environment
v. Bureaucratic Lobby
vi. Changing nature of Government Schemes
vii. Lack of Knowledge

12. RECOMMENDATIONS

1. The state has to take lead action in the form of enabling policies, provision of resources for the establishment of support mechanism which can multiply and monitor the process and monitor the devolution of powers and responsibilities to local communities and the poor.
2. Social mobilisation and people's participation should be the key strategy of the government for poverty eradication. It should occupy the highest priority of the Government
3. The process of empowerment of women at the political level has already begun, but it needs to be carried forward into the social and economic spheres as well. Special emphasis would have to be placed on ensuring that control of social infrastructure in the public domain is vested in women and women's organisations;
4. The Government should formulate a "National Women's Empowerment Policy" by drawing various experts working in this field. Various interventions which are required at the macro and micro level should be worked out and suitable amendments can be carried out in existing laws, rules, regulations, procedures and Government orders which come in the way of poverty alleviation;
5. There is a need for more and better coordination between the Government and the NGOs working in this area. Both should be partners in development. The NGOs should not undertake specialized programmes which the Government is already undertaking eg., construction of houses, sanitary latrines, wasteland development etc. NGOs should concentrate on social mobilization. There should be a common set of guidelines for all the SHGs.
6. All the Government functionaries should be trained and sensitized on the processes involved in social mobilisation and community empowerment.
7. Continuous training, motivation and exposure of the community volunteers, network leaders, group leaders and members is required to sustain the groups. A fixed annual training calendar should be designed by identifying proper training centres and resource persons. NIRD and SIRDs should draw up exclusive training programmes for social mobilisation and community empowerment;
8. Banks and implementing agency should take steps to avoid under financing and for verification of assets periodically. This type of verification helps the misuse of funds by the beneficiaries;
9. While selecting the groups, preference may be given to those groups, in which the members have crossed the eligible age limit to secure government jobs;

10. The rate of interest. charged by commercial banks is considered very high therefore, it may be reduced for the benefit of the poor women entrepreneurs;
11. The major problems of raw material shortage, lack of common work-shed, irregular marketing etc., need to be solved for the steady growth and successful functioning of the units;
12. Rural industrial products, handicrafts by women should be promoted and supported by adequate marketing arrangements;
13. Encouragement of co-operative ventures will promote and secure greater female participation at all levels.
14. Amravati district is a area inhabited by *Adivasi* forest dwellers particularly the Melghat area is full of various issues and problems which need be taken cognizance. Efforts should be taken to remove the deep rooted ignorance and negative attitude regarding women's role. It is necessary to provide special centers in this area for training and information of the *Adivasi* women.

At present, the climate in India is ripe for promoting the economic status of women particularly in Amravati district of Maharashtra. It is widely believed that with the growth of education and communication, opening up of new employment opportunities, Indian women will move steadily towards more equal status with men. Thus, she should be treated with equality of opportunities and it is the sole responsibility of the government to protect her interests in the wake of liberalisation.

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Review of Research
UGC APPROVED
International Online Multidisciplinary Journal

Volume - 7 | Issue - 7 | April - 2018

5.2331(UIF) 2249-894X

"AN ANALYTICAL STUDY OF GOVERNMENT SCHEMES FOR WOMEN EMPOWERMENT IN AMRAVATI DISTRICT"

P. G. Dammani

P. G. Dammani

Assistant Professor, Department of Management, Vidyabharati Mahavidyalaya, Camp Road, Amravati, Maharashtra, India.

Abstract: In the process of poverty eradication and reducing gender discrimination, the governments have been implementing various schemes and

Editor - In - Chief - Ashok Yakkaldevi

VOL. 5 SPECIAL ISSUE 4 APRIL 2018 UGC Approved Journal No. 45886 ISSN: 2348-1390

NEWMAN

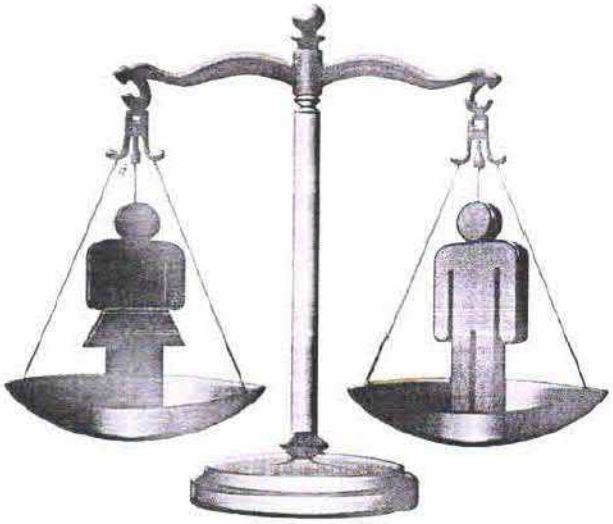
International Journal of Multidisciplinary Studies

A Refereed and Indexed Journal

SPECIAL ISSUE
on the Occasion of

National Conference on
Gender Isonomy: A Societal Onus-2018
(GISO-2018)

19th April 2018



Organized by

Pratibha Women's Studies Center,
Vidya Bharati Mahavidyalaya

C.K. Naidu Marg, Camp, Amravati - 444602, Maharashtra, India.

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Website: www.vbmv.ac.in

New Man International Journal of Multidisciplinary Studies
(UGC Approved Journal No. 45886)
ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

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Gender Inequality In Education

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Introduction: We proud Indians of 21st century rejoice in celebrations when a boy is born, and if it is a girl, a muted or no celebrations is the norm. Love for a male child is so much so that from the times immemorial we are killing our daughters at birth or before birth, and if, fortunately, she is not killed we find various ways to discriminate against her throughout her life. Though our religious beliefs make women a goddess but we fail to recognize her as a human being first; we worship goddesses but we exploit girls. We are a society of people with double-standards as far as our attitude towards women is concerned; our thoughts and preaching are different than our actions.

Definition And Concept Of Gender Inequality: 'Gender' is a socio-cultural term referring socially defined roles and behaviors assigned to 'males' and 'females' in a given society; whereas, the term 'sex' is a biological and physiological phenomenon which defines man and woman. In its social, historical and cultural aspects, gender is a function of power relationship between men and women where men are considered superior to women. Therefore, gender may be understood as a man-made concept, while 'sex' is natural or biological characteristics of human beings.

Gender Inequality, in simple words, may be defined as discrimination against women based on their sex. Women are traditionally considered by the society as weaker sex. She has been accorded a subordinate position to men. She is exploited, degraded, violated and discriminated both in our homes and in outside world. This peculiar type of discrimination against women is prevalent everywhere in the world and more so in Indian society.

Journey from Ancient to Present : In the ancient India women were held in high esteem and the the position of a woman in the Vedas and the Upanishads was that of a mother (maata) or goddess (Devi). In the Manusmriti, woman was considered as a precious being and in the early Vedic age, girls were looked after with care. Then practice of polygamy deteriorated the status of woman and in the medieval period, the practices of purdha system, dowry and sati came into being. With the passage of time, the status of woman was lowered. After the development of science and technology, female foeticide is being practiced on a large scale. This has led to a drop in the female ratio. And then dowry have become common and started female infanticide practices in few areas.

In many parts of India, women are viewed as an economic liability despite contribution in several ways to our society and economy. The crime graph against women is increasing at an alarming rate. The condition of an Indian widow is quite deplorable. At home, the woman's contribution towards home as a housewife is not recognized. Domestic Violence, Rape, Sexual Exploitation, molestation, eve-teasing, forced prostitution, sexual harassment at work places etc are a common affair today and in some cases its too tragic that it gets the global attention. The major reasons for this inequality are identified as the need of a male heir for the family, huge dowry, continued financial support to girl child, poverty, domestic violence, farming as major job for poor and the caste system.

Gender Inequality In India: Important Data: Global Indices: Gender Inequality is also reflected in India's poor ranking in various global gender indices.

- **UNDP's Gender Inequality Index- 2014:** India's ranking is 127 out of 152 countries in the List. This ranking is only above Afghanistan as far as SAARC countries are concerned.
- **World Economic Forum's Global Gender Gap Index- 2014:** India's ranks at 114 in the list of 142 countries of the world. This Index examines gender gap in four major areas:
- Economic participation and opportunity.
- Educational achievements.
- Health and life expectancy.
- Political empowerment.

India's position on these indicators was as follows:

- Economic participation and opportunity: **134th**
- Educational achievements: **126th**
- Health and Life expectancy: **141st**
- Political empowerment: **15th**

These two important Global Indices show the sorry state of affairs in India as far as gender equality is concerned. Only in case of 'Political Empowerment' India is doing fine which is a welcome sign. But other indices are very poor and a lot need to be done to improve the same.

Gender Inequality And Significance Of Education: Education is a gate way of all the values, sincerity, equality and character. It is a best weapon to fight all challenges related with human society. The gender inequality can be handled with the help of promoting gender equality through education. The school, classroom and teachers are all part and parcel of a society. In a society people are suffering from various problems related with gender such as gender discrimination, oppression, inequalities, biasedness and various other issues. Therefore, by keeping in mind to all these issues, government of India time to time has worked on the education for women equality and has launched various scheme as;-SarvaShikshaAbhiyan; Kasturba Gandhi BalikaVidyalya Scheme (KGBVS); District Primary Education Programme (DPEP); MahilaSamakhy a (MS);Mid-day Meal Scheme (MDMS); The Total Literacy Campaign (TLC); Non formal Education System etc. Moreover, in India gender equality issues in education have been studied for several decades. But, gender equality in education based on systematic research is necessary precondition forformulation of inclusive educational policies that would not leave out a single girl or boy. It is therefore important to gain insight into the overall situation of teachers as well as their behaviour and attitudes towards their pupils (NarayanraoandGingine: 2016).

Thus, the above mention scheme helps the girl children to access education on priority bases. With the help of education, genderequality in educational institutes can create awareness among the children, parents and other members of the community about their roles in future as the men and women in the society. Although, presently,gender has been accepted as a main category in the formulation of policy and curricula framework in India. Moreover, women and gender studies also becomes the main subject and a stream to study at higher level of education.

Gender Inequality And Educational Institutes: This is the responsibility of educational institutes to ensure that all the students should be sensitized to gender and learned to respect each-other without gender bias. Children in a school come from such types of societies where there is a male dominate societies. Usually father is head of the family; male child is given more freedom rather than girl child. There may be possibilities of gender discrimination within the school promises between peer groups or by teachers. Thus, with the help of educational institutes can create awareness towards gender equality in schools and make the children to understandable their roles for presentand future about as the men and women in the society. The main concern of educational institutes should be to increase the sensitivity of people at large towardswomen equality and their problems, so that students can develop right perception about women who have equal role, rights, status and significance in decision making at every field of life. Overall stereotypical image related with women should not be seen longer in the mind-set of men. Gender sensitization is first instance, tends to change the perception that men and women have equal to each other. Education institutes should also promote leadership qualities among the girls so that they can get strengthen to fight with every challenge in their life.

A comprehensive school programmes should be introduced that address to thegender issues and can make a constructive impact on the minds of the studentsregarding gender equality. The various co-curricular activities like discussion, seminar, plays, slogan writing, fancy dress competitions, elocution, debate,essay writing, story writing, poem writing, workshops and campaigns, clubs activates focus related issues on current women problems & gender sensitization issues & introduced self defence lessons etc. should be organized on the possiblethemes and related activities to promote gender sensitivity and also complementto co-existence of men and women.

As well as educational institutes shouldorganize some community based activities and programmes on gender equalitywithin the institutes and also outside of the institutes that involve the parents, stakeholders and teachers. Thus, both kinds of activities inside and outsideof institutes can play a significance role for gender equality. Moreover, the Education institutes should involve the media in sensitizing gender based issues sothe awareness can be created in among the masses. In the same line, Gingine andNarayanrao (2016), described that "gender sensitivity in early childhood education-equal encounter in nursery schools to plan and implement training for kin-dergarten professionals about equality education. The goal was the promote gender equality in the pedagogical work in finish speaking kindergartens throughresearch, education and engagement in the debates of educational policy."To sensitize the people towards gender, all of the educational institutes' administrations, teaching and other staff and also students should treat with dignity andequality to men and women both. The institutes should also arrange discussionson the all concerns related with female rights and their roles in the society duringthe parents' teacher meetings. Thus, if all educational institutes take care of theseactivities then gender inequality will not be an issue to think and work for along time. Moreover, this is the power of education that can make a great socialchange in the society at large. Presently, a gender and women study has become amain subject of study at higher level of education. It is also included in the syllabus of teacher education, so that pupil teacher can learn how to deal with issuesrelated with gender inequality in a smooth manner. Thus, all the possible concerns should be made by the educational institutions to promote the genderequality in education access, learning process and educational outcomes.

ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

Conclusion: India needs to deactivate the gender inequality. The needs of the day are trends where women are able notonly to break out of the culturally determined patterns of employment but also to offer advice about careerpossibilities that look beyond the traditional list of jobs. It is surprising that in spite of so many laws, womenstill continue to live under stress and strain. According to Barodia (2015) that "gender sensitization through education can be as a forceful, effective and primary tool to bringchange in the thought process of students through formal school education. Themain focus should be on breaking the stereotypes and set patriarchal notions prevalent in the society. The time has come for women to rise up and force the patriarchal society to underline the importance and necessity of the role played bywomen in cultivating a strong, rational and progressive society."To ensure equality of status for our women we still have miles to go.Man and Woman are like two wheels of a carriage. The life of one without the other is incomplete.

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New Man International Journal of Multidisciplinary Studies
(UGC Approved Journal No. 45886)
ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

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g) Promote basic and applied researches on Ecosystems and Biodiversity Conservation and help the institutions through guiding information to conserve ecosystems, biodiversity and mobilize its benefits.

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04

BIODIVERSITY IN BUSINESS AND ENTERPRISES

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Introduction

All companies can have an impact on biodiversity in the course of their business because they use natural resources, produce or consume products, own and manage areas of land, or finance other activities which have direct and indirect impacts. Biodiversity is recognized as being key in ensuring a stable environment for businesses to operate in. All business depends on biodiversity and ecosystem services, directly or indirectly; most businesses also have impacts on nature, positive or negative. Some business like forestry, fishing, agriculture, ecotourism, and pharmaceuticals are direct dependants whereas there are sectors which have a direct impact on ecosystems and biodiversity through their operations, such as mining, construction, and energy. In our country India, the lives and livelihoods of a large number of rural poor people is dependent on the sustainable use of biological resources. The business case for biodiversity management is strong and so are the challenges.

Dependence on Biodiversity and Ecosystem Services

The links between business, biodiversity and ecosystem services vary across sectors and even within sectors. These links depend on the location of the business, the source of its raw materials, in some cases the location of its

customers, and the production technology employed. Broadly, these links can be grouped into business impacts on biodiversity, on the one hand, and business dependence on ecosystem services on the other. In each case it is important to look beyond direct impacts and dependence, to consider the indirect links arising through business value chains. This section provides an overview and some concrete examples of business impacts and dependence on biodiversity and ecosystem services, across a range of sectors.

• **Agriculture**

The agriculture sector faces a growing dilemma: it needs to feed a rapidly growing and increasingly comfortable global population while also conserving biodiversity and sustainably managing natural resources on an increasingly exhausted planet. The need for increased food production is meanwhile constrained by poor land management and lack of means financial and technological to maintain let alone enhance productivity. Agriculture as a sector is the biggest land manager in the world and provides important habitats for many wild plant and animal species. At the same time, extensive land clearing for farming, and especially for large-scale intensive crop production and livestock, is one of the main drivers of biodiversity loss. Agricultural productivity is heavily dependent on numerous species and ecosystem services, including soil micro-organisms, natural and domesticated pollinators and pest predators, the genetic diversity of crops and livestock, as well as freshwater supplies, climate regulation and nutrient cycling.

• **Forestry**

Forest ecosystems are important habitats for many wild plant and animal species, and the forestry industry depends on numerous ecosystem services, including freshwater supply, climate regulation and nutrient cycling. Sustainable forest management has a large role to play in biodiversity conservation and mitigating climate change. On the latter point, not only do forests and wood products act as carbon sinks, but the main industrial outputs of the forest products industry timber and pulp are renewable if managed sustainably. In addition, compared to other common building materials like cement, steel and aluminum, wood-based building materials require less energy for production, have higher thermal efficiency, and can be reused, recycled, or used as bio-mass for energy. While forest loss is primarily driven by expanding agriculture, unsustainable commercial logging activities are nevertheless a significant contributor to forest and biodiversity loss around the world. Both legal and illegal logging activities can also indirectly affect biodiversity through the construction of logging roads habitat fragmentation, which can facilitate small-scale mining, hunting, illegal logging, fishing and settlement within previously untouched forests. The forestry industry, especially the pulp and paper sector, is relatively energy intensive. However, wood-based biomass is often used as a fuel that, if sourced from a sustainably managed forest, is carbon neutral or near carbon neutral. Overall, production processes in the forest products industry make a relatively small contribution to climate change.

• **Mining and Quarrying**

With the exception of supplies of freshwater for mineral processing, the mining industry is not directly dependent on biodiversity or ecosystem services. However, it has a number of significant direct and indirect impacts on BES which if ignored can create major risks to mining operations. One of the main direct impacts comes from surface mining, whereby overlying habitats and geological features are removed during the extraction of minerals. Other disturbances to plants and animals during the quarrying process include noise, dust, pollution and removal and storage of waste. While the

process of quarrying itself is mainly associated with negative impacts, a growing number of companies are beginning to use biodiversity offsets to compensate for residual impacts that cannot be mitigated onsite, while also investing in ecological restoration and rehabilitation on former mine sites.

The indirect impacts of mining on biodiversity and ecosystems include pollution and water used during refining and smelting processes. Mining operations can also have significant indirect impacts on biodiversity sensitive areas by developing roads that provide access to areas that were previously underdeveloped and inaccessible, leading to immigration and accelerated conversion of habitat.

• **Oil and Gas**

The oil and gas sector delivers a range of products to end-users, including fuel, electricity and derivatives of oil-like plastics and lubricants. Like the mining sector, most parts of the oil and gas sector are not directly dependent on biodiversity and ecosystems services except for supplies of freshwater. In terms of direct biodiversity impacts, the industry can be split between upstream exploration, production, downstream, marketing and distribution activities. The most obvious impacts on biodiversity are from upstream activities seismic studies, drilling, construction, production, maintenance and transportation. Although significant progress has been made to reduce these impacts, environmental gains have been overwhelmed by increased consumption and demand for energy, and increasing exploration and production in sensitive environments, such as deep water drilling, oil sands and the arctic. The industry also has significant indirect impacts on biodiversity due to the emission of greenhouse gases from upstream and downstream activities, and from the consumption of oil and gas products.

• **Cosmetics**

The cosmetics sector relies on biodiversity for many natural ingredients. As the variety of species and habitats continue to decline, both the quality and quantity of these natural ingredients may be jeopardized. This example illustrates that compensation for adverse environmental impacts is not only an important means for companies to maintain their license to operate, but can deliver overall improvements in ecosystem services with substantial economic benefits at modest expense. A renewed focus on natural ingredients is apparent throughout the food and cosmetics sectors. Consumer concerns about health and adoption of more 'wholesome' lifestyles are important market drivers, as affluent consumers are keen to buy products that enhance or are perceived to enhance their well-being.

• **Water Supply and Sanitation**

The water sector is highly dependent on ecosystems for sustainable and cost-effective operations. The quantity and quality of water depends on functioning aquatic ecosystems, including lakes, rivers, streams and wetlands, as well as local bio-physical processes and land-use practices. Ecosystem services important to water utilities include:

- Protection of water quality and quantity through the water cycle and hydrological processes throughout a catchment area
- Riparian vegetation filtering water, removing impurities and reducing erosion
- Catchment rehabilitation processes following natural events such as flood and fire Flood protection
- Assimilative capacity of large waterways and the ocean for waste water discharge and treatment
- Microbiological purification of wastewater
- Other ecosystem services associated with intact watershed catchments e.g., carbon sequestration, pollination, bio-banking and

biodiversity offset value, recreational and cultural values.

• **Transport**

Transport within business comprises specialist transport and logistics companies as well as distribution, logistics and transport departments within larger companies. Covering air, road, rail and sea transport, this sector is characterized more by its impacts on biodiversity than by its dependence on ecosystem services. Typical risks to biodiversity relate to transport infrastructure e.g. land take and pollution associated with developing and operating roads, ports and depots, incidents such as ship groundings on corals and oil spills, and operational externalities such as emissions of carbon and particulates.

• **Manufacturing**

The impacts of manufacturing industry on biodiversity are both direct and indirect, reflecting the footprint of facilities and the pollution arising from production processes, as well as the impacts of suppliers of raw materials or semi-finished goods.

• **Finance**

The impacts of the financial services industry on biodiversity are indirect but nevertheless can be very significant. While financial institutions are not directly dependent on ecosystem services, they are exposed to BES risks through the loans, investments and insurance cover they provide to companies and projects. The banking sector uses at least four strategies to manage biodiversity risks: 1) 'Red-lining' investments in areas of high biodiversity; 2) Developing sector guidelines for environmentaliy sensitive sectors; 3) Refraining from financing sectors in which a bank lacks specialist knowledge; and 4) Working together with borrowers to improve their environmental performance and mitigate harm through an engagement policy.

Conclusion

The conservation community should work to improve techniques for monitoring conservation outcomes of specific measures, and should remain vigilant about the quality of impact assessments and subsequent implementation of mitigation actions. The biodiversity and impact assessment community should seek opportunities to work with those companies within the private sector that are positioned to take action in integrating biodiversity into impact assessment practices and guidance. This can benefit the conservation community both by delivering conservation outcomes on the ground around the projects that develop under this improved planning process, and by gaining access to more and better information about the status and trends of biodiversity. At the same time, the biodiversity and impact assessment community should be looking to work with governments to establish stronger regulatory frameworks that require biodiversity to be integrated into all impact assessments, regardless of which company is implementing the project.

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Available Online at www.ijcsmc.com

International Journal of Computer Science and Mobile Computing

A Monthly Journal of Computer Science and Information Technology

ISSN 2320–088X
IMPACT FACTOR: 6.017

IJCSMC, Vol. 7, Issue. 2, February 2018, pg.33 – 41

An Empirical Study on 'CLOUD COMPUTING'

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Abstract: In the last few years there has been a rapid exponential increase in computer processing power, communication and data storage. But still many complex and computation intensive problems, which cannot be solved by supercomputers. In the field of computing, a lot of changes have been observed due to the increased use and popularity of the Internet and the availability of high-speed networks. Resource sharing in a pure plug and play model that dramatically simplifies infrastructure planning is the promise of "Cloud computing". Cloud computing[1] is the development of parallel computing, distributed computing, grid computing and virtualization technologies which define the shape of a new era. Cloud computing is an emerging model of business computing. The paper aims to provide a means of understanding the model and exploring options available for complementing your technology and infrastructure needs. Also explore some of the basics of cloud computing with the aim of introducing aspects such as: Realities and risks of the model, Components in the model, Characteristics and Usage of the model. This work aims to provide the ways to reduce security risk & also promotes the performance of cloud computing.

Keywords: Cloud computing, architecture, VM, SLA, SaaS, Paas, Iaas, daas, Cloud Service Provider, Cloud computing metaphor.

Introduction:-

The term "Cloud Computing"[2] is everywhere. Simply put, cloud computing is computing based on the Internet. In the past, people would run application or programs from software downloaded on a physical computer or server in their building. Cloud computing allows access from the same kinds of applications through the internet on a virtual server.

It is the new computing example which provides large pool of dynamical scalable and virtual resources as a service on demand. Cloud computing is a complete new technology. It is the development of parallel computing, distributed computing grid computing, and is the combination and evolution of Virtualization, Utility computing. The main principle of cloud computing representation is to offer computing, storage, and ***software as a service, (SaaS)****,*

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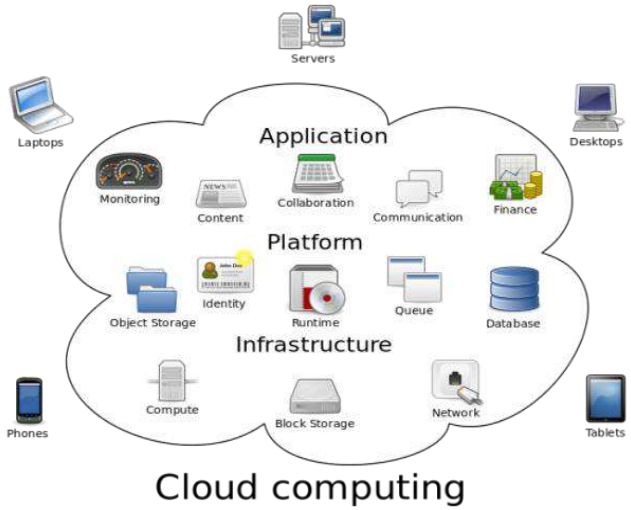
Platform as a Service (PaaS), ***Infrastructure as a Service (IaaS)***,) *or as a utility*, ***Data as a Service(Daas)***. *We just by using the need internet.*



Cloud computing metaphor: Cloud is a metaphor[9] to describe web as a space where computing has been preinstalled and exist as a service; data, operating systems, applications, storage and processing power exist on the web ready to be shared. The group of networked elements providing services need not be individually addressed or managed by users; instead, the entire provider-managed suite of hardware and software can be thought of as an amorphous cloud.

"Cloud is a parallel and distributed computing system consisting of a collection of inter-connected and virtualized computers based on service-level agreements (SLA) which established through cooperation between the service provider and consumers."

Cloud computing is a computing example, where a large pool of systems are connected in private or public networks which provide dynamically scalable infrastructure for application, data and file storage.

Cloud computing is a practical approach for to experience direct cost benefits and it has the potential to transform a data center from a capital-intensive set up.

The idea is based on a very fundamental principal of reusability of IT capabilities'. The difference is that to bring compared to traditional concepts of "grid computing", "distributed computing", "utility computing", or "autonomic computing".

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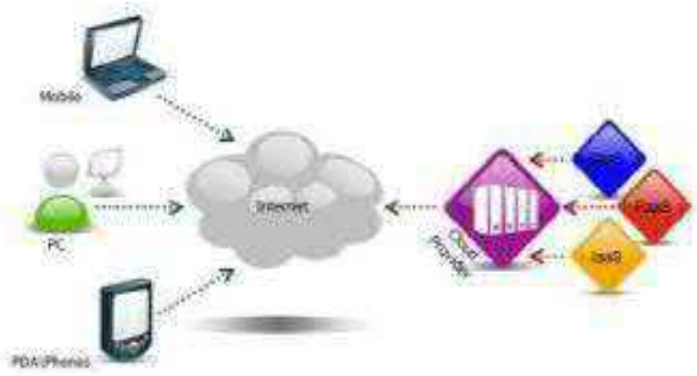
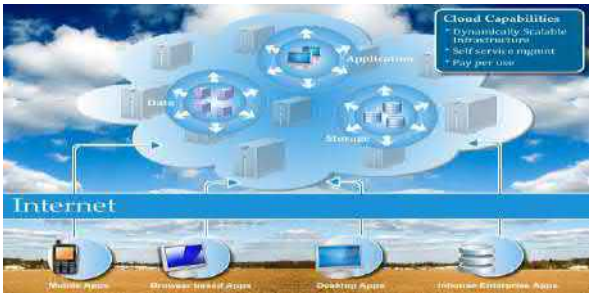


Fig. 1: Cloud computing concept

Fig. 1 shows [8] that how users can connect to the cloud services which are provided by cloud service provider by using any device over the internet. It includes scalable resources in storage, network, and compute & also contain virtualized infrastructure and provide that services to the users.

Forrester defines cloud computing as:

"A pool of abstracted, highly scalable, and managed compute infrastructure capable of hosting end-customer applications and billed by consumption."



It cuts the operational and capital costs and permits the IT departments to focus on strategic projects instead of keeping the datacenter running. It provides the services on Infrastructure level, Platform level, and Software level, many features such as speed, scalability of resources, parallel processing, to choose another technology at any time to further work like 24/7 availability of services, device and location independent and security etc. Cloud computing has five essential features such as rapid elasticity, measured services, on-demand self-service, resource pooling, and board network access. as shown in Fig. 2.

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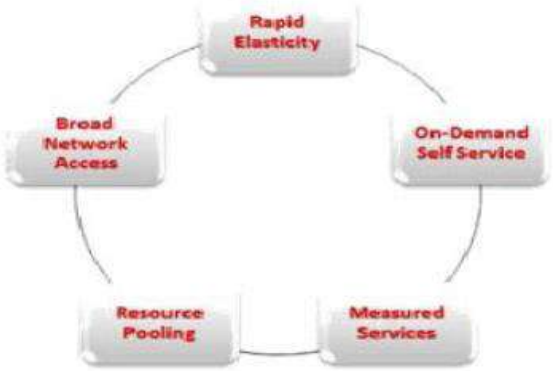

Fig. 2: Five features of cloud computing

Cloud Computing Models:

Cloud service Providers [4] following 4 types of Models:-

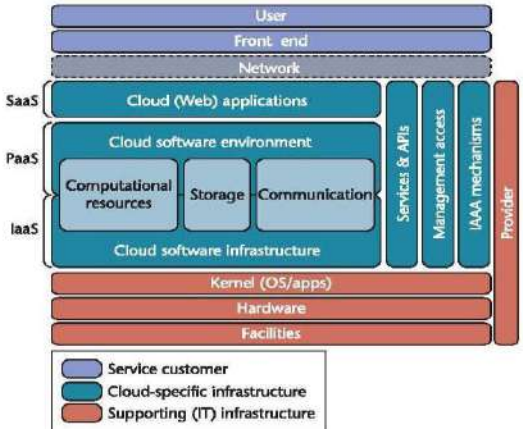

Fig.3: The Cloud reference architecture

Cloud reference architecture [11] that makes the most important security-relevant cloud components explicit and provides an abstract overview of cloud computing for security issue analysis.

1. ***Software as a Service (SaaS):*** *In this model,[12] a complete application is offered to the customer, as a service on demand. A single instance of the service runs on the cloud & multiple end users are serviced. Today SaaS is offered by companies such as Googlemail, Salesforce.com, Microsoft, Zoho, etc.*

2. ***Platform as a Service (Paas):*** *a layer of software or development environment is encapsulate & offered as a service, upon which other higher levels of service can be built. In this model the customer has the freedom to build his own applications, which run on the*

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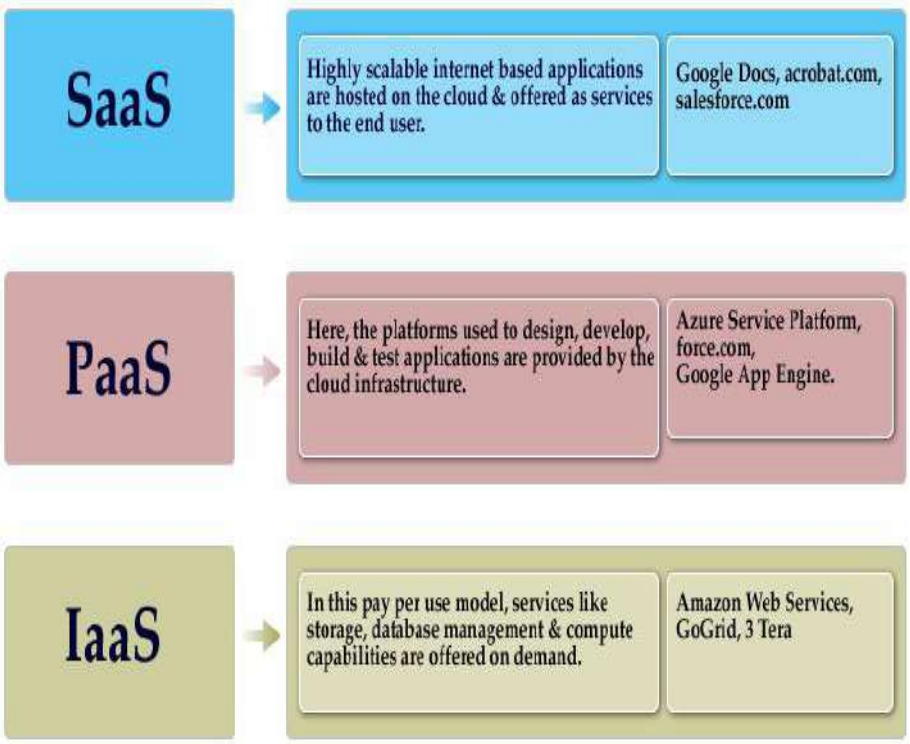
provider"s infrastructure. PaaS providers offer a predefined combination of OS and application servers, such as LAMP platform (Linux, Apache, MySql and PHP), classified J2EE, Ruby etc. Google's App Engine, Force.com, etc

3. ***Infrastructure as a Service (Iaas):*** *IaaS provides basic storage and computing capabilities as standardized services over the network. The basic strategy of virtualization is to set up independent virtual machines (VM) that are isolated from both the underlying hardware and other VMs. Servers, storage systems, networking equipment, data centre space etc. The customer would typically deploy his own software on the infrastructure. Some common examples are Amazon'EC2, GoGrid, 3 Tera, etc.*

4. ***Data as a Service (Daas):*** *Daas*
Delivery of virtualized storage on demand becomes a separate Cloud service - data storage service. Notice that DaaS could be seen as a special type IaaS. DaaS allows consumers to pay for what they are actually using rather than the site license for the entire database. In addition to traditional storage interfaces such as RDBMS and file systems.
Some common examples are Amazon S3, Google BigTable, and Apache HBase, etc.



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Public, Private & Hybrid Cloud:-

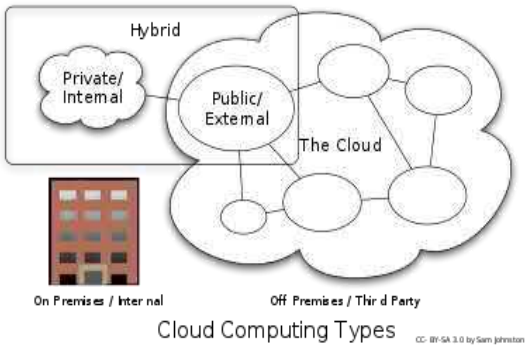

Fig. 3: cloud computing Types

Public Cloud

Public clouds are owned and operated by third parties; they deliver better economies of scale to customers, as the infrastructure costs are spread among a mix of users, giving each individual client an attractive low-cost, "Pay-as-you-go" model. One of the advantages of a Public cloud is that they may be larger than an enterprises cloud, thus providing the ability to scale seamlessly, on demand.

Private Cloud

Private clouds are built exclusively for a single enterprise. They aim of Private Cloud is to address concerns on data security.

There are two variations to a private cloud:-

*- **On-premise Private Cloud:** also known as internal clouds are hosted within one own data center.*

*- **Externally hosted Private Cloud:** This type of private cloud is hosted externally with a cloud provider.*

Hybrid Cloud

Hybrid Clouds combine both public and private cloud models.. The Hybrid cloud environment is capable of providing on-demand, externally provisioned scale.

Cloud Computing Characteristic:-

1: Dynamic computing infrastructure
2: IT service-centric approach
3: Self-service based usage model
4: Minimally or self-managed platform

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5: Consumption-based billing
6. Reduced Cost
7. Increased Storage
8. Flexibility
9. Data Protection
10 Data Recovery and Availability
11. Management Capabilities
12. Disaster Recovery
13. Automatic Software updates
14. Free Capital- expenditure
15. Work from anywhere
16. Document control
17. Security

Advantages of Cloud Computing

(1) Shared Resources:

it shares resources to provide the services to multiple users.

(2) Pay-As-You-Go:

Users only need to pay those resources which are used by them. They can demand for more resources if they required

(3) Better Hardware Management:

It is easy for cloud service provider (CSP)[4] to manage the hardware easily because all computers run the same hardware.

Area of Cloud Computing:

1. Banking

2. Insurance

3. Weather Forecasting

4. Space Exploration

5. Software as a service

6. Platform as a Service

7. Infrastructure- as -a-Service

8. Data-as-a-service

APPLICATIONS:-

There are a few applications of cloud computing [6] as follows:

1) Cloud computing provides dependable and secure data storage center.

2) Cloud computing can realize data sharing between different equipments.

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3) The cloud provides nearly infinite possibility for users to use the internet.

4) Cloud computing does not need high quality equipment for the user and it is easy to use.

Scope:-

Cloud computing is a tremendous innovation in the digital landscape that has changed the way IT solution are delivered and how end-users put them tom use. The cloud computing aspect is growing and will continue to do so.

Conclusion:-

Cloud computing is a new technology of computer network, providing the web services at lower cost comparing to normal technique. It contribute to improve the service in other related technologies like,

Grid Computing, Cluster Computing,

Utility Computing / Automatic Computing

Distributed Computing

With cloud computing, to the interface between service suppliers and multiple groups of service consumers. Cloud services will demand expertise in distributed services, procurement, risk assessment and service negotiation — these are the areas that many enterprises are only modestly equipped to handle.

Cloud Computing initiatives could affect the enterprises within two to three years as it has the potential to significantly change IT.

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IJIRR

International Journal of Information Research and Review
Vol. 05, Issue, 03, pp.5310-5313, March, 2018

REVIEW ARTICLE

A COMPREHENSIVE STUDY ON CLOUD COMPUTING

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ARTICLE INFO

Article History:

Received 25th December, 2017
Received in revised form
23rd January, 2018
Accepted 04th February, 2018
Published online 30th March, 2018

Keywords:

Cloud computing, architecture,
VM, SLA, SaaS, Paas, Iaas, daas,
Cloud Service Provider,
Cloud computing metaphor.

ABSTRACT

In the last few years there has been a rapid exponential increase in computer processing power, communication and data storage. But still many complex and computation intensive problems, which cannot be solved by supercomputers. In the field of computing, a lot of changes have been observed due to the increased use and popularity of the Internet and the availability of high-speed networks.

Resource sharing in a pure plug and play model that dramatically simplifies infrastructure planning is the promise of "Cloud computing". Cloud computing (1) is the development of parallel computing, distributed computing, grid computing and virtualization technologies which define the shape of a new era. Cloud computing is an emerging model of business computing. The paper aims to provide a means of understanding the model and exploring options available for complementing your technology and infrastructure needs. Also explore some of the basics of cloud computing with the aim of introducing aspects such as: Realities and risks of the model Components in the model and Characteristics and Usage of the model. This work aims to provide the ways to reduce security risk & also promotes the performance of cloud computing.

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INTRODUCTION

The term "Cloud Computing" (https://en.wikipedia.org /wiki/Cloud_computing) is everywhere. Simply put, cloud computing is computing based on the Internet. In the past, people would run application or programs from software downloaded on a physical computer or server in their building. Cloud computing allows access from the same kinds of applications through the internet on a virtual server. It is the new computing example which provides large pool of dynamical scalable and virtual resources as a service on demand. Cloud computing is a complete new technology. It is the development of parallel computing, distributed computing grid computing, and is the combination and evolution of Virtualization, Utility computing. The main principle of cloud computing representation is to offer computing, storage, and software as a service, (SaaS), Platform as a Service (PaaS), Infrastructure as a Service (IaaS),) or as a utility, Data as a Service (Daas). We just by using the need internet. Cloud computing metaphor: Cloud is a metaphor (http: //en.wikipedia. org/wiki/Cloud_computing#/media/File:Cloud_computing.svg) to describe web as a space where computing has been pre installed and exist as a service; data, operating systems, applications, storage and processing power exist on the web ready to be shared. The group of networked elements providing services need not be individually addressed or managed by users; instead, the entire provider-managed suite of hardware and software can be thought of as an amorphous cloud. "Cloud is a parallel and distributed computing system consisting of a collection of inter-connected and virtualized computers based on service-level agreements (SLA) which established through cooperation between the service provider and consumers." Cloud computing is a computing example, where a large pool of systems are connected in private or public networks which provide dynamically scalable infrastructure for application, data and file storage. Cloud computing is a practical approach for to experience direct cost benefits and it has the potential to transform a data center from a capital-intensive set up. The idea is based on a very fundamental principal of reusability of IT capabilities'. The difference is that to bring compared to traditional concepts of "grid computing", "distributed computing", "utility computing", or "autonomic computing". Fig. 1 shows (Jadeja Yashpal Singh and Modi Kirit, 2012) that how users can connect to the cloud services which are provided by cloud service provider by using any device over the internet. It includes scalable resources in storage, network, and compute & also contain virtualized infrastructure and provide that services to the users.

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Department of MCA, Vidya Bharati Mahavidyalaya, SGB University, Amravati, India.

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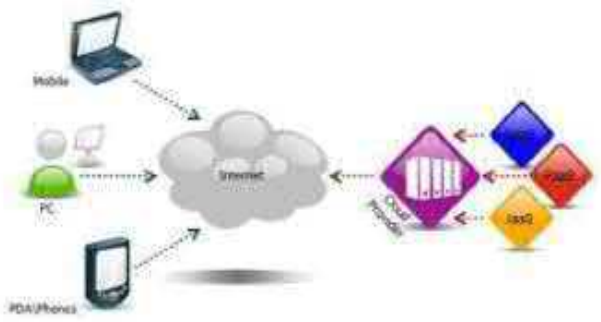
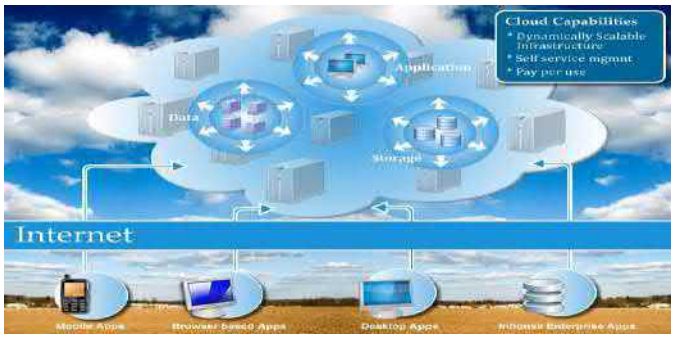


Fig. 1. Cloud computing concept



Conceptual View of Cloud Computing

It cuts the operational and capital costs and permits the IT departments to focus on strategic projects instead of keeping the datacenter running. It provides the services on Infrastructure level, Platform level, and Software level, many features such as speed, scalability of resources, parallel processing, to choose another technology at any time to further work like 24/7 availability of services, device and location independent and security etc. Cloud computing has five essential features such as rapid elasticity, measured services, on-demand self-service, resource pooling, and board network access. as shown in Fig. 2.

Fig. 2. Five features of cloud computing

Cloud Computing Models

Cloud service Providers (4) following 4 types of Models

Cloud reference architecture (Grobauer *et al*., 2011) that makes the most important security-relevant cloud components explicit and provides an abstract overview of cloud computing for security issue analysis.

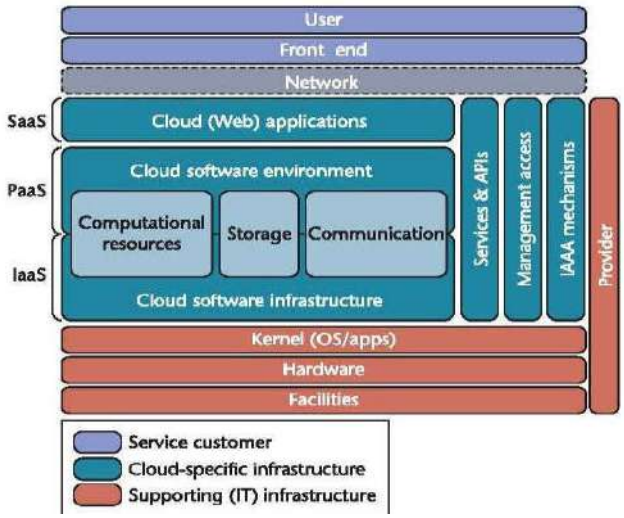


Fig. 3. The Cloud reference architecture

- Software as a Service (SaaS): In this model, (https://en.wikipedia.org/wiki/software_as) a complete application is offered to the customer, as a service on demand. A single instance of the service runs on the cloud & multiple end users are serviced. Today SaaS is offered by companies such as Googlemail, Salesforce.com, Microsoft, Zoho, etc.
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- Data as a Service (Daas): Daas Delivery of virtualized storage on demand becomes a separate Cloud service - data storage service. Notice that DaaS could be seen as a special type IaaS. DaaS allows consumers to pay for what they are actually using rather than the site license for the entire database. In addition to traditional storage interfaces such as RDBMS and file systems.

