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E-LIBRARY IN DEVELOPING NATIONS

Preeti Abrol*, Mrunalini Nandanwar and Mohit Gupta

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Abstract

In the twenty first century when e-commerce, e-voting, e-governance is catching on in every walk of life, the role of Electronic library can't be denied for very long. Actually, the concept is already catching up in the west where premier educational institutes like M.I.T, Harvard and Princeton are making online lectures available to their students. The technology gives an edge in delivery of things in the far flung areas. In the developing nations as India, Bhutan etc. where literacy rate is low and audience is widely distributed, it's difficult to bring the audience for a message where e-libraries makes it very easy. e-library is already built into the concept and a country like India has a lot of potential in this area. India has a big rural base where a large fraction of population does not have access to good education. In case of distributed audiences (student / teacher) it's difficult to reach everywhere on time who needs to be updated regularly. The good trainers may not be available for each subject in all schools/colleges but virtually they can be made digitally available to every student at his location. e-libraries will increase the speed to spread the information and reduces the cost involved in printing and distributing. E-library is the solution to many issues as non availability of text books, updated material and delivery to vast audiences. It's time to grow a virtual connection between students and teachers. In this paper, a real scenario has been created in Bhutan where e-library is allowed to reach out to much bigger audience thereby accelerating their participation in modern economy and nation building.

Keywords: E-Library, Digital Education, Online Learning.

INTRODUCTION

E-Library means an electronic library with the digital objects which includes e-books in form of pdf / epub format, recorded lectures / practical in audio or video format and other relevant material in digital format, which is stored and organized in an electronic collection. An elibrary application means an application (web based portal) used to organize, store and retrieve the content from the collection (Database).

In traditional libraries which are bulky, expensive and distributed, it's hard to find the particular resource and requires a lot of efforts and can be served to limited users only. A student having access to e-library doesn't need to be dependent on the physical resources and have no limitation to visit the library to access resources at a particular place and for specific time duration. Digital resources are accessible on the devices as laptops, tablets, etc at anytime and anyplace which creates a big demand for the digital resources where there is no physical or time limitation.

Every student must be given the right to study quality material for which it is required to go beyond the traditional white chalk and black board teaching. Education with e-libraries is more interesting, personalized and enjoyable. Teacher should target to create more of digital content to enchance the e-library resources which will motivate the students. This will broaden the scope of learning. Students will have wide range of study material from the subject matter experts across the globe.

Initial implementation hurdles and slow beginning are no doubt to be faced but experience in the west shows that once the e-library picks up the momentum it get self-propelling.

RELATED WORKS

There are many projects already implemented for digital resources as textbooks, video and audio lecture series, simulations, journals, research articles etc. to cater the needs of a wide range of users as students and teachers at school and university levels. Some of the projects include, The National Digital Library (NDL) which is an initiative from Ministry of Human Resource Development, Government of India, under National Mission on Education through Information and Communication Technology. A project to develop a framework for repository of resources with a single-window search facility, multilingual support for all academic levels including researchers and life-long learners, all disciplines, all popular form of access devices.

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NPTEL (National Programme on Technology Enhanced Learning) which is an initiative by Indian Institutes of Technology (IIT) and Indian Institute of Science (IISc) a project funded by the MHRD (Ministry of Human Resource Development) for provides e-learning through online Web and Video courses in Engineering, Sciences, Technology, Management and Humanities. The content in NPTEL includes 100 courses as web based supplements and 100 complete video courses, for forty hours of duration per course. Contents for the above courses were based on the model curriculum suggested by All India Council for Technical Education (AICTE) and the syllabi of major affiliating Universities in India.

e-PG Pathshala, an MHRD initiative, under its National Mission on Education through ICT (NME-ICT), has assigned work to the UGC for development of e-content in 77 subjects at postgraduate level. The content and its quality is the key component of education system. Besides this, there are many other initiatives for digital education as National Digital Literacy Mission or Digital Saksharta Abhiyan (Disha) etc. by Government of India.

E-LIBRARY IN SCHOOLS AND COLLEGES AT BHUTAN

In Bhutan, there was no e-library concept in the schools and colleges. The only medium to study in the schools was books which were supplied by Education Department, Bhutan. In Bhutan there is no concept of buying school books. Complete study material is provided by the government for free, which is a good approach to educate the students but there can be some common problems as non-availability, delay in transportation and difficult to update material on regularly basics in remote areas.

Knowing importance of e-library in Bhutan Hon'ble Prime Minister of India, Sh. Narendra Modi announced Government of India's assistance for establishment of e-library in Bhutan during his first visit to Bhutan in June 2014. This is a testimony to the importance India gives to e-library. The goals of the project include making the educational contents accessible to students across Bhutan. This involved deployment of modern information technology in a reliable way. The project envisages students of Bhutan getting access to world class education content including curriculum from NCERT in order to gain best knowledge in the best way.

SCOPE OF INDO-BHUTAN E-LIBRARY PROJECT .

Total 63 key locations spread all over hilly terrains on Bhutan including 49 central schools, 12 colleges, 1 Data Center (For making portal public) and 1 Central Studio (for content creation) were the destinations where IT infrastructure was deployed beside this a web based portal was developed to access the resources at these identified locations and rest of the world. The portal provides a framework to access (online and offline) collaborative e-content from central repository or local cache for utilization by students, scholars, teachers and other citizens in the form of e-books, rich media as audio-video and other innovative contents. The framework provides anytime-anywhere access to e-contents through desktops, laptops, tablets etc using web and local network. It has a vast variety of content uploaded which is categorized based on standards, subject, author, education level and publisher. The project was awarded to Center for Development of Advanced Computing for its implementation.

IMPLEMENTATION OF INDO-BHUTAN E-LIBRARY PROJECT.

Preliminary Study: For successful implementation of the project, study visits were conducted by CDAC officials for collection of user inputs from students and teachers. To inspect the kind of infrastructure installed at schools and college. All the inputs were considered while designing the project. Currently installed IT infrastructure and its scope of explanation were also considered. During the study, it was found that internet is a major issue at many schools in Bhutan. IT infrastructure was not present in the majority of school libraries. There was also a need for web based portal which can be accessed from anywhere and anytime locally on school network. Digitization of content and content correction was also the requirement of the project.

Implementation of Project: For the ease of implementation of this project, a Project office was setup in the capital city of Bhutan to monitor all the project activities. During the initial meeting with the stake holders as school teachers, students it was observed that

DIGITAL EDUCATION

they lacked clarity about this project at the ground level. For better understanding about the project one of the co-author who was deputed in Bhutan visited all the schools and colleges including in far flug areas of the Bhutan to make the interaction with the teachers, students to help them know about the project along with the roles and responsibilities and showed them the elibrary portal on staging environment. These meetings were very beneficial for the schools and colleges as it resulted in much clarity which was required at the ground level. Everyone was aware about the project but doesn't have the knowledge what exactly is covered in this project. The contribution of Project Engineer who is also the co-author was appreciated by the Royal government of Bhutan and Ambassador of India to Bhutan, Government of India.

Few words from those appreciation/ Recognition are:

"I take this opportunity to commend you for your hard work and sincere efforts in the successful implementation of the Indo-Bhutan e-Library project funded by the Government of India"

By: Ambassador India to Bhutan.

"*You travelled and vested all the project locations, including the far flung area of Bhutan. We would like to thank you for all your concerted efforts towards ensuring the launch of the project on 5th September, 2016.*"

By: Secretary, Gross National Happiness Commission, Royal Government of Bhutan.

After the successful meetings with all the school and colleges coordinators IT infrastructure for schools and college was dispatched from India for Bhutan towards end locations in schools and colleges. After successful delivery and installation at school and colleges the project was inaugurated by Minister of Education, Royal government of Bhutan and Ambassador of India to Bhutan, Government of India on 5th September, 2016. The project was also appreciated in local media of Bhutan and few of its glimpses are:

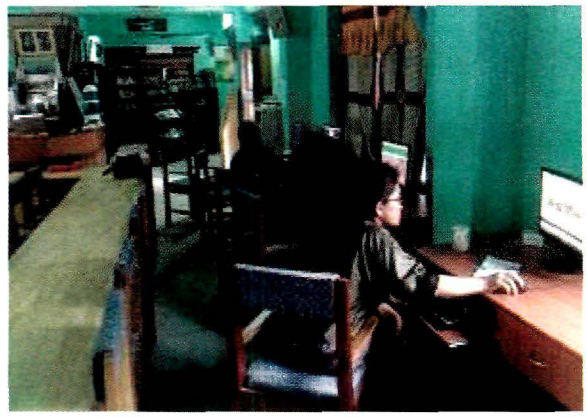
Indo-Bhutan e-Library project launched: Ministry of Education launched Indo-Bhutan e-Library Project at Motithang Higher Secondary School in Thimphu, today. The digital library will have study materials, newspapers and journals in the form of text, video, and audio images.

Source: BBS News, dated 5th September 2016

Students can access 2 million books with launch of e-library: Students and teachers in five colleges under the Royal University of Bhutan, two medical colleges, Royal Thimphu College, Royal Institute of Management and 21 schools across the country can now access 118 text books, reading resources, and other curriculum materials on an electronic library.

Source: Kuensel Newspaper, dated 6th September 2016

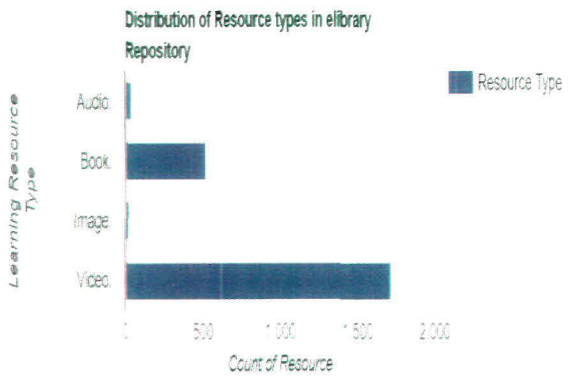
FEW GLIMPSES OF E-LIBRARY IN SCHOOLS AND COLLEGES AT BHUTAN.



PERPESTIVES OF E-LIBRARY PORTAL

RICH KNOWLEDGE SOURCE

The e-library portal provided National Council of Educational Research & Training (NCERT) resources in the form of e-books from K- 12th standard in e-pub format and 1700+ videos of NCERT teachers on various topics. These resources were useful for the Bhutan students specially those who are studying in remote areas. Prior to this framework the students were not aware of what was being taught in Indian schools. This is just a beginning to digital content and it will increase with the collaboration of students and teachers. A large amount of storage is already installed in the data center to cater the future needs.



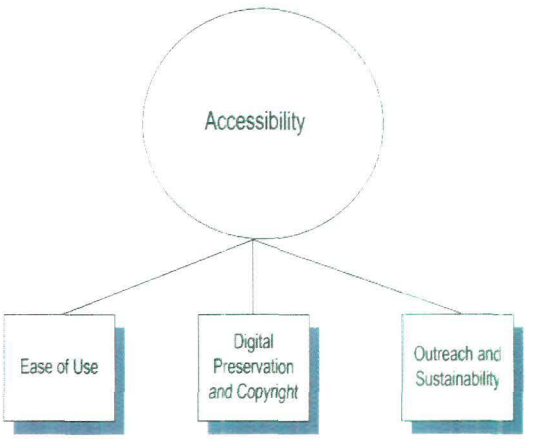
TREASURE OF BOOKS

In addition to the NCERT repository, the portal also contains 139 titles from Bhutan school curriculum. The local teachers were very excited to see that their students no longer have to wait for the printed books especially in the remote areas of the country where distribution was difficult. Availability of these books on e-library framework will help the students in completing their curriculum.

In Bhutan, all the books are provided by the schools in the beginning of the school session and the school session start in February and ends in November. The students were not able to make the best use of this vacation. Now they can start self study of the coming standard which will help them in course time.

EASE OF ACCESSIBILITY

The web portal developed for e-library contains study material which is very easy to access keeping in view the level of understanding of its audience, as it may be vary from a small school kid to a college graduate student. Each user is comfortable in using it and getting best useful resource.



For making the content available easily from the repository several measures were taken as:

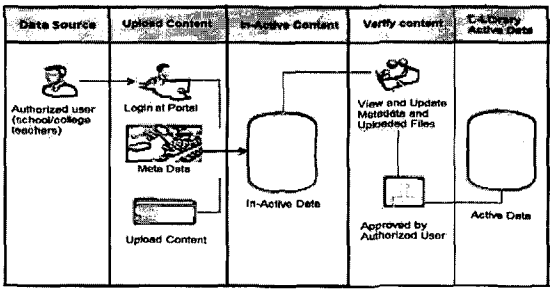
- **Catalogue:** Different classifications are made in the portal under the catalogue as Subject, File Type, Author, Education level and Publisher.
- **Search:** There is an unified search option in the portal where the material can be searched based on the metadata with the additional filter.
- **Meta-Data:** Meta data is a data about the data which means the keywords which a student will enter to find the particular material. Meta-data creation is an important task as a student should be able to find the books from a universal search in the framework without its meta data. The content is in pdf / e-pub format but the search keywords need to be added which are related to that particular book so that student may not find difficulty in finding content. Without proper meta-data the content will be of no use, as if a student is not able to search that book from the repository.

  In the framework, the forms are designed to capture all the relevant fields for metadata creations while uploading the content through authorized user.

USER CLUSTERING

Hierarchy of authorized users is developed in e-library portal for uploading and approving the content. For the content to be visible on portal, it's mandatory to be approved by the authorized user. For viewing of content no authorization is required.

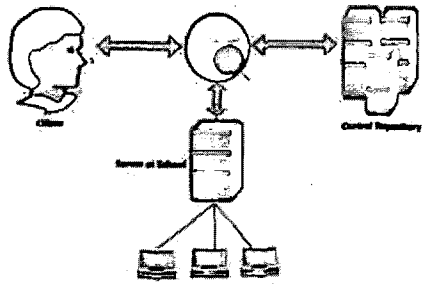
The process of uploading resources goes as shown in below diagram:



INTERNET INDEPENDENT FRAMEWORK

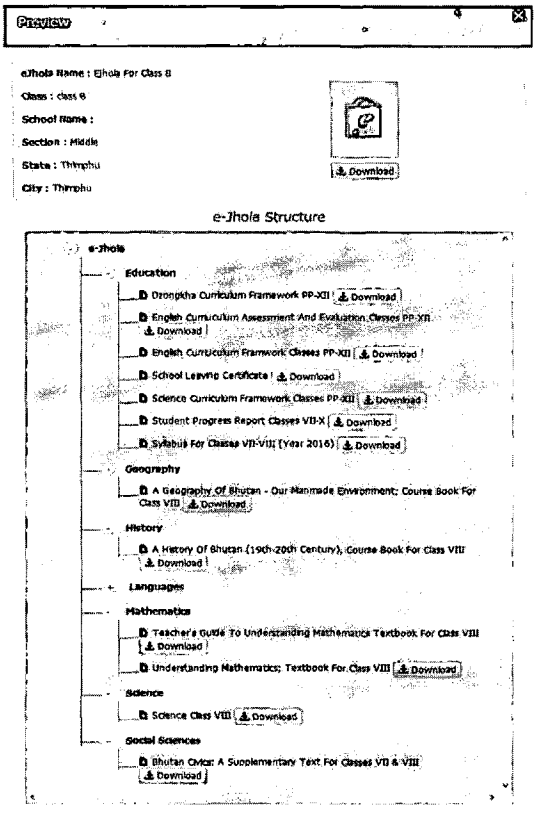
There is no dependency on internet to access the portal in schools and colleges as internet connectivity is a major issue at many remote areas. For making the application accessible on LAN (local area network) of school / college, a server has been installed at each location (school / college).

To update the content from central repository internet is required; in case where internet is not available a portable hard drive was also provided in the schools and colleges so that they could download material from central repository using internet from some other location and later same can be uploaded in the school/college local server which will then be accessible on their local network.



e-JHOLA

This concept was added in framework for making it more useful for students of a particular category. e-jhola is a collection of study material based on standard, author and publisher etc, to get bunch of material relevant for them in just one click. A school child may find some difficulty in finding all content for his own standard, so to ease out, the study material was clubbed so that student navigation is minimum. The same can be viewed online or can be downloaded to view on a personal device at home.



CENTRAL REPOSITORY

A central repository is deployed in data center at Bhutan to make framework accessible through internet. The portal can be accessed through web at http://www.elibrarybhutan.com/

CONTENT DIGITIZATION AND CREATION (RECORDING OF LECTURES / PRACTICAL)

For this purpose a studio is setup in capital city for content creation where different matter experts could record their lectures / practical. Later after processing and editing those lectures, same would be uploaded in the central repository in e-library framework for wider audience.

COST

The entire framework (IT hardware setup and software) is a onetime investment and later its just maintenance. The schools and colleges need to make their involvement by increasing the resources and making it more useful.

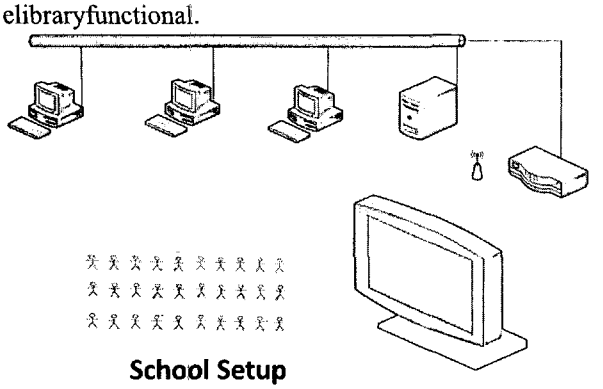
Only non-IT infrastructure as furniture, electricity etc. is required from the schools and colleges rest everything is funded by Government of India.

IT INFRASTRUCTURE INDO-BHUTAN E-LIBRARY

For making the elibrary portal accessible to students in library the IT infrastructure was installed at each location keeping in view the limitation of internet, the onsite servers were also installed at each location through which the portal was accessible on local area network. Similarly the appropriate hardware was installed in the data center, to make the application accessible through internet and a recording studio was setup for recording of lectures and digitizing the content.

INFRASTRUCTURE AT SCHOOL

In each school (total 49) IT hardware included three desktop computers to access the elibrary portal, one local server for keeping the application and repository, one 42' LED TV for showing videos to students, one portable hard drive to transfer data. Apart from this, Antivirus, UPS and Microsoft office for the computer system was also provided. For networking the equipment installed were one router, one switch, two WiFi points, one rack and cat6 cabling with casing. This whole bunch of hardware was installed at each school for making elibraryfunctional.

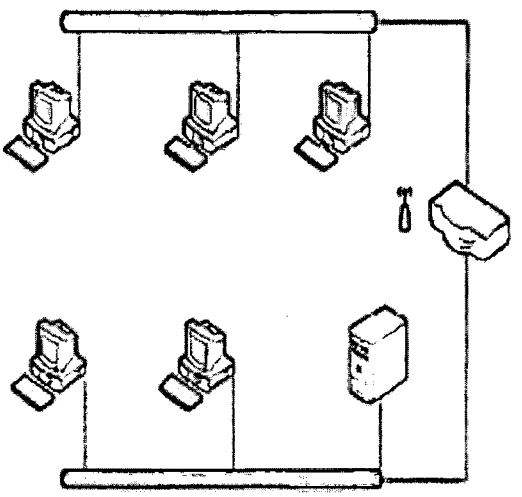


School Setup

ELIBRARY SETUP AT COLLEGES

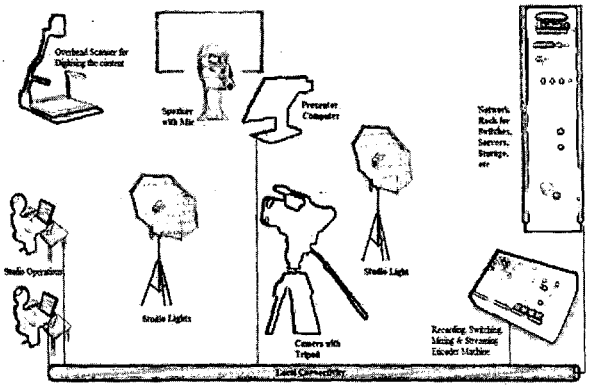
In each college (Total no. of colleges - 12) IT hardware included five desktop computers to access the elibrary portal, one local server for keeping the application and repository, one portable hard drive to carry data. Apart from this, Antivirus, UPS and Microsoft office for the computer system was also provided. For networking the equipment installed was a router, a switch,two WiFi points, one rack and cat6 cabling with casing. This whole bunch of hardware was installed at each college for making elibrary functional.

