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Evolutionary Study Of Moray Eel With In-Silico Drug Design

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ABSTRACT

Phylogenetic is the study of evolutionary relationships among groups of organisms (e.g. Species, populations), which are discovered through molecular sequencing data and morphological data matrices.The family Muraenidae is one of the largest and most recognizable eel groups. Moray eels are key components of marine ecosystems but their relationships remain poorly understood. The phylogenetic relationships of the morays are examined herein using mitochondrial 12S and 16S sequence data, totalling 1673 bp for 139 taxa. In this study Moray eel and other 22 fish nucleotide sequences were compare and the phylogenetic tree was constructed by using POWER software. Moray eels, as well as many other eel like fish of the order Aguilliformes have toxic proteins in their blood. They are usually referred to as ichthyotoxins. These substances is there in moray eel serum. Serum Ichthyotoxin is very useful for curing kidney inflammation, heart problems and burning sensation of the kidneys with doubt of uremia. Fish is known to contain certain polyunsaturated fatty acids that can regulate prostaglandin synthesis and hence, induce wound healing. Insilico drug designing was done by using several Bioinformatics tools such as POWER, Clustal W, Chem Sketch, Openbabel GUI, Autodock 4, Cygwin Terminal, Chimera, Toxnet etc.

Keywords: Moray eel, Mitochondrial DNA or Protein,Ichthotoxin, Kidney Inflammation.

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INTRODUCTION

Evolution is the change in the inherited characteristics of biological populations over successive generations. Evolutionary processes give rise to diversity at every level of biological organisation, including species, individual organisms and molecules such as DNA and proteins [3, 4]. Change in the genetic composition of a population during successive generations, as a result of natural selection acting on the genetic variation among individuals, and resulting in the development of new species. The historical development of a related group of organisms; phylogeny. All Life on Earth evolved from a universal common ancestor approximately 3.8 billion years ago. Repeated speciation and the divergence of life can be inferred from shared sets of biochemical and morphological traits, or by shared DNA sequences [5, 8]. These homologous traits and sequences are more similar among organisms (species) that share a more recent common ancestor, and can be used to reconstruct evolutionary histories, using both existing species and the fossil record. Existing patterns of biodiversity have been shaped both by speciation and by extinction [2, 9].

Phylogenetic is the study of evolutionary relationships among groups of organisms (e.g. Species, populations), which are discovered through molecular sequencing data and morphological data matrices.

Moray eels are cosmopolitan eels of the family Muraenidae. The approximately 200 species in 15 genera are almost exclusively marine, but several species are regularly seen in brackish water, and a few, for example the freshwater moray (Gymnothoraxpolyuranodon), can sometimes be found in freshwater [4,10].With a maximum length of 11.5 cm (4.5 in), the smallest moray is likely the Snyder's moray (Anarchiasleucurus) [1], while the longest species, the slender giant moray (Strophidonsathete) reaches up to 4 m (13 ft) [5]. The largest in terms of total mass is the giant moray (Gymnothoraxjavanicus), which reaches 3 m (9.8 ft) in length and 30 kg (66 lb) in weight [6, 7].

Insilico drug design uses computational chemistry to discover, enhance, or study drugs and related biologically active molecules. The most fundamental goal is to predict whether a given molecule will bind to a target and if so how strongly. Molecular mechanics or molecular dynamics are most often used to predict the conformation of the small molecule and to model conformational changes in the biological target that may occur when the small molecule binds to it. Semi-empirical, ab initio quantum chemistry methods, or density functional theory are often used to provide optimized parameters for the molecular mechanics calculations and also provide an estimate of the electronic properties (electrostatic potential, polarizability, etc.) of the drug candidate that will influence binding affinity [11,12].

Dimericferredoxin-like protein from an unidentified marine microbe.This is the first structure of a protein derived from the metagenomic sequences collected during the Sorcerer II Global Ocean Sampling project. The crystal structure shows a barrel protein with a ferredoxin-like fold and a long chain fatty acid in a deep cleft (shaded red).

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MATERIALS AND METHODOLOGY

DATABASE USED

1. NCBI - NATIONAL CENTER FOR BIOTECHNOLOGICAL INFORMATION.
2. PDB – Protein Data Bank
3. GLIDA – Identify the ligand of proteins.