Some common examples are Amazon S3, Google BigTable, and Apache HBase, etc.

Public, Private and Hybrid Cloud

Public Cloud

Public clouds are owned and operated by third parties; they deliver better economies of scale to customers, as the

infrastructure costs are spread among a mix of users, giving each individual client an attractive low-cost, "Pay-as-you-go" model. One of the advantages of a Public cloud is that they may be larger than an enterprises cloud, thus providing the ability to scale seamlessly, on demand.

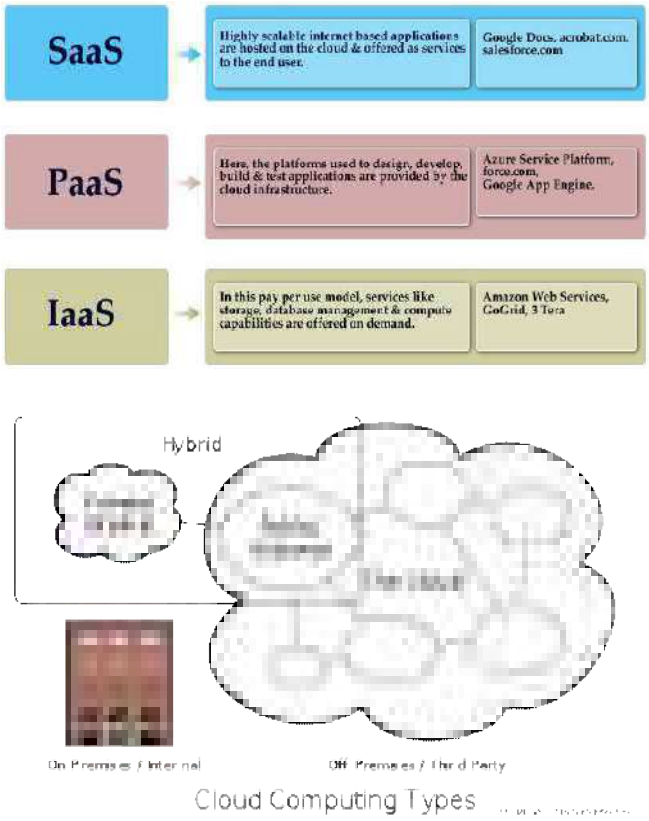

Fig. 4. Cloud computing Types

Private Cloud

Private clouds are built exclusively for a single enterprise. They aim of Private Cloud is to address concerns on data security.

There are two variations to a private cloud

- On-premise Private Cloud: also known as internal clouds are hosted within one own data center.
- Externally hosted Private Cloud: This type of private cloud is hosted externally with a cloud provider.

Hybrid Cloud

Hybrid Clouds combine both public and private cloud models. The Hybrid cloud environment is capable of providing on-demand, externally provisioned scale.

Cloud Computing Characteristic

1: Dynamic computing infrastructure
2: IT service-centric approach
3: Self-service based usage model
4: Minimally or self-managed platform
5: Consumption-based billing
6. Reduced Cost
7. Increased Storage
8. Flexibility
9. Data Protection
10 Data Recovery and Availability
11. Management Capabilities
12. Disaster Recovery
13. Automatic Software updates
14. Free Capital- expenditure
15. Work from anywhere
16. Document control
17. Security

Advantages of Cloud Computing

Shared Resources: It shares resources to provide the services to multiple users.

Pay-As-You-Go: Users only need to pay those resources which are used by them. They can demand for more resources if they required

Better Hardware Management: It is easy for cloud service provider (CSP) (4) to manage the hardware easily because all computers run the same hardware.

Area of Cloud Computing

- Banking
- Insurance
- Weather Forecasting
- Space Exploration
- Software as a service
- Platform as a Service
- Infrastructure- as -a-Service
- Data-as-a-service

Applications

There are a few applications of cloud computing (Zhang *et al.*, 2010) as follows

- Cloud computing provides dependable and secure data storage center.
- Cloud computing can realize data sharing between different equipments.
- The cloud provides nearly infinite possibility for users to use the internet.
- Cloud computing does not need high quality equipment for the user and it is easy to use.

Scope

Cloud computing is a tremendous innovation in the digital landscape that has changed the way IT solution are delivered and how end-users put them tom use. The cloud computing aspect is growing and will continue to do so.

Conclusion

Cloud computing is a new technology of computer network, providing the web services at lower cost comparing to normal technique. It contribute to improve the service in other related technologies like, Grid Computing, Cluster Computing, Utility

Computing / Automatic Computing Distributed Computing With cloud computing, to the interface between service suppliers and multiple groups of service consumers. Cloud services will demand expertise in distributed services, procurement, risk assessment and service negotiation — these are the areas that many enterprises are only modestly equipped to handle. Cloud Computing initiatives could affect the enterprises within two to three years as it has the potential to significantly change IT.

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Aayushi International Interdisciplinary Research Journal (AIIRJ)
ISSN 2349-638x Impact Factor 4.574 Special Issue No. 25
UGC Approved Sr.No.64259 **Website :-** www.aiirjournal.com **Email id:-** aiirjpramod@gmail.com

THE CONCEPT OF 'CLOUD COMPUTING'

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ABSTRACT

In the field of computing, a lot of changes have been observed due to the increased use and popularity of the Internet and the availability of high-speed networks.
Resource sharing in a pure plug and play model that dramatically simplifies infrastructure planning is the promise of "Cloud computing".
Cloud computing is becoming an increasingly popular enterprise model in which computing resources are made available on-demand to the user as needed.
Cloud computing[1] is the development of parallel computing, distributed computing, grid computing and virtualization technologies which define the shape of a new era. Cloud computing is an emerging model of business computing.
The paper aims to provide a means of understanding the model and exploring options available for complementing your technology and infrastructure needs. Also explore some of the basics of cloud computing with the aim of introducing aspects such as:
Realities and risks of the model
Components in the model
Characteristics and Usage of the model.
This work aims to provide the ways to reduce security risk & also promotes the performance of cloud computing

Keywords: *Cloud computing, architecture, Cloud systems, SLA, SaaS, Paas, Iaas, daas, Cloud Service Provider, Cloud computing metaphor.*

INTRODUCTION

The term "Cloud Computing" [2] is everywhere. Simply put, cloud computing is computing based on the Internet. In the past, people would run application or programs from software downloaded on a physical computer or server in their building. Cloud computing allows access from the same kinds of applications through the internet on a virtual server.
It is the new computing example which provides large pool of dynamical scalable and virtual resources as a service on demand. Cloud computing is a complete new technology. It is the development of parallel computing, distributed computing
grid computing, and is the combination and evolution of Virtualization, Utility computing. The main principle of cloud computing representation is to offer computing, storage, and software as a service,(SaaS), Platform as a Service (PaaS), Infrastructure as a Service (IaaS),) or as a utility, Data as a Service(Daas). We just by using the need internet.

Cloud computing metaphor: Cloud is a metaphor[9] to describe web as a space where computing has been pre installed and exist as a service; data, operating systems, applications, storage and processing power exist on the web ready to be shared. the group of networked elements providing services need not be individually addressed or managed by users; instead, the entire provider-managed suite of hardware and software can be thought of as an amorphous cloud.

"Cloud is a parallel and distributed computing system consisting of a collection of inter-connected and virtualized computers based on service-level agreements (SLA) which established through cooperation between the service provider and consumers."

Cloud computing is a computing example, where a large pool of systems are connected in private or public networks which provide dynamically scalable infrastructure for application, data and file storage.

Cloud computing is a practical approach for to experience direct cost benefits and it has the potential to transform a data center from a capital-intensive set up.

The idea is based on a very fundamental principal of reusability of IT capabilities'. The difference is that to bring compared to traditional concepts of "grid computing", "distributed computing", "utility computing", or "autonomic computing".

Fig. 1: Cloud computing concept

Fig. 1 shows [8] that how users can connect to the cloud services which are provided by cloud service provider by using any device over the internet. It includes scalable resources in storage, network, and compute & also contain virtualized infrastructure and provide that services to the users.

Forrester defines cloud computing as:

"A pool of abstracted, highly scalable, and managed compute infrastructure capable of hosting end-customer
applications and billed by consumption."

It cuts the operational and capital costs and permits the IT departments to focus on strategic projects instead of keeping the datacenter running. It provides the services on Infrastructure level, Platform level, and Software level, many features such as speed, scalability of resources, parallel processing, to choose another technology at any time to further work like 24/7 availability of services, device and location independent and security etc. Cloud computing has five essential features such as rapid elasticity, measured services, on-demand self-service, resource pooling, and board network access. as shown in Fig. 2.

Fig. 2: Five features of cloud computing

CLOUD COMPUTING MODELS

Cloud service Providers [4] following 4 types of Models:-

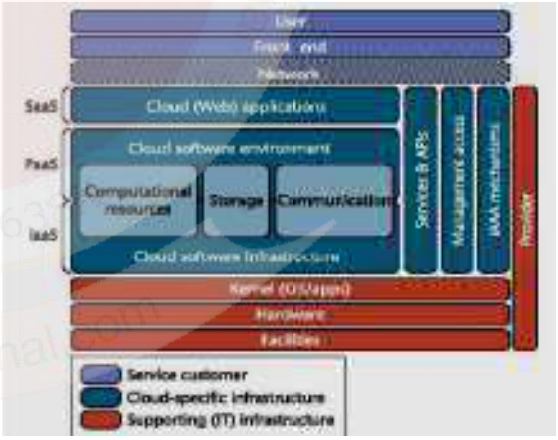

Fig.3: The Cloud reference architecture

Cloud reference architecture [11] that makes the most important security-relevant cloud components explicit and provides an abstract overview of cloud computing for security issue analysis.

1. Software as a Service (SaaS): In this model,[12] a complete application is offered to the customer, as a service on demand. A single instance of the service runs on the cloud & multiple end users are serviced. Today SaaS is offered by companies

such as Googlemail, Salesforce.com, Microsoft, Zoho, etc.

2. Platform as a Service (Paas): a layer of software or development environment is encapsulate & offered as a service, upon which other higher levels of service can be built. In this model The customer has the freedom to build his own applications, which run on the provider"s infrastructure. PaaS providers offer a predefined combination of OS and application servers, such as LAMP platform (Linux, Apache, MySql and PHP), classified J2EE, Ruby etc. Google's App Engine, Force.com, etc

3. Infrastructure as a Service (Iaas): IaaS provides basic storage and computing capabilities as standardized services over the network. The basic strategy of virtualization is to set up independent virtual machines (VM) that are isolated from both the underlying hardware and other VMs. Servers, storage systems, networking equipment, data centre space etc. The customer would typically deploy his own software on the infrastructure. Some common examples are Amazon'EC2, GoGrid, 3 Tera, etc.

DATA AS A SERVICE (DAAS): DAAS

Delivery of virtualized storage on demand becomes a separate Cloud service - data storage service. Notice that DaaS could be seen as a special type IaaS. DaaS allows consumers to pay for what they are actually using rather than the site license for the entire database. In addition to traditional storage interfaces such as RDBMS and file systems.

Some common examples are Amazon S3, Google BigTable, and Apache HBase, etc.

Public, Private & Hybrid Cloud:-

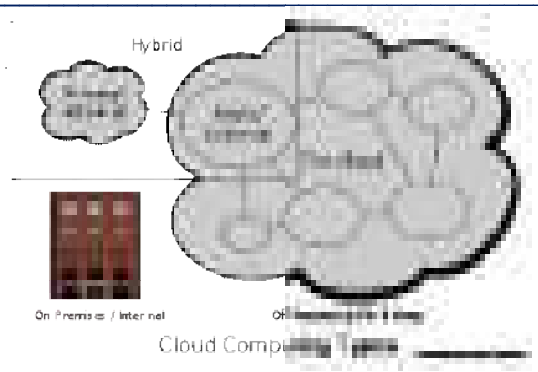

Fig. 3: Types of Cloud Deployment Model

Public Cloud

Public clouds are owned and operated by third parties; they deliver better economies of scale to customers, as the infrastructure costs are spread among a mix of users, giving each individual client an attractive low-cost, "Pay-as-you-go" model. One of the advantages of a Public cloud is that they may be larger than an enterprises cloud, thus providing the ability to scale seamlessly, on demand.

Private Cloud

Private clouds are built exclusively for a single enterprise. They aim of Private Cloud is to address concerns on data security.

There are two variations to a private cloud:-

- On-premise Private Cloud: also known as internal clouds are hosted within one own data center.
- Externally hosted Private Cloud: This type of private cloud is hosted externally with a cloud provider.

Hybrid Cloud

Hybrid Clouds combine both public and private cloud models.. The Hybrid cloud environment is capable of providing on-demand, externally provisioned scale.

Cloud Computing Characteristic:-

1: Dynamic computing infrastructure
2: IT service-centric approach
3: Self-service based usage model
4: Minimally or self-managed platform
5: Consumption-based billing
6. Reduced Cost
7. Increased Storage
8. Flexibility
9. Data Protection
10 Data Recovery and Availability
11. Management Capabilities
12. Disaster Recovery
13. Automatic Software updates
14. Free Capital- expenditure
15. Work from anywhere

16. Document control
17. Security

ADVANTAGES OF CLOUD COMPUTING

(1) Shared Resources:
it shares resources to provide the services to multiple users.

(2) Pay-As-You-Go:
Users only need to pay those resources which are used by them. They can demand for more resources if they required

(3) Better Hardware Management:
It is easy for cloud service provider (CSP)[4] to manage the hardware easily because all computers run the same hardware.

Area of Cloud Computing:
1. Banking
2. Insurance
3. Weather Forecasting
4. Space Exploration
5. Software as a service
6. Platform as a Service
7. Infrastructure- as -a-Service
8. Data-as-a-service

MOTIVATING FACTORS AND CHALLENGES

Cloud systems [15] are not just another form of supply provisioning transportation and in fact, have multiple opportunities from the principles for cloud infrastructures that will enable further types of applications, compact development and provisioning time of different services.

APPLICATIONS

There are a few applications of cloud computing [6] as follows:
1) Cloud computing provides dependable and secure data storage center.
2) Cloud computing can realize data sharing between different equipments.
3) The cloud provides nearly infinite possibility for users to use the internet.
4) Cloud computing does not need high quality equipment for the user and it is easy to use.
Scope:-
Cloud computing is a tremendous innovation in the digital landscape that has changed the way IT solution are delivered and how end-users put them tom use. The cloud computing aspect is growing and will continue to do so.

CONCLUSION

Cloud computing is a new technology of computer network, providing the web services at lower cost comparing to normal technique. It contribute to improve the service in other related technologies like,
Grid Computing, Cluster Computing,
Utility Computing / Automatic Computing
Distributed Computing
With cloud computing, to the interface between service suppliers and multiple groups of service consumers. Cloud services will demand expertise in distributed services, procurement, risk assessment and service negotiation — these are the areas that many enterprises are only modestly equipped to handle.

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Aayushi International Interdisciplinary Research Journal (AIIRJ)
ISSN 2349-638x Impact Factor 4.574 Special Issue No. 25
UGC Approved Sr.No.64259 **Website :-** www.aiirjournal.com **Email id:-** aiirjpramod@gmail.com

FIDOOP ALGORITHM : DATA HIERARCHY AND PARALLEL MINING OF FREQUENT ITEMSETS USING MAP REDUCE

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ABSTRACT

In Existing parallel mining algorithms are deficient in some of the features like parallelization of sequential code, distribution of data over computers in a cluster and balancing load over cluster of computers. To overcome these problems, FIDoop uses parallel mining algorithms on the basis of I/O overhead, data distribution, storage, scalability, load balancing, automatic parallelization and fault tolerance. FiDoop algorithm uses the ultrametric tree pattern for storage of data. This technique incorporates three MapReduce job to mine the large amount of data conventionally and economically.
In first MapReduce job , it minimizes I/O overhead by scanning the database twice ,all frequent itemsets are discovered.
In second MapReduce job is FIU-tree an improved way to partition a database, which results from clustering transactions, and significantly reduces the search space, it removes infrequent itemstes.
Third MapReduce is most important, it construct small ultrametric trees which is helpful to mine the frequent data conventionally and economically which significantly reduces computing time.
FiDoop algorithm is implemented in Hadoop cluster. For high dimensional data, FiDoop-HD is used, it is an improved version of FiDoop. FiDoop using FIUT and Map Reduce programming model

Key words: *Automatic parallelization, Scalability , Frequent item sets, frequent items ultrametric tree (FUIT), Map Reduce, FiDoop,load balance.*

INTRODUCTION

The existing mining algorithm lacks in some areas like it is expensive to mine the required data, the time required to mine the data is more, it require more storage while processing the data. The existing system uses the FIUT(frequent itemset ultrametric tree), but it lacks some of the features like parallelizing the data. To overcome this problem FiDoop algorithm is introduced.
FiDoop algorithm overcomes these problems. In FiDoop algorithm the data is decomposed and with the help of ultrametric tree the data is stored. With ultrametric tree we can mine our data or we can FIU-tree is a tree structure constructed as follows, the FIU-tree to enhance the efficiency of mining frequent itemsets.
After the root is labeled as null, an itemset p1, p2, . . . , pm of frequent items is inserted as a path connected by edges (p1, p2), (p2, p3), . . . , (pm−1, pm) without repeating nodes, beginning with child p1 of the root and ending with leaf pm in the tree. An FIU-tree is constructed by inserting all itemsets as its paths, each itemset contains the same number of frequent items. Thus, all of the FIU-tree leaves are identical height. Each leaf in the FIU-tree is composed of two fields: named item-name and count. The count of an item-name is the number of transactions containing the itemset that is the sequence in a path ending with the item name. Non leaf nodes in the FIU-tree contains two fields: named item-name and node-link. A node-link is a pointer linking to child nodes in the FIU-tree.
The FIUT algorithm consists of two key phases. The first phase involves two rounds of scanning a database. The first scan generates frequent one-itemsets by computing the support of all items, whereas the second scan results in k-itemsets by pruning all infrequent items in each transaction record. Note that, k denotes the number of frequent items in a transaction. In phase two, a k-FIU-tree is repeatedly constructed by decomposing each h-itemset into k-itemsets, where $k + 1 \leq h \leq M$ (M is the maximal value of k), and unioning original k-itemsets. Then, phase two get our data very easily, we do not have to scan the tree again and again to get our data. FiDoop uses some special scheme to distribute the data over nodes of the cluster. For high-dimentional data, FiDoop-HD is used. The FiDoop has some special features like parallization of sequential data which improve the performance of data mining.
To distribute the data over nodes so that it does not degrade the performance by over loading the data at one node in a cluster.
The three Map Reduce jobs are performed in FiDoop.

FIUT

starts mining all frequent *k*-itemsets based on the leaves of *k*-FIU-tree without recursively traversing the tree. Compared with the FP-growth method, FIUT significantly reduces the computing time and storage space by averting overhead of recursively searching and traversing conditional FP trees.

Scan results in *k*-itemsets by pruning all infrequent items in each transaction record. Note that, *k* denotes the number of frequent items in a transaction. In phase two, a *k*-FIU-tree is repeatedly constructed by decomposing each *h*-itemset into *k*-itemsets, where $k + 1 \leq h \leq M$ (*M* is the maximal value of *k*), and unioning original *k*-itemsets. Then, phase two starts mining all frequent *k*-itemsets based on the leaves of *k*-FIU-tree without recursively traversing the tree. Compared with the FP-growth method, FIUT significantly reduces the computing time and storage space by averting overhead of recursively searching and traversing conditional FP trees.

MAPREDUCE FRAMEWORK

MapReduce is a promising parallel and scalable programming model for data-intensive applications and scientific analysis. A MapReduce program expresses a large distributed computation as a sequence of parallel operations on datasets of key/value pairs. A MapReduce computation has two phases, namely, the Map and Reduce phases. The Map phase splits the input data into a large number of fragments, which are evenly distributed to Map tasks across the nodes of a cluster to process. Each Map task takes in a key-value pair and then generates a set of intermediate key-value pairs. After the MapReduce runtime system groups and sorts all the intermediate values associated with the same intermediate key, the runtime system delivers the intermediate values to Reduce tasks. Each Reduce task takes in all intermediate pairs associated with a particular key and emits a final set of keyvalue pairs. Both input pairs of Map and the output pairs of Reduce are managed by an underlying distributed file system. MapReduce greatly improves programmability by offering automatic data management, highly scalable, and transparent fault-tolerant processing. Also, MapReduce is running on clusters of cheap commodity servers—an increasingly attractive alternative to expensive computing platforms. Thanks to the aforementioned advantages, MapReduce has been widely adopted by companies like Google, Yahoo, Microsoft, and Facebook.

Hadoop—one of the most popular MapReduce implementations—is running on clusters where Hadoop distributed file system (HDFS) stores data to provide high aggregate I/O bandwidth. At the heart of HDFS is a single Name Node—a master server that manages the file system namespace and regulates access to files. The Hadoop runtime system establishes two processes called Job Tracker and Task Tracker. Job Tracker is responsible for assigning and scheduling tasks; each Task Tracker handles Map or Reduce

FIDOOP

In light of the MapReduce programming model, we design a parallel frequent itemsets mining algorithm called FiDoop. The design goal of FiDoop is to build a mechanism that enables automatic parallelization, data distribution and load balancing for parallel mining of frequent itemsets on large clusters. To facilitate the presentation of FiDoop. Aiming to improve data storage efficiency and to avert building conditional pattern bases, FiDoop incorporates the concept of FIU-tree .

1. METHODOLOGY

first MapReduce job is responsible for creating all frequent one-itemsets. A transaction database is partitioned into multiple input files stored by the HDFS over data nodes of a Hadoop cluster. Each mapper sequentially reads each transaction from its local input split, where each transaction is stored in the format of pair. Then, mappers compute the frequencies of items and generate local one-itemsets.

Second MapReduce Job: Given frequent one-itemsets generated by the first MapReduce job, the second subsequent MapReduce job applies a second round of scanning on the database to prune infrequent items from each transaction record. The second job marks an itemset as a k-itemset if it contains k frequent items ($2 \leq k \leq M$, where M is the maximal value of k in the pruned transactions).

Third MapReduce Job: The third MapReduce job,a computationally expensive phase is dedicated to: decomposing itemsets; constructing k-FIU trees; mining frequent itemsets. The main goal of each mapper is twofold: 1) To decompose each k-itemset obtained by the second MapReduce job into a list of small-sized sets, where the number of each set is anywhere between 2 to $k - 1$ and 2)to construct an FIU-tree

by merging local decomposition results with the same length.

6. LOAD BALANCE

The *decompose*() function of the third MapReduce job accomplishes the decomposition process. If the length of an itemset is *m*, the time complexity of decomposing the itemset is *O(2m)*. Thus, the decomposition cost is exponentially proportional to the itemset's length. In other words, when the itemset length is going up, the decomposition overhead will dramatically enlarge. The data skewness problem is mainly induced by the decomposition operation, which in turn has a significant performance impact on FiDoop. The first step toward balancing load among data nodes of a Hadoop cluster is to quantitatively measure the total computing load of processing local itemsets. We achieve this first step by developing a workload-balance metric to quantify load balance among the data nodes.

7. PERFORMANCE ANALYSIS

The efficiency of the system can be analyzed in terms of time taken by the FP-Tree and FIU-Tree algorithms in generating the Frequent Itemsets. We compare the performance of the system with the Fidoop system.

In Table 7.1 shows the time taken to create the Frequent Itemsets of different transactions size. From the Table, it is clear that the amount of time taken to generate frequent itemsetsby FP-Tree algorithm is around 1.5 times slower than the FIU-Tree for the same input.

FP-Growth Tree				FIU- Tree			
S. No	No. of Records	Support Value	Time	S. No	No. of Records	Support Value	Time
1.	10	0.1	10.002	1.	10	0.1	1.31
2.	20	0.1	20.00	2.	20	0.1	2.44
3.	50	0.1	100.05	3.	50	0.1	6.54
4.	100	0.1	212.04	4.	100	0.1	14.98

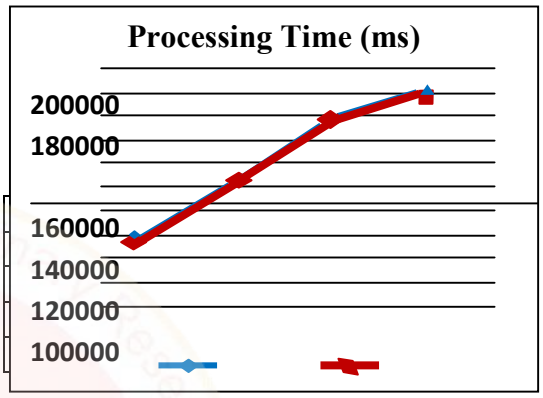
Table :7.1

8. ADVANTAGES

8.1 Processing time

Processing time is defined as the time it takes to complete a prescribed procedure.

This graph shows the processing time. When compared to the existing method, there is less processing time in the proposed method.



9. CONCLUSION

This paper, proposed the FiDoop based parallel mining of frequent item set using map reduce. To solve the scalability and load balancing challenges in the existing parallel mining algorithms for frequent itemsets,the MapReduce programming model to develop a parallel frequent itemsets mining algorithm called FiDoop. FiDoop incorporates the frequent items ultrametric tree or FIU-tree rather than conventional FP trees, thereby achieving compressed storage and avoiding the necessity to build conditional pattern bases. FiDoop seamlessly integrates three MapReduce jobs to accomplish parallel mining of frequent itemsets.

An important role of the third MapReduce job plays in parallel mining; its mappers independently decompose itemsets whereas its reducers construct small ultrametric trees to be separately mined. We improve the performance of FiDoop by balancing I/O load across data nodes of a cluster. We enhance the execution of FiDoop by adjusting I/O load crosswise over information hubs of a group.

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How to Raise Kids who will Believe in Gender Equality

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Introduction: *As we all are aware of a well known quote by Simone de Beauvoir from her book 'The Second Sex' is " One is not born but becomes a woman". With this famous phrase Beauvoir first articulated what has come to be known as the sex-gender distinction, that is, the distinction between biological sex and the social and historical construction of gender and its attendant stereotypes. The fundamental source of woman's oppression, Beauvoir notes its historical and social construction as the quintessential Other. De Beauvoir defines women as the " second sex" because women are defined in relation to men. In other words sex is determined by nature but gender is determined by society. Thus in modern time awareness for gender equality in society is going to start in various ways. Among them there is a stream of thought that achieving gender equality through art of parenting i.e. to raise kids who believe in gender equality. We all want our children to grow up to be caring, thoughtful and socially conscious people. Part of this means raising them to believe in and stand up for gender equality.*

There are number of stages of upbringing of kids in natural way and as a parent these stages can be used for the kids to become more humane socially . A gist of the present paper is that how parents can give their children both girls and boys- the solid foundation they need to become the feminists of tomorrow.

Learning through observation: Social learning science teaches us that children's development happens through observation and imitation. Modeling parents own feminism can mean anything from showing love for their body to filing a complaint with a local retailer for running a sexist ad compaign. No matter where parents are on the activist spectrum. Let your kids see your feminism in action.

Find everyday opportunities to walk your talk. A parent can raise their kids in a household where there always use gender neutral pronouns . For example in Marathi language " aag tikde ja" instead of using "aag" we as a parent can use " tu tikde ja" . Instead of buying doll as a toy for girls and plane or helicoptor for boys as a parent we must buy any toys whatever girls like rather we should promote them to buy plane, car, etc.

Acknowledge the parenting power of fathers: Break the biological determinism that says women means parenting and men means working out. Today's dads come in many forms : they can be single or married ; externally employed or stay at home gay or straight; adoptive or step-parents. What do we know is that dad's affection and increased family involvment help promote children's social and emotional development.

Start early: It is never too early to start talking about equality with your children. Find opportunities in everyday life for teachable moments.

Teach them that gender is fluid: Gender is one of the first social categories children become aware of . By the time they are 3 years old, they have formed their gender identity. So much of what limits boys and girls is rooted in socially constructed ideas about what one is or isn't permitted to do within their gender. Let your children take the lead and experience their gender with as much fluidity as they wish.

Teach them about healthy sexuality: Teaching your kids about healthy sexuality is as important as teaching them about safety, nutrition and acceptable social behaviour. It's important to be both helpful and approachable as a parent .

*Start conversations about sexuality rather than waiting to be asked.

*Give them real names for their body parts.

*Give honest answers about sex and sexuality.

*Assure them that you will answer any question about sex no matter how awkward or uncomfortable the topic might be.

Teach them about body autonomy and how to exercise their own consent.

Body autonomy is the right control over own body and to decide what happens to it. Allowing your kids to exercise their own consent (in ways that are age appropriate) ensures that they grant the same body autonomy to others. Some ways to empower your kids to practice body autonomy include:

*Giving them a say when it comes to when they eat or sleep (within reason)

*Telling them they have right to say stop when they feel uncomfortable, regardless of who the person is .

*Giving them real names for body parts.

*Never forcing them to hug or kiss people (includinng grown- up and family members)

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*Teach them to respect others when they say no or stop .

*Trusting their abilities in age-appropriate ways.

Teach them emotional intelligence: According to psychology today emotional intelligence is the ability to be aware of, control and express one's emotions. Children with high EQ become empathetic, engaged and nurturing adults who respect and value others.

Parent can teach their son empathy by making gender equality issues personal to them by asking such type of questions " How would you feel if that happened to him\ his mom \ dad and their family members".

Encourage them to celebrate diversity: " kids don't come with instructions but they do come with open minds " said Dr. Christopher Metzler. As parents, we are positioned to guide our children to appreciate the differences that make each of us unique. Explaining diversity in a way that is understandable to kids can be challenging, but is integral to raising kids who treats others fairly.

Conclusion: Here are a few tips to get started:

- Recognize that you may hold your own conscious or unconscious biased and work on addressing them.
- Talk to your kids about stereotypes : how they can be divisive and don't always tell the whole story.
- Find age appropriate ways to bring diversity into your children's lives. And not just of thought, experience, socio-economic status, sexual orientation and identity- etc.

Thus through above mentioned ways, we, as parents can raise our children with the basic ideals of gender equality. Welcoming, adopting and practicing such patterns of behaviour has become must today. In the globalized world, things are changing in a fast rate. The age old norms, definitions and codes of behaviour are changing with a fast rate. In order to keep a pace with the changing time, we need to nurture these ideologies for the betterment of future generation. After all it is well said, "Charity Begins at Home".

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Changing Language Teaching Methodologies: The Need of the Day

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Abstract:

Language is a complex specialized proficiency which gets developed spontaneously without conscious effort or formal instruction without awareness of its underlying logic. So language teachers need to use some strategies to teach effectively. Apart from it, English language teachers need to utilize innovative ideas in their teaching because in our country English is learnt as a second language. This paper analyses the innovative and quite interesting methods we have in teaching English language. We may have a number of teaching methods in between traditional and modern. Everybody has his own understanding and conclusions on teaching English language. But this paper portrays combining this two types how we can make our teaching very effective. We have been completely bounded with traditional methods of teaching and understanding where the present day learners felt uncomfortable a bit. Learner's mind will never be static it is ever growing and ever changing. The study is based on secondary data.

Keywords: Language, strategies, innovative, portrays, traditional, growing, changing,

1.1 Introduction:

The importance of language cannot be underestimated, because it is the vehicle of thought and communication. The English language is a national and international medium of communication. By so doing, it has led to the exchange of feelings and effects which has contributed tremendously to the socio-economical and political development of any state. The poor performances in English language in most schools/colleges are due to the fact that the teaching is textbook-based. Teachers do not have regular supply of the teaching aids and where they are available they are inadequate and obsolete. This paper stresses the need for making English language lessons easy and enjoyable through the use of instructional aids/ improvisations. It presents innovative methods and techniques to teach English language by using various teaching aids. It also aims to make English teachers aware of the strategies to use it in an effective manner.

1.2 Advantages of Using Innovative Methods:

" Adds interest, involvement and brings the world into the classroom;
" Makes learning permanent;
" Develops greater understanding;
" Stimulates self-activity;
" Fosters continuity of thought;
" Makes teaching effective;
" Helps in overcoming language barriers; and
" Provides a great variety of methods.

1.3 Problems with Current Methodologies:

It is of paramount importance that the teacher should know what his/her task is and what he/she is trying to achieve by teaching English. They go on with their job of teaching without knowing the difficulties of the learner. The teacher should be fully aware of the fact that his student's proficiency in English is not up to mark owing to the deteriorating standard of teaching in schools. In today's world English is taught in a very orthodox manner. The basic teaching is needed. Teaching the alphabets and

the formation of the words is essential and a must. But there is something that is even more important. The student must be able to speak the words and understand their meaning before writing them down. The foundation to teach English can only be taught using the orthodox methods of teaching the alphabets and the words and the rules. But then teaching only the grammatical rules is found to be boring by most students and it is because of this that they lose interest in learning the language. Although there is no way other than the traditional one to teach the basics of the language these methods must be tweaked a bit so as to appeal to the students. When it comes to teaching English to students of higher classes who are supposed to have the basics the traditional methods generally tend to yield poorer results that innovative methods. This has already been proven by methods implemented like use of stories, poems, movies, books and newspapers etc. These methods help the students learn the language better without them actually realizing and also it keeps their interest. This paper will provide a few of such methods to teach English Language.

1.4 Use of Innovative Methods, Materials and Practices in ELT

Innovative teaching is necessary for the present and future of education to help students to reach their full potential. In most of the class rooms in India conventional teaching methods, materials and teaching techniques based on prescribed texts and syllabus are used homogeneously in spite of vast differences in class rooms and level of students. The traditional methods which largely depend on lecturing and rote learning reduce English language learning to mechanical memorization and miserably fail in developing language competency among the students. These stereotyped methods and teaching material makes the learning a monotonous activity and creates distaste among the students by reducing them to mere passive receptors of language and not active participants in the learning process.

1.4.1 Task-based teaching/Activity-centered teaching:

Students always look for opportunities to be active participants in tasks which is required to practice language in communication with their teacher, their peers, and others. It is adventurous for them by using projects and everyday materials to teach English. It involves shared experiences in a particular situation. Through active discussion, students discover language principles at work in the situation. Through debriefing, students are able to sort and order the information gathered and relate it to the lesson. The teacher guides the students but it is the students who actually discover for themselves what is being taught.

1.4.2 Transactional reading

Transactional reading strategies can be used at specific intervals during or between other activities in order to encourage students to read a wider range of sources rather than just one textbook. It will help students to make the transition from passive listener to active reader.

1.4.3 By Using Language Laboratory:

Technological aids in language teaching are a major force today, and among these aids, the language laboratory occupies the most prominent place. The language laboratory is very useful for assessing students' speech. It provides students with the technical tools to get the best samples of pronunciation of the language.

1.4.4 Teaching through word games:

It is one of the interesting method of teaching. Traditional methods dictated for study and games to be separate but the fact remains that the students tend to be more interested in playing games rather than using traditional method for study. Any logical reasoning would dictate us to combine the two aspects to solve the problem. The most important part of any language is the vocabulary. To understand the meaning of the words and to use them in day to day life is a very difficult task and games can

help the students overcome this difficulty. Games like scrabble, housie etc. have been designed for this specific purpose. These games are just based on words and help the students develop their vocabulary.

1.4.4 Teaching through arranging various competitions:

Most of the times competitions like debates and elocutions, group discussions, role playing also help the students a lot in learning the language as the aspect of the competitions keep them at the best in conversations. It forces them to use the best possible construction of sentences to put forward their opinions and to use good vocabulary

1.4.5 Teaching through various multimedia sources:

Multimedia sources like songs, movies, TV series, magazines, newspapers play a very vital role in improving our language. Such sources can be used to help the students improve their language. This is something that the students will do in their spare time. Traditional methods of reading newspapers and books, novels are also very good methods to teach the language. When the traditional methods are modified along with some innovative ideas the entire learning and the teaching process is enriched and guarantees a success in efficient learning.

CONCLUSION:

Since English is the official language of this world it has to be taught in such a way that it will help us not just to speak and write and listen but to communicate. That is the purpose of the language and that is what it must be used for. Hence innovative methods help in bringing a change and most of the times for the better. So, innovative methods help in bringing a change which helps the students to learn in an efficient, interesting and an interactive manner. And it is responsibility of teacher not only to use traditional methods but for using new and better methods for the students benefit. This can bring a much awaited and much required change in teaching techniques.

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International Journal of Research in Advent Technology, Vol.6, No.5, May 2018
E-ISSN: 2321-9637
Available online at www.ijrat.org

Axially Symmetric Cosmological Models In $f(R,T)$ Gravity With Time Varying Deceleration Parameter

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Abstract: In the present paper an attempt has been made to study an axially symmetric space-time is considered in the presence of a perfect fluid source in the framework of $f(R,T)$ gravity. We consider two types of scale factors (i) $a(t)=\sinh(\alpha t)$ and (ii) $a(t)=te^{t}$ which yield time dependent DP. To get deterministic solution, expansion scalar θ is proportional to the shear scalar σ have been used. Some physical behavior for both models have been discussed by using physical parameters.

Keywords: $f(R, T)$ gravity, Axially symmetric space-time, Deceleration Parameter

1. INTRODUCTION

During last decade, there has been several modifications of general relativity to provide natural gravitational alternative for dark energy. It has been suggested that cosmic acceleration can be achieved by replacing the Einstein-Hilbert action of general relativity with a general function Ricci scalar, *f (R)*. Modification of general relativity are attracting more and more attention to explain late time acceleration and dark energy. There have been several modified theories like *f* (*R*) gravity, *f* (*G*) gravity f(T) gravity or *f* (*R*,*G*) gravity and so on investigated by several researchers. A generalization of *f* (*R*) modified theories of gravity was proposed in [1]. Among the various modifications, *f* (*R*) theory of gravity is considered as the most suitable due to the cosmologically important *f* (*R*) models. It has been suggested that cosmic acceleration can be achieved by replacing the Einstein–Hilbert action of general relativity with a general function Ricci scalar, *f* (*R*). Nojiri *et al* [2] have studied *f* (*R*), *f* (*G*) or *f* (*R*,*G*) gravity in various contexts. Many researchers [3–11] have investigated *f* (*R*) gravity in different contexts. Shamir [12] has proposed a physically viable *f* (*R*) gravity model, which shows the unification of early-time inflation and late-time acceleration. Paul et al. [13] obtained FRW models in f(R) gravity while Sharif and Shamir [14,15] have studied the solutions of Bianchi type I and V space-times in the frame work of f(R) gravity. Shamir [16] studied the exact vacuum solutions of Bianchi type I, III and Kantowski-Sachs space-times in the metric version of f(R) gravity. Adhav [17] has obtained LRS Bianchi type I cosmological model in f(R, T) gravity. Reddy et al. [18] have discussed Bianchi type III cosmological model in f(R, T) while Reddy et al. [19], Reddy and Shanthikumar [24] studied Bianchi type III dark energy model and some anisotropic cosmological models, respectively, in f(R, T) gravity. Chaubey and Shukla [20] have constructed a new class of Bianchi cosmological model in f(R, T) gravity. The exact solutions of the Einstein-Rosen cosmological model filled with perfect fluid have been derived in f(R, T) gravity by Rao and Neelima [21].

Axially symmetric cosmological models with string dust cloud source developed by Bhattacharaya and Karade [22]. Axially symmetric space-times representing material distribution were obtained by Marder [23].

Axially symmetric space-times play an important role in the study of universe on a scale in which anisotropy and inhomogeneity are not ignored [24]. Kilinc [25] showed that axially symmetric cosmological models have made significant contributions in understanding some essential features of the universe such as the formation of galaxies during the early stages of the evolution. Jain et al. [26] studied axially symmetric space-time with wet dark fluid in bimetric theory. Energymomentum localization in Marder's axially symmetric space-time has been studied by Aygun et al. [27]. Recently Rao et al. [28] have obtained axially symmetric cosmological model with perfect fluid in general relativity and in f(R, T) gravity. Sahoo et al. [29] obtained the exact solution of the field equations in f(R, T) theory with the help of special law of variation for Hubble parameter. Two fluid axially symmetric cosmological models in f(R, T) theory obtained by Pawar et al. [30].

The constant DP is commonly used by cosmologist in literature with various aspects. In order to make more detailed description of the kinematics of cosmological expansion, it is useful to consider various forms of time dependence deceleration parameter. One of the most popular form is known as linearly varying deceleration parameter (LVDP). Linear parametrization of the DP represents quite naturally. The next logical step towards the behaviour of future model is either it expands forever or ends with a Big Rip in finite future. This can be parametrized with redshift parameter z, cosmic scale factor a and with cosmic time t. Transition of the universe from the decelerated phase to the present accelerating phase motivate us to consider variable DP. Several researchers (Pradhan *et al.* [31], Amirhashchi *et al.* [32], Akarsu and Dereli [33]) have discussed the evolution of the universe with variable DP. Also Mishra et al [34] have proposed a linearly varying deceleration parameter and using it they have investigated Bianchi Type-II dark energy model in f(R, T) gravity. It is used in Bianchi type-V cosmological model with of holographic dark energy to escape the Big Rip singularity [35]. Singh et al.[36] have been studied the homogeneous and anisotropic Bianchi type-I cosmological model in the presence of viscous uid source of matter, which starts with a big bang and ends in a Big Rip. The kinematical behaviour of LVDP along with null energy condition (NEC) has been explored in the framework of f(R; T) gravity for Bianchi type -I and V space-time[37]. Akarsu et al.[38]have described the fate of the universe through parametrization $q = q0+q1(1-t/t_0)$, which is linear in cosmic time t, along with two well-known additional parametrization of the DP $q = q_0+q1(1-a/a_0)$ and $q = q_0 + q_1z$, where z and a are the redshift parameter and scale factor respectively. Furthermore, they have studied the dynamics of the universe in comparison with the standard ^CDM model. Sahoo and Sivakumar [39] have obtained the model for perfect fluid source coupled with strange quark matter with linearly cosmic time parametrization of the deceleration parameter.

The present paper is organized as follows. In sect.1, a brief introduction is given. The field equations in metric version of $f(R, T)$ gravity is given in sect. 2. In section 3, explicit field equations in $f(R, T)$ gravity are obtained by using the particular form of the functions $f(T) = \lambda T$, which are used by Harko et al. [40], with the general class of axially symmetric metric in the presence of perfect fluid. Section 4 deals with cosmological solutions of the field equations using the linearly varying deceleration parameter by considering physically relevant assumptions and also discuss some

physical properties of the model. Conclusions are given in sect.5.

2. GRAVITATIONAL FIELD EQUATIONS OF $f(R,T)$ GRAVITY

The $f(R,T)$ theory of gravity is the modifications of General Relativity (GR). The field equations of $f(R,T)$ gravity are derived from the Hilbert-Einstein type variational principle. The action for the modified $f(R,T)$ gravity is

$$S=\frac{1}{16\pi}\int\left[f(R,T)+L_m\right]\sqrt{-g}\,d^4x, \tag{1}$$

where $f(R,T)$ is an arbitrary function of the Ricci scalar R, T is the stress energy tensor T_{ij} of the matter and L_m is the matter Lagrangian density, The energy momentum tensor T_{ij} is defined as

$$T_{ij}=-\frac{2}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\right)L_m}{\delta g^{ij}}. \tag{2}$$

Here we assume that the dependence of matter Lagrangian is merely on the metric tensor g_{ij} rather than its derivatives.

In this case, we obtain

$$T_{ij}=g_{ij}L_m-\frac{\partial L_m}{\partial g^{ij}}. \tag{3}$$

The $f(R,T)$ gravity field equations are obtained by varying the action S with respect to metric tensor g_{ij}.

$$f(R,T)R_{ij}-\frac{1}{2}f(R,T)g_{ij}+\left(g_{ij}\otimes-\nabla_i\nabla_j\right)f_R(R,T)=8\pi T_{ij}-f_T(R,T)T_{ij}- \tag{4}$$

where $\theta_{ij}=-2T_{ij}+g_{ij}L_m-2g^{\alpha\beta}\frac{\partial L_m}{\partial g^{ij}\partial g^{\alpha\beta}}$. (5)

Here

$$f_R(R,T)=\frac{\partial f(R,T)}{\partial R},\quad f_T(R,T)=\frac{\partial f(R,T)}{\partial T},\ \otimes=\nabla^i\nabla_i$$

where ∇_i denotes covariant derivative.