Setup at college is shown below



STUDIO SETUP

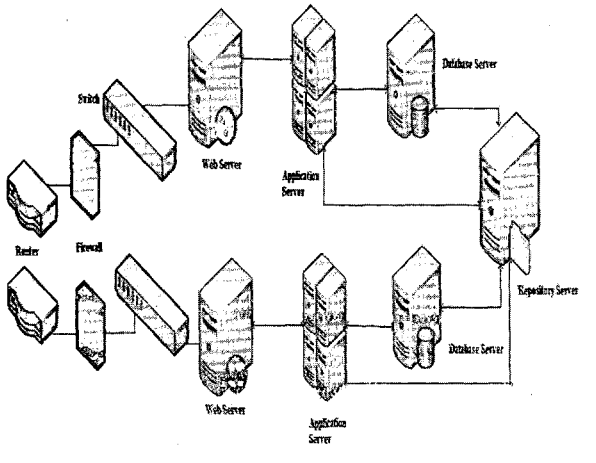
One studio was setup in the capital city for recording and digitizing the content. The hardware at studio included: one Edge Router with Firewall, one Edge Switch, two high end desktop with Windows OS , Antivirus , UPS and MS Office Prof for desktops, one USB Hard Drive and one Scanner A3 (Overhead) with Image processing software. Along with this there were some other equipments as Full HD video Camera with Tripod, Presenter Desktop , Touch Screen Monitor for annotation on Presentation, Hardware Annotation Processor , Recording, Switching, Mixing & Streaming Encoder Machine , AV Server , Microphone Mixer with Feedback Suppression, Preview display monitor, Lavelier Mic (Receiver), Lavelier Mic (Transmitter), Lavelier Mic (Microphone), AV Control System, Headset, HDMI Cables, Studio Light.



Studio Setup

DATA CENTER SETUP

One central repository was created in the data centre at Tech Park in the capital city for making the application accessible through web. The hardware at data centre included: Database Servers , Portal Application Server (in cluster) and Web Portal Authentication Server (in Cluster) Antivirus Server and NMS Server, HIPS for Servers, Object Storage, Virtual Tape Library, Backup Software, NMS software , DC Router, DC Firewall, Core Switch, 17" Rack Monitor with KB and Mouse for Servers, IP KVM 16 ports with command control software, Datacenter infra with five racks with fiber and cat6 cabling, Edge Switch, Desktops with windows OS, Antivirus; MS Office Prof and UPS for Desktops, Data Centre Infrastructure.



Data center Setup

Each request will hit the router which will be filtered in the firewall and passed to web servers. Web servers are configured in the active passive clustering configuration where in case one goes down due to some issue the second web server gets live. The frontend user will make the request on the web server which will filtered through firewall in request will be passed on to internal switches for communication with other servers. For security reasons the database and repository cannot be approached directly. The request from internal switches will access the java api server where java api will get the appropriate results from repository and database.

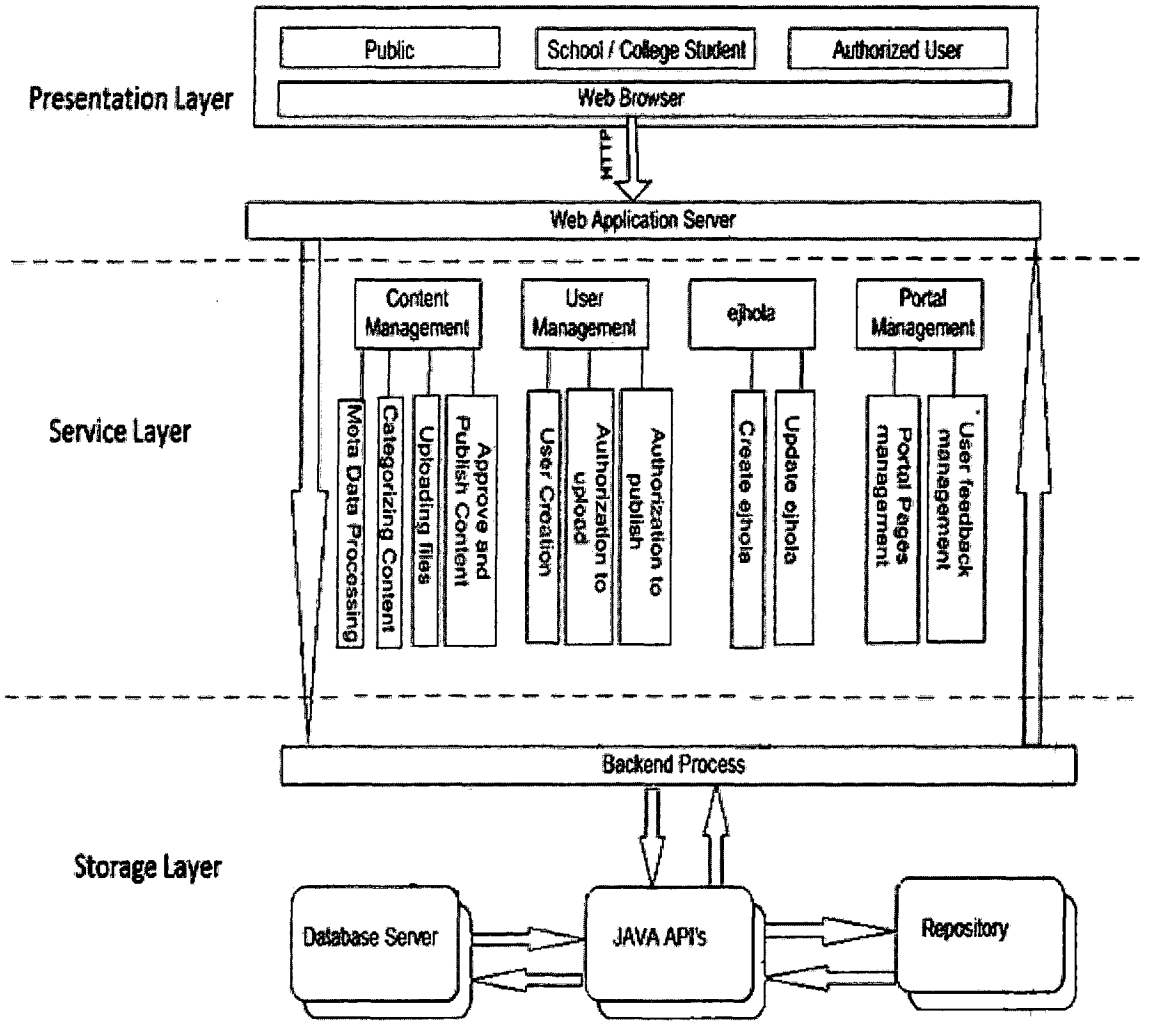
ARCHITECTURE OF E-LIBRARY PORTAL

E-library has been developed in three layers as Presentation layer, Service layer and Storage layer. The request will flow in a two way direction from one layer to other. The brief about each layer is explained below:

Presentation Layer: A graphical interface / GUI acts as a presentation layer which present the complete application to user. Any type of user can send request on web browser through http for any kind of action. Depending on the user type, there are different types of services to be called. Few services require authorization but to view the content, no authorization is required.

Service Layer: Based on the type of user, there are many services available in the portal as content management, user management, e-jhola (Collection of Books), portal management. To get the desired result, the presentation layer calls the backend process. The request made through presentation is passed on to the storage layer.

Storage layer: The http request from presentation layer sends parameters to the backend process where API's provides the desired results from the repository and the database. For security reasons repository and database can't be called through http. The request from API's can only get the results from database and repository.



Information model of Indo-Bhutan Elibrary

CHALLENGES IN IMPLEMENTATION

COST

A certain amount of cost is involved in every project. The budgets need to be managed and allocated for developing and maintaining digital libraries. In case of Indo-Bhutan e-library project complete funding is made by Government of India.

PRELIMINARY TRAINING

To make schools and colleges understand about the project it was required to visit each location so that end user was comfortable about the framework and know about their roles and responsibilities. For the same visits were made to all the project locations as 49 central schools and 12 colleges across the Bhutan for better implementation of project.

LOCATION

The schools and colleges are distributed in the whole country and it's not easy to approach all the locations, except the central locations. Maintaining from a central location was required for better implementation of this project. This was achieved by creating a central repository in the capital city.

RESISTANCE TO ADAPT DIGITAL EDUCATION/ DIGITAL LITERACY

E-library is not yet common in the education system. There is certain amount of resistance that can be seen to adapt digital education which can only be removed after its use and making user friendly system which can be easily adapted. It is a common myth that the digital content is difficult to read and understand as compared

to books. The importance of the digital content needs to be understood, as the storage space required is much less and can be at any time and from any place. Students can access the whole library while he is travelling which will never be possible in case of printed books.

LACK OF INFRASTRUCTURE

In many developing nations there is a shortage of IT infrastructure in educational institutions but can be overcome by using old or refurbished computers, keeping maximum amount of data on the local area network or use of the personal digital devices as laptops, smart phones etc.

LACK OF INTERNET CONNECTIVITY

Internet connectivity is major issue for the schools in remote areas. For making it internet independent solution the installation of servers at each location was done. For getting the updated content internet was required but in case there is no internet connectivity available in school one portal hard drive was provided to each school so that the teachers could download the content from some other internet source and later uploaded the same in their local server for making it accessible on local area network of school.

CONCLUSION

In spite of poor infrastructure, illiteracy, language dominance and all the other reasons there are many award winning e-governance projects. E-library needs to be promoted in schools and colleges for students, so that they can learn beyond the books and compete with world. This would be initial one time investment of IT hardware and building the framework but it can save printing and other costs. The study through digital portal will also give better understanding of the concepts as human brain has good video graphic memory as compared to printed textbooks.

The subject matter experts from entire nation can add their own resources which will be made available to wide range of students at different geographical locations. This will also help the government to share things with the students quickly and easily. To make the digital learning successful all the challenges must be overcome with the support and best practice solutions. Teachers and students must be motivated to upgrade from the traditional libraries practice to elibrary approach in education.

Now it's high time to use digital education to replace bulky bags with the electronic devices. Digital education will decrease gaps between student and teacher and will make the learning easier and better.

FUTURE SCOPE

There is a lot of future scope in this project. Presently only 61 locations are covered in this project in Bhutan, but this can i.e. increased to large number of schools in India and Bhutan. The scope of portal can also be increased by introducing some other modules as attendance, student assessment, live lectures/video conferencing etc.

Content will always be the golden line in e-library, teachers should make their best efforts to add more and more content to the database so that students always get to see something new and get connected.

ACKNOWLEDGEMENT

The elibrary project was implemented by CDAC with the support of Ministry of External Affairs, Government of India and Royal Government of Bhutan.

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ULTRASOUND ASSISTED SYNTHESIS, DFT AND DOCKING STUDIES OF SOME PYRAZOLYLTHIAZOLES BASED MOLECULAR HYBRIDS

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ABSTRACT

We have developed an efficient procedure for the synthesis of a series of aryl and heteroaryl moieties linked pyrazolylthiazole derivatives using α-bromomethyl ketones under ultrasonic irradiation as non-conventional heating source. This protocol offers several advantages over conventional method. The structure of all compounds has been optimized using HF method with 631+g basis set. Docking studies of all compounds with human serum albumin has been done to explore the mode of binding. Some compounds show binding energy comparable with standard drug Warfarin.

Keywords: Coumarin, Thiazole, DFT, Docking, Human Serum Albumin

INTRODUCTION

A large number of naturally occurring compounds contain five-membered heterocyclic rings as an important part of their structure. Among the heterocycles, thiazole is a prevalent scaffold in a number of naturally occurring and synthetic molecules with attractive biological activities such as antiviral, anticancer, antibacterial, antifungal, anticonvulsant, antiparkinsonian and anti-inflammatory activities [Stankova et al, Solimana et al, Vicini et al, Amin et al and Azam et al]. The thiazole ring is present also in various marine or terrestrial natural compounds. Pyrazoles are another important class of 5-membered heterocyclic compounds having remarkable activities against bacteria, fungi, tumors, viruses and especially against HIV proteases [Jaen et al, Rudolph et al] 3,5-Dimethylpyrazole displays hypoglycemic activity in diabetic rats because it metabolizes to the corresponding 5-carboxylic acid [Windholz et al].

Therefore, thiazole and pyrazole comprises of an important class of heterocyclic componds found in many potent biologically active molecules such as bleomycin, meloxicam **(I)**, abafungin **(II)**, tiazofurin **(III)**, lonozolac **(IV)**, celecoxib **(V)**, ramifenazone **(VI)** etc. (**Figure 1**)

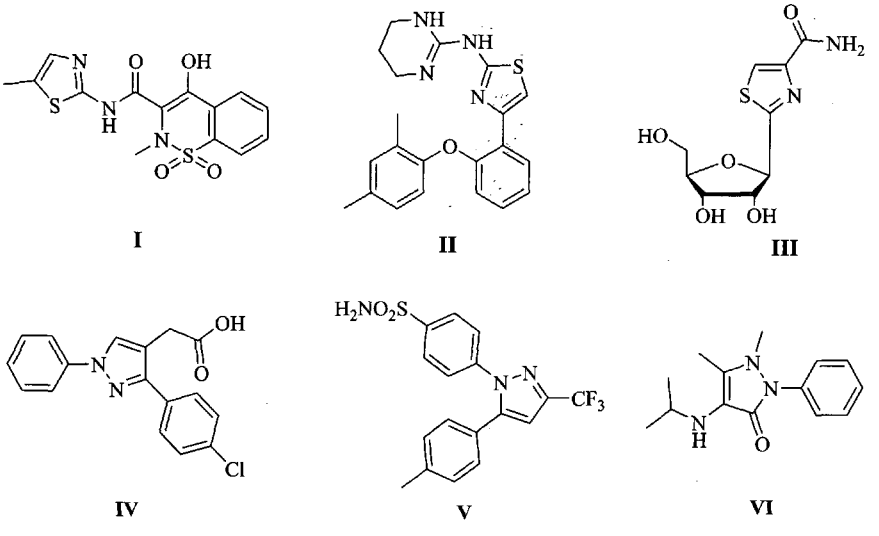

Figure 1. Some biologically important azoles.

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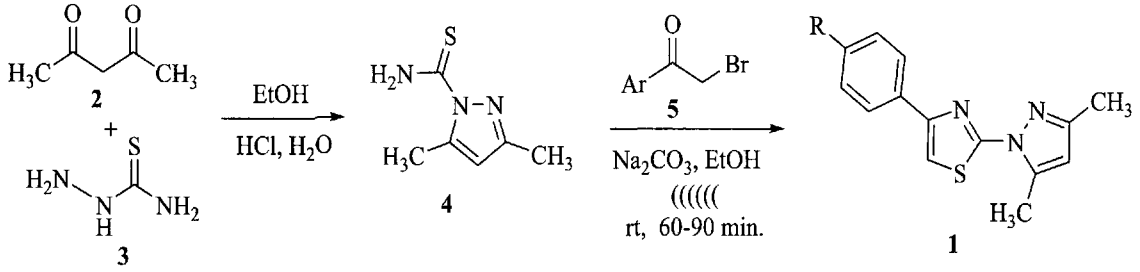
Thus, a careful literature survey revealed that thiazole and pyrazole ring systems have occupied a unique position in the design and synthesis of novel biological active agents with remarkable biological activities [Holla et al and Karegoudar et al]. The chemistry of thiazole, pyrazole and most of their derivatives has been well studied. However, the chemistry of pyrazolylthiazoles is still essentially in the development stage.

Human serum albumin (HSA) is the most abundant protein in blood plasma and is responsible for many physiological functions of the body. It is a widely studied protein for over 40 years due to its ability to extraordinary binding capacity, availability, stability and altered pharmacokinetic properties [Nicoletti et al]. The main function of human serum albumin is to act as a carrier for many endogenous and exogenous ligands such as hormones, fatty acids and metabolites to particular biological targets [He et al]. Therefore, serum albumin plays an important role in the distribution, free concentration, excretion, metabolism and interaction with the target tissues of these ligands. The activity level of a pharmaceutical drug depends on the interaction with targeting molecules, mode of action and affinity size, while the structural differences in drug often lead to changes in its biological activity [Xie et al]. Thus, the investigation of bioactive molecules binding to HSA is of important significance [Pastukhov et al].

In view of the above discussed facts and in continuation of our work on the development of molecular hybrids of biological importance [Kumar et al and Aggarwal et al], we have developed thiazole-pyrazole based molecular hybrids to explore their mode of binding with human serum albumin.

RESULTS AND DISCUSSION

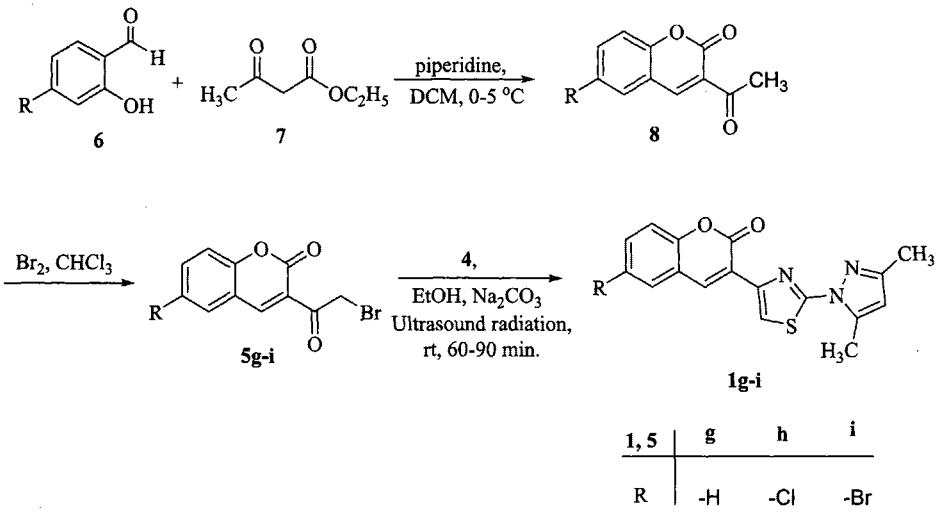
Synthesis of **1a** was accomplished by sonication of an equimolar mixture of α-bromoacetophenone **5a** with **4** in the presence of sodium carbonate in ethanol under ultrasonic radiations at room temperature for 60-90 minutes (**Scheme 1**). The starting material, 3,5-dimethylpyrazole-1-thiocarboxamide (**4**) was obtained by the condensation of acetylacetone (**2**) and thiosemicarbazide (**3**). α-Bromoacetophenones **5a-f** were synthesized by the bromination of acetophenones in acetic acid/chloroform and their formation was confirmed by comparison with literature melting points [Heilborn et al and Miyahara et al].



1, 5	a	b	c	d	e	f
R	-H	-CH_3	4-Cl	4-Br-	4-F-	4-NO_2-

Scheme 1. Synthesis of 4-aryl-2-(3,5-dimethylpyrazol-1-yl)thiazoles

Scope of this reaction was further extended by employing heterocyclic α-bromomethyl ketones **5g-5i**. 3-Acetylcoumarins **8g-8i** were synthesized by the reaction of corresponding salicylaldehydes (**6**) with ethyl acetoacetate (**7**) in presence of catalytic amount of piperidine at low temperature [Gursoy et al.]. Further, synthesis of **1g-1i** was accomplished by sonicating an equimolar mixture of α-bromoacetophenone **5g-5i** with **4** for 60-90 min in the presence of sodium carbonate in ethanol under ultrasonic irradiation. (**Scheme 2**)

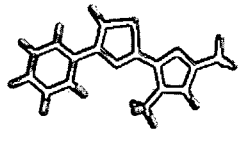
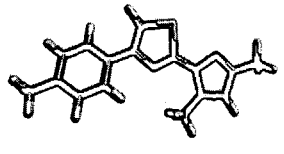
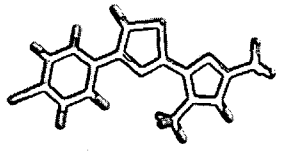


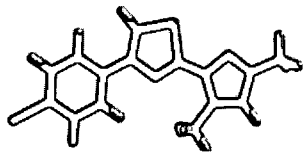
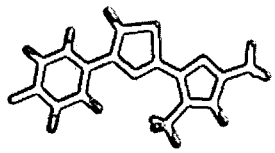
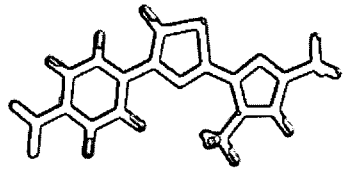
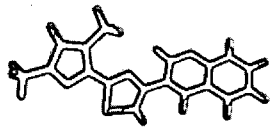
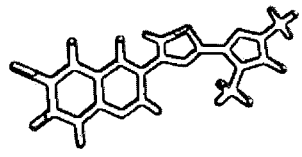
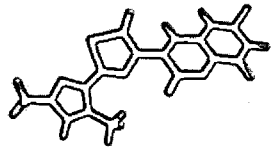
Scheme 2. Synthesis of 4-(coumarin-3-yl)-2-(3,5-dimethylpyrazol-1-yl)thiazoles

Electrostatic Results

The HOMO and LUMO energy of a molecule represents its electron donating and receiving ability. Higher the energy of HOMO higher will be its electron donating ability. For all compounds (**1a-1i**), a full geometry optimization was performed using HF and the 6-31+g basis set. In all the compounds, no much difference in HOMO energy has been observed for all the compounds, even though compounds have different substituents. However, the LUMO orbital energies were affected by the presence of coumarin moiety on the thiazole ring; consequently, there was a change in energy according to attached groups. HOMO-LUMO energy gap (E gap) have significant importance as far as pharmaceutical studies were concerned. The energy gap between HOMO-LUMO can be correlated further with docking studies. Table 1 summarized the theoretical electronic parameters for investigating the thiazole-pyrazole (TP) based molecular hybrids.

