

**FUNCTIONAL ANNOTATION AND STRUCTURAL CHARACTERISATION OF OPSIN
PROTEIN IN *LEPTUCA PUGILATOR***S. Harshini¹ and Dr. K. Shoba^{*2}¹M.Sc., Biochemistry, P.G Research Department of Biochemistry, D.K.M College for Women (Autonomous), Vellore – 632001.²Assistant Professor, P.G. Research Department of Biochemistry, D.K.M College for Women (Autonomous), Vellore – 632001.***Corresponding Author: Dr. K. Shoba**

Assistant Professor, P.G. Research Department of Biochemistry, D.K.M College for Women (Autonomous), Vellore – 632001.

Article Received on 24/02/2023

Article Revised on 14/03/2023

Article Accepted on 04/04/2023

ABSTRACT

Fiddler crabs, which belong to the Ocypodidae family and subfamily Ucinae, are prevalent across the world's tropics and subtropics. Decapod crustaceans in the Uca family include *Leptuca pugilator* (Fiddler crabs), often known as the Atlantic sand fiddler crab or calling crab. They are brachyuran crabs from the Ocypodidae family, which are among the most recent aquatic organisms to reach the shore. Fiddler crabs are easily recognised by their distinctly asymmetrical claws, and they can be found in the Algarve regions of Portugal, West Africa, the Western Atlantic, the Eastern Pacific, and the Indo-Pacific. These species are present in seacoasts and brackish intertidal mud flats, lagoons and swamps, mangroves, salt marshes, and sandy or muddy coasts. Opsin, a photoreceptor protein found in fiddler crab species, functions as a fundamental piece of molecular machinery for colour perception and maybe trichromatic vision. The Protein and Nucleotide sequence of opsin protein from *Leptuca pugilator* were retrieved using NCBI database in fasta format. The Functional analysis were done through using AmiGO and T-COFFEE followed by Gene Expression analysis using JCAT Server. The Structural and Biophysical Characterization done through using SWISS-MODEL and Dipole Moment Server. Furthermore, our study investigates which shows the different insilico analysis of the Opsin protein in *Leptuca pugilator* which will increase the Opsin protein characteristics for the range of various medicinal applications.

KEYWORDS: Bioinformatics; *Leptuca pugilator*; Opsin; Photoreceptor protein; Functional Analysis; Structural Analysis; Medicinal applications.

INTRODUCTION

Crustacea (phylum Arthropoda), a group of invertebrate animals consisting of some 45,000 species distributed worldwide. Crabs, lobsters, shrimps, and wood lice are among the best-known crustaceans, but the group also includes an enormous variety of other forms without popular names.

Fiddler crabs, which are widespread throughout the world's tropics and subtropics, are members of the Ocypodidae family and subfamily Ucinae. The males' feeding behaviour, which comprised a tiny claw that travelled from the ground to its mouth in a manner like how a bow would be moved across a fiddle, gave rise to the name "Fiddler Crab" (the large claw). They are most closely related to the ghost crabs of the "sister genus", Ocypode. There are currently 97 recognised species and subspecies of fiddler crabs. Using a data matrix made up of 236 discrete morphological features, a phylogenetic analysis of 88 species was conducted after researching the systematic history of the genus and its members. Fiddler crabs have five pairs of legs, like other crabs do.

The first pair was known as chelipeds due to the presence of claws. The remaining four pairs are called legs or ambulatories and are utilised for walking. Fiddler crabs typically inhabit intertidal areas with muddy or sandy open flats of protected shoreline, river banks, salt marshes, and mangrove muck. While certain species can be found upstream to the highest intertidal limits of mangroves, others can be found in close contact to the sea.

Antimicrobial peptides and proteins form an important means of host defense in eukaryotes. Antimicrobial peptides serve as endogenous antibiotics as well as being involved in inflammation, wound healing, and adaptive immune system modulation. Many antimicrobial peptides have been identified and discovered in crabs over the past few years.

Leptuca pugilator (Fiddler crabs) also called Atlantic sand fiddler crab or calling crab are decapod crustaceans belong to the Uca family. They belong to the brachyuran crab family Ocypodidae and are the most recent species

of aquatic animal to reach the shore. In this Ocypodidae crab family, there are more than 100 species of fiddler crabs, which are divided among 11 of the 13 genera. Fiddler crabs are easily recognised by their distinctly asymmetrical claws, and they can be found in the Algarve regions of Portugal, West Africa, the Western Atlantic, the Eastern Pacific, and the Indo-Pacific. These species are present in seacoasts and brackish intertidal mud flats, lagoons and swamps, mangroves, salt marshes, and sandy or muddy coasts.

Rhodopsin and its relatives are photosensitive molecules composed of a protein component called an opsin and a non-protein moiety termed the chromophore retinal. GPCRs, also referred to as opsins, are found in animals. More than a thousand opsins have been found so far.

Opsins are membrane proteins that primarily function as light sensors in animals. They have molecular weights of 30–50 kDa and are related to the protein moiety of the photoreceptive molecule rhodopsin. Opsins are the common photoreceptor molecules found in all animal visual systems. During light absorption, they have the ability to switch from a resting state to a signalling state, activating the G protein and triggering a signalling cascade that results in physiological reactions. Opsins are proteins that bind to substances that react to light and are the basis for circadian rhythms, phototaxis, and other light-mediated responses in living things. Type I opsins, common in bacteria, evolved separately from type II opsins that are common in animals. This protein which is essential for normal colour vision. Photoreceptor cells are responsible for transduction of visual signals, and in arthropod compound eyes are clustered together ommatidia. Opsin protein present in *Leptuca pugilator* contains 380 amino acids with the molecular weight of 42.13926 KDA or 42139.26 g/mol. **Formula:** C₁₉₅₀H₂₉₆₂N₄₈₀O₅₁₇S₂₃

A collection of uncommon eye conditions known as retinitis pigmentosa (RP) affect the retina (the light-sensitive layer of tissue in the back of the eye). RP causes the retinal cells to gradually deteriorate over time, resulting in visual loss. RP is a hereditary condition that affects people from birth.

