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Marine Bioinformatics

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Introduction

The bioinformatics field is growing astoundingly during last decade due to the advancement of biotechnology combined with the development of computational skills and the network effort developed by different countries in sharing information. It further enhanced by grouping and compiling of huge data by means of revolutionizing internet concepts with various interpretations made out using the power of algorithms. Even in today's technological world no man-made structure is as complex as biological systems. Thus the foremost aim of bioinformatics is solving multifaceted biological problems i.e. from molecular biology to physiological processes by the exchange of information, databases through network. Our views in biology starting from systematic classification of organisms to genomics and proteomics are now changing or progressing due to the availability of various high-tech software tools and databases for bioinformatics. New insights are made often with these tools to explore molecular biology through the logics of computation. In India, presently attempts have been taken for the use of bioinformatics in marine biology related research. This article discusses the scope of bioinformatics applications in marine biology based research i.e. marine bioinformatics (MBi) in the global and Indian context.

Life in the marine environment

About 70% of our planet Earth is covered by Oceans with 1370.323 million cubic km of water and therefore oceans influences the climate of entire planet. Since, the ocean water is a rich medium with lot of unique properties; it supports 90 % of world's living biomass. The marine environment provides various ecological conditions to a wide variety of organisms living in the intertidal region to offshore and surface to deeper parts of oceans' depth. Hence, marine organisms are adapted to varying physicochemical conditions ranging from low to high saline habitats, freezing to very high temperature (hydrothermal vents), normal to extreme pressure at depths and normal light regimes to complete dark regions in deep sea, normal oxygen to methanogenic environment (gas hydrates) etc. Similarly, the diverse marine

organisms living in normal to extreme environments (extremophiles) have useful characteristics yet to be discovered from their wide array of biomolecules. The marine environment is the exceptional reservoir of bioactive natural product, many of which exhibit structural or chemical features not found in terrestrial natural products (Carte, 1996). The protein, DNA and other compounds isolated from these organisms holds the key for useful enzymes, biomolecules, biomaterials, bioprocess etc., could be used for the development of industrial and pharmaceutical products.

Marine bioinformatics

The bioinformatics developed during eighties and defined as “the scientific discipline that encompasses all aspects of biological information acquisition, processing, storage, distribution, analysis and interpretation”. It combines the tools of Biology, Chemistry, Mathematics, Statistics, and Computer Sciences to understand life and its processes. The term Marine Bioinformatics refers to the use of computer and networking technologies to gather, store, integrate, analyse, interpret and disseminate the marine organism's data such as organism's distribution, description, systematic classification, phylogeny, and their biomolecular structure and sequence data along with the functional aspects using marine proteomics and genomics. (Vinithkumar, 2004).

The bioinformatics field offers specialised analytical technology tools for both laboratory and networking technology fields to achieve the goal of finding natural bioactive compounds from marine organisms as potential drugs, antifouling compounds, biomaterials etc. It has highest implication in marine based ecology, biology, biotechnology and molecular biology, which are integrated for the gene based discovery and development of marine drugs. The marine bioinformatics includes marine genomics and marine proteomics. Marine genomics refers to any attempt to analyze or compare the entire genome complement of a species of marine origin. Similarly marine proteomics is the study of protein family derived from marine organisms. The proteome is defined as the PROTEin complement of the genOME. Proteomics is concerned with qualitative and quantitative studies of gene expression at the level of the functional proteins themselves. The pharmacogenomics is the application of genome approach and technology to the identification of drug target protein and particularly useful in the development of drugs from marine organisms.

Need and use of marine bioinformatics

The successful sequencing of entire human genome in the Human Genome project opened up our understating on biological systems in an unprecedented way. This was made possible due to the advancement of molecular biotechnology combined with information technology. Presently, bioinformatics techniques are widely being applied to study the land based animals, plants and humans, and also to an extent in marine based systematics, phylogenetics, genomics and proteomics.

As the volume of databases for biomolecules, proteins and genes of various land and marine organisms are growing amazingly, analyzing the data and getting required results for marine organism from the common database of land, air and water is increasingly becoming complex. This is being felt when every time a search was

made for some biomolecules in the existing databases, the search results showed entries for organisms living in different environments. Hence, there is a need for separate storage, retrieval and analysis of marine organism database, which would reduce much time for the students and scientists doing data mining in marine based research.

