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In silico analysis of proteins of *Curcuma aromatica* Salisb

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Abstract: From ancient times, many scientists have been exploring the nature, specifically plants to discover novel drugs which are used to treat various diseases. *Curcuma aromatica* Salisb. Commonly known as Wild Turmeric is indulged in treatment of various diseases related to skin, cardiovascular and respiratory system. So the medicinal plants have a promising role in to prevent and as well as to cure the diseases. In this study three proteins of *Curcuma aromatica* were analysed using different bioinformatics tools. By using the tools like protparam (Expasy), SOPMA, SOSUI, TMHMM, structural predictions and functional characterisation were done. The primary information like molecular weight, pI etc., were obtained by protparam and the secondary structures like alpha helix, beta strand were obtained by SOPMA. Transmembrane proteins were identified by SOSUI and TMHMM. Homology modelling was done using swiss model and finally Rasmol was used to visualise the tertiary structure of the proteins.
Keywords: *Curcuma aromatica*, Expasy, Swiss model, Rasmol.

Introduction

The presence of bioactive constituents in medicinal plants plays a major role in healing as well as curing the diseases. For this reason pharmaceutical company uses the medicinal plants in production of the new drugs against various diseases[1]. Medicinal plants possess anti-inflammatory, anticancer, anti-viral, anti-malarial, anti-bacterial, antianalgesic and anti-fungal activities. Our mother nature is the major source of potential drugs and the drugs derived from these medicinal plants are easily available, safe, efficient and less expensive [2].

The phytochemicals which acts against the disease are naturally occurring in the medicinal plants in different parts including leaves, vegetables and roots .The presence of defense mechanism in those substances are responsible in protection from various diseases. Phytochemicals are primary and secondary compounds. The primary constituents include chlorophyll, proteins, common sugars and secondary compounds consist of terpenoid, alkaloids and phenolic ompounds[3].

Curcuma aromatica Salisb. (Family: Zingiberaceae) commonly known as wild turmeric or yellow zedoary is also a widely used curcumin species in addition to the common turmeric (*Curcuma longa* Linn.). *Curcuma aromatica* is distributed throughout India and cultivated mainly in Kerala and West Bengal[4].It is widely used as a flavouring agent, tonic, carminative and used against snakebite[5]and also to enhance complexion. This wild and aromatic turmeric is the most useful species among the other turmeric members for its unique medicinal values.

Curcuma aromatica rhizome is a rich source of volatile oil, which consists of several anti-tumor ingredients including demethoxycurcumin, β-elemene, curcumol, curdione, etc. [6, 7] and also promotes blood circulation to remove blood stasis [8].

In traditional medicine the rhizome is also used against various bacterial and fungal diseases. Its extract possesses a significant repellent activity against mosquitoes[9]. When compared to curcuma longa it has a higher level of volatile content (4- 8%) and the chemical and aroma characteristics of the volatile oil of two species are also different. Curcumin, the active ingredient in *C. aromatica*, acts as a promising agent in the treatment and/or prevention of Alzheimer'sdisease[10]. There are many parameters like deforestation, improper cultivation practices and the greater dependency of pharmaceutical industries on sources make this plant threatened in many South Asian countries [11]. In this study three protein sequences of *Curcuma aromatica* were selected and analysed with the help of computational tools. In silico approach provide useful information by identifying the primary, secondary and tertiary structure predictions which can be used for further analysis.

Materials and Methods

The FASTA sequence of the proteins (Table 1) were retrieved from Genbank database hosted by the NCBI (http://www.ncbi.nlm.nih.gov)

Table 1: Proteins of curcuma aromatica

S.No	Accession number	Protein	Length
1	AEF58784.1	Chalcone Synthase	189
2	AHG98410.1	PsbZ	62
3	AET36762.1	RNA polymerase	175

Primary Structure Prediction

The primary structure prediction i.e., the physical and chemical parameters for the given protein sequence was computed with Expasy's protparam server (http://web.expasy.org/protparam/). The computed parameters include the molecular weight, theoretical pI, amino acid composition, atomic composition, extinction coefficient, instability index, aliphatic index and grand average of hydropathicity (GRAVY)[12].

Secondary structure prediction

Self-Optimized Prediction Method with Alignment (SOPMA) tool predicts the secondary structures of the protein using the FASTA sequence which gives the various secondary structures like alpha-helix, beta-sheet and coil.

