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RESEARCH ARTICLE

HOMOLOGY MODELING AND INSILICO APPROACH OF *CLEOME GYNANDRA - AN* INDIGENOUS MEDICINAL PLANT

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ABSTRACT

Cleome gynandra is a widespread medicinal plant belonging to the family Capparaceae. In Ayurvedic medicine *C. gynandra* is a main component in Narayana Churna. It has numerous properties like Anthelmintic, in ear diseases, pruritis and several other diseases like gastro intestinal disorders and gastrointestinal infections etc. This is an effort to gather and document evidence on different features of *C. gynnadra* and highlight the need for survey and development. In this current study, nine proteins of *C. gynandra* were identify by using of bioinformatics tools. The bioinformatic study of the characterization of proteins of *C. gynandra* were using Expasy Protparam server, 3D structure was done using SWISS MODEL. Plants of different family show uniqueness 98% and above were particular and its sequences retrieved, aligned using Clustal Omega. Secondary Structure prediction exhibited that α – helix, random coil, β – turn and long strand leads. Phylogenetic analysis of Glyceraldehyde 3 PO4 of *C. gynandra* exposes that the Capparaceae families are closely related. *Insilco* sequence analysis of *C. gynandra* showed that these proteins taken from different organisms linked organized evolutionarily as they possess conserved regions in their protein sequences. These results will be helpful to further study on *C. gynandra* protein functions at molecular or structural levels and also valuable in homology modelling and insilico approach.

Keywords: *Cleome gynandra,* Phylogenetic analysis, Homology modelling, Secondary structure, Capparaceae.

1. INTRODUCTION

Cleome gynandra is a common, plant and its native of Africa and now largely distributed in tropical and subtropical regions throughout the world [1]. *C. gynandra* is a richly current species and produces as a weed in common barren land and in crop fields throughout India. In all over the world in diverse countries it is used to treat many ailments in their traditional system and it is also used in many traditional food systems for its notable nutritional and antioxidant properties. In India alone it is used by the traditional therapists for many diseases e.g... epilepsy, irritable bowel syndrome and in protozoal and worm infections [2].

In the process of novel drug discovery, the application of virtual screening and network pharmacology can improve active compounds among the applicants and effectively indicate the mechanism of action of medicinal plants, reducing the cost and increasing the efficiency of the whole procedure [3]. We also review common databases, software programs and website tools that can be used for virtual screening and pharmacological network construction. Furthermore, we accomplish with a simple example that illustrates the whole methodology, and we present outlooks on the development and application of this in silico methodology to reveal the pharmacological basis of the effects of traditional medicinal plants [4].

The lot of protein sequences that can be modelled, as well as the exactness of the prediction, is growing gradually because of the growth and number of known protein sequences and structures as well as advances in the modelling software. It is now possible to model, with useful exactness. Significant parts of approximately one half of all known protein sequences [5]. Despite progress in an initio protein structure prediction, qualified modelling remains the only process that can constantly predict the 3-D structure of a protein with accuracy comparable to a low-resolution experimentally determined structure. Even models

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with mistakes may be useful, because some features of function can be predictable from only coarse structural features [6].

However there remains still a huge scope for use of current scientific methods - genomics, proteomics and bioinformatics in the *C. gynandra.* Bioinformatics shall enable study and integration of information from these linked fields to enable the identification of genes and gene products and explain the useful relationships between genotype and observed phenotype [7]. This study report affords a state-of-the-art overview of bioinformatics study of *C. gynandra* with importance on the new development and future plans, which shall provide tools and properties essential to know and help advances in this vital field [8].

2. MATERIALS AND METHODS

2.1. Sequence Retrieval

The FASTA sequence of the proteins was retrieved by using of Genbank database hosted by the NCBI [9].

2.1.1. Primary Structure Prediction

For Physio-chemical description, theoretical Isoelectric Point (pI), molecular weight, total number of positive and negative residues, extinction coefficient, instability index, aliphatic index and grand average of hydropathy (GRAVY) were computed using the Expasy Protparm server [10]

2.1.2. Secondary Structure Prediction

SOPMA (Self Optimized Prediction Method with Alignment) was used for the secondary structure prediction.

2.1.3. Functional Characterization

SOSUI tool used to describe whether the protein is soluble or transmembrane in nature. InterPro is a combined resource for protein families, domains and functional sites. Inter Pro incorporates the major protein signature databases into a single resource. Superfamily and molecular function were predicted by Inter pro protein sequencing and classification.

Sequence alignment of was performed using pair wise sequence alignment tool (NCBI- BLAST) (http://blast.ncbi.nlm.nih.gov/Blast.cgi) and multiple sequence alignment was done using the EBI-CLUSTAL OMEGA (http://www.ebi.ac.uk/Tools/msa/clustalo/) tool. Clustal Omega also has powerful features for adding sequences to and exploiting information in existing alignments, making use of the vast amount of precomputed information in public databases like Pfam [11].The importance of this work was to novelty the regions of sequence comparison, which in other words allows us to yield functional and evolutionary relationships among the proteins considered in this study.