In this context the multi-linked approach would be much helpful for the analysis of marine organisms, i.e., instead of having single data base (protein, gene or other biomolecules databases) for all organisms from different environments, the databases could be compartmentalized with defined structure based on the environment and geographical boundaries they live, but at the same time all databases could be linked or integrated with one another. For this, provision should be made in the flat files of biomolecules databases, to describe the required environmental and other background information such as biology, ecology etc., from the same database or from other linked databases. For example the COML (Census of Marine Life) or OBIS (Ocean Biodiversity Information System) data on biodiversity could be interlinked with the existing biomolecular databases.

Since our search for organisms is limited, many of the species in marine environment are yet to be discovered. The data and information regarding marine resources remain distributed with several organizations and individuals, making it difficult to access adequate and accurate information about them, easily and efficiently (Chavan *et al.*, 2004). Hence there is an urgent need to integrate marine organisms' database which are existing and to be developed further.

International initiatives on marine bioinformatics

The bioinformatics approach is used in genome approach and technology to the identification of target protein as drugs from marine organisms. It is also used for phylogenetic classification of marine organisms by comparing the sequence of various organisms, which is considered as supporting method for systematic classification of marine organisms. This approach could be used in protein structure prediction, studies on basic biological processes in marine organism using functional and comparative molecular methods on marine models, functioning of marine bio ecosystem and development of aquaculturally important species through gene manipulation etc.

As the search for natural bioactive molecules from marine organism as potential drugs, bioinformatics offers many high technology tools to stepping up new drug discovery. Without bioinformatics, new application oriented research in many fields of marine drug discovery and marine biology would come to a standstill. Globally many pharmaceutical company looking for potential drugs from extremophilic marine organism as the sea has extreme conditions like, high pressure in deep sea, high temperature about 350°C hot hydrothermal vents, deep cold conditions in the depth of the oceans, higher saline conditions in some places and anoxic conditions in the sediments and water column, higher poisonous dissolved and solidified (gas hydrates) gaseous sedimentary conditions. Already many DNA primers have been developed from the sequence of deep sea bacteria living in the hydro thermal vents. The DNA primers found to be highly stable in varying temperature conditions, its potential in the PCR based primers development was utilized effectively and marketed by US based companies. Recently the European Network of Excellence (NoE) was mainly devoted

for marine genomics. In line with this many of the European, US and Japanese universities and companies are working on various aspects of marine bioinformatics.

Indian initiatives on marine bioinformatics

The nucleotide and protein sequences of marine organisms distributed in Indian seas and also in other seas are being published regularly. Many of the sequences are published mostly with the online databases and journals from other countries. Little initiatives have been taken in this regard to create the genomic and proteomic databases of Indian organisms. However, Indian contribution to marine bioinformatics field is increasing in the recent years. Therefore, our knowledge to cope up with the modern tools and techniques for the Indian marine organisms is also increasing. Thus it is highly essential to establish the niche for marine bioinformatics particularly to serve the areas of marine biology in the context of Indian and global level.

India was the first country in the world to establish in 1987 a distributed Biotechnology Information System Network (BTIS net) by Department of Biotechnology (DBT, Govt. of India) to create an infrastructure that enables the scientific community to solve biotechnology problems through the application of bioinformatics. To integrate the national resources and promote tandem research, the department has also established a high speed and large bandwidth network in the form of Biogrid India. The grid has been designed to act as a knowledge pathway for discoveries in biotechnology. There is also a provision for marine bioinformatics related issues. In addition to this the Ministry of Environment and Forests (MoEF, 2004) sponsored many Environmental Information System (ENVIS) in various universities and other institutions. Similarly the Agricultural Research Information Network (ARISNET) is also working on different issues related to biodiversity informatics (Chavan, 2005).