Cancer is any of a wide range of illnesses characterised by the growth of aberrant cells with the capacity to invade and damage healthy bodily tissue while dividing uncontrollably. It is frequently possible for cancer to spread throughout your body. Cancer is the second-leading cause of death in the world.

Lung adenocarcinoma is the most common primary lung cancer seen in the United States. Adenocarcinoma of the lung usually evolves from the mucosal glands and represents about 40% of all lung cancers. Lung adenocarcinoma usually occurs in the lung periphery, and in many cases, may be found in scars or areas of chronic inflammation.

In this research, functional analysis and structural analysis of opsin protein in *Leptuca pugilator* were done using various bioinformatics tools. So it will be very useful for further research process in drug designing for life threatening diseases.

METHODOLOGY

- Target protein sequence of Opsin in *Leptuca pugilator* were retrieved from NCBI database.
- Functional Annotation of Opsin protein in *Leptuca pugilator* were analysed using AmiGO.
- Phylogenetic relationships of annotated sequence were identified using T-COFFEE.
- The Gene Expression Analysis of Opsin protein were examined using JCAT Server.
- Structural Characterization like primary, secondary and tertiary structure of Opsin protein were done through using SAPS, PSIPRE and SWISS – MODEL.
- Biophysical characterization of Opsin protein in *Leptuca pugilator* were done using.

Dipole movement server

Results and Discussion

1. NCBI

PROTEIN SEQUENCE

>ADQ01811.1 opsin protein [Leptucapugilator]

MMAAMKVLNATGPQAMAYSGGYSFGFPEGVSVD
TDFVPDHIKHMHPHWEKFPFVNPMWHYLLGVVY
LFL
GAISLFGNGMVLFFFMKNNLRSPANLVANLAIF
DFIMMLKTPVFIVNSFNPEGVWGLGCDVFALMG
S
YAGIGGAVTNAAIAYDRYKTIKPFKMSRSTAF
LMVVGWVAYASPWSLLPLFGIWGRFVPEGFLTTC
FDYLSDELNTRSFVGAIFVFSYILPGMLIVFYFSQIF
SHVKSHEKAMHEQAKKMNVNLRNNAEANAQSA
EVRIAKVAMTNVALWLVCTWTPYAAVVVQGLFFN
QEDITPIVSMLPALLAKSASVYNPIIYAINHTKFR
LALTKQMPGFCIHEEEEEKASGADSKSTDTQKA

NUCLEOTIDE SEQUENCE

>HM765427.1:103-1245 Celucapugilatoropsin protein (Rh3) mRNA, complete cds

ATGATGGCTGCTATGAAGGTGCTTAACGCGACT
GGCCACAGGCCATGGCCTACGGCTCAGGAGGA
TATT
CTTTCGGTTTTTCCCGAAGGTGTATCTGTCACTGA
CTTTGTTCTGACCACATTAAGCATATGATTCAC
CC
TCACTGGGAAAAATTTCCACCCGTTAACCCCAT
GTGGCACTACCTTCTGGGTGTTGTGTATCTCTTC
CTC
GGCGCCATTTCTTGTTCGGCAACGGAATGGTG
CTGTTGTTGTTTCATGAAGAATAAGAATCTACGG
AGTC
CAGCCAACTACCTTGTAGCCAACCTGGCGATAT
TCGACTTCATAATGATGCTGAAAACGCCTGTGTT
CAT

TGTTAACTCCTTCAACGAGGGGCCGGTGTGGGG
 CAAGCTAGGATGTGACGTGTTTGCCTCATGGG
 CTCC
 TACGCTGGTATTGGCGGCGCTGTGACCAACGCT
 GCCATCGCCTATGATAGATATAAAACCATCGCC
 AAGC
 CGTTTGAAGCTAAGATGTCCCGCAGCACAGCCT
 TCCTCATGGTGGTGGGAATCTGGGCCTACGCCTC
 ACC
 ATGGTCCCTCCTTCCACTCTTTGGGATATGGGGA
 AGATTTCGTGCCAGAGGGCTTCCTGACAACTGC
 AGC
 TTCGACTACCTATCAGAGGACCTCAACACTCGCT
 CCTTCGTCGGTGCCATCTTCGTGTTCTCATACAT
 CC
 TGCCGGGGATGCTAATTGTCTACTTCTACAGCCA
 GATTTTCAGTCACGTCAAGAGCCACGAGAAGGC
 GAT

GCACGAACAGGCCAAGAAGATGAACGTCACCA
 ACCTCAGGTCCAATGCCGAGGCTAACGCTCAGT
 CTGCT
 GAGGTTTCGCATCGCCAAGGTGGCCATGACCAAC
 GTGGCTCTGTGGCTCGTCTGCTGGACGCCATACG
 CCG
 CCGTTGTTGTTTCAGGGTTTGTCTTCAACCAGGA
 GGACATCACTCCCATCGTTTCCATGTTGCCTGCC
 CT
 GCTGGCCAAAAGTGCCTCTGTCTACAATCCAAT
 AATTTACGCCATCAACCATAACCAATTCCGTCTG
 GCC
 CTCACGAAGCAGATGCCCCGGCTTCTGCATTTCAT
 GAGGAAGAGGAGAAGGCGTCCGGTGCTGACAG
 CAAGT
 CCACGGATACCCAAAAGCGTAA

The above results shows the protein and Nucleotide sequence of opsin protein in *Leptuca pugilator*.