Table 1: Electrostatic results of compounds 1a-1i

Compound	Optimized structure	HOMO-1 (eV)	HOMO (eV)	LUMO (eV)	LUMO+1 (eV)	E_{gap} (eV)
1a		-9.330	-8.169	1.720	1.896	-6.44
1b		-9.256	-7.993	1.734	1.906	-6.25
1c		-9.640	-8.394	1.578	1.720	-6.81

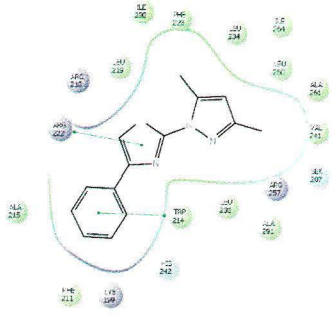
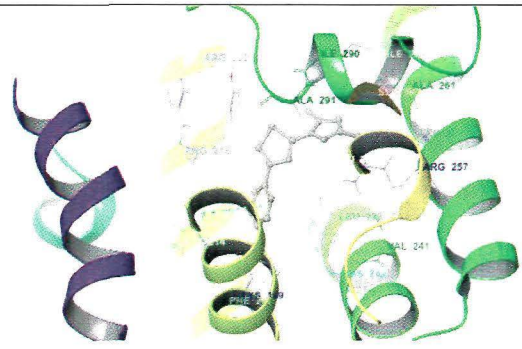
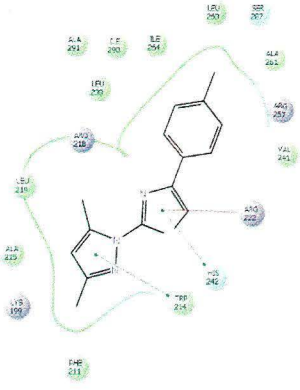
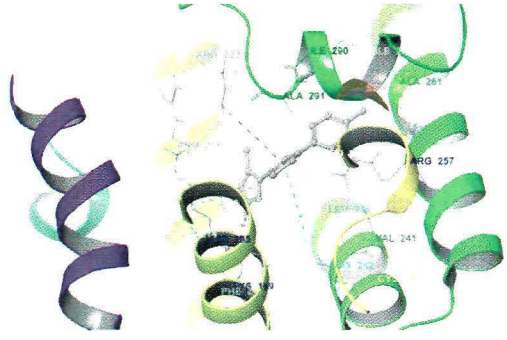
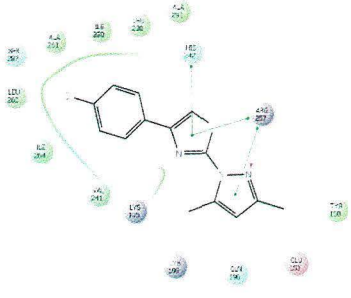
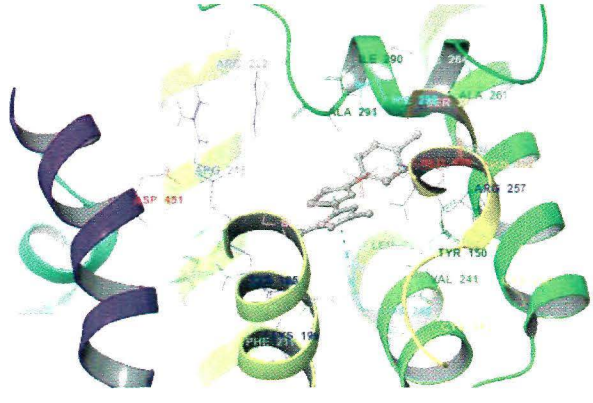
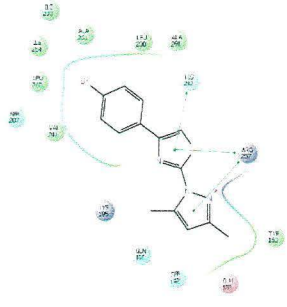
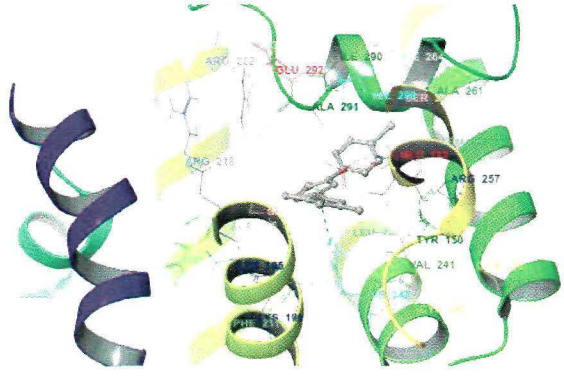
1d		-9.571	-8.315	1.518	1.602	-6.79
1e		-9.664	-8.383	1.616	1.792	-6.76
1f		-9.930	-8.817	0.357	1.439	-8.46
1g		-9.231	-8.608	1.209	1.486	-7.39
1h		-9.440	-8.768	0.915	1.393	-7.85
1i		-9.364	-8.749	0.943	1.331	-7.80

Molecular Docking Studies

Molecular docking is an important tool to explore the possible binding mode between ligand and protein complex. In the present work, we have attempted to study the interactions of thiazole-pyrazole (TP) hybrids with Human serum albumin (HSA). For this purpose molecular docking studies of all the synthesized compounds **1a-1i** were performed in the binding pocket of HSA (PDB ID:1H9Z). The binding affinity of ligands **1a-1i** for HSA are discussed on the basis of four major parameters-Glide score, Glide energy, H-bonds and non-bonded interactions (van der Waals and Coulombic). The more negative value of Glide score and minimum energy for the formation of complex between ligand and receptor (Glide energy) indicates a good binding affinity. The results of docking studies and the docked conformations of all compounds are shown in Table 2. These docking results clearly indicate that the most active compounds exhibited significant binding affinities towards Human serum albumin (Glide energy range -72.05 $kcalmol^{-1}$ to -55.49 $kcalmol^{-1}$). Analysis of the docking pose for all synthesized compounds **1a-1i** shows that all of them cozily fit into the active site of HSA and the binding energy obtained for all these compounds is comparable with warfarin i.e., -75.03 $kcalmol^{-1}$(Table 3).In case of all componuds van der waals and coulombic interactions are more prevalent over the electrostatic contribution in the binding of molecules **1a-1i** to HSA. Extensive van der Waals and coulombic interactions have been observed with residues Leu 260, Ser 287, Ala 261, Arg 257, Val 241, Arg 222, His 242, Trp 214, Phe 211, Lys 199, Ala 215, Leu 219, Arg 218, Leu 238, Ala 291, Ile 290 and Ile 264 lining the active site of HSA. The binding pattern predicted by Glide clearly indicates that these thiazole-pyrazole (TP) based hybrids have a high affinity toward active site

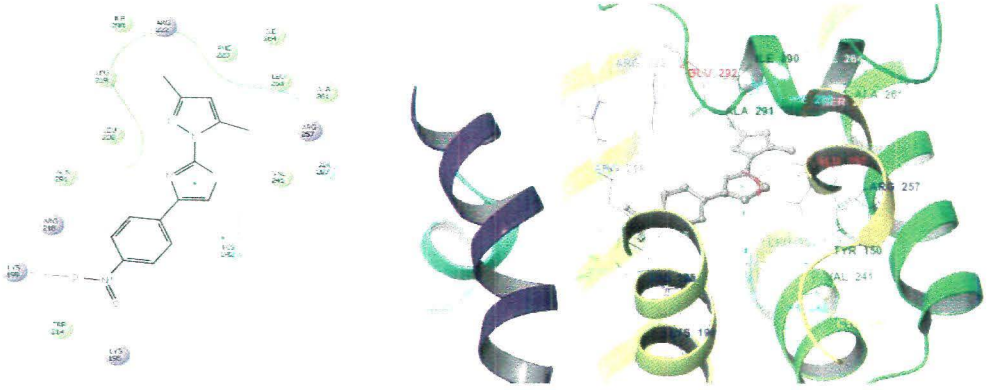
of HSA which provides a strong platform for new structure-based design efforts.

Table 2: 2D and 3D binding poses of lead compounds and standard drug warfarin with HSA

Compound	2D Docking Pose	3D Docking Pose
1a		
1b		
1c		
1d		

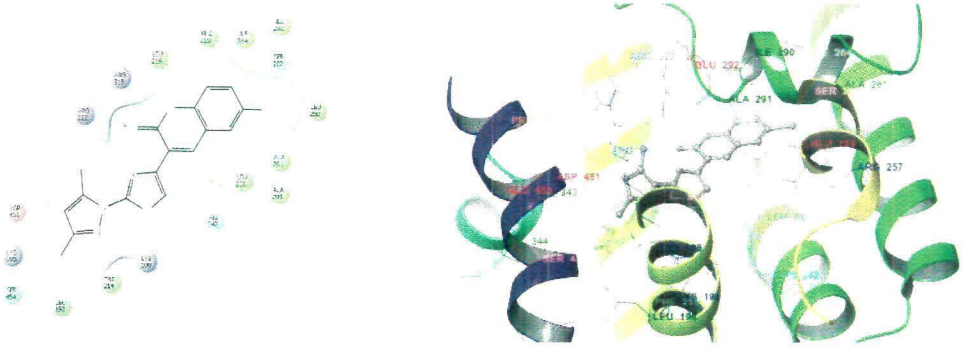
1e

1f

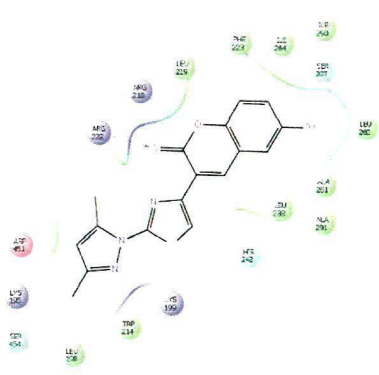


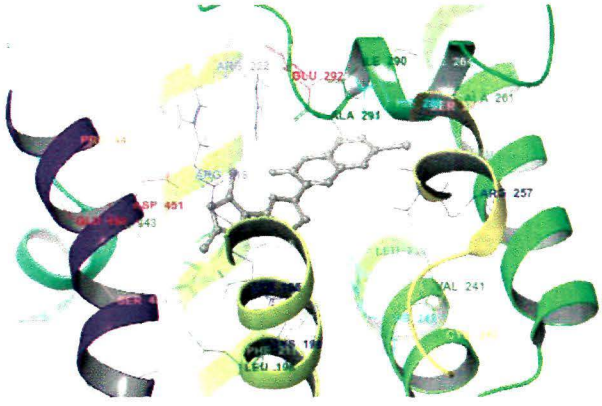
1g

1h

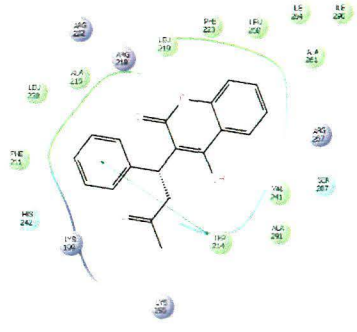


1i





Warfarin



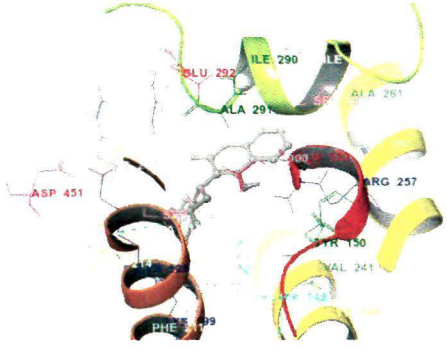


Table 3: Binding data of lead compounds based on MMGB-SA binding energy study

Entry	GScore	δG_Bind (Kcal/mol)	δG_Bind Coulomb (Kcal/mol)	δG Bind H bond (Kcal/mol)	δG_Bind Lipo (Kcal/mol)	δG_Bind vdW (Kcal/mol)	Key Protein ligands interaction
1a	-6.0	-56.84	-1.21	0	-39.38	-35.58	Leu 260, Ser 287,Ala 261, Arg 257, Val 241, Arg 222, His 242, Trp 214, Phe 211, Lys 199, Ala 215, Leu 219, Arg 218, Leu 238, Ala 291, Ile 290, Ile 264, Phe 223, Leu 234
1b	-6.3	-58.57	-0.92	0	-37.98	-40.41	Leu 260, Ser 287, Ala 261, Arg 257, Val 241, Arg 222, His 242, Trp 214, Phe 211, Lys 199, Ala 215,

							Leu 219, Arg 218, Leu 238, Ala 291, Ile 290, Ile 264
1c	-5.1	-59.64	0.59	-0.70	-32.59	-37.06	Leu 260, Ser 287 Ala 261, Arg 257,Val 241, His *242,Lys 199, Leu* 238,Ala 291, Ile 290,Ile 264, Lys 195,Gln 196, Glu 153
1d	-4.8	-59.19	0.05	-0.80	-32.10	-37.63	Leu 260, Ser 287 Ala 261, Arg 257,Val 241, His 242,Lys 199, Leu 238,Ala 291, Ile 290,Ile 264, Lys 195,Glu 153, Ser 192
1e	-5.9	-57.59	-1.99	0	-33.76	-39.31	Leu 260, Ser 287, Ala 261, Arg 257, Val 241, Arg 222, His 242, Trp 214, Phe 211, Lys *199, Ala 215,* Leu 219, Arg 218, Leu 238, Ala 291, Ile 290, Ile 264
1f	-4.8	-55.49	7.56	-0.09	-27.53	-37.38	Leu 260, Ser 287, Ala 261, Arg 257,Val 241, His 242,Phe 223, Arg 222, Leu 219, Arg 218, Trp 214, Leu 238, Ala 291, Ile 290, Ile 264, Lys 199
1g	-5.1	-56.83	-17.02	-1.09	-22.75	-38.58	Leu 260, Ser 287, Ala 261, Arg 257, Val 241, Arg 222, His *242, Trp 214,* Phe 223, Lys 199, Ala 215, Leu 219, Arg 218, Leu 238, Ala 291, Ile 290,

							Ile 264, Leu 198, Ser 454, Lys 195, Asp 451
1h	-5.5	-70.57	-15.51	-1.08	-32.29	-42.56	Leu 260, Ser 287, Ala 261, Arg 257, Val 241, Arg 222, His 242, Trp 214, Phe 223, Lys 199, Ala 215, Leu 219, Arg 218, Leu 238, Ala 291, Ile 290, Ile 264, Leu 198, Ser 454, Lys 195, Asp 451
1i	-5.5	-72.05	-15.35	-1.08	-32.63	-44.15	Leu 260, Ser 287, Ala 261, Arg 257, Val 241, Arg 222, His 242, Trp 214, Phe 223, Lys 199, Ala 215, Leu 219, Arg 218, Leu 238, Ala 291, Ile 290, Ile 264, Leu 198, Ser 454, Lys 195, Asp 451
Warfarin	-7.4	-75.03	-11.91	-0.51	-35.60	-43.52	Leu 260, Ser 287 Ala 261, Arg 257,Val 241, His 242,Lys 199, Leu 238,Ala 291, Ile 290,Ile 264, Lys 195,Glu 153, Ser 192

Pharmacokinetic Effect of Synthesized Compounds 1a-1i

Pharmacodynamics results indicated that compounds (**1a-1i**) may prove good lead as drug because of their strong binding affinity towards HSA. For drug formulation pharmacokinetic properties are also an important aspect and should be taken into consideration. The pharmacokinetic parameters of all nine lead molecules have been studied along with standard drug warfarin using QikProp application available with Maestro 9.2.73 [Maestro et al]. All the synthesized compounds (**1a-1i**) were seems to be acceptable with respect to all the major parameters which were incorporated in Table 4. Prediction of oral drug absorption (Percent Human Oral Absorption) was highly satisfactory for all the test compounds **1a-1i** with a high percentage (>80 %) of Human Oral Absorption as compared to the reference compounds warfarin, indicating that thiazole-pyrazole (TP) hybrids could be developed as an orally dosed drug.

Lipinski's rule of 5 could be another parameter which could be viewed more likely to have good intestinal absorption or permeation and is confirmed by the predicted Caco-2 cells permeability (QPPCaco), used as a model for the gut-blood barrier [Lu et al]. QPPCaco predictions for all the test compounds showed very good values compared to the standard warfarin. Further, QPlogKhsa which is the prediction for human serum albumin binding, shows that the predicted values for all the inhibitors lie within the expected range (-1.5 to 1.5). Also, the QikProp descriptor for brain/blood partition coefficient (QPlogBB) show satisfactory predictions for all the test compounds and the reference compounds. Furthermore, QPlogHERG descriptor for the prediction of IC50 value of HERG K+ channel blockage was predicted for the test compounds. Compounds have been predicted to possess QPlogHERG values in below concern range (< -5) comparable to reference warfarin (Table 4).

Table 4: Predicted ADME properties of synthesized compounds **1a-1i** and standard drug Warfarin

Compounds	QP logPo/w[a]	QP logHERG[b]	QPPCaco[c]	QP logBB[d]	QPPMDCK[e]	QP logKp[f]	QPlog Khsa[g]	Percent Human Oral Absorption[h]	Lipinski's rule of five
Acceptable range	**(-2.0 to 6.5)**	**> -5.0**	**<25 poor > 500 great**	**(-3 to 1.2)**	**<25 poor > 500 great**	**(-8.0 to -0.1)**	**(-1.5 to 1.5)**	**> 80% High, > 25% low**	**< 5**
1a	3.84	-5.74	1578.9	-0.0	3128.8	-2.175	0.332	100	0
1b	4.39	-5.44	5495.3	0.38	4879.7	-1.178	0.657	100	0
1c	4.57	-5.43	5499.3	0.56	10000	-1.148	0.611	100	0
1d	4.64	-5.46	5499.7	0.57	10000	-1.151	0.637	100	0
1e	4.30	-5.38	5499.5	0.51	8838.4	-1.115	0.53	100	0
1f	3.30	-5.44	657.4	-0.6	491.54	-2.885	0.384	96.75	0
1g	3.33	-5.81	1578.8	-0.1	1267.5	-2.007	0.204	100	0
1h	4.01	-5.50	5496.3	0.39	4880.5	-0.981	0.483	100	0
1i	3.92	-5.77	1579.0	-0.0	3364.2	-2.177	0.358	100	0
Warfarin	2.70	-5.62	913.0	-0.7	448.36	-1.839	0.078	95.75	0

[a] Predicted octanol/water partition co-efficient logp. [b] Predicted IC_{50} values to block HERG K^+channels. [c] Predicted Caco-2 cell permeability. It represents the ability of drug to cross gut blood barrier. [d] Predicted brain/blood partition coefficient. [e] Predicted apparent MDCK cell permeability. It represents the ability of drug to cross blood-brain barrier. [f] Predicted skin permeability. [g] Predicted binding to human serum albumin. [h] Predicted oral absorption of drug in percentage term.

CONCLUSION

In conclusion, we have developed a simple and efficient procedure for the synthesis of a series of aryl and heteroaryl moieties linked pyrazolylthiazole derivatives. α-Bromomethyl ketones and thiocarboxamides were condensed under ultrasound irradiation at room temperature. When compared to the conventional method, this approach has several and important advantages including milder conditions, shorter reaction times and higher yields. Structure of all compounds has been optimized using HF method with 631+g basis set. Energy gap between the HOMO and LUMO were found high for all the molecules. Docking studies of all compounds with human serum albumin has been done to explore the mode of binding. Compounds **1a** and **1b** show high binding energy which is comparable with standard drug Warfarin.

EXPERIMENTAL SECTION

General

Melting points were determined in open capillaries in electrical apparatus and are uncorrected. The ^1H and ^{13}C NMR spectra were recorded on a Bruker instrument at 400 MHz and 75 MHz, respectively. D_2O exchange was

applied to confirm the assignment of the signals of OH protons. Mass spectra were measured in EI mode on a Kratos MS-50 spectrometer at MS Facilities at SAIF, Panjab University, Chandigarh, India. Elemental analyses were performed at NIPER (Mohali), Chandigarh, India. All the compounds gave C, H and N analysis within 0.5 of the theoretical values. Ultrasound for sonication is generated with the help of ultrasonic instrument (Digital Ultrasonic Cleaner LMUC-2). The specifications, operating frequency and details of set up are as follows: Operating frequency 40±3 KHz, Wattage 1.8 L, Tank Size 175mm x 165mm x 200mm.

Acetylacetone, thosemicarbazide, aldehydes and ethyl acetoacetate were commercially available. 3,5-Dimethylpyrazole-1-thiocarboxamide and 3-(2-bromoacetyl)coumarins were synthesized according to literature procedure [Heilborn et al, Miyahara et al and Gursoy et al]. Literature melting points of **1a-i** were compared with Aggarwal et al.