Marine genomics

The marine genomics applied in three different areas viz., a. Comparative genomics – the study of representative marine organisms across the different phyla of life, b. Functional genomics - for the exploration of complex relationships between stimuli and gene expression, c. Environmental genomics – The delineation of structure and dynamics of biodiversity in marine ecosystems, including microbial diversity and ecology, the functional and adaptive aspects of intraspecific biodiversity and management of biodiversity. In the case of functional genomics the ultimate goal is to identify the function of all genes in an organism and to understand how those genes are coordinated to respond to the marine environment.

Functional genomics involves using a new technology, called DNA micro arrays, or DNA ‘chips’, to monitor the level of gene products of nearly all the genes in a tissue on a single chip so that researchers can have a better picture of the interactions among thousands of genes simultaneously. While chips measure the level of gene products, the DNA sequencing performed to fabricate the chips also to identify normal genes and novel gene mutations. The gene expression studies using DNA micro arrays are being used to study the characteristics of land and marine organisms and also humans.

DNA micro array technique is increasingly being used to study the commercially important coastal aquaculture species and for the development of new drugs. In this context, the Marine Genomics project is a functional genomics initiative developed to provide a pipeline for the curation of Expressed Sequence Tags (ESTs) and gene expression micro array data for marine organisms. It provides a unique clearing-house for marine specific EST and micro array data and is currently available at <http://www.marinegenomics.org> (McKillen *et. al.*, 2006). As of 2005 it contained 19 marine species databases (over 46,000 EST sequences) which included *Anas platyrhynchos* (mallard), *Crassostrea gigas* (Pacific oyster), *Callinectes sapidus* (blue crab), *Crassostrea virginica* (eastern oyster), *Eubalaena glacialis* (Northern Atlantic right whale), *Fundulus* species (killifish), *Homarus americanus* (American Atlantic lobster), *Karenia brevis* (red tide algae), *Leucoraja erinacea* (little skate), *Litopenaeus setiferus* (white shrimp), *Litopenaeus stylirostris* (blue shrimp), *Litopenaeus vannamei* (white shrimp), *Montastraea annularis* (lobed star coral), *Oculina varicosa* (stony coral), *Porites Porites* (clubbed finger coral), *Palaemonetes pugio* (daggerblade grass shrimp), *Squalus acanthias* (spiny dogfish) and *Tursiops truncatus* (bottlenose dolphin) that are maintained by registered users from local and remote locations in Europe and South America in addition to the USA. A collection of analysis tools are implemented include a pipeline upload tool for EST FASTA file, sequence trace file and micro array data, an annotative text search, automated sequence trimming, sequence quality control (QA/QC) editing, sequence BLAST capabilities and a tool for interactive submission to GenBank. Another feature of this resource is the integration with a scientific computing analysis environment implemented by MATLAB (McKillen *et. al.*, 2006).

Table 1: Institutions and projects working on marine genomics

Sl. No.	Description	URL
	The Marine Genomics Project	http://www.marinegenomics.org/
	The Hollings Marine Laboratory (HML) - Charleston , South Carolina	http://www.nccos.noaa.gov/about/hml.html
	Marine Genomics Europe Network	http://www.marine-genomics-europe.org/
	Marine Genomics Laboratory	http://crawford.rsmas.miami.edu/
	Göteborg University Marine Research Centre	http://www.gmf.gu.se/english/index.htm
	Marine Biomedicine and Environmental Sciences (MBES) Centre	http://www.musc.edu/mbes/home.htm
	Scripps Institution of Oceanography	http://scripps.ucsd.edu/about
	Institute for Marine Bioscience	http://imb-ibm.nrc-cnrc.gc.ca/index_e.php
	Marine Biology.Org	http://www.marinebio.org/
	Kristineberg Marine Research Centre	http://www.kmf.gu.se/index_eng.html
	Center for Biotechnology (Cebitec)	http://www.cebitec.uni-bielefeld.de/groups/brf/cooperations/marine_genomics_bioinformatics.html
	Warwick Marine Genomics Web server	http://nerc.bio.warwick.ac.uk/
	Genoscope	http://www.genoscope.cns.fr/externe/English/corps_anglais.html
	Groningen Genomics Centre	http://www.genomics.rug.nl/
	National Facility for Marine Cyanobacteria, India	http://www.nfmc.res.in/

