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Tructural Evaluation and Insilico Study Of Protein Of *Morinda Citrifolia* In Phenylalanine Ammonialyase For Phenylketoneuria

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Abstract: *Morinda citrifolia* is a fruit-bearing tree in the coffee family of Rubiaceae. *Morinda* is considered to have biological properties in traditional medicine. *Morinda citrifolia* is contain many protein structure but specially take a limited protein and study a insilico analysis.Morinda citrifolia is contain many enzymes but especially in phenylalanine ammonialyase. Phenylalanine ammonia lyase is cure for the inborn error of protein metabolism(phenylketoneuria). Phenylalanine ammonia lyase is found widely in plants, as well as some bacteria, yeast, and fungi, with isoenzymes existing within many different species. This study is usually facilitated by accurate three-dimensional (3-D) structure of the protein. Number of known protein sequences and structures as well as improvements in the modeling software.

Keywords: *Morinda citrifolia* , Bioinformatics , traditional medicine, Phenylalanine ammonia lyase.

I. INTRODUCTION

Medicinal plants are very useful source of various bioactive compounds which have direct or indirect use in the treatment of various human ailments. From the time immemorial, human civilizations have been exploring and using various plants and plant products to cure the deadly diseases [1].Ten percent of all vascular plants are used as medicinal plants and there are estimated to be between 350,000 and almost half a million species of them. Since ancient times, plants have been used in medicine and are still used today. Morinda citrifolia L. (Rubiaceae), popularly known as noni, is widely used in Tahiti, Hawaii, Polynesia and different Asian countries to treat and prevent different pathophysiology such as high blood pressure, bacterial, fungal and viral infections, wounds, dyslipidemia and diabetes, cancer, among others. In some countries, including Brazil, the use of noni (all plant parts and/or noni herbal medicines) has been banned by the National Health Surveillance Agency[4]. Phenylalanine ammonialyase is an enzyme that catalyzes a reaction converting L-phenylalanine to ammonia and trans-chinnamic acid. Phenylalanine ammonia lyase (PAL) is the first and committed step in the phenyl propanoid pathway and is therefore involved in the biosynthesis of the polyphenol compounds such as flavonoids, phenylpropanoids, and lignin in plants. It has a molecular mass in the range of 270–330 kDa. The activity of PAL is induced dramatically in response to various stimuli tissue wounding, pathogenic attack, light, low temperatures, and hormones. PAL has recently been studied for possible therapeutic benefits in humans afflicted with phenylketonuria[2]. Bioinformatics shall facilitate analysis and integration of information from these related fields to enable the identification of genes and gene products and elucidate the functional relationships between genotype and observed phenotype. This research report provides a state-of-the-art overview of bioinformatics study of *Morinda citrifolia* with emphasis on the current progress and future directions, which shall provide tools and resources necessary to understand and promote advances in this important field.

II.MATERIALS AND METHODS

SEQUENCE RETRIEVAL

The FASTA sequence of the proteins were retrieved from Genbank database hosted by the NCBI (http://www.ncbi.nlm.nih.gov).

PRIMARY STRUCTURE PREDICTION:

For Physio-chemical characterization, 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)

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were computed using the Expasy Protparm server. (http://us.expasy.org/tools/protparam.html).

SECONDARY STRUCTURE PREDICTION

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

FUNCTIONAL CHARACTERIZATION

SOSUI and TMHMM v.2.0 tools were used to characterize whether the protein is soluble or transmembrane in nature. InterPro is an integrated resource for protein families, domains and functional sites. InterPro incorporates the major protein signature databases into a single resource. These include: PROSITE, which uses regular expressions and profiles, PRINTS, which uses Position Specific Scoring Matrix-based (PSSM-based) fingerprints, ProDom, which uses automatic sequence clustering, and Pfam, SMART, TIGRFAMs, PIRSF, SUPERFAMILY, Gene3D and PANTHER, all of which use hidden Markov models (HMMs). Superfamily and molecular function were predicted by Interpro protein sequencing and classification. (http://www.ebi.ac.uk/interpro/).

SEQUENCE ALIGNMENT

Sequence alignment of was performed using pairwise 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 recomputed information in public databases like Pfam .The emphasis of this work was to find the regions of sequence similarity, which in other words allows us to yield functional and evolutionary relationships among the proteins considered in this study.

PHYLOGENETIC ANALYSIS

The phylogentic analysis of ten proteins were performed to determine the number of proteins that share common structural and functional features. As an input to Clustal Omega all sequences in fasta formats were supplied with default options. The output was analyzed 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 . The stability of the internal nodes was assessed by bootstrap analysis with 1000 replicates.