Standard procedure for the preparation of 2-(3,5-dimethylpyrazol-1-yl)-4-substitutedthiazoles **1a-i**:
An ethanolic solution (10 ml) of sodium carbonate (2 mmol), 3-(α-bromoacetyl)coumarin (**5g**) (2 mmol) and 3,5-dimethylpyrazole-1-thiocarboxamide (**4**) (2 mmol) was added to a flask. The reaction mixture was kept under sonication by an ultrasonic probe at room temperature for the specified period (60-90 min) until complete consumption of starting materials monitored by TLC. When the reaction was completed, the mixture was poured over ice-water (10 ml). The resulting solid compound **1g** was filtered and washed with water.

4-(Coumarin-3-yl)-2-(3,5-dimethylpyrazol-1yl)thiazole (**1g**): Mp 221-223 °C (lit[19] mp 222 °C); yield 85%; ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.32 (s, 3H, 3-CH_3), 2.82 (s, 3H, 5-CH_3), 6.06 (s, 1H, pyrazole 4-H), 7.42 (m, 2H, coumarin 7,8-H), 7.59 (m, 1H, coumarin 6-H), 7.67 (d, 1H, *J*=7.8 Hz, coumarin 5-H), 8.24 (s, 1H, thiazole 5-H), 8.58 (s, 1H, coumarin 4-H). ^{13}C NMR (75 MHz, $CDCl_3$, δ): 13.32, 24.64, 106.73, 114.36, 116.41, 119.14, 122.74, 122.81, 124.52, 125.67, 128.48, 130.26, 137.94, 143.49, 145.91, 159.84, 163.27; MS (m/z): 323, 308, 299, 295, 281, 145.

Similarly other compounds were prepared using the same procedure.
Characterization data of the compounds:
1a: 4-Phenyl-2-(3,5-dimethylpyrazol-1-yl)thiazole
Mp 99-101 °C (lit mp 102 °C); yield 90%; ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.32 (s, 3H, 3-CH_3), 2.80 (s, 3H, 5-CH_3), 6.03 (s, 1H, pyrazole 4-H), 7.23 (s, 1H, thiazole 5-H), 7.37 (m, 1H, 4-H of Ph), 7.47 (m, 2H, 3,5-H of Ph), 7.92 (d, 2H, *J*=7.2 Hz, 2,6-H of Ph).

1b:4-(*p*-Methylphenyl)-2-(3,5-dimethylpyrazol-1-yl)thiazole
Mp 118-119 °C (lit mp 119 °C); yield 84%; ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.31 (s, 3H, 3-CH_3), 2.40 (s, 3H, *p*-CH_3), 2.79 (s, 3H, 5-CH_3), 6.03 (s, 1H, pyrazole 4-H), 7.16 (s, 1H, thiazole 5-H), 7.26 (d, 2H, *J*=7.8 Hz, 3,5-H of Ph), 7.81 (d, 2H, *J*=8.1 Hz, 2,6-H of Ph).
1c:4-(*p*-Chlorophenyl)-2-(3,5-dimethylpyrazol-1-yl)thiazole
Mp 150-152 °C (lit mp 151 °C); yield 92%; ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.32 (s, 3H, 3-CH_3), 2.79 (s, 3H, 5-CH_3), 6.04 (s, 1H, pyrazole 4-H), 7.21 (s, 1H, thiazole 5-H), 7.42 (d, 2H, *J*=8.7 Hz, 2,6-H of Ph), 7.85 (d, 2H, *J*=8.4 Hz, 3,5-H of Ph).
1d:4-(*p*-Bromophenyl)-2-(3,5-dimethylpyrazol-1-yl)thiazole
Mp 148-149 °C (lit mp 149 °C); yield 90%; ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.31 (s, 3H, 3-CH_3), 2.78 (s, 3H, 5-CH_3), 6.04 (s, 1H, pyrazole 4-H), 7.22 (s, 1H, thiazole 5-H), 7.57 (d, 2H, *J*=8.4 Hz, 2,6-H of Ph), 7.79 (d, 2H, *J*=8.1 Hz, 3,5-H of Ph).
1e:4-(*p*-Fluorophenyl)-2-(3,5-dimethylpyrazol-1-yl)thiazole
Mp 118-120 °C (lit mp 120 °C); yield 93%; ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.32 (s, 3H, 3-CH_3), 2.80 (s, 3H, 5-CH_3), 6.05 (s, 1H, pyrazole 4-H), 7.26 (s, 1H, thiazole 5-H), 7.56 (m, 2H, 2,6-H of Ph), 7.81 (m, 2H, 3,5-H of Ph).
1f:4-(*p*-Nitrophenyl)-2-(3,5-dimethylpyrazol-1-yl)thiazole
Mp 188-190 °C (lit mp 192 °C); yield 92%; ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.32 (s, 3H, 3-CH_3), 2.80 (s, 3H, 5-CH_3), 6.06 (s, 1H, pyrazole 4-H), 7.43 (s, 1H, thiazole 5-H), 8.06 (d, 2H, *J*=8.4 Hz, 2,6-H of Ph), 8.31 (d, 2H, *J*=8.4 Hz, 3,5-H of Ph).
1h: 4-(6-Chlorocoumarin-3-yl)-2-(3,5-dimethylpyrazol-1-yl)thiazole
Mp 194-195 °C (lit mp 195 °C); yield 90%; IR (cm^{-1}): ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.33 (s, 3H, 3-CH_3), 2.80 (s, 3H, 5-CH_3), 6.07 (s, 1H, pyrazole 4-H), 7.36 (d, 1H, *J*=8.7 Hz, coumarin 8-H), 7.53 (dd, 1H, *J*=8.7 Hz, 2.4 Hz, coumarin 7-H), 7.66 (d, 1H, *J*=2.4 Hz, coumarin 5-H), 8.26 (s, 1H, thiazole 5-H), 8.50 (s, 1H, coumarin 4-H).
1i: 4-(6-Bromocoumarin-3-yl)-2-(3,5-dimethylpyrazol-1-yl)thiazole
Mp 260-262 °C (lit mp 262 °C); yield 88%; ^{1}H NMR (300 MHz, $CDCl_3$, δ): 2.32 (s, 3H, 3-CH_3), 2.80 (s, 3H, 5-CH_3), 6.06 (s, 1H, pyrazole 4-H), 7.30 (m, 1H, coumarin 8–H), 7.63 (dd, 1H, *J*=8.4 Hz, 2.1 Hz, coumarin 7-H), 7.80 (d, 1H, *J*=2.1 Hz, coumarin 5-H), 8.25 (s, 1H, thiazole 5-H), 8.49 (s, 1H, coumarin 4-H).

Computational Methods

The theoretical calculations were performed using HF method. For each structure, a full geometry optimization was performed using this function and the 6-31+g basis set as implemented by Gaussian 03 package [Trucks et al]. All geometries were visualized either using Avogadro 1.2 software packages.

Molecular Docking

The protein preparation wizard was used to clean and optimize the protein–ligand crystal structure. All the water molecules were removed during preprocess and missing side chains of residues have been added using prime module incorporated within the package. The hydrogen atoms were added to the protein structure corresponding to the physiological pH 7.0 considering the appropriate ionization states for the acidic as well as basic amino acids. Finally energy minimization with root-mean-square deviation (RMSD) value of 0.30 was carried out using optimized potentials for liquid simulations (OPLS-2005) force field after assigning charge and protonation state. All ligands were prepared using the Schrodinger LigPrep utility (Schrodinger, LLC, USA) which generates a low energy 3D structures.

The active site of protein was defined by a bounding box (grid) that was centered on the native ligand in the crystal complex. Extra-precision glide docking (Glide XP) which docks ligands flexibly was used to rank the docking poses and to gauze the binding affinity of these ligands toward the protein.

ADME Prediction

ADME properties were predicted for synthesized compounds **1a–1i** using computational methods. In this study, we have calculated Qp LogPo/w, QP LogHERG, QPPCaco, Qp LogBB, QPPMDCK, QPlogKp, QpLogHSA, Percentage Human oral absorption and Lipinski's rule of five using QikProp.

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SIGNIFICANCE OF ETHICS IN RESEARCH

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Abstract

The paper aims to give a glimpse of genesis of ethical guidelines and the circumstances which led to the formation of these guidelines. Although the ethical codes mark their origin from the 5th century B.C. but after the World War II, the states began to take more interest in science and research. This resulted in the inception of colossal, methodical investigations to gain knowledge for effective ethics in research. Research involving human participants raises unique and complex ethical, legal, social and political issues. The ethical guidelines were initially formulated to protect the rights of humans from being treated as guinea pigs for medical research, but with the advent of research, ethics have spread their wings in all horizons of research including chemical synthesis, economics and environment. Ethical guidelines play a key role in deciding whether an ongoing research is ethically acceptable or not. The present report summaries the origin and highlights the importance of ethics in all domains of research.

Keywords: Ethics, Clinical, Chemical synthesis, Environment Research

INTRODUCTION

Ethics are self-realized and pre-arranged ordinances involving alignment, screening, forefending and commending perceptions of right and wrong execution. It is a philosophical term derived from an ancient Greek term "ethos" (Internet). It was the end of World War II that marked the need for ethical principles underlying the research endeavors. In the emblematic event of the Nuremberg War Crimes Trial (Grodin, 1992) following World War II, the hideous act of German scientists of using their captives as experimental subjects were exposed. This led to the development of a common belief about the need of key ethical principles that should be the fundamental guiding light of all research endeavors. It was in the mid and late 19th century, some gruesome acts of unethical practices came into picture which underlined the necessity for developing set of guidelines monitoring the research practices. The experiments by the Nazi doctors which included the dreadful acts of keeping their prisoners in compression chambers and creating gun shots to analyze the response were the cruelest of all of them. Most of these experiments terminated with the death of the subjects. The hideous act by the German scientists of using the captive human subjects for experimentation questioned the credibility and morality of the scientific research and laid foundation and consensus for the fabrication of the key ethical principles. Further in 1950s-60s, the efficacious remedy for Syphilis was refused to the infected African-American participants. Such events led the states to take more interest in science and research thereby enforcing the re-examination of ethical standards. Further, this led to the formation of cautious rule and regulations protecting the human subject from being treated as 'guinea pigs' in scientific research. By 1990s, the kinetics had changed and people had become more aware. The ethical principles were no longer only confined to medicine and clinical research but had expanded its horizons to all vistas of research. The synthesis of chemical substances and their fate and utility became a question of debates and discussions. Man is a social animal always affected by the economy. Justice, character and efficiency became the three pillars of ethics in economics. The moral relationship between the man and environment became more intense in the beginning of 1970s. As a result, environmental ethics appeared as new sub division of philosophy. There are a number of articles in literature on specific topics elaborating subject based ethical guidelines, but an overall review is missing (to the best of our knowledge). As the world is becoming interdisciplinary and the research has become multifaceted, the aim of this paper is to bridge the guidelines governing the four major aspects of research. Starting from the synthesis of the new product, evaluating its clinical implications, measurements of its economical outputs to its impact in the environment is described in the present work.

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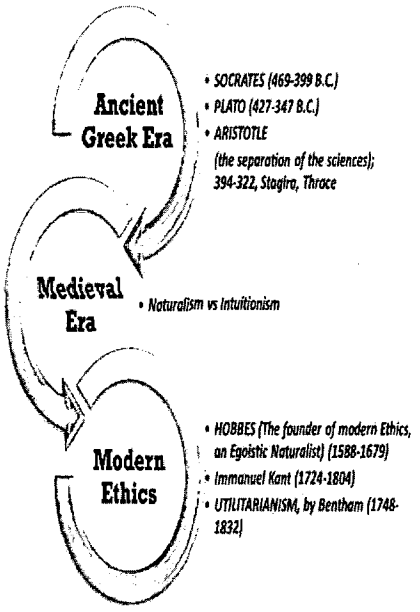

Figure 1 Flow Chart depicting different phases in History of Ethics (Rogers, 1911)

Ancient Greek Ethics: The ethical codes mark their origin from the 5th century B.C. with the itinerant teachers called Sophists. The words from parents and elders were the ethical tenets but as societies learned the power of writing words, they began to set down their ethical beliefs. Socrates, Plato and Aristotle laid the foundation of ancient ethics. It was centred on scepticism and egoism.

Socrates: ***(Athens, 469-399 B.C.)*** Socrates is known as founder of Science of Ethics. He raised his voice against the egoism of Sophists like Gorgias. He supported the virtue of knowledge. He strongly believed and supported his thoughts about the facts of nature, which are the basis of all knowledge (James, 2007). Socrates objected the unexamined, traditional values of the aristocrats. The dubious practicality of the commercial class came to light. The focal point of ethical philosophy was questioned by Socrates. Both aristocratic and marketplace morality faced his logical criticism and catastrophic fate.

Plato: ***(427-347 B.C.)*** Plato was the student of Socrates at the Socratic schools of thought. Plato (Austin, 2016) established an organised pattern of God, nature and human, which became the genesis of his ethical ideologies. He laid four paramount virtues associating to the "STATE"; Wisdom, Fortitude, Temperance and Justice. An ideal ruler is symbolic of an ideal state, according to him. He was philosopher, a lover of wisdom, and a perfect combination of intellectual insight and practical comprehension.

Aristotle: ***(384-322, Stagira, Thrace)*** Aristotle (Trompoukis,2007) illustrated "Political Science" as superlative of all sciences. He stimulated the naturalistic traditions with great value in the fundamental needs, liabilities and potential of man. He gave the idea of the separation of the sciences.

Medieval Era: Stoicism and Neoplatonism framed a new era in history of ethics and gave rise to Christian philosophy. The Stoics laid emphasis on justice and promoted self-mastery. On the other hand, the Neoplatonic supported the ancient Jew's belief in personal God. The divine rules were the primitive source of moral authority and following them was the goal of human life. The philosophies saw neck to neck with each other which lead to tense and conflicted interpretations of theological principles. In modern era, there were primarily two schools of thought:

- Naturalizm: Ethical ideas arise from and natural laws.
- Intuitionism: Ethical ideas and obligations are intuitive.

Early Modern Ethics: Philosophy blossomed when the preconceived notions of morals and culture were shaken in periods of rapid social transformation. The basic concepts, principles, and standards of values, all were redefined in this Era.

Hobbes (1588-1679): Hobbes was the founder of modern Ethics and an Egoistic Naturalist. Traditional notions were challenged by Galilean natural science. But they were supported by authority and strategy casting doubt on the basics of natural law. Hobbes described Philosophy as a game of cause and effect (Manent, 1994) i.e. the anticipation of effects by the knowledge of causes. Hobbes underlined principle is Exclusive Egoism (Ego being the "soul"). He brought forward the approach of equality of all humans. They all possess equal powers of self-defence and he proclaimed that men are in war with men. Nothing is right or wrong, black or white. The two virtues of Force and fraud are in war and when they become rational, peace comes. Without social harmony happiness is impossible.

Immanuel Kant (1724-1804): The modern ethics define themselves with the name of Immanuel Kant. The attack on the natural laws and tradition by the ethics driven by authority in favour of individual reason took a non-utilitarian form. "Duty" and "Self-love" were the two cardinal virtues of Kant's teachings. It is the criteria of action that ought to be obeyed by all rational means, under all situations and for its own sake. The laws are independent of the people. Kantian emphasis on "Categorical Imperative" and advocated the need of the persons to act on those principles. Diligent adherence of these principles will make them a universal law.

Kant based his theory on three postulates of morality

- The presence of lord
- The liberty of will
- The endurance of the Soul

Rational intuition is known by general principle and duties that can never be doubted. He ascertained that man could do what he ought to do but unless he knows what he ought to do, he cannot do it. He also stated that a collision of duties is impossible. Morality of action is driven by motive not the effects.

Utilitarianism: Utilitarianism is basis of ethical standard that is focused on "great happiness" of the people in general. It was founded by Bentham (1748-1832) and further followed by Stuart Mill and Sidgwick. Nature placed human under the domain of two masters i.e. pain and pleasure. It is matter of their choice what they want to opt for. To make a choice or to disapprove and approve every action i.e. indirectly related to happiness of party is governed by principle of utility. How can we measure the pain and pleasure? There are many factors affecting these emotions. The personal pleasure is measured by time span, intensity, positively, affinity, purity (freedom from pain). Second comes the community, it follows like how many persons are there to share your pleasure. Equality according to Bentham is the seventh measure. In his terms, "everyone is to consider equal irrespective of anything".

So, it is true if pure ethical concepts are not applicable to real-life problems persisting in society then they are useless. The basis of applied ethics is to deal with more concrete subjects like State/Politics, Family and Profession. There is a very small invisible difference between applied and pure Ethics. To achieve social good, the special interests of human should be regulated. But the question is "How'? Here the actual fundamental problem of applied ethics comes. In actual practice, the individual has to use its own sixth sense to make a right judgment, i.e. to construct his own system of Applied Ethics. The complete knowledge of ethics history and pure ethical theory helps the individuals to evaluate right and wrong in practical life. Science and Research, Economics and Environmental ethics are parts of the Applied Ethics that will be discussed thoroughly in further sections. Although there are many other spheres of ethics like Arts, artificial intelligence, business, geology, law etc. but they are out of scope of this paper.

Chronology of Ethical Guidelines

The following are the Ethical guidelines constructed on the basis of incidents that occurred in past and were not acceptable in any aspect. Table 1 summarizes the Ethical guidelines.

Table : Ethical Guidlines

1.	 Nuremberg Code	1947	∘ Official permission of the individual is absolutely essential. ∘ Research designs for qualified researchers. ∘ The ratio: Risk/Benefit should be acceptable. ∘ No forceful practice on participant at any time and he/she should be free to move at any time.
2.	 WMA's Declaration of Helsinki	1964	∘ The well-being of the individual should be the priority over the interests of science and society. ∘ The consent letter is to be signed by participant only. ∘ Special attention is to be paid if participant is in dependent relationship with researcher. ∘ Placebo use should be limited. ∘ The research should be assessable to society to benefit others.
3.	 Belmont Report (USA)	1979	∘ Respect for individuals: proclaiming respect for persons as autonomous agents with self-reliance. ∘ To protect persons from harm and to maximize possible benefits and minimize harms. ∘ Selection of subjects: Justice
4.	Council for International Organizations of Medical Sciences	1993	∘ Official permission ∘ Safeguard: Vulnerable population ∘ Burdens and benefits should be distributed among population ∘ Ethical committees should know their role and responsibilities

Ethics, an essential dimension of human research, is defined by the scientific community as guidelines to administer their professional strivings. It is considered both as discipline and practice in harmony with each other. Sincere perusal of the principles of education, mentoring, experimentation, review and submission of results delineates the ethical demeanour. Ethics demand the credential sample fabrication, precise and reproducible sampling of data, accurate measurements and reporting,etc. It acts like a selectively permeable membrane separating the moral and the immoral. Technical faults in the research design, wrong recruitment process, insufficient sample size, and weak statistica analysis of the data often lead to non-publishable research and are considered ethically punishable.

Meta-ethics, Normative ethics and Applied ethics are the three zone of ethics. 'Meta-ethics' works on the basic understanding of the ethical principles along with their accessible social invention and their origin from individual emotions. Normative ethics have been particularly significant in unfolding the of drug policy. Where, applied ethics is the examination of precise controversial actions/issues using the concepts of meta-ethics and normative ethics. They try to resolve these issues by applying the concepts. This indirectly means that an individual's behaviour or judgements can be considered wrong even if quite sufficient and acceptable outcomes are obtained.