TOOLS USED

1. CLUSTAL W – Multiple Sequence Alignment.
2. POWER - PhylOgenetic Web Repeater
3. CHEM SKETCH - To produce professional looking structures and diagrams for reports and publications.
4. OPENBABEL GUI - Open Babel is a chemical toolbox designed to speak the many languages of chemical data.
5. AUTODOCK 4 - AutoDock is a molecularmodeling simulation software.
6. CYGWIN TERMINAL - is a Unix-like environment and command-line interface for Microsoft Windows.
7. CHIMERA - is an extensible program for interactive visualization and analysis of molecular structures and related data.

METHODS

STEP 1: Collect the sequences of selected species by using NCBI
STEP 2: Align the sequences of selected species: by using CLUSTAL W
STEP 3: Analyse the tree of selected species by using POWER
STEP 4: Find the protein structure for selected Fatty Acid for disease Kidney Inflammation by using PDB.
STEP 5: Find the ligand structure for selected protein by using GLIDA
STEP 6: Draw the Ligand molecule in Chem Sketch tool, which is an advanced drawing tool for chemicals.
STEP 7: Convert the ligand from mol file to PDB file by using openbabel.
STEP 8: Selected Protein 2OD6.
STEP 9: Work with Autodocksoftwate for docking the protein.
STEP 10: Work the Biological process like Docking, Molecular Modelling by using CYGWIN TERMINAL
STEP 11: Add input Docked protein in CHIMERA.

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RESULT AND DISCUSSION

Fig 1 :Multiple Sequence Alignment For SelecteSeqence:

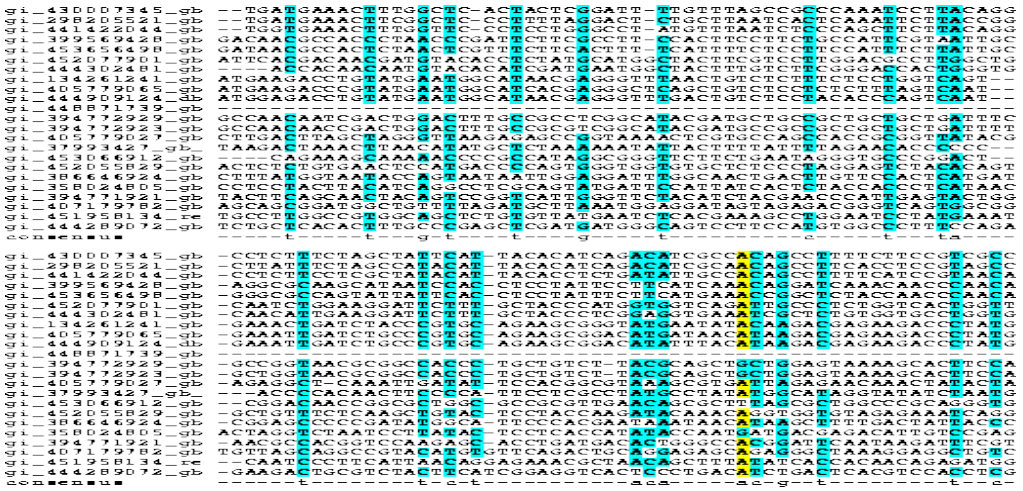
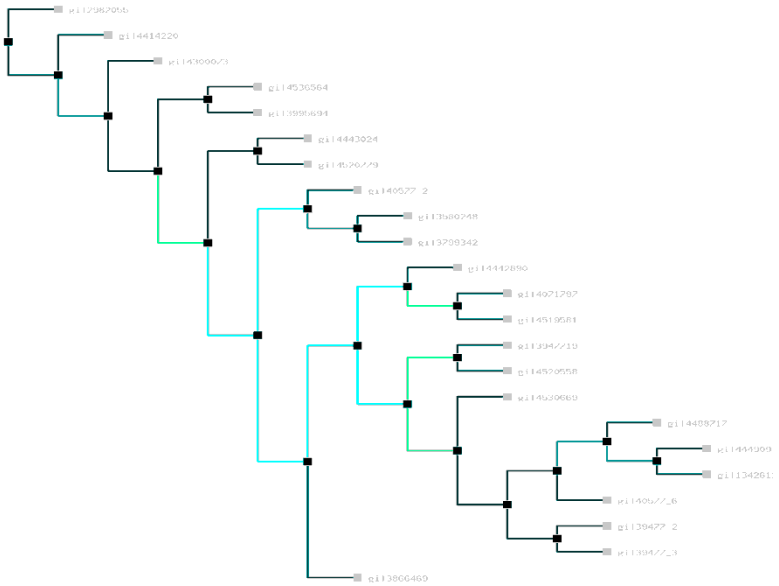