TOOLS

Primary tools for sequence comparison and assembly have grown in line with an expansion of the datasets that they analyze. Insilico contain a many tools for the primary ,secondary and tertiary structures. Without basic local alignment search tool (BLAST) and related sequence comparison tools, much of the data coming from the many high-throughput sequencing laboratories would be nothing more than strings of letters. BLAST remains the fastest means by which to identify specific sequences in large datasets and enables the rapid annotation of novel sequences. Although BLAST is the standard tool for identifying sequence similarities in large datasets, there are several options for assembling sequence datasets, the choice of which depends on hardware availability, dataset size, data format, structure and the genetic structure of the organism. Sequence similarity search and assembly tools are the foundation of many software applications for analyzing plant genomic information. The ability to rapidly identify similarities to previously characterized sequences greatly enhances the sequence annotation process. This has led to the development of comparative sequence databases, whereas sequence assembly packages both reduce the high level of redundancy in datasets and enable variations in sequence to be identified.

III.RESULT AND DISCUSSION

Herbal medicine is based on the premise that plants contain natural substances that can promote health and alleviate illness. Plant products are frequently considered to be less toxic and more free from side effects than synthetic ones. Natural products are chemical compound found in nature and they have pharmacological and biological activity, they are generally used in drug discovery and drug design.The use of these plants has been gradually refined over the generations, and this has become known in many contexts as traditional medicine. In the beginning, the trial and error method was used to treat illnesses or even simply to feel better, and in this way, to distinguish useful plants with beneficial[3].Morinda citrifolia article is a review of the literature, which aims to present the latest findings on the therapeutic potential of this plant according to studies already developed mainly on its pharmacological activity and toxicity, aiming to contribute to the disclosure of the risk and benefit of empirical use of this plant and its derivatives and biological constituents. Natural products are chemical compound found in nature and they have pharmacological and biological activity, they are generally used in drug discovery and drug design. This plant possessing a multitude utility could be well exploited for its phytoconstituent responsible for the activity and characterized for the bio safety level which later could be developed into a value added commercial product[4].

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Table 1: PARAMETERS COMPUTED USING EXPASY'S OF PHENYLALANINE AMMONIALYASE IN *MORINDA CITRIFOLIA*

.S.No	Accession number	Protein	Length	Mol.wt	PI	-R	+R	EC	II	AI	GRAVY
1	A0A6H1PS87	phenylalanine ammonialyase	717	77980.80	5.81	85	71	45100	30.19	90.52	-0.175

Mol. Wt – molecular weight(Daltons), pI – Isoelectric point, -R - Number of negative residues, +R – Number of Positive residues, EC – Extinction Coefficient at 280 nm, II – Instability Index, AI – Aliphatic Index, GRAVY – Grand Average Hydropathicity, * - No Trp, Tyr or Cys residue should not be visible by UV spectrophotometry.

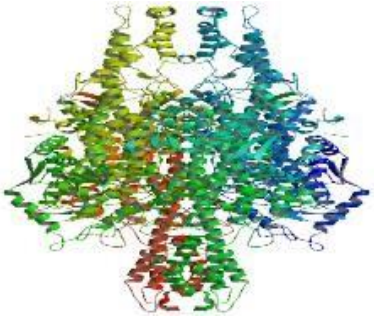
The primary structure prediction was done with the help of protparam tool (Table 1). The parameters were computed using Expasy's protparam tool which revealed that the molecular weights for 77980.80 (phenylalanine ammonialyase).

TABLE 2: SECONDARY STRUCTURE RESULT OF PHENYLALANINE AMMONIALYASE IN *MORINDA CITRIFOLIA*

S.NO	Secondary structure	PAL
1	Alpha helix	55.51
2	Extended strand	9.07
3	Beta turn	5.30
4	Random coil	30.13

Secondary structure prediction of *Morinda citrifolia* proteins by SOPMA revealed that α – helix, random coil, β – turn and extended strand were more prevalent. TMHMM v.2.0 and SOSUI predicted that phenylalanine ammonialyase is soluble protein.

TERTIARY STRUCTURE OF PHENYLALANINE AMMONIALYASE IN *MORINDA CITRIFOLIA*:



PHYLOGENITIC AND RAMACHANDRAN PLOT ANALYSIS OF PHENYLALANINE AMMONIALYASE IN MORINDA CITRIFOLIA:

Phylogeny is the history of descent of a group of taxa such as species from their common ancestors including the order of branching and sometimes the times of divergence. In molecular phylogeny, the relationships among organisms or genes are studied by comparing homologues of DNA or protein sequences. Dissimilarities among the sequences indicate genetic divergence as a result of molecular evolution during the course of time. In brief, while classical phylogenetic approach relies on morphological characteristics of an organism, the molecular approaches depend on nucleotide sequences of RNA and DNA and sequences of amino acids of a protein which are determined using modern techniques.