2. AMIGO TOOL

AmiGO 2 Home Search Browse Tools & Resources Help Feedback About

Quick search Search

Information about Genes and gene products search

Filter results

Total gene product(s): 782

opsin

No current user filters.

Your search is pinned to these filters

- document_category: bioentity

Source

Organism

Total gene product(s): 782; showing: 1-10

Results count: 10

«First» «Prev» «Next» «Last» Custom DL (up to 100000)

Bookmark

Gene/product	Gene/product name	Organism	PANTHER family	Type	Source	Synonyms
<input type="checkbox"/> Cl-opsin1	Opsin	Ciona intestinalis	opsin pthr24240	protein	UniProtKB	UniProtKB:Q95P33 PTN000662302
<input type="checkbox"/> opsin3	G_PROTEIN_RECEP_F1_2 domain-containing protein	Ciona intestinalis	b2 bradykinin receptor/angiotensin II receptor pthr24228	protein	UniProtKB	UniProtKB:F6VG01 PTN000659602
<input type="checkbox"/> Gpr88	G-protein coupled receptor 88	Mus musculus	opsin pthr24240	protein_coding_gene	MGI	Strg
<input type="checkbox"/> Sag	S-antigen, retina and pineal gland (arrestin)	Mus musculus	arrestin pthr11792	protein_coding_gene	MGI	A930001K18Rik Arr1 arrestin 1 rod arrestin visual arrestin 1
<input type="checkbox"/> Opn4	opsin 4 (melanopsin)	Mus musculus	opsin pthr24240	protein_coding_gene	MGI	1110007J02Rik

S. No.	SPECIES	PROTEIN NAME
1.	<i>Leptucapugilator</i>	Opsin
2.	<i>Cionaintestinalis</i>	Opsin
3.	<i>Bostaurus</i>	Opsin, partial
4.	<i>Canis lupus familiaris</i>	Opsin 4
5.	<i>Gallus gallus</i>	Opsin
6.	<i>Strongylocentrotuspurpuratus</i>	Opsin, ultraviolet-sensitive-like
7.	<i>Gorilla gorillagorilla</i>	Short-wave-sensitive opsin 1
8.	<i>Anopheles gambiae</i>	Opsin, partial
9.	<i>Triboliumcastaneum</i>	Ultraviolet sensitive opsin
10.	<i>Xenopustropicalis</i>	Blue-sensitive opsin

The above results shows the Functional Annotation of Opsin protein in *Leptuca pugilator*.

3. PHYLOGENETIC ANALYSIS: T-COFFEE

T-Coffee

Input form | Web services | Help & Documentation | Bioinformatics Tools FAQ | Feedback