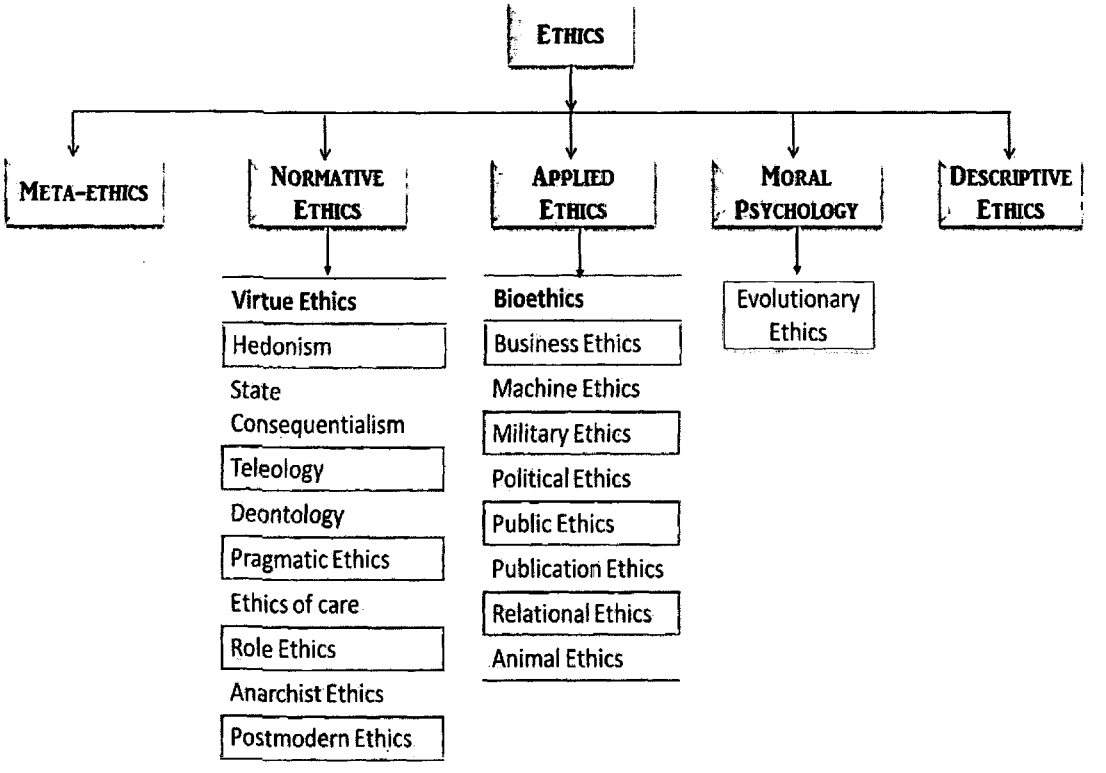

Figure 2 Types of Ethics

Ethics, a necessary evil for Synthetic Chemists

The field of chemistry has allowed mankind to conquer diseases, has enabled modern lifestyles, and has generated new industries. Fabrication and synthesis is the heart of research in all fields of science. Although chemistry has underpinned progress across various disciplines and in various areas but at the same time synthesis of novel chemical compounds raises numerous ethical questions generally neglected by chemists. The fate of these synthesized products sometimes cast a doubt and is questionable in their commercial worth. The primitive Bohr's quadrant model was based on the basic research where the eventual application was not considered. But with the evolution of research, need and application became the basis, leading to more objective Pasteur's and Edison's quadrants (Stokes, 1997). Here, the synthesis is stimulated by the practical use of the pristine substance. The synthetic research flourishes and amplifies with the manufacturing of novel compounds leading to the expansion of the library of new compounds. However, novelty also leads to uncertainty. On one hand, it intensifies the inquisitiveness thereby the research blossoms, while on the other the unpredictability and risk factors also elevates. The potential risks associated with creation of new substances are often ignored which sows the seeds of requirement of ethics in chemical synthesis. The fundamental understanding of a particular subject/chemical compound is profitable for research and is of vital importance. But the complications regarding chemical synthesis is always a matter of concern. Perhaps there is a possibility that a synthesized compound is an effective explosive or a precursor to such a substance or neurotoxin. So, there is nothing which can be said with certainty, so basic research is of vital importance which enlightens the community with good and bad outcomes. Roald Hoffmann annotates, "There is no fun in invention or practising something prior considering its use, that is purely a waste of time and resources" (Hoffmann, 2012a). In chemical synthesis, there are numerous ethical questions like the very question is; "What is the application of synthesized compound"? In modern society, at least six wide range of categories of chemicals exist (Fig. 3). Within this broad category of chemicals, there are many other types of chemicals which chemists try to make without being aware of its effect on humans and its economic value. He is even not aware of its effects on environment. Although research must continue and novel compounds with unique properties is the demand of progressing research but its effect on humankind and environment should not be ignored. Rather, deep analysis of the repercussions in terms on economic outcomes, translations applications and environmental implications.

The decision is taken by considering science/research, economic and environmental ethics. All these factors will be considered separately if research is at laboratory, at governmental or university level where researcher has ample control over what she/he does or is it done at industrial level where the research design is dependent upon company policies. In this section, the ethical component is being discussed. Chemistry comes under the shadow of philosophers in applied ethics. The logicians are aware of the ethical values regarding chemistry such as ill effects on environment, chemical hazardous impacts on human, chemical accidents etc. According to community, chemistry seems to equate with all evils. However, logicians found no link of these issues with the chemistry. Chemistry is like any other subject which has equal importance. It is dependent upon the interactions, behaviours, and aspirations of each one in order to work properly. Each social system has a set of rules i.e. compose of behavioural norms that means a code of practises which governs acceptable and unacceptable behaviour.

But the question is how these ideas relate to science. The relationship is quite simple; science includes humans directly or indirectly which are related to numerous decisions. To exemplify, development in science depends on the honesty of those researchers who report the experimental results as these results are key to the understanding of natural phenomenon under investigation. Ethics demand the credential sample fabrication, precise and reproducible sampling of data, accurate measurements and reporting, etc. The scientific results are actually accessible to all so the results should be reported with honesty. If the results are not reported honestly, then the follower who carries the reported experiment and try to work on it has wasted his/her time and other resources on it and his/her trust is violated. But when the results impact a field like medicine or it comes to product safety or environment safety, a number of people life are at risk because finding are made relying on the false information. Personal gain at the expense of others is ethically not acceptable.

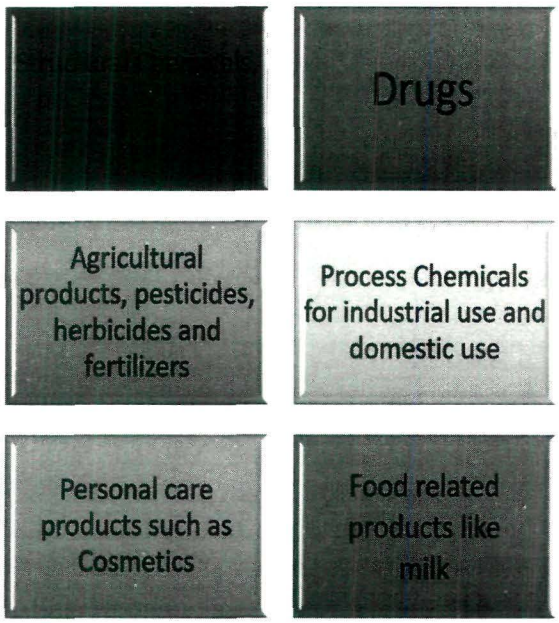

Figure 3 Six broad categories of chemicals prevailing in modern society

So, it is the responsibility of scientific community that ethical decision making encompass a wide range of responsibilities like design of experiment, reporting of data and interactions between collaborators. It was first in 1994 that the American Chemical Society (ACS) started publishing a series of articles entitled "Ethical Guidelines to Publication of Chemical Research" in ACS journals (American Chemical Society, 1994). The guidelines were revised in January 2000 which defines the ethical obligations of each and every participant in scientific community who is responsible for bringing a scientific publication to the community of editors, reviewers, scientists and general readers. The editors have greater share of responsibility because they need to give an unbiased consideration to all scientific reports submitted for publication in a timely and fair manner. After the editor, reviewers must also be sensitive to conflicts of interest for instance; a reviewer should not be in close relationship with the person whose manuscript is to be evaluated or a relationship which would otherwise force him/her mentally to take a bias judgment in reviewing the manuscript honestly. It is also the duty of authors, those have the privilege of reviewing unpublished results should not disclose that information prior to the publication. Authors are obliged to report an accurate and honest work with enough information so that reviewers and readers can properly evaluate the results reported in manuscript and reproduce them.

Let us analyse a case in history: The case involving the synthesis of Agent Orange and various effects related to it can be examined to address the various ethical issues. The history of Agent Orange and its dioxin contamination was of prime importance as it was used as a constituent in herbicides for agricultural usage and also in Vietnam. The unsolicited side reaction was of utmost concern as its contamination led to severe complications to mankind as well as to the environment. A chemist has synthesized a groundbreaking and an earlier unexplored compound without prognosticating its applications but with an exclusive and pragmatic motive of a new and innovative fabrication. Now, further let us presuppose that the talked about compound comes out to be pernicious and somebody pilfers or pirates its synthesis from the laboratory and utilizes that compound with the purpose to harm people. So the big query now is: Who shall be answerable for it? The moral conclusion not only challenges the individual chemist who synthesizes new compounds/substance, it is also a moral challenge to the whole community of synthetic chemists for which synthesis is actually an end in itself. The internal norms of that community aren't in accordance with the mainstream moral standards. This and the various obligations put forward by this community reflect their non-realization of the general moral responsibilities. They, on the other hand, erroneously label their activities as morally neutral. The ethical norms should be fomented in the researchers from the onset of their careers and the government should corroborate that the rules are followed with paramount sincerity and these recommendations should foster and enhance the quality of research.

Ethics in clinical research

Any novel potential therapeutic agent or technique becomes a drug or an accepted treatment only after successfully undergoing the clinical trials. The exposure of the gruesome, horrendous and inhumane conduct during such research experiments in the Second World War lead to the fabrication of ethical guidelines. Although we do agree that trials on humans are necessary to verify the actual effect of the therapy but risking the lives of some vulnerable individuals to inspect and scrutinize the adequate conditions for the betterment of the society is objectionable and atrocity. The ethical committees consolidate the gap between the investigators and the ethical protocols of the country. The ethical board establishes a self-reliant and skilful determination of all ethical facets. It shields the virtue, rights, benefits, comfort and wellbeing of the research subjects. Research ethics are mainly concerned with the research participants who act as subjects to improve the human health by being test subjects to new and better treatments and cures. It takes into account the benefit of the society at large. Ethics is a meticulous approach to segregate true from the fallacious.

India is a country with pregnable, uneducated and unaware audience. So the virtual reality of ethics needed a concrete structure. To safeguard the rights

of the research subjects, the first official guidelines were released by The Indian Council of Medical Research (ICMR) in 1980. With time, the improvement in the guidelines were done by Council for International Organization of Medical Sciences (Council for International Organizations of Medical Sciences, 2016). These were a common set of rules for establishment of ethical committees covering all medical colleges and research centres in world. But, sadly there are still hundreds of reports exhibiting the controversial research and abatement of these guidelines. A famous controversy exposed at the Institute for Cytology and Preventive Oncology (Srinivasan, 2005), New Delhi in 1980s where as a result of experimental study conducted on 1158 women, 71 women developed malignancies, 9 suffered and died of invasive cancer. Incidents like these reflected the ambiguity of the earlier existing rules and 'Ethical Guidelines for Biomedical Research on Human Subjects' were formulated and finalized in the year 2000. With the changing milieu and the protocols were revised in 2006. These guidelines serve a four dimensional purpose of safeguarding respect for person, philanthropy, neutrality and fair play by obscuring twelve general principles. Now the question arises, are these guidelines act as stumbling blocks in the path of advancement of research? How should the research be conducted? The research should be planned and executed in such a way that benefits the patients and the doctors alike. All the aspects of health care should be keenly envisioned. The ecological and environmental aspects should also be given identical weightage because the wellbeing of the planet is the first and foremost responsibility of every man alive. The volunteer should be well aware of the nature, complexity and predictable repercussions of the experiments. It should be an impartial and unbiased decision without the influence of the treating doctor. Also, extreme care and cautions should be taken at each stages of the research from its initiation to the formulation of research design and finally the conduct of the research to prevent research participant from any harm and adverse events.

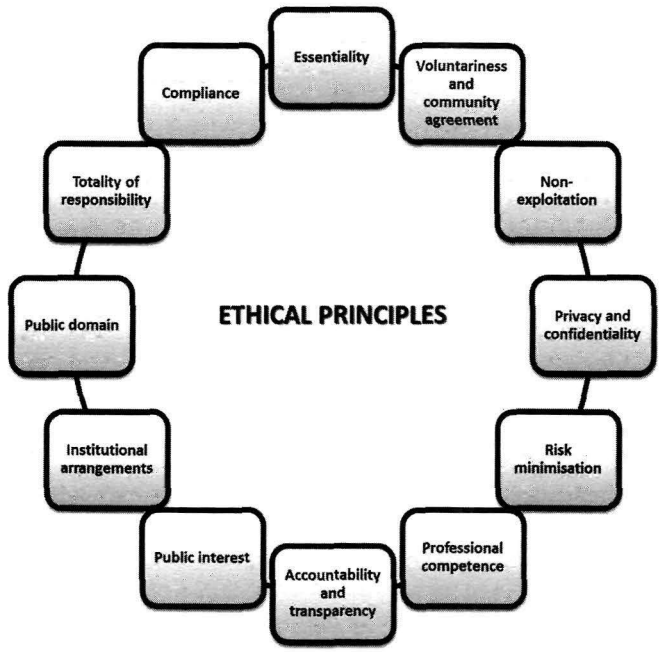

Figure 4 Principles of Clinical Ethics

The ethical committees help in risk minimization and permits only highly competent and well qualified persons in their respective field to conduct clinical research. But it is the inner conscious of each researcher which makes these guidelines successful. The researcher should conduct experiments in fair and transparent manner after complete revelation of his/her interests in research. The research data should be retained for at least 5 years, and the principles of privacy and confidentiality should be followed. The results of the research should be used for benefit of all humans in general and the research participants themselves in particular. The community at large should be at the receiving end and not only to those who are socially better off.

Ethics and Economics: Rivals or Supporting Companions

Although it is a common notion that ethics and economics are the two sides of an ever expanding river which never meets. The society always depicts the troubled relationship between the two and the general public remains under the false impression that economics is all about making and multiplying wealth. But the true reality is that economics is an integral follower of ethics. It involves the decision making under the realms of social environment with coherent and calculated self-interest. The relation is strained due the inherent difference in the thinking lines of ethical philosophers and Ethicists. Ethicists considers economists to be obsessed money makers with low regard for the general good and morality while ethicists are the protectors of explicitness and fair society. The controversy is incessant but when understood properly, ethics and economics are the two sides of the same coin. Economics is all about ethics; it involves the management, understanding and fulfilment of a large population with diverse ideas, interests and values. It stands on the triad of Justice, Character and Efficiency. The assessment in economics is done keeping in mind the social relations and divergent criteria and aspects of ethics. This fortify the point that ethics is an integral part of doing economics

Now the interrogations are based on the question, "Are economists only driven by self -interest? The rebuttal to this question is NO! It's the "Rational Self-Interest". Economics administer strategic and procedural support to ethics. It weighs the unplanned but accountable consequences of the actions. Economical modelling tests the strength of the ethical principles and makes the moral reasoning more practical and financially beneficial. It ensures better Utilitarianism. It adds rationale to moral values. There is therefore a comprehensible difference in the ideologies but the ultimate purpose of benefiting the society at large remains the same.

Ethics in environment

Environmental ethics is a branch of ethics that learns the moral relation of human with the environment. This section is focussed on how ethics play its role in evaluating the relation. Environmental ethics consider humans are a part of community as other living creatures, which includes animals and plants. Actually, it is a department of applied ethics that studies the conceptual foundations of environment values. It also concentrate on issues surrounding the societal attitudes, actions and policies to assure the safety of bio-diversity and ecological systems. The environmental ethics cover issues that deals with the rights of individuals that are fundamental to life and well-being. Figure 5 elaborates upon the regions that are covered by environmental ethics.

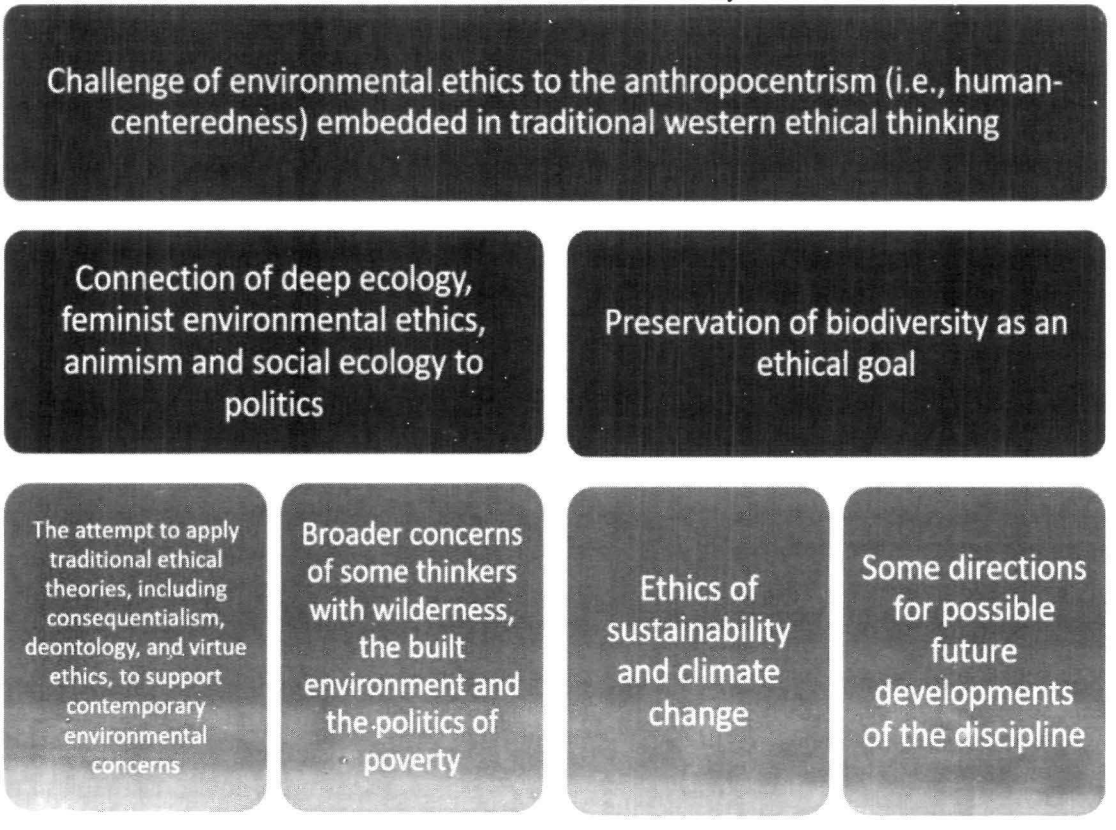

Figure 5 Regions covered by environmental ethics

Let us assume, putting out the natural fires, culling wild animals is essential for the preservation of molarity of certain ecosystem. But there is a question "Will these activities be morally permissible or even required?" Is it morally agreeable for farmers in countries to practise slash and burn techniques to clear their areas of farming? Is it acceptable if a mining company execute open pit mining in an area which is not meant for that purpose? This give arise to moral questions that actually originate by these kind of practices occurring in the countries. The big question is "What is the value of humanly restored environment when it is compared with originally natural environment?" Deforestation is one of the major issues persisting in the society which is creating nuisance to environment, animals and human being themselves. Global warming is primarily caused by human beings as they are actually responsible for increase in carbon dioxide into the environment.

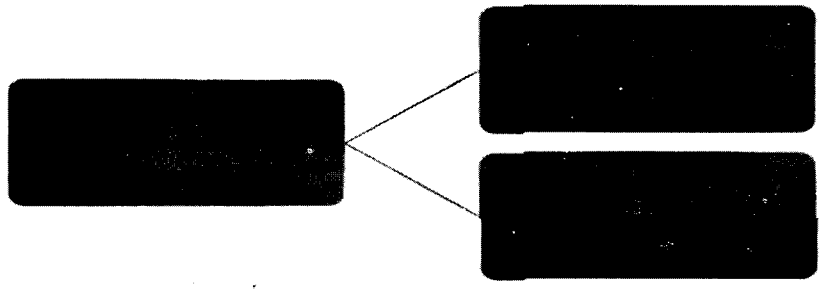

Figure 6 Type of ethics in environment

The above mentioned activities are incorrect and solution to above problems is sustainable environment which is the need of the hour i.e. present as well as future. The environment has certain values in their hands so that these values should be respected and protected in any case. The origin of environmental ethics emerges in early 1970s. It occurs by posing a claim to historic anthropocentrism. At the first, it questioned the supposed moral superiority of humans to other living beings on earth. (Fig. 6) Then the second one, it inspected the feasibility of rational debates for appointing intrinsic charge to the natural environment and its non-human ingredients. Briefly, this is the prospective that all the moral values that we have towards the environment are derived from our responsibilities to human inhabitants.

Let us assume that day-to-day non-anthropocentrist tends to act more generous towards the non-human environment on which human well-being depends. This is the main reason to boost non-anthropocentric thinking. It is acceptable to those who really thinks that the concept of non-anthropocentric intrinsic value hard to swallow.

Environmental ethics build on scientific understanding by uplifting human values, moral principles and improved by making judgments regarding conversation with science. It was the "Earth Day" in 1970 which marked to develop environmental ethics in developed and non-developed countries. This is very much important because ethics regarding natural environment are major concern these days. In today's scenario, environment ethics have a major interest for the mankind. "Industrialization" has risen pollution which imbalances our ecological balance. If the industry is creating such kind of problems, it is not only their duty but also humans has to make up for the losses. All the answers to the problems are very difficult to find but environmentalists are trying their hard to find it.