Functional characterization

SOSUI and TMHMM tools were used to characterize whether the protein is soluble or transmembrane in nature.

Tertiary structure prediction

Homology modeling was performed with fully automated protein structure modeling server, Swiss model and the structure was visualized and analyzed by using the visualization software Rasmol.

Results and Discussion

The primary structure prediction was done with the help of protparam tool (Table 2). The parameters were computed using Expasy's protparam tool which revealed that the molecular weights for three different proteins as 20283.2(Chalcone Synthase), 6587.8 (PsbZ) and19428.6(RNA polymerase). The pI of two proteins was less than 7 which indicated that they are acidic and one protein was greater than 7 which showed that it is basic in character. The proteins are found to be compact and stable at their pI[13].All the three proteins of *Curcuma aromatica* showed instability index lesser than 40, indicating that the proteins are stable. Aliphatic index of the proteins ranged between90.85-147.74. The range of GRAVY (Grand Average of Hydropathicity) of *Curcuma aromatica* proteins was found to be -0.031to 1.387. The lowest value of GRAVY indicates the possibility of better interaction with water [14].

Table 2:Parameters computed using protparam tool

Protein	MolWt	pI	-R	+R	EC	II	AI	GRAVY
Chalcone Synthase	20283.2	5.03	21	14	22125	30.56	90.85	0.143
PsbZ	6587.8	5.59	1	1	11000	38.33	147.74	1.387
RNA polymerase	19428.6	8.89	18	21	8605	35.05	109.71	-0.031

Mol. Wt – Molecular weight(Daltons), pI – Isoelectric point, -R - Number of negatively charged residues, +R – Number of Positively charged residues, EC – Extinction Coefficient at 280 nm, II – Instability Index, AI – Aliphatic Index, GRAVY – Grand Average of Hydropathicity

The secondary structure prediction of *Curcuma aromatica*proteins was analysed by SOPMA which revealed that alpha helix, extended strand,beta turn andrandom coil, were more predominant. In all the three proteins alpha helix dominates which isfollowed by random coil, extended strand and beta turn(Table 3).

Table 3: Secondary structures predicted using SOPMA tool

Secondary structures	Chalcone Synthase	PsbZ	RNA polymerase
Alpha helix	43.39%	41.94%	38.29%
3_{10} helix	0.00%	0.00%	0.00%
Pi helix	0.00%	0.00%	0.00%
Beta bridge	0.00%	0.00%	0.00%
Extended strand	16.93%	27.42%	14.86%
Beta turn	10.05%	1.61%	12.57%
Bend region	0.00%	0.00%	0.00%
Random coil	29.63%	29.03%	34.29%
Ambiguous states	0.00%	0.00%	0.00%
Other states	0.00%	0.00%	0.00%

SOSUI andTMHMM predicted that chalcone synthase and RNA polymerase were soluble protein, on the other handPsbZ found to have transmembrane region (Fig 1) with 23 residues length (Table 4).