Now contraction of equation (4) gives

$$f_R(R,T)R+3\otimes f_R(R,T)g_{ij}-2f(R,T)=8\pi T-f_T(R,T)(T+\theta), \tag{6}$$

Where $\theta=\theta_i^i$. Equation (6) gives a relation between Ricci scalar R and the trace T of energy momentum tensor. Using matter Lagrangian L_m the stress energy tensor of the matter is given by

$$T_{ij}=(\rho+p)u_iu_j-pg_{ij}, \tag{7}$$

where $u^i=(0,0,0,1)$ is the four velocity in commoving coordinates which satisfies the condition $u^iu_i=1$ and $u^i\nabla_ju_i=0$. ρ and p are energy density and pressure of the fluid, respectively, and the matter Lagrangian can be taken as $L_m=-p$ since there is no unique definition of the matter Lagrangian. Then with the use of (5) we obtain the variation of stress energy of perfect fluid expression

$$\theta_{ij} = -2T_{ij} - pg_{ij},$$

(8)

On the physical matter of the matter field, the field equations also depend through the tensor θ_{ij}. Hence in the case of $f(R, T)$ gravity depending on the nature of the matter source, we obtain several theoretical models corresponding to different matter contribution for $f(R, T)$ gravity are possible. However, Harko et al. [40] gave three cases of these models.

$$f(R, T) = \begin{cases} R + 2f(T) \\ f_1(R) + f_2(T) \\ f_1(R) + f_2(R) f_3(T) \end{cases}$$

(9)

In this paper, we are focused to the first class, i.e. $f(R, T) = R + 2f(T)$

where $f(T)$ is an arbitrary function of stress energy tensor of matter. We get the gravitational field equations of $f(R, T)$ gravity from equation (4) as

$$R_{ij} - \frac{1}{2}Rg_{ij} = 8\pi T_{ij} - 2f'(T)T_{ij} - 2f'(T)\theta_{ij} + 2f(T)g_{ij}$$

(10)

where the prime denotes differentiation with respect to the argument. If the matter source is a perfect fluid then the field equations (in view of equation (8)) becomes

$$R_{ij} - \frac{1}{2}Rg_{ij} = 8\pi T_{ij} + 2f'(T)T_{ij} + [2pf'(T) + f(T)]g_{ij}$$

(11)

3. METRIC AND FIELD EQUATIONS

We consider the axially symmetric metric (Bhattacharya and Karade [22]) as

$$ds^2 = dt^2 - A^2(t)\left[d\chi^2 + f^2(\chi)d\phi^2\right] - B^2(t)dz^2,$$

(12)

with the convention $x^1 = \chi,\ x^2 = \phi,\ x^3 = z \quad and \quad x^4 = t$, *and* A, B are functions of the proper time t alone while f is a function of the coordinate χ alone . In view of equation (7) for axially symmetric space-time (12) , the field equations (11) leads to

$$\frac{\ddot{A}}{A} + \frac{\dot{A}\dot{B}}{AB} + \frac{\ddot{B}}{B} = p(8\pi + 3\lambda) - \rho\lambda,$$

(13)

$$2\frac{\ddot{A}}{A} + \left(\frac{\dot{A}}{A}\right)^2 - \frac{f''}{A^2 f} = p(8\pi + 3\lambda) - \rho\lambda,$$

(14)

$$\left(\frac{\dot{A}}{A}\right)^2 + 2\frac{\dot{A}\dot{B}}{AB} - \frac{f''}{A^2 f} = -\rho(8\pi + 3\lambda) + p\lambda,$$

(15)

where an overhead dot and dash represents differentiation with respect to t and χ respectively.

The functional dependence of the metric together with equation (14) and (15) imply that

$$\frac{f''}{f} = m^2, \quad m^2 = cons\tan t.$$

(16)

If $m = 0$, then $f(\chi) = c_1\chi + c_2, \ \chi > 0$

(17)

where c_1 *and* c_2 are integrating constants. Without loss of generality, by taking $c_1 = 1$ *and* $c_2 = 0$ we get $f(\chi) = \chi$ resulting in the flat model of the universe (Hawking and Ellis [41]).

Now the field equations (13)-(15) reduces to

$$\frac{\ddot{A}}{A} + \frac{\dot{A}\dot{B}}{AB} + \frac{\ddot{B}}{B} = p(8\pi + 3\lambda) - \rho\lambda,$$

(18)

$$2\frac{\ddot{A}}{A} + \left(\frac{\dot{A}}{A}\right)^2 = p(8\pi + 3\lambda) - \rho\lambda,$$

(19)

$$\left(\frac{\dot{A}}{A}\right)^2 + 2\frac{\dot{A}\dot{B}}{AB} = -\rho(8\pi + 3\lambda) + p\lambda.$$

(20)

The spatial volume is given by

$$V = a^3 = A^2B$$

(21)

where a is the mean scale factor.

The mean Hubble parameter H for axially symmetric metric is given by

$$H = \frac{\dot{a}}{a} = \frac{1}{3}\left[2\frac{\dot{A}}{A} + \frac{\dot{B}}{B}\right]$$

(22)

The directional Hubble parameter in the directions of χ, ϕ *and* z are

$$H_\chi = H_\phi = \frac{\dot{A}}{A} \text{ and } H_z = \frac{\dot{B}}{B}$$

(23)

The deceleration parameter is

$$q = -\frac{a\ddot{a}}{\dot{a}^2}$$

(24)

4. SOLUTIONS OF THE MODEL

Equations (18)-(20) are three independent equations in four unknowns A, B, p, ρ . Hence to find a determinate solution, we assume expansion scalar θ is proportional to the shear scalar σ which yields

$$A = B^n$$

(25)

Subtracting (18) from (19) and taking second integral, we obtain the following relation

$$\frac{A}{B} = k_2 e^{k_1 \int \frac{1}{a^3} dt}$$

(26)

Thus equation (26) gives values of A, B as

$$A = k_2^{\frac{n}{(n-1)}} e^{\frac{k_1 n}{(n-1)}\int \frac{1}{a^3}dt} \quad n \neq 1$$

(27)

$$B = k_2^{\frac{1}{(n-1)}} e^{\frac{k_1}{(n-1)}\int \frac{1}{a^3}dt} \quad n \neq 1$$

(28)

Thus the metric functions are found explicitly in terms of average scale factor a.

4.1. Case I: $a(t) = \sinh(\alpha t)$

As suggested by Pradhan et al. [42], firstly we consider the variation of scale factor a with cosmic time t by the relation

$$a(t) = \sinh(\alpha t)$$

(29)

where α is an arbitrary constant.

Using equation (29) into (27) and (28), we have the following set of expressions for the scale factors

$$A = k_2^{\frac{n}{(n-1)}} e^{\frac{k_1 n}{(n-1)}\int [\sinh(\alpha t)]^{-3} dt} \qquad n \neq 1$$

(30)

$$B = k_2^{\frac{1}{(n-1)}} e^{\frac{k_1}{(n-1)}\int [\sinh(\alpha t)]^{-3} dt} \qquad n \neq 1$$

(31)

The physical quantities of observational interest in cosmology such as directional Hubble parameters (H_i), spatial volume (V), mean anisotropy parameter (Δ), shear scalar (σ^2) and expansion scalar (θ) are respectively given by

$$H_\chi = H_\phi = \frac{k_1 n}{(n-1)\sinh(\alpha t)}$$

(32)

$$H_z = \frac{k_1}{(n-1)\sinh(\alpha t)}$$

(33)

$$V = \sinh^3(\alpha t)$$

(34)

$$\Delta = \frac{2}{3}\frac{(3n^2 + 2n + 1)}{(2n+1)^2}$$

(35)

$$\sigma^2 = \frac{k_1^2(3n^2 + 2n + 1)}{(n-1)^2 \sinh^2(\alpha t)}$$

(36)

$$\theta = \frac{3k_1(2n+1)}{(n-1)\sinh(\alpha t)}$$

(37)

The deceleration parameter as

$$q = -\tanh^2(\alpha t)$$

(38)

Using equations (30) and (31) in (19) and (20), we obtain the values of pressure and energy density as

$$p = \frac{k_1 n}{(n-1)^2 \sinh^2(\alpha t)\left[(8\pi + 3\lambda)^2 - \lambda^2\right]}\left[(8\pi + 3\lambda)(3k_1 n - 2\alpha(n -$$

(39)

$$\rho = \frac{k_1 n}{(n-1)^2 \sinh^2(\alpha t)\left[(8\pi+3\lambda)^2-\lambda^2\right]}\left[\lambda(3k_1 n - 2\alpha(n-1)\cosh(\alpha t)) - (8\pi+3\lambda)k_1(2+n)\right]$$

(40)

4.2. Physical Behavior of the model

When $t=0$ the scalar expansion and shear scalar are infinity but at $t=\infty$ the scalar expansion and shear scalar are zero. The model of the universe start with big bang Spatial volume expands exponentially as t increases and becomes infinitely large as $t\to\infty$.The directional Hubble parameters H_χ, H_ϕ, H_z are infinite at $t=0$ and vanishing at $t\to\infty$.The shear scalar become zero as $t\to\infty$. We observe pressure and energy density remains always positive and it converges to zero as $t\to\infty$. From equations (30) and (31) we observe that the spatial scale factor become constant at the initial epoch $t=0$. Since $\lim_{t\to\infty}\frac{\sigma}{\theta}\neq 0$ the model does not approach isotropy for large value of t.

4.3. CASE II: $a(t)=te^t$

Following Amirhashchi et al.[43], we consider the following scale factor

$$a(t)=te^t$$

(41)

Using equations (41) in (27) and (28), we have the following set of expressions for the scale factors

$$A = k_2^{\frac{n}{(n-1)}} e^{\frac{k_1 n}{(n-1)}\int\left[te^t\right]^{-3}dt} \quad n\neq 1$$

(42)

$$B = k_2^{\frac{1}{(n-1)}} e^{\frac{k_1}{(n-1)}\int\left[te^t\right]^{-3}dt} \quad n\neq 1$$

(43)

The physical parameters as described in the case I are expressed as

$$H_\chi = H_\phi = \frac{k_1 n}{(n-1)t^3 e^{3t}}$$

(44)

$$H_z = \frac{k_1}{(n-1)t^3 e^{3t}}$$

(45)

$$V = t^3 e^{3t}$$

(46)

$$\Delta = \frac{2}{3}\frac{\left(3n^2+2n+1\right)}{(2n+1)^2}$$

(47)

$$\sigma^2 = \frac{k_1^2\left(3n^2+2n+1\right)}{(n-1)^2 t^6 e^{6t}}$$

(48)

$$\theta = \frac{3k_1(2n+1)}{(n-1)t^3 e^{3t}}$$

(49)

The deceleration parameter as

$$q = -\frac{t(t+2)}{(t+1)^2}$$

(50)

Using equations (42) and (43) in (19) and (20), we obtain the values of pressure and energy density as

$$p=\frac{k_1 n}{(n-1)^2 t^6 e^{6t}\left[(8\pi+3\lambda)^2-\lambda^2\right]}\left[(8\pi+3\lambda)\left(-6(n-1)(t+1)t^2e^{3t}+3k_1n\right)-\lambda k_1(2+n)\right] \quad (51)$$

$$\rho=\frac{k_1 n}{(n-1)^2 t^6 e^{6t}\left[(8\pi+3\lambda)^2-\lambda^2\right]}\left[\lambda\left(-6(n-1)(t+1)t^2e^{3t}+3k_1n\right)-(8\pi+3\lambda)k_1(2+n)\right] \quad (52)$$

4.4. *Physical Behavior of the model*

We observe that the spatial volume is zero at $t=0$ and expansion scalar is infinite, which shows that the universe starts evolving with zero volume at $t=0$ which is big bang scenario. We observe that the spatial volume increases exponentially with time. The physical quantities pressure (p), energy density (ρ), Hubble factor (H), shear scalar (σ^2) and expansion scalar (θ) diverge at $t=0$. As $t\to\infty$ volume becomes infinite whereas $p,\ \rho,\ H,\ \theta$ approaches to zero. We observe that the average scale factor $a(t)\to 0$ as $t\to 0$ and $a(t)\to\infty$ as $t\to\infty$ .This indicates that there exists inflation. Since $\lim_{t\to\infty}\frac{\sigma}{\theta}\neq 0$ the model does not approach isotropy throughout the evolution of the universe.

5. CONCLUSION

In this paper, we have considered a cosmological model in the presence of perfect fluid and variable deceleration parameter in *f* (*R*, *T*) theory of gravity. According the choice of *f* (*R*, *T*), we are focused to the first class, i.e. $f(R,T)=R+2f(T)$.

The exact solutions of the modified Einstein's field equations are obtained for the axially symmetric universe with perfect fluid. We assumed two types of scale factors (i) $a(t)=\sinh(\alpha t)$ and (ii) $a(t)=te^t$ which yield time dependent DP.

The observations of both the model are as follows:
The mean anisotropy parameter becomes constant for both models. It can be observed that our models are expanding and accelerating universe which starts at a big bang singularity. In both the cases energy density is positive valued and decreasing function of time. It is interesting to notice that q decreases very rapidly and then after it remains constant. It is observed that, our derived model has accelerated expansion at present epoch which is consistent with recent observation of type Ia supernova and CMB anisotropies.

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International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064
Index Copernicus Value (2016): 79.57 | Impact Factor (2017): 7.296

Dark Matter and Holographic Dark Energy Models in Different Scenarios of the Universe

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Abstract: ***In this paper we examine homogeneous and anisotropic Bianchi type-V universe filled with interacting Dark matter and Holographic dark energy. Here we express a scale factor in emergent, logamediate, and intermediate scenarios, under which the universe expands differently. It is shown that for suitable choice of interaction between dark matter and holographic dark energy there is no coincidence problem (unlike ΛCDM). Also, in all the resulting models the anisotropy of expansion dies out very quickly and attains isotropy after some finite time. The physical and geometrical aspects of the models are also discussed.***

Keywords: Dark energy; Bianchi Type V Space-time; Emergent; Logamediate; Intermediate; Deceleration Parameter

1. Introduction

The most attractive subject in cosmology is the accelerating expansion of the universe which is based on the recent astronomical observations as Type Ia supernovae (SNe) Riess et al. [1], Wilkinson Microwave Anisotropy Probe (WMAP) Observations Spergel [2], cosmic microwave background (CMB) anisotropy Tegmark et al.[3] and large scale structure (LSS) Enqvist et al. [4]. This implies that there is a mysterious component in the universe, which has a large negative pressure called dark energy (DE).

An approach to the problem of DE arises from holographic principle that states that the number of degrees of freedom related directly to entropy scales with the enclosing area of the system. As an application of holographic principle in cosmology, it was studied by Li [5] that consequence of excluding those degrees of freedom of the system which will never be observed by that effective field theory gives rise to IR cut-off L at the future event horizon. Based on cosmological state of holographic principle, proposed by Fischler and Susskind [6], the Holographic model of Dark Energy (HDE) has been proposed and studied widely in the literature Setare and Shafei [7]. In Huan and Gong [8] using the type Ia supernova data, the model of HDE is constrained once when c is unity and another time when c is taken as free parameter. It is concluded that the HDE is consistent with recent observations, but future observations are needed to constrain this model more precisely.

Holographic dark energy models have been tested and constrained by various astronomical observations Zhang and Wu [9]; Shen et al. [10]; Chang et al. [11]. A special class are models in which holographic DE is allowed to interact with DM Pavón and Zimdahl [12]; Wang et al. [13-14]; Carvalho and Saa [15];Perivolaropoulos [16]; Gong [17]; Gong and Zhang [18];Huang and Li [19]; Nojiri and Odintsov [20]; Guberina et al. [21-22]; Guo et al. [23-25]; Hu and Ling [26]; Li et al. [27]; Setare [28-29]; Sadjadi [30]; Banerjee and Pavón [31]; Kim et al. [32]; Zimdahl and Pavón [33]; Zimdahl [34]; Adhav et al.[35]. Furthermore, the holographic dark energy model has been extended to include the spatial curvature contribution, i.e. the holographic dark energy model in non-flat space Sarkar [36-38]. Recently, Sarkar [36-38] have studied non-interacting holographic dark energy with linearly varying deceleration parameter in Bianchi type-I and V universe and interacting holographic dark energy in Bianchi type-II respectively. Besides, some interacting models are discussed in many works because these models can help to understand or alleviate the coincidence problem by considering the possible interaction between dark energy and cold dark matter due to the unknown nature of dark energy and dark matter. In addition, the proposal of interacting dark energy is compatible with the current observations such as the SNIa and CMB data . Currently, an interesting attempt for probing the nature of dark energy within the framework of quantum gravity is the so-called "holographic dark energy". This principle is enlightened by investigations of the quantum property of black holes. Roughly speaking, in a quantum gravity system, the conventional local quantum field theory will break down. The holographic dark energy model has been tested and constrained by various astronomical observations. We focus in this paper on the holographic dark energy in a non-flat universe. The anisotropy plays a significant role in the early stage of evolution of the universe and hence the study of anisotropic and homogeneous cosmological models becomes important. The Bianchi type universe models are spatially homogeneous cosmological models that are in general anisotropic. The Bianchi type-I space-time is the straight forward generalization of Robertson-Walkar (RW) metric. However, Bianchi type I, V, VII models isotropy at late times even for ordinary matter, and the possible anisotropy of the Bianchi metrics necessarily die away during the inflationary era. The Bianchi type-I space-time reduces to flat FRW soon after inflation.

According to the accelerating expansion of the universe, we work on three kinds of scenarios which are based on different eras in the evolutionary process of the universe which all of them consist of a kind of expanding exponential scale factor. Motivated by the above discussion, in the present paper, we consider spatially homogeneous and anisotropic Bianchi type-V universe filled with interacting Dark matter and Holographic dark energy. The geometrical and physical aspects of the models are also studied. The

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physical parameters that are of cosmological importance for Bianchi type-V space-time are

- The mean Hubble parameter:

$$H = \frac{\dot{a}}{a} = \frac{1}{3}\frac{\dot{V}}{V} \tag{1.1}$$

- The deceleration parameter:

$$q = -\frac{\ddot{a}a}{\dot{a}^2} = \frac{d}{dt}\left(\frac{1}{H}\right) - 1 \tag{1.2}$$

Where a is the average scale factor and $H_1 = \frac{\dot{A}}{A}$, $H_2 = \frac{\dot{B}}{B}$, $H_3 = \frac{\dot{C}}{C}$ are the directional Hubble parameters in the directions of x, y, z axes respectively.

2. Metric and Field Equations

We consider the Bianchi type-V metric given by

$$ds^2 = -dt^2 + A^2dx^2 + B^2e^{-2mx}dy^2 + C^2e^{-2mx}dz^2 \tag{2.1}$$

where A, B, and C are the metric functions of cosmic time t and m is constant.

The Einstein's field equations are $(8\pi G = 1 \; and \; c = 1)$

$$R_{ij} - \frac{1}{2}R\,g_{ij} = -T_{ij}^{M} + T_{ij}^{\Lambda} \tag{2.2}$$

where

$$T_{ij}^{M} = \rho_m u_i u_j \;\; T_{ij}^{\Lambda} = \left(\rho_\Lambda + \bar{p}_\Lambda\right)u_i u_j + g_{ij}\bar{p}_\Lambda - 2\eta\sigma_{ij} \tag{2.3}$$

with $\bar{p}_\Lambda = \left(p_\Lambda - \xi u^i_{;i}\right)$

are matter tensor for dark matter (pressure less i.e. $\omega_m = 0$) and holographic dark energy. Here ρ_m is the energy density of dark matter and ρ_Λ and p_Λ are the energy density and pressure of holographic dark energy. $\eta \geq 0, \; \xi \geq 0$ are the coefficients of shear and bulk viscosity respectively, v_i, the four-velocity vector of the fluid satisfying, $v_i v^i = -1$, θ is the expansion scalar and σ_{ij} is the shear tensor.

The Einstein's field equations (2.2) for metric (2.1) with the help of Eqs. (2.3) can be written as

$$-\left[p_\Lambda - \left(\xi - \frac{2}{3}\eta\right)\theta\right] + 2\eta\frac{\dot{A}}{A} = \frac{\ddot{B}}{B} + \frac{\ddot{C}}{C} + \frac{\dot{B}\dot{C}}{BC} - \frac{m^2}{A^2} \tag{2.4}$$

$$-\left[p_\Lambda - \left(\xi - \frac{2}{3}\eta\right)\theta\right] + 2\eta\frac{\dot{B}}{B} = \frac{\ddot{A}}{A} + \frac{\ddot{C}}{C} + \frac{\dot{A}\dot{C}}{AC} - \frac{m^2}{A^2} \tag{2.5}$$

$$-\left[p_\Lambda - \left(\xi - \frac{2}{3}\eta\right)\theta\right] + 2\eta\frac{\dot{C}}{C} = \frac{\ddot{A}}{A} + \frac{\ddot{B}}{B} + \frac{\dot{A}\dot{B}}{AB} - \frac{m^2}{A^2} \tag{2.6}$$

$$\rho_m + \rho_\Lambda = \frac{\dot{A}\dot{B}}{AB} + \frac{\dot{B}\dot{C}}{BC} + \frac{\dot{A}\dot{C}}{AC} - \frac{3m^2}{A^2} \tag{2.7}$$

$$0 = \frac{2\dot{A}}{A} - \frac{\dot{B}}{B} - \frac{\dot{C}}{C} \tag{2.8}$$

where overhead dot (.) represents derivative with respect to time t. The volume scale factor V is given by

$$V = a^3 = ABC \tag{2.9}$$

θ is the expansion scalar defined by

$$\theta = u^i_{;i} \tag{2.10}$$

Subtracting (2.4) from (2.5), we get

$$2\eta\left(\frac{\dot{B}}{B} - \frac{\dot{A}}{A}\right) = \frac{\ddot{A}}{A} - \frac{\ddot{B}}{B} + \frac{\dot{A}\dot{C}}{AC} - \frac{\dot{B}\dot{C}}{BC} \tag{2.11}$$

On integrating (2.11), We obtain

$$\frac{A}{B} = d_1 \exp\left[x_1 \int a^{-3}e^{-2\int \eta\, dt}dt\right] \tag{2.12}$$

Similarly, Subtracting (2.5) from (2.6) and (2.4) from (2.6), and integrating we get

$$\frac{A}{C} = d_2 \exp\left[x_2 \int a^{-3}e^{-2\int \eta\, dt}dt\right] \tag{2.13}$$

$$\frac{A}{B} = d_3 \exp\left[x_3 \int a^{-3}e^{-2\int \eta\, dt}dt\right] \tag{2.14}$$

Where the relations $d_1 d_2 d_3 = 1$ and $x_1 + x_2 + x_3 = 0$ are satisfied by the constants $d_1, d_2, d_3, x_1, x_2, x_3$.

From equations (2.12)-(2.14), the metric functions can be written explicitly as

$$A = aa_1 \exp\left[b_1 \int a^{-3}e^{-2\int \eta\, dt}dt\right] \tag{2.15}$$

$$B = aa_2 \exp\left[b_2 \int a^{-3}e^{-2\int \eta\, dt}dt\right] \tag{2.16}$$

$$C = aa_3 \exp\left[b_3 \int a^{-3}e^{-2\int \eta\, dt}dt\right] \tag{2.17}$$

In order to introduce an interaction between dark energy and dark matter, we assume that both components do not conserve separately but interact with each other in such a manner that the balance equations take the form

$$\dot{\rho}_m + \frac{\dot{V}}{V}\rho_m = Q \tag{2.18}$$

$$\dot{\rho}_\Lambda + \frac{\dot{V}}{V}\left(\rho_\Lambda + \bar{p}_\Lambda\right) = -Q \tag{2.19}$$

where $\omega_\Lambda = \frac{p_\Lambda}{\rho_\Lambda}$ is the equation of state parameter for holographic dark energy and $Q > 0$ measures the strength of the interaction. A vanishing Q implies that matter and dark energy remain separately conserved. In view of continuity equations, the interaction between dark energy and dark matter must be a function of the energy density multiplied by a quantity with units of inverse of time, which can be chosen as the Hubble factor H. Models featuring an interaction matter-dark energy were introduced by Wetterich [39-40] (see also Billyard and Coley [41]) and first used alongside the holographic dark energy by Horvat [42]. Further, there is no known symmetry that would suppress such interaction and arguments in favour of interacting models have been put forward recently (Farrar and Peebles [43]). There is freedom to choose the form of the energy density, which can be any combination of dark energy and dark matter. Thus, the interaction between dark energy and dark matter could be expressed phenomenologically in forms such as (Amendola et al. [44-45])

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$$Q = b^2 \frac{\dot{V}}{V} \rho_m = 3b^2 H \rho_0 V^{(b^2-1)} \quad (2.20)$$

Where b^2 is coupling constant.

From Eqs. (2.20) and (2.18), we get the energy density of dark matter as

$$\rho_m = \rho_0 V^{(b^2-1)} \quad (2.21)$$

Where $\rho_0 > 0$ is constant of integration.

Using Eqs. (2.20) and (2.21), we get the interacting term as

$$Q = 3b^2 H \rho_0 V^{(b^2-1)} \quad (2.22)$$

3. Cosmological Solution

To solve the cosmological coincidence problem, we consider the interaction between the components on phenomenological level. Generally, interaction could be considered as a function of energy densities and their derivatives: $Q(\rho_i, \dot{\rho}_i ...)$.According to the accelerating expansion of the universe, we consider three kinds of scenarios which are based on different eras in the evolutionary process of the universe which all of them consist of a kind of expanding exponential scale factor as the followings.

3.1. Emergent Scenario

The scale factor in this scenario is given by,

$$a(t) = a_0 \left(\lambda + e^{\mu t}\right)^n \quad (3.1)$$

Where $a_0 > 0$, $\lambda > 0$, $\mu > 0$ *and* $n > 1$ **(**Fabris, Gonsalves and de Sonza [46]).

we assume that the coefficient of shear viscosity is proportional to the scale of expansion, i.e. $\eta \propto \theta$

That is

$$\eta = \eta_0 \theta \quad (3.2)$$

Integrating, we get

$$\int \eta \, dt = 3\eta_0 n \log\left(\lambda + e^{\mu t}\right) \quad (3.3)$$

Using Eq. (3.1) and (3.3) in Eqs. (2.15)–(2.17), we obtain the exact value of scale factors as

$$A = a_0 a_1 \left(\lambda + e^{\mu t}\right)^n \exp\left[\frac{b_1 a_0^{-3} \left(\lambda + e^{\mu t}\right)^{-3n(1+2\eta_0)+1}}{(-3n(1+2\eta_0)+1)\mu e^{\mu t}}\right] \quad (3.4)$$

$$B = a_0 a_2 \left(\lambda + e^{\mu t}\right)^n \exp\left[\frac{b_2 a_0^{-3} \left(\lambda + e^{\mu t}\right)^{-3n(1+2\eta_0)+1}}{(-3n(1+2\eta_0)+1)\mu e^{\mu t}}\right] \quad (3.5)$$

$$C = a_0 a_3 \left(\lambda + e^{\mu t}\right)^n \exp\left[\frac{b_3 a_0^{-3} \left(\lambda + e^{\mu t}\right)^{-3n(1+2\eta_0)+1}}{(-3n(1+2\eta_0)+1)\mu e^{\mu t}}\right] \quad (3.6)$$

Using Eqs. (3.4)–(3.6) in Eqs. (2.21) and (2.22), we get

$$\rho_m = \rho_0 a_0^{3(b^2-1)} \left(\lambda + e^{\mu t}\right)^{3n(b^2-1)} \quad (3.7)$$

$$Q = 3b^2 \mu n \rho_0 a_0^{3(b^2-1)} e^{\mu t} \left(\lambda + e^{\mu t}\right)^{3n(b^2-1)-1} \quad (3.8)$$

Using Eqs. (3.4)–(3.6) and (3.7) in Eq. (2.7), we obtain the energy density of holographic dark energy as

$$\rho_\Lambda = (k_1 k_2 + k_2 k_3 + k_1 k_3)\left(\lambda + e^{\mu t}\right)^{2h} \left(he^{\mu t} - \lambda\right)^2 + 2n(k_1 + k_2 + k_3)\mu e^{\mu t} \left(\lambda + e^{\mu t}\right)^{h-1} \left(he^{\mu t} - \lambda\right)$$
$$+ 3n^2 \mu^2 \; e^{2\mu t} \left(\lambda + e^{\mu t}\right)^{-2} - 3m^2 (a_0 a_1)^{-2} \left(\lambda + e^{\mu t}\right)^{-2n} \exp\left[\frac{-2k_1 \left(\lambda + e^{\mu t}\right)^{h+1}}{\mu e^{\mu t}}\right]$$
$$- \rho_0 a_0^{3(b^2-1)} \left(\lambda + e^{\mu t}\right)^{3n(b^2-1)} \quad (3.9)$$

where $h = -3n(1+2\eta_0)$, $k_1 = \frac{b_1 a_0^{-3}}{-3n(1+2\eta_0)+1}$, $k_2 = \frac{b_2 a_0^{-3}}{-3n(1+2\eta_0)+1}$, $k_3 = \frac{b_3 a_0^{-3}}{-3n(1+2\eta_0)+1}$.

Using Eqs. (3.3) and (3.6) Eq. (2.4), we obtain the pressure of holographic dark energy as

$$p_\Lambda = -\left(k_2^2 + k_3^2 + k_2 k_3\right)\left(\lambda + e^{\mu t}\right)^{2h} \left(he^{\mu t} - \lambda\right)^2 - (k_2 + k_3) h\mu e^{\mu t} \left(\lambda + e^{\mu t}\right)^h$$
$$- \left[(k_2 + k_3) h\mu e^{\mu t} + 2(k_2 + k_3) + k_2 e^{\mu t} + n\mu k_3 - \sigma\eta_0 \mu n e^{\mu t} k_1\right]\left(\lambda + e^{\mu t}\right)^{h-1} \left(he^{\mu t} - \lambda\right)$$
$$- \left[-2n\mu^2 e^{2\mu t} + n^2 \mu^2 e^{2\mu t} + \sigma\eta_0 \mu^2 n^2 e^{2\mu t}\right]\left(\lambda + e^{\mu t}\right)^{-2}$$
$$- e^{\mu t}\left|\eta\mu^2 - 3\mu n\left|\xi - 2\eta_0 \mu n e^{\mu t} \left(\lambda + e^{\mu t}\right)^{-1}\right|\right|\left(\lambda + e^{\mu t}\right)^{-1} \quad (3.10)$$

The EoS parameter of holographic dark energy is given by

$$\omega_\Lambda = \frac{-\left(k_2^2 + k_3^2 + k_2 k_3\right)\left(\lambda + e^{\mu t}\right)^{2h} \left(he^{\mu t} - \lambda\right)^2 - (k_2 + k_3) h\mu e^{\mu t} \left(\lambda + e^{\mu t}\right)^h}{(k_1 k_2 + k_2 k_3 + k_1 k_3)\left(\lambda + e^{\mu t}\right)^{2h} \left(he^{\mu t} - \lambda\right)^2}$$
$$\frac{- \left[(k_2 + k_3) h\mu e^{\mu t} + 2(k_2 + k_3) + k_2 e^{\mu t} + n\mu k_3 - \sigma\eta_0 \mu n e^{\mu t} k_1\right]\left(\lambda + e^{\mu t}\right)^{h-1} \left(he^{\mu t} - \lambda\right)}{+ 2n(k_1 + k_2 + k_3)\mu e^{\mu t} \left(\lambda + e^{\mu t}\right)^{h-1} \left(he^{\mu t} - \lambda\right)}$$

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$$\frac{-\left[-2n\mu^2 e^{2\mu t}+n^2\mu^2 e^{2\mu t}+\sigma\eta_0\mu^2 n^2 e^{2\mu t}\right]\left(\lambda+e^{\mu t}\right)^{-2}}{+3n^2\mu^2\ e^{2\mu t}\left(\lambda+e^{\mu t}\right)^{-2}-3m^2\left(a_0a_1\right)^{-2}\left(\lambda+e^{\mu t}\right)^{-2n}\exp\left[\frac{-2k_1\left(\lambda+e^{\mu t}\right)^{h+1}}{\mu e^{\mu t}}\right]}$$
$$\frac{-e^{\mu t}\left[\eta\mu^2-3\mu n\left[\xi-2\eta_0\mu n e^{\mu t}\left(\lambda+e^{\mu t}\right)^{-1}\right]\right]\left(\lambda+e^{\mu t}\right)^{-1}}{-\rho_0 a_0^{3\left(b^2-1\right)}\left(\lambda+e^{\mu t}\right)^{3n\left(b^2-1\right)}} \quad (3.11)$$

Using Eqs. (3.2)–(3.4) in Eqs. (1.1) and (1.2), we get the mean Hubble parameter, deceleration parameter of expansion as

$$H=\frac{\mu n e^{\mu t}}{\left(\lambda+e^{\mu t}\right)} \quad (3.12)$$

$$q=-\left[1+\frac{\lambda}{ne^{\mu t}}\right] \quad (3.13)$$

The coincidence parameter $\bar{r}=\frac{\rho_m}{\rho_\Lambda}$ i.e. the ratio of dark matter energy density to the dark energy density is given by

$$\bar{r}=\frac{\rho_0 a_0^{3\left(b^2-1\right)}\left(\lambda+e^{\mu t}\right)^{3n\left(b^2-1\right)}}{\left(k_1k_2+k_2k_3+k_1k_3\right)\left(\lambda+e^{\mu t}\right)^{2h}\left(he^{\mu t}-\lambda\right)^2+2n\left(k_1+k_2+k_3\right)\mu e^{\mu t}\left(\lambda+e^{\mu t}\right)^{h-1}\left(he^{\mu t}-\lambda\right)}$$
$$\frac{1}{+3n^2\mu^2\ e^{2\mu t}\left(\lambda+e^{\mu t}\right)^{-2}-3m^2\left(a_0a_1\right)^{-2}\left(\lambda+e^{\mu t}\right)^{-2n}\exp\left[\frac{-2k_1\left(\lambda+e^{\mu t}\right)^{h+1}}{\mu e^{\mu t}}\right]}$$
$$\frac{1}{-\rho_0 a_0^{3\left(b^2-1\right)}\left(\lambda+e^{\mu t}\right)^{3n\left(b^2-1\right)}} \quad (3.14)$$

First, we consider the simplest case of modified holographic dark energy interacting with dark matter in emergent era and reconstruct the coincidence parameter and equation of state parameter numerically. By imposing the coefficient of shear viscosity is proportional to the scale of expansion, and variable parameter λ in the equation of state, we have the holographic dark energy, which is in general form. In this case the behavior of equation of state parameter is like minimal coupling case. The equation of state parameter $\omega_\Lambda<-1$, which means the phantom-like behavior. This shows that the Emergent scenario is useful for describing the universe because it is in agreement with the real data. The coincidence parameter has a faster decreasing time. The universe at large scale is isotropic and homogeneous and there is no time-like singularity. Cosmological solutions for phantom matter which violates the weak energy condition were found by Dabrowski et al.[47]. Caldwell [48], Srivastava [49], Yadav [50] have investigated phantom models with $\omega_\Lambda<-1$ and also suggested that at late time, phantom energy has appeared as a potential DE candidate which violets the weak as well as strong energy condition.

3.2. Logamediate Scenario

The Logamediate scenario of the universe is motivated by considering a class of possible cosmological solutions with indefinite expansion. In this model the scale factor showing the accelerating expansion of the universe is given by,

$$a(t)=e^{A_1(\log t)^\alpha} \quad (3.15)$$

where $A_1>0,\ \alpha>1$(Bilic, Tupper and Violler [51]).

we assume that the coefficient of shear viscosity is proportional to the scale of expansion, i.e.

$$\eta\ \alpha\ \theta \quad (3.16)$$

That is

$$\eta=\eta_0\theta \quad (3.17)$$

Integrating, we get

$$\int\eta\,dt=3A_1\eta_0(\log t)^\alpha \quad (3.18)$$

Using Eq. (3.15) and (3.18) in Eqs. (2.15)–(2.17), we obtain the exact value of scale factors as

$$A=a_1e^{A_1(\log t)^\alpha}\exp\left[\frac{b_1e^{-3A_1(1+2\eta_0)(\log t)^\alpha t}}{-3A_1(1+2\eta_0)\alpha(\log t)^{\alpha-1}}\right] \quad (3.19)$$

$$B=a_2e^{A_1(\log t)^\alpha}\exp\left[\frac{b_2e^{-3A_1(1+2\eta_0)(\log t)^\alpha t}}{-3A_1(1+2\eta_0)\alpha(\log t)^{\alpha-1}}\right] \quad (3.20)$$

$$C=a_3e^{A_1(\log t)^\alpha}\exp\left[\frac{b_3e^{-3A_1(1+2\eta_0)(\log t)^\alpha t}}{-3A_1(1+2\eta_0)\alpha(\log t)^{\alpha-1}}\right] \quad (3.21)$$

Using Eqs. (3.19)-(3.21) in (1.1), (1.2), the Hubble parameter, its derivative, deceleration parameter and expansion scalar are given by

$$H=\frac{A_1\alpha(\log t)^{\alpha-1}}{t} \quad (3.22)$$

$$\dot{H}=\frac{A_1\alpha(\log t)^{\alpha-2}(\alpha-1-\log t)}{t^2} \quad (3.23)$$

$$q=-\left[\frac{A_1\alpha+(\log t)^{3\alpha-4}(\alpha-1-\log t)}{A_1\alpha}\right] \quad (3.24)$$

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$$\theta = \frac{3A_1\alpha(\log t)^{\alpha-1}}{t} \quad (3.25)$$

Using Eqs. (3.19)–(3.21) in Eqs. (2.21) and (2.22), we get

$$\rho_m = \rho_0 e^{3A_1(b^2-1)(\log t)^{\alpha}} \quad (3.26)$$

$$Q = 3b^2 A_1\alpha(\log t)^{\alpha-1}\rho_0 e^{3A_1(b^2-1)(\log t)^{\alpha}} t^{-1} \quad (3.27)$$

Using Eqs. (3.19)–(3.21) and (3.26) in Eq. (2.7), we obtain the energy density of holographic dark energy as

$$\rho_\Lambda = 3\left(\frac{A_1\alpha(\log t)^{\alpha-1}}{t}\right)^2 - 2(b_1+b_2+b_3)\frac{e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}}{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}}\left(1-3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}-\frac{\alpha-1}{\log t}\right)$$
$$-\frac{3m^2}{a_1^2\exp 2\left[A_1(\log t)^{\alpha}-\frac{b_1 e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}t}{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}}\right]}-\rho_0 e^{3A_1(b^2-1)(\log t)^{\alpha}} \quad (3.28)$$

Using Eqs. (3.18)-(3.20) in Eq. (2.4), we obtain the pressure of holographic dark energy as

$$p_\Lambda = \left(\xi-\frac{2\eta_0 A_1\alpha(\log t)^{\alpha-1}}{t}\right)\frac{3A_1\alpha(\log t)^{\alpha-1}}{t}+3(2\eta_0-1)\left(\frac{A_1\alpha(\log t)^{\alpha-1}}{t}\right)^2+(b_2+b_3-2\eta_0 b_1)e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}$$
$$\left(1-\frac{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}}{t}-\frac{(\alpha-1)}{\log t}\right)-\frac{2A_1\alpha}{t^2}\left((\alpha-1)t(\log t)^{\alpha-2}-(\log t)^{\alpha-1}\right)$$
$$+\frac{(b_2+b_3)}{3A_1\alpha(1+2\eta_0)}e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}\left\{\frac{1}{t}-\frac{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha}}{t}\right.$$
$$\left.-\frac{3A_1\alpha(1+2\eta_0)}{t^2}\left[-3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}-1\right]-\frac{(\alpha-1)}{(\log t)^{2\alpha}t}\left[-3A_1\alpha(1+2\eta_0)(\log t)^{2\alpha-1}-\alpha(\log t)^{\alpha-1}\right]\right\}$$
$$-\frac{(b_2^2+b_3^2+b_2b_3)}{\left(3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}\right)^2}e^{-6A_1(1+2\eta_0)(\log t)^{\alpha}}\left(1-\frac{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}}{t}-\frac{(\alpha-1)}{\log t}\right)^2 \quad (3.29)$$

The EoS parameter of holographic dark energy is given by

$$w_\Lambda = \frac{\left(\xi-\frac{2\eta_0 A_1\alpha(\log t)^{\alpha-1}}{t}\right)\frac{3A_1\alpha(\log t)^{\alpha-1}}{t}+3(2\eta_0-1)\left(\frac{A_1\alpha(\log t)^{\alpha-1}}{t}\right)^2+(b_2+b_3-2\eta_0 b_1)e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}}{3\left(\frac{A_1\alpha(\log t)^{\alpha-1}}{t}\right)^2-2(b_1+b_2+b_3)\frac{e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}}{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}}\left(1-3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}-\frac{\alpha-1}{\log t}\right)}$$
$$\left(1-\frac{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}}{t}-\frac{(\alpha-1)}{\log t}\right)-\frac{2A_1\alpha}{t^2}\left((\alpha-1)t(\log t)^{\alpha-2}-(\log t)^{\alpha-1}\right)$$
$$-\frac{3m^2}{a_1^2\exp 2\left[A_1(\log t)^{\alpha}-\frac{b_1 e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}t}{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}}\right]}-\rho_0 e^{3A_1(b^2-1)(\log t)^{\alpha}}$$
$$+\frac{(b_2+b_3)}{3A_1\alpha(1+2\eta_0)}e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}\left\{\frac{1}{t}-\frac{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha}}{t}\right.$$
$$\left.-\frac{3A_1\alpha(1+2\eta_0)}{t^2}\left[-3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}-1\right]-\frac{(\alpha-1)}{(\log t)^{2\alpha}t}\left[-3A_1\alpha(1+2\eta_0)(\log t)^{2\alpha-1}-\alpha(\log t)^{\alpha-1}\right]\right\} \quad (3.30)$$

The coincidence parameter is given by

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$$\bar{r}=\frac{\rho_0 e^{3A_1\left(b^2-1\right)(\log t)^{\alpha}}}{3\left(\frac{A_1\alpha(\log t)^{\alpha-1}}{t}\right)^2-2\left(b_1+b_2+b_3\right)\frac{e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}}{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}}\left(1-3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}-\frac{\alpha-1}{\log t}\right)}$$

$$-\frac{3m^2}{a_1^2\exp 2\left[A_1(\log t)^{\alpha}-\frac{b_1 e^{-3A_1(1+2\eta_0)(\log t)^{\alpha}}t}{3A_1\alpha(1+2\eta_0)(\log t)^{\alpha-1}}\right]}-\rho_0 e^{3A_1\left(b^2-1\right)(\log t)^{\alpha}} \quad (3.31)$$

The Coincidence parameter and total equation of state parameter in this era with the intermediate scale factor reveals the quintessence-like behavior which is based on the $\omega_\Lambda > -1$. In this case Equation of state parameter is vanishes slower than coincidence parameter. the quintessence model is consistent with present and expected future evolution of the universe. The quintessence model approaches to isotropy at late time.