Fig 2: Phylogenetic relationship for selected species:

Color of line indicates how many times the group which consists of the species to the right of the fork occurred. :<=20 :>20 &<=40 :>40 &<=60 :>60 &<=80 :>80



SCREENING METHOD

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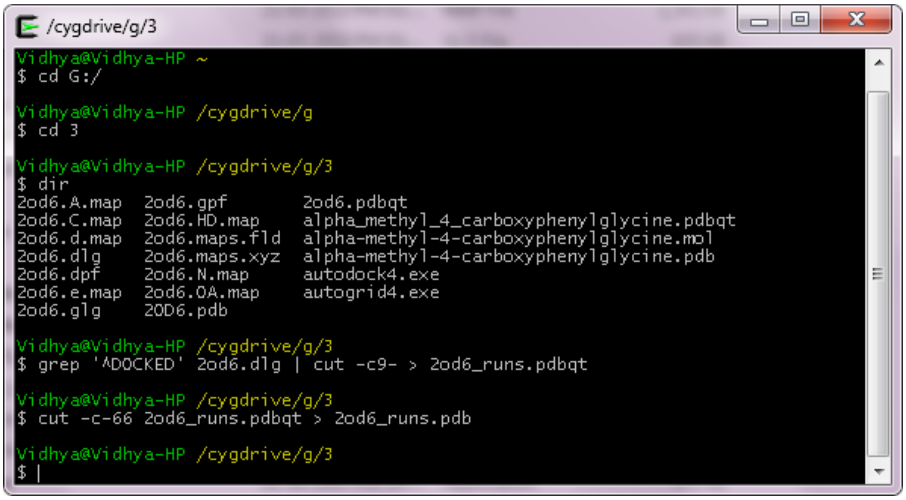
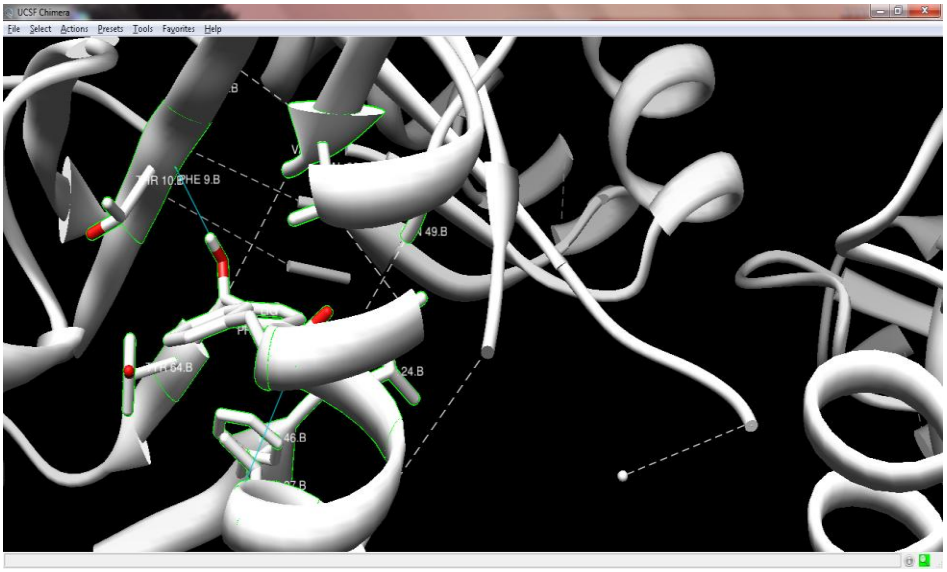
Fig 3: Cygwin is exclusively works for 2OD6 protein:



VISUALISATION METHOD

Fig 4: Chimera is a graphics program designed for the display and analysis of macromolecules, in a wide range of rendering styles.