The phylogenetic analysis of ten proteins was completed to determine the number of proteins that part common structural and functional features. As an input to Clustal Omega all sequences in FASTA formats were supplied with default options. The output was analysed for sequences that are aligned for the complete length, scores, alignment, conserved residues, substitutes and semi conserved substituted residue patterns. The phylogenetic tree was constructed based on the bootstrap Neighbour Joining (NJ) method [12]. The steadiness of the internal nodes was assessed by bootstrap analysis with 1000 replicates.

3. RESULTS AND DISCUSSION

The plant is an herb Caparaceae family. It is commonly known as African spider. The plant is natural to tropical forest Tropical and subtropical dry broadleaf forests habitats *C. gynandra* contains vast number of bioactive constituents.

In addition, it has extensive variety of pharmacological activities. Hence the plant can be used to treat numerous diseases, and can be used in numerous pharmaceutical inventions and drug development studies [13].

The primary structure prediction was complete with the help of protparam tool (Table 2). The parameters were computed using Expasy‘s protparam tool which showed that the molecular weights for two different proteins as 18612.15 (Ribulose bisphosphate carboxylase), 50287.84 (Maturase K), 50287.84 (Replication associated protein), 24910.25 (Transcription activator protein), 37330.21 (Capsid Protein), 19733.29 (Protein V2), 24212.76 (Replication enhancer), 15527.41 (C4 Protein), 15636.60 (AC4). The pI of five protein was less than 2 which specified that they are acidic and one protein was greater than 7 which exhibited that it is basic in character. The proteins are created to be compact and stable at their pI. Among the nine five proteins are presented instability index lesser than 40, signifying that the protein is stable.

Table 1.Primary structure of *Cleome gynandra*

S.NO	ACCESSION NUMBER	PROTEIN NAME	LENGTH	MOLECULAR WEIGHT	P I	R-	R+	E C	I I	A I	GRAVY
1.	ALH24879.1	RIBULOSE BIS PHOSPHATE CARBOXYLASE LARGE CHAIN (RuBisCo large Subunit)	169	18612.15	5.75	20	18	27515	27.43	79.11	-0.299
2.	ACB15320.1	MATURASE K	558	66321.02	9.56	45	73	81305	37.22	94.82	-0.203
3.	ACG60169.1	REPLICATION ASSOCIATED PROTEIN	438	50287.84	6.56	51	49	59860	38.05	72.97	-0.545
4.	ACG60168.1	TRANSCRIPTIONAL ACTIVATOR PROTEIN	214	24910.25	9.85	17	28	19855	51.42	62.48	-0.632
5.	ACI15834.1	CAPSID PROTEIN	318	37330.21	9.80	29	49	41745	43.19	64.62	-0.558
6.	ACT75667.1	PROTEIN V2	169	19733.29	5.62	23	17	11960	39.51	63.43	-0.586
7.	ACG60167.1	REPLICATION ENHANCER	202	24212.76	8.34	19	21	34170	27.71	85.45	-0.336
8.	ACT75672.1	C4 PROTEIN	138	15527.41	6.65	12	12	5625	58.34	57.25	-0.609
9.	ACG60170.1	AC4	136	15636.60	8.61	12	14	12615	56.30	56.03	-0.655

Table 2. Secondary structure results of C*leome gynandra*

S.NO:	ACCESSION NUMBER	STRUCTURE			
		ALPHA HELIX	EXTENDED STRAND	BETA CHAIN	RANDOM COIL
1.	ALH24879.1	27.22%	22.49%	2.96%	47.34%
2.	ACB15320.1	50.10%	17.10%	4.17%	28.63%
3.	ACG60169.1	31.39%	16.39%	5.56%	46.67%
4.	ACG60168.1	14.18%	14.93%	5.22%	65.67%
5.	ACI15834.1	20.70%	24.61%	3.52%	51.17%
6.	ACT75667.1	44.35%	4.35%	4.35%	46.96%
7.	ACG60167.1	40.30%	29.10%	4.48%	26.12%
8.	ACT75672.1	21.18%	14.12%	3.53%	61.18%
9.	ACG60170.1	23.54%	9.41%	3.53%	63.53%