The answer to all these questions lies in the concept of sustainable development which can help to achieve the goals in environmental ethics. Sustainable development is development that meets the needs of the present without negotiating the ability of future to meet their present demands. There are number of common principles embedded in action plan to achieve sustainable development. These include:

1. Dealing transparently and systematically with risk and uncertainty.
2. Living within environmental limits
3. A sustainable economy
4. A commitment to good practise
5. Create a global alliance
6. No net loss of human capital
7. Ensuring a good, healthy environment within the society

Thus the goal of sustainable development is much more than the environmental protection because it is joint collaboration of scientists, economists and ecologists by parallel care of ecosystem. Interpretations will vary but we must flow from a general agreement on the basic concept of sustainable development and on a broad framework with an aim to achieve it. (Routledge, 2012)

Headway in Ethics

Ethics and morality touch all walks of human life starting from the fundamental of protection of well-being of human subjects, to the modern day ethics of protecting the mother earth. The future of ethics caters the debatable questions of sustainability and social justice. The tree of research will only bear fruit if nurtured with the water of honesty and sincerity. The ethical guidelines act as sunlight which shines alike on the researcher and the receiver (society). These guidelines should not be taken as stern protector, but these should become the way of living. We should leave the planet better than how we received it from our ancestors. Modernization and advancement should not define with pollution and global warming but the God given intelligence should be amalgamated with morals and ethics to produce a better, cleaner and peaceful planet earth. At the end, liberty of research is dependent upon freedom of moral choice.

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SEASONAL VARIATION OF PHYTOPLANKTON ASSEMBLAGES AND ITS RELATION TO ENVIRONMENTAL VARIABLES IN A FRESHWATER LAKE SITUATED IN THE ZOOLOGICAL PARK, CHATTBIR, PUNJAB, INDIA.

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Abstract

Seasonal variation of phytoplankton assemblages was examined in a natural freshwater lake (India) with regard to some major physical and chemical variables. Samples were collected at three stations from October 2014 to September 2015. A total of 26 species of phytoplankton were recorded, represented by diverse groups comprising Cyanophyceae (7), Chlorophyceae (12), Bacillariophyceae (4), Xanthophyceae (1), Zygnemophyce ae (1) and Trebouxiophyceae (1). This indicated diverse nature of phytoplanktons in general as well as of the lake in particular. The order of dominance was Cyanophyceae> Chlorophyceae> Bacillariophyceae. The Shannon-Weiner diversity index was higher in autumn (2.58) and the lowest in summer (0.5) whereas Berger Parker index of dominance showed maximum dominance during monsoon (0.89) and minimum during pre and post monsoon (0.31 and 0.33 respectively). Results of Pearson's correlation showed that nitrate, phosphate and water temperature were the most important environmental factors influencing the variation of phytoplankton community structure. It is suggested that changing water temperature and availability of nutrients may lead to dominance of one particular species leading to toxic algal blooms.

Key words: Phytoplankton, seasonal variation, abiotic, allelopathy, water bloom.

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1. Introduction
2. Materials and Methods
   - Study area
   - Physicochemical analysis
   - Biological parameters
   - Statistical analysis
3. Results and Discussion
   - Abiotic parameters
   - Phytoplankton composition
   - Diversity indices
   - Relationship between physicochemical characteristics and Diversity indices
4. Conclusion
5. Acknowledgement
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INTRODUCTION

Lakes are important component of inland aquatic resources of India, especially because of their potential for fishery. Despite the ecosystem services they provide, their biological diversity has been poorly investigated. Biological diversity (biodiversity) refers to the degree of variation of life forms within a given species, ecosystem, biome or planet. Phytoplanktons are sensitive aquatic organisms, and their community structure can reflect the eutrophic status of a waterbody (Oberholster et al., 2010; Serrano et al.,

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2010; Marwood et al., 2011; Yates and Ragers, 2011; Weithoff and Gaedke, 2016). Moreover, algae species occur in a wider variety of waters (at least a few can be found in almost any condition) and their distribution is cosmopolitan (Ahluwalia, 1993; Beyene et al., 2009; Renuka et al., 2014). Therefore, the phytoplanktons are often used to estimate the impact of aquatic ecosystem (Walsh et al., 2001; Omar, 2010; Pomati et al., 2017) and it makes use of the sensitivity of plankton to envirionmental change as an early warning indicator of the health of the aquatic ecosystem (Hosie et al., 2003). Algae are even suitable for monitoring very extreme conditions where other types of organisms are absent (Taylor et al., 2007; Kohshima et al., 2007; Riedel et al., 2008; Holzinger and Karsten,2014; Hallmann et al., 2016). In order to find a way to solve the environmental problems of nutrient enrichment and eutrophication and to develop new tools for building restoration strategies in the lake, it is necessary to understand the processes of plankton production and bioresources (Huang et al., 2004).

MATERIALS AND METHODS

Study area

Chattbir zoo lake is situated in Mahender Chaudhary Zoological Park, Zirakpur, Punjab, India at longitude- 76.7928° E and latitude- 30.6036° N. (Fig 1) The total area of the lake is approximately 20,416 square meter, with maximum depth of 8m. Lake is a source of drinking water for many wild/zoo animals and an important habitat for migratory birds. Two seasonal inlets and one perennial outlet exist with definite boundaries bordered by thick patches of macrophytic vegetation.

Algal sample collection was done by Random Sampling Technique for which three sites were selected on the basis of water inlet and outlet of the water body.

Physicochemical analysis

Water temperature (WT), pH, Electrical conductivity (EC) and Total Dissolved solids (TDS) were determined in-situ employing various instruments. The samples were stored in plastic containers for analysis of chemical characteristics and for measuring other parameters. In Laboratory, nitrate (N), phosphate (P), sulphate and total alkalinity were measured using standard methods (APHA,2005).

Biological parameters

For taxanomic determination of phytoplankton, water samples from each site were collected. The water sample (one liter) from each site was also fixed with Lugol solution for phytoplankton identification and counting in the laboratory. The fixed samples were enumerated and counted using a Sedgwick-Rafter counting slide on a light microscope as per procedure given by Wetzel and Likens (1991). The samples were allowed to settle in the counting chamber for 3-5 min prior to their enumeration. More than ten fields of view were randomly selected across each slide and the process repeated three times with different microscope fields.

Statistical analysis

Mean values, standard deviation and standard error from different replicates per treatment (n=3) were calculated. Correlation coefficents were calculated using Statistical package for Social Sciences (SPSS16.0) and analyzed for their significance using Pearson's tables.

RESULTS AND DISCUSSION

Abiotic Parameters

Monthly variations in physic-chemical parameters of Chattbir Zoo Lake are depicted in Table 1. The seasonal changes in phytoplankton productivity are related to variation in temperature and the nutrient conditions. Maximum temperature was recorded during July and August and minimum in December and January. The variation in the water temperature may be due to the difference in sampling time and the season (Jayaraman et al., 2003; Tiwari et al., 2004; Renuka et al., 2014).Similar observations were also made by Lv et al., (2014); Spencer and King (1989) and Chen et al.(2016). Temperature is an important factor, which regulates the biogeochemical activities in the aquatic environment. Water temperature influence aquatic weeds, algal blooms (Zafer, 1968) and surrounding air temperature (Gupta and Sharma. 1993). All metabolic and physiological activities and life prcesses such as feeding, reproducting, movements and distribution of aquatic organisms are greatly influenced by water temperature. The pH of lake water varied from 8.5 to 9.4 (alkaline eange) with a minimum in march and maximum in November to December. Wani and Subla (1990) reported that the pH values above eight in natural waters in a result of high photosynthetic rate that demands more carbon dioxide than quantities furnished by respiration and decomposition. pH is one of the most important factors that serves as an index of pollution. pH value of majority of lakes and reservoirs in India has been found to be between 6 to 9. The higher range of pH (alkaline) indicates higher productivity of water (Khan and Khan,1985).

The maximum electrical conductivity (EC) was observed in May and minimum in September. High

value of EC indicated pollution status of the lake (Kadam, 1990). Throughout the investigation period, a relatively lower value of TDS was recorded in September (216.6 mg/L), and higher value in the month of June (353.3 mg/L).

The presence of higher amounts of nitrogen (1.82 mg/L) and phosphorous (28.3 ug/L) indicate a eutrophic nature, leading to subsequent algal blooms. High nitrate values in the water body indicated higher biological productivity. The presence of inorganic phosphorus at 30 ug/L concentrations is sufficient to cause algal blooms (Sheela et al. 2011). The range of phosphorous to the tune of 2-28 ug/L during the year of study clearly indicated eutrophic nature of the lake. Significantly higher values of alkalinity were also observed throughout the investigation period (Tables 1). Das et al. (2009) have concluded that high alkalinity indicates pollution of a water body.

Phytoplankton Composition

A total of 26 species of phytoplankton (Table 2) were recorded. They were represented by diverse groups like Cyanophyceae (7), Chlorophyceae (12), Bacillariophyceae (4), Xanthophyceae (1), Zygemophyceae (1) and Trebouxiophyceae (1) indicating diverse nature of phyto planktons in the lake. The order of dominance was found to be Cyanophyceae > Chlorophyceae > Bacillariophyceae (Fig2).

Cyanophyceae constituted the most dominant group of phytoplankton. The monthly per cent contribution of cyanophyceae on the basis of number of cells/ mL is shown in the Figure 3. Monthly per cent contribution varied from minimum of 0% (September 2015) to maximum of 92% (July 2015). The most abundant species in terms of population density were *Microcystis aeruginosa, Anabaena sp., Oscillatoria sp., Spirulina sp., Gloeocapsa sp., Chrococcus sp. and Merismopedia sparsa.*

Microcystis aeruginosa was recorded to be the most dominant species amongst Cyanophyceae. Cyanophyceae are more efficient in utilizing carbon dioxide at relatively higher levels of pH and thus their abundance indicates eutrophic nature of the water body (Lin, 1972).

Blue green algal (cyanophyceaen) was major portion of phytoplankton community during monsoon. The reasons behind this result may be the high temperature, alkaline pH, humid conditions and bright sunlight which create favorable conditions for better propagation of this group of phytoplankton (Fig 3).

Chlorophyceae formed the second most diverse group on the basis of number of cells/mL but it also had the most diverse number of species amongst all the groups. The monthly per cent contribution of Chlorophyceae in terms of population density amongst different phytoplankton groups at the selected site is shown in Fig 3. Monthly per cent contribution varied from a minimum of 6.3% (July 2015) to maximum of 80.8% (April 2015). The most abundant species in term of population density were *Chlorella sp., Monoraphidium sp., Scendesmus sp. and Tetraedron sp.*

Unni (1993) analyzed the data from a large number of studies and observed that the species diversity (50 to 100 species) of hypertrophic reservoirs is higher (and similar to that of tropical lakes in Southeast Asia) than that of the oligotrophic reservoirs (about 15 species). In a short term comparative study of nine south India reservoirs, Uhlmann et al. (1982) also observed surprisingly a large number of phytoplankton taxa (mostly green algae) evenin waters deficient in orthophosphate. A number of workers have reported some algal species as indiators of water quantity (Naik et al., 2005; Nandan and Aher, 2005; Zargar and Ghosh, 2006; El-Kassas and Gharib, 2016). Zargar and 7Ghosh (2006) in a study on Kadra reservoir of Kamataka listed few algal forms belonging to Chlorophyceae, Cyanophyceae, Euglenophyceae and Bacillariophyceae as indicators of water pollution. Progressive enrichment of water with nutrients leads to mass production of algae, which in turn leads to the increased productivity and other undesirable biotic changes.

Nandan and Aher (2005) had shown that species of algal genera, (*Euglena, Oscillatoria, Scenedesmus, Navicula, Nitzschia and Microcystis*) were found in organically polluted waters. Some of these genera were recorded in the present investigation thereby indicating that the lake is organically polluted. The epilithic and epiphytic algae are excellent indicators of water pollution (Round, 1965). In the present study, occurrence of *Oscillatoria* as epilithic algae and certain diatoms like *Nitzschia* and *Navicula* as epiphytics have been recorded. Thus, algal communities can be used as indicators of pollution for assessing the water quality of this lake of international importance. The alga like Microcystis aeruginosa was used as the best single major indicator of pollution and it was associated with the highest degree of civic pollution (Nandan and Aher, 2005). In the present study, *Microcystis* was also recorded as dominant form.

It is reported that excessive growth of certain algal genera, viz., *Scenedesmus, Anabaena and Oscillatoria* indicate nutrient enrichment of aquatic bodies (Kumar, 1990: Zargar and Ghosh, 2006). The present study on Chattbir Zoo Lake also supported the earlier findings. Studies show that the dominant phytoplankton and their seasonality are highly variable in different water bodies according to their nutrients status, age, morphometry and other locational factors (Gopal and Zutishi, 1998). The study revealed that the water quality parameters such as temperature, pH, nitrate and phosphate play a very important role in altering the phytoplankton distribution.

Diversity Indices

An important application of diversity indices in phytoplankton studies is their usage in the assessment of pollution. Species diversity is a function of species richness and evenness with which the individuals are distributed in these species (Margalef, 1958). For Indian lakes, the Shannon-Weiner diversity index greater than (> 4) indicates clean water; value between 3-4 is for mildly polluted water and value less than 2 (< 2) indicates heavily polluted water (Shekhar *et al.*, 2008). As, the Shannon-Weiner diversity index in the present study ranged between 0.4-2.58 for the study period (Fig. 4a), therefore, this water body is highly polluted. The maximum species diversity was observed during pre-monsoon and the minimum in post monsoon. The range of evenness was from 0.05 to 0.25 (Fig 4b). Berger Parker Dominance index (BPD) values ranged from 0.31 to as maximum of 0.89 (Fig 4c), so that an increase in the value of the index correlated with an increase in dominance by one particular species.

Relationship between Physicochemical characteristics and diversity Indices

The study revealed that water temperature had significant effect on diversity, richness, evenness and dominance of species. Water temperature exhibited a negative correlation with Shannon diversity (r=-0.563), evenness (r= -0.701) and positive correlation with Berger Parker index (r=0.335). (Fig 5 a,b,c). The dominance index exhibited a positive correlation with Nitrate (r= 0.407) and Phosphate (r= 0.667) (Fig. 6 a,b) that with increase in water temperature, N and P of water, dominance by single species increases.

CONCLUSION

The phytoplankton community in the freshwater lake showed distinct seasonal shifts at taxanomic level. The succession patterns of dominant taxa were different based on abundance. However, species of cyanophyta were mostly abundant during low temperature period and high humid weather and their dominance was closely co-related to other physicochemical parameters. Our results demonstrated that water temperature and nutrients availability together were the most important key factors in shaping the composition of phytoplankton community. Our findings further suggest that with the rise in water temperature, Shannon-Wiener index and Evenness decreases at the species level while Berger Parker Dominance index increases. Therefore, it can be concluded that changing temperature, and also availability of nutrients and other biotic factors altogether may leads to dominance of one particular species, resulting in algal bloom.

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DIVERSITY OF FRESH WATER NATURAL LAKE IN TERMS OF PHYTOPLANKTON AND ENVIRONMENTAL VARIABLES AND THEIR COORELATION

LEGENDS TO FIGURES:

Fig. 1: Location of sampling site

Fig. 2: Pattern of monthly variation in phytoplankton groups during the study period (Oct, 14 to Sep, 15)

Fig. 3: Monthly per cent contribution of different phytoplankton groups on the basis of number of cells of each group.

Fig. 4: Monthly Variations in Phytoplankton a) Species Richness (Shannon Wiener diversity) b) Evenness c) Berger Parker Dominance index (BPD)

Fig.5: Correlation between water temperature and microalgal diversity a) Water temperature (WT) and Shannon diversity b) Water temperature and Evenness c) Water temperature and Berger Parker Dominance index.

Fig. 6: Correlation between Dominance and a) Nitrate (N) and b) Phosphate (P)

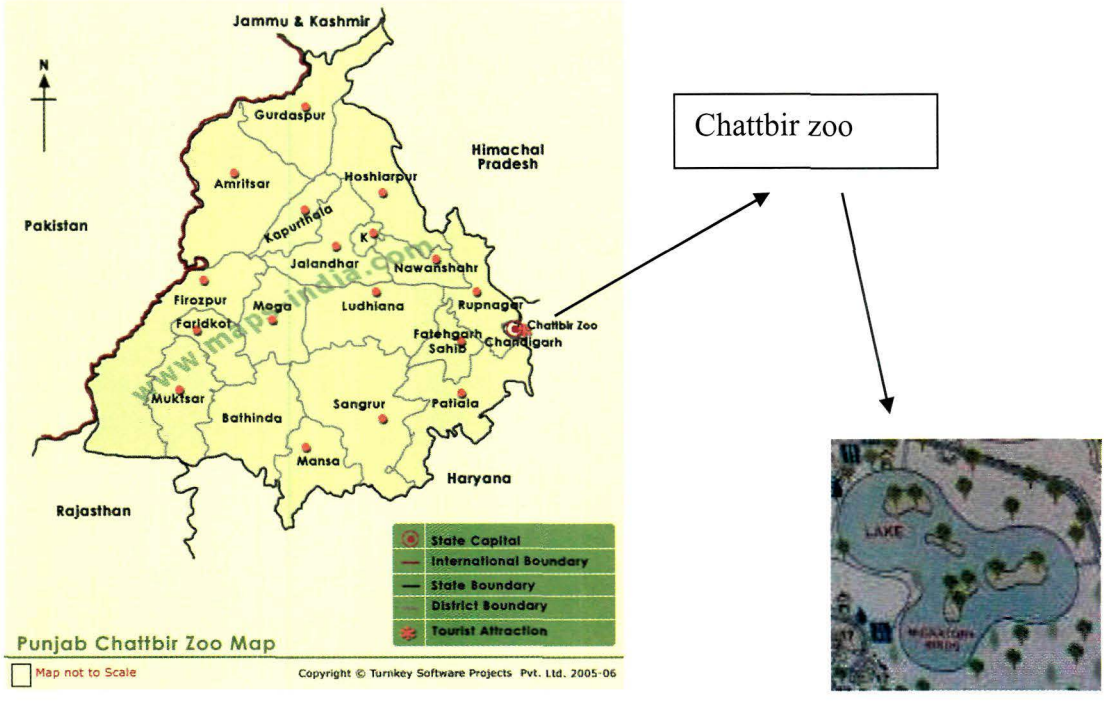
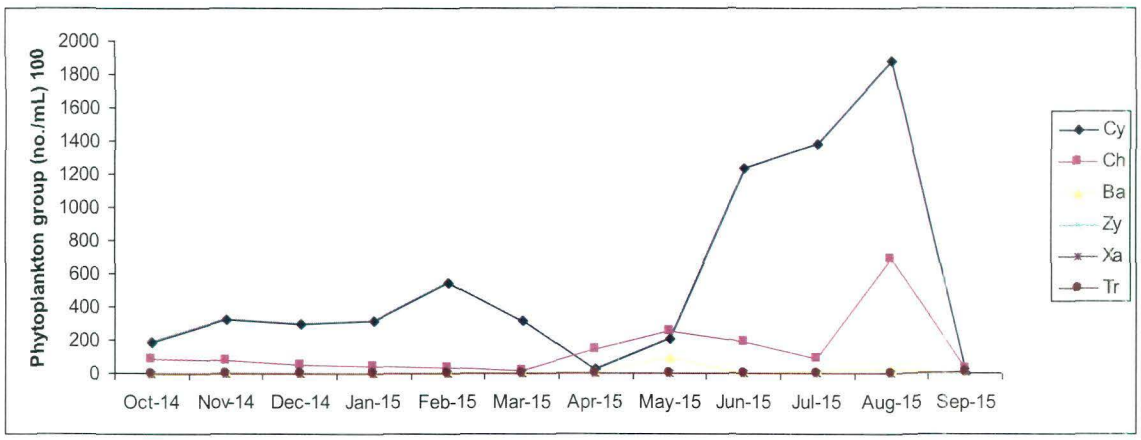
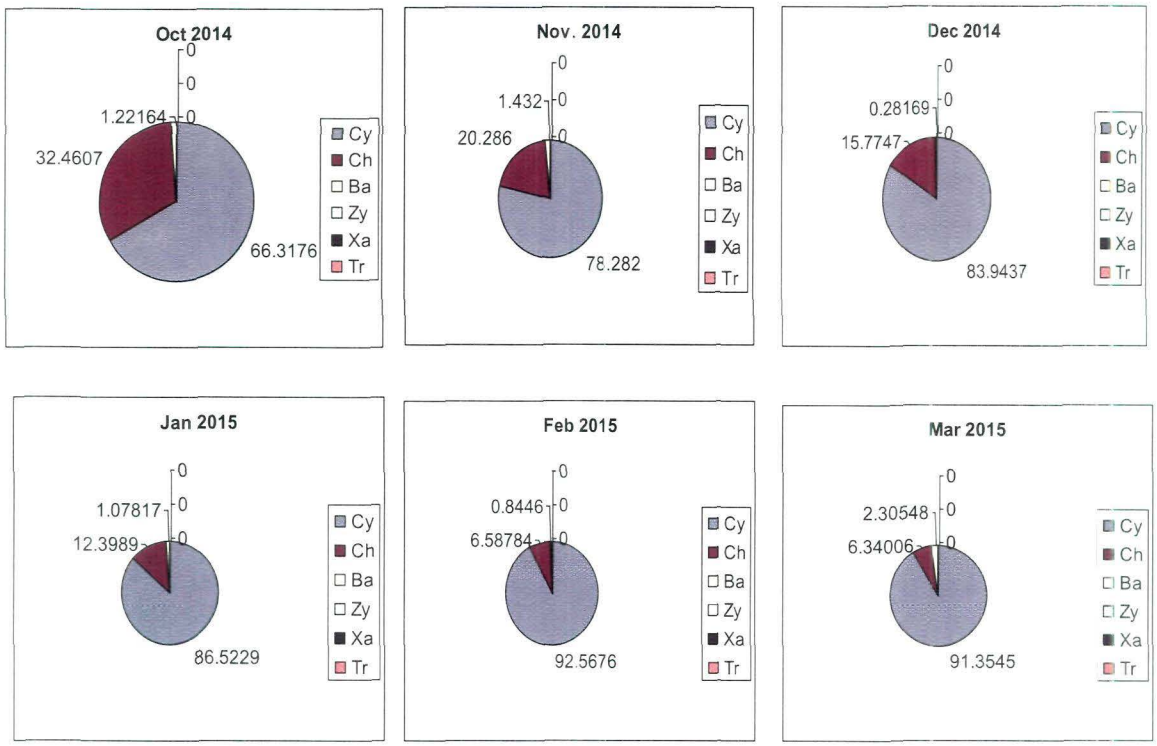