The nucleic acid of wide variety of organisms are analysed to understand the mechanisms involved in protein synthesis and subsequent downstream processes. The Nucleic Acids Research Molecular Biology Database Collection is public online resources that are freely available to the public. The 2005 update includes 719 databases (Galperin, 2005). The database list and summaries are available online at the Nucleic Acids Research web site (<http://nar.oupjournals.org/>). Among the database list provided, very few are found to be of marine based research e.g. GeneNest – Gene indices of human, mouse, zebra fish, etc., (<http://www.genenest.molgen.mpg.de/>), ZFIN – Zebra fish information network (<http://zfin.org>) (Galperin, 2005). This clearly indicates that there is an immediate requirement for marine organism based genome and nucleic acid database development.

Marine proteomics and drugs discovery

The marine proteomics resources are widely scattered. The protein structural database, the protein data bank (PDB) contains about 28,000 structures as of 2006. PDB itself contains many structure files of protein derived from marine organisms. The protein structural database is growing in an enormous speed with a total count reaching about 36012 molecules and the rate of deposits per year is also increased very rapidly. This is going to be one of the burgeoning field in molecular biology, to find out answer for different disease with use of various tools and databases is already finding its applications in drug industries. Marine organisms like sponges, corals, sea weeds and starfish etc. have various functional properties like antibacterial, anti fungal and antiviral which can be used as a potential drug target. Thus finding bioinformatics could be widely used for the prediction of potential activities of marine drugs.

Tools and databases for marine bioinformatics

There are many software tools available, which includes Blast, Cn3D, Swiss PDB viewer, Hex, Vega, Bioeditor, Bioviewer, Protein explorer, Chime, Rasmol, Emboss etc., based on different operating systems like Linux and Windows. Also more than a hundreds software tools are available for bioinformatics could be used well for MBI applications. There are many databases which also include the marine based molecular sequences and some of them are NCBI, EMBL, DDBJ, PIR, GenBank, KEGG etc. The NCBI web (National Center for Biotechnology Information) which includes GenBank, PubMed also contains marine organisms based nucleotides and protein sequences.

The GenBank includes the sequences of marine bacteria, fungi, virus, invertebrates, vertebrates and plants. These are kept with corresponding protein and gene records and hints to other NCBI database. GenBank is a comprehensive database that contains publicly available DNA sequences for more than 165000 named organisms (Benson, *et. al.*, 2005). GenBank also contain large number marine organism based DNA sequences. In addition to maintaining the GenBank nucleic acid sequence databases, the National Center for Biotechnology Information (NCBI) provides data

retrieval systems and computational resources for the analysis of data in GenBank and other biological data made available through NCBI's website (Wheeler *et. al.*, 2005).

Protein Data Bank (PDB) contains about more than 30,000 worldwide repositories for the distribution on 3D biology macromolecules structural data which include many marine organism's protein sequences and structures. Also, complete or partial genome sequences of some marine invertebrate organisms such as sea urchins, shrimps and molluscs are available in the net and many are in the pipeline (<http://www.marinegenomics.org/>).

The Micro-Mar database of marine microbial genome (<http://egg.umh.es/micomar/>) is recently been created to collect DNA diversity information from marine prokaryotes for biographical and ecological analyses. The database currently includes 11874 sequences corresponding to high resolution taxonomic genes (16s rRNA, ITS and 23S rRNA) and many other genes including CDS of marine prokaryotes together with available biogeographical and ecological information. This database aims to integrate molecular data and taxonomic affiliation with biogeographical and ecological features that will allow to have a dynamic representation of marine microbial diversity embedded in a user friendly web interface.

Marine biodiversity informatics

Computer aided taxonomy (CAT) is getting importance due to the endless necessity for the proper identification of species. There are over 50 million species are projected to exist on the Earth and about 1.5 million species are known to us so far (Chavan *et. al.*, 1998). In order to conserve the natural living resources, a thorough understanding and identification of individual species and its role in ecology are highly imperative. It is highly applicable in the case of marine biota, since they constitute about 70% of known fauna and flora (Chavan *et. al.*, 1998).