Tools > Multiple Sequence Alignment > T-Coffee

CLUSTAL W (1.83) multiple sequence alignment

```

AAA19495.1
AAB47565.1
ADQ01811.1
APU53810.1
APY20675.1
CAA76825.1
NP_001027727.1
XP_002937272.2
XP_004046224.1
XP_030842286.1

MSSNSSQAPP
MMAAMKVLNATGPGQAMAY-G-----SGGYSFGF-PEG-VSVTDVFV
MNPPSGPG-AQEPGCVATAA-----SPGR-WHGSPRSTVGLDQAL
MLHNLATPFFHQARTMETMA-----NHLG-WNV-PKD-
PD-
MNQWLETIMNE-RK-FEIVNSSLQGLLKPDLSLGMDDHV-TPT-VDLTDGV
MMSKGRADVRL-----EM-PD-DFYI-PI
MRKMSEEEFY-----L-F-
MKLLTRRDANQGPCD-----P-

-----N-----GTPGPFDPGPWPYQAPW-STYVGVAVLMTGTVVACASV
PDH--IKHMIHPH-----WEKFPFVN--PMWHYL-LGVVYFLGALISLF
PTGPTAAGARAAA-----WAPFPTVDVPDHAHYI-LGTVILLVGLTGML
-----ELIHIPQH-----WLVEPEPE-ASMHL-LALIYIGFFIMATI
PQC--K-DLNPPYVLKGDGWVPHISRANRSTYSF-LCVYMTFVFLSCS
PLE--TT-NI--SSLSPLVPQTHLGTGP-IFMS-ISAFMLFTIIFGFP
-----K-NI--SPVGPWDGPQYHIAPVW-AFYL-QAAFMTGTVFLIGFP
-----ESVGLF

VNLGLVIVVSIKYKKLRSPNLNLYILVNLAVADLLVTLGSSVS--LSNNING
GNGMVLFFFMKNNLRSPANLYLVANLAIFDFIMMLK-TPVF--IVNSFNE
GNLMVIYTFCTRGLRTPSNMFIINLAVSDFFMSFTQAPVF--FASSLHK
GNGLVWIFSTSKSLRTASNMFVVNLATCDFAMMIK-TPIF--IYNSFYR
-----VAEPLVHHHLR-----H-
LNILVIVATLKNKVLQRPLNYIIVNLAVVDLLSGFVGGFIS--IAANGAG
LNLLTIICTAKYKKLRSHLNYILVNLAVANLIVICFGSTTA--FYSFSQM
LNAMVLVATLRYKKLRQPLNYILVNVSFGGFLLCIFSVPV--FVASCNG
GNALVVISVIVGKKLRITITNVLVVNLAFADFMACIL-LPFQSAGLLSQTG

FFVFGRRMCELEGFMVSLTGIVGLWSLAILALERYVVVCKPLGDFQF--Q
GPVWGKLGCDVFALMGSYAGIGGAVTNAIAYDRYKTIKPFEEA-KM--S
RWLFGEAGCEFYAFCCGALFGITSMITLTAIALDRYLVITHPLAAVGV-VS
GFALGHLGCQIFAFIGSLSGIGAGMTNACIAYDRYTTITRPFDDG-KI--T
CAA76825.1
NP_001027727.1
XP_002937272.2
XP_004046224.1
XP_030842286.1

-----LRVLAADHLLVHLHPEGCVRS--R
YFFWGKTMQCIIEGYFVSNFVGVTGLLSIAVMAFERYFVICKPFPGVRF--E
YFSMGTLACKIEGFTATLGGIIGLWSLAVAFERFLVICKPMGSFTF--R
YFVFGRHVCALEGFLGTAGLVAGLVGWSLAFALAFERYIVICKPFGNFRF--S
GYPLDEAVCATVAAGVYISVCCSVHTLVATFVRWYVITRSIRGHRGLHT

RRHAVSGCAFTWGWALLWS-APPLLG-WSSYVPEGLRTSCGPNWYTGG--
RSTAFLMVVGIIWYASPS-LLPLFGIWGRFVEGFLTTCSFDYLS--
KRRALVLLGWLYALAWS-LPPFFG-WSAYVPEGLLTSCSWDYMSFT--
RTKALVMIIFVWGYTIPWA-VMPLLEIWGRFAPEGFLTACSFDTLDT--
EEHARAGQ-----EG-
EKHSIFGIVITWVSMFWN-TPPLIF-WDGYDEGLGTSCAPNWFVKE--
ESHAVLGCILTWMGLLAA-TPPLLG-WSRYIPEGLQCSCGPDWYTVNNK
SKHALTVLATWTIGIGVS-IPPPFG-WSRYIPEGLQCSCGPDWYTVGTK
PKKIAIMVLIWIFSISFMVVPFVG-VGKFGYSTYYGTCSL---TDT--

-----SYMIVLMVTCCFIPLSVIILCYLQVWLAIKRAVAKQ-----
SNNNSYILSLFVTCFVPLPLSLILFSYTNLLTLRAAAAQ-----
LNTRSFVGAIFVFSYILPGMLIVFYFSQIFSHVKSHEKAMHEQAKKMNVT
PSVRAYTMLLFCFVFFPLPLLVIVYCYVFIFRAIRETGQALQTF--RACEG
FDNHMFVTSIFICSYVIPMSMIIYFYSQIVSKVFSHEKALREQAKKMNVE
-----NVA
KRERLFIILYFYFCFVIPLAVIMICYGKILTLRQIAKE-----
WNNESYVIFLFCFCFGFPLAIIVFSYGRLLTLHAVAQK-----
YRSESYTWFLFIFCFIVPLSLICFSYQTLRLAKAVAAQ-----
NELEFYFILLQGTLVANALLFVIFYIRILCHVLRHNKQFRDKYA-VDEH

```

AAA19495.1	---	Q-KDSESTQKAEKEVTRMVMVMIFAYCLCWGPYTFACFAAAQPGYA
AAB47565.1	---	Q-KEADTTQRAEREVTRMVIIVMMAFLLCWLPYSTFALVVATHKGI
ADQ01811.1	---	NLRS-NAEANAQSAEVRIAKVAMTNVALWLCWTPYAAVYVQGLFFNQED
APU53810.1	---	GARS-PRQRQLQREWKMAKMEILLVILLFVLSWAPYSAVALTAFAGYSHV
APY20675.1	---	SLRSNQSQQASQSAELRIAKAAIAICSLFVASWTPYAVLALIGAFGDQSL
CAA76825.1	---	SLRT-QEAQNTSTEMKLAKVALVTISLWFMWTPYLVINFTGIF-KAAP
NP_001027727.1	---	S-SLSG-GTSPGEVTKMVVVMVTAFAVFCWLPYAAFAMYNVNVNPEAQ
XP_002937272.2	---	Q-EQSATTQKAEREVTRMVIIVMAGFLVCWLPYASFALWSVTHRGEL
XP_004046224.1	---	Q-QESATTQKAEREVSVMVVMVGSFCVCYVPYAAFAMYMVNNRNHG
XP_030842286.1	---	TCSN-STEAHQDKASSSIA---

AAA19495.1	FH---	---
AAB47565.1	IQPVLASLPYSYFSKTATVYNPIIYVFM-NKQFQSCLEMLCCGYQPQ-RT	---
ADQ01811.1	ITPIVSMPLALLAKSASVYNPIIYAIN-HTKFRLLALTQKMPGFCIHE-EE	---
APU53810.1	LTPYMNSVPAVIAKASAIHNPPIIYAIT-HPKYRMAIAQHLPCLGVLLGVS	---
APY20675.1	LTPGVTMVPACACKFVACLDPYVYVYIS-HPKYRLELQKRLPWLAIKE-TA	---
CAA76825.1	ISPLATIRGSLFAKANAVYNPIVYG---	---
NP_001027727.1	IDYALGAAPAFFAKTATIYNPLIYIGL-NRQFRDCVVRMIFNGRNPWVDE	---
XP_002937272.2	FDLRMASIPSVFSKASTVYNPFIYIFM-NRQFRSCMMKMFVCGKNPLGDD	---
XP_004046224.1	LDLRLVTIPSFSSKACIYNPIIYCFM-NKQFQACIMKMCVCG-KA-MTDE	---
XP_030842286.1	---	AGSRPPLNYCLILNTE---