Fig. 1: Location of sampling site



Cy= Cyanophyta, Ch= Chlorophyta, Ba= Bacillariophyta, Zy=Zygnemophyta, Xa= Xanthophyta, Tr= Trebouxiophyta

Fig. 2: Pattern of monthly variation in phytoplankton groups during the study period (Oct, 2014 to Sep, 2015)



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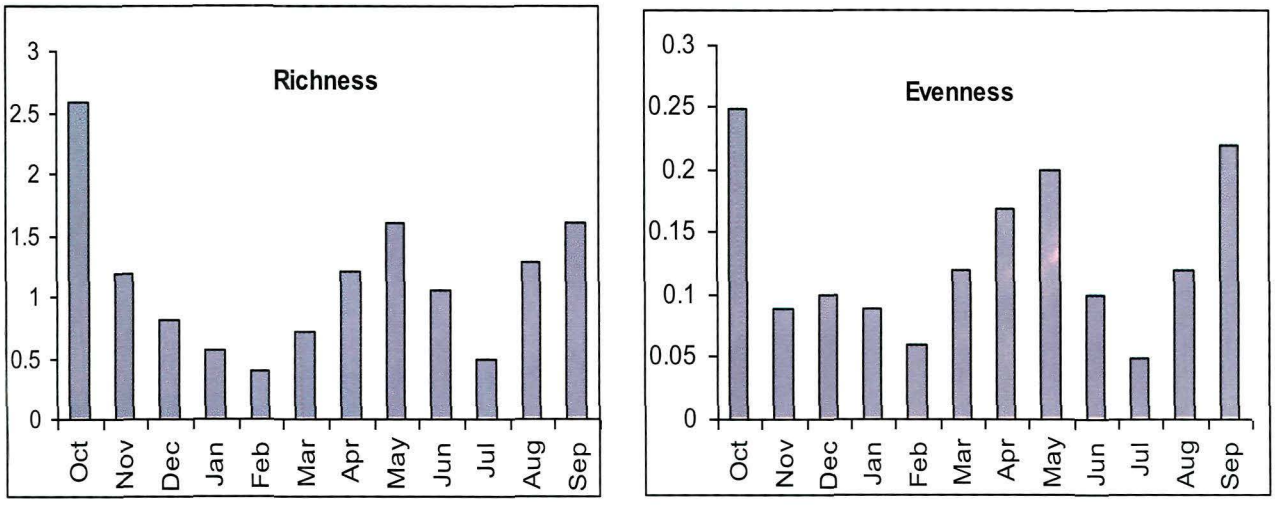
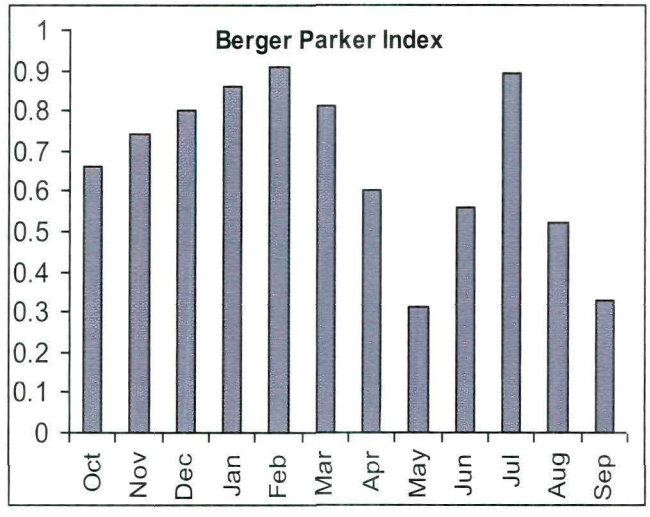
Cy= Cyanophyta, Ch= Chlorophyta, Ba= Bacillariophyta, Zy=Zygnemophyta, Xa= Xanthophyta, Tr= Trebouxiophyta

Fig. 3: Monthly per cent contribution of different phytoplankton groups on the basis of number of cells of each group.

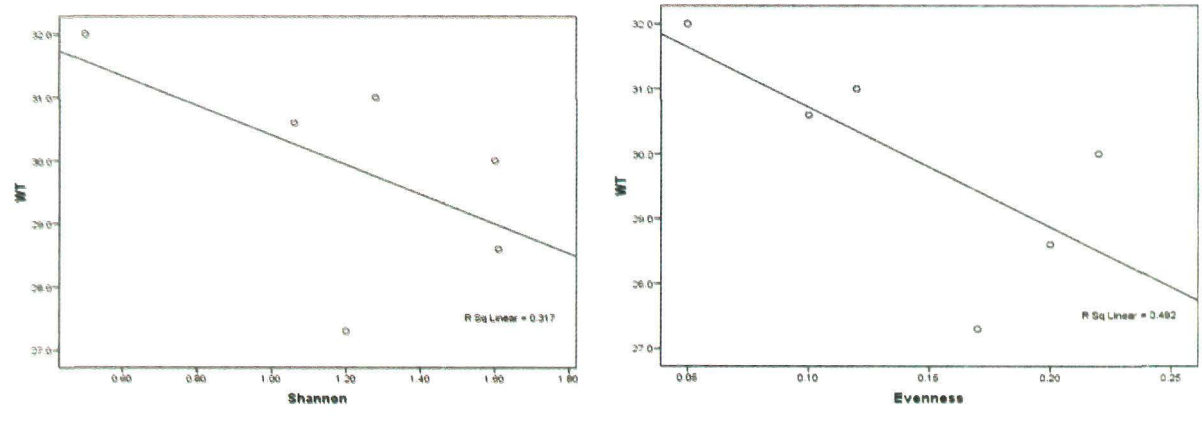


(a) (b)



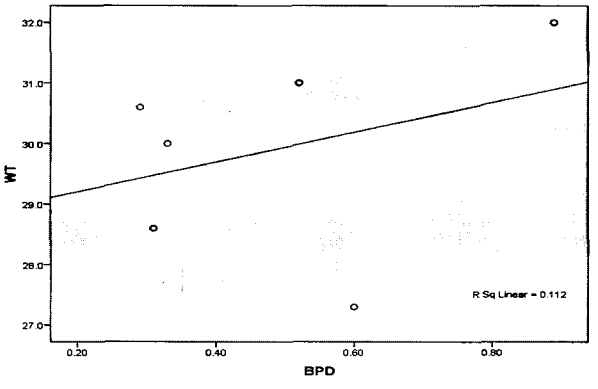
(c)

Fig. 4: Monthly Variations in Phytoplankton a) Species Richness (Shannon Wiener diversity) b) Evenness c) Berger Parker Dominance index



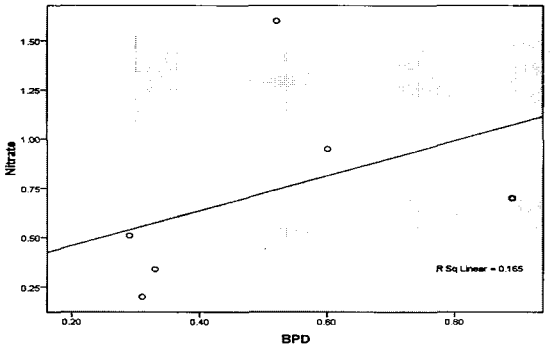
(a) (b)

DIVERSITY OF FRESH WATER NATURAL LAKE IN TERMS OF PHYTOPLANKTON AND ENVIRONMENTAL VARIABLES AND THEIR COORELATION

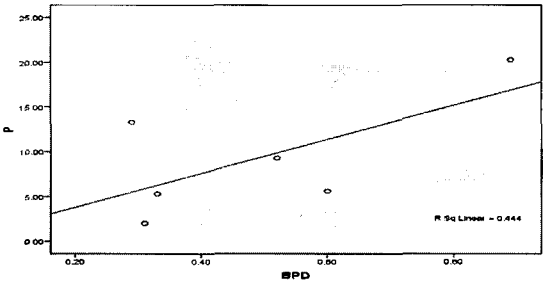


(c)

Fig.5: Correlation between water temperature and microalgal diversity a) Water temperature and Shannon diversity b) Water temperature and Evenness c) Water temperature (WT) and Berger Parker Dominance index (BPD)



(a)



(b)

Fig. 6: Correlation between Dominance (BPD) and a) Nitrate (N) b) Phosphate (P)

Table 1 : Physicochemical parameters of Chattbir Zoo lake water recorded during October 2014 to September 2015

Month	WT (°C)	pH	EC (μ S/cm)	TDS (mg/L)	Nitrate (mg/L)	Phoshate (μg/L)	Sulphate (μg/L)	Total Alkalinity (mg/L)
Oct-14	23.1±0.1	9.06±0.03	40.3±1.3	283.3±8.8	0.1±0.03	5±1	-	218.6±8.7
Nov-14	16±0.0	9.4±0.06	44.6±1.2	326.6±12.0	0.3±0.1	10.3±2.3	-	255.3±2.4
Dec-14	11.3±0.3	9.4±0.1	44.3±0.6	296.6±18.5	1.82±0.8	28.3±5.2	-	252±2.9
Jan-15	11±0.5	9.2±0.05	43.3±0.3	296.6±6.6	0.26±0.04	2.6±0.3	-	-
Feb-15	15.6±0.5	8.8±0.1	36.6±0.3	270±5.7	0.65±0.29	4±0.0	-	-
Mar-15	19.3±0.3	8.06±0.2	43±0.5	286.6±3.3	0.91±0.3	3.3±0.3	98.6±8.8	252.8±1.6
Apr-15	27.3±1.2	8.3±0.0	39.6±1.3	296.6±6.6	0.95±0.3	5.6±1.2	141.3±6.4	253.6±16.8
May-15	28.6±0.3	9.3±0.03	49.3±0.8	343.3±3.3	0.20±0.09	2±0.0	-	357.3±8.7
Jun-15	30.6±0.3	8.5±0.1	53±1.1	353.3±8.8	0.51±0.1	13.3±3.3	76.6±10.6	326.6±3.5
Jul-15	32±0.0	8.7±0.03	43.6±0.8	300±5.7	0.7±0.1	2.3±0.11	45.2±8.4	300±2.3
Aug-15	31±0.0	8.5±0.06	38±0.5	256.6±8.8	1.6±0.4	9.3±0.3	61.2±7.1	248±6
Sep-15	30±0.0	9.2±0.03	30.6±0.8	216.6±3.3	0.34±0.01	5.3±0.6	143±16.2	214.6±2.6

n=3, mean±SE

Table 2: Monthly variations in population density of phytoplankton in Chattbir zoo lake, Punjab from October 2014 to September 2015.

Months	Oct 14	Nov	Dec	Jan 15	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
Genera												
Microcystis aeruginosa	+	+	+	+	+	+	-	-	+	+	+	-
Anabaena	-	+	+	-	-	-	-	-	-	-	-	-
Gloeocapsa	-	-	+	-	-	-	+	+	-	-	-	-
Spirulina	-	+	+	-	-	-	+	-	-	+	+	-
Oscillatoria	-	-	-	-	-	+	-	-	+	+	+	-
Chroococcus	-	-	-	-	+	+	-	-	-	-	-	-
Merismopedia sparsa	-	-	-	-	-	-	-	+	-	-	-	-
Scenedesmus obliquus	+	+	+	+	+	+	+	+	+	+	+	+
Pediastrum tetras	+	+	-	-	-	-	-	-	-	-	+	-
Pediastrum boryanum	-	-	-	-	-	-	-	-	-	-	-	+
Monoraphidium komarkovae	+	+	+	+	-	-	+	+	+	+	+	+
Tetraerdon muticum	+	+	-	-	-	-	-	+	+	+	+	-
Tetraedron limneticum	-	+	-	+	-	-	-	+	+	+	-	-
Chlorella	+	+	+	+	+	-	-	-	-	+	+	-
Golenkinia	+	+	-	-	-	-	-	-	-	-	-	-
Selenestrum	+	-	-	-	-	-	-	-	+	-	-	-
Pandorina	-	+	+	-	+	+	-	-	+	-	-	-
Elakatothrix	-	-	-	-	-	-	-	-	+	-	-	-
Tetraedron trigonum	+	-	-	-	-	-	-	+	+	-	+	+
Nitzschia acicularis	+	-	-	-	-	-	-	-	-	-	-	-
Nitzschia palea	-	+	-	+	-	-	+	+	-	+	+	-
Navicula	-	-	+	-	+	+	+	-	-	-	-	-
Synedra	-	-	-	-	-	-	+	-	-	-	-	-
Cosmarium portianum	-	-	-	-	-	-	-	-	-	-	-	+
Oocysitis	-	-	-	-	-	-	-	-	-	-	-	+
Charciopsis pyriformis	-	-	-	-	-	-	-	-	-	-	-	+

+ Presence, - Absence

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SEARCH-BASED SOFTWARE ORGANIZATION

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Abstract

Organization Software refers to the process of decomposing software system into more manageable smaller clusters with an aim to simplify its structure as well comprehension. It is one of the techniques that have been used to develop more maintainable and understandable software systems. In this paper, categorizations of software organization techniques have been discussed with ample emphasis on the importance of use of search-based software organization with an aim of software comprehension or software re-organization. Further, metrics to measure quality of software organization have been depicted with illustrations. The existing available organization of the software under investigation has been used as reference in this study.

Keywords: Software Modularisation; Nature-Inspired Algorithms; Precision; Recall.

INTRODUCTION

Software organization refers to the process of decomposing software into more maintainable smaller subsystems called modules/clusters in such a way that the software units (function/variable/class) within a subsystem (module/cluster/package) are more similar to one another in terms of a set of predefined features as compared to those in other modules/clusters. The entity could be a class, file or a function and a feature could be a function call, inheritance, use of variables etc (Mitchell and Mancoridis 2008). It is useful during the process of the development as well as during maintenance phase of software (Sullivan, Griswold et al. 2001). Various applications of different techniques for software organization are available in literature. It has been mentioned by Myers et al. (Myers 1978) "Modularity is the single attribute of software that allows a program to be intellectually manageable". So, major principle that could be followed behind software organization is that entities are clustered in such a way that the entities in a module/cluster are always used together.

Categorization of Software Organization Techniques

Räihä et al. (Räihä 2010) used some of the search based techniques for the process of software design problems along with software organization. Software organization approaches has been classified as:

- Hierarchal Organization
- Concept-Based Software Organization
- Graph-Based Software Organization
- Search-Based Software Organization

Hierarchal Organization

One of the hierarchal organization techniques that has been applied by Hutchens and Basili (1985) for the re-organization of software is performed by using linkage to modularize procedures on the basis of variables they used. Procedures are grouped together such that the procedures that use similar variables together are grouped together. Schwanke (1991) used a heuristic based approach for hierarchal software organization on the basis of coupling among the functions and types. Design coupling is achieved by the interdependence of functions on types and observes the effect of altering a type on its intedependent functions. In order to perform the similarity measure, interdependency between a function and each type is exploited. The author further remarked that the single linkage algorithm produced best results. Along with this unsupervised organization, supervised modes of organization have also been studied in which an expert may be the developer approves merge operations before being actually performed. If the developer feels by experience that the merge should not be made, the algorithm does not attempt to merge the pair again.
The ability of variety of hierarchical organization has also been investigated by the research community for re-organization of software systems. Anquetil and Lethbridge (1999) analyzed different types of linkage based algorithms on the basis of features such as return out of a function call, reference types etc. in identifiers obtained by a method based on identification of concepts. On the basis of the combinations of attribute as well as linkage type, similarity measure leads to organization algorithms which are used on four samples including Linux, and Mosaic, The result were evaluated on the basis of

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design quality as well as authoritativeness. Authoritativeness was measured with measure called "precision and recall". The directory structure of the software is used as the expert decomposition.

Concept-Based Software Organization

Deuresen and Kuipers (1999) studied the application of concept analysis for decomposition of identifiers of a software system. In this approach, concept lattice has been used in which each possible grouping of elements has been placed. Each of the candidates organization is obtained on the basis of a universal concept such as the presence of an element in the program. The concepts are stored in the form of partial ordering from most general concerpt to the least one.. This type of organization produces only one feasible organization. Further each element could be allocated to more than one cluster which is a more realistic approach to handle elements.

Tonella (2001) also applied to concept analysis for re-organization. They performed organization of functions according to their use of structures in C, changing memory heaps and global identifiers. This approach works to modularise the systems while taking care of organization expenses including Encapsulation violations and effectiveness of organization. This effectiveness cost is calculated from the quantity of work needed to acclimatize to the new organization which is calculated by the amount of difference between the re-modularised system and the original system. Modularization Quality is calculated by the count of the number of clusters produced. This approach has the potential to produce a large number of candidate partitions.

Graph-Based Software Organization

Rigi Müller et al. (1993) also investigated graph-based techniques (called Rigi) for semi-automatic hierarchical organization of software. Rigi intends to make hierarchies from basic components. Rigi is based on the composition dependency graph (CDG) which is built to represent the complete decomposition of the system. The leaf nodes of the RFG (Resource Flow Graphs) are developed by generalising dependency graphs which are meant to involve any fact whose resource relations are defined. An element could be part of any number of clusters leading to CDGs as acyclic directed graphs and not trees.

Search Based Software Organization

Search-based methods have been a source of inclination for the process of software organization. The process of software organization is formulated as an optimization problem that is further joined by the features including relaxation of populating candidate solutions and the capacity to generate fitness values for these solutions. There is numerous search based software organization techniques that have been developed in the past two decades. These could be broadly classified in two different classes depending on the goal that they strive to attain:

Comprehension Approaches

The classes of software systems are clustered into smaller more manageable subsystems without taking into account the original organization of the classes in such a way that the resulting structure is more understandable. One of the remarkable tools in the area of search based software organization is Bunch. The tool leads to produce hierarchical decompositions obtained by the application of either Hill Climbing (Mancoridis, Mitchell et al. 1999), Simulated Annealing (Mitchell 2002), or Genetic Algorithm (Doval, Mancoridis et al. 1999). The process of software organization starts with clusters of small size followed by subsequent searches performed with an aim to join the clusters from the previous execution to generate a layered decomposition.

For improving the performance of Bunch tool, Harman et al. (2002) proposed an alternative representation which diminishes the search space by reducing the possible representations of a candiate. Use of the novel crossover operator performs better the previous one, but it very soon gets rafted at local optima. It performa worse tham a Hill-Climbing algorithm.

Harman et al. (2005) further proposed EVM fitness function and compared its performance with fitness function used in Bunch. Seng et al. (2005) proposed GA based approach to decompose software classes into subsystems (packages). They modularized classes so as to increase internal dependencies of the packages thus generated. They also consider cyclic dependencies between packages to be negative for design quality of the resultant package structure. The main drawback of this approach is the ambiguity in the definition of the organization/package quality (Abdeen 2010).

In another work, the authors (Praditwong, Harman et al. 2011) used the concept of multi-objective for automating the process of software module organization. They found that low coupling and high cohesion when used as an objective (MQ) leads to poor quality decomposition. They introduced a set of objectives and found that this approach outperforms traditional Hill-Climbing and GA techniques. The two techniques of the multi–objective organization problem include Maximum Organization Approach (MCA) and Equal Organization Approach (ECA). It is empirically evaluated that ECA approach optimizing the number of intra-edges, the number of inter-edges, the number of clusters, MQ, the difference between the maximum and minimum

number of modules/clusters in a cluster outperforms the MCA approach (optimizing the number of isolated clusters in place of the difference between the maximum and minimum number of entities in a cluster) in most of the cases.

Glavas et al. (2011) proposed an automatic approach for software organization based on four different algorithms (GA, Hill Climbing, PSO and SA) using class coupling and cohesion attributes. The approach is based on optimization of cohesion and coupling only. Barros (2012) described the negative impacts of using unnecessary objective functions in multi-objective optimization algorithms designed for software organization. They observed an increase in the quality of software organization after eliminating unnecessary and repeated objectives.