There is an urgent requirement for developing Electronic Catalogues (ECAT) of marine organisms by integrating through internet. Wheeler *et. al.*, 2004 acknowledge with a cautious stance, that the world wide web presents a perfect medium for exploring how to undertake collaborative taxonomic studies. Specialized online software such as digital libraries of biodiversity literature is being developed to collect and show the details of a species or a group of organisms from different websites or databases in a single query page. This would help the scientist to find out the required information in a reasonably short period of time.

Establishing the range of most taxa, which is desirable for purposes such as fisheries, conservation, and Biogeographic analyses, requires consulting the original literature (Fautin, 2000). Thanks for the efforts being done, that there are already environment based biodiversity databases are being developed and few example includes marine biodiversity databases such as Global Biodiversity Information Facility (GBIF; <http://www.gbif.org>), Census of Marine Life (CoML; <http://www.coml.org/colm.htm>), Indian Ocean Census of Marine Life (IO-CoML), Ocean Biodiversity Information System (OBIS; <http://www.obis.org>), Indian Ocean Biogeographic Information System (IndOBIS; <http://www.indobis.org>) etc.

Table 2: Some of the global and regional online marine biodiversity catalogue

Sl. No.	Description	URL
1.	Fish base- for identification of fishes	http://www.fishbase.org/home.htm
2.	Larval base Global Information system about fish larvae	http://www.larvalbase.org/
3.	Reef base A global information system on coral reefs	http://www.reefbase.org/
4.	A global database of coral reef systems and their resources	http://www.wcmc.org.uk/data/database/reefbase.html
5.	California artificial reef base	http://www.msi.ucsb.edu:16080/CARB/
6.	Reef base GIS - Interactive world map for coral reefs	http://reefgis.reefbase.org/mapper.asp
7.	Hawaii coral reef bibliography - reference listings of surveys, studies, technical reports, atlases etc.	http://home.hawaii.rr.com/cpie/CoralReefBib.html
8.	Great Barrier Reef Marine Park Authority, Australia	http://www.gbrmpa.gov.au/
9.	Plankton Image Library	http://192.171.163.165/pil/plankton_image_database_homepage.htm
10.	An annotated list of Illustrated plankton resources - Estuarine Ecology Lab, Texas A&M University	http://www-ocean.tamu.edu/~pinckney/plankton.htm
11.	The user-friendly guide to coastal planktonic ciliates	http://www.liv.ac.uk/ciliate/
12.	Department of Marine Ecology, Marine Botany - Göteborg University, Sweden	http://www.marbot.gu.se/
13.	Protist information server - Japan	http://protist.i.hosei.ac.jp/Protist_menuE.html
14.	Protist Image Data , Canada	http://megasun.bch.umontreal.ca/protists/
15.	Cladocera web page	http://www.cladocera.uoguelph.ca/default.htm
16.	of Type Specimens of Foraminifera	http://www.ucmp.berkeley.edu/foram/types/types.html
17.	The plankton net	http://www.biosci.ohiou.edu/faculty/currie/ocean/
18.	Harmful Algae and Phycotoxins Information Links	http://cbr-rbc.nrc-cnrc.gc.ca/issaha/New_ISSHA/Links_Gen.htm
19.	A resource site for Seaweeds	http://www.seaweed.ie/
20.	European Molluscs database	http://www.mnhn.fr/base/malaco.html .
21.	Bryozoans database	http://www.civgeo.mit.edu.au/bryozoan/index.html/
22.	Sea anemones	http://www.biocomplexity.nhm.ukans.edu/edu/anemones/images/index.html .
23.	OBIS	http://marine.rutgers.edu/obis/
24.	Molluscs, OBIS	http://www.amonline.net.au/invertebrates/
25.	Species 2000	http://www.sp2000.org
26.	ETI World Biodiversity Databases	http://www.eti.uva.nl
27.	Database on Algae	http://www.algaebase.org/
28.	Census of Marine Life (CoML)	http://www.coml.org/
29.	Marine Species Index- Marine Biological Laboratory	http://www.database.mbl.edu/SPECIMENS/phylum.taff?function=form&page=2
30.	UNESCO-IOC Register of Marine Organisms	http://www2.eti.uva.nl/database/urmo/default.html
31.	IndFauna-Electronic Catalogue of Known Indian Fauna	http://www.ncbi.org.in/biota/fauna
32.	European Register of Marine Species (ERMS)	http://erms.biol.soton.ac.uk/