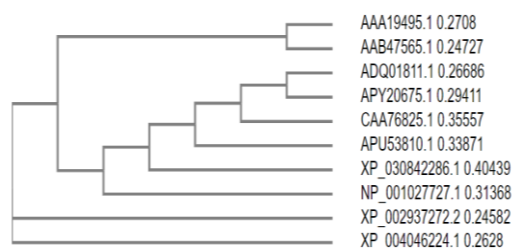
AAA19495.1	GK--AS--	PGTGPHADVTAA
AAB47565.1	-E-KA--	SGAD--SKSTDT
ADQ01811.1	GQ--RTG	PGYASYRSTHRSTLSSQA--SDLSWISGRRRQASLGSESEVGVW
APU53810.1	AS--ET--	QSTT--TENTTT
APY20675.1	---	---
CAA76825.1	---	---
NP_001027727.1	LVGSQV	S--STGSQTLTAV
XP_002937272.2	EE--TS--	V--SGSTQVSSV
XP_004046224.1	SD--TC--	S--SQKTEVSTV
XP_030842286.1	---	---

AAA19495.1	---	GLR--	---	N
AAB47565.1	---	QK--	---	---
ADQ01811.1	---	---	---	---
APU53810.1	---	MDTEAAAVWGAAQ	PAGGRFLCTQGLEDAEAKAPLRPRGQAVETPGKVVT	---
APY20675.1	---	QSAT--	---	---
CAA76825.1	---	---	---	---
NP_001027727.1	---	SS--	---	N
XP_002937272.2	---	SS--	---	S
XP_004046224.1	---	SS--	---	T
XP_030842286.1	---	---	---	---

AAA19495.1	KVMP--	AHPV--	---
AAB47565.1	---	---	A
ADQ01811.1	ATAAWDPPLHPGWAFQ	---	---
APU53810.1	---	T--T--	T
APY20675.1	---	---	---
CAA76825.1	---	---	---
NP_001027727.1	KVAP--	A--	---
XP_002937272.2	QVAP--	S--	---
XP_004046224.1	QVGP--	N--	---
XP_030842286.1	---	---	---

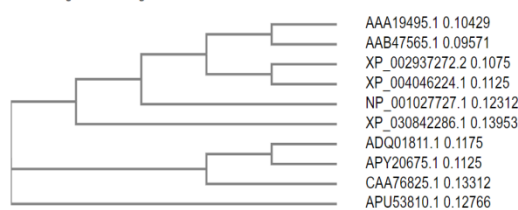
Phylogenetic Tree

Branch length: ☒ Cladogram ☐ Real



Phylogram

Branch length: ☒ Cladogram ☐ Real



Guide Tree

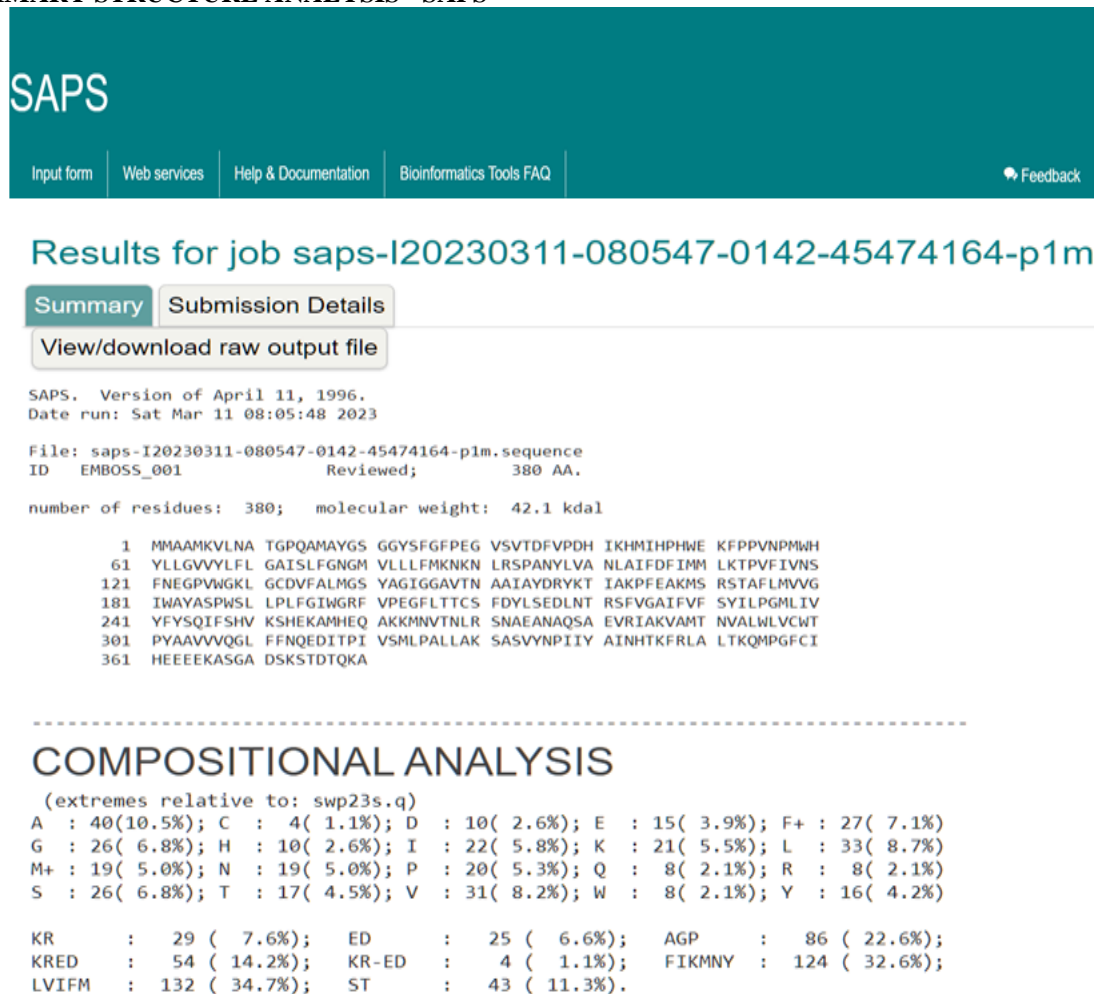
The above resultsshow the evolutionary relationship of opsin protein with annotated sequence.