Deepika et al. (2012) used MCA and ECA formulations (Praditwong, Harman et al. 2011) and optimized multiple objectives using multi-objective GA. Kumari et al. (2013) used Multi-objective Hyper-heuristic Evolutionary Algorithm (MHypEA) for the cause of software organization. They used MQ, cohesion and coupling as fitness function to be optimized. In another work (Chhabra 2014), sensitivity of MCA and ECA formulations for software organization has been analyzed using NSGA-II algorithm. It is seen that the MCA formulation is less sensitivity and a better choice for multi-objective software organization. In another work (Ibrahim, Rayside et al. 2014), copperative organization based on MQ has been utilized for automated software organization. This work has a drawback as using just single objective may not lead to efficient organization. This is seen that the efficiency of this technique degrade with increase in problem size. In addition, the authors used MQ as an objective for software organization as well as a motivation in the approach used for its validation.

In another work, PSO algorithm has been implemented for the process of software organization using MQ (Hussain, Khanum et al. 2015) as the fitness function. Paixao et al. (2015) investigated the application of MCA and ECA approaches of multi-objective Two-Archive algorithm for the organization of C/C++ based editor (Kate) for KDE platform and observed improved software organization quality metrics.

Re-organization Approaches.

The classes of the software system are re-modularized taking into account the original organization of the classes so that certain properties of the software system such as its maintainability or evolvability are improved.

In another work in the field of software organization, Abdeen et al. (2013) used the cohesion in all subsystems, the coupling amount among clusters and the different between the original and evolved organization as objectives to be optimized using NSGA-II. This technique is helpful in re-organization. It does not apply to organization of newly developed software.

In another advancement, Mkaouer et al. (2015) used NSGA-III for organization of software system using seven objectives including the number of subsystems, total cohesion, total coupling, the number of nodes per subsystem, the number of code changes, the vocabulary based similarity and the similarity between history of code changes as objectives to be optimized. This technique is helpful for software re-organization. Some of the objectives could not be utilized for the organization of newly developed software.

Quality Metrics

Automated organization has been performed by a variety of methods in the past few decades. There are numerous methods to assess the quality of these automatically generated criteria. One of the popular ways of assessing the authoritativeness quality of software organization that is widely used in literature is by using an existing available decomposition to assess the similarity between automated organization and the organization proposed by the original developer. A large numbers of frequently used similarity measures such as MeCl, EdgeSim, MoJo have been discussed.

Precision and Recall

It has been widely used for information retrieval approaches (Anquetil and Lethbridge 1999). It is measured as the ratio between relevant retrieved documents and total documents. It has the ability to predict correct positive and correct negatives.

$$Precison = \frac{True\ Positives}{True\ Positives + False\ Positives}$$

$$Recall = \frac{True\ Positives}{True\ Positives + False\ Negatives}$$

In case of software organization, positive means elements in the same clusters and negative mean the elements are in different clusters. In other words, precision is the amount of pairs of entities in the same subsystem which are also in the same subsystem in the given organization and recall is the amount of pairs of entities actually organized together which were organized pair wise by the algorithm. It has observed usage by large number of researchers (Maqbool and Babri 2007; Beck and Diehl 2010).

For the organization shown in Figure 1. Precision and recall is calculated as shown below.

Together (a) = ([C1 C2], [C1 C3], [C1 C4], [C2 C3], [C2 C4], [C3 C4] for package P1; [C7 C8], [C6 C7], [C6 C8] for package P2)
Together (b) = ([C1 C2], [C1 C3], [C1 C4], [C2 C3], [C2 C4], [C3 C4], [C1 C6], [C2 C6], [C3 C6], [C4 C6], for package P1; [C7 C8) for package P2)
Apart(a) = ([C1 C5],[C2 C5],[C3 C5],[C4 C5],[C6 C5],[C7 C5], [C8 C5] [C1 C8] [C2 C8],[C3 C8],[C4 C8], [C1 C7] [C2 C7],[C3 C7],[C4 C7], [C1 C6] [C2 C6],[C3 C6],[C4 C6])
Apart(b) = ([C1 C5],[C2 C5],[C3 C5],[C4 C5],[C6 C5],[C7 C5], [C8 C5] [C1 C8] [C2 C8],[C3C8],[C4 C8],[C6 C8], [C1 C7] [C2 C7],[C3 C7],[C4 C7], [C6 C7])

$$Precisio = \frac{Together(a) \cap Together(b)}{Together(a)} = \frac{7}{9} = 0.777$$

$$Recall = \frac{Together(a) \cap Together(b)}{Together(b)} = \frac{7}{11} = 0.6363$$

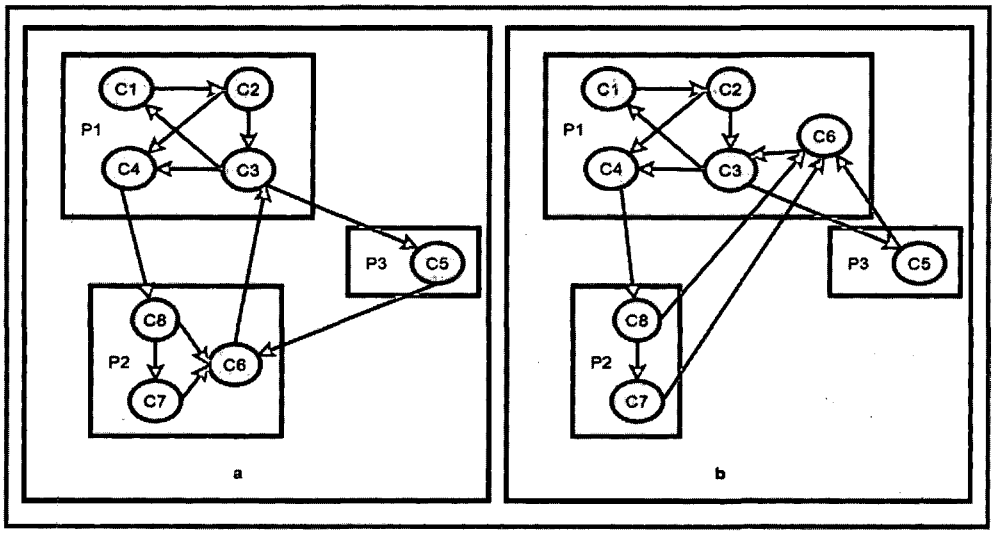

Figure 1: Automatic and reference decomposition

It has been accompanied by some drawbacks also. One of the undesirable aspects of Precision/Recall is that it is susceptible to the size and number of subsystems. In other words, for the organization of small sized system (with a few entities), a few misplaced entities in a cluster has a larger emphasis on Precision/Recall than if the subsytems that has large number of entities. In addition, the number of clusters has also been observed to have an impact on Precision/Recall. There should be no association between the size and number of subsystem for the measuring of authoritatbeness (Mitchell and Mancoridis 2001). Sometimes precision and recall measures are also found to provide contrasting results especially in extreme cases.

MoJo

MoJo (**Mo**ve and **Jo**in) is a technique (Wen and Tzerpos 2003) for calculating the degree of authoritativeness among automatic and reference organization. It has observed a wide variety of use in literature for comparison of software organization partitions. It is basically used to calculate the effects required to alter one subsystem into another. The calculations are based on the number of move and join operations. Move operation is described as the process of moving one element from one cluster to another (this cluster is created if does not exist already). The join operation is described as the process of combing two clusters to make a new cluster. Each of these operations is assigned a weight of 1. It has been used in a wide variety of software organization approaches (Kim and Bae 2008; Naseem, Maqbool et al. 2011).

For the MDGs shown in Figure 2, number of move operations= 1 (C6 moved from package P2 to package P1 from Figure 2 (a) to get organization shown in Figure 2 (b)) and number of join operations=0. MoJo is accompanied by a number of defects. MoJo quality metric is non-symmetric measure. It means the minimum number of Move or Join action required to alter organization X to Y may be different from the minimum number of Move

or Join actions required to transform Y to X. Tzerpos (Wen and Tzerpos 2004) further enlightened other defects associated with MoJo which hinders its use as a quality metric.

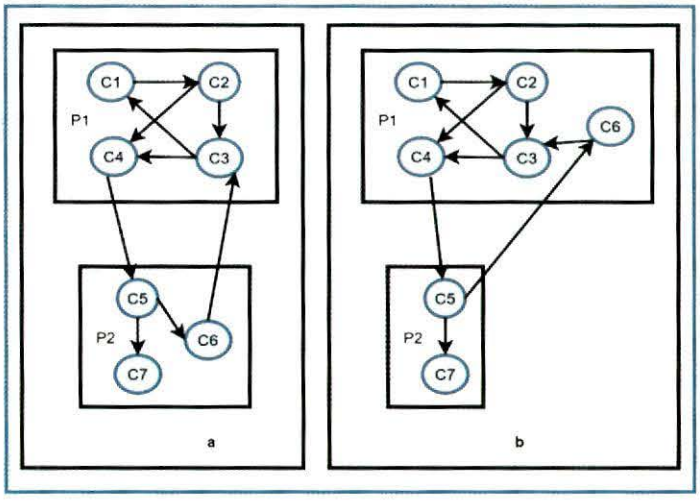

Figure 2: Module Dependency Graph to calculate MoJo

MeCl

MeCl (Mitchell and Mancoridis 2001) (**Me**rge **Cl**usters) is a method of measuring similarity of two partitions in terms of the difference between two organization of a graph. Let M and N be two given partitions whose similarity is to be calculated. MeCl works by dividing subsystem in M by intersecting each Subsystem with each of the subsystem in N. These subsystem are then combined to obtain organization N.

The weightage of inter-edge relationships thus developed due to the merging of clusters is calculated and described as a ratio of the total weight of all edges. This is used to measure the amount of restructuring required which is further calculated by Mitchell as normalisation obtained by subtracting it from 1 (Mitchell 2002).

Further, no new inter-edges are created when its clusters are combined to form reference partition B. It has been extensively used for software organization in variety of techniques (Mitchell 2002; Wu, Hassan et al. 2005; Maqbool and Babri 2007). In general, MeCl(a,b) != MeCl(b,a). So, for the transformation in which its course is not vital then MeCl is calculated as

$MeCl_{min}(a,b) = min[(MeCl(a,b);MeCl(b,a)]$.

Figure 3 (a) and Figure 3 (b) represents two partitions of graph G = (V;E) where

V=[C1,C2,C3,C4,C5,C6,C7,C8]

E=[(C1,C2); (C2,C3); (C3,C4); (C2,C4); (C3,C1); (C3,C5); (C6,C3); (C4,C8); (C8,C6); (C8,C7); (C7,C6)]

G_a=[P1,P2,P3] from Figure 3 (a)

G_b=[P1,P2] from Figure 3 (b)

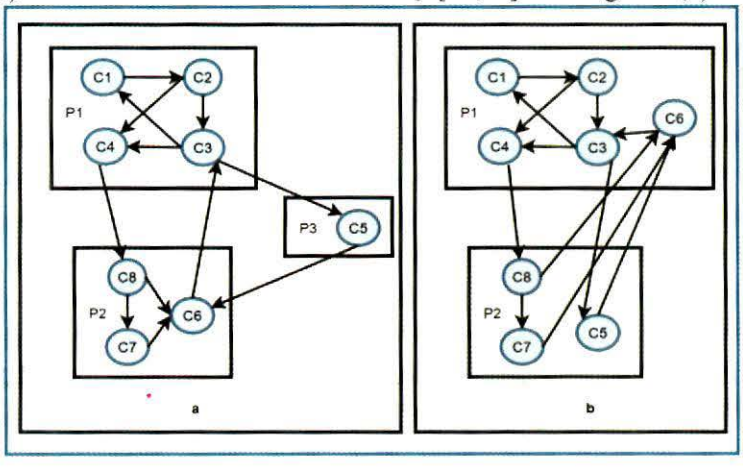

Figure 3: Module Dependency Graph to calculate MeCl

In order to calculate MeCl, distance between Figure 3 (a) and Figure 3 (b) is calculated on the basis of each P_i in Figure 3 (a) with respect to each of the clusters P_j in Figure 3(b) represented by C_{ij}.

$C_{ij}= (V_{ij}; E_{ij})$

$V_{ij}= V_i \cap V_j$

$E_{ij}= E_i \cap E_j$

MeCl(a,b)=C11 C12 C21 C22 C31 C32

It is required to calculate a set of intra-edges φ *in* Figure 3 (a) that are inter-edges θ in Figure 3 (b).

$\gamma_{ij} = \varphi_i \cap \theta_j$

C_{11} is obtained from package P1 in Figure 3 (a) and P1 in Figure 3 (b).

C_{11}=([C1,C2,C3,C4],[C1,C2); (C2,C3); (C3,C4); (C2,C4); (C3,C1)]);

C_{12}=(Φ,Φ);

C_{21}=([C6], Φ);

C_{22}=([C7,C8], [C8,C7]);

C_{31}=(Φ, Φ);

C_{32}=([C5], Φ);

$\gamma_{11} = 0$

$\gamma_{12} = 0$

$\gamma_{21} = ([C8\ C6],[C7\ C6])$

$\gamma_{22} = 0$

$\gamma_{31} = 0$

$\gamma_{32} = 0$

The clusters thus obtained are shown in Figure 4. In order to obtain the organization shown in Figure 3 (b), obtain $C11 \cup C21$ *and* $C22 \cup C32$

In order to calculate MeCl, the overall cost of this combination operation is calculated as the total coupling edges introduced during the merging operation.

$$MeCl(a,b) = \left[1 - \frac{Weight(\gamma)}{Weight(E)}\right] * 100$$

$$Weight(\gamma) = \bigcup_{i=1}^{2} \bigcup_{j=1}^{3} \gamma_{ij} = \left[1 - \frac{2}{12}\right] * 100 = 83.33\%$$

MeCl(b,a)=C11 C12 C13 C21 C22 C23

C_{11}=([C1,C2,C3,C4],[C1,C2); (C2,C3); (C3,C4); (C2,C4); (C3,C1)]);

C_{12}=([C6],Φ);

C_{13}=(Φ, Φ);

C_{21}=([C7,C8], [C8,C7]);

C_{22}=(Φ, Φ);

C_{23}=([C5], Φ);

$\gamma_{11} = ([C6,C3])$

$\gamma_{12} = 0$

$\gamma_{13} = 0$

$\gamma_{21} = 0$

$\gamma_{22} = 0$

$\gamma_{23} = 0$

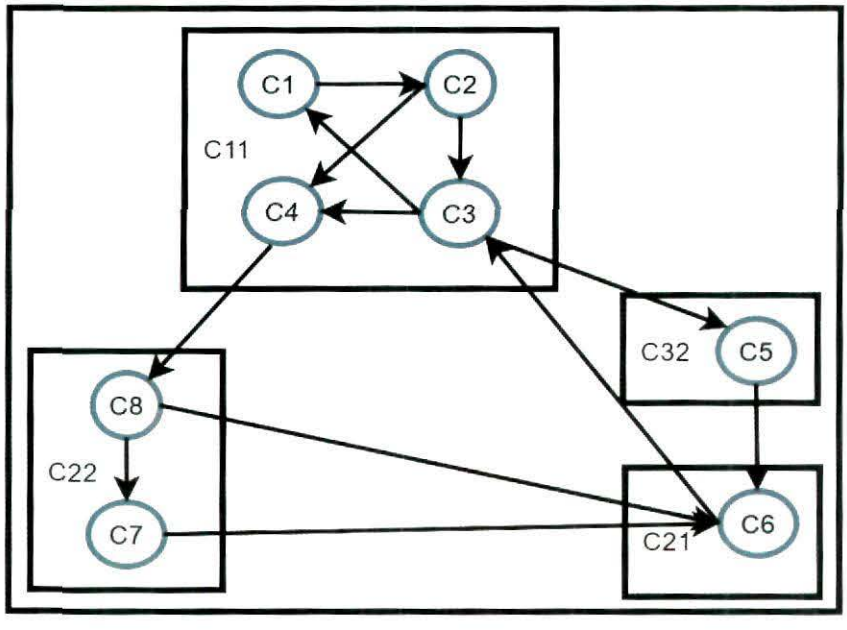

Figure 4: Sub-partition of **Figure 3** (a) and **Figure 3** (b)

It is observed that MeCl have the tendency to favour organization which form cohesive sub-clusters as far as reference partition is concerned.

EdgeSim

EdgeSim (Mitchell and Mancoridis 2001) works on the edges in the MDG. It includes both cohesion and coupling of the primary organization. For two organization A and B, EdgeSim is calculated as

$$\mathbf{EdgeSim} = \frac{\mathbf{Weight(\gamma)}}{\mathbf{Weight(E)}} * \mathbf{100}$$

Where E is the set of all edges in a given MDG and γ is the set of all edges which are inter-edges (inter-edges in A are inter-edges in B) or intra-edges (intra-edges in A are intra-edges in B) in both A and B. So higher the value of EdgeSim, better is the organization obtained. For the sample MDG shown in Figure 3, EdgeSim is calculated to be

$$\boldsymbol{EdgeSim} = \frac{\mathbf{9}}{\mathbf{12}} * \mathbf{100} = \mathbf{75}$$

MeCl and EdgeSim have been used extensively in a large number of software organization techniques (Shtern and Tzerpos 2011; Shtern and Tzerpos 2012). The main drawback of both is that they take into consideration the misplacement of edges and do not consider the misplacement of the entities in the wrong clusters.

MoJoFM

MoJo is associated with various defects as discussed above. Tzerpos updated MoJo to develop MoJoFM (Wen and Tzerpos 2004). Let A be the automatic organization and B be the reference package structure in which entities are clustered in the given application. For B, the package structure developed by its developers has been used (Beck and Diehl 2013).

$$MoJoFM = \left(1 - \frac{mno(a,b)}{\max(mno(\forall a,b))}\right) * 100$$

mno(a,b)=min(move and join actions to convert a to b)max(mno($\forall$a,b))=most distant decomposition from reference decomposition b.

So, higher the value of MoJoFM, better is the organization obtained (Corazza, Di Martino et al. 2016). MoJoFM is an improvement over MoJo as it is based on the fact that organization farthest from the "gold standard" has a value of 0%, while a organization similar to the "gold standard" has a quality of 100%. Further, MoJo is a non-symmetric measure because it takes minimum number of Move or Join operations to convert organization a to b or b to a. It has been used most popularly till date to measuring the effectiveness of software organization (Hall, Khojaye et al. 2014) (Naseem, Maqbool et al. 2011).

For MDG shown in Figure 2, value of mno(a,b) is equal to 1 and $\mathbf{max(mno(\forall a,b))}$ is calculated as follows. Most distant decomposition from Figure 2 (b) is shown in Figure 5. So, $\mathbf{max(mno(\forall a,b))}$ is 6 because it needs 3 and 2 move operations to transform most distant organization to organization shown in b. It means

$$\text{MoJoFM} = \left(1 - \frac{1}{5}\right) 100 = 80.$$

CONCLUSIONS

Software organization refers to the placements of software entities into appropriate clusters and has been observed to be useful in both the development and maintenance of a software system. Various kinds of software organization techniques have been studied in literature including Hierarchal Organization, Concept-Based software Organization, Graph-Based software Organization and Search-Based software Organization. In this paper, Search-Based software organization techniques are extensively studied and further classified as comprehensive and re-clustering techniques. Techniques to evaluate authoritativeness quality of software clustering obtained by Search-Based software organization techniques have been discussed along with appropriate illustrations.

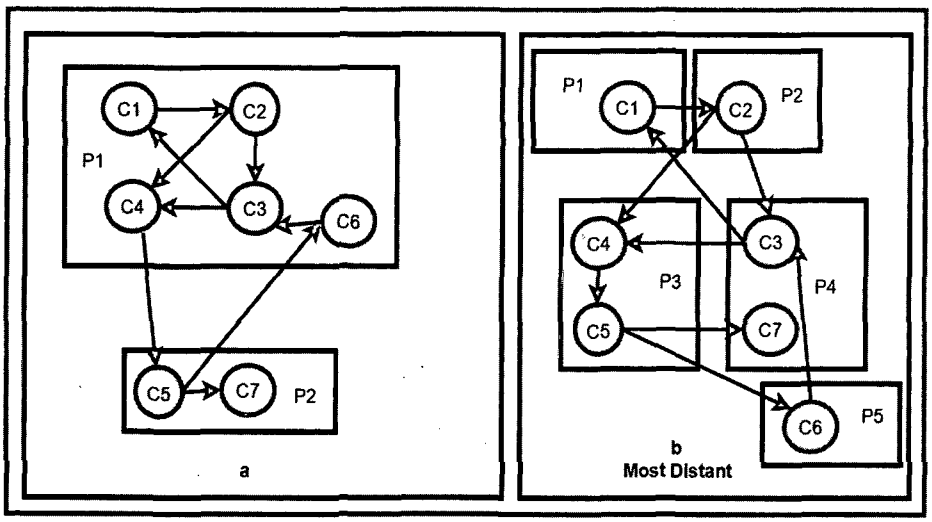

Figure 5: Most distant organization from reference organization for MoJoFM

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