OBIS is a component of the Census of Marine Life (CoML) an International program to assess and explain the diversity, distribution, and abundance of marine life (Grassle, 2000). OBIS an online service provider of global georeferenced information on accurately identified marine organisms. OBIS databases on species and habitat level provide a spectrum of spatial query tools for visualizing the relationships between species and environment. European Register of Marine Species (ERMS), a register of marine species in Europe to facilitate marine biodiversity research and management (www.erms.biol.soton.ac.uk). It produced a checklist of over 29,000 marine fauna and flora species in Europe (Costello, 2000).

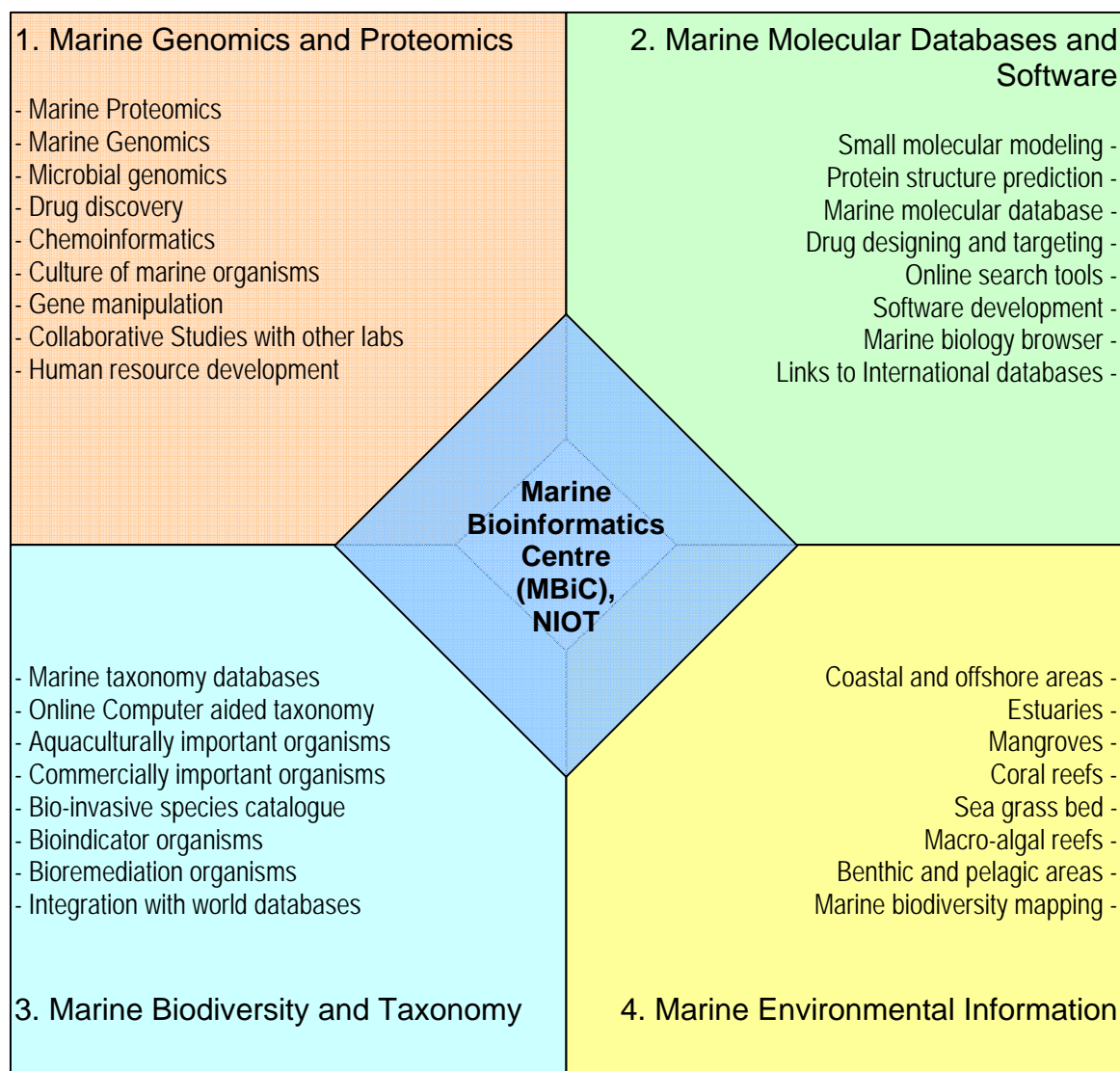
Fautin, (2000) assembled the database on sea anemones of the world from primary literature, which contains all definitive lists of nominal species, each in its original binomen, with full bibliographic citation and associated data. Even the most popular “Google Earth” software also integrating the biodiversity information in their Geographical Information System (GIS) based layer. Also similar efforts are underway to integrate bioinformatics with geoinformatics. GIS is successfully used for georeferenced biodiversity mapping.