3.3. Intermediate Scenario

For the scale factor corresponding to intermediate scenario we have,

$$a(t)=e^{B_1 t^{\beta}} \quad (3.32)$$

Where $B_1>0,\ 0<\beta<1$(Bento, Bertolami and Sen [52]).

we assume that the coefficient of shear viscosity is proportional to the scale of expansion, i.e. $\eta\ \alpha\ \theta$

$$\eta=\eta_0\theta \quad (3.33)$$

$$\int \eta\, dt=3\eta_0 B_1 t^{\beta} \quad (3.34)$$

Using Eq. (3.32) and (3.34) in Eqs. (2.15)–(2.17), we obtain the exact value of scale factors as

$$A=a_1\exp\left[B_1 t^{\beta}-\frac{b_1 e^{-3B_1(1+2\eta_0)t^{\beta}}}{3B_1(1+2\eta_0)\beta t^{\beta-1}}\right] \quad (3.35)$$

$$B=a_2\exp\left[B_1 t^{\beta}-\frac{b_2 e^{-3B_1(1+2\eta_0)t^{\beta}}}{3B_1(1+2\eta_0)\beta t^{\beta-1}}\right] \quad (3.36)$$

$$C=a_3\exp\left[B_1 t^{\beta}-\frac{b_3 e^{-3B_1(1+2\eta_0)t^{\beta}}}{3B_1(1+2\eta_0)\beta t^{\beta-1}}\right] \quad (3.37)$$

Using Eqs. (3.35)-(3.37) in (1.1), (1.2), the Hubble parameter, its derivative, deceleration parameter and expansion scalar are given by

$$H=B_1\beta t^{\beta-1} \quad (3.38)$$

$$\dot{H}=B_1\beta(\beta-1)t^{\beta-2} \quad (3.39)$$

$$q=-\left[1+\frac{(\beta-1)}{te^{B_1 t^{\beta}}}\right] \quad (3.40)$$

$$\theta=3B_1\beta t^{\beta-1} \quad (3.41)$$

Using Eqs. (3.35)–(3.37) in Eqs. (2.21) and (2.22), we get

$$\rho_m=\rho_0 e^{3B_1\left(b^2-1\right)t^{\beta}} \quad (3.42)$$

$$Q=3b^2B_1\rho_0\beta t^{\beta-1}e^{3B_1\left(b^2-1\right)t^{\beta}} \quad (3.43)$$

Using Eqs. (3.35)–(3.37) and (3.41) in Eq. (2.7), we obtain the energy density of holographic dark energy as

$$\rho_\Lambda=3\left(B_1\beta t^{\beta-1}\right)^2+\frac{2\left(b_1+b_2+b_3\right)}{3(1+2\eta_0)t^{\beta-1}}e^{-3B_1(1+2\eta_0)t^{\beta}}\left[3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right]$$

$$\frac{2\left(b_1b_2+b_2b_3+b_1b_3\right)}{3B_1\beta(1+2\eta_0)t^{2(\beta-1)}}e^{-3B_1(1+2\eta_0)t^{\beta}}\left[3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right]$$

$$-\frac{3m^2}{a_1^2\exp 2\left[B_1 t^{\beta}-\frac{b_1 e^{-3B_1(1+2\eta_0)t^{\beta}}}{3B_1\beta(1+2\eta_0)t^{\beta-1}}\right]}-\rho_0 e^{3\left(b^2-1\right)B_1 t^{\beta}} \quad (3.44)$$

Using Eqs. (3.35)-(3.37) in Eq. (2.4), we obtain the pressure of holographic dark energy as

$$p_\Lambda=3B_1\beta\left(\xi-2\eta_0B_1\beta t^{\beta-1}\right)t^{\beta-1}+6\eta_0\left[\left(B_1\beta t^{\beta-1}\right)^2+\frac{b_1e^{-3B_1(1+2\eta_0)t^{\beta}}}{3(1+2\eta_0)t^{\beta-1}}\left(3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right)\right]$$

$$-\Big[2B_1\beta(\beta-1)t^{\beta-2}-3(b_2+b_3)B_1(1+2\eta_0)\beta t^{\beta-1}e^{-3B_1(1+2\eta_0)t^{\beta}}$$

$$-\frac{(\beta-1)(b_2+b_3)}{3(1+2\eta_0)B_1}e^{-3B_1(1+2\eta_0)t^{\beta}}t^{-2\beta}\left(3B_1(1+2\eta_0)t^{2\beta-1}+t^{\beta-1}\right)\Big]$$

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$$-\left[3\left(B_1\beta\ t^{\beta-1}\right)^2+3(b_2+b_3)B_1\frac{t^{\beta-1}e^{-3B_1(1+2\eta_0)t^\beta}}{3(1+2\eta_0)t^{2(\beta-1)}}\left(3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{(\beta-2)}\right)\right]$$

$$+\left(b_2^2+b_3^2+b_2b_3\right)\frac{e^{-6B_1(1+2\eta_0)t^\beta}}{\left(3B_1\beta(1+2\eta_0)t^{2(\beta-1)}\right)^2}\left(3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right)^2$$

$$+\frac{m^2}{a_1^2\exp 2\left[B_1t^\beta-\frac{b_1e^{-3B_1(1+2\eta_0)t^\beta}}{3B_1\beta(1+2\eta_0)t^{\beta-1}}\right]} \quad (3.45)$$

The EoS parameter of holographic dark energy is given by

$$w_\Lambda=\frac{3B_1\beta\left(\xi-2\eta_0B_1\beta t^{\beta-1}\right)t^{\beta-1}+6\eta_0\left[\left(B_1\beta t^{\beta-1}\right)^2+\frac{b_1e^{-3B_1(1+2\eta_0)t^\beta}}{3(1+2\eta_0)t^{\beta-1}}\left(3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right)\right]}{3\left(B_1\beta t^{\beta-1}\right)^2+\frac{2(b_1+b_2+b_3)}{3(1+2\eta_0)t^{\beta-1}}e^{-3B_1(1+2\eta_0)t^\beta}\left[3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right]}$$

$$\frac{-\left[2B_1\beta(\beta-1)t^{\beta-2}-3(b_2+b_3)B_1(1+2\eta_0)\beta t^{\beta-1}e^{-3B_1(1+2\eta_0)t^\beta}\right.}{\frac{2(b_1b_2+b_2b_3+b_1b_3)}{3B_1\beta(1+2\eta_0)t^{2(\beta-1)}}e^{-3B_1(1+2\eta_0)t^\beta}\left[3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right]}$$

$$\left.-\frac{(\beta-1)(b_2+b_3)}{3(1+2\eta_0)B_1}e^{-3B_1(1+2\eta_0)t^\beta}t^{-2\beta}\left(3B_1(1+2\eta_0)t^{2\beta-1}+t^{\beta-1}\right)\right]$$

$$-\frac{3m^2}{a_1^2\exp 2\left[B_1t^\beta-\frac{b_1e^{-3B_1(1+2\eta_0)t^\beta}}{3B_1\beta(1+2\eta_0)t^{\beta-1}}\right]}-\rho_0e^{3\left(b^2-1\right)B_1t^\beta}$$

$$-\left[3\left(B_1\beta\ t^{\beta-1}\right)^2+3(b_2+b_3)B_1\frac{t^{\beta-1}e^{-3B_1(1+2\eta_0)t^\beta}}{3(1+2\eta_0)t^{2(\beta-1)}}\left(3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{(\beta-2)}\right)\right]$$

$$+\left(b_2^2+b_3^2+b_2b_3\right)\frac{e^{-6B_1(1+2\eta_0)t^\beta}}{\left(3B_1\beta(1+2\eta_0)t^{2(\beta-1)}\right)^2}\left(3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right)^2$$

$$+\frac{m^2}{a_1^2\exp 2\left[B_1t^\beta-\frac{b_1e^{-3B_1(1+2\eta_0)t^\beta}}{3B_1\beta(1+2\eta_0)t^{\beta-1}}\right]} \quad (3.46)$$

The coincidence parameter is given by

$$\bar{r}=\frac{\rho_0e^{3B_1\left(b^2-1\right)t^\beta}}{3\left(B_1\beta t^{\beta-1}\right)^2+\frac{2(b_1+b_2+b_3)}{3(1+2\eta_0)t^{\beta-1}}e^{-3B_1(1+2\eta_0)t^\beta}\left[3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right]}$$

$$\frac{}{\frac{2(b_1b_2+b_2b_3+b_1b_3)}{3B_1\beta(1+2\eta_0)t^{2(\beta-1)}}e^{-3B_1(1+2\eta_0)t^\beta}\left[3B_1\beta(1+2\eta_0)t^{2(\beta-1)}+(\beta-1)t^{\beta-2}\right]}$$

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$$-\frac{3m^2}{a_1^2\exp 2\left[B_1 t^{\beta}-\frac{b_1 e^{-3B_1(1+2\eta_0)t^{\beta}}}{3B_1\beta(1+2\eta_0)t^{\beta-1}}\right]}-\rho_0 e^{3(b^2-1)B_1 t^{\beta}} \quad (3.47)$$

It is observed that at t = 0, the parameters θ, H diverge. Hence the model starts with a big bang singularity at t = 0. This is a Point Type singularity (MacCallum [53]) since directional scale factor A, B and C vanish at initial time. The Coincidence parameter and total equation of state parameter in this era with the intermediate scale factor reveals the quintessence-like behavior which is based on the $\omega_\Lambda > -1$. In this case Equation of state parameter is vanishes slower than coincidence parameter.

4. Conclusion

In this paper we have studied the anisotropic and homogeneous Bianchi type-V universe filled with interacting Dark matter and Holographic dark energy. Here we discussed three different scenario. $w_\Lambda < 0$ is necessarily accompanied by the decay of the dark energy component into pressureless dark matter $(b^2 > 0)$. It is shown that for suitable choice of interaction between dark matter and holographic dark energy i.e. Eq. (2.20) with $(b^2 = 1)$, there is no coincidence problem in case of exponential volumetric expansion model and special form of deceleration parameter which matches with the observations as we now live in the stationary coincidence state of the universe, whereas there is coincidence problem in case of power-law volumetric expansion model. In the Emergent case, we found the phantom-like behavior due to the w_Λ, leads to uncommon cosmological scenarios and quintessence-like behaviors in the Intermediate and Logamediate era is obvious. Since the Phantom-like behavior is more consistent with the observational data, Then the Emergent scenario is better than the Logamediate and Intermediate ones. It is observed that such DE models are also in good harmony with current observations. Thus, the solutions demonstrated in this paper may be useful for better understanding of the characteristic of anisotropic DE in the evolution of the universe within the framework of Bianchi type-V space-time.

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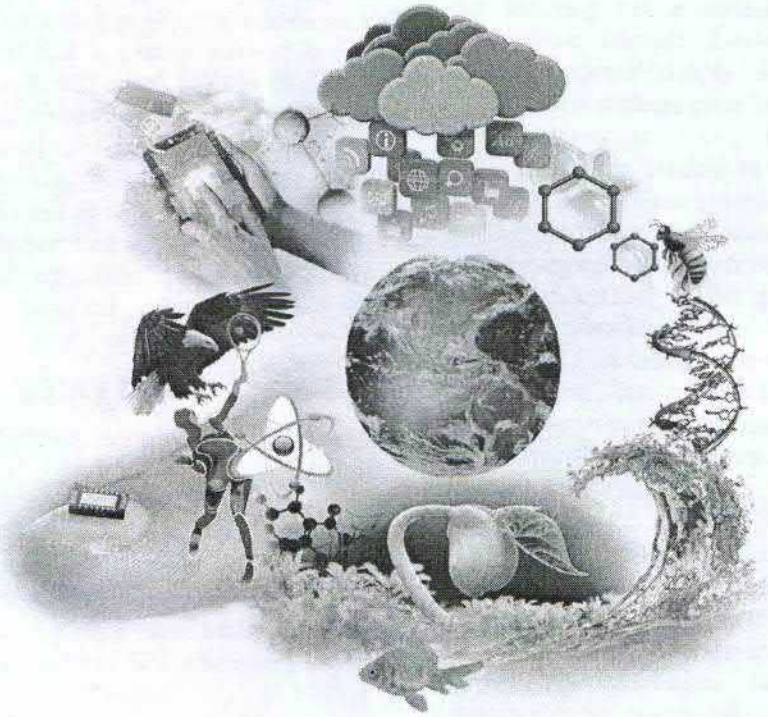

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Aayushi International Interdisciplinary Research Journal (AIIRJ)
ISSN 2349-638x Impact Factor 4.574 Special Issue No. 25
UGC Approved Sr.No.64259 **Website :-** www.aiirjournal.com **Email id:-** aiirjpramod@gmail.com

USE OF INFORMATION TECHNOLOGY IN PHYSICAL EDUCATION & SPORT

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INTRODUCTION

In a modern & Technical era in the field of physical education & sports it is most to use new technique, new equipments & new tools to improve the standards & performance for this. Hi-Tech Technology is the most important factor in the field of physical education & sports.

Hi technology important roles for delivering physical education & sports around the world, ICT has changed the development planning and management of coaching in physical education and sport. The use of ICT is easiest method & gets a effectiveness result. ICT available for all any time & any where implementation of ICT in physical education & sports are enhanced he performance of player & achieving best level, for this purpose paper focused on use of ICT in physical education & sports, new concept of ICT application of ICT, role of physical education Teacher & coaches, suggestion for physical education teacher & coaches etc.

WHAT IS ICT

ICT is an umbrella term that includes any communication device or application, encompassing radio, cellular phone, computer, network & software satellite system & so on, as well as the various services & application associated with them such as video conferencing & distance learning ICT are often spoken in particular context, such as ICT education, physical education, sports & health care.

DEFINATION OF ICT

Information Technology is an application & commodity support through which or by means of which information is transferred, recorded, edited, sotred manipulated or disseminated.

According to UNESCO information technology as scientific, technology & engineering disciplines & management techniques used in information handling & processing information & their application, computer & their interaction with man & machine & associated social, economic & cultural matters.

ICT TO IMPROVE STUDENT LEARNING

ICT should to be utilized selectively within the learning context & should focus upon improving students understanding & enthusiasm. The prime goal must reside with effective teaching & learning with ICT contributing to such a dynamic process.

It is important to remember that ICT is not a tool for learning but a medium for delivering pre determined content. Lessons must be avoided where students simply search for & retrieve information with no prior learning outcomes being set by the teacher.

ICT allows the teacher to reconsider teaching & learning & frees the teaching form the constraints of the classroom & traditional teaching strategies. ICT is appealing to students & must surely be the preferred learning mode, given that the computer is often viewed as the 'Child's Machine'. If learning materials are designed around technologies, the students should be motivated by such opportunities as use of technologies in physical education & sports.

TALEMATICS

Telematics typically is any integrated use of telecommunications & informatics, also now as ICT telematics is originally coined to mean the convergence of telecommunication & information processing, the term later evolve to refer automation in automobiles. This includes dial up services to the internet as well as all type of networks with Global positioning system (GPS) tracking data processing is very sophisticated system of handling software & language.

MULTIMEDIA

Computer have integrated learning with multimedia presentations.

- Internet : A global network providing the capability to communicate, share ideas & access information & resources from around the globe.

- Intranet : Similar to the internet, but information from within a school or organization.
- World wide web : The world wide web is that part of the internet supporting graphics audio, video & hyperlinks (the ability to connect form on computer site to another) as well as standard text.
- Local area network : The development of local area networks (LANs) allows computer users to communicate with each other without leaving their location or without the need of a telephone conversation.
- Technology in physical education & sports in Physical education & sport field. Technology helps physical education teachers) coaches/ Trainers to enhance the learning process in academics & sports performance by employing innovative techniques/ methods. Technology is used an effective tool to enhance I the authenticity of the decisions & results.

The learning process in academics and sports performance by employing innovative techniques/methods. Technology is used as an effective tool to enhance I the authenticity of the decision and results.

Assisting the Umpires/Referees : In the field of sports instant replay and other high-tech aids are used to help referees in order to make the right call. Basketball referees use replay systems to make sure players are shooting within the time allotted by the shot clock. In international cricket, the third umpire sitting off the ground with access to TV replays of certain situations (such as disputed catches and boundaries) to advise the central umpires. The umpires out on the field are in communication via wireless technology with the other umpire. The Third umpire is also asked to adjudicate on am out decisions, which he makes without consultation with the two central umpires. Replays could be used to decide off-side decisions, whether a ball passes over the goal line, and clarify penalty decisions in football.

Hawk-Eye Technology : Hawk-Eye is revolutionary sports tracking device. Hawkeye is the name of computer and camera system which traces a ball's trajectory. This has helped transform coverage of Test Cricket and other sports, including tennis. Hawke- eyes used in Wimbledon providing both stats and line call coverage for the BBC and ESPN. The system is the most technologically advanced cricket coaching system in the world. It provides valuable information to players, coaches and umpires to enable them to identify faults, measure performance and improvement, focus on specific areas and improve tactical awareness. Hawk-Eye is currently developing a system to have correct decisions in any kind of game. HawkEye is a computer system used in cricket tennis, snookers, volleyball, basketball, hockey, wushu, cycle polo and other sports to visually track the path of the ball and display a record of its most statistically likely path as a moving image Hawk-Eye can track any type of bounce, spin, swing and seam movement of the ball. Give as prediction as accurate as 99.99 percent Hawk-Eye was used for referring decisions to the third umpire in LB,W. They track the ball's entire trajectory, right from the point where it is released from the bowler's hand to the point the ball is considered dead.

Authentic Substitute for Human Error: In the earlier days, whatever decision was made by the match officials was considered the last word. Though efforts had been made by all the great sports governing bodies of the world to do away with bias, yet the element of human error still remained and will continue to exist. What technology strives to do is to remove the element of human error in the course of a match been played.

Technological Advancement in Equipments: Equipment is constantly changing in all sports. It has become to increase power and reduce injury, it is now stronger and provides better protection in certain sports.

Technological Advancement in facilities : Technology has improved the materials that are available to sports manufacturers making the athlete more aerodynamic in swimming cycling, skating and has improved the quality of surfaces in football, hockey tennis athletics and gymnasium halls. Improvement in playing surfaces has made the sports safer and attractive. Fitness Gyms are full of computerized training Equipment, Stadiums are being updated to make spectators Safer.

Technology Applied to athlete's Health : Ranging from nutrition to the treatment of injuries, as'She knowledge of the human body has deepened over time, an athlete's potential has beini, increased[1]:, Athletes are now able to play to an older age, recover more quickly from injuries and train more effectively than previous generations of athletes.

Encourage Research : Advance technology Created new opportunities for research in physical education and sports. Being able to use motion

capture to capture an athlete's movement or advanced computer simulations to model physical scenarios has greatly increased an athlete's ability to understand what they are doing and how they can improve themselves.

Technology Advancements in Sports:

Technology continues to transform many aspects of our lives. Today with the advent of mobiles phones we can communicate with the rest of the world no matter where we are, micro sensors can detect an imminent car crash and deploy airbags in the instant before a collision, and computes that once filled a room can be carried in our pockets and owned by everyone. Technology has gone a long way in proving its mettle in sport. It has created a niche for itself in every major sport on the planet. Be it the outdoor sports like soccer, tennis or cricket or their indoor counterparts like snooker, badminton or basketball technology is used in each one of them. Treadmills swimming flumes, cycling and rowing machines replace the usual athletic environment so that they can be more easily assessed. Ventilators can be used to monitor lung function and consumption of oxygen. Pedometers, heart rate monitors and trip computers for bicycles today are common place and represent some of the earliest technological innovations popular with elite and recreation athletes alike. A runner, swimmer or rower wearing these devices can have examined in detail their performance on the track or even on race day itself.

Hot Spot : Hot spot is an infra-red imaging system used in cricket to determine whether the ball has struck the batsman, bat or pad . Hot spot is new technology that requires two infrared cameras on opposite sides of the ground above the field of play that are continuously recording an image. With the use of this technology we can help the batsman in knowing the truth that the ball had stuck the pad and not the bat, with the help of the white spot which is produced on the pad.

The White Spot : Whenever we slap a person, we are applying some force and at this instant the heats is produced due to the friction that occurs between the face and hands and if we use the IR cameras we could easily detect this.

Hypcndc Tent : An altitude tent, also known as an altitude simulation tent or hypoxic tent, is an enclosed living space which simulates high altitude by maintaining a lower oxygen concentration. It is used by •athletes and by high altitude mountain climbers to stimulate the body's natural adaptations to altitude $_{M}$ including an increase in the number of red blood cells and enzymes, Red blood cells carry oxygen to the body; athletes benefits from increased delivery of oxygen to the muscles, and mountain climbers can avoid altitude sickness by better utilizing the diminished amount of oxygen found at high altitudes.

Automated Boxing Scoring System : The Automated boxing scoring system (ABSS) is a research and development project being developed by a group of Australian institutions and private companies. It aims to provide a training aid and unbiased scoring for the sport of Amateur Boxing and potentially other Combat and Martial are sports.

Pre Cool Vest: A cooling vest or ice vest or "pre cool vest" is a piece of equipment worn to cool a person down. Cooling vests are used by many athletes, industry workers, doctors working dogs, people with Multiple Sclerosis or Hypo hidrotic ectodermic dysphasia and by military pilots and tank crew. Olympic athletes use the lightweight body cooling vest to pre-cool before events.

Cyclops : Cyclops is computer system conceived by British inventor Bill Carlton of Malta, which is used on the ATP and WTP professional tennis tours to help determine whether a serve is in or out. The system, which must be activated by the chair umpire before each serve, projects five or six infra-red horizontal becams of light along the court 10 mm above the ground. One beam covers the good (short) side of the service line and others cover the fault (long) side.

Desso Grass Master : Desso Grass Master is a sports playing field surface composed of natural grass combined with artificial fibres. The artificial grass fibers are injected 20 centimeters (7.9) in deep and cover about 3% of the surface. While the grass is growing. The roots inter wine with the artificial fibers. The designers claim this anchors the field to create a solid, even structure with good drainage and 'playing comfort'

Goal-Line Technology : Goal-line technology is proposed technology which determines when the ball has crossed the goal -line thus indicating whether a goal has been scored or not. Goal-line technology has not yet been implemented in a competitive game of association football.

Point Tracker : Point Tracker created by IBM, is an application featured in grand slam tennis tournaments that presents an animated 3D view of each shot played in a singles match.

Global Position Systems : High precision GPS or Global positioning systems now have accuracy better than 1 Ocm and can be used to monitor

runners, skiers, football players and rowing sculls position and even velocity. **Rail Cam** : The camera is fastened to rail system that runs on the top of the glass on one side of the ice rink. As the play shifts from end to end, the motorized mount allows the camera to follow the action, sliding rapidly down the side of the ice. Though there is an ongoing dehiic *on* the feasibility of the use of technology in sports, it has certainly provided man with a useful tool to reduce human error and increase performance and as far as its scope is concerned, it is definitely here to stay.

EMG Biofeedback : EMG stands for electromyography, measures the electrical response of the muscles when contracting. The electrical response is measured with pads placed on the skin and results are displayed visually and /or indicated by a tone sound. By indirectly measuring muscle contraction, this allows the used to see and/or hear their level of muscular tension; EMG biofeedback produces rapid and significantly greater development of strength when combined with more traditional form of strength training. It is used for muscle reeducation and strengthening in sports rehabilitation following surgery or trauma, selective training of a particular muscle after injury and to remediate neck, scapular and lower back pain.

SUMMARY

At last, it is to be said that technology has become a part and parcel of entire physical education and sports environment, other than the area of broadcasting and televising sports events. Technology in the form of teaching aids (wind gauge, underwater camera, photo finish camera, various measuring tools, foul indicators, electronic gadgets, overhead and LCD Projectors, laser beam technology, adobe Photoshop etc.) helps the physical education teacher and sports trainers to make their teaching and coaching more interesting and also improves the teacher-taught relationship.

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Aayushi International Interdisciplinary Research Journal (AIIRJ)
ISSN 2349-638x Impact Factor 4.574 Special Issue No. 25
UGC Approved Sr.No.64259 Website :- www.aiirjournal.com Email id:- aiirjpramod@gmail.com

THE ROLE OF TECHNOLOGY IN THE AGRICULTURE DEVELOPMENT OF INDIA

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ABSTRACT

In the development of our country technology has been proving very resourceful for all round development of the society at large. In short technology has the potential to play an important role in economic growth and social development, . India has come up with various technological innovations in every sector. This paper reviews several aspects of role of technology in the evolution of Indian Economy.

Keywords: Agriculture, Technology, India

INTRODUCTION

Technology has been spreading all over the world by leaps and bounds. It has encroached every walk of life. India as a country has made progress in every sector after her independence. In the last seven decades, in the fields of industry, agriculture, education and banking, our country has made tremendous progress. India is a mixed economy and its base is agriculture. Our nation cannot progress unless we make development in the field agriculture. The complete raw materials are sought from agricultural resources. Thus, every industry runs with the support of agricultural products only.

It has changed the face of industry, banking, agriculture, education and means of transportation. The Indian economy has geared up its speed in present context. Indian industry has growth many manifold since 1980s. The industry has contributed considerably to the economic in terms of GDP employments and foreign exchange earnings. Because of spread of technology the competence of industry is increasing and almost all sectors of the economy like services and at banks, post offices, railways airports etc.

Information technology is a knowledge based industry, IT industry embraces production, manipulation, storage and dissemination of information. IT sector has a remarkable potential for accelerating economic growth of the nation. It has made our governance efficient. It enhances excess to information, excess to government services, protects consumers, makes skill development and training more effective, progresses delivery health services and promotes transparency. Thus the role of IT industry in enhancing the economic development of country has been acknowledged by the government.

Beside IT Biotechnology has brought radical changes in agriculture. Use of Biotechnological tools in agriculture could make food crops high yielding and more robust to biotic and a - biotic stresses. This could stabilized and increase food supplies which is important against the background of increasing food demand, climate change and land and water scarcity. Due to biotechnological tools the productivity of the food crops have increased immensely, such as soybean, corn, cotton etc. Bt cotton has certainly increased the profitability of the farmers and at the same time it reduced the use of chemical pesticides in this crop drastically. Studies suggest that the introduction of Bt technology has reduced food insecurity by 15-20% among Indian cotton growers. The country has also developed golden rice which is rich in B-carotene. This is a great solution for India as nearly Five Thousand children go-blind every year because of deficiency of B-carotene. Thus biotechnology has supported the Indian Economy.

Nanotechnology can be used in agriculture in many ways. It can help in promoting soil fertility and balanced crop nutrition, effective weed control, enhancing seed emergence using carbon nanotubes, delivery of agriculture chemicals, field sensing system to monitor the environmental stressed and crop conditions and improvement of plant trades against environmental stresses and diseases. Application within animal husbandary might include improving feeding efficiency and nutrition of agricultural animals, minimizing losses from animal diseases, and turning animal by products and waste and environmental concerns

into value added products. In short, nanotechnology after considerable opportunities for the development of innovative products and application for agriculture, water treatment, food production, processing, preservation and packaging. Its use may bring benefits to farmers, food industry and consumers alike. Thus, nanotechnology has huge potential in revolutionizing the food packaging.

Protected cultivation or greenhouse cultivation is the most promising area where productions of horticultural crops has improved qualitatively world over in the last few decades. At present Spain, the Netherland and Israel are the leaders in cultivation of crops in polyhouses and greenhouses. The application of plasticulture can decrease the costs and therefore can lead to high productivity with a better quality of crops. In India the area under protected cultivation is around 25000 ha while the greenhouse vegetable cultivation area is about 2000 ha. India and the Netherlands having more or less same land under flower cultivation but in flower export, the contribution of Netherlands is 70% and India's contribution is just 1% because of advanced technology of polyhouses in the Netherlands. There technology based methods of cultivation have made a great revolution in the world market. Gradually, India is making a more in that direction of technology.

Technology has geared up the use of modern irrigation methods because of which the agricultural income has been increased immensely. Availability of enough water for crops in India is very critical. Raining in India is uncertain. Without water expected yield can not be achieved from agricultural sector. In India 78% water goes to the agriculture sector while the remaining goes to drinking, industry and other usage. But in modern times by using science and technology different irrigation system have been developed, such as dripping sprinkling and water guns, mechanisms have been devised. It has helped the country like India to save water on large scale. These modern techniques of irrigation will increase irrigation potential in the direction of the optimal utilization of water resources to optimum irrigation scheduling. Micro irrigation is advance techniques of irrigation and it will increase water used efficiency and crop productivity.

Indian agriculture market is flourishing compared to that of past because modern technology has developed fastest transfer tools. Now most of the action and work related to farming have become technology supported the sowing of the seed, crop protection, harvesting, post harvest management to marketing have become sophisticated. Central government of India has under taken a program of connecting every Grampanchyat of the country with internet facilities. These Grampanchyat should become technology transfer hubs to the farmers.

Internet and mobile phones are powerful tools to impart knowledge on new developments, improve methods of cultivation in the field of agriculture. These tools can help in understand weather data and agro-climate condition, information of prices of agricultural products to the farmer. Throughout the country in each district KVKs have been established to make spread of latest technology in agriculture.

Variety of new methods is brought in force to make farming easy going business. Pesticides, fertilizers, micronutrients and computer assisted regulation have become a big boon to the Indian agriculture system.

In a way the use of technology in agriculture have supported the nation at large enhancing the ill-health of Indian economy. Technology has added its huge contribution in the general national income of our country.

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VOL. 5 SPECIAL ISSUE 4 APRIL 2018 UGC Approved Journal No. 45886 ISSN: 2348-1390

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International Journal of Multidisciplinary Studies

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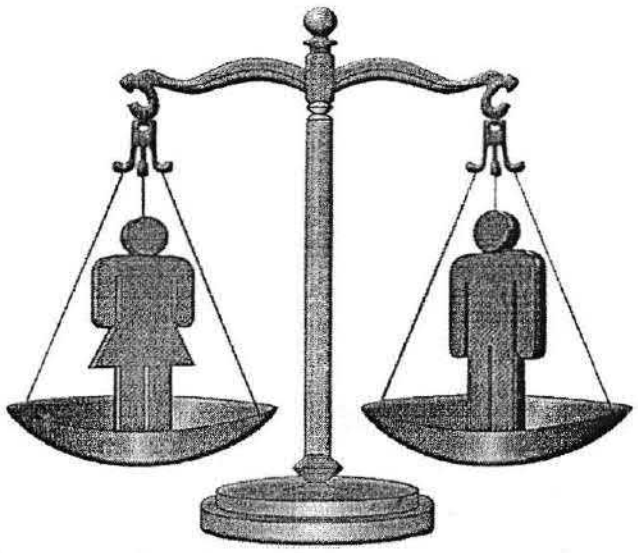

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New Man International Journal of Multidisciplinary Studies
(UGC Approved Journal No. 45886)
ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

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स्त्रियांनो - सुर्योदय होत आहे

डॉ. मीनल खेरडे

विद्याभारती महाविद्यालय, अमरावती.

प्रस्तावना :- 'दोन घडीचा डाव याला जीवन ऐसे नाव' हा डाव आपण रडीचा की चिडीचा खेळणार हे आपण ठरवायचे. वैदिक काळात स्त्री स्वातंत्र्य अबाधित होते. पण उत्तर वैदिक काळात स्त्रियांवर बंधने लादण्यात आली. रामायणात सितेला लक्ष्मण रेषा आखून दिली होती. पण महाभारतात प्रत्येक स्त्री पात्र व्यासाने स्वयंपूर्ण साकारलेले आहे. ती स्वयंभूपणे जगणारी आहे. मानवी समाजात स्त्रियांचा सहभाग पुरुषांच्या बरोबरीने असला तरी स्त्रियांना समान दर्जा मात्र मिळालेला नाही. पुरुष प्रधान व्यवस्थेत जगाचा उध्दार करणारी स्त्री ही रजस्त्रावाच्या वेळी वेगळी मानल्या जावू लागली. मातृत्व आणि लैंगिकता यांच्या सीमा रेषा ठरविल्या गेल्या आणि स्त्रियांना दुय्यम स्थानात बंदिस्त केले.

इ.स.पुर्व ६ व्या शतकात स्त्री दास्यत्वाची कहानी सुरु झाली. शुद्रकाचे मुच्छकटिकम्, मनुस्मृती याज्ञवाल्यकल्य स्मृतीवरुन तत्कालिन स्त्रियांचे शैक्षणिक, राजकीय, आर्थिक हक्क, अधिकार लोप पावलेले दिसतात. मध्यकाळात तिच्या व्यक्ती स्वातंत्र्याची कल्पनाच समाजाने अमान्य केली. भारतीय समाजाने स्त्रियांची स्थिती दयनीय केली. तिच्या सर्वांगीण उन्नतीच्या अधिकारांची पायमल्ली झाल्याने कौटुंबिक व्यवस्थेत तिचे स्थान दुय्यम दर्जाचे झाले. तथापि झाशीची राणी लक्ष्मीबाई, अहिल्याबाई होळकर ही काही अपवादात्मक उदाहरण आहेत.

पुढे १९ व्या शतकात मात्र ब्रिटींशाच्या शैक्षणिक धोरणामुळे आधुनिक शिक्षण प्रणालीचा प्रारंभ होवून स्त्रियांना आशेचा किरण दिसू लागला. नवशिक्षित तरुण पाश्चात्यांच्या आधुनिक विचारांनी प्रभावित होवून त्यांनी स्त्रियांच्या अनेक प्रश्नांना वाचा फोडण्याचे काम केले. यात राजाराम मोहनरॉय, ज्योतिबा फुले, धोंडो केशव कर्वे, विठ्ठल रामजी शिंदे, राष्ट्रसंत तुकडोजी महाराज, महात्मा गांधी, डॉ. बाबासाहेब आंबेडकर यांनी पोषक वातावरण निर्माण केले. राष्ट्रसंत तुकडोजी महाराज म्हणतात, स्त्रीला हीन समजणे तिचा अनादर करणे हे जर समाजाला मान्य असेल तर भारत कदापि शक्तीशाली राष्ट्र बनणार नाही. वरील सर्व महापुरुषांनी स्त्रियांची सामाजिक बंधनातून मुक्तता करण्याकरीता शिक्षणास प्राधान्य देवून परंपरांना मुठमाती दिली. स्त्रीचा सामाजिक दर्जा नाकारुन समाजाची ५०% क्षमता वाया घालवणे हे समाज आणि राष्ट्राच्या उन्नतीकरिता अत्यंत घातक आहे. यावर उपाय म्हणून अनेक कायदे अस्तित्वात आलेत. महिलांच्या उन्नतीच्या दृष्टीने डॉ. बाबासाहेब आंबेडकरांनी हिंदू कोड बील आणले. हिंदू कोड बील हा एक महत्त्वपूर्ण टप्पा समजल्या जातो. या बिलामुळे स्त्रियांना घटस्फोटाचे अधिकार, घटस्फोटीत स्त्रीला पोटगीचा अधिकार, संपत्तीचा अधिकार, आंतरजातीय विवाहास मान्यता हे अधिकार मिळाले म्हणजे स्त्रियांनी आता अर्धी लढाई जिंकली होती. सतीबंदी कायदा १८२९, विधवा विवाह कायदा १८५६, बालविवाह प्रतिबंध कायदा १९२९, मुलींचा अनैतिक व्यापार विरोधी कायदा १९५६, दत्तक घेण्याचा कायदा १९५६, हुंडा प्रतिबंध कायदा १९६१, हिंदू विवाह कायदा १८७२,समान वेतन विरोधी कायदा १९७६, कौटुंबिक हिंसाचार प्रतिबंध कायदा २००५. हे सर्व कायदे पारीत करुन भारतीय लोकशाहीने स्त्रियांना केवळ कौटुंबिक स्तरावर नव्हे तर आर्थिक, सामाजिक बाबतीत ही संरक्षण दिले. आज स्त्रिया ज्या प्रकारे कर्तृत्व गाजवत आहेत हे त्या कायद्याचे फलित आहे.

स्वातंत्र्यापूर्वी अबला समजल्या जाणारी स्त्री जात सबला बनली होती. कौटुंबिक जबाबदाऱ्या सांभाळून स्त्री यशस्वीपणे यशाची शिखरे गाठत होती. या सर्व बदलामुळे समान काम, समान वेतन स्त्रियांना मिळावे याची जाणीव झाली. १९७५ मध्ये ही मागणी केली. १९८८ नंतर मार्क्सवादी कम्युनिष्ट पक्षाने स्त्री मुक्ती संस्थेने पुरुषाइतकेच स्त्रीला वेतन मिळावे म्हणून लढा दिला. स्त्री संघटनांनी समान वेतनावर भर दिला. कायम स्वरुपात असलेल्या स्त्री कामगारांना त्याचा फायदा मिळाला. पण कायमस्वरुपी काम नसलेल्या कष्टकरी स्त्रिया मात्र वंचित आहे. आज गरज आहे अशा स्त्रियांचा प्रश्न सोडविण्याची. याशिवाय अनेक कायदे स्त्रियांसाठी पारीत करण्यात आले.

काही निवडक कायदे खाली नमुद करण्यात आले आहे.

१. **स्त्रियांना अटक करु शकत नाही -** सुप्रिम कोर्टाच्या आदेशानुसार सुर्यास्तानंतर स्त्रियांना अटक करता येत नाही. अगदी महिला शिपाही सुध्दा स्त्रीला अटक करु शकत नाही. फारच गंभीर गुन्हा असल्यास न्यायालयास अटकेचे लेखी कारण दयावे लागते.

२. **प्रायव्हीचीचा अधिकार -** रेप पिडीत महिला खाजगी जबाब देवू शकते. त्यावेळी मॅजिस्ट्रेट सोबत असतात पिडीत स्त्री कॉन्स्टेबल आणि पोलीस सर्वासमोर जबाब देण्यासाठी दबाव आणू शकत नाही.

३. **कितीही काळानंतर नोंदवू शकता तक्रार -** बऱ्याचशा महिला समाजाच्य, कुटुंबाच्या व इतर तत्सम कारणामुळे पोलिसांकडे तक्रार करत नाहीत पण कितीही उशीर झाला तरी स्त्री तक्रार करु शकते. ही तक्रार नोंदवायला पोलीस तक्रार देवू शकत नाहीत मात्र महिला ईमेलच्या माध्यमातूनही तक्रार देवू शकते.

पटलावर सतत संघर्ष करुन उच्चपद प्राप्त केले. त्या भारताच्या प्रथम महिला राष्ट्रपती बनल्या तर सिंधूताई सपकाळ ह्या अडचणीवर मात करुन हजारोंची आई झाल्या. जिला स्वतःचे घर नव्हते तीने हजारोंना आश्रय दिला. रझिया सुलतान, नलिनीताई लढके, यशोमती ठाकूर, राणी बंग, अशा अनेक स्त्रियांची नावे नमुद करता येतील. यांनी प्रश्न सोडविण्याचे काम केले म्हणून त्यांच्या नावाची नोंद आपणास प्रेरणादाई वाटते.

समाजाचा दुसरा वर्ग म्हणजे कष्टकरी समाज कष्टकरी स्त्रियांचे आयुष्य पाहता परिस्थितीवर मात करुन धडपडत राहण्याची प्रेरणा त्यांना कशातून मिळते. स्त्री स्वांतत्र्य, स्त्री मुक्ती समानता या प्रश्नावर विचार तर सोडाच पण हे शब्दही त्यांच्या कानावरुन गेलेले नसतात. पण परिस्थितीचे आव्हान स्वीकारुन दारुडा नवरा, आर्थिक विवंचना, आजारी सासू सासरे, पडकी घरे, गलिच्छ वस्ती, कायमस्वरुपी नसणारे काम, एक ना अनेक प्रश्न घेवून केवळ इच्छा शक्तीच्या बळावर परिस्थितीवर मात करुन उरले सुरले सामाजिक भानही त्या जोपासतात. अशा स्त्रियांशी संभाषण केल्यास आपल्या जीवनातील लहान सहान दुःख कुरवाळीत बसणाऱ्या आम्हा मध्यमवर्गीय स्त्रियांमध्ये काही जिद्द करारीपणा आणि चौकटी पलिकडे काही करण्याची उर्मी निर्माण होईल का? मला माहित नाही पण हे सर्व परिषदेस उपस्थित असणाऱ्यांना विचार करायला लावणारे आहे.

सारांश :-आज समाजात स्त्रियांना शिक्षण आहे पण त्यांचा स्त्रियांनी वापर करणे शिकले पाहिजे. सरकारने सर्व सुविधा दिल्या तरी त्याची माहिती स्त्रियांनी स्त्रियांपर्यंत पोहचविली पाहिजे. काही कायद्यामध्ये सुधारणा घडवून आणली पाहिजे. यासाठी स्त्रियांनी पुढाकार घेतला पाहिजे. तलाक विरोधी कायद्याला स्त्रियांच मोर्चा काढून विरोध करतात. स्त्रियांनी या मुस्लिम समाजातील स्त्रियांच्या पाठीशी उभे राहून तिला मदतीचा हात दिला पाहिजे. सर्वात महत्त्वाचे तिने कायदे वाचून समजून घेतले पाहिजे. समान वेतनाचा कायदा किती कष्टकरी स्त्रियांना माहित आहे तो समजावून सांगण्याचे काम सुशिक्षित स्त्रियांचे आहे. समान काम समान वेतन हे रुजविण्याचे काम आता शिक्षित स्त्रियांनी केले पाहिजे. आज मुलींना शिक्षणाबरोबर घरातील कामे शिकविण्याची गरज आहे. कुटूंब व्यवस्था टिकवून ठेवायची असेल तर मुलामुलींच्या कामाची वाटणी करु नका. विधवा स्त्रियांना कमी लेखू नका. तुमच्या समारंभात त्यांनाही वाटेकरी करा. स्त्रीने स्त्रियांची बाजू समाजाला पटवून सांगायला हवी. स्त्रीने स्त्रीचा द्वेष करु नये.

स्त्रियांमध्ये नैसर्गिकरित्या दोन हार्मोन्स असल्यामुळे ती पुरुषांपेक्षा अनेक कामे एकाच वेळी करु शकते. स्त्रीमध्ये व्यवस्थापन असते. पुर्णब्रम्ह हॉटेल हे एका मराठी स्त्रीने काढलयं. आय.टी. क्षेत्रात तिने १७ वर्षे नोकरी करुन ती सोडून तिने हॉटेल टाकल. जगातले सर्वात मोठे शाकाहारी रेस्टॉरंट एका स्त्रीने सुरु केले. तेथे ५० टक्के स्त्री कामगार आहेत. तिच्या अंगभूत गुणांचा उपयोग करुन आदर्श गाव प्रकल्प, वसुंधरा बचाव, प्लॉस्टिक निर्मुलन, पाण्याचे नियोजन अशी अनेक कामे स्त्री करु शकते. स्त्रियांच्या अंगभूत गुणांना महत्त्व देवून स्त्रियांनीच आता स्त्रियांना प्रोत्साहन देण्याची गरज आहे. पाककलेत निपुण असणाऱ्या स्त्रियांनी व्यवसाय करावेत, गृहउद्योग करावेत, कर्ज काढण्यासाठी इतर सुशिक्षित स्त्रियांनी त्यांना मदत करावी.

आपल्या घरी काम करणाऱ्या बाईलाही महत्त्व दया. तिच्या सुखादुःखात आर्थिक भार सोसाण्याकरीता तिला मदतीचा हात दया नाहीतरी, ती कामाला आली नाही, तर घर कशी होतात हे आपण सर्वच जाणतो, नाहीतर संत कबीर एका दोह्यात म्हणतात,

माटी कहे कुम्हार से, तू क्या रौंदे मोहें |
इक दिन ऐसा होयेंगा, मै रौदूंगी तोहे ||

शासनाने महिलांच्या उन्नतीकरिता तसेच त्यांना समाजात पुरुषांबरोबर स्थान प्राप्त करण्याकरिता विविध कायदे आणून त्यांच्या सामाजिक परिस्थितीची सुर्योदय होत असल्याची त्यांना जाणीव करुन दिलेली आहे.

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४. **झीरो FIR चा अधिकार -** रेप पिडीत महिलेला झीरो FIR नोंदविण्याचा अधिकार आहे. अशा केसमध्ये महिला कोणत्याही पोलीस स्टेशनमध्ये तक्रार नोंदवू शकते.

५. **चौकशीसाठी बोलवू शकत नाही -** कोणत्याही महिलेला चौकशीसाठी पोलीस स्टेशला बोलावले जावू शकत नाही, महिलेची चौकशी तिच्या घरीच एखाद्या महिला पोलिसांच्या उपस्थित करु शकता.

६. **गोपनीयतेचा अधिकार -** रेप केसमध्ये महिलेची ओळख गोपनीय ठेवणे गरजेचे आहे. पोलीस व मिडिया कोणीही पिडीताचे नाव उजागर करु शकत नाही.

७. प्रेग्नंट गरोदर कर्मचाऱ्यांची कंपनी कामावरुन हकालपट्टी करु शकत नाही.

८. कोणत्याही वेळी कोणत्याही हॉटेलमध्ये तुम्हाला पिण्याच्या पाण्याची मागणी करता येईल. तसेच वॉशरुमचा वापरही करु शकता तेही मोफत.

९. कायद्यानुसार एखाद्या हॉटेलमध्ये एखाद्या अविवाहीत जोडप्यांना प्रवेश नाकारण्याचा अधिकार नाही.

१०. महिलांना एखाद्याच्या विरोधात थेट पोलीस आयुक्त किंवा आयुक्ताकडे इमेल किंवा रजिस्टर्ड पोस्टाच्या माध्यमातून तक्रार नोंदवता येतो.

११. एखाद्याला अटक केल्यानंतर २४ तासात कोर्टात हजर करावे लागते. नसता पोलीस त्याला ताब्यात ठेवू शकत नाही.

१२. एखाद्या विवाहीत पुरुषाने अविवाहीत महिलेबरोबर संबंध ठेवल्यास तो गुन्हा ठरत नाही.

१३. मुली आणि मुलांना कायद्यानुसार समान हक्क असतो.

१४. लग्नाला किमान एक वर्ष झाल्याशिवाय एखाद्या दाम्प्त्याला घटस्फोटासाठी अर्ज करता येत नाही.