4. GENE EXPRESSION ANALYSIS - JCAT

S.No.	Protein Name	Species	CAI Value
1.	Opsin	<i>Leptucapugilator</i>	0.955261450769427

The above results shows the CAI Value of opsin protein (*Leptuca pugilator*) where the value indicates that gene expression is highly expressed.

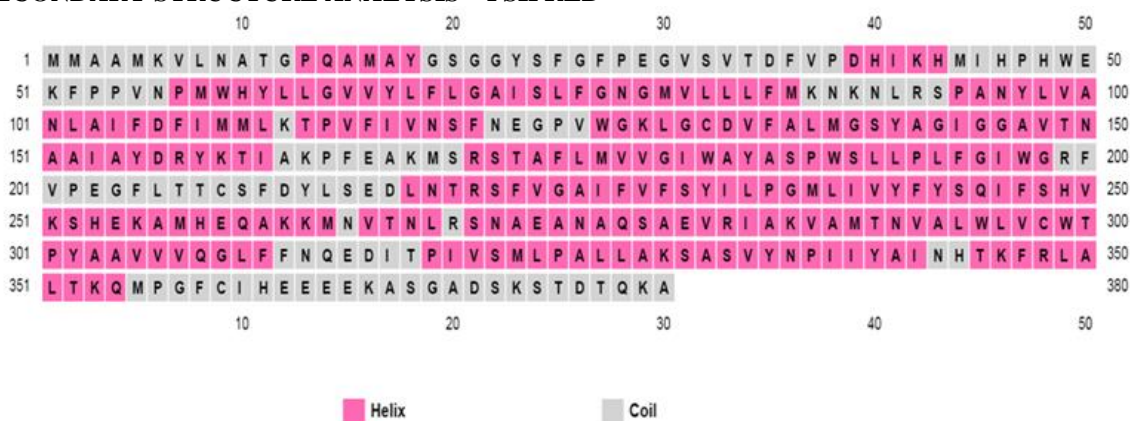
5. PRIMARY STRUCTURE ANALYSIS - SAPS



The above results shows the primary structure analysis like molecular weight, number of amino acids and

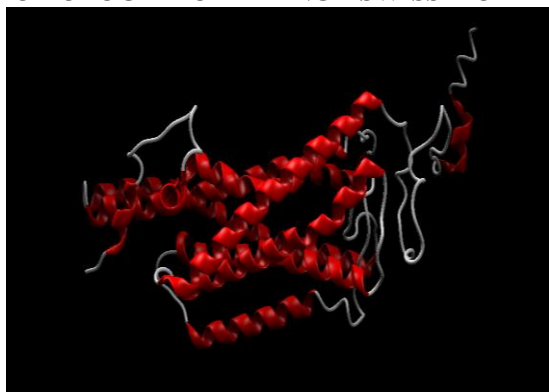
compositional analysis of opsin protein in *Leptuca pugilator*.

6. SECONDARY STRUCTURE ANALYSIS – PSIPRED

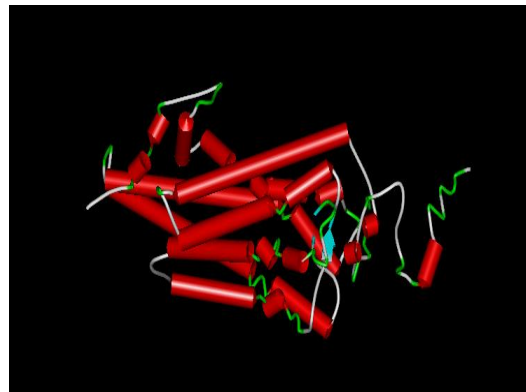


The above resultsshow the secondary structure analysis of opsin protein in *Leptuca pugilator*. i.e., pink colour indicates the Helix region and grey colour indicates the coil region identified in opsin protein.

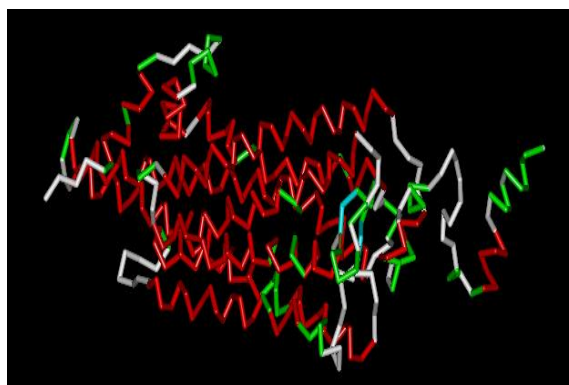
7. HOMOLOGY MODELLING – SWISS MODEL



Ribbon Structure



Pipeline Structure



Stick Structure


Swiss model - Discovery studio


The above results shows the 3 D Structure of Opsin Protein in *Leptuca pugilator*.