In order to catalogue the marine species available in India, National Chemical Laboratory, Pune has initiated excellent work on marine biodiversity information. The collection in IndOBIS provides information about 35,000 marine species (www.ncbi.org). Also efforts are underway to catalogue the specimens available in Indian museum. For this a special software name “SAMPADA” has been developed by NCL (Chavan, *et. al.* 2005). Earlier few biodiversity catalogues of Indian marine species like crabs and shrimps were compiled by the Bioinformatics Center of National Institute of Oceanography (NIO). Presently NIO involved in carrying out the Indian part of Census of Marine life project. National Institute of Ocean Technology initiated work in marine bioinformatics during 2003. A website was launched for this purpose during October 2004.

Marine Bioinformatics Center (MBiC) of NIOT

In the ongoing program of Ocean Science and Technology for Islands (OSTI), NIOT a variety of biological, ecological, biodiversity, biochemical and biomolecular data are being collected for different projects from coastal and offshore areas of mainland India and Islands including Andaman and Nicobar, Lakshadweep and Gulf of Mannar. Also OSTI is carrying out the DOD sponsored multi-institutional programme of “Development of Potential Drugs From Sea” with the aim of isolation and identification of potential drug compounds for human diseases from the marine organisms collected from Andaman and Nicobar Islands. Also different biofouling related programme such as “Development of potential antifouling compounds from marine organisms” is also being carried out.

In the process of collecting and cataloguing marine organism for above purposes, the biodiversity data are being compiled in the form of database using marine bioinformatics approach. Also in support of laboratory research, various molecular biology databases on protein, gene and other biomolecules particularly from marine organism are being exploited with the open source database and software available through internet.



In the backdrop of above, in order to store, retrieve, process and disseminate data, the Marine Bioinformatics Centre (MBiC) was developed as first of its kind in India, as the supporting facility for the ongoing programmes of OSTI of NIOT during July 2003. MBiC is integrating the four subject areas such as (1) Biodiversity and Taxonomy of marine organisms, (2) Software and molecular databases for marine organism, (3) Laboratory studies on marine genomics and proteomics and (4) Marine environment. MBiC is planning to serve as one of the linking point for other institutions working in similar subject areas in India and abroad. The biology related information collected is being updated and made available for all user agencies with or without restriction, based on the importance of the data to OSTI and other sponsoring agencies. The selective distribution of database will serve the public as well as students and scientific community working in the areas of marine biology, biotechnology and bioinformatics. Based on the experience gained from different projects, OSTI is also conducting short term, wet-lab training programme for the students, researchers and lecturers of various institutions. The MBiC site can be visited with the link: <http://www.niot.res.in:82/mbic/index.html>.

To integrate the laboratory based research facilities, computer hardware with networking facilities have planned to be created in order to analyze and distribute the

databases of biodiversity, molecular sequence and structure, particularly for marine organisms.

Conclusions

The prospects for development of marine bioinformatics in India are tremendous. Since our search for useful genes such as potential drugs could be located from the organisms living in marine environment, development of separate database would be much helpful in getting quick results. At the same time the data could be used to compare with the land based organisms by interlinking different environment based databases. Thus in line with the development of bioinformatics elsewhere in the world, it is time to develop marine bioinformatics set up in the country, as we are fast developing our infrastructure in Information Technology and Biotechnology.

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