१५. पोलीस अधिकाऱ्याने एखाद्याला अटक करतांना एखाद्या महिलेवर थेट व्यभिचाराचा आरोप लावता येत नाही.

१६. तुमची तक्रार नोंदवण्यास तक्रार देणाऱ्या किंवा टाळाटाळ करणाऱ्या पोलिसांला ६ महिने ते २ वर्ष या तुरुंगवासापर्यंत शिक्षा होऊ शकते.

भारत सरकारने स्त्रियांशी संबंधित वाईट प्रथा संपविण्यासाठी आणि स्त्रियांच्या उत्थानासाठी विविध कायदे केले. या सर्व कायद्यांनी स्त्रियांना संपूर्ण प्रकारचे संरक्षण प्राप्त झाले. स्त्रियांना संपूर्ण स्वातंत्र्य व हक्क मिळाले. सर्व क्षेत्रात पुढे जाण्याची संधी मिळाली. एकेकाळी अनेक बंधनात असलेल्या अबला म्हणून हिनवल्या गेलेल्या स्त्रीने आज प्रगतीची सर्व शिखरे पुरुषाच्या बरोबरीचे किंबहूना काही ठिकाणी त्याही पेक्षा जास्त प्रमाणात पादाक्रांत केलेली आहेत. भारत सरकारने केलेल्या कायद्यामुळे स्त्रियांना संरक्षण प्राप्त झाले. खऱ्या अर्थाने कायद्याने स्त्री मुक्त झाली. भारतीय राज्यघटनेने स्त्रियांना दिलेले अधिकार स्त्रियांच्या उन्नतीसाठी अथक परिश्रम करणाऱ्या समाजातील थोर स्त्री पुरुषांच्या प्रयत्नांना आलेले यश हे नाकारता येत नाही.

मुलींसाठी शासनाने पुरस्कार, सवलती, शिष्यवृत्या जाहीर केलेल्या आहेत. वसतीगृहे स्थापन करुन स्त्रियांना प्रोत्साहन दिले. आर्थिक दृष्टया मागास वर्गातील विद्यार्थ्यांना मिळणारी गुणवत्ता शिष्यवृत्ती, मागासवर्गीय मुलींसाठी कल्याणकारी योजना सार्वजनिक आरोग्यविषयक योजना, सावित्रीबाई फुले दत्तक पालक योजना अशा अनेक योजना सरकारने राबविल्या. या सर्व योजनांचा स्त्रियांनी फायदा करुन घेतला आहे.

आज कोणत्याही विद्यापीठाच्या विविध परीक्षेत मुली सर्वाधिक सुवर्ण पदके प्राप्त करुन उत्तीर्ण झालेल्या दिसतात. महाविद्यालयालयीन स्तरावरही मुली विविध उपक्रमात पुढे आहेत. शहरी भागाची टक्केवारी पाहता शिक्षणाचे प्रमाण अधिक आहे. यात मुस्लिम स्त्रियांचे शिक्षणाचे प्रमाण नगण्य आहे. गरज आहे त्यांचे मानसिक परिवर्तन करण्याची. यासाठी हमीद दलवाई यांनी महाराष्ट्रातील प्रतिगामी मुस्लिम समाजास आधुनिकतेच्या मुख्य प्रवाहात आणण्याचे काम जोमाने केले. मुस्लिम समाजांचे प्रबोधन घडवून आणून त्यांना सेक्यूलर राष्ट्रवादी बनविणे, त्यांच्यात वैज्ञानिक दृष्टी निर्माण करणे. मुस्लिम स्त्रियांचे सशक्तीकरण करणे हे कार्य जोमाने सुरु केले. ही प्रेरणा त्यांनी महात्मा फुले कडून घेवून २२ मार्च १९७० साली मुस्लिम सत्यशोधक मंडळ स्थापन केले. अनेक चळवळी राबविल्या. याद्वारे समान नागरी कायदा चळवळ, मुस्लिम स्त्रियांना मिळणारा एकतर्फी तोंडी तलाक, तसेच प्रार्थना स्थळी स्त्रियांना प्रवेश मिळावा याकरीता देखील स्त्रियांनी यशस्वी आंदोलने केली.

मुस्लिम समाजात होणारे बहुविवाह, त्यामुळे घरातील स्त्रियांचे कमी होणारे महत्त्व. मुस्लिम स्त्रीचे कायद्याद्वारे संरक्षण व्हावे म्हणून भारतातील अनेक शहरामध्ये तलाक विरोधात स्त्रियांना एकत्र आणून त्यांना संघटीत करुन लढा देण्यास सशक्त बनविले. कलम १२५ अन्वये पोटगीचा अधिकार मिळवून दिला. कुटुंब नियोजनाचा कायदा मुस्लिम स्त्रियांनी स्विकारावा. १९८६ ला काही प्रमाणात मुस्लिम स्त्रियांना पोटगी मिळाली. २०१८ ला त्रितलाक बंद झाला. वरील संदर्भ पाहता आजही भारतात पुरुष प्रधान संस्कृती आहे हे अमान्य करुन चालणार नाही. याही परिस्थितीत सुध्दा स्त्रियांनी मोठया प्रमाणात आपल्या कार्याचा ठसा उमटविला हेही नाकारुन चालणार नाही.

स्त्रियांनी सामाजिक भान जोपासून केलेले कार्य :- गोदावरी परुळेकर यांनी (१९०७-१९९६) भारतीय समाजातील अतिशय उपेक्षित आदिवासी समाजात राहून त्यांचे प्रश्न समजून त्यांना न्याय हक्क मिळवून दिले. १९१०-१९९२ यांनी आदिवासी समाजाच्या उध्दारासाठी संपुर्ण आयुष्य खर्ची घातले. आदवासी समाजाच्या मुलामुलींना समाजाच्या मुख्य प्रवाहात आणण्यासाठी अनुताई वाघ जीवनभर संघर्ष करीत होत्या. कुसुमताई पटवर्धन यांनी महिलांच्या अधिकारासाठी सतत संघर्ष करीत राहिल्या. साधनाताई आमटे यांनी बाबा आमटे यांच्या खांदयाला खांदा लावून कुष्ठरोग्यांसाठी कार्य केले आहे. महामहिम राष्ट्रपती प्रतिभाताई पाटील यांनी राजकीय

Aayushi International Interdisciplinary Research Journal (AIIRJ)
ISSN 2349-638x Impact Factor 4.574 Special Issue No. 25
UGC Approved Sr.No.64259 Website :- www.aiirjournal.com Email id:- aiirjpramod@gmail.com

IS SOCIAL MEDIA CONTAGION TO EMOTIONAL STATES OF COLLEGIANS OFFERING VARIOUS STUDY STREAMS?

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ABSTRACT

Life of young collegians is highly influenced by social media. It has led to develop e-identity and e-personality. Now a day emotions of the youngsters are no more personal experience, but has become e-emotions. The present study aimed to study whether social media addiction is contagion to emotional states of the collegians. The sample comprised of 161 college students (Male-56, Female-105). Social Media Disorder Scale and Eight State Questionnaire were used. Mean scores obtained on both measures shows little variation. T value of between correlated means of emotional states exhibited non significant result. Correlation coefficient between media addiction and emotional states was negative and non-significant. Even Chi square test across study stream and gender exhibited non significant results. It is concluded that social media is not contagion to emotional states. Changes in emotional states are only temporary and can be attributed to the factor of chance.

Keywords: Social media disorder, emotional states, body dissatisfaction, emotional contagion.

INTRODUCTION

Recently, social media was in media due to its adverse effects on teenagers and the youngsters. The internet games like 'Blue whale challenge', 'Pink whale challenge', 'Pokoman go', taking selfies at risky places like on running railways or at the overflow dams indicates that in younger generation internet addiction is increasing day by day and they are becoming over conscious about their presence in social media. Even in interpersonal relationships, social media has caused tremendous change. One-to-one contact is replaced by virtual relationship and this has led to e-identity, e-personality and have divulged the emotional life of youngsters.

The speed of forwarding the message and posting selfie is so fast that it seems like a contagion. Even the emotional states can be transferred to other via emotional contagion, leading people to experience the same emotions without their awareness. In other words, due to social media emotional world of an individual is now no more private, but emotions have become e-emotions.

Emotional contagion is well established in laboratory experiments. In such experiments it is found that without knowing people transfer positive and negative emotions to others. Data from large real-world social network, collected over a 20 year period suggests that longer lasting moods (e.g. depression, happiness) can transferred through networks, but the results are controversial (Flower and Christakis, 2008).

OPERATIONAL DEFINITIONS

Social media disorder- Social media disorder means preoccupation with instagram, facebook, selfie taking behavior that enable the user to continuous chatting on computer and smart phone. In the present work, nine factors related to social media have been incorporated. They are preoccupation, tolerance, withdrawal, persistency, escapism, problems, deception, displacement and conflict.

Emotional states-Emotional states are a mixture of psychological and physiological reactions. In the present work eight emotional states are taken into consideration. They are anxiety, stress, depression, regression, fatigue, guilt, extraversion and arousal.

SOCIAL MEDIA ADDICTION AND EMOTIONAL STATES

Over the past decade, social media addiction has emerged two major arena of research. First, use of internet for gambling and pornography are common among youngsters (Kuss and Griffiths, 2012; Griffiths, 2012). Secondly, excessive use of social media has manifest a range of certain psychological problems such as depression, attention deficit, hyperactivity disorder, social

isolation and low self esteem (Guangheng, et al. 2011).

Young collegians, both males and females, are more conscious about physical appearance. However, intense desire to be physically attractive leads to discrepancy between real and ideal body image which ultimately results in certain psychological problems including body dissatisfaction and disturbances in emotional states. Researchers have cited that mass media is a culprit behind the growing trend of body dissatisfaction among young women (Dittmar, 2009). Fredrickson and Roberts (1997) asserted that body image is important for both men and women; however, women are more prone to body dissatisfaction because they are more likely to be seen as physical and sexual objects whose social values can be inferred from bodily appearance. Young women who experience a large amount of body dissatisfaction might take and post selfies in an attempt to garner affirming messages that might boost their own self confidence.

Research on gender differences in use of social media and selfie behavior are equivocal. Fox and Rooney (2015) found that males are more prone to selfie posting than females. On the contrary, Manago, Graham, Greenfield and Salimkhan, (2008) have reported that females are more prone to use social media for posting selfies. This is mainly because frequent posting of selfies by women could be related to their need for physically attractive for self-presentation or an elevated need to belong in a group, which may be as less important to men. Dhir, et al. (2016a) have reported preponderance of women in use of social media and they are less likely to use privacy – preserving strategies compared to young male adults. Their selfie photos to make them look impressive before posting them on social media. It tends to portray women of below average thinness and retouches and airbrushes their subjects until they reach unrealistically perfect level of physical beauty (Hass, et al., 2012). Young women might develop body image issues if they compare themselves to social norms of beauty as displayed in these media representation (Bergstorm, et al., 2009). Peer pressure is also one of the important variables in selfie behavior. Tandoc, Ferrucci and Duffy (2015) have reported that individuals who are in peer groups are characterized by high degrees of social comparison and competition among members are more likely to take selfies and post photos on social networking sites to make themselves look more outstanding than their peers.

The foregoing review states that excessive use of social media may be particularly problematic to young people. Therefore, in the present work the factor of social media addiction, study stream and gender were incorporated. It aimed to find whether social media is contagion to emotional states of youngsters offering various study streams.

AIM AND OBJECTIVES OF THE STUDY

Main aim of this study is to find impact of social media on emotional states of youngsters from various study streams.

Objectives- Major objectives of the study are...

1- To explore the social media contagion on emotional states of collegians.
2- To find the strength of association between social media disorder and emotional states of youngsters.
3- To study differences in the use of social media among students offering different study courses.
4- To study gender differences in the use of social media among college youngsters.
5- To study differences in the emotional states of collegians offering different study courses.
6- To study gender differences in the emotional states of college youngsters.

Hypotheses:

Assuming other factors are kept constant it is hypothesized that

H1- Social media addiction is contagion to emotional states of collegians.
H2- There will be strong positive strength of association between social media disorder and emotional states.
H3- Students offering various study courses will not differ significantly in the use of social media.
H4- Gender will not be a significant factor in the use of social media.
H5- There will not be significant difference in the emotional states of collegians offering different study courses.
H-6 Gender will not be significant factor in the emotional states of college youngsters.

Sample: The sample comprised of 161 (Male- 56 and Female- 105) under graduate and post graduate students from science, computer, pharmacy and management stream.

Tools: The Social Media Disorder Scale by Ringa, et al. (2016) was used. The scale comprised 27 items and nine subscales including preoccupation, tolerance, withdrawal, persistency, escapism,

problems, deception, displacement and conflict. IPAT Eight States Emotional State Questionnaire was used to assess emotional states of the subjects. The test comprised of 96 items. It measures anxiety, stress, depression, regression, fatigue, guilt, extraversion and arousal. The validity and reliability reported by the authors of the tools is quite high.

STATISTICAL INTERPRETATION

In the present study three independent variables were incorporated, they are social media addiction, gender and study stream. A social media disorder scale and emotional states questionnaire were administered in group form. The average scores obtained by the subjects are given in following tables.

Table: 1 Faculty-wise distribution of Mean values on sub-tests of Social Media Disorder Scale.

Faculty/Sub-tests	Preoccupation	Tolerance	Withdrawal	Persistency	Escapism	Problems	Deception	Displacement	Conflict
Science	9.85	9.55	8.39	9.07	9.16	7.85	7.83	7.67	7.32
BCA	10.28	9.66	9.33	9.46	9.3	9.25	8.92	8.61	8.35
Pharmacy	9.14	8.02	7.32	7.91	8.41	7.08	5.82	6.91	6.73
MBA	9.78	9.64	8.67	9.28	9.92	8.82	7.85	7.64	7.21

Table No. 2 Faculty-wise distributions of Mean values on sub-tests of Emotional States Questionnaire

Faculty/Sub-tests	Anxiety	Stress	Depression	Regression	Fatigue	Guilt	Extraversion	Arousal
Science	16.30	14.07	16.58	14.98	17.55	16.25	15.19	7.32
BCA	16.30	15.30	15.12	15.28	16.97	16.48	16.41	8.35
Pharmacy	17.05	15.79	14.97	13.58	18.00	17.02	16.17	6.73
MBA	16.35	14.46	15.32	13.57	18.39	15.96	15.50	7.21

Values depicted in table no. 1 and table no. 2 are average scores obtained by students offering various study courses. Careful observation of the values in the above tables shows that there is considerable variation in the responses of all groups. However, in the present work only total test/scale values are incorporated for interpretation.

Table: 3 Stream-wise Mean and Standard Deviation values obtained on the basis of total score on Social Media Disorder Scale and Emotional States Questionnaire.

		Social Media Disorder		Emotional States	
Faculty	N	Mean	SD	Mean	SD
Science	56	69.41	21.00	124.75	20.73
BCA	39	74.84	19.05	126.56	17.04
Pharmacy	34	60.64	22.46	125.26	22.06
MBA	32	71.64	19.60	121.71	14.75

Table: 4 Gender-wise Mean and Standard Deviation values obtained on the basis of total score on Social Media Disorder Scale and Emotional States Questionnaire.

		Social Media Disorder		Emotional States	
Gender	N	Mean	SD	Mean	SD
Male	56	73.90	19.02	122.17	17.04
Female	105	73.99	24.61	126.05	11.22

The values depicted in table no 3&4 shows that, stream-wise there is a greater variation in average performance on Social Media Disorder Scale. Whereas in emotional states there is not much variation except MBA students exhibiting lowest score. Gender-wise distribution shows that on Social Media Disorder Scale, male and female subjects exhibiting almost similar scores. In emotional states, females surpassing males, exhibiting higher average score but less variation.

Table: 5 Mean, Correlation Coefficient and t values obtained on the basis of total score on Emotional States Questionnaire and Social Media Disorder Scale.

	Social Media Disorder	Emotional states
Mean	76.20	123.28
SD	24.69	21.62
r	-0.05 (N=161)	
t *	1.67	

*Between correlated means of Emotional States Scores

Table: 6 Chi square values obtained across faculty and gender on Emotional States Questionnaire and Social Media Disorder Scale.

Faculty/Gender	Social Media Disorder	Emotional States	df
Faculty	1.60	0.1	3
Gender	0.001	0.06	1

The main objective of the present work was to find out the whether social media addiction is contagion to emotional states of the college youngsters. In order to reveal this effect Social Media Disorder Scale was administered between two sessions of Emotional States Questionnaire. t value (Table-5) between two correlated means of Emotional States Questionnaire yielded non significant result ($p>.05$, $df= 160$). It means that social media contagion is occurred by chance only, in other words changes in emotional states are temporary.

In order to fetch the strength of association between Social Media Disorder and Emotional Sates Pearson Product Moment Correlation was computed. The obtained value is -0.05, it is negative and non significant ($p>.05$, $df=160$). For further interpretation the data were treated by Chi Square test of significance. Faculty wise on Social Media Disorder Scale and on Emotional Sates Questionnaire the obtained values are 1.6 and 0.1 respectively and are non significant ($P>.05$ $df=3$). In case of gender differences they are 0.0001 and 0.06, respectively (Table-6), on both measures are non significant ($p>0.06$ and $p>0.0001$, $df=1$). It indicates that differences in obtained scores are attributed to the factor of chance only.

DISCUSSION

The younger generation is quite aware about their physical appearance, status and position in the group and quite conscious about their e-personality and internet profile. Many researchers have examined the role of social media and personality traits. The results of these studies suggest that social media activity is related to several obsessed personality traits including emotional problems. This is a big avenue to investigate whether these traits are developed out of the influence of social media or such traits enable an individual to use this media at great extent.

The present work entailed to test six different hypotheses. On the basis of the data as well as test of significance (t test and Chi Square) it is concluded that first two hypotheses were not strongly supported. It was hypothesized that social media addiction is contagion to emotional states of collegians. The results were not as per expectations. On the contrary, previous studies revealed that excessive use of internet and social networking platforms could weaken the connections between individuals and their families, friends and loved ones. And it makes an individual to feel lonelier, depressed and certain problems related to emotional states (Pantic, 2014; Yellowes and Marks, 2007). The second hypothesis was there will be strong positive strength of association between social media disorder and emotional states. The data did not support the hypothesis. It means that social media does not play significant role in emotional states. Therefore, whatever the differences in average score observed they are attributed to the factor of chance only and variations in emotional moods are temporary.

Remaining four hypotheses (H3, H4, H5 and H6) were related to stream-wise and gender-wise differences in the use of social media and differences in the emotional states of young collegians. All these hypotheses were strongly supported by the data. This is mainly because communication technology is changing vary rapidly. As far social media is concerned, this change is fast. It appears that there is a synchrony between media generation (i.e., 1-G, 2-G, 3-G, 4-G ....) and human generation. Even new generation is more techno-savvy than the previous one, college students are not exception to this. Secondly, the virtual platforms such as internet and social media allow the young collegians to be anonymous by disguising their identity, they can act as a person they are not and express themselves more comfortably (Kurtalan, 2008). However, Xu and Tan (2012) suggest that the transition from normal to problematic social networking use

occurs when social networking is viewed by the individual as an important mechanism to relieve stress, loneliness or depression. They contended that those who frequently engage in social networking are poor at socializing in real life. For these people, social media use provides continuous rewards (e.g., self-efficacy, satisfaction) and they end up engaging in the activity more and more, eventually, leading to many problems (e.g., ignoring real life relationships, work/educational conflicts etc.). These resulting problems may then exacerbate individuals' undesirable moods. This then leads such individuals to engage in the social networking behavior even more as a way of relieving unhappy mood states.

CONCLUSIONS

On the basis of findings and statisticalinterpretation it is concluded that...

1) Social media addiction is not contagion to emotional states.

2) Strength of association between social media disorder and emotional states is very poor and negative.

3) There was no significant difference in the use of social media among students offering different study courses.

4) Male and female students exhibited similar trend in the use of social media.

5) There were no significant differences in the emotional states of collegians offering different study courses.

6) There were no significant gender differences in the emotional states of college youngsters.

LIMITATIONS

The study has several limitations. Firstly, the scope is limited to the collegians offering various study courses enrolled in a single college affiliated to SGB Amravati University. Secondly, the investigation is based on responses given by the collegians. To study the contagion effect, laboratory study is required. Thirdly, inspite of the validity and reliability of the tools, the gravity of respondents is the major constraint in drawing conclusions. Finally, due to the space restrictions, interpretation and conclusions are drawn only on the basis of total test/scale score. Sub-test/scale scores are not incorporated

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VOL. 5 SPECIAL ISSUE 4 APRIL 2018 UGC Approved Journal No. 45886 ISSN: 2348-1390

NEWMAN

International Journal of Multidisciplinary Studies

A Refereed and Indexed Journal

SPECIAL ISSUE
on the Occasion of

National Conference on
Gender Isonomy: A Societal Onus-2018
(GISO-2018)

19th April 2018

Organized by

Pratibha Women's Studies Center,
Vidya Bharati Mahavidyalaya

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New Man International Journal of Multidisciplinary Studies
(UGC Approved Journal No. 45886)
ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

Revealing Gender Isonomy with Respect to Capacity, Domestic Chores and Domestic Violence.

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Abstract : Gender isonomy is one of the most studied and discussed phenomena. The issue is multidimensional in nature and widely affected by socio-cultural norms. Present work aimed to search the extent of gender isonomy in the form competency, interest, domestic chores and domestic violence among collegians. Sixteen itemscale was used. Total sample was comprised of 110 students (58 female & 52 Male). Their age range was 18-20 years. Mean, SD and item wise percentage was computed. A Chi square test was used to test the significance of difference in the responses of boys and girls.

Results revealed that in capacity and interest domain there are strong belief. 73.52% boys and only 20.63% girls have accepted that 'boys are naturally better at maths and science than girls' whereas35.29% boys and 84.48% girls agreed that 'girls are naturally better at social studies and language than boys'. Data supported the hypothesis.

Second domain was related to domestic chores. In case of 'changing diapers, giving a bath, and feeding kids is the mother's responsibility', 44.11% boys and 56.89% girls answered affirmatively. However, the difference was non significant. The hypothesis was partially accepted.

Last domain was related to domestic violence. Interestingly in case of all six items the percentage to 'yes' response was at lower end. This shows that still there is a trend that domestic violence should not be discussed openly. The hypothesis was not accepted.

Key words: Capacity domain, domestic chores, domestic violence.

Introduction: In ancient times, Indian women were in the position of high esteem and were treated in the form of 'Mata' or 'Devi'. However, the practice of polygamy deteriorated the position of women and in the medieval period, certain practices came into force like purdha, dowry and sati system. With the passage of time the status of women has lowered. The situation became more pathetic in two decades. In 1980s sex selection phenomenon and in 1990s due to urbanization lot of families have moved to cities to look for work. People became much wealthier but at the same time there is pressure to produce sons as an heir. This has worsened the women's position in our society (Jha& Nagar, 2015).

Gender is a common term generally refers to the socially constructed roles, activities and attributes that a particular society considers appropriate for men and women (Shastri, 2014). Traditionally in every society, a female role is to look after house, children, family relatives and on the other hand men are made to earn a bread and hardship. Such type of societal outlook makes women weaker and deprived from basic things. The distinct role and behavior may give rise to gender discrimination which is a prejudicial treatment of an individual or group due to gender.

The process of gendering and gender discrimination starts right from the birth of a child. Birth of a male child is celebrated with fun just like a festival; whereas birth of a female child is considered as a burden, which they have to carry till her marriage. In a nation-wide study Anandlakshmy (1994)has noted, "the birth of a girl child tends to be greeted with devilishjoy, if not grief and that she continues to be treated within the family and outside as a second-class citizen" (p. 43). In Maharashtra, especially the in villages in Western Maharashtra, there are some girls named as 'Nakusa' (unwanted), 'Dagadi' and 'Dhondi', which means 'stone' (Times of India, 4th Sept, 2011).Such nomenclature shows how girl is treated as an unwanted child.

Gender discrimination is observed in various forms like competency, interest, domestic chores etc. In every society there are certain gender based beliefs and stereotypes. It is believed that girls are weak in mathematics and in some cognitive as well as physical abilities. Boys have higher competence beliefs than girls for Maths and sport and girls have higher competence beliefs for language, reading and social activities. These differences increase after puberty (Eccleset al.1993). Even domestic responsibilities and roles are also fixed as per gender.

Gender-based violence (GBV) is one of the burning issues discussed and studied throughout the world. In our constitution there are several legal provisions for men and women (eg. article 14, article 15(3), article 16, and article 39(d)). In 2005, for the protection of women from

different types of violence, Domestic Violence Act, 2005 passed by parliament. However, only making laws and enforcing them is not enough but there is a need of social awakening and change in the attitude of masses. According to United Nations Development Program Human Development Report-2013 (cf. Jha& Nagar, 2015), India ranks 132 out of 187 countries on gender inequality index, lowers than Pakistan. Report states that all countries in South Asia, with the exception of Afghanistan, were a better place for women than India. Considering these realities this study was aimed to search the extent of gender isonomy in the form competency, interest, domestic chores and domestic violence among collegians.

Aim: Main aim of the study was to search the extent of gender isonomy with respect to competency, interest, domestic chores and domestic violence among collegians.

Objectives: Major objectives of the study are...

- To study gender differences in capacity and interest domain of the collegians.
- To study the attitude of collegians towards domestic chores and daily life responsibilities.
- To study the attitude of the collegians towards domestic violence.

Hypotheses: Assuming other factors as constant, it is hypothesized that...

- There willbe a significant difference in the attitude of boys and girls towards capacity and interest belief.
- There willbe a significant difference among boys and girls regarding attitude towards domestic responsibilities.
- There will a significant gender difference in the attitude towards domestic violence.

Methodology:

Sample: Initially, the sample was comprised of 135 under graduate students from Social Science and Science streams. After scrutiny it was found fifteen respondents have not attempted the scale properly. Hence, effective sample was comprised of 110 students (58 female & 52 Male). Their age range was 18-20 years. The scale was administered in group form, containing 25-30 students in each.

Variables: Gender is treated as independent variable. Belief towards capacity, domestic chores and violence were considered as dependent variables.

Operational definitions: Capacity and interest domain: In every society there are certain gender specific stereotypes. Girls are assumed to be better in language and arts; whereas boys are good in mathematics and sports. In the present work the respondent's belief towards maths, science, sports and computer were treated as capacity and interest domain.

Domestic chores and daily life domain: It involves attitudes towards gender specific domestic responsibilities assigned to a mother and a father.

Violence domain: It involves certain beliefs towards domestic violence like violence against wife is a private matter and it should be tolerated by her to keep family together.

Tool used for data collection: Gender Equitable Men (GEM) Scale by Geeta Nanda (2011) was used. Items related to Domestic chores and daily life and violence were incorporated. Capacity and interest related items were added separately.

Statistical Treatment: First Mean, Standard Deviation and item wise percentage were computed. Then the data were treated by Chi Square Test of significance.

Delimitations: The study is based on Under Graduate students only. The tool used for data collection was English version. Only single independent factor, i.e. gender was incorporated.

Findings, Interpretation and Discussion: Throughout the world, the culture what so ever it may be, societyis dominated by the males. Activities or duties outside the home are performed by males while household activities are to be carried out by females. Males have better opportunities of receiving different types of experiential interactions through which they could develop their potentialities. Experiential field of the females is limited; their interactions with different kinds of environments are also restricted. Obviously, they could not get more opportunities to develop different kinds of cognitive abilities. Even though the scenario in India had changed radically, yet the functions and duties of males and females are gender specific. This has led to develop specific beliefs and stereotypes towards capacity, domestic responsibilities and domestic violence.

Table 1: Mean, SD and Chi Square values obtained on three domains

	Male				Female		
Domain	D1	D2	D3	Domain	D1	D2	D3
Mean	3.64	2.67	2.64	Mean	2.58	2.29	2.96
SD	0.93	1.04	1.3	SD	0.94	1.14	1.35
Chi Square Value	.02, df = 2, p>.05			Chi Square Value	.35df = 2, p>.05		
Chi Square Value.001df = 1, p<.05							

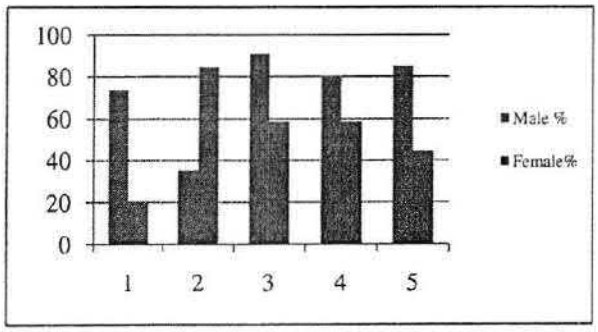
Figures depicted in table no. 1 are Mean, SD and Chi square values obtained by male and female students on three domains, namely capacity and interest (D1), domestic chores and daily life (D2) and domestic violence (D3). Careful observation of the above table shows that male respondents have obtained highest Mean score on capacity and interest domain, whereas in remaining areas male and female have obtained more or less similar

scores. It means that on the basis of sub scale scores views of the respondents are almost similar. For further treatment the data were treated by Chi square test of significance. Domain wise obtained values are .02 and .35 for boys and girls, respectively. These values are non significant (df = 2, p> .05). Even male female difference is also non significant(df = 1 .001, p> .05). It means that the responses of boys and girls are almost similar. And whatever the differences in opinion occurred, they are attributed to the factor of chance only.

For more interpretation the data were treated by domain-item wise percentage and Chi square test of significance.This is the major concern of this study. These values are depicted in table no. 2, 3, and 4.

Table 2: Item wise percentage and Chi square values obtained on Capacity and Interest Domain.

Item No.	1	2	3	4	5
Male %	73.52	35.29	91.17	79.41	85.29
Female%	20.68	84.48	58.62	58.62	44.82
Chi Square Values	29.63 **	20.19 **	7.07 **	3.13	12.58 **



In capacity and interest domain, item no. 1 stands for 'boys are naturally better at maths and science than girls'. It was found that 73.52% boys and only 20.63% girls have answered this statement affirmatively and the difference is significant (29.63**, df = 1, p<.01). This shows that there is a firm belief that maths and science are meant for boys.

Second statement was 'girls are naturally better at english, social studies and language than boys'. In this case 35.29% boys and 84.48% girls have answered affirmatively. The difference between these two groups is significant (20.19**, df = 1, p<.01).

Third statement was 'boys are naturally better at most sports'. Here 91.17% boys and 58.62% girls have answered 'yes'. The difference is significant (7.07**,df = 1, p<.01).

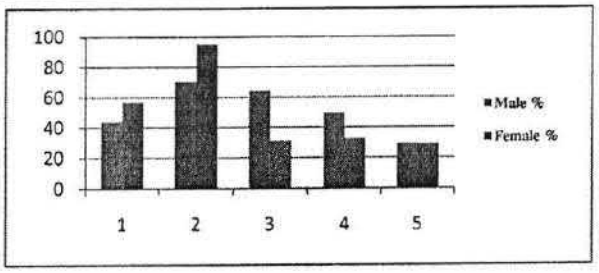
Fourth item was 'boys need sports activities for their psychological development more than girls do'. Here 79.41% boys and 58.62% girls have answered 'yes'. Though there is a difference in the opinion, but it is non significant (3.13,df = 1, p>.05).

Last statement in this domain was 'boys are naturally better at learning to use computers'. In this case 85.29% boys and 44.82% girls have replied positively. The difference is significant (12.58**, df = 1, p<.01).

The first hypothesis was related to capacity and interest domain. It was hypothesized that'there will be a significant difference in the attitude of boys and girls towards capacity and interest belief'.The hypothesis was strongly supported by the data. Referring to item no. 1, 2, 3 and 5 the difference is significant. Subject related beliefs are highly favorable to boys. Even with respect to item no. 4 the responses are more favorable to boys but the difference is non significant. This is mainly because in our society since childhood boys are prepared and educated to have a good profession which is believed to be possible by offering maths, science and computer. Whereas girls are trained for domestic responsibilities and low capacity jobs hence they are forced to offer social science and language. Secondly, masculinity meant for boys and therefore, they are inspired to have games and sports. This distinction is caused due to the parents, teachers and social attitude. Parents and teachers give boys more attention and instructions than girls (yet boys get lower grades than girls, Board and University examinations show the same trend). This results in lower self-esteem of girls (Santrock, J. W., 2007). All these findings and trends show that there are several gender specific differences in cognitive abilities and academic achievement. However, socio-cultural variables along with personality dispositions decide the extent and severity of such differences.

Table 3: Item wise percentage and Chi square values obtained on Domestic chores and daily life domain.

	1	2	3	4	5
Male %	44.11	70.58	64.7	50	29.41
Female %	56.89	94.82	31.03	32.75	29.31
Chi Square Values	0.65	3.55	11.85 **	3.6	0.00001



Second dependent variable in this study was belief related domestic chores and daily life domain. Item no. 1 was 'changing diapers, giving a bath, and feeding kids is

the mother's responsibility.' In this case 44.11% boys agreed that it is mother's responsibility whereas more number of girls (56.89) girls answered positively. Nevertheless, boys are also accepting that it is their responsibility, though % of response is rather low. The Chi Square value is non significant (.65,df = 1, p>.05). It means that though there is a difference in the opinion of boys and girls, but it is not very large, it is occurred by the factor of chance only. In other words regarding baby care boys and girls have accepted that baby care is a combine responsibility. It is a changing outlook of the youngster.

Next item was 'a woman's role is taking care of her home and family.' 70.58% boys and 94.82 % girls are agreed with this statement. Percentage of boys and girls is at higher end. This shows the traditional outlook of our society that a women's role is bound to household activities. Even girls are accepting this reality. However, obtained Chi square value is non significant (3.55,df = 1, p>.05) which indicates that the difference in opinion can be attributed to chance factor, otherwise regarding women's role the views of boys and girls are similar.

Third statement was 'the husband should decide to buy the major household items.' Here 64.70% boys and 31.03% have answered positively. Chi square value was found significant (11.85**, df = 1, p<.01). It means that regarding financial decisions still male are dominant and women has to accept it.

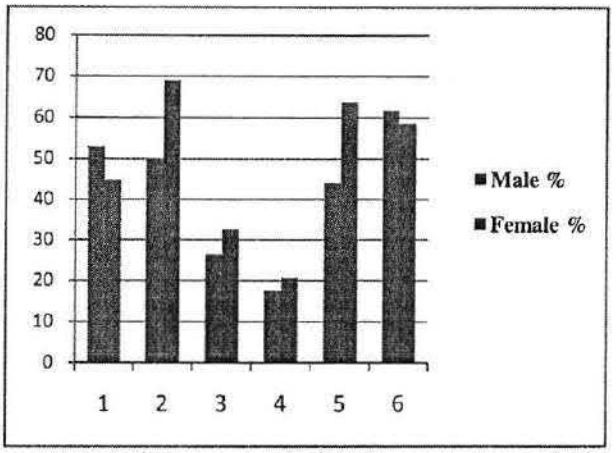
Fourth item in this domain was'a man should have the final word about decisions in his home.' 50% boys and 32.75% girls answered affirmatively. Higher percentage of boys shows male domination in decision making at home. However, Chi square value is nonsignificant (3.6, df = 1, p>.05). The difference has occurred due to chance otherwise, the opinions of boys and girls are similar.

Last item in this domain was 'a woman should obey her husband in all things.' Referring to this statement it was observed that gender wise percentage is almost similar (Boys= 29.41% and girls = 29.31%). This lower percentage shows changing attitude of the youngsters. The Chi square value is also non significant (.00001, df = 1, p>.05).

Second hypothesis in this study was related to domestic responsibilities. It was hypothesized that'there will be a significant difference among boys and girls regarding attitude towards domestic responsibilities'. This hypothesis was partially supported by the data. Only in terms of item no. 3 supportive evidences were observed; whereas in remaining items (1, 2, 4 and 5) the differences were non significant. This shows changing outlook of the youngsters. But careful observation indicates that still there is a difference in the attitudeof boys and girls. It is assumed that baby care is the mother's responsibility whereas financial and major domestic decisions are rest on male member of the family. This is mainly due to patriarchal nature of our society. In India, when women's role is discussed emphasis is given on reproduction, family planning and childbearing, while women's independent personality has been relatively neglected. And this is imprinted on her mind since childhood.

Table No. 4 Item wise percentage and Chi square values obtained on Domestic violence domain.

	1	2	3	4	5	6
Male %	52.94	50	26.47	17.64	44.11	61.76
Female %	44.82	68.96	32.75	20.68	63.79	58.62
Chi Square Values	0.67	3.02	0.66	0.24	3.58	0.08



Domain no. three was related to domestic violence. It was assessed with the help of six items. Item no. 1 was 'there are times when a woman deserves to be beaten.' With respect to this item,percentage of boys and girls is rather moderate (boys = 52.94%, girls = 44.82%). The Chi square value is non significant (0.67, df = 1, p>.05). Higher percentage of boys indicates that to beat a woman is natural a thing.

Item no. 2 was 'a woman should tolerate violence to keep her family together.' 50% and 68.96 % girls agreed affirmatively. The Chi square value is non significant (3.02, df = 1, p>.05). Higher percentage of girls shows that they are acceptingviolence as natural thing in domestic life.

Item no. 3 was 'it is alright for a man to beat his wife if she is unfaithful.' Here 26.47% boys and 32.75% girls answered 'yes'. The Chi square value is non significant (.66,df = 1, p>.05). This lower percentage shows that the issue of 'unfaithfulness' is not openly discussed.

Item no. 4 was 'a man can hit his wife if she won't have sex with him'. In accordance to this statement 17.64% boys and 20.68% girls answered positively. Chi square value is non significant (.24, df = 1, p>.05). This

lower percentage shows a mental set that private issues like 'sex' are not openly discussed.

Item no 5 was 'if someone insults a man, he should defend his reputation with force if he has to'. Here 44.11% boys and 63.79% girls answered positively. Chi square value is non significant (3.58, df = 1, p>.05). This higher percentage of girls shows typical Indian feminine psychology that in case of insulta woman takes an initiative to protect the reputation of her husband.

Last item was 'man using violence against his wife is a private matter that shouldn't be discussed outside'. For this statement 61.76% boys and 58.62% girls answered 'yes'. Obtained Chi square value is non significant (0.08, df = 1, p> .05).Higher percentage shows that boys and girls are accepting domestic violence but they do not want to discuss this issue openly, hence the difference is non significant.

Third hypothesis in this study was related to domestic violence. It was hypothesized that 'there will a significant gender difference in the attitude towards domestic violence'. The data did not support this hypothesis. In case of all six items obtained Chi square values were non significant. This shows that whatever the differences in the opinion towards domestic violence they are attributed to chance factor, otherwise the opinions of boys and girls are more or less similar. Another interesting thing observed in this domain was that percentage of boys and girls with respect to all six items were rather low as compared to first two domain. This shows that the issue of domestic violence still is not openly accepted. The reasons are deep rooted in socialization process because we treat boys as masculine and prepare him for outside world. On the contrary, girls are prepared for domestic responsibilities and taught to develop tolerance.Generally psychological consequences of gender based violence (GBV) on women and children living in povertyare openly discussed. However, in affluent families, due to social prestige, the incidents of GBV are repressed easily. The problems of women who face domestic violence from husband and in-laws have not been openly reported and discussed in society because the system considers these acts of violence as acceptable Due to religious, cultural and social bindings they are forced to remain in the vicious circle of religious and cultural bindings(**Shubha Kumar, et al. 2005).**

Conclusions: On the basis of statistical findings and test of significance it is concluded that...

1. In case of capacity and interest there are firm beliefs. Boys are considered as superior in maths, science, computer and sports, whereas social studies and language are considered as suitable subjects for girls.
2. In domestic chores still male-female roles are fixed, however, the difference was not significant. But regarding financial decisions still male are dominant and his words are final, there is no gender isonomy.
3. Percentage regarding all six items of domestic violence is at lower end which indicate that domestic problems and violence should not be discussed openly.

Limitations: There are several limitations imposed on the study. Firstly, the sample size was small, though statistically, it was large. Secondly, the respondents were from a single college only. Therefore, findings cannot be generalized. Thirdly, only single independent variable, i.e. gender was incorporated in the study. Finally, the tool used for data collection was in English version. Inspite of atmost care, there is some possibility of misinterpretation on the part of the respondents.

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VOL. 5 SPECIAL ISSUE 4 APRIL 2018 UGC Approved Journal No. 45886 ISSN: 2348-1390

NEWMAN

International Journal of Multidisciplinary Studies

A Refereed and Indexed Journal

SPECIAL ISSUE
on the Occasion of
National Conference on
Gender Isonomy: A Societal Onus-2018 (GISO-2018)
19th April 2018

Organized by

Pratibha Women's Studies Center,
Vidya Bharati Mahavidyalaya

C.K. Naidu Marg, Camp, Amravati - 444602, Maharashtra, India.

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Website: www.vbmv.ac.in

New Man International Journal of Multidisciplinary Studies
(UGC Approved Journal No. 45886)

ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

18

Gender Equality and Women Empowerment of India in Current Scenario

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Abstract: Gender is seen closely related to the roles and behaviour assigned to women and men based on their sexual differences. As soon as a child is born, families and society begin the process of gendering. The birth of the son is celebrated, the birth of a daughter filled with pain; sons are showered with love, respect, better food and proper health care.

Female foeticide is heinous and a process opposed to Natural Laws. Every alive being has a right to survive. So how do us negeclect girls. They are equal in status in society. None has authority to distinguish between girl and boy child. In overall comparison, women are at par with men in all arenas. There are numerous examples which also show that they have excelled at work when compared to men.

Today's age is an age of globalization. With respect to age there is need to change us and our mentality about gender inequality. Women reflected the expression of her work in every field.

(Key Words-Culture, religion, progress, unity, efforts etc)

Introduction- Women are the backbone of society. Society never complete without women. Men and women are the two wheels of the life. There should be uniformity in both parties. But when we see the structure of Indian society, it always gives the secondary status to the women. As per the development of education, the changes have been taking place in the position of women.

India is predominately a patriarchal society has a child sex ratio of 914, according to the census of 2011,which is even lower than all over female sex ratio it decreased 1.40% during last decade. In 2001 child sex ratio was 927. The women were treated as the deity and the one, who gives birth to the men, now is struggling for survival.

Gender inequality can further be understood through the mechanisms of sexism and discrimination which is takes place in this manner as men and women are subject to prejudicial treatment on the basis of gender. Sexism occurs when men and women are framed within two dimensions of social cognition. Objective rules applied rigidly to women but leniently to men. Economical, social, psychological and cultural differences between men and women is the part of Indian society. Literacy for females stands at 65.46%, compared to 82.14% for males. Behind 1000 men there are 933 women. Means in comparison both factors are unequal. Job profile is shown the effect of gender bias. Women do not own property under their own names and usually do not have any inheritance rights to obtain a share of parental property. Carry forward of race is the name of sons only.

The bias against female in India is related to the facts that sons are called upon to provide the income. They are the ones who do most of the work in field. In this way sons are looked to as a type of insurance .This problem is also intimately tied to the institution of dowry, in which the family of a prospective bride must pay enormous sum of money to the family in which the women would live after marriage. After independence, the gender inequality in India had not been emphasized so much. The current scenario reports many cases at various parts of India. For eradication and sorting out the problems, there is need to do collective efforts and work at all the levels of society. Collective efforts, role of intellectual class and education can eradicate the gender inequality related issues in India.

Women Problems in current scenario-

Un-attraction of Female Education: Since ancient time we have been seen that generally women ignored from the education. 'Ladki to paraya dhan hoti hai' is common tendency observe among the Indians. Accordingly, much attention is paid to the education of women after

ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

independence. The female literacy level is also increasing steadily. It has increased from 18.7% in 1971 to 39.42% in 1991 and to 64% in 2001. In spite of this change in the trend towards literacy, some problem has cropped up.

Dowry a curse: At the time of marriage ceremony, the gift or amount given by the parents of girl is general trend in India. In later stage it became problem called dowry. Every year so many cases of dowry exposed in India. It is a very serious problem faced by Indian women and their parents.

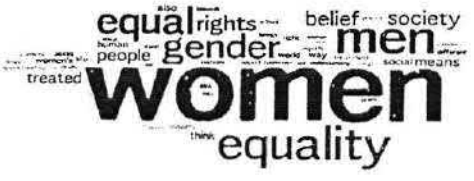
Violence against women: Sexual exploitation, female foeticide, dowry, domestic violence etc are the common practices can see in Indian society. The rate of such problems is high in rural society. Main cause of it is that spoil mentality with old customs and traditions.