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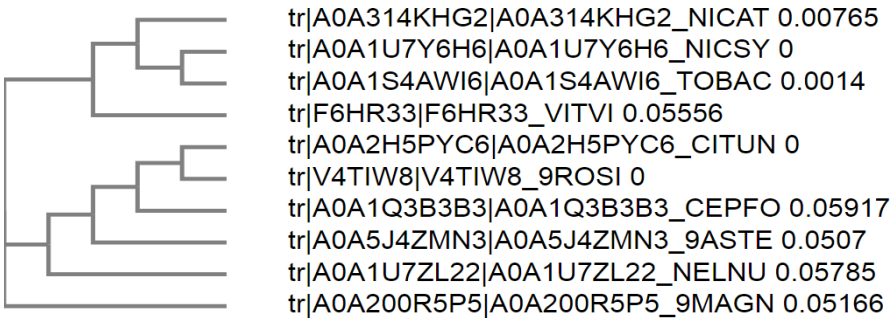
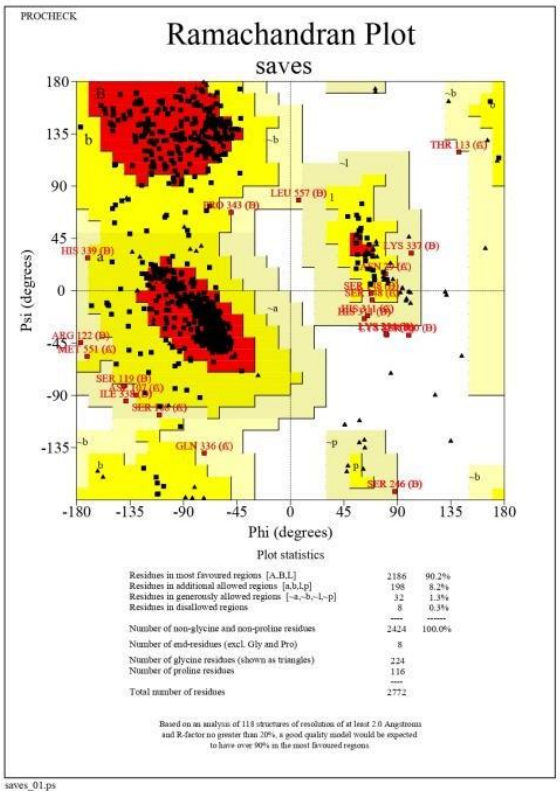
Table 3: lists of plant species showing similarity of 84% and above with the (PAL)

S.NO	Species containing PAL protein	Family	AccessionNumber	Identity
1	Nyssa sinensis	Cornaceae	A0A5J4ZMN3	87.3
2	Cephalotus follicularis	Cephalotaceae	A0A1Q3B3B3	86.3
3	Vitis vinifera	Vitaceae	F6HR33	85.7
4	Nicotiana attenuata	Solanaceae	A0A314KHG2	85.5
5	Nicotiana sylvestris	Solanaceae	A0A1U7Y6H6	85.4
6	Nicotiana tabacum	Solanaceae	A0A1S4AWI6	85.3
7	Macleaya cordata	Papaveraceae	A0A200R5P5	85.2
8	Nelumbo nucifera	Nelumbonaceae	A0A1U7ZL22	85.0
9	Citrus unshiu	Rutaceae	A0A2H5PYC6	84.2
10	Citrus clementina	Rutaceae	V4TIW8	84.2

Fig-:PHYLOGENITIC TREE OF PAL PROTEIN CONTAINING PLANTS:





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II. CONCLUSION

Morinda citriofolia having various pharmacological properties and is a source of beneficial secondary metabolites. Computational studies of its key biosynthetic enzymes may provide valuable insights into the mechanism of action of the enzymes aiding in the ultimate aim of improving quality and quantity of the reaction products. Consequently, the use of appropriate computing and bioinformatics tools to allow automated data storage and efficient non-labor intensive data analysis may further help in metabolomics analysis of phenylalanine ammonialyase in *morinda citriofolia.* This may then be used either for 'fingerprinting' samples to perform comparative analyses to detect differences for 'profiling' where individual differential secondary metabolites like alkaloids, phenolic components, are identified for further analysis. In this study, proteins of *morinda citriofolia* were selected. Expasy's ProtParam tool predicted the physio-chemical characters of the proteins. Phylogenetic study revealed the close and distant relationship protein of *morinda citriofolia* of Moraceaeeae family with the plants of other family. Further analyses are required for drug target identification. To best of our knowledge, ours is the first study to show these functional aspects of proteins of *morinda citriofolia.* Further investigations are needed to determine how protein functions in these plant processes and to provide a more comprehensive understanding of the evolution of this unusual gene.

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REFERENCES

[1]. Shyma TB, Devi PAG. Traditional use of medicinal plants and its status among the tribes in Mananthavady of Wayanad district, Kerla. World Res. J. Med. Arom. Plants. 1(2):22-26 ,2020.

[2]. Jones DH . Phenylalanine ammonia-lyase: regulation of its induction, and its role in plant development. *Phytochemistry.* ;23:1349–1359, 1984.

[3]. Taur DJ, Patil RY. Some medicinal plants with antiasthmatic potential: a current status. Asian Pac. J. Trop. Med. 413-418 . 2019.

[4]. Ubirajara lanza ,Shafaz nisar . Chemical compounds ,pharmalogical activity and toxicity of morinda citrifolia.University of agriculture ,Pakistan.11-14 , 2020.