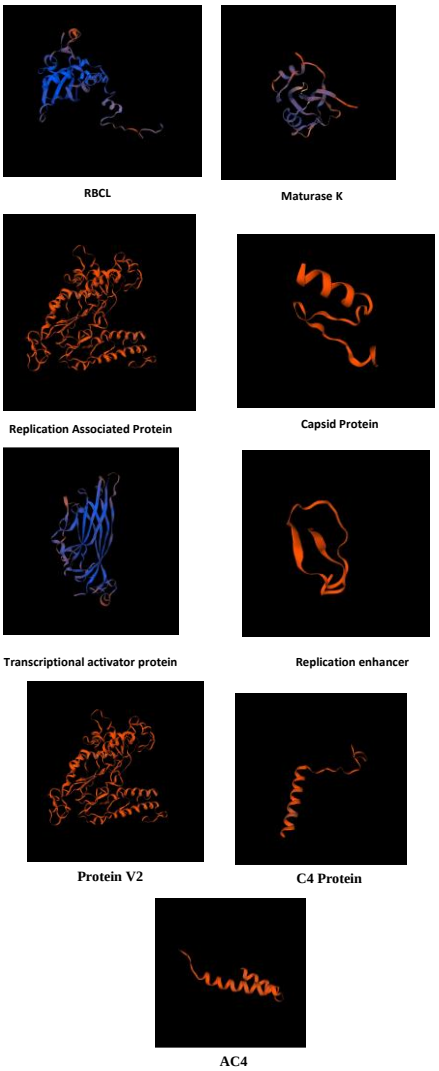
Aliphatic index of the proteins extended between 56.03 - 94.82. The computed extinction coefficients help in the quantifiable study of protein–protein and protein–ligand relations in solution. The range of GRAVY (Grand Average of Hydropathicity) of *C. gynandra* proteins was found to be -0.023 to –0.655. The lowest value of GRAVY shows the possibility of better interaction with water.

The secondary structure prediction of *C. gynandra* proteins (Table-3) was exhibit by SOPMA which revealed that alpha helix, extended strand, beta turn and random coil, were more main. In all the three proteins alpha helix dominates which is tracked by random coil, extended strand and beta turn. The secondary structure was using default parameters (Window width: 17, similarity

threshold: 8 and number of states: 4). TMHMM v.2.0 and SOSUI predicted that 2 proteins were soluble protein.

Secondary structure of proteins by SOPMA revealed that α – helix, random coil, β – turn and extended strand were more predominant. In rbcL , maturase K, capid protein α – helix predominates, whereas V2 protein L32, C4 protein random coil region was frequent (Table: 2). In Replication enhancer, A4 protein Beta subunit, Ribosomal protein II, Replication enhancer extended strand controls followed by random coil and α – helix. Domains are evolutionary units, frequently known as repeated sequence or 3D structure [14].

Fig. 1. Tertiary Structure

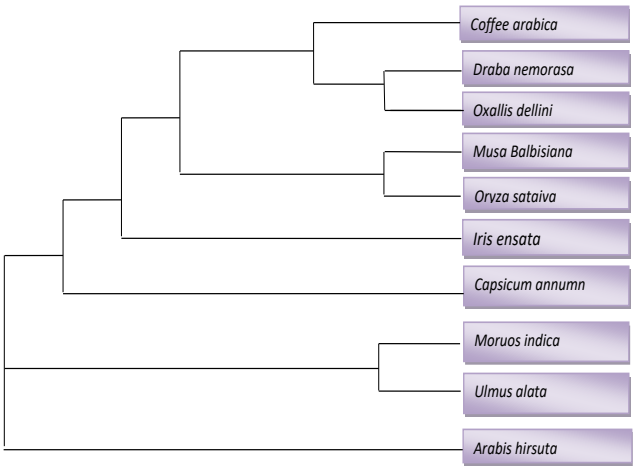


Phylogenetic analysis of *cleome gynandra*

Table 3. Lists of plant species showing similarity of 98% and above with the (RBCL)

S.NO.	PLANT SPECIES CONTAINING RBCL	FAMILY NAME	ACCESSION NUMBER	IDENTITY (%)
1.	*Coffea arabica*	*Arabian coffee*	ABJ89687.1	98.2
2.	*Draba nemorosa*	Woodland willow grass	BAF50382.1	98.1
3.	*Oxalis dillenii*	*Gray-green wood sorrel*	AAA84534.2	98.3
4.	*Musa balbisiana*	Banana	THU42669.1	98.5
5.	*Oryza sativa*	Rice	AAS46190.1	98.0
6.	*Iris ensata*	*Iris kaempferi*	BAA05704.1	98.6
7.	*Capsicum annum*	Capsicum pepper	PHT78021.1	98.2
8.	*Morous indica*	Morous	ABB20966.1	98.3
9.	*Ulmus alata*	*Winged elm*	AAA20538.1	98.4
10.	*Arabis hirsuta*	*Turritis hirsuta*	BAF50031.1	98.5

Fig: 2 PHYLOGENETIC TREE OF RIBULOSE BIS PHOSPHATE CARBOXYLASE LARGE CHAIN (EC 4.1.1.39)



The evolutionary relations between the plants were evaluated by phylogenetic analysis of the ranged amino acids sequence of *C. gynandra* protein sequences with neighbour-joining (NJ)

method (Fig 2.). Merging and separation are two vital phylogenetic properties, which can be valuable to novelty and closely as well as distantly related group containing *C. gynandra* protein sequences [15]. The minimum degree of divergence was found between *Capisicum annumn*, while the maximum degree of divergence was found between *Ulmus alata* unicolor. This outcome suggests that *C. gynandra* protein sequences are conserved and they are developed from a common ancestor [16].