Sexual Harassment: Now days so many cases are exposing related to sexual harassment of women. Delhi gang rape and so many incidents' taking place in India. Child abuse, sexual exploitation, human trafficking, child labour etc are the various problems are present in Indian society.

Organizational problems: In working place, women face a lot of problems regarding various matters. May be some times sexual harassment and other conflicts can creates at working place. Excessive bossing, unequal shifts, unwanted demands by high authority etc are the factors responsible for women exploitation in organization.

Familiar and Social Problems: Family and society quickly takes the cognizance about women issues. The intensity and proportion of works is always more than men. In religious and cultural activities women generally ignore and put secondary place. Whatever the situation is there the women assume a responsible for that act. Also there is a tendency that women are the factories of child creation.

Marginalization and women in India



Marginalization is a individual level as well as group wise process. Marginalization of aboriginal communities is a product of colonization. In marginal groups, aboriginal communities lost their land, were forced into destitute areas, lost their sources of income, and were excluded from the labor market. This situation can see in India everywhere in society.

The full development of personality and fundamental freedoms and equal participation by women in political, social, economic and cultural life are concomitants for national development, social and family stability and growth culturally, socially and economically is important.

Suggestions-

1. Strict action and provision of punishment-Affected persons should be booked with full proof charge sheets and exemplary actions be executed on them. This strict action can be the lesion to others in society.
2. Provision of awards and incentives-The special schemes and plans should be executed and spread the awareness in society those family are having only daughters. Maharashtra government already started and that can be model for other states.
3. Government record maintaining -institutions operating USG machines should be made more accountable towards record keeping and reporting towards higher authority.Government, semi government and private hospital should be under observation.
4. Overall observation and cognizance regarding sex discrimination and gender bias various groups in society.
5. All births should be registered under the relevant Act.
6. Health staff to be made accountable for tracking all pregnancies and their outcomes.
7. Self motivated pregnant women should not be entertained for sex selective procedures, and any influence of family pressure and relatives.
8. The positive role of family education and planning with women empowerment
9. Change the structure and framework of society regarding gender inequality.
10. Emphasis on the role of NGOs, social thinkers, sociologists and social workers.

Recommendations-

1. Strict application of legal provisions.
2. Women empowerment and development.
3. Proper education for awareness and spread the message in society.
4. Dowry prohibition act should be implemented effectively.
5. Reaching the masses through religious/spiritual leaders
6. Role of media and entertainment.
7. Social awareness for changing public mind-set

ISSN: 2348-1390
Impact Factor: 4.321 (IIJIF)

8. Strict implementation of PNDT and MTP Acts
9. Curbing quackery, sensitization of doctors. NGOS, govt. machinery, panchayat leaders.
10. Protect unborn girl child.
11. Educating/sensitizing male members of family.
12. Equal treatment, dignity and respect for girl child
13. Fight against social evils.
14. Women empowerment: to make it a reality.
15. Role of NGO's administration and Government.

Some of the plans for women implemented by Government of India-

1. Mahila cosh yojana-
2. Training and employment programme for women (TEPW)
3. Rashtriya Mahila Kosh (RMK)
4. Rajiv Gandhi Scheme for Empowerment of Adolescent Girls (RGSEAG)
5. Central Social Welfare Board (CSWB)
6. Indira Gandhi Matritva Sahyog Yojana (IGMSY)
7. Swayam Siddha yojana
8. Short Stay Home for Women and Girls (SSH)
9. Swadhar

Conclusion: Community awareness on the benefits of empowering women should be carried out in order that the empowerment may be supported by the community as whole. For the proper construction of society there is needed to give special attention on women empowerment in India. Also traditional attitude has to change regarding women. Awareness programme, education and positive role of every indivisible will help to development in women empowerment in India. Indian government is always fewer rebel and conscious about women development. Time to time different schemes and planning have been implemented for the success of women. Behind this problem, many root causes are responsible and affect on social system. Suitable social structure can be maintain with following suggestions and recommendations-

For adequate social change, development and social control, there is a need of time to eradicate this problem as early as possible and maintain the developmental tract in society.

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REVIEW OF RESEARCH
ISSN: 2249-894X
IMPACT FACTOR : 5.2331(UIF)
VOLUME - 7 | ISSUE - 6 | MARCH - 2018

BASIC KNOWLEDGE AND ATTITUDE AMONG COLLEGE STUDENTS TOWARDS SNAKES IN AMRAVATI

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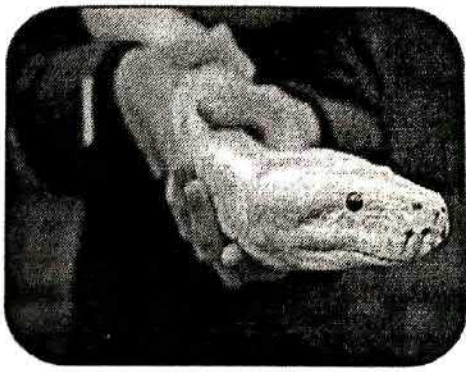
ABSTRACT



Snakes belongs to class reptilian, plays a vital and critical role in any ecosystem as a prey as well as a predator. Due to lack of knowledge and misguidance snakes can be categorized under threatened species. Students and youths are important part of any society. They play an important role in framing the society. Their perspective towards environmental education is very crucial for conservation and preservation of any flora and fauna especially the snakes. A cross-sectional study was conducted among the under graduate students of Vidya Bharati Mahavidyalaya College Amravati, Maharashtra during the period of January 2018 to know their knowledge of snakes and attitude toward snakes. In the present study majority of the participants had basic knowledge about venomous snake, snake bite and their conservation and they show a positive attitude towards snake

KEYWORDS : *Snakes, Conservation, Venomous, Attitude, Amravati.*

INTRODUCTION:

Snakes belongs to class reptilian, plays a vital and critical role in any ecosystem as a prey as well as a predator. Humans in various cultures have feared snakes, provoking an aversion and persecution that hinders conservation efforts for these reptiles (Alves *et al.*, 2014). Snakes may be keystone predators especially in agricultural and grassland ecosystems, because snakes are effective predators of rodents and they indeed likely help to regulate food webs in important ways that other predators cannot (Mills *et al.*, 1993, and Kotliar *et al.*, 1999). Snakes are also excellent ecological indicators due to their sensitivity to temperature and climate change (Beaupre and Douglas, 2009). Therefore, disappearance of snakes can have negative impacts on interactions in ecosystems and may affect predator–prey population dynamics in different ways. Snakes were the fifth most dislike fauna in animal kingdom due to fear (Kellert, 1980). The lack of knowledge is dangerous for both human and snakes because when people get frightened they tend to make irrational decisions that often results in snake death or increased risk of snake bite, this also became a human snakes conflict (Chrstoffel, 2007).

In India most of the people have lack of proper knowledge about snakes. They have learned about snakes more by traditional knowledge, through movies than factual knowledge from books and literatures.

Snakes provide a variety of ecosystem services to human but their populations are decreasing globally and locally. There can be both positive and negative attitude towards snakes from human. Due to lack of knowledge and misguidance snakes can be categorized under threatened species. We should ensure that future conservation planners and policymakers, who determine the future of snakes, express positive

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attitude towards snakes or demonstrate a capacity to view snakes objectively (Calderon-Arrieta 2017). In order to ensure the need of conservation of snakes which directly or indirectly affects the health of an ecosystem, we need to develop an informed population to understand the need and importance of snakes in an ecosystem.

Students and youths are important part of any society. They play an important role in framing the society. Their perspective towards environmental education is very crucial for conservation and preservation of any flora and fauna especially the snakes. Through Environmental Education, students can be agents of change as well as future decision makers on sustainable use of biodiversity. Such education will make them become active and responsible environmental to value our biodiversity.

The present study was undertaken to assess the knowledge, current attitude and myths about snakes in undergraduate students of Vidyabharti Mahavidyalaya College Amravati (M.H).

MATERIAL AND METHODS

Prior the study, permission was taken from the Principal Vidyabharti Mahavidyalaya College. This cross-sectional study was conducted among the under graduate students of Vidya Bharati Mahavidyalaya College Amravati, Maharashtra during the period of January 2018. Simple random survey method was adopted. Questionnaire was used to interview the study participants and various in depth questions regarding knowledge, current attitude and myths about snakes were asked. Three pictures of venomous snakes were shown to study participants for identification based questions. Statistical analysis was done by using Microsoft Excel and the results were calculated in percentages.

RESULTS

Out of the total 200 study participants, 88 (44%) were males and 112 (56%) were females. To assess the knowledge regarding species identification and venomosity of snakes, four images of locally prevalent venomous and non-venomous snakes were shown to the respondents. Among the 3 venomous snake 175 (87.5%) of the study participants correctly identified Indian spectacled Cobra, 37 (18.5%) identified common Krait correctly, 30 (15%) study participants identified Russell viper correctly and 22 (11%) study participants were not able to identify any one of three venomous snake.

From the venomous snakes 167(83.5%) study participants correctly identified Indian Spectacled Cobra as venomous and 17 (8.5%) identified viper correctly as venomous and 5 (2.5%) identified krait correctly as venomous.

When asked about measures taken upon encountering a snake near human settlement, maximum number of respondents 147 (73.5%) opined calling a forest official or a snake friend, followed by leaving the snake as it is 39 (19.5%) and kill 16 (8%).

When asked about the immediate measures taken by the study participants if a person is bitten by a snake, 136 (68%) of the study participants stated that they would prefer to take the victim to the nearest health facility while 64 (32%) of the study participants stated that they would prefer first aid measure. 156 (78%) of the study participants knew that medical treatment is available for snakebite while 130 (68.5%) participants knew about antivenom. Nearly 191 (95.5%) of the total study participant opted myth instead of fact for the question that snake's drinks milk and 196 (98%) opted myth for the question that snakes seek revenge when somebody harms them.

178 (89%) study participants know about that snakes are protected under wild life protection act 1972 but none of the students know about that under which schedule of wild life protection act they are protected. 147 (73.5%) of student participants opined that if they found someone trafficking snake they will inform the forest official and 53(26.5%) will ignore it.

100% of the study participants believed that snakes are very important for our ecosystem and removal of snake from any area can have direct or indirect negative impact on the health of that ecosystem. When asked about the knowledge they acquired about snakes, 78(39%) study participants opted knowledge

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from books and lectures, 87 (43.5%) opted from movies and 35 (17.5%) opted traditional knowledge and folklore knowledge.

DISCUSSION

In the present study 175 (87.5%) of the total study participants could identify the Spectacled Cobra correctly and 167 (83.5%) correctly identified it to be venomous which was significantly more as compared to other snakes. This could be due to the fact that Spectacled Cobra has a prominent hood which makes them easily identifiable and also they are mentioned and portrayed in many Indian religious literatures and also in many Indian movies and daily soaps. Similar results have been found in the studies done by Duminda *et al.*, (2014) in Sri Lanka. According to study done by Pandey (2015) in Nepal, 95% study participants were aware that Common spectacled Cobra is venomous. Alves *et al.*, (2014) assumed that the cultural beliefs associated with snakes might be related with the fear of snakes that they found in their primary-education student sample size.

One of the major positive findings in our study was that 156 (78%) of the participants knew about medical treatment being available for snake bite which was quite similar to the study done by Pandey *et al.*, (2016).

It was noted that 136 (68%) study participants opted that they will rush to the nearest hospital if someone is bitten by Snake followed by first aid measures 64 (32%). Also, it was wonderful to know that in the present study all participants would prefer going to hospital than considering a traditional healer as a treatment option after snake bite, this finding was similar to the study done by Pandey *et al.*, (2016). While in other similar studies 86% of snakebite victims in Bangladesh, 75% in Pakistan, and 61% in Maharashtra, India still visit traditional healers (Inamdar *et al.*, 2007 and Chandio *et al.*, 2000).

CONCLUSION

In the present study majority of the participants had basic knowledge about venomous snake, snake bite, their conservation and myths related to snake. Majority of the students were in the favor that snakes should be protected and conserved, which shows a positive attitude. Most correctly identified venomous Snakes were Spectacled Cobra followed by Russell's viper and common krait respectively. All the participants knew that there is medical treatment available for snakebite, although majority of the participants were not aware about antivenom. Also most of the participants considered the concept of snake's drinks milk and take revenge if they are harmed as a myth as they were aware of the fact that snakes are strictly carnivores. Most of the participants believed that Snakes are important part of the ecosystem and also know the importance of snake to the ecology and ecosystem and also they are protected under Indian wild life protection Act 1972 but they were not aware about the schedule of wild life protection Act 1972 under which they are protected.

Students play an important role in the society therefore their proper knowledge is important for the conservation of any wildlife. Therefore awareness camps, seminars and workshop on basic knowledge about snake identification, snakebite prevention, conservation strategies of snakes and clearing misconceptions should be held in schools, colleges, universities several other institutions. Proper first aid measures for snakebites should be demonstrated through various outreach activities, workshop and increased awareness about snake and snakebite identification among students and general population should also be done for conservation of the snake fauna.

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Aayushi International Interdisciplinary Research Journal (AIIRJ)
ISSN 2349-638x Impact Factor 4.574 Special Issue No. 25
UGC Approved Sr No 64259 Website :- www.aiirjournal.com Email id:- aiirjpramod@gmail.com

ANURAN INVENTORY OF VIDARBHA REGION, MAHARASHTRA

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ABSTRACT

The use of some drugs during pregnancy may causes abnormalities to the embryo. Sometime the drug also effect to the new born if the drug transferred through lactation. The present experiment used the Clarias batrachus as model to check the effect of norfloxacin on hatching rate of eggs. The 10, 20, 50, 100 µg/ml concentrations of drug were used. No significant mortality or malformations were observed in fish embryos. Hatching was stared from 36 hr. In control group, 90% hatching rate was observed. Lowest hatching rate was observed in highest concentration (100µg/ml). Present investigation suggests the possibility that high dosage can harm the unborn baby or new born babies, if the mothers use norfloxacin.

Key words: Anuran fauna, diversity, Maharashtra, Vidarbha.

INTRODUCTION

The diversity of flora and fauna on the earth and its genesis has long been a source of questionable curiosity (Joshi *et al.*, 2015). The study of biodiversity includes both the inherent and anthropocentric principles allied with it. The importance of these incredible biological factors is renowned in relation of the ecosystem services (Baumgartner 2007). Biodiversity is the foundation for maintaining the ecosystem and the operative facets of the species that offers many goods and services to for human well being. Examinations of species diversity of a region facilitate the evaluation of potential serviceable role of the species. In any ecosystems, observing the species diversity can be used as a contrivance to minimize the mismanagement and contamination in urbanized, industrial, rural, and managed areas by human (Wilson 1997). Extending this view, the species diversity review in any ecosystems is essential to understand the effect of anthropocentric development on the integrity and sustenance of ecosystem.

The inventories of species diversity are immense resource that provides recent and previous information on their topographic distribution. The elementary species occurrence data have various applications. Species inventories that contain such elementary and collective species-occurrence data, plays a fundamental role in providing information on the status of species transpire in different spatial scales. These inventories have been used for taxonomic and biogeographic studies as well for conservation planning, reserve selection, climate change studies, agriculture, forestry and fishery, and species translocation studies (Chapman 2005a). The meticulousness of the taxonomic and spatial information is valuable reflection for determination of data quality and validation of the species occurrence data. Hence the significance of the data excellence in the inventory of Indian fauna hardly needs emphasis (Chapman 2005b).

The anuran diversity has been focused in many studies explaining their dominance in the terrestrial and aquatic ecosystems and also the provision of ecosystem services (Joshi *et al.*, 2014). In this perspective, the present communication is part of an effort to verify the validity of anuran species based on a review of the earlier checklists published over the past two decades. Finally, a comprehensive anuran inventory of Vidarbha region of Maharashtra has been provided along with source literature.

MATERIALS AND METHODS

Study area: Vidarbha is one of the most diversified Regions in Maharashtra State of India, with respect to biodiversity. Its healthy climate, mountainous terrain, rugged configuration and sudden fall in elevation are phenomenal. It is located between 20.9374° north and 77.7796° east. It has a total area of 97,321 square

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kilometers. The climatic condition of this district is characterized by a hot summer, well-distributed rainfall during the south-west monsoon season and generally dry weather during rest of the year. The cold season is from December to February. The average annual rainfall in the district is 795.7 mm. During summer the mean daily maximum temperature in summer was 44.2° C to minimum as 26.7° C while it decreased toward winter with the mean daily maximum temperature was 27.8° C and minimum 14.9° C.

Primary inventory: The present inventory of fauna has been compiled primarily from articles and technical reports published in scientific journals. However reports in newsletters, unpublished reports, personal field observations and personal communications with other herpetologists and field workers have also been taken into account. Information on species distribution and taxonomy has been compiled from literature published until July 2017.

Taxonomic Treatise: The list provided, is at the species level and the taxonomy follows, Daniel (2002) and Ahmed *et al.*, (2009).

Validity of species listed: Based on the distributional records available, the validity of the species listed in the earlier checklists of India, particularly Maharashtra and neighborhood published in the past two decades has been reviewed.

RESULTS AND DISCUSSION

The present comprehensive inventory is based on a review of the earlier checklists of the anuran fauna published over a past decade. The review cleared the presence of following twelve species belongings to Five families (Table 1).

Table 1: Anuran inventory of Vidarbha region, Maharashtra, India

Sr.	Family	Species	Common name
1.	Bufonidae	*Duttaphrynus melanostictus* (Schneider,1799)	Asian common toad
2.		*Duttaphrynus stomaticus* (Lutken, 1864)	Indian marbled toad
3.	Dicroglossidae	*Euphlyctis cyanophlyctis* (Schneider, 1799)	Indian skipper frog
4.		*Euphlyctis hexadctylus* (Lesson, 1834)	Indian green frog
5.		*Fejervarya limnocharis* (Gravenhost, 1829)	Asian grass frog
6.		*Hoplobatrachus tigerinus* (Daudin,1803)	Indian bullfrog
7.		*Hoplobatrachus crassus* (Jerdon,1853)	Jerdon's bullfrog
8.		*Sphaerotheca breviceps* (Schneider, 1799)	Indian burrowing frog
9.	Microhylidae	*Microhyla ornata* (Dumeril and Bibron, 1841)	Asian ornate frog
10.		*Kaloula taprobanica* (Parker 1934)	Asian painted frog
11.	Ranidae	*Hylarana malabarica* (Tshudi, 1838)	Fungoid frog
12.	Rhacophoridae	*Polypedatus maculatus* (Gray, 1830)	Indian tree frog

Vidarbha is most diversified region with lush green deciduous forests through large protected areas which are home to variety of flora and fauna. It has approximately 37,251 km^2 forest cover. Vidarbha also has many popular wildlife sanctuaries and parks *viz.* Melghat in Amaravti, Amba-barwa and Nalganga in Buldhana, Tadoba-Andhari in Chandrapur, Nagzira and Navegaon Bandh in Gondia, etc. The region is represented with rich faunal diversity. The utility of species as indicators of environmental conditions is a basis for preparation of present inventory.

The present inventory of anuran fauna of Vidarbha region is based on available locality records by providing relevant source literature on specimens that would be ensuring its quality. Because, the accurate and precise quality data on species occurrences are imperative for the assessment of conservation status and drawing management considerations hence used for further research purposes such as predictions on species distributions, habitat suitability, and threat assessments etc.

Many researchers from Vidarbha region had given their valuable contribution in development of anuran studies. The monumental works on anuran fauna of Vidarbha region mainly includes the Dhande and Khandare (2013), Pandharikar *et al.* (2015), Sawarkar and Kasambe (2009), Wagh *et al.* (2017) to name a few.

According to Joshi *et al.* (2017), the fauna is always threatened by anthropogenic and environmental factors. The diverse habitats of the

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Vidarbha Region are rapidly changing due to new irrigation projects and industrialization. Forest areas are being de-notified for implementing development projects such as mining, industry, communication and tourism. This has resulted in alternating climate as well shrinkage, fragmentation, degradation and destruction of natural habitats. Road accidental killing on highways across wildlife refuges are an intrusion and affect the wildlife and its habitats adversely. Misconceptions and fear about these species especially about snakes are also threatening this important creature of the ecosystem.

In parity with the anuran species observed in Vidarbha region, Maharashtra, India, it may be assumed that the species carry out diverse functional roles for the sustenance of the ecosystems. The availability of the green space and the heterogeneity of the habitats in terms of the available vegetation and allied factors that render stability to the population and species assemblages in the landscapes are possibly important contributors to the observed variations in the saurian species observed in the present study. The present diversity study is confined to limited area and selected habitats. There are, in future, chance of more species being reported because of few pockets and habitats in the studied area required more extensive exploration.

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Current Global Reviewer

UGC Approved International Research Refereed Journal For

ISSN 2319-8648 | Impact Factor - 2.143 | Indexed (IIJIF | UGC Approved Sr. No. 64319

Spcial Issue

24 Feb. 2018, ISSUE I VOL II

Todays challeges

Edited by
Prof. Dinesh Jaronde
Prof. Prashant Jawade

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निराकरण / उपाय / सल्ला :-

- तणाव, चिंता, नैराश्य यातून सुटका होण्यासाठी योगा आणि प्राणायाम यांचा उपयोग नियमित करावा.
- नैराश्य दूर करण्यासाठी परिस्थितीशी जुळवून घेणे व समस्येचे भावनीक समायोजन करण्यास शिकणे.
- जीवनशैली साधी व गरजा कमी ठेवणे.
- बालमनावर कुटुंब व शाळांमधून सकारात्मक स्वसंकल्पनेची बीजे रुजविणे.
- स्वत:ची बलस्थाने आणि उणिवा ओळखून त्याचा स्वीकार करणे.
- नकारात्मक विचार, गैरसमजुती, व्यसनाधीनता यापासून दूर राहणे. रागावर नियंत्रण ठेवावे.
- विनोदबुध्दी, छंद जोपासणे, मैत्रीपुर्ण नातेसंबध ठेवणे, साजेसा जीवनसाथी शोधणे, आपले काम प्रामाणिकपणे करणे व आनंदी राहणे.
- स्वआदरभाव राखून स्वत:चा व इतरांचा मानसन्मान करणे.
- अपमान सहन करायला शिकले पाहीजे.
- सकारात्मक प्रेरणा देणाऱ्या महामानवांच्या जीवनावरील पुस्तकाचे वाचन करावे. जसे छत्रपती शिवाजी महाराज, महात्मा ज्योतीराव फुले, सावित्रीबाई फुले, डॉ. बाबासाहेब आंबेडकर, डॉ. ए.पी.जे. अब्दुल कलाम, बाबा आमटे इ.
- स्वत:चा आत्मविश्वास वाढवावा, मी माझे मानसिक आरोग्य उत्तम ठेऊन आनंदाने आयुष्य जगू शकतो असे स्वत:ला सुचवित राहावे.
- सकारात्मक विचार देणाऱ्या चित्रपट , टी.व्ही. मालिका पाहाव्या.

ताणतणाव, चिंता व नैराश्य यावर मात करुन सुखी व आनंदी जीवन जगण्यासाठी प्रत्येकांनी प्रयत्न करावा व सकारात्मक विचारधारेचा अंगीकार करावा.

Current Global Reviewer
Impact Factor 2.143 UGC Approved Sr. No. 61524 ISSN 2320-4685

विदर्भातील सार्वत्रिक लोकसभा निवडणूक २०१४ : एक दृष्टिक्षेप

नितीन वसंतराव खोब्रागडे
विद्याभारती महाविद्यालय, कॅम्प, अमरावती.

भारतीय लोकशाही ही एक सर्वोत्तम व्यवस्था असून आदर्शाच्या स्वरुपात सर्वमान्य झाली आहे. लोकशाहीत चालू वर्तमानकाळाचा आवाज असल्यामुळे जनतेकडुन नैतिक समर्थन प्राप्त झाले आहे. लोकशाही व्यवस्थेमध्ये निवडणूका ह्या राजकीय इच्छा आकांक्षेची अद्वितीय माध्यम असल्यामुळे आधुनिक युगात विशिष्ट भुप्रदेश निश्चित करुन प्रतिनिधीद्वारे लोकशाही निवडणूकीच्या माध्यमातून क्रियान्वित केली जाते.

जनतेच्या भावना लक्षात घेवून राजकीय व्यवहाराची समीकरणे मांडली जातात. ज्यामध्ये लोकशाही यशस्वितेकरीता जनतेकडुन निवडून दिलेला प्रतिनिधी हा लोकांच्या भावी योजना, आशा, आकांक्षा पूर्ण करण्यासाठी राजकीय लोकशाहीचं अस्तित्व टिकविण्यासाठी स्विकृत मार्गाने लोकशाहीचा अवलंब करीत असतो. त्याअनुषंगाने आपण विदर्भातील निवडणूक 2014 चा विचार करुन भारतीय राजकीय लोकशाही मुल्यव्यवस्थेत भारतीय इतिहासाचे पाळेमुळे रुजली आहेत का? असतील तर त्याचा विदर्भावर काय परिणाम होतो, ते जाणून घेण्याकरीता आदर्श लोकशाहीचा वापर करुन विदर्भातील निवडणूक यशस्वी झाली आहे का? त्याचे उत्तर शोधण्याचा प्रयत्न केला जात आहे.

विदर्भातील सोळावी लोकसभा निवडणूकीची पार्श्वभूमी लक्षात घेतांना विदर्भाचे एकुण क्षेत्रफळ 97.321 चौ.कि.मी. असून त्याची लोकसंख्या 23003,179 इतकी आहे. भारतातील राज्यांमध्ये एक प्रमुख राज्य असलेल्या महाराष्ट्र राज्यामध्ये एकुण 35 जिल्हे व सहा प्रशासकीय विभाग आहेत, त्यापैकी नागपूर महसूल विभाग व अमरावती महसूल विभागाचा प्रामुख्याने विदर्भ प्रांतामध्ये समावेश होतो. विदर्भामध्ये असलेला अमरावती महसूल विभाग हा 'पश्चिम विदर्भ' नावाने परिचीत आहे, तर नागपूर महसूल विभाग हा पूर्व विदर्भ या नावाने नावरुपास आहे. अमरावती महसूल विभागामध्ये अनुक्रमे अमरावती, अकोला, यवतमाळ, बुलढाणा व वाशिम या जिल्ह्यांचा समावेश होतो. तर नागपूर विभागामध्ये प्रामुख्याने नागपूर, वर्धा, भंडारा, गोंदिया, गडचिरोली व चंद्रपूर या जिल्ह्यांचा समावेश होतो. एका अभ्यासिकेनुसार या दक्षिण पट्ट्यातील एका भूभागावर राजश्री यादवाचा पुत्र विदर्भ याने विदर्भ नगराची स्थापना केली, या नगरीला राजधानी बनवून विदर्भाने सभोवतालच्या भूभागावर राज्य केले, अशाप्रकारे हा भूभाग 'विदर्भ' या

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नावाने ओळखला जातो. विदर्भातीलं लोकसभा क्षेत्र 10 आहेत, तर विधानसभा क्षेत्र हे 67 आहे.

विदर्भातील जिल्हानिहाय लोकसंख्येचे विवरण पुढील तक्त्याद्वारे दर्शविता येईल.

अ.क्र	जिल्हा	स्त्री	पुरुष	एकुण
1	अमरावती	1482845	1404981	2887626
2	अकोला	966226	882391	1818617
3	वाशिम	621228	575486	1196714
4	यवतमाळ	1525593	1341864	2775457
5	बुलढाणा	1342152	1245887	2588039
6	नागपूर	2388558	2264613	8653171
7	चंद्रपूर	1120316	1073946	2194262
8	भंडारा	603471	594431	1198810
9	गोंदिया	662524	659807	1322331
10	गडचिरोली	542813	28982	1071795
11	वर्धा	665925	630232	1296157

सोळावी लोकसभा निवडणूकीमध्ये मतदारांनी 66.38 टक्के एवढे विक्रमी मतदान केले आहे. प्रचार–प्रसार माध्यमे आणि मतदारांचा नव्या उमेदवारांसंबंधीचा दृष्टिकोण यांचा अंतर्भाव सोळावी लोकसभा निवडणूक दिसून आला आहे. त्यात प्रामुख्याने राष्ट्रीय काँग्रेसपक्ष आणि दुसरीकडे भारतीय जनता पार्टीने तयार करुन नविन चेहरा दिलेली मोदी लाट यांच्यातील संघर्ष प्रकर्षाने दिसतो. मोदींचा प्रभाव अधिक आणि काँग्रेसचे पूर्वाश्रमीचे आरोप प्रत्यारोप त्यामुळे भारतीय राष्ट्रीय काँग्रेस पक्षाला मतदारांनी बाजूला सारुन भाजपा व राष्ट्रीय स्वयंसेवक संघ यांना मतदारांनी सत्ताकेंद्री स्थापन केले. भविष्यात कधीही न होणारा विजय हा नरेंद्र मोदीच्या बाजूने मतदारांनी कौल दिला आहे. त्यामुळे सोळावी लोकसभा निवडणूक जात, धर्म, पंथ, पक्ष बाजुला सोडून नवोदितांना संधी देणारी ठरली.

सोळावी लोकसभा निवडणूकीमध्ये राजकीय वर्तुळामध्ये नव्याने विचार करावयाची संधी मिळाली आहे. दीर्घकाळ सत्ता असलेली राष्ट्रीय काँग्रेस व त्याचे सहयोगी पक्ष मिळून बनलेली संयुक्त पुरोगामी आघाडी (युपीए) यांच्या विरोधात भाजपच्या नेतृत्वाखालील राष्ट्रीय लोकशाही आघाडी (एन.डी.ए.) ला नवमतदारांनी संधी देवून त्यांना सत्तेवर विराजमान केले आहे. नरेंद्र मोदी यांचे नेतृत्व भाजपाला पर्यायाने एन.डी.ए.ला संधी देण्यास कारणीभूत ठरले.

Current Global Reviewer
Impact Factor 2.143 UGC Approved Sr. No. 61524 ISSN 2320-4685

विदर्भातील सोळावी लोकसभा निवडणूक 2014 यांचे सैध्दातिक विश्लेषण केले असता विदर्भातील लोकसभा मतदारसंघ व त्या दहा लोकसभा मतदारसंघातील व्यवहारवादी विश्लेषण केले असता संबंधित लोकसभा निवडणूकीत परंपरागत मुल्यव्यवस्था नाकारुन नव्या सरकारची नवी व्यवस्था हा मतदारांचा दृष्टिकोण व्यवहारवादी जरी दिसत नसला तरी एकसंघ सत्ता एकाच्या हाती जास्त काळ दिली तर तो पक्ष हुकूमशाहीला आव्हान करीत असते आणि ते आव्हान मतदारांनी नाकारले आहे. त्यामुळे राष्ट्रीय काँग्रेस पक्ष मागे पडून, नवा पक्ष, नव्या जाणीवा घेवून मतदारांना काय देवू शकतो हे येणारा काळच त्याची ग्वाही देईल असे वाटते.

संशोधन क्षेत्रामध्ये लोकशाहीच्या अंगाने विचार करतांना अनेक अडथळे येतात अनेक क्षेत्रात खोट्या अफवा, व्यक्तींचे हितसंबंध, जातीय हितसंबंध, धार्मिक व सामाजिक, राजकीय पक्ष आणि त्या पक्षप्रमुखाची मक्तेदारी ही निवडणूक प्रक्रियेत सक्रिय होतांना दिसते, त्यामुळे कधी जातीच्या, धर्माच्या नावावर निवडणूक लढविण्याचा व प्रतिनिधी देण्याचा मानस राष्ट्रीय पक्ष करीत असतात. ते सत्तेच्या दृष्टीकोणातून योग्यही आहे. थोडक्यात सत्ता संघर्ष हाच लोकशाहीचा मुलाधार असल्यामुळे जनतेचा कौल लोकप्रतिनिधीला शेवटपर्यंत समजत नाही. कारण ही लोकशाही गुप्त मतदान पध्दतीची आहे.

विदर्भातील सोळावी लोकसभा निवडणूक 2014 यांचे व्यवहारवादी विश्लेषण केले असता प्रामुख्याने भौगोलिक परिस्थितीचा विचार करुन धार्मिक, सामाजिक, आर्थिक व राजकीय परिस्थिती विचारात घेवून मागील निवडणूकीचा इतिहास आणि त्याचे परिणाम आणि 2014 च्या लोकसभा निवडणूकीतील परिणाम यांचा तुलनात्मक अभ्यास केला असता विदर्भ हा राष्ट्रीय काँग्रेस पक्षाचा बालेकिल्ला असला तरी लोकसभा निवडणुकीत तो हादरलेला दिसत आहे. भारतीय जनता पक्षाने प्रयत्नाची पराकाष्टा करुन विदर्भातील एकुण दहा लोकसभा मतदार संघातून भाजप सहा लोकसभा मतदारसंघात विजय प्राप्त केला आहे. तसेच शिवसेना व घटक पक्षांने चार लोकसभा मतदार क्षेत्र भाजपाच्या प्रभावशाली नेतृत्वामध्ये प्राप्त केले आहे, आणि राष्ट्रीय काँग्रेस पक्षाचा दारुण पराभव करुन भारतीय जनता पक्ष प्रणीत एन.डी.ए. ला बहुमत मिळवून विजय संपादन करुन दिला आहे.

विदर्भातील सोळावी लोकसभा निवडणूक 2014 चे विश्लेषण अभ्यासिले असता लोकशाही प्रवृत्तीच्या मानवी संस्कृतीमध्ये प्रगल्भ व विकसित लोकशाही मुल्यांचा लोकमानसाने यथायोग्य वापर केलेला आहे. लोकतांत्रिक प्रणालीमध्ये सहभागी होवून जे दुर्गुण राज्यकर्त्यामध्ये, पुढाऱ्यांमध्ये जे दिसत होते, ते डावलण्याचा खरा प्रयत्न मतदारांनी केला आहे. त्यात प्रामुख्याने भ्रष्टाचार, महागाई, बेरोजगारी, कुपोषण,

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आरोग्य आदि ठिकाणी सरकारने निष्क्रियता दाखविल्यामुळे जागृत झालेला मतदार 66. 38 टक्के मतदार करुन नव्या मतदारांचा उत्साह दिसून आला आहे.

सोळावी लोकसभा निवडणूक 2014 मध्ये विजयी झालेले उमेदवार त्यांचे मतदारक्षेत्र, पक्ष, मिळालेली मते व टक्केवारी खालीलप्रमाणे आहे.

अ. क्र.	मतदार क्षेत्र	उमेदवाराचे नाव	पक्ष	मिळालेली मते	टक्केवारी
1	अमरावती	आनंदराव अडसूळ	शिवसेना	467212	46.72
2	अकोला	संजय धोत्रे	भाजपा	456472	
3	बुलढाणा	प्रतापराव जाधव	शिवसेना	509145	52.01
4	यवतमाळ–वाशिम	भावना गवळी	शिवसेना	477905	46.27
5	नागपूर	नितिन गडकरी	भाजपा	577766	54.17
6	रामटेक	कृपाल बालाजी तुमाने	शिवसेना	519892	44.48
7	गडचिरोली–चिमूर	अशोक नेते	भाजपा	433982	52.18
8	वर्धा	रामदास तडस	भाजपा	537518	53.04
9	भंडारा–गोंदिया	नानाभाऊ पटोले	भाजपा	606129	50.62
10	चंद्रपूर	हंसराज अहिर	भाजपा	508049	45.77

वरील सर्व उमेदवार हे भाजपा तसेच भाजपाप्रणित राष्ट्रीय लोकशाही आघाडीचे विजयी उमेदवार आहेत.

प्रस्तुत शोधनिबंधामध्ये भारतीय लोकशाहीतील निवडणूक प्रक्रिया आणि मतदार व्यवहार यांचा संयुक्तपणे अभ्यास करुन काही निष्कर्ष हाती लागले आहेत. राष्ट्रीय कॉंग्रेस पक्ष प्रणीत (यु.पी.ए.) व भारतीय जनता पक्ष प्रणीत (एन.डी.ए.) यांमध्ये मुख्य लढत दिसुन आली. रा.कॉं. पक्ष (यू.पी.ए.) या पक्षाने वर्षानुवर्ष सत्ता उपभोगूनसुध्दा लोकसभेत दारुण पराभव स्विकारावा लागला असून, साधे विरोधी पक्षनेतेपद सुध्दा टिकविता आले नाही. नरेंद्र मोदींचे विकासतंत्र, गुजरात मॉडेल, आणि प्रभावी भाषाशैली मतदारांना प्रभावित करण्यात कारणीभूत ठरली. हिंदुत्ववादी संघटना व रा.स्व.सं. च्या परिणामुळे भाजपाला स्पष्ट बहुमत मिळविण्यात मदत झाली. गांधी परिवाराचा मतदारांवरील प्रभाव कमी झाल्याचे दिसून आले. कॉंग्रेस पक्षाचा भ्रष्टाचार राष्ट्रीय नेतृत्वाचा अभाव प्रामुख्याने दिसून आला. प्रादेशिक पक्षांना झुगारुन मतदारांनी राष्ट्रीय पक्षाला दिलेली पसंती, नवमतदारांनी निवडणूकीमध्ये दाखविलेला उत्साह व त्यामुळे वाढलेली मतदारांची टक्केवारी भाजपला विजयश्री खेचून आणण्यास यशस्वी ठरली.

Current Global Reviewer
Impact Fact .143 UGC Approved Sr. No. 61524 ISSN 23 4685

सोळावी लोकसभा निवडणूक ही लोकप्रतिनिधीचे गुणदोष यांचे अध्ययन करणारी असली तरी तिचे अंतरंग तपासले असता 1991 पासून एकहाती सत्ता असलेला पक्षाला युतीचे संमिश्र सरकार आणि बहुमताचे सरकार यात मतदात्यांनी संयुक्त पुरोगामी आघाडीला बाजुला ठेवून भाजपाचे मोठ्या प्रमाणात उमेदवार निवडून दिले. आजपर्यंत ज्या पक्षाला अपेक्षित यश मिळाले नाही, त्यांच्या हातात एक हाती सत्ता देवून सोळावी लोकसभा निवडणूक खऱ्या अर्थाने सार्वत्रिक ठरली. तसेच नवनियुक्त प्रथमच लोकसभेत पोहचलेली व्यक्ती पंतप्रधानपदी विराजमान झाली. हे यश मोदींच्या राजकीय चातुर्यामुळे मिळाले हे नाकारता येत नाही.

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ISSN: 2348-1390

NEW MAN

INTERNATIONAL JOURNAL OF MULTIDISCIPLINARY STUDIES

VOL. 5 SPECIAL ISSUE 4 APRIL 2018

A REFEREED AND INDEXED E-JOURNAL

IMPACT FACTOR: 4.321 (IIJIF)

(UGC Approved Journal No. 45886)

Special Issue

On the occasion of National Seminar on

Gender Isonomy: A Societal Onus—2018

Organized by

Pratibha Women's Studies Centre

Vidya Bharati Mahavidyalaya, Amrawati

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New Man International Journal of Multidisciplinary Studies
(UGC Approved Journal No: 45886)
ISSN: 2348-
Impact Factor: 4.321 (

Gender Inequality in Political System - A Global Problem

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Absract: Gender inequality is a problem not only across India but also all over the world, there is a power gap between men and women. Women have less access to parliamentary and executive power. They are less educated, have fewer good jobs and are less wealthy than men. Gender inequality can be found in the patriarchal structure of the cultural background of every ethnicity, nation or people. Also all religious communities, whether Jewish, Muslim, Hindu, traditional or Christian, give more power to men than to women. We think that gender inequality is not as much of a problem in our generation as it was in our parents' and grandparents' generations. This article aims to analyze gender inequality in the political system.

Key words : Gender inequality, political system, women enpowerment

Introduction: Gender inequality leading to deprivation of power among women continues to be a political reality in India today. Women are perpetually excluded from decision-making at every step of the ladder, starting from the household to the top layer of policy making. Although the Constitution of India attempts to remove gender inequalities by interdicting discrimination based on sex and class, and enshrining fundamental rights for all citizens, women still have only *de jure* rather than *de facto* access to these rights.

There is no denying the fact that greater participation of women in the political process would be a pre-condition for their economic and social emancipation. However, even though a significantly large number of women vote in the country, yet only a few of them assume the reins of power..

Measuring Gender Inequality: To measure inequality the United Nations Development Programme (UNDP) developed two indicators: the Gender-related Development Index (GDI) and the Gender Empowerment Measure.The GDI measures (the same as the Human Development Index, HDI) life expectancy, knowledge and the quality of life. The indicators are (1) the life expectancy at birth; (2) the adult literacy rate and the combined gross enrolment ratio for primary, secondary and tertiary schools; and (3) the Gross Domestic Product (GDP) per capita in purchasing power parity (PPP).

Electoral Systems: Elections, generally to choose amongst political parties or candidates for a house of representatives, can be held in different systems. There are two main systems of representation: proportional and majoritarian representation. From a gender perspective th proportional Generally women don't participate as muc as men due to the aforementioned reasons. If the participate they use more non-conventional ways. The are more engaged in social movements and non governmental organizations than in governments parliaments or political parties. Generally the parliamen should be a mirror of the society. All groups should b represented equally.

Data Analysis and Discussion : One instrument for th empowerment of women in the government is a quot system, since aside from the aforementioned cultural economic and social and historical reasons, femal participation also depends on the electoral system. On reason for the huge gender inequality is the lack o empowerment of women which is also reflected i women's representation in parliament. Women's representation in India parliament was only 4.9%, whic is almost the lowest among its neighbors the onl exceptions being Sri Lanka and Bhutan where th representation was only 4.9%. In contrast women's representation was 13% in Myanmar, 20% each i Bangladesh and Pakistan, 23.6% in China and 29.5% i Nepal.

To remedy the low participation of women electors India in 1994 established quotas (reservations) vide th 73rd and 74th constitutional amendments to reserve 3 per cent of the seats in local governments for women. Th Women's Reservation Bill (108th amendment) has als been introduced in the national Parliament to reserve 3 per cent of the LokSabha seats for women, but the bill i yet to be passed. It is believed that though increasing th number of women in national government may no guarantee an impact on governance, a critical mass o women in power can bring about transformation i leadership

The core idea of quotas is to increase the politica participation of women or religious or ethnic or othe minorities. Quotas are an instrument against under-representation and especially they are helpful to realise critical minority instead of only a few token women i political life.

Conclusion : Equal participation of women and men i politics is an important condition for effective democrac and good governance. Apart from strengthening an enhancing the democratic system, the participation o more women in political decision-making has man positive effects on society that can help improve the live

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AARHAT MULTIDISCIPLINARY INTERNATIONAL EDUCATION RESEARCH JOURNAL (AMIERJ)

Volume–VII, *Special Issue–XXIII,* *22nd September, 2018*

Peer Reviewed Journal *ISSN 2278-5655* *EduIndex Impact Factor 5.18*

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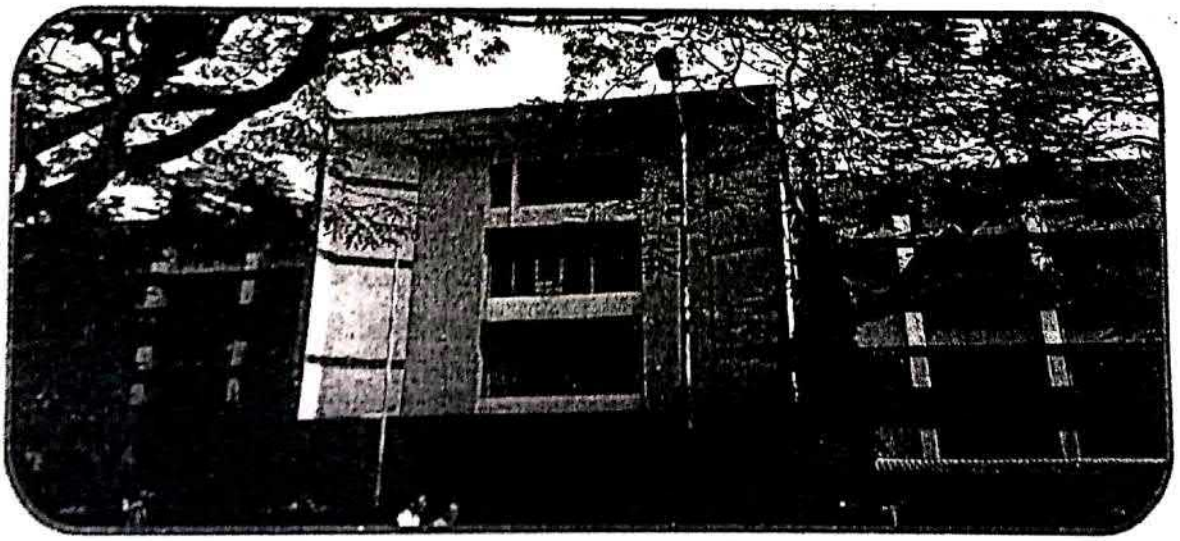

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Chief Editor

Dr. Yashodhara Varale

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Combinatorial Chemistry & High Throughput Screening, **2018**, *21*, **204-214**

1 RESEARCH ARTICLE

QSAR Analysis for Antioxidant Activity of Dipicolinic Acid Derivatives

Vesna Rastija[*a], Maja Molnar[b], Tena Silađi[b], and Vijay Hariram Masand[c]

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ARTICLE HISTORY

Received: September 21, 2017
Revised: November 17, 2017
Accepted: February 3, 2018

DOI:
10.2174/1386207321666180213092352

Abstract: ***Aim and Objective*:** The aim of this study was to derive robust and reliable QSAR models for clarification and prediction of antioxidant activity of 43 heterocyclic and Schiff bases dipicolinic acid derivatives. According to the best obtained QSAR model, structures of new compounds with possible great activities should be proposed.