8. BIOPHYSICAL CHARACTERIZATION – DIPOLE MOMENT SERVER

Dipole moment for

	No. of Chains=1		Elongated							
	No.Atoms	No.Res.	R _M	Pos.Res.	Neg.Res.	Charge	Dipole	Quadrupole	Crg./Nat.	Dip./Nat.
Value	2483.	314.	376.77	22.	18.	4.	1180.	2235.	0.0016	0.4751
No.Dev.Units	0.61	0.60	0.76	-0.16	-0.50	0.95	1.52	-0.07	0.53	0.37

 Dipole vector (in atomic units): -56.20 -239.10 2.93

 Mass Moments vector: 415.67 917.53 512.83

 Open a larger Jmol window.



Biophysical characterization of Opsin protein in *Leptuca pugilator* were done using dipole movement server. The dipole movement server shows the net charge, dipole moment and mean radius of 3D protein structure and its

constituents peptide chains and display the dipole vector superimposed on a ribbon backbone of the protein.

CONCLUSION

In Humans, the overexpression of opsin protein (Melanopsin / OPN 4) in lung cancer cells and tissues which leads to **Lung Adenocarcinoma**. People with this condition suffers from breathing difficulties, pneumonia, pleural effusion, metastasis and Horner's syndrome (eye muscle problems). Retinal degeneration is brought on by the genetic condition known as **retinitis pigmentosa**, or RP. Those who have this condition face a gradual loss of vision. It is brought on by the deterioration of photoreceptors. Over time, it is inevitable to experience central visual impairment, reduced rods and cones, colour perception, and restricted vision. Rhodopsin, a photopigment, will decline as a result of the damage in the rods. So there will be lacking of Opsin in the retina. Opsin protein is one of the most important antimicrobial protein. It is also responsible for many life threatening diseases. In this study opsin protein in *Leptuca pugilator* was selected. The Sequence of Opsin protein in *Leptuca pugilator* were retrieved using NCBI Database in fasta format and the protein were subjected to several insilico analysis like Functional Annotation, Phylogenetic relationship, Gene expression Analysis, Structural and Biophysical Characterization. Therefore, the Antimicrobial Protein Opsin in *Leptuca pugilator* may have potential application in the treatment of Lung Adenocarcinoma and Retinitis Pigmentosa.

REFERENCE

- G. Vidal-Gadea; M.D. Rinehart; J.H. Belanger (March). "Skeletal adaptations for forward and sideways walking in three species of decapod crustaceans". *Arthropod Structure & Development*, 2008; 37(2): 179 – 194. doi:10.1016/j.asd.2007.06.002. PMID 18089130
- Adams DC, Collyer A, Kaliontzopoulou A. 2020. Geomorph: software for geometric morphometric analyses. R package version 3.2.1. <https://cran.r-project.org/package=geomorph>. Accessed, 27 January 2020.
- B.Kavipriya, T.Nalini, K.Shoba, &B.Deevika, Protein Designing studies and Biophysical Characterization of Gaucher Disease, *International Journal of Pharmacy and Biological Sciences*, 2019; 9(2): 303-313. ISSN: 2230-7605.
- Capparelli MV, Abessa DM, McNamara JC. Effects of metal contamination in situ on osmoregulation and oxygen consumption in the mudflat fiddler crab *Ucarapax* (Ocypodidae, Brachyura). *CompBiochemPhysiol C Toxicol Pharmacol*, 2016 Jul-Aug; 185-186: 102-111.
- Dr Leo W H Tan and Peter K L Ng, Fiddler Crab, A Guide to Seashore Life, Singapore Science Centre.
- Dr. K. Shoba, S. Haritha and S. Harshini, Antimicrobial Peptides and its functional studies on *Austrucaannulipes*, *Recent Advancements in commerce and management, Innovation and Entrepreneurship, Science and Technology, Pharmacy and health, Humanities and social science, education, language and literature, & Environment and Sustainability*, International Publications, August 2022; 1: 186-194. ISBN - 978-93-94819-06-1.
- Epub Mar 16.crabs of the world (Ocypodidae: genus Uca). Princeton University Press, Princeton, New Jersey, 2016; 736.
- Guaní-Guerra E, Santos-Mendoza T, Lugo-Reyes SO, Terán LM, Antimicrobial peptides: general overview and clinical implications in human health and disease, *Clin. Immuno*, 2010; 135: 1-11.
- Guinot, Danièle (11-14). "New hypotheses concerning the earliest brachyurans (Crustacea, Decapoda, Brachyura)". *Geodiversitas*, 2019; 41(1): 747. doi:10.5252/geodiversitas2019v41a22.
- H L Clark, P R Y Backwell Territorial battles between fiddler crab 1. 1. species, *Affiliationsexpand*, PMID: 28280560.
- Hale JD, Hancock RE, Alternative mechanisms of action of cationic antimicrobial peptides on bacteria, *Expert Rev. Anti. Infect. Ther*, 2007; 5: 951-959.
- Hsi-Te Shih , Joseph Poupin A New Fiddler Crab of *AustrucaBott*, Closely Related to *A. perplexa* (H. Milne Edwards, 1852) (Crustacea: Brachyura: Ocypodidae), from the South Pacific Islands, *Affiliationsexpand*, PMID: 33262849, PMCID: PMC7688405, 1973.
- Klingenberg CP, Barluenga M, Meyer A. Shape analysis of symmetric structures: quantifying variation among individuals and asymmetry. *Evolution*, 2002; 56: 1909–1920. doi:10.1111/j.0014-3820.2002.tb00117.x. [PubMed]
- Lanfear R, Frandsen PB, Wright AM, Senfeld T, Calcott B. PartitionFinder 2: new methods for selecting partitioned models of evolution for molecular and morphological phylogenetic analyses *MolBiolEvol*, 2017; 34: 772–773. doi:10.1093/molbev/msw260. [PubMed]
- Mangale V. Y. and Kulkarni B. G Biodiversity Of Fiddler Crabs In Mumbai Region, *Trends in life sciences*, 2013; 2,4.
- N Zolkhiflee, S Shuhaida & KYahya Carapace width-weight relationship and condition factor of *Austrucaannulipes* in mangroves of Penang Island. *IOP Publishing*, 2020; 736: 1-3.
- P. Chen; A.Y. Lin; J. McKittrick; M.A. Meyers (May). "Structure and mechanical properties of crab exoskeletons". *ActaBiomaterialia*, 2008; 4(3): 587– 596. doi:10.1016/j.actbio.2007.12.010. PMID 18299257.
- Rafael D Rosa and Margherita A Barracco Antimicrobial peptides in crustaceans, *Invertebrate Survival Journal*, 2010; 7: 262-284.
- Roy AK, RumpiGhosh, Upadhayay AD. In silico analysis, structure modeling and phosphorylation site prediction of vitellogenin protein from *Gibelioncatla*. *JApplBiotechnolBioeng*, 2017; 3(1): 265-270. DOI: 10.15406/jab,2017.03.00055.
- Shoba K., Manjuladevi M, Dr. Mazher sultana, Biochemical analysis and gene expression profiling on collagenase protein in fiddler crab, *World journal*

