IN-SILICO ANALYSIS OF FENUGREEK (TRIGONELLA FOENUM-GRAECUM) PROTEIN

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Abstract - In-silicoanalysis and development of protein models in Fenugreek (*Trigonella foenum-graecum*) has paved a new path in the advancement of seed spice research using the modern computational tools. The present study is an effort to yeild more valuable scientific information related to fenugreek.In this study, the physiochemical properties, secondary structure and three-dimensional structure of available protein sequences were determined. The estimated molecular weight of identified for fenugreek protein was 11372.8 and was predicted as a basic protein. We have identified a channel in fenugreek transmembrane protein, through which a ligand might pass. The present finding may be a valuable addition to the proteomic information available on fenugreek.

Keywords - Fenugreek, Protein, Physiochemical, Secondary, Tertiary Structure

I. INTRODUCTION

Fenugreek (Trigonella foenum-graecum) is amember of the Fabaceae family meaning Greek hay, as the plant was traditionally used to scent inferior hay (Helambe and Dande, 2012). Fenugreek contains protein, fibre, vitamin C, niacin, potassium, iron and alkaloids. It also contains a compound diosgenin which has oestrogen-like properties, as well as steroidal saponins. These compounds impart many benefits to fenugreek. Fenugreek seeds are rich in protein (25·5%), fat (7·9%), unavailable carbohydrate (48%), mucilaginous matter (20%) and saponins (4·8%). Spices and aromatic herbs are considered to be essential in diets or medical therapies for delaying aging and biological tissue deterioration (Bukhari *et al.,* 2008).

The state of Rajasthan supplies 83-90% of this and ranks first in fenugreek production in India (Mathur*et al*., 2009). Inspite of large potential and high content of protein in fenugreek seeds, however, no reports on molecular structure predictions is available on Trigonella spp. native to this region. The present study was therefore aimed to focus on understanding the molecular structure and its characterization based on its stability and different physiochemical properties.

II. MATERIALS AND METHODS

2.1. Translation

National Centre for Biotechnology Information (NCBI) a public domain database (http://www.ncbi.nlm.nih.gov/) was used to retrieve sequenced data available and to prepare a protein structure using different translation tools (Transeq and Sixpack) and perl script was developed to get six reading frames.

2.2. Physiochemical properties and Secondary structure prediction

The physiochemical properties of like- molecular weight, theoretical isoelectric point, extinction coefficients (Gill, *et al.,* 1989), instability indexes (Guruprasad*et al.,* 1990), aliphatic index (Ikai, 1980), grand average of hydropathicity (GRAVY) (Kyte, *et al.,* 1982) etc. were calculated for ten protein sequences of fenugreek usingProtparam. Also the secondary structures for the protein sequences were predicted using GOR version IV (Guermeur, *et al.,* 1999).

2.3. Model building and evaluation

Ab-initio and threading Meta servers (Zhang, 2008) were used for modeling the three dimensional structure of the protein.

III. RESULTS AND DISCUSSION

3.1. Primary structure prediction

In the present study, Expasy'sProtParam server (http://expasy.org/cgi-bin/protparam) was used to determine the physiochemical properties or the primary structure of fenugreek protein. The translated primary sequence, with 102 amino acid residues of protein used for primary structure prediction its estimated molecular weight was 11372.8. The isoelectric point (pI) was also calculated which is useful because at pI, solubility is least and mobility in an electro focusing system is zero. The computed pI value of fenugreek protein was predicted basic in nature. The Aliphatic index determined for the protein sequence was 68.82.

Total number of negatively charged residues (Asp + Glu) and total number of positively charged residues (Arg + Lys) were estimated to be 8 and 15 respectively. The computed extinction coefficients help in the quantitative study of protein–protein and

protein–ligand interactions in solution (Jethra, *et al.*, 2012).

The instability index provides an estimate of the stability of protein in a test tube. The instability index value for fenugreek protein, indicates that the identified protein was a stable protein. The Grand Average hydropathicity (GRAVY) value for a peptide or protein was calculated as the sum of hydropathy values of all the aminoacids, divided by the number of residues in the sequence.

3.2. Secondary structure prediction

Secondary structure of protein was predicted using ProteinPredict, SOPMA PSIPRED and JPRED3. The protein sequences in FASTA format were used to derive secondary structure of protein (Mihasan, 2010). The results revealed that random coil (69.61%) dominated among secondary structure elements and alpha helices (4.90%) and extended strand (25.49%) were also present.

3.3. Tertiary structure prediction

SAVES server was used for further verification and stability check for 3D structure of fenugreek protein which showed 78.4% residues or empirically distributed data-points present in the structure lie in most favored region and 14.2% residues in additional allowed region of Ramachandran plot showing the stability and good quality of protein 3D structure (Figure 1).

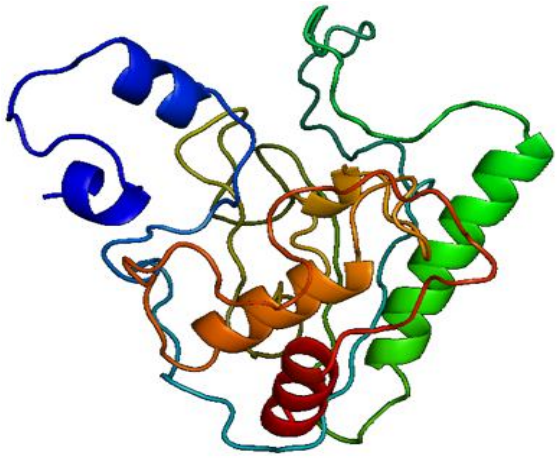

Fig. 1: Three dimensional Structure for fenugreek

CONCLUSION

The present finding is first report of in-silico protein modeling for fenugreek and showed homology only with the reported bacterial and human protein domains. Which have happened due to low strength of cellular database available on fenugreek or other related crops.

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