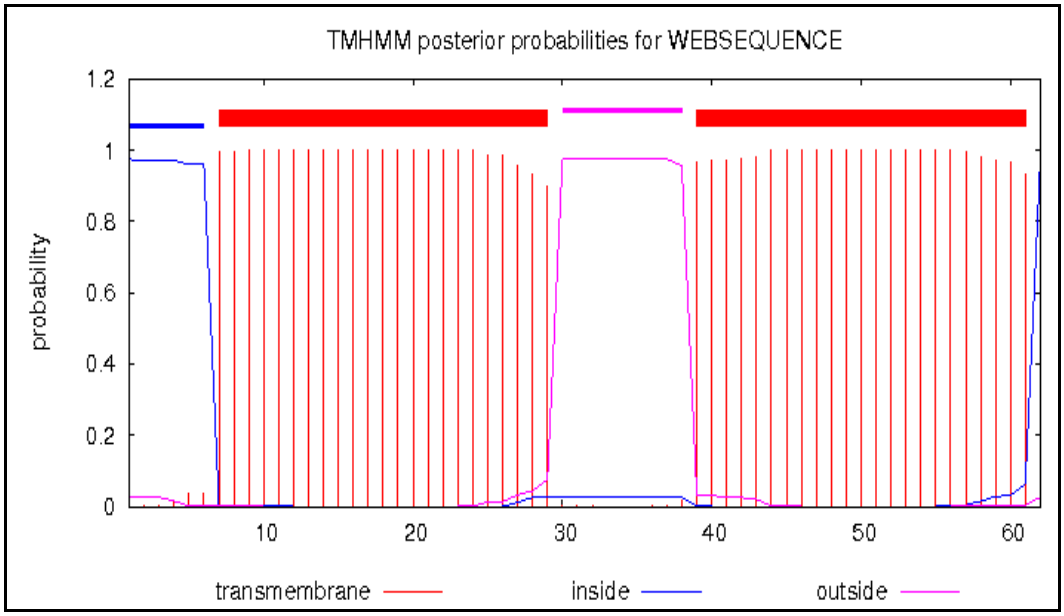

Fig 1: TMHMM showing the transmembrane region of PsbZ

Table 4: Transmembrane region predicted by SOSUI

Protein	Transmembrane region	Type	Length
PsbZ	QLAVFALIATSSVLLISVPVVFA	PRIMARY	23
	IVFSGTSLWIGLVFLVAILNSLI	PRIMARY	23

The tertiary structure was modelled by Swiss model workspace for all the three proteins (Figure 2, 3.4). The proteins were visualised and analysed with the help of Rasmol.The modelled structure of chalconesynthase showed 218, PsbZ with 52 and RNA polymerase with 92 hydrogen bond. Disulphide bridge was absent in all the three proteins.