***Methods*:** Molecular descriptors were calculated by DRAGON and ADMEWORKS from optimized molecular structure and two algorithms were used for creating the training and test sets in both set of descriptors. Regression analysis and validation of models were performed using QSARINS.

***Results*:** The model with best internal validation result was obtained by DRAGON descriptors (*MATS4m*, *EEig03d*, *BELm4*, *Mor10p*), split by ranking method (R^2 = 0.805; R^2_{ext} = 0.833; F = 30.914). The model with best external validation result was obtained by ADMEWORKS descriptors (*NDB, MATS5p*, *MDEN33, TPSA*), split by random method (R^2 = 0.692; R^2_{ext} = 0.848; F = 16.818).

***Conclusion*:** Important structural requirements for great antioxidant activity are: low number of double bonds in molecules; absence of tertial nitrogen atoms; higher number of hydrogen bond donors; enhanced molecular polarity; and symmetrical moiety. Two new compounds with potentially great antioxidant activities were proposed.

Keywords: QSAR, antioxidant activity, dipicolinic acid, polar surface area, hydrogen bond donors, derivatives.

1. INTRODUCTION

Dipicolinic acid (DPA) (2,6-pyridinedicarboxylic acid) is naturally inherent in the spores of *Bacillus* [1] and *Clostridium genusus* [2] that exists in the core in the form of chelates with calcium ions [3]. DPA contributes to the spore resistance to UV radiation [4], wet heat [5], and protecting spore DNA from damage [6]. DPA forms stable chelates with metal ion, and these complex compounds show a variety of biological activities, such as antimicrobial, antifungal [7-9], anticancer [10] and antioxidant activities [11].

It was discovered that a series of substituted mono- and bis-dipicolinic derivatives possessed antimicrobial and antioxidant activities [12-15]. In our previous work, we have reported synthesis of Schiff bases [16] and heterocyclic compounds [17] derived from DPA. Many of the obtained compounds exhibited significant antifungal and antioxidant activities. The above-mentioned studies identified significant chemical features for the most active compounds. In a series of synthesized mono- and bis-dipicolinic acid heterocyclic derivatives – thiosemicarbazides, triazoles, oxadiazoles and thiazolidinones, and thiosemicarbazides showed predominant antioxidant activity. Influence of different substituents is obvious, since in almost all compounds phenyl substitution results in a better 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging activity compared to the alkyl substitution [17]. In a series of Schiff bases derived from dipicolinic acid, compounds derived from di-hydrazide showed higher antioxidant activity than the ones derived from mono-hydrazide [16].

The structure-activity relationship (SAR) of the antibacterial and antiproliferative potential of some 1-pyridinecarbonyl-4-substituted thiosemicarbazide derivatives showed that substitution at the position 2 of the pyridine ring enhances biological activity.

In the present study, the main goal was to build robust and reliable QSAR models for the description and prediction of antioxidant activity of heterocyclic and Schiff bases dipicolinic acid derivatives. The relevance of the best QSAR model should also be to provide a chemical and structural explanation of antioxidant activities of the most active compounds. Also, the aim of this study was to compare the statistical performance of different algorithms for splitting data into training and test set, as well as models obtained by two sets of descriptors calculated by different computer programs.

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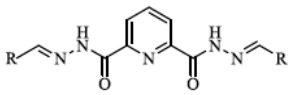
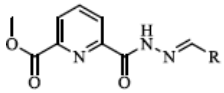
Table 1. Structures along with experimentally determined antioxidant activities (expressed as log % DPPH) of 2,6-pyridinedicarboxylic acid derivatives [16, 17].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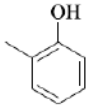
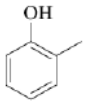
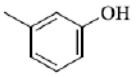
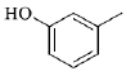
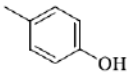
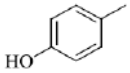
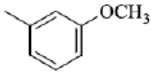
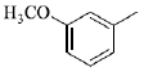
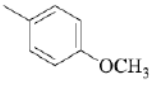
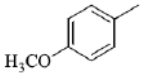
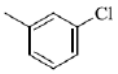
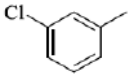
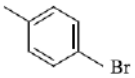
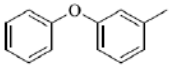
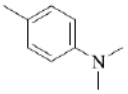
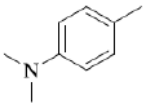
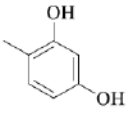
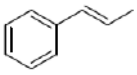
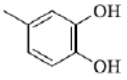
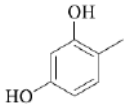
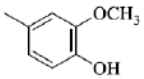
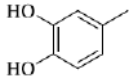
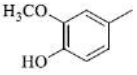
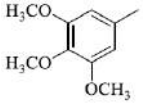
1		-0.31	2		0.894
3		0.782	4		0.582
5		0.701	6		0.845
7		0.834	8		0.786
9		0.671	10		0.68
11		0.748	12		0.705
13		0.768	14		0.656
15		0.608	16		-0.495
17		-0.854	18		0.955
19		0.874	21		0.856
20		-0.42	23		1.692
22		0.874	25		1.429
24		1.732			
26		1.621			
27		0.736			

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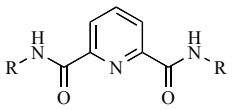				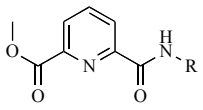	
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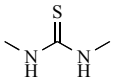
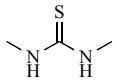
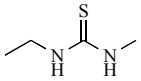
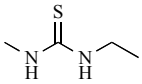
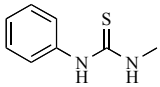
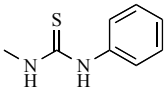
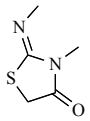
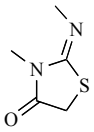
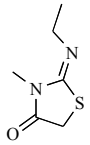
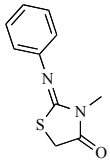
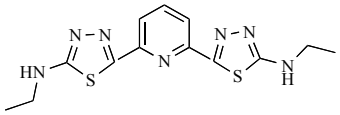
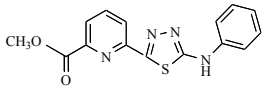
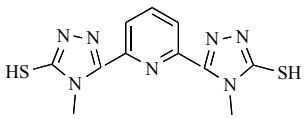
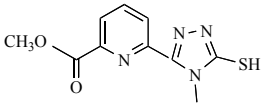
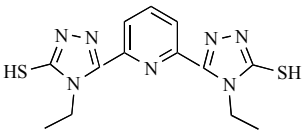
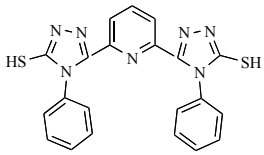
31		1.061	**28**		1.583
32		1.566	**29**		1.68
33		1.688	**30**		1.936
41		0.301	**40**		0.114
42		0.996			
43		0.362			
36		1.134	**34**		1.1
37		1.487	**35**		1.401
38		1.504	**39**		1.49

2. MATERIALS AND METHODS

2.1. Data Set

The synthesis and antioxidant evaluation of 43 DPA derivatives have been described in our previous studies [16, 17]. Antioxidant activities, expressed as % scavenging activity on DPPH (using ascorbic acid as standard), were converted in the form of the logarithm (log %DPPH). Higher value of log %DPPH means more powerful antioxidant activity. Structural details of all studied molecules along with experimental log %DPPH are shown in Table **1**.

2.2. Descriptor Calculation and Selection

The three-dimensional (3D) structures of 43 DPA derivatives were optimized using the molecular mechanics force field (MM+) [18] applying the Avogadro 1.2.0. (University of Pittsburgh, Pittsburgh, PA, USA). Subsequently, all structures were submitted to the geometry optimization using semiempirical AM1 method [19]. The molecular structures were optimized using Polak-Ribiere algorithm until the root mean square gradient (RMS) was 0.001 kcal/(Åmol).

The Polar Surface Area (PSA) surface was generated from an optimized structure by VEGA ZZ (Department of Pharmaceutical Sciences of the University of Milan, Milan, Italy) [20]. The Polar Surface Area (PSA) was calculated considering polar and apolar atom surfaces, as dotted shape, with probe radius 1.4 and density 60.

Two set of descriptors were calculated by two different softwares 1. DRAGON descriptors – were calculated using Parameter Client (Virtual Computational Chemistry Laboratory, an electronic remote version of the Dragon program [21]. Seventeen groups of two-dimensional (2D) and three-dimensional (3D) Dragon's descriptors were used to generate QSAR models: constitutional, topological, walk and path counts, connectivity, information, 2D auto-correlations, edge adjacency, BCUT (Burden eigenvalues), topological charge, eigenvalue-based, geometrical, RDF (Radial Distribution Function), 3D-MoRSE (3D-molecular representation of structures based on electron diffraction), WHIM (WeigHted Covariance Matrices), GETAWAY (Geometry, Topology, and Atom-Weights AssemblY) descriptors, functional group counts, and molecular properties [22]. In order to reduce huge number of calculated descriptors (about 1260), firstly, zero values descriptors were excluded from initial pool. Further exclusion was performed using QSARINS-Chem 2.2.1 [23]: constant and semi-constant descriptors, i.e. those having chemical compounds with a constant value for more than 80 %, and too inter-correlated descriptors (> 85%) were rejected.

2. ADMEWORKS descriptors – calculated by ADMEWORKS ModelBuilder, tool for building mathematical models (Version 7.9.1.0(build.187.4934.2102) Enterprise Edition Copyright (C) 2011 Fujitsu Kyushu Systems Limited). Numerous groups of 2D and 3D molecular descriptors have been calculated, such as: charged partial-surface-area (CPSA) descriptor, atom-specific CPSA descriptor (DATOM), carbon type (CTYPE), molecular distance edge descriptor (DEDGE), fragment descriptors generation routine (DMFRAG), hydrogen bond specific descriptors for pure (HBPURE) and mixed (HBMIX) compounds, measure of the conformational flexibility, Hückel molecular orbital calculation (HMO), MOPAC descriptor, molecular strain energy calculation (STRAIN), etc. [24]. Elimination of irrelevant descriptors was performed using Feature Selection command of ADMEWORKS ModelBuilder that includes following tests: a) missing values test - which excludes descriptors with missing values; b) zero test - which excludes descriptors with less than the specified percentage of non-zero values; c) automated correlations test - deletes all parameters that have single or multiple correlations to other parameters, with the R^2 value larger than the specified threshold (0.7).

2.3. Training and Test Set Compounds Selection

Two algorithms were used for creating the training and test sets in both set of descriptors:

1. Data sets were randomly divided into training (80 %, N_{train} = 35) and prediction (20 %, N_{test} = 8) set using QSARINS.

2. Data sets were split by ranking method: Compounds were ranked by the activities from the most active to the least active compound. Then, the activities were divided into the bins by grouping the values into the six class intervals. Finally, one or two compounds were selected randomly from each class for the test set (N_{train} = 35, N_{test} = 8) [25].

2.4. Regression Analysis and Validation of Models

The best QSAR models were obtained by using a Genetic Algorithm (GA) using QSARINS. In order to avoid the overfitting the smallest number of descriptors that can adequately model the activity of the compounds in the study should be used. According the Topliss-Costello rule [26], the number of variables should be higher or equal to 5. In this study, considering we worked with the small data set (35 compounds in the training set), the number of descriptors (k) in the multiple regression equation was limited to four. Additional descriptors, will be resulted in overfittied and not predictive models. The models have been assessed by: fitting criteria; internal cross-validation using leave-one out (LOO) method and Y-scrambling; and external validation. Fitting criteria included: the coefficient of determination (R^2), adjusted R^2 (R^2_{adj}), cross-validate R^2 using leave-one-out method (Q^2_{LOO}), global correlation among descriptors (Kxx), difference between global correlation between molecular descriptors and y the response variable, and global correlation among descriptors (ΔK), standard deviation of regression (s), and Fisher ratio (F) [27-29]. Collinearity among the descriptors has also validated by variance inflation factor (VIF). VIF is the reciprocal of tolerance: $1/(1-R^2_i)$ where R^2_i is the squared multiple correlation of the ith independent variable regressed on the other independent variables in the analysis [30].

Internal and external validations also included the following parameters: the coefficient of determination of test set (R^2_{ex}), root-mean-square error of the training set ($RMSE_{tr}$); root-mean-square error of the training set determined through cross validated LOO method ($RMSE_{cv}$), root-mean-square error of the external validation set ($RMSE_{ex}$), concordance correlation coefficient of the training set (CCC_{tr}), test set using LOO cross validation (CCC_{cv}), and of the external validation set (CCC_{ex}) [27], mean absolute error of the training set (MAE_{tr}), mean absolute error of the internal validation set (MAE_{cv}) and mean absolute error of the external validation set (MAE_{ex}) [27], predictive residual sum of squares determined through cross-validated LOO method ($PRESS_{cv}$) in the training set and in the external prediction set ($PRESS_{ex}$). The analysed external validation parameters also include. Robustness of QSAR models was tested by Y-randomisation test.

Investigation of the applicability domain of a prediction model was performed by leverage plot (plotting residuals vs. leverage of training compounds). The warning leverage h^* is defined as $3p'/n$, where n is the number of training compounds and p' is the number of model adjustable parameters [31]. Tools of regression diagnostic as residual plots and Williams plots were used to check the quality of the best models and define their applicability domain using QSARINS.

3. RESULTS AND DISCUSSION

Four models were obtained by two different sets of descriptors (calculated by Dragon and ADMEWORKS software) and two different methods (random and ranking) for creating training and prediction set.

Models obtained by DRAGON descriptors:

The random splitting model

log %DPPH = -1.073 – 0.492 *IVDE* – 0.492 *Mor08u* – 11.755 *Dp* + 1.736 *R5u* (1)

Compounds in the test set: **15**, **20**, **23**, **31**, **33**, **36, 37**, **42**

The ranking splitting model

log %DPPH = 2.954 – 1.427 *MATS4m* + 1.093 *EEig03d* – 4.2 *BELm4* + 0.974 *Mor10p* (2)

Compounds in the test set: **1**, **2**, **7**, **16, 29**, **33**, **34**, **35**

Models obtained by ADMEWORKS descriptors:

The random splitting model

log %DPPH = 0.545 – 0.4 *NDB* – 2.2 *MATS5p* – 0.182 *MDEN33* + 0.014 *TPSA* (3)

Compounds in the test set: **1**, **4**, **6**, **7**, **11**, **13**, **28, 29**

The ranking splitting model

log %DPPH = 3.361 – 0.281 *NDB* – 0.432 *GATS8v* – 1.235 *MATS5p* + 0.129 *NUMHBD* (4)

Compounds in the test set: **1**, **2**, **7**, **16, 29**, **33**, **34**, **35**

The statistical results for the obtained models are presented in Table **2**.

Description of descriptors included is given in Table **3**. In order to exclude collinearity of descriptors included in same model, correlation matrix was generated (Tables **4-7**). Descriptors included in models (1-4) are not mutually correlated (correlation coefficient, $R \leq 0.7$). *VIF* values of individual descriptors from each model were also presented in Tables **4-7**. Linear dependence within the correlation descriptors sets has been rejected since the all *VIF* < 5 [32]. Low collinearity is also verified by the low values of *Kxx* (Table **2**). The molecular descriptor values have been tabulated in Supplementary File 1 (SF 1). Experimental and calculated log %DPPH by model (1-4) are shown in Supplementary File 2 (SF 2).

Satisfaction of fitting criteria implies the following: the closer R^2 values are to unity, the more similar calculated values are to the experimental ones, that is, $R^2 \geq 0.60$. The minimum acceptable statistical parameters for internal and external predictivity include the following conditions: $R^2_{ext} \geq 0.60$; $CCC \geq 0.85$; *RMSE* and *MAE* close to zero; and $RMSE_{tr} < RMSE_{cv}$. Robust QSAR models should have R^2_yscr and Q^2_yscr < 0.2, as R^2_yscr > Q^2_yscr [33]. Also, larger *F* statistic and lower standard deviation means that the model is more significant. Analysis of Table **2** indicates that all four models satisfy threshold for most of the internal validation parameters. However, models (1) and (2), created by Dragon descriptors, have better fitting performances (higher R^2, R^2_{adj}, *F*, and CCC_{tr}, and lower *s*, $RMSE_{tr}$, MAE_{tr} than models (3) and (4), obtained by ADMEWORKS descriptors. Also, models (1) and (2) showed a better performance in the

Table 2. The statistical results for the QSAR models for antioxidant activity.

	Model (1)	Model (2)	Model (3)	Model (4)
N_{tr}	35	35	35	35
N_{ex}	8	8	8	8
Fittinig criteria				
R^2	0.821	0.805	0.692	0.646
R^2_{adj}	0.797	0.779	0.650	0.599
s	0.281	0.278	0.381	0.374
F	34.455	30.914	16.818	13.689
p	$< 10^{-5}$	$< 10^{-5}$	$< 10^{-5}$	$< 10^{-5}$
Kxx	0.357	0.325	0.251	0.192
ΔK	0.034	0.004	0.031	0.074
$RMSE_{tr}$	0.260	0.257	0.353	0.257
MAE_{tr}	0.212	0.19	0.290	0.257
CCC_{tr}	0.902	0.892	0.818	0.785
Internal validation criteria				
Q^2_{LOO}	0.753	0.725	0.576	0.522
$RMSE_{cv}$	0.306	0.305	0.414	0.403
MAE_{cv}	0.250	0.226	0.340	0.300
$PRESS_{cv}$	3.268	0.849	5.989	5.670
CCC_{cv}	0.866	0.849	0.750	0.715
R^2_Yscr	0.118	0.118	0.119	0.116
Q^2_Yscr	-0.224	-0.232	-0.208	-0.215
External validation criteria				
$RMSE_{ext}$	0.674	0.550	0.231	0.520
MAE_{ext}	0.611	0.365	0.197	0.381
$PRESS_{ext}$	3.637	2.424	0.426	2.160
R^2_{ext}	0.717	0.833	0.848	0.639
Q^2_{F1}	-0.009	0.55	0.842	0.562
Q^2_{F2}	-0.078	0.507	0.84	0.56
Q^2_{F3}	-0.203	0.106	0.868	0.203
CCC_{ext}	0.678	0.657	0.908	0.666
$\overline{r_m^2}$	0.261	0.083	0.765	0.26
Δr_m^2	0.366	0.651	0.12	0.4
Applicability domain				
N compounds outlier	2 (**16**,**17**)	3 (**1**,**16**,**27**)	0	2 (**16**,**17**)
N compounds out of app.dom.	3 (**39**, **42**, **20**)	1 (**17**)	0	0

internal validation (higher Q^2_{LOO}, CCC_{cv}, and lower $RMSE_{cv}$, MAE_{cv}, and $PRESS_{cv}$. The results of Y-scrambling demonstrated that all models were not obtained by chance correlation (Q^2yscr < 0.2, and R^2yscr< 0.2; R^2yscr > Q^2yscr). In spite of a good fitting performance and good internal validation, the real predictive power of model (1) and (2) is failed according to the external validation parameters and outliers and compounds outside of applicability domain. Moreover, negative values of Q^2_{F1}, Q^2_{F2} and Q^2_{F3} of model 1, as well as very low values (< 0.7) of model (2) and (4), including values of $\overline{r_m^2}$ < 0.6 indicate these models are useless for external predictivity.

Model (3) was generated by ADMEWORKS descriptors and random splitting methods. In spite of its powerless fitting and internal performances, model possess real predictivity for the chemicals in the validation set according to high values of parameters for external validations (R^2_{ext} = 0.848; CCC_{ext} = 0.908) and small difference between $RMSE_{tr}$ and $RMSE_{ex}$, and between MAE_{tr} and MAE_{ex}.). Also, Williams plot for same model reveals no outliers, and no compounds outside of applicability domain (Fig. **1**). A scatter plot of experimentally obtained antioxidant activity by model (3) is shown in Fig. (**2**). Model (4) has weakest parameters of external validation, as well as one outlier (**16**), and one compound out of the applicability domain (**17**).

Despite of difference in predictive potential of the proposed models, included molecular descriptors may relieve in elucidation of important physicochemical and structural requirements for the antioxidant activity of heterocyclic and Schiff bases dipicolinic acid derivatives. Negative sign of variable that represents a number of double bonds (*NDB*) in equations (3) and (4), means that this type of covalent bond is unfavourable for the antioxidant power (except double bonds in phenyl or heterocyclic ring). Thus, the most active compound **30** (log %DPPH = 1.936) has 3 double bonds, while the compounds with low antioxidant activity have 6 double bonds (**41,** log %DPPH = 0.301; **17**, log %DPPH = -0.854). Negative sign of descriptor *MDEN33* in model (3) indicates that higher distance between tertial nitrogen atoms negatively influences on the antioxidant activity. Compounds without tertial nitrogen atoms have a higher antioxidant potential, such as thiosemicarbazides (**28-33**). Since DPPH test is based on the capability of stable free radical 2,2-diphenyl-1-picrylhydrazyl to react with H-donors [34], positive coefficient of hydrogen bond donors (*NUMHBD*) in model (4) is expected. That implies that higher number hydrogens attached to the oxygen, nitrogen or sulphur atoms, positively influences on antioxidant activity, such as secondary nitrogen atoms in thiosemicarbazides (**28-33**). This supports our recent findings that enhanced value of hydrophilic factor, which is related with number of –OH, –NH_2, and >NH groups in molecule, is favourable for antioxidant activity of coumarinyl Schiff bases [35]. Also, it corresponds with previously statement about negative influence of enhanced number of tertial nitrogen atoms on antioxidant activity. However, five compounds (**22**, **24**, **31-33**) have more than five hydrogen bond donors, and according the Lipinski's rule of five [36], as potential drug, they could have poor absorption or permeation. Topological polar surface area (*TPSA*) in model (3), is descriptor that also characterized drug absorption, including intestinal absorption, bioavailability and blood–brain barrier penetration. Polar surface area (*PSA*) is sum of surface of polar atoms (oxygen, nitrogen, sulphur, etc.) [37]. Although model (3) implies that molecules with enhanced values of *TPSA* have higher antioxidant activity, these molecules could poorly penetrate through the cell membranes [15, 38]. According the data presented in Supplementary File 1, value of *TPSA* for the most active compound (**30**) is larger (124.44) than for the least active (**17**) (114.27). *TPSA* is a useful descriptor in QSAR models, which a sign its coefficient can indicate whether a more polar ligand is favoured or disfavoured for enhanced activity. However, it is based only on the contribution of tabulated polar fragments, not from the 3D conformations of these chemical groups. Also, *TPSA* does not include the influence of positional changes of functional groups [38]. In order to additionally clarify sense of PSA for antioxidant activity of Schiff bases dipicolinic acid derivatives, we were calculated and compared PSA of the most active (**30**) and the least active compound (**17**). Apolar atom surface takes into account C and H atoms bonded to C atoms. Polar atoms are O, S, N, P and H, not bonded to C. Because of higher number of polar atoms in molecule (**30**), their PSA (203.4 $Å^2$) is much higher than molecule (**17**) (165.6 $Å^2$). Moreover, apolar surface area of the most active compound (**30**) is significantly lower (590.3 $Å^2$) than at least active compound (**17**) (983.2 $Å^2$). Fig. (**3**) shows a mapped PSA of the most active molecule (**30**) and the least active molecule (**17**), for comparison. Apolar and polar surfaces are presented as gradient of two color codes: black (apolar surface) and grey (polar surface).

3D-MoRSE descriptors, *Mor08u* and *Mor10p*, are involved in models (1) and (2). These descriptors were generated from electron diffraction studies and reflect the three-dimensional arrangement of atoms in a molecule [39]. Descriptor *Mor08u* denotes unweighted descriptors with scattering parameter s = 7 $Å^{-1}$. Since it is unweighted, the descriptor has no discriminative ability and treats each atom equally. It has the possibility to distinguish the difference between the bond lengths of any kinds of atoms at least 0.12 Å. Consider that their final values are derived mostly from long distances atoms, it has great power to distinguish mono- from bis-substituted dipicolinic derivatives (Table **S1**). Negative coefficient of *Mor08u* in Eq. (1) implies that lower values of that descriptor are favourable for the exhibition of antioxidant activity. Descriptor *Mor10p* reflects the contribution of 3D distribution of atomic polarizability (p) at a scattering parameter s = 9 $Å^{-1}$. According to model (2), it is expected that increased values of *Mor10p* indicates higher antioxidant activity. As can be noticed from Table **S1**, this descriptor is extremely sensitive to the position of the sulphur atoms (atom with higher polarizability, p = 19.6) in molecules.

MATS5p, *MATS4m* and *GATS8v* belong to the 2D autocorrelation molecular descriptors that describe how a considered property is distributed along a topological molecular structure. *MATS5p* corresponds to the Moran autocorrelation –lag 5 / weighted by atomic polarizability, while *MATS4m* is the Moran autocorrelation descriptor –lag 5 / weighted by atomic masses.

Table 3. Summary table for descriptors included in models 1-4.

Symbol	Descriptor name	Groups of descriptors
IVDE	Mean information content on the vertex degree equality	Information
Mor08u	3D-MoRSE signal 08 / unweighted	3D-MoRSE
Mor10p	3D-MoRSE signal 10 / weighted by polarizability	3D-MoRSE
Dp	D total accessibility index / weighted by polarizability	WHIM
R5u	R autocorrelation of lag 5 / unweighted	GETAWAY
MATS4m	Moran autocorrelation of lag 4 weighted by mass	Autocorrelations
MATS5p	Moran autocorrelation of lag 4 weighted by atomic polarizabilities	Autocorrelations
GATS8v	Geary autocorrelation of lag 8 weighted by van der Waals volume	Autocorrelations
EEig03d	Eigenvalue 03 from edge adj. matrix weighted by dipole moments	Edge adjacency
BELm4	Lowest eigenvalue 4 of Burden matrix / weighted by atomic masses	BCUT
NDB	Number of double bonds	DMFRAG
MDEN33	Molecular distance edge between all tert tert N	EDGE
TPSA	Topological polar surface area	Mol. properties
NUMHBD	Number of hydrogen bond donors	H acceptor/donor

Table 4. Correlation matrix for the descriptors included in model 1 and variance inflation factor (VIF) for individual descriptor.

	VIF	***IVDE***	***Mor08u***	***Dp***	***R5u***
IVDE	1.45	1.00			
Mor08u	1.69	0.38	1.00		
Dp	1.23	0.00	0.01	1.00	
R5u	1.45	0.18	0.33	0.37	1.00

Table 5. Correlation matrix for the descriptors included in model 2 and variance inflation factor (VIF) for individual descriptor.

	VIF	***MATS4m***	***EEig03d***	***BELm4***	***Mor10p***
MATS4m	1.49	1.00			
EEig03d	1.49	0.43	1.00		
BELm4	1.11	-0.28	0.09	1.00	
Mor10p	1.37	-0.41	-0.34	0.17	1.00

Table 6. Correlation matrix for the descriptors included in model 3 and variance inflation factor (VIF) for individual descriptor.

	VIF	**NDB**	**MATS5p**	**MDEN33**	**TPSA**
NDB	1.96	1.00			
MATS5p	1.15	-0.20	1.00		
MDEN33	1.96	-0.49	-0.01	1.00	
TPSA	1.49	0.21	-0.01	0.34	1.00

Table 7. Correlation matrix for the descriptors included in model 4 and variance inflation factor (VIF) for individual descriptor.

	VIF	NDB	GATS8v	MATS5p	NUMHBD
NDB	1.49	1.00			
GATS8v	1.35	-0.13	1.00		
MATS5p	1.39	-0.20	0.01	1.00	
NUMHBD	1.85	0.43	-0.38	-0.02	1.00

GATS8v is Geary autocorrelation of lag 8 weighted by van der Waals volume [22]. These descriptors reflect contribution of pairs of atoms different polarizability/mass/ van der Waals volume at the defined topological distance or spatial lag. Therefore, *MATS5p*, *MATS4m* and *GATS8v* indicate dependence of one atom on value of polarizability /mass/ van der Waals volume of other atoms at the topological distance 5, 4, and 8, respectively. Their negative regression coefficients in models (3) and (4) suggest in unfavorable effect of increased autocorrelation contents of five-, four-, eight-member structural graphs weighted by atomic polarizability, mass, and van der Waals volume for the activity.

WHIM is geometrical descriptor calculated on the projections of the atoms along principal axes [24]. Descriptor *Dp* is total accessibility index weighted by atomic polarizability, which values are strongly influenced by kind and position of substituents on phenyl ring. Negative coefficient of *Dp* in model (1) implies that 3D distribution of substituents with the increased atomic polarizability (Cl, Br atoms) could negatively influenced to the antioxidant power. It explains weak antioxidant activity of compounds with Br (**16**) and Cl atoms (**14**, **15**). Descriptor *IVDE* is mean information content on the vertex degree equality [24]. Since it is a measure of the lack of structural homogeneity or the diversity of a molecule [40], its negative coefficient in model (1) suggests that molecules with symmetrical moiety are potentially more active.

Descriptor *BELm4* in model (2) belongs to the BCUT descriptors. BCUT descriptors are the eigenvalues of a modified connectivity matrix, the Burden matrix, which capture useful measurement of molecular diversity [41]. Highest value of *BELm4* have most inactive compounds, **17** and **20** (*BELm4* = 1.894 and 1.607, respectively, Table **S1**), which correspond with a negative coefficient of that variable in model (2). Descriptor *EEig03d* in model (2) is related to the molecular polarity, which mainly described the electronic effect of molecule and the hydrophobic properties. Same as *TPSA* in model (3), positive regression coefficient of *EEig03d* in model (2) suggests that enhanced molecular polarity positively influence on antioxidant activity of compounds.

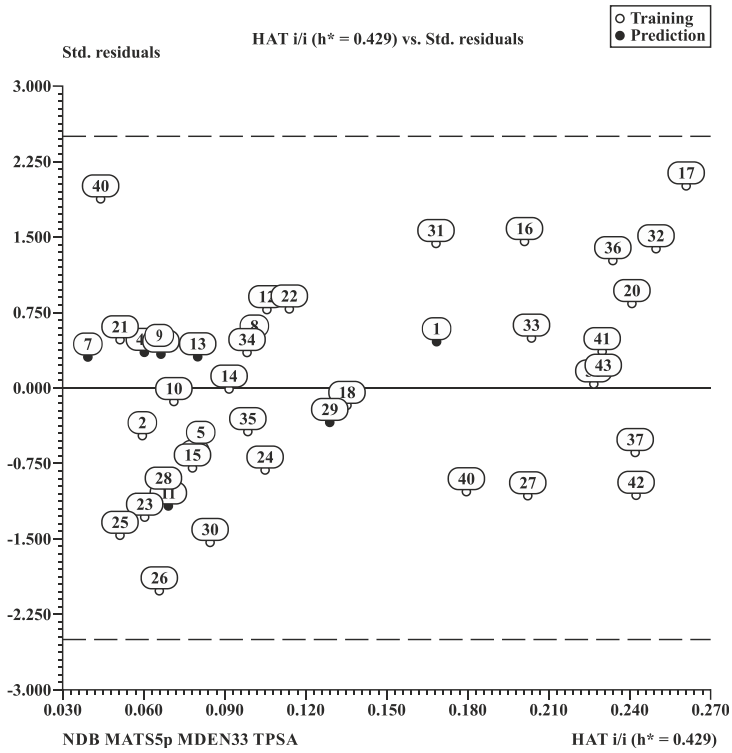


Fig. (1). Applicability domain of the QSAR model for antioxidant activity calculated by model (3).

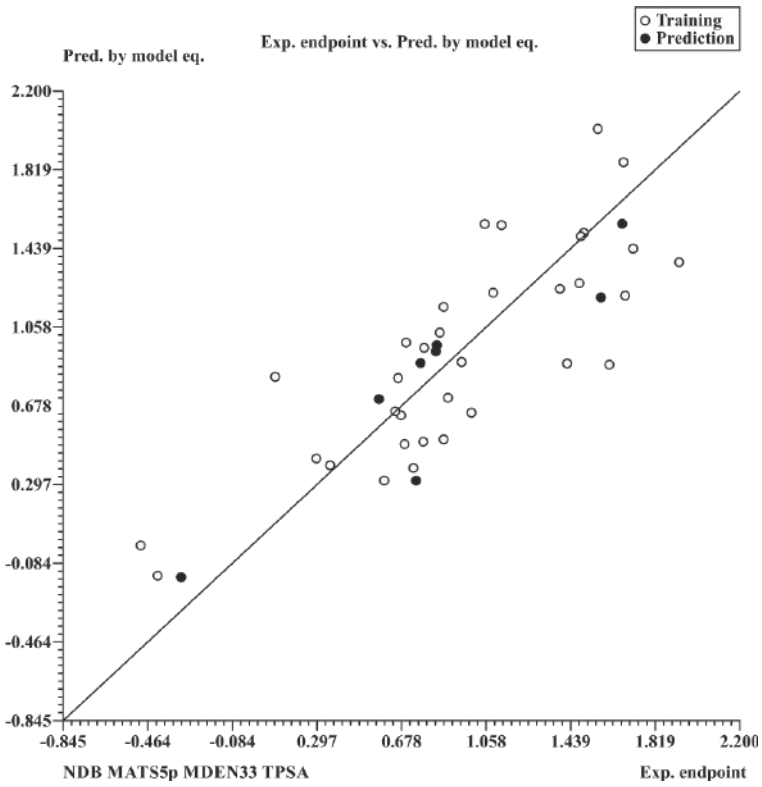


Fig. (2). Observed versus predicted log %DPPH for the 43 dipicolinic acid derivatives calculated by model (3).

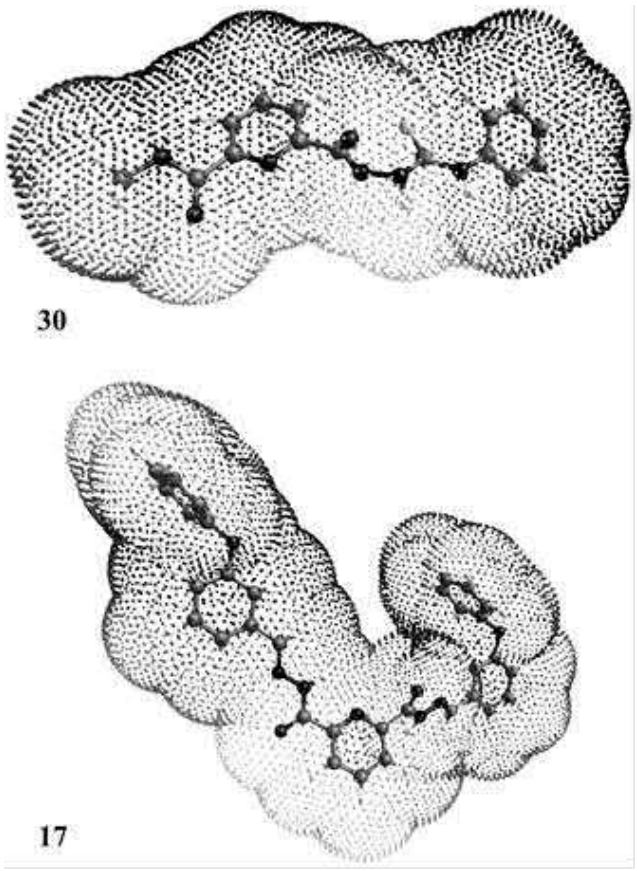
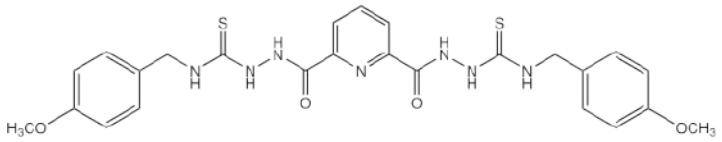
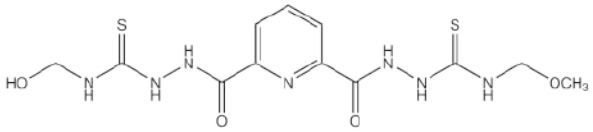


Fig. (3). Dotted polar surface area (PSA) for the compound with highest (30), and compound (17) with lowest antioxidant activity. PSA is presented as gradient of two colors: black (apolar surface) and grey (polar surface).



44 log %DPPH$_{pred.}$ = 1.953



45 log %DPPH$_{pred.}$ = 2.015

Fig. (4). Structures of the proposed molecules as promising antioxidant agents. Antioxidant activities have been predicted according the model (3).

Based on the conclusions given in the QSAR analysis, structures of two new compounds (**44**, **45**) with possible great activity are proposed (Fig. **4**). Antioxidant activities of the proposed compounds have been predicted by means of the model (3) (log %DPPH = 1.953 and 2.015, for **44** and **45**, respectively). Calculated descriptors are shown in Supplementary File 1. Applicability domain of the proposed new potentially active derivatives has been verified. Leverage (HAT) values of both compounds are inside the applicability domain of a model (0.267 for **44,** 0.321 for **45**; h^* = 0.429). The Williams plot of the regression is presented in Supplementary File 3 (SF 3).

CONCLUSION

The results of the QSAR analysis suggest that derivatives of dipicolinic acid with the following structural feature may exhibit great antioxidant activity: low number of double bonds in molecules; absence of tertial nitrogen atoms; higher number of hydrogen bond donors; enhanced molecular polarity; substituents without halogen atoms; and symmetrical moiety. Model with the best external validation result was obtained by ADMEWORKS descriptors, and the test set was generated by random method. Obtained models could help in suggesting design of novel molecules with improved activity profile. According to developed model, structures of two new compounds with possible great activities were proposed. Thus, the model provides a practical tool for the prediction of antioxidant activity of new and untested antioxidant.

CONSENT FOR PUBLICATION

Not applicable.

CONFLICT OF INTEREST

The authors declare no conflict of interest, financial or otherwise.

ACKNOWLEDGEMENTS

This work was supported in by the two J. J. Strossmayer University Grants: INGI-2015-20 and „Synthesis and biological activity of dipicolinic acid derivatives“ (2013).

SUPPLEMENTARY MATERIAL

Supplementary materials are available on the publisher's web site along with the published article:

SF 1. Values of the most relevant descriptors in QSAR models (1)-(4).

SF 2. Values of the experimental and calculated log %DPPH by QSAR models (1)-(4).

SF 3. Applicability domain of the proposed new potentially active derivatives (44, 45) calculated by model (3).

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REVIEW OF RESEARCH
IMPACT FACTOR : 5.2331(UIF) UGC APPROVED JOURNAL NO. 48514 ISSN: 2249-894X
VOLUME - 7 | ISSUE - 7 | APRIL - 2018

"AN ANALYTICAL STUDY OF GOVERNMENT SCHEMES FOR WOMEN EMPOWERMENT IN AMRAVATI DISTRICT"

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ABSTRACT:

In the process of poverty eradication and reducing gender discrimination, the governments have been implementing various schemes and programmes providing ways and means towards women development and empowerment, SHG movement, one among such programmes which has been proved successful in fulfilling its objectives. However, it is felt that the other schemes and programmes do have their prominent part in the process of women development and empowerment and which are being successfully implemented. The present proposal is an attempt to develop conceptual clarity of the term empowerment delineating it with several other overlapping concepts of gender equality, social inclusion, powerful etc. and suggest and advocate an inclusive approach of policy measures whereby the Government working towards an empowerment approach develop ways enabling women themselves to critically review their own situation and participate in creating and shaping the society as agents of change and economically empowering themselves.

The participation of women is important to make a significant impact on their empowerment both in social and economical aspects therefore this study addresses impacts and problems of Economic empowerment of women through Government schemes in Amravati District of Maharashtra. The information required for the study has been collected from primary sources through structured questionnaire and personal interview and secondary sources. The research will be based on various statistical tools, techniques and methods such as collection, classification, tabulation, graphic presentation, percentages, averages, correlation and regression analysis etc. The researcher has also applied, wherever necessary and possible, tests of significance such as Chi-square Test for drawing inference and testing of hypothesis. Women participation through various government schemes have obviously created tremendous impact upon the life pattern and style of poor women and have empowered them at various levels not only as individuals but also as members of the family members of the community and the society as whole. The results of the study revealed that the Government schemes have had positive impact on both economic and social aspects of the beneficiaries.

KEYWORDS : *Government Schemes, Economic Empowerment, Empowerment of Women.*

1. INTRODUCTION:

Women are the part of our society but they have less authority. Society cannot be created without women contribution. Empowerment has many elements which depend upon and relate to each other i.e. economic, social, political and personal. Economic empowerment means to give woman her rights in the economy. Social empowerment means status of woman in the society should be equal to man by eliminating injustice and inequity. Women should have respectable value in the society. Political empowerment means

women should have seats in provincial and national assemblies and giving one woman right of one vote. Personal empowerment means women should have freedom in their personal matters. Women can change their status in the economy, and also of the societies and countries. Often contributions of women in the economy are ignored, and their work is underestimated.

Economic empowerment is thought to allow poor people to think beyond immediate daily survival and to exercise greater control over both their resources and life choices. For example, it enables households to make their own decisions around making investments in health and education, and taking risks in order to increase their income. There is also some evidence that economic empowerment can strengthen vulnerable groups' participation in the decision-making. For example, microfinance programmes have been shown to bolster women's influence within the household and marketplace. The evidence also suggests that economic power is often easily 'converted' into increased social status or decision-making power.

The literature on economic empowerment is vast, and a large part of this focuses on the economic empowerment of women - a key strategy in addressing gender inequality. More generally, the discourse on economic empowerment centers around four broad areas: a) the promotion of the assets of poor people; b) transformative forms of social protection; c) microfinance; and d) skills training.

In the words of ex. President Dr. A.P. J. Abdul Kalam, "Empowering women is a prerequisite for creating a good nation, when women are empowered, society with stability is assured". Empowerment of women is essential because their thoughts and value systems leads to the development of a good family, good society and ultimately a good nation.

In India women development has carved out a prominent figure in the development planning right from the dawn of independence. But the concept of women development has been changing. The welfare-oriented approach adopted in the First Plan continued till the end of the Fourth-Five Year Plan. During the Fifth Plan there was a shift from welfare to development approach. However, during the 6th plan (1980-85) a multi-disciplinary development approach emphasizing on women's health, education and employment was adopted. During the 7th plan, there was a paradigm shift of development approach to empowerment.

But despite all these constitutional safeguards and colossal investment on women development in India, women are lagging much behind than men, which can be visualized from the following analysis. It exhibits the role of women in different social activities. Thus, the researcher has therefore attempted to study the Analysis of government schemes in economic empowerment of women during the 10th and 11th Five Year plan with reference to Amravati district, Maharashtra.

2. IMPORTANCE & NEED OF STUDY:

Despite impressive contributions to the society, women in India have only secondary status in the society. They are generally under employed due to limited command over resources. Their position can be improved only by providing employment opportunities. The successful functioning of these enterprises provides economic independence to women.

Women are generally under employed due to their limited command over resources. Hence several programmes have been introduced by the central and state governments by recognizing that women empowerment is the best strategy for poverty alleviation and for ensuring gender equality.