- of pharmacy and pharmaceutical sciences, issn 2278 – 4357, 6(3): 747-756.
21. Shoba K., Sowmiya S and Dr. Mazher sultana, World Journal of Pharmaceutical and Life Sciences, ISSN 2454-2229, 3(1): 427-436.
 22. Shoba K., Hebsibah Elsie B. And Bavyasri S. Insilico Peptide Modeling Studies And Structural Analysis On Ribulose -1, 5 Bisphosphate Carboxylase In *GracilariaEdulis*, World Journal Of Pharmacy And Pharmaceutical Sciences, 2018; 7(3): 1086- 1095, Issn 2278 – 4357.
 23. Shoba K., Kalpana K., Protein Modeling and Drug Docking Studies on Potential Protein Target (E. coli–dosP) and Compound Aldehyde (Sumatriptan) using Bioinformatics Tools. Research & Reviews: A Journal of Bioinformatics, 2018; 5(3): 9–18.
 24. Shoba. K, Hebsibah Elsie. B and Jayakumari. S. Sathya. R. Insilico Structural Analysis and Drug Docking Studies On Ribulose -1, 5 Bisphosphate Carboxylase In *GracilariaEdulis*. International journal of advanced research, 2018; 6(9): 159-165] (ISSN 2320- 5407).
 25. Shoba. K, Nithya.G and Deepa.L. Biochemical Analysis and Peptide Modeling of Lysozyme in Indian Fenneropenaeusindicus shrimp species. International journal of advanced research, 2018; 6(9): 159-165. (ISSN 2320-5407).
 26. Shoba.k and Dr. Mazher sultana, Three - dimensional structure and motif prediction studies on collagenase protein in fiddler crab, International journal of novel trends in pharmaceutical sciences, Issn: 2277 – 2782, 6(4): 79 – 83.
 27. Shoba.K and Moganapriya.S, Insilico homology structure and functional site prediction studies on collagenase protein in fiddler crab, Journal of University of Shangai for Science and Technology, 2022; 24(4): 323-330. ISSN:1007-6735.
 28. Shoba.K, Hebsibahelsie.B, insilico homology modeling ofribulose-1, 5bisphosphate carboxylase protein in *gracilariaedulis*, world journal of pharmacy and pharmaceutical sciences, 2017; 6(8): 396-406. issn 2278 – 4357.
 29. Shoba.K, Lavanya.G, Identification Of De Novo Peptide And Motif Prediction On Porphyrin Protein (Hmbs) Using Insilico Tools, Universal Journal Of Pharmacy, 2018; 8(1). Issn2320-303x.
 30. Shoba.K, Lavanya.G, Tertiary Structural Prediction And Drug Binding Studies On Mutated Gene (Hmbs) In Human Porphyrin, International Journal Of Novel Trends In Pharmaceutical Science, 2018; Issn 2277 -2782, 8(1).
 31. Swathi.D, Sangeetha.D, and Shoba.K, Biophysical characterization & functional annotation of enolase protein in *Anustrcaannlipes*, International journal of Pharmaceutical sciences and Research, 2023; 14(1): 366-372, ISSN: 2320 – 5148.
 32. Usha.K and Shoba.K, Functional analysis & peptide structure modeling of sphystatin protein in *scyllaparamamosain*, International Journal of Current Science and Technology, 2019; 701(A): 666-669, January, ISSN: 2320-8090.
 33. UthaiKuhapong a, FahmidaWazedTinaa, KiadtisakLimsakuna SurananWatthanaphonga, EkapoteLuckbana, TeethatPiyakuna (2020), Temporal variations in the air, soil and fiddler crab (*Austrucaerplexa*) burrow temperatures in southern Thailand. Journal of Animal Behaviour and Biometerology, 2113; 1.