4. CONCLUSION

Now-a-days designing and developing Medicinal plants built on ethanobotanical and traditional systems of medicine is fast extra importance. The use of *in silico* methods for drug discovery in natural products has enhanced during the past decade. However, even the application of currently existing chemo- and bioinformatics capitals and approaches provide valuable data for finding of new applications of conservational and industrial wastes beyond their traditional use. The bioinformatics studies, which overwhelmingly and broadly confirms its therapeutic potential. Hence, the vital to exploit the abilities of these plants particularly in areas of traditional medicine and therapeutic industries growths.

REFERENCES

1. Refaz Ahmad Dar, Mohd Shahnawaz, and Parvaiz Hassan Qazi. (2017). General overview of medicinal plants: A review. *J. Phytopharmacol.* 6(6): 349-351.

2. Gupta, P. and Wagh, R.D. (2014). A Review on morphology, phytochemistry, pharmacology and Folk-lore uses of *Cleome gynandra*. *Int. J. Pharm. Life Sci.* 5(6): 3622-3626.

3. Bhat, R., Sridhar, K.R. and Yokotani, K.T. (2007). Effect of ionising radiation on antinutritional features of velvet bean seeds (*Mucuan pruriens*). *Food Chem.* 103: 860-866.

4. Francis and Rita, (1986). Colorimeteric assay for cell growth and survival modifications of tetrazolium dye procedure giving sensitivity and realability. *J. Immunol. Methods.* 89: 271-277.

5. David, B., Wolfender, J.-L. and Dias, D.A. (2014). The pharmaceutical industry and natural products: historical status and new trends. *Phytochem. Rev.* 14: 299-315.

6. Fabina Sievers. (2011). Fast, Scalable generation of high – quality protein multiple sequence alignments using Clustal Omega.

7. Márcio Dorn, Mariel Barbachane Silva, Luciana S. Buriol and Luis C. Lamb, (2014). Three-dimensional protein structure prediction: Methods and computational strategies, *Computat. Biol. Chem.* 53: 251–276.

8. Dao, V., Langella, I. and Carbo, J. (2011). From green to sustainability: Information technology and an integrated sustainability framework. *J. Strategic Information Systems* 20(1): 63-79.

9. Gasteiger E., Hoogland C., Gattiker A., Duvaud S., Wilkins M.R., Appel R.D. and Bairoch A.; (In) John M. Walker (ed). (2005). Protein Identification and Analysis Tools on the EXPASY Server The Proteomics Protocols Handbook, Humana Press, 571-607.

10. Perriere, G. and Gouy, M. (1996) WWW-Query: An on-line retrieval system for biological sequence banks. *Biochimie* 78: 364-369.

11. Upgade Akhilesh, Bhaskar, Anusha, Issar Sakshi and Senthamarai Selvi V. (2012). In Silico Characterization of Keratitis Causing Herpes Simplex Virus (HSV 1) Membrane Proteins using Computational Tools and Servers. *Res. J. Recent Sci.* 1(11): 27-31.

12. Bézivin C, Tomasi F, Lohézic-Le Devehat F, and Boustie J. (2003). Cytotoxic activity of some lichen extracts on murine and human cancer cell lines. *Phytomedicine* 10: 499–503.

13. Lee, E.B. (1973). Pharmacological studies on *Platycodon grandiflorum* A. DC. IV. A comparison of experimental pharmacological effects of crude platycodin with clinical indications of Platycodi radix. *Yakugaku Zasshi* 93: 1188–1194.

14. Daisy, P., Winfan Celes, J. and Pon Nivedha, R. (2014). HPLC, GC-MS and in silico analysis of *Cucurbita maxima* methonolic extract for its activity against Prostate Cancer. *Int. J. Pharm Tech Res.* 6(2): 500-505.

15. Vadnere Gautam, P., Pathan Aslam, R., Kulkarni Bharti, U. and Abhay Kumar Singhai, (2013). Diplocyclos Palmatus: A Phytopharmacological Review. *Int. J. Res. Pharm. Chem.* 3: 157-159.

16. Kebila Venkatasamy, (2013). In silico Analysis and Homology Modeling of Putative Hypothetical Protein Q4QH83 of Leishmania major. *Advanced BioTech* 13(3): 1-4.

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