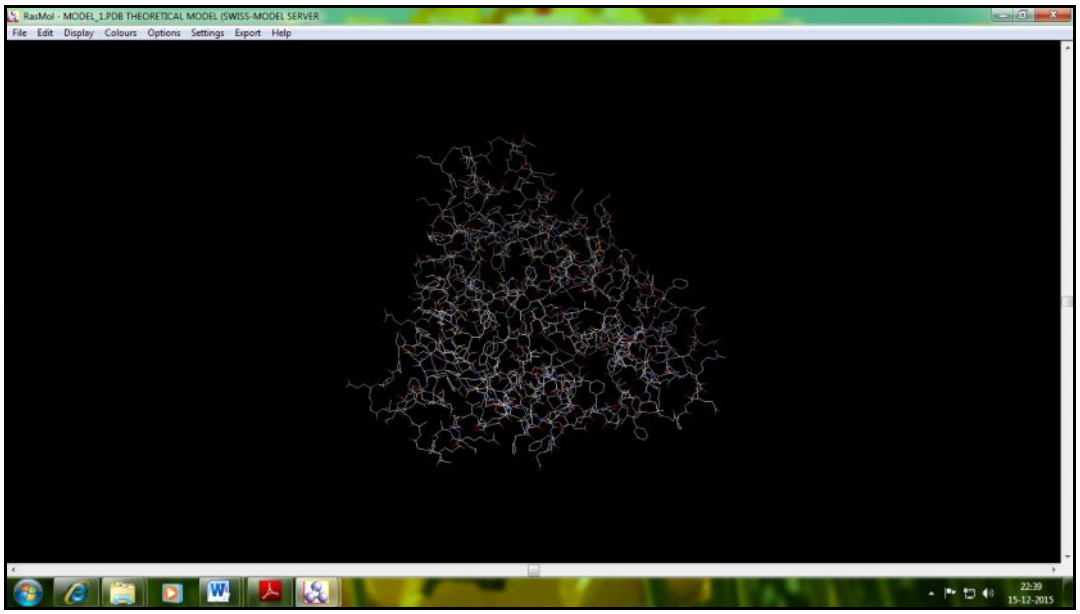

Fig 2: Three dimensional structure of Chalcone Synthase

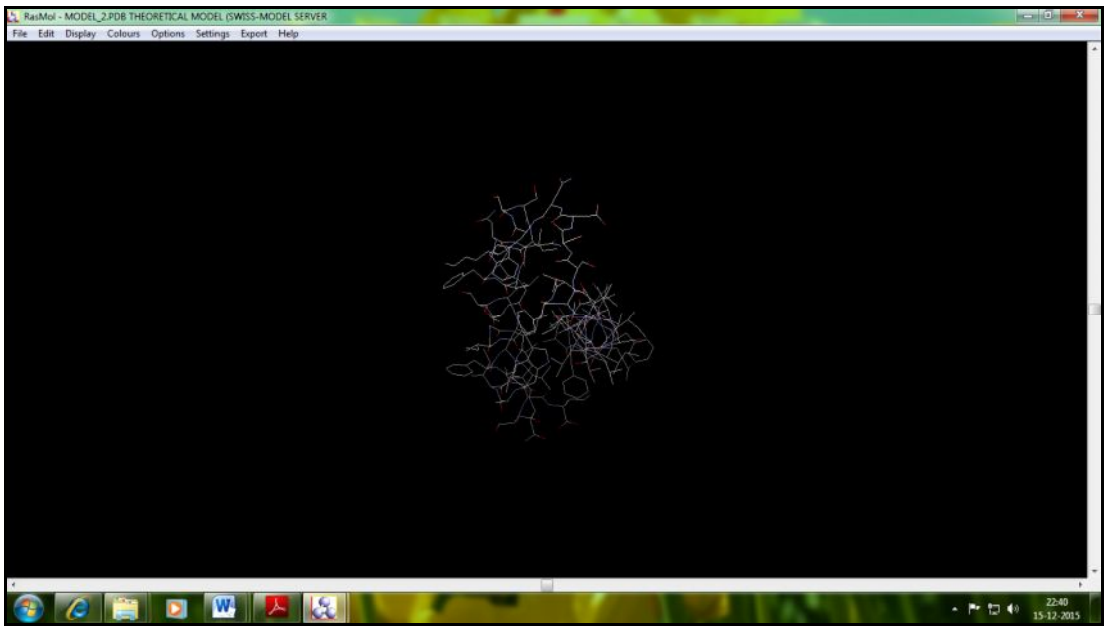

Fig 3: Three dimensional structure of PsbZ

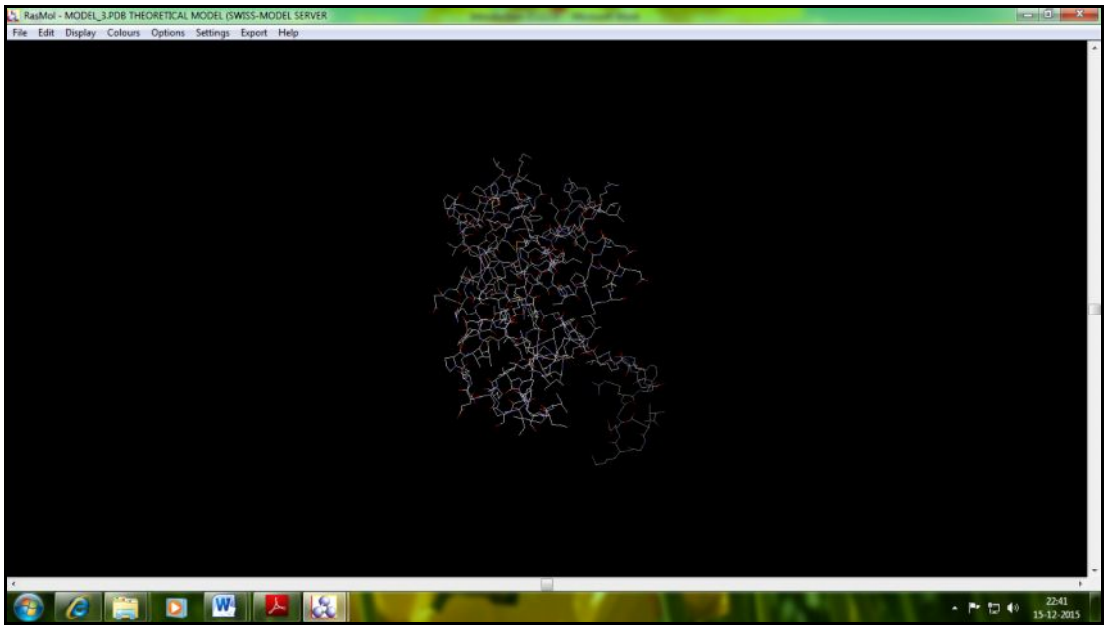

Fig 4: Three dimensional structure of RNA polymerase

Conclusion

In this study, three proteins of *Curcuma aromatica* were selected.

Primary, secondary and tertiary predictions were done with help of various bioninformatics tools which has provided the useful information . This can be further analysed for the process of drug discovery.

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