Entrepreneurial development is also one of the important area majority countries has been focus upon as a part of over all Human Resource Development. It is well ascertained by policy makers across the countries that strategic development of an economy required equal participation and equal opportunities to all sectors and genders. Entrepreneurial development is one the significant factor for sustainable socio-economic development. Especially, development of women is inviting special significance because many small and medium firms are well operated through women and though it is less recognized. In order to ensure better support from various levels, it is necessary to understand, what are the motivational factors which influence women to become entrepreneurs? Contemporarily less research has been conducted in

rural and semi urban areas that give specific focus on women entrepreneurs' motivational factors and awareness regarding different employment schemes.

Hence it is necessary to explore what are the factors which influences the motivation of women and to what extend it influence their entrepreneurial aspirations? How rural women looks on entrepreneurial opportunities and what are their concerns to enter into such ventures? Are they conducive that the schemes provided by government for their empowerment will help economic growth & self-reliance? This particular research tries to understand the motivational factors, effectiveness of various government schemes for women which influence on entrepreneurial factors, and how it facilitate the educators and educational institutions to develop infrastructure, design programs and course ware, ensure training and development activities that in tune with the requirement of entrepreneurial education in rural and semi urban areas where small and medium scale industries are more located. Hence there is need to increase awareness about government schemes for self-employment and economic empowerment among women.

3. RESEARCH PROBLEM

Most of the Government schemes are executed effectively, as the statistics revealed. But it is noted that still major portion of the population, especially women are unaware about these policies and programmes. Hence the present study was conducted to look into the awareness and knowledge of women on these women empowerment schemes.

4. HYPOTHESIS OF THE STUDY

1. The role of government schemes in economic empowerment of women during 10^{th} and 11^{th} Five Year Plan is positive.
2. There is a positive impact of government schemes in economic empowerment of women with reference to their occupational activity during 10^{th} and 11^{th} Five Year Plan.
3. There is a positive impact of government schemes in economic empowerment of women with reference to their Expenditure Pattern during 10^{th} and 11^{th} Five Year Plan.
4. There is a positive impact of government schemes in economic empowerment of women with reference to their Educational Expenditure during 10^{th} and 11^{th} Five Year Plan.
5. The implementation of government schemes for economic empowerment of women during the 10^{th} and 11^{th} plan faces a number of problems and there is an urgent need of training the government officials as well as the women folk with a view to change their approaches and mindsets.

5. PROBABLE IMPLICATIONS:

1 When women's participation in the labor force grew fastest, the economy experienced the largest reduction in poverty rates.

2 When women farmers can access the resources they need, their production increases, making it less likely that their families are hungry and malnourished.

3 When women own property and earn money from it, they may have more bargaining power at home. This in turn can help reduce their vulnerability to domestic.

4. When women have access to time-saving technologies & Skill training programmes they increase their productivity as well as launch income-generating pursuits and entrepreneurial ventures. Those kinds of outcomes empower women to become stronger leaders and to more effectively contribute financially to their families, communities and countries.
5. Investing in women helps speed up the development of local economies and creates more equitable societies.
6. Increased income controlled by women gives them self confidence, which helps them obtain a voice and vote in for empowerment

7. Household decisions such as domestic well-being decisions as women tend to use income clout for more equitable decisions about sons and daughters' diet, education and health.
8. Economic empowerment makes conducive the Economic decisions of acquiring, allocating, and selling assets.
9. Increasing the role of women in the economy is part of the solution to the financial and economic crises and critical for economic resilience and growth.

6 REVIEW OF LITERATURE

According to Roy and Niranjan (2004), Empowerment is associated with indirect indicators like Education and work participation of women, and direct indicators of female autonomy (empowerment) such as decision-making, mobility and access to economic resources that can be viewed both as an outcome and a process.

According to Malhotra, Schuler & Boender 2002, Empowerment is a dynamic process. Separating the process into components (such as enabling factors, agency and outcomes)

According to Prahlad Kumar and Tinku Paul, Empowerment cannot be defined in terms of specific activities or end results because it involves a process whereby women can freely analyze, develop and voice their needs and interests, without them being pre-defined, or imposed from above.

According to Naila Kabeer, empowerment is "the expansion in people's ability to make strategic life choices in a context where this ability was previously denied to them." Empowerment cannot be reduced to a single aspect of process or outcome. Moreover, impacts on empowerment perceived by outsiders might not necessarily be those most valued by women themselves.

Dr.vasanthakumari (2012) in his study he recognized that by organizing poor women into groups, they not only expand options available to them for their development but also provide them with opportunities to develop their confidence and skills to improve their status and to bring about a change in the attitude of the society towards women.

According to Golla, A. M., Malhotra, A., Nanda, P. and Mehra, R., 2011 their paper provided an Understanding and Measuring of Women's Economic Empowerment with a framework to guide the design, implementation and evaluation of economic advancement programmes, schemes and various policies.

According to Kabeer, N., Mahmud, S. and Tasneem, S. 2011, in his paper 'Does Paid Work Provide a Pathway to Women's Empowerment?**,** describes combination of survey data and qualitative interviews to explore the impact of paid work on various indicators of women's empowerment, ranging from shifts in intra-household decision-making processes to women's participation in public life. It finds that forms of work that offer regular and relatively independent incomes hold the greatest transformative potential.

According to Reena , Rajdeep Kaur , Nikita who studies a Comparative Analysis of Women's Economic Empowerment through Self Help Groups to evaluate the level of Women's economic empowerment through SHG i.e. income, expenditure and saving of the member after joining SHG.

7 OBJECTIVES OF STUDY:

1. To present an overview of role, Functioning and Performance of government schemes in economic empowerment of women in India particularly with reference to Amravati District of Maharashtra State.
2. To study the awareness & effectiveness of Government schemes for economic empowerment of women
3. To study the socio-economic impact of economic empowerment of women through government schemes during the 10^{th} and 11^{th} Five Year Plan with special reference to Amravati district of Maharashtra.

4. To study the performance and impact of various government schemes with reference to economic empowerment of women during the 10th and 11th Five Year Plan with special reference to Amravati district of Maharashtra.
5. To study the problems of economic empowerment of women during the 10th and 11th Five Year Plan with special reference to Amravati district of Maharashtra.

8. RESEARCH METHODOLOGY:

The said study is based on primary as well as secondary data. Primary Data has been collected through well structured questionnaire and survey method wherein the questionnaire was distributed among 50 members of different Women Beneficiaries of various state and central Government schemes in Amravati district with the help of Stratified Random sampling technique as the selection of the sampler requires the separation of defined target population into different groups based on some strata like income groups (Low, Middle, high), rural & urban area, age, profile of beneficiaries, kind of employment etc., which represents the entire population. The secondary data is collected from various published sources such as published data of various government agencies, Research journals and periodicals, Newspapers; other sources etc. also will be used to support the conclusions. The major source of secondary data is the published annual reports of the sample banks under study.

9. LIMITATIONS OF STUDY:

1. The study will be limited to Amravati city. As such the finding of the study may not be totally applicable to other cities.
2. The study will be limited for empowerment of Women Beneficiaries of various Central and state Government schemes run in Amravati District.
3. Conclusions and suggestions are drawn on the basis of information provided by women beneficiaries only.
4. Sample size is of 50 only

10. DATA ANALYSIS AND INTERPRETATION:

The data after collection has been analyzed, arranged in tabular form followed by Analysis and Interpretation of data in a general way involves a number of closely related operations, which are performed with the purpose of summarizing the data that fulfill the research objective.

Table No. 1 Education-Wise Details of Women Beneficiaries:-

Sr. No.	Particulars	Responses	%
A	Upto SSC	21	46.6%
B	Under Graduate	18	36%
C	Graduate and Above	7	14%
D	Illiterate	4	08%
Total		50	100%

Table No.2 Age-wise Distribution of Women Beneficiaries

Sr.No.	Particulars	Responses	%
A	Below 30 years	15	30%
B	30-40 Years	24	48%
C	Above 40 years	11	22%
Total		50	100%

Table No.3 Income Group wise Classification of the Sample

Sr.No.	Particulars	Responses	%
1	Low Income Group	16	32.00
2	Medium Income Group	28	56.00
3	High Income Group	6	12.00
Total		50	100%

Table No .4 Utilization of Income wise Classification of the Sample

Sr.No.	Particulars	Responses	%
1	Household Expenses	23	46.00
2	Child's Education	12	24.00
3	Saving & Investment	7	14.00
4	Repayment of Loans	4	8.00
5	Medicinal Expenses.	4	8.00
Total		50	100%

Table No.5 Reasons of Working of Sample Respondents

Sr.No.	Particulars	Responses	%
1	Economic Empowerment	33	66.00
2	Use of Skills	12	24.00
3	Self-Identity	4	8.00
4	Other	1	2.00
Total		50	100%

Table No.6 Treatment Given by the Family of the Sample Respondents

Sr.No.	Particulars	Responses	%
1	Normal	10	20.00
2	Good	8	16.00
3	Force for Earning	20	40.00
4	Always Helping	7	14.00
5	Cruel	5	10.00
Total		50	100%

Table No.7 Sources of Capital of the Sample Respondents

Sr.No.	Particulars	Responses	%
1	Personal Savings	13	26.00
2	Friends & Relatives	18	36.00
3	Financial Institutions	37	74.00
4	Government Schemes	43	86.00
5	Sale of Personal Property	28	56.00
6	Money Lenders	23	46.00
Total		50	100%

Table No. 8 Financial Security Status of the Sample Respondents

Sr.No.	Particulars	Responses	%
1	Partly Secured	12	24.00
2	Fully Secured	28	56.00
3	Not Secured	10	20.00
Total		50	100%

Table No.9 Awareness of Government Schemes to the Sample Respondents

Sr.No.	Particulars	Responses	%
1	Partly Aware	9	18.00
2	Fully Aware	30	60.00
3	Not Aware	11	22.00
Total		50	100%

Table No.10 Participation in the Scheme by the Sample Respondents

Sr.No.	Particulars	Responses	%
1	MNREGA	13	26.00
2	NRLM-SGSY-SHG's Initiative	14	28.00
3	MAVIM-CAIM, Tejaswini	32	64.00
4	PMKVY	22	44.00
5	DDU-GKV Yojana	6	12.00
6	MSRLM-UMED	14	28.00
7	EDTP	14	28.00
8	DIC Loan Scheme	9	18.00
9	PMEGP/PMKY	12	24.00
10	Seed Money Scheme	12	24.00
11	Any Other	19	38.00
	Total	50	100.00

11. MAJOR FINDINGS

Following Are the Conclusions of the Present Study

1. It is concluded that, majority of the respondents are form low income group.
2. It is concluded that, Majority of the respondents are utilizing their income for household expenses
3. It is concluded that, majority of the respondents are working for Economic Empowerment.
4. It is concluded that, majority of the respondents have reported that the treatment given by their family is Force for Earning.
5. It is concluded that, majority of the respondents have reported that the source of capital is Government Schemes, whereas very few have reported that the source of capital is Personal Savings.
6. It is concluded that, majority of the respondents have reported that the financial security is fully secured.
7. It is concluded that, majority of the respondents have reported that they are fully aware of the government schemes.
8. It is concluded that, majority of the respondents have reported that they are participated in MAVIM-CAIM, TEJASWINI Scheme
9. It is concluded that, there is significant difference between the opinions of sample respondents before and after Government Schemes for Economic Empowerment of Women about

i. The impact of Government Schemes for Economic Empowerment of Women on occupational activity.

ii. The impact of Government Schemes for Economic Empowerment of Women on expenditure pattern.
iii. The impact of Government Schemes for Economic Empowerment of Women on Health Care Expenditure.
iv. The impact of Government Schemes for Economic Empowerment of Women on Education Expenses.
v. The impact of Government Schemes for Economic Empowerment of Women on Leisure Expenses.
vi. The impact of Government Schemes for Economic Empowerment of Women on Social Status Expenses.
vii. The impact of Government Schemes for Economic Empowerment of Women on Expenses on Consumer Durables.

10. It is concluded that, out of the total 50 sample respondent majority of women beneficiaries have reported the problem of Following aspects:

i. Security Aspects
ii. Lack of training and Communication Skills
iii. Lack of Marketing Skills
iv. Negative social environment
v. Bureaucratic Lobby
vi. Changing nature of Government Schemes
vii. Lack of Knowledge

12. RECOMMENDATIONS

1. The state has to take lead action in the form of enabling policies, provision of resources for the establishment of support mechanism which can multiply and monitor the process and monitor the devolution of powers and responsibilities to local communities and the poor.
2. Social mobilisation and people's participation should be the key strategy of the government for poverty eradication. It should occupy the highest priority of the Government
3. The process of empowerment of women at the political level has already begun, but it needs to be carried forward into the social and economic spheres as well. Special emphasis would have to be placed on ensuring that control of social infrastructure in the public domain is vested in women and women's organisations;
4. The Government should formulate a "National Women's Empowerment Policy" by drawing various experts working in this field. Various interventions which are required at the macro and micro level should be worked out and suitable amendments can be carried out in existing laws, rules, regulations, procedures and Government orders which come in the way of poverty alleviation;
5. There is a need for more and better coordination between the Government and the NGOs working in this area. Both should be partners in development. The NGOs should not undertake specialized programmes which the Government is already undertaking eg., construction of houses, sanitary latrines, wasteland development etc. NGOs should concentrate on social mobilization. There should be a common set of guidelines for all the SHGs.
6. All the Government functionaries should be trained and sensitized on the processes involved in social mobilisation and community empowerment.
7. Continuous training, motivation and exposure of the community volunteers, network leaders, group leaders and members is required to sustain the groups. A fixed annual training calendar should be designed by identifying proper training centres and resource persons. NIRD and SIRDs should draw up exclusive training programmes for social mobilisation and community empowerment;
8. Banks and implementing agency should take steps to avoid under financing and for verification of assets periodically. This type of verification helps the misuse of funds by the beneficiaries;
9. While selecting the groups, preference may be given to those groups, in which the members have crossed the eligible age limit to secure government jobs;

10. The rate of interest. charged by commercial banks is considered very high therefore, it may be reduced for the benefit of the poor women entrepreneurs;
11. The major problems of raw material shortage, lack of common work-shed, irregular marketing etc., need to be solved for the steady growth and successful functioning of the units;
12. Rural industrial products, handicrafts by women should be promoted and supported by adequate marketing arrangements;
13. Encouragement of co-operative ventures will promote and secure greater female participation at all levels.
14. Amravati district is a area inhabited by *Adivasi* forest dwellers particularly the Melghat area is full of various issues and problems which need be taken cognizance. Efforts should be taken to remove the deep rooted ignorance and negative attitude regarding women's role. It is necessary to provide special centers in this area for training and information of the *Adivasi* women.

At present, the climate in India is ripe for promoting the economic status of women particularly in Amravati district of Maharashtra. It is widely believed that with the growth of education and communication, opening up of new employment opportunities, Indian women will move steadily towards more equal status with men. Thus, she should be treated with equality of opportunities and it is the sole responsibility of the government to protect her interests in the wake of liberalisation.

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International Journal of Engineering Technology Science and Research
IJETSR
www.ijetsr.com
ISSN 2394 – 3386
Volume 5, Issue 4
April 2018

Digitalization of Ecotourism and Allied Services in Melghat Tiger Reserve of Vidarbha

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ABSTRACT

Ecotourism is an alternative form of tourism whose sole purpose is holiday activities and the core elements of this type of tourism is natural-based. The basic intention of this type of tourism is to raise awareness amongst travelers about the natural place they visit for and at the same time minimize any corrosive impact of human activity along with the upliftment of the localites of the particular area. In the digital era of technology, travel agendas rarely rely on trusted word-of-mouth recommendations and physical guidebooks; breakthroughs in digitalisation have given customers independence and choice in a really big way. Let's not forget that travel is essentially about connecting – places, people, experiences and memories. One thing that technology does well, is connect things.Before going on a trip, most people research the place they're about to visit. Once they arrive at the destination, the search for the best places to visit continues. Thankfully, the power of Wi-Fi allows travelers to use their devices anywhere from the hotel room to coffee shops and touristic attractions. As a result, planning any trip becomes as easy as visiting a review website and choosing the next destination point. A Descriptive approach was adapted to conduct the study on digitalization of ecotourism and other related services in the Melghat Tiger Region, the researcher could that digital services has in a way created varied sources of revenue generation and employment opportunities for the local people called as 'korku'. It is due to the vision of making India digital Melghat is crowned with Harisal- India's first digital village.

Keywords: Digitalisation, Ecotourism, Employment, Services, Tiger Reserves.

What is Ecotourism?

Ecotourism (also called sustainable tourism) can be defined by a variety of travel practices, but it all comes down to a general set of ideas. As an eco-tourist, you decide to travel in a way that shows respect to nature and does not contribute to its degradation.

Additionally, ecotourism is a part of environmental conservation, and understanding what the needs of the people are who are local to the area so that you can help to improve their quality of life. It also involves learning more about the history of other cities and preserving the historical landmarks.

As per The International Ecotourism Society,

"*Ecotourism is now defined as "responsible travel to natural areas that conserves the environment, sustains the well-being of the local people, and involves interpretation and education. Education is meant to be inclusive of both staff and guests.*"

Ecotourism is a responsible tourism which conserves the environment and sustains the well being of local people. It...

- Builds environmental awareness
- Provides direct financial benefits for conservation
- Provides financial benefits and empowerment for local people
- Respects local culture
- Supports human rights and democratic movementssuch as:

International Journal of Engineering Technology Science and Research
IJETSR
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ISSN 2394 – 3386
Volume 5, Issue 4
April 2018

- conservation of biological diversity and cultural diversity through ecosystem protection
- promotion of sustainable use of biodiversity, by providing jobs to local populations
- sharing of all socio-economic benefits with local communities and indigenous peoples by having their informed consent and participation in the management of ecotourism enterprises
- tourism to unspoiled natural resources, with minimal impact on the environment being a primary concern.
- minimization of tourism's own environmental impact
- affordability and lack of waste in the form of luxury
- local culture, flora, and fauna being the main attractions
- local people, who benefit from this form of tourism economically, and often more than mass tourism

Objectives of Ecotourism:

Eco tourism or sustainable tourism is designed to make travelers aware of the environment and carry out all tourism operations in an eco-friendly manner. We have listed down a few aims and objectives of ecological tourism. Have a look:

- Maintaining the Sanctity of the Environment
- Utilizing All Types of Resources Efficiently
- Preserving the Biological Diversity
- Ensuring the Economic Progress
- Increasing the Scope of Employment
- Strengthening the Cultural Bonding

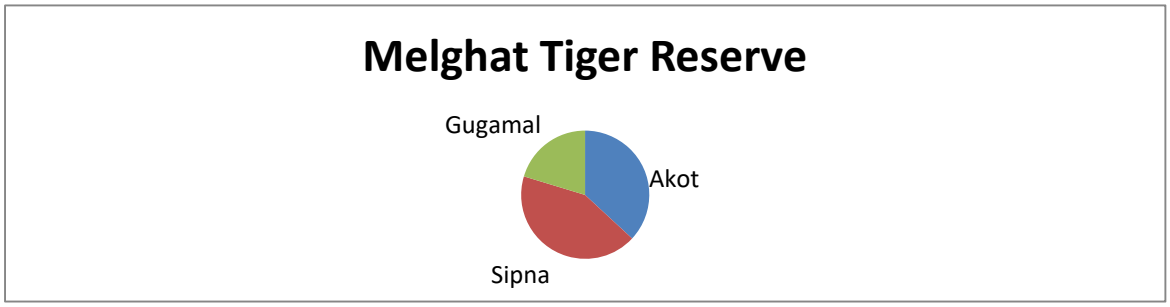
Melghat Tiger Reserve:

Melghat means ‘meeting of the ghats’ which is just what the area is, a large tract of unending hills and ravines scarred by jaggesd cliffs and steep climbs. The exquisite hill forests, thick undergrowth and moss-covered trees underscore its virgin confines.

Melghat was declared a tiger reserve and was among the first nine tiger reserves notified in 1973-74 under the Project Tiger. It is located inAmravati District of Maharashtra State in India. The Tapti River and the Gawilgadh ridge of the Satpura Range form the boundaries of the reserve. In 1985 Melghat Wildlife Sanctuary was created. The Tapi river flows through the northern end of the Melghat Tiger Reserve, through a forest which lies within the catchment area of the river system. Many different kinds of wildlife, both flora and fauna, are found here.

Melghat Tiger Reserve Division:

The Melghat Tiger Reserve is divided under three sub-divisions namely,



There are various rest houses at-

International Journal of Engineering Technology Science and Research
IJETSR
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ISSN 2394 – 3386
Volume 5, Issue 4
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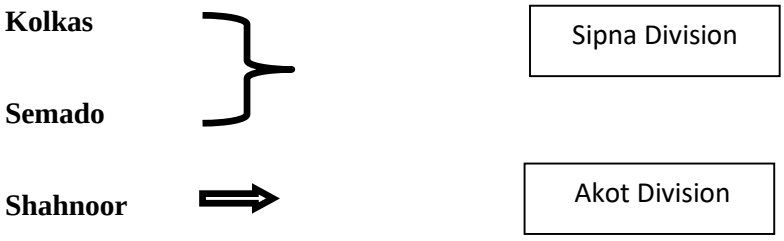

Korku tribes of Melghat:

Korku have derived their name from the combination of the word 'Koru' meaning Man and 'Ku' which make it plural meaning tribal men.

Forming an important part of its identity, India remains home to a large number of aboriginals, untouched by the modern lifestyle of the city these people continue to live in the remotest of location with dense forest, raging rivers and varied wildlife. Living so close to nature, these people are filled with love, compassion and warmth.

Digitalization in Ecotourism:

There's no denying that technology plays a pivotal role within the travel and tourism sector.

Along with the exponential growth of extension and using the Internet and the World Wide Web, both at home and at work, have increased also the opportunities for travel providers to distribute information and to process bookings for potential buyers. The development processes within the information technology, communications and Internet, have revolutionized the entire tourism industry, creating new business models, changing the structure of distribution channels of the tourism and reprojecting all products of this industry and last but not least, influencing the touristic packages suppliers , destinations and stakeholders. (Organism or group of people with major interests in the conduct and results of the company). Some hotels have implemented a fully automated check-in process, stepping back from personal contact and relying on an electronic process to meet the customer's needs. As long as the small tourism operators can be reached on the Internet, the trend will grow up in their direction, because the Internet is similar to a "playground" in which with a well done web site, the small businesses can advertise as professional as their larger competitors. In this context, we assist to a more and more emphasized development of the electronic commerce, hence of the electronic tourism (or e-tourism).

Our day-to-day lives are made easier through the use of the internet and technology – whether it be on our mobile devices, at home or in the work place using a desktop or laptop. Significant developments in technology have now made this achievable on a global scale.

It's seen by many that technology – namely social media – has created a global village, connecting everybody to everyone, everywhere. Some argue that this has made us less sociable, inhibiting face to face and physical interaction. However, the concept that globalisation and technology allows us to overcome the limitations of physical distance through our finger tips, presents countless opportunities for the travel and tourism industry to flourish.

People always have and always will continue to travel around the world to experience new things… and advances in technology are there to influence and inspire this: not prohibit.

Websites, booking platforms, apps and using social media all provide the opportunity to engage and connect with customers on a variety of levels to allow an enhanced travel experience. Now that this information for customers is easily accessible (through various mediums), it inevitably means that it's important for companies to get smarter and adapt to remain competitive.

International Journal of Engineering Technology Science and Research
IJETSR
www.ijetsr.com
ISSN 2394 – 3386
Volume 5, Issue 4
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The digitalization impact has spread its wings to the nearby villages and its people too. Harisal, about 270km from Nagpur, is going to be India's "first smart village". The state and central governments have big plans for the hamlet, located in a hilly area deep inside the Melghat Tiger Reserve and inhabited by 2,000 people, mostly Korku Adivasis. They plan to provide each of the 406 households with solar electricity and Internet connections.

So far, Harisal has been known mainly for its malnutrition deaths. Now the words "digital" and "smart" are on everybody's lips - right from unlettered villagers to the few who have been to school. The government wants to introduce the Internet and computers to the villagers, mostly farmers, to put the village on the digital map. On the agenda are cashless markets, WiFi zones, mobile connectivity, health cards and telemedicine facilities.

In summary, developments in technology have led to big changes in the way that customers use it to enhance their full travel experience. Consequently, travel companies must adapt to continue providing their customers with the best customer experience possible along with the upliftment of the localites in the region.

Research Methodology:

Research in common parlance refers to a search for knowledge. Once can also define research as a scientific and systematic search for pertinent information on a specific topic.

The process used to collect information and data for the purpose of coming to a conclusion giving suggestion and taking decision for which the methodology included books, publication research, interviews with official at the Forest Office of Melghat Tiger Reserve and Maharashtra Tourism Development Corporation Amravati.

Statement of Problem:

The traditional method of providing information and services are limiting the growth of tourism industry. Digitalization of these services will save the time and cost of the tourist which will result into the higher satisfaction level and increase in their number.

Hence the researcher under took the study “Digitalization of ecotourism and allied services in Melghat Tiger Reserve of Vidarbha”.

Objectives of the Study:

1. To study the various segment of forest tourism.
2. To analyze the Traditional and Digital Methods of tourism.
3. To analyze the impact of digitalization on the related services and tourist.
4. To study the impact of digitalization on the growth of tourism in Melghat Tiger Reserve.
5. Ti study the impact of digitalization on providing employment opportunities to localites.

Tiger Reserve- An Introduction:

India is home to 70% of tigers in the World. There are around 50 tiger reserves in India which are governed by Project Tiger administrated by the National Tiger Conservation Authority (NTCA).

Initially 9 Tiger Reserves were created for Project Tiger in 1973-74

1. Manas Wildlife Sanctuary (Assam)
2. Palmau Tiger Reserve (Bihar)
3. Similipal National Park (Orissa)

International Journal of Engineering Technology Science and Research
IJETSR
www.ijetsr.com
ISSN 2394 – 3386
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4. Corbett National Park (Uttar Pradesh now UttaraKhand)
5. Kanha National Park (Madhya Pradesh)
6. Melghat Tiger Reserve (Maharashtra)
7. Bandipur National Park (Karnataka)
8. Ranthambore (Rajasthan)
9. Sunderban Wildlife Sanctuary (West Bengal)

List of Tiger Reserves in Maharashtra

Tiger Reserve	Year declared	Core Area(km^2)	Buffer Area(km^2)	Total Area (km^2)
Melghat	1974	1,500	1,268	2,769
Tadoba	1993	626	1,102	1,728
Pench	1977	257	484	741
Sahyadri	2007	600	565	1,166
Nawegaon-Nagzira	2013	654	1241	1895
Bor	2014	138	678	816
Total		**3775**	**5338**	**9113**

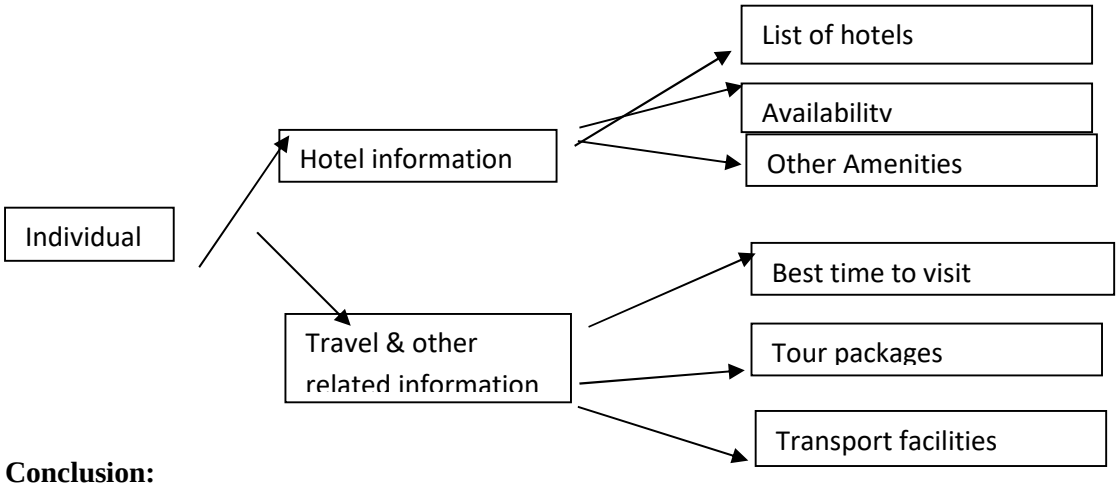
(Source: https://en.wikipedia.org/wiki/Tiger_reserves_of_Maharashtra)

Findings:

It is found that the traditional method of tourism included various middlemen and lot of tedious structure of the booking and reservation process. Whereas, the world of technology have enhanced the reservation system by Douglas Foster- Do-it-yourself reservation system, wherein all the information and booking are available at just one click.

The digital initiative has, among other things, focused on providing Internet facilities to schools. Students and teachers will be given online training. Computer labs are being set up, along with a digital library with the help of Sant Gadge Baba Amravati University.

It is also found that the digital method have given a boost to the tourism sector in the region as compared to the traditional methods of tourism with help of Do-it-yourself model.



Conclusion:

International Journal of Engineering Technology Science and Research
IJETSR
www.ijetsr.com
ISSN 2394 – 3386
Volume 5, Issue 4
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From the above findings and survey done during the research process it can be concluded that-

- There are various avenues available in the region of Melghat Tiger Reserve, such as jungle safari, adventure sports at Shahnoor rest house.
- The digital methods of tourism have given a boost to the ecotourism in the last 3 years as a result a new gate for jungle safari has been opened from Chikhaldara from February 2017.
- The digital growth in the the region is been such that the local people are been given training and computer literacy so that they can sell their handmade bamboo items online globally.
- Melghat is one of the oldest tiger reserves in India and is now acknowledged world wide due to digitalization.
- There is almost a hike of 8-10% annually in the number of visitors in the region.
- It can also be concluded that the digitalization of ecotourism and their allied services have generated moderate employment opportunities for the localites- such as tour guides, catering, handicrafts, various sports activities tutors etc.

Suggestions:

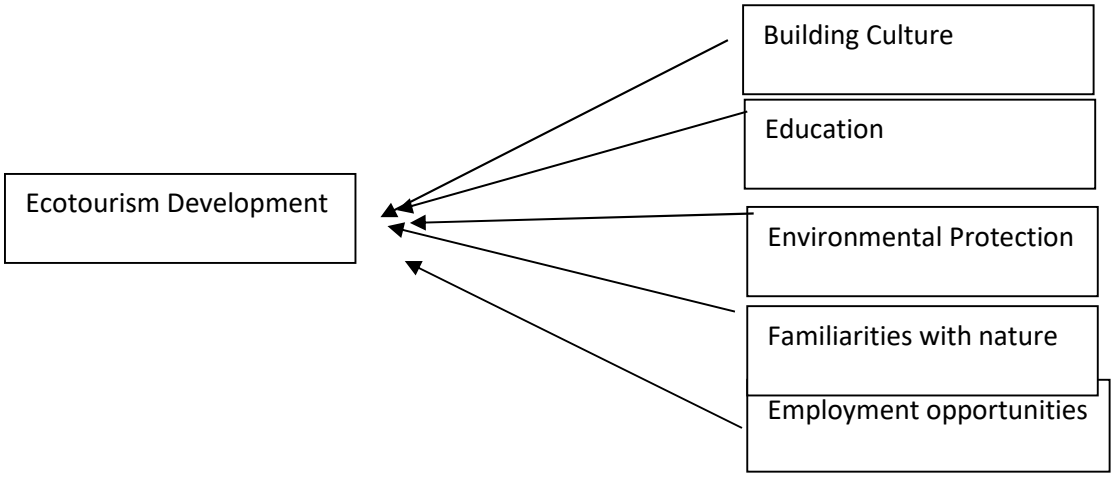
There is huge scope of growth in the tourism industry in the region of Melghat.

Adequate supply of electricity

More number of mobile and wifi towers.

Residential facilities in Korku huts for proper understanding of the local culture and environment.

The ecotourism can develop when the other related factors are in proper coordination with it.



Proper synchronization of the above factors will channelize the ecotourism in an effective manner for a better tomorrow for the people in the region of Melghat and the generation to ccome in the digital era.

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UGC Approved Journal No: 49229
SJIF Impact Factor(2016) :5.708
Print ISSN: 2321 - 6247

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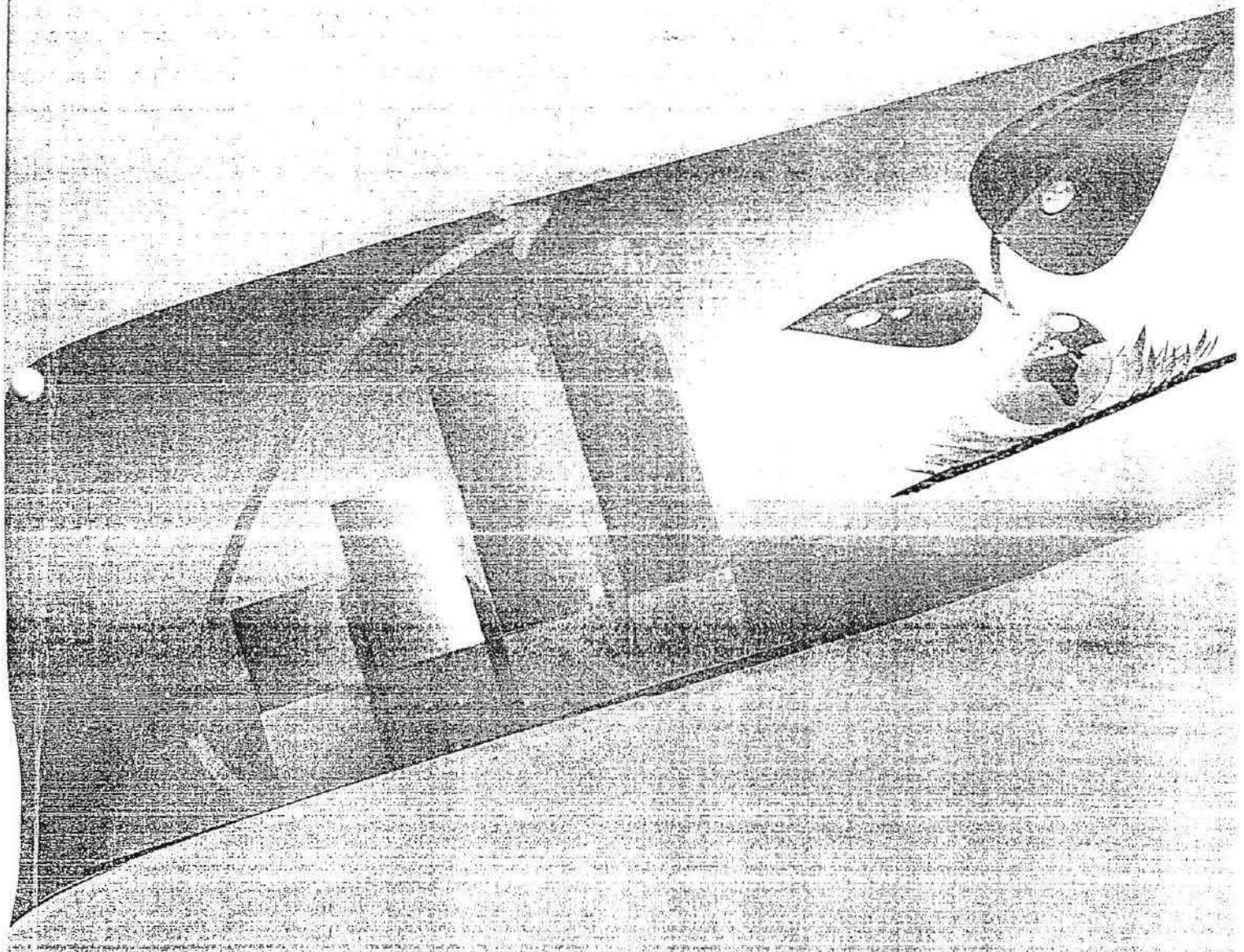

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ISSN: 2321-6247

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ROLE OF MULTICULTURALISM, PROFESSIONAL ETHICS AND HUMAN VALUES IN CURRENT SCENARIO

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ABSTRACT

Multiculturalism is a feature of the modern age. Heterogeneous of various types of culture is called as multiculturalism. Macro theory in anthropology is related to the concept multiculturalism. As per the Darwin's theory, the realm of social cultural phenomenon explains the application of technology with environmental aspects for the production and distribution of goods in society. On the Materialism process, Marx and Engel, enlightened with detailed illustration. Multicultural society characterized by cultural pluralism. Basically in the multiculturalism gives the place to cultural variety like linguistic, religious, ethnic diversity of culture which has material and nomadic dimensions.

KEYWORDS: *Multiculturalism, Multicultural society, global culture*

INTRODUCTION

Multiculturalism is a feature of the modern age. Heterogeneous of various types of culture is called as multiculturalism.

Macro theory in anthropology is related to the concept multiculturalism. As per the Darwin's theory, the realm of social cultural phenomenon explains the application of technology with environmental aspects for the production and distribution of goods in society. On the Materialism process, Marx and Engel, enlightened with detailed illustration. Multicultural society characterized by cultural pluralism. Basically in the multiculturalism gives the place to cultural variety like linguistic, religious, ethnic diversity of culture which has material and nomadic dimensions.

Multiculturalism is nature of cultural variation multiculturalism.

Following are the various aspects of multiculturalism

1) Sub culture
2) Caste sub culture.
3) Regional sub culture
4) Occupational sub culture
5) Centro culture.

Marvin Harris has proposed the theory of cultural materialism. In which he has mentioned the various aspects related to race, religion, cast which try to accept the life and frame geographical structure.

India is the well-known example of cultural pluralism and multiculturalism in the world. Multiculturalism is filled towards the cultural diversity.

It is a universal and cultural determination phenomenon in world.

Multiculturalism means place to the civilization. Civilization means coming towards modern process like modernization, urbanization and industrialization. It is a symbol of refinement and progress. Existence of large number of people in cities, specially stratified and governing and ruling by elites in organized political system.

SCOPE OF MULTICULTURALISM

Today, the global culture concept has been raised in society. Migration, development, natural calamities bind to people to move other places. Technology, transportation, communication, connectivity, hypermedia cultural effect etc are responsible for increasing the dimension of global culture. The world coming together and that's why multiculturalism is coming up is current scenario.

Ethnic resurgence and cultural assimilation are the main components of multiculturalism. Multiculturalism is an advance part of cultural pluralism. Pluralistic societies moving towards modern life style are a main cause of multiculturalism.

Definition-

Coping and curbing the divisive pressure in pluralistic or multi- ethnic societies is the adaptation of a public policy based on mutual respect and tolerance for cultural differences called as multiculturalism. It involves the public policy for managing the societal cultural diversity. There is common difference between cultural pluralism and multiculturalism. Globalization is also resulted the multiculturalism phenomenon.

Multiculturalism explains the existence, promotion of multi cultural traditions. It allows people to truly express within society for acceptance of other things for better social issues.

Multiculturalism is formed to the migration of various ethnic groups in one society.

Components of Multiculturalism

1) Religious
2) Linguistic
3) Territory
4) Race

There is need to adopt following points for betterment of multiculturalism-

1) Awareness
2) Empathy
3) Tolerance
4) Compassion
5) Non Discrimination

PROFESSIONAL ETHICS

Morals and values are important to maintain social control and dignity in the society. Moral are standard norms which help to guide our behaviors and accept behavior of value reflect own behavior attitude judgment and self esteem.

Ethic is a philosophical term represents the positive human action in society. Morality, integrity, sincerity and responsibility are the pillars of ethics. It is one type of applied moral science.

Human Values = Morals + Values + Ethics

Human values are integral and core part to maintain the status in society. Human values are form and values of life.

Today is the age of globalization. Many organizations and management provide the job to the job seekers. In organization, work culture promotes the work ethics of particular organization. There is a particular code of conduct. Good work, suitable working method controls the result into the expected productivity. Team work service, attitude, learning, respect to others, courage sharing and caring are important in every organization.

Profession is a self job or occupation and service. After stipulated time, man become perfect in his work and acquires professionalism, expertise and try to maintain quality work in professional ways.

ETHICS

Ethics Means identification of good and rights for society. Every organization expects

professional ethics. Corporate values are common phenomenon and to indulge in today's age. Ethics and virtues, law, facts, rights, environment responsibility etc are the co related terms. Avoidance of professional ethics is dangerous to each organization.

Engineering ethics is inserted in the engineering area. Ethics promote the ethics and values among the engineers. There should be suitable correlations about safely responsibilities and rights. To take risk is harmful work but it is essential in organization to follow the duty and role of management. Today there is most important to professional ethics in engineering.

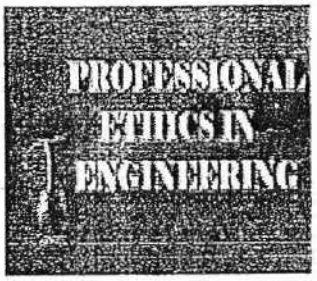
Professional ethics start from family. Professional ethics carry forward through socialization process. Life in school, college, family and friend are components of ethics. The value education getting in childhood impress on future life. Therefore the most schools and colleges provide value education to the students. Value education is based on universal, rational and harmony pillars.

Professional ethics is cause of nation development through public administration. Transparent and professional administration of organization boosts the quality of work. Ethics and human interface reflect on working culture.

Professional ethics and values are the two sides of same coin.

Socialization is refers to the inculcation of new things and carry forward to others. Human values and directives principle of state policy have some similarity. In chapter 4th of Indian constitution as per the article 14, mentioned the directive principle of state policy.

Emotional intelligence, social competence, social skills, influence on job performance etc are some of the examples of professional ethics.



For promotion or development of professional ethics, following points are essential-

1) Leadership qualities and team work
2) Developing self awareness and mindfulness
3) Efficiency, expertise and equality in own field.
4) Truth
5) Work dedication
6) Honesty
7) Non violence
8) Courage and daring
9) Self discipline
10) Faith and responsibility
11) Impartiality and objectivity.
12) Concentration and mindfulness
13) Emphasis on political professional and personal responsibility.
14) Fallowness of legislation and code of conduct
15) Diligence and respect of law
16) Position of legal, personal, organization values.
17) Quality and excellence
18) Tolerance and openness
19) Creativity and Service
20) Humanity and Neutrality
21) Implementation of code of ethics and conduct

Professional Ethics are effective and useful in following ways-

1. Corruption related issues.
2. Nepotism
3. Administrative lacunas, loopholes, secrecy
4. Leaking of information
5. The imperative related to legality accountability and responsibility.
6. Red tapizem
7. Solution of ethical conflict and negligence
8. Compromise in work due to personal issues.
9. Cases on violations rules and regulation.
10. Dysfunctional system
11. Lack of transparency and poor incentive structure.

Ethics are the principles of right conduct.

Professional ethics help to promote improvement in work culture and quantity of service delivery.

Ethics maintain standard of living, awaking about responsibilities. moral delusions. Ethics is a system of accepted behavior, mores and values. As per the Latin a word, ethics is eticus means morals rule of conduce towards humanity. Ethics is a part of philosophy. Ethics suggested in Ramayana, Mahabharata, Bhagvad Gita, Buddha Charita, Arthashastra, Panchtantra, Kuran , Kadambari and Hitopadesh.

In professional ethics, need of the following factors-

1) Seek to acquire professional code of conduct.
2) Acquired knowledge, skills and duties.
3) Setting target of own work and performance.
4) Positive collaboration between machine and man.
5) Not influence by social economical, political afflation in performance of their duties and role.
6) Positive behaviour with soft skills, dignity and alertness with standard of performance..
7) Pursuit of excellence and expertise in own field with suitable training.
8) Encouragement and recognition about creativity and initiative among subordinate.
9) Maintaining of confidentiality in working organization.
10) Trust full with legitimate confidence about towards work.
11) Update self and maintain the dignity in own organization.
12) Promote the effective, positive control system.
13) Suitable life style, social relation, cultural identity, physical power and social interaction.
14) Prestige and status in society
15) Authority, ability utilization and achievement.
16) Stress management effectively.

Under professional ethics following are the mainly considerable points-

1) Healthy interaction with family member
2) Right code of conduct with higher authority and subordinates.
3) Place to truth, love, peace, tolerance, and non violence, morality, Goodness, understanding, liberal, motivation, and balancing about emotional intelligence
4) Prompt leadership towards conceptual frame work.

Types of Ethics-

1) Metal ethics
2) Normative ethics
3) Applied ethics
4) Descriptive ethics

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