DISCUSSION

From this study I came to know the closest relatives to the Mediterranean Moray are the many other species of morays. They are also closely related to bone fish, tarpon, ladyfish and saxpharynx fish. People commonly think that the electric eel and the Mediterranean moray must be very similar but in fact bony tongues, butterfly fish, elephant fish and featherbacks are closer on the tree of life. The electric eel and the Mediterranean moray do not show any relation until you go right back to its phylum, Chordata. And this serum Ichthyotoxin is very useful for curing kidney inflammation, heart problems and burning sensation of the kidneys with doubt of uremia.The bite of the Mediterranean moray

can be dangerous mainly due to the mildly toxic slime of its skin. It can be utilized fresh and eaten broiled, boiled and baked. The skin can be used for leather.

SUMMARY AND CONCLUTION

- Evolution study of moray eel with Insilco drug design was done by Phylogenetic Web Repeater and Auto Dock.
- Moray eels, as well as many other eel like fish of the order Aguilliformes have toxic proteins in their blood.
- They are usually referred to as ichthyotoxins. These substances are also haemolytic It is there in moray eel serum.
- Ichthyotoxin is very useful for curing kidney inflammation, heart problems and burning sensation of the kidneys with doubt of uremia.
- Fish is known to contain certain polyunsaturated fatty acids that can regulate prostaglandin synthesis and hence, induce wound healing.
- During the last two decades Polyunsaturated Fatty Acids (PUFA) has attracted great interest among scientists for their medicinal and nutritional properties.
- PUFA have been shown to have positive effects on cardiovascular diseases and cancers.
- Moray eels are having barrel protein with a ferredoxin-like fold and a long chain fatty acid.
- This protein can be used to create a new drug for kidney inflammation, cancer, cardiovascular.
- This protein was carried out using the method of drug design.
- Minimum the Binding Energy, Maximum will be its stability.
- The Protien-ligand complex showed the Bindind energy as -6.4
- 2Hydrogen bonds were formed with the Protein-ligand complex
- In future eel has to be used as a supplement in the products or it has to be used in the form of value added products or by-products.
- Consumption of this nutritious and less popular fishes, we can able to prevent over exploitation of other food fishes and can conserve the fish stock for future generations.
- These fishes may provide an alternate source of protein and fat for the population of developing countries.

REFERENCES

[1] Bshary R, Hohner A, Ait-el-Djoudi K, Fricke H. PLoS Biol. 4 (12): e431. doi:10.1371/journal.pbio.0040431. PMC 1750927. PMID 17147471.
[2] Cracraft, J.; Donoghue, M. J., eds. (2005). Oxford University Press. ISBN 0-19-517234-5.
[3] Dobzhansky, T.; Hecht, MK; Steere, WC (1968). Evolutionary biology volume 2 (1st ed.). New York: Appleton-Century-Crofts. pp. 1–34
[4] Froese, Rainer, and Daniel Pauly, eds. (2010). In FishBase. January 2010 version.
[5] Froese, Rainer, and Daniel Pauly, eds. (2010). In FishBase. January 2010 version.
[6] Froese, Rainer, and Daniel Pauly, eds. (2010). In FishBase. January 2010 version.
[7] Froese, Rainer, and Daniel Pauly, eds. (2012). in FishBase. May 2012 version.

[8] Hall, B. K.; Hallgrímsson, B., eds. (2008). Strickberger's Evolution (4th edition.). Jones & Bartlett. p. 762. ISBN 0-7637-0066-5.
[9] Panno, Joseph (2005). Facts on File INC.ISBN 0-8160-4946-7.
[10] P Sasal et al. Mar Ecol Prog Ser 1997;149: 61-71.
[11] Rajamani R, Good AC. Curr Opin Drug Discov Devel 2007;10(3):308–15.
[12] Wang R, Lai L, Wang S. J. Comput. Aided Mol Des 2002;16(1):11-26.