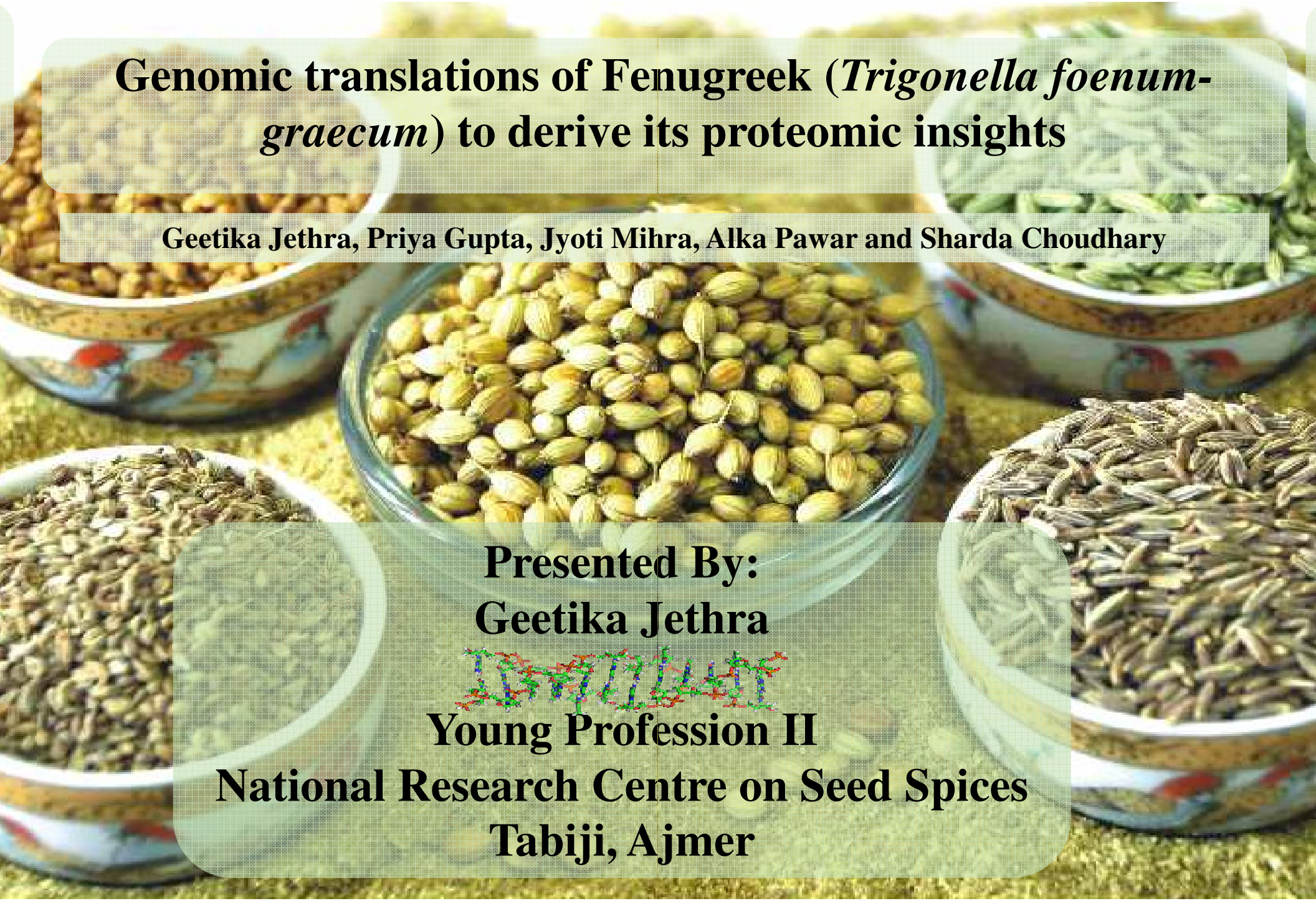
Genomic translations of Fenugreek (*Trigonella foenum-graecum*) to derive its proteomic insights

Geetika Jethra, Priya Gupta, Jyoti Mihra, Alka Pawar and Sharda Choudhary



Presented By:
Geetika Jethra
Young Profession II
National Research Centre on Seed Spices
Tabiji, Ajmer

Seed Spices

- Indian spices include a variety of spices grown across the Ind subcontinent and mostly categorised under Apicaeae family.

- Spices are used for flavour, colour, aroma and preservation of fooc beverages in almost all of the Indian Cuisines.

- But the database available on Apicaeae and Fabaceae family is spars populated with sequences.



Statistics of Seed Spices

	Fenugreek	Cumin	Coriander	Fennel	Celery	Ajowan	Anise	Caraway	Nigella
de	91	57	85	398	676	-	36	29	114
	33	38	47	4643	591	-	8	6	48
	-	-	-	-	18	-	-	-	-
	-	-	-	-	1122	-	-	-	-
	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-
es	-	-	-	-	-	-	-	-	-
	1	-	-	-	10	-	-	-	-

Fenugreek (Trigonella foenum-graecum)

Fenugreek is commonly known as *methi* in Hindi

t is an important leguminous spices and well known aromatic and medicinal herb.

Fenugreek is used as both seed and leaf.

Fenugreek seed contains carbohydrate (48%), protein (25.5%), mucilaginous ma
20%), fat (7.9%), and saponin (4.8%).

nspite of large potential and high content of protein in fenugreek seeds, however
eports on molecular structure predictions is available on Trigonella spp. native to
egion.



An Introduction to Bioinformatics

oinformatics is the application of computer technology for the managemen
ological information.

omputers are used to gather, store, analyse and integrate biological and ge
formation which can then be applied to gene-based sequence determination
ructure prediction.

the present study, Fenugreek (*Trigonella foenum-graecum*)protein models w
esigned and generated using in-silico tools.



NCBI

National Centre for Biotechnology Information

(http://www.ncbi.nlm.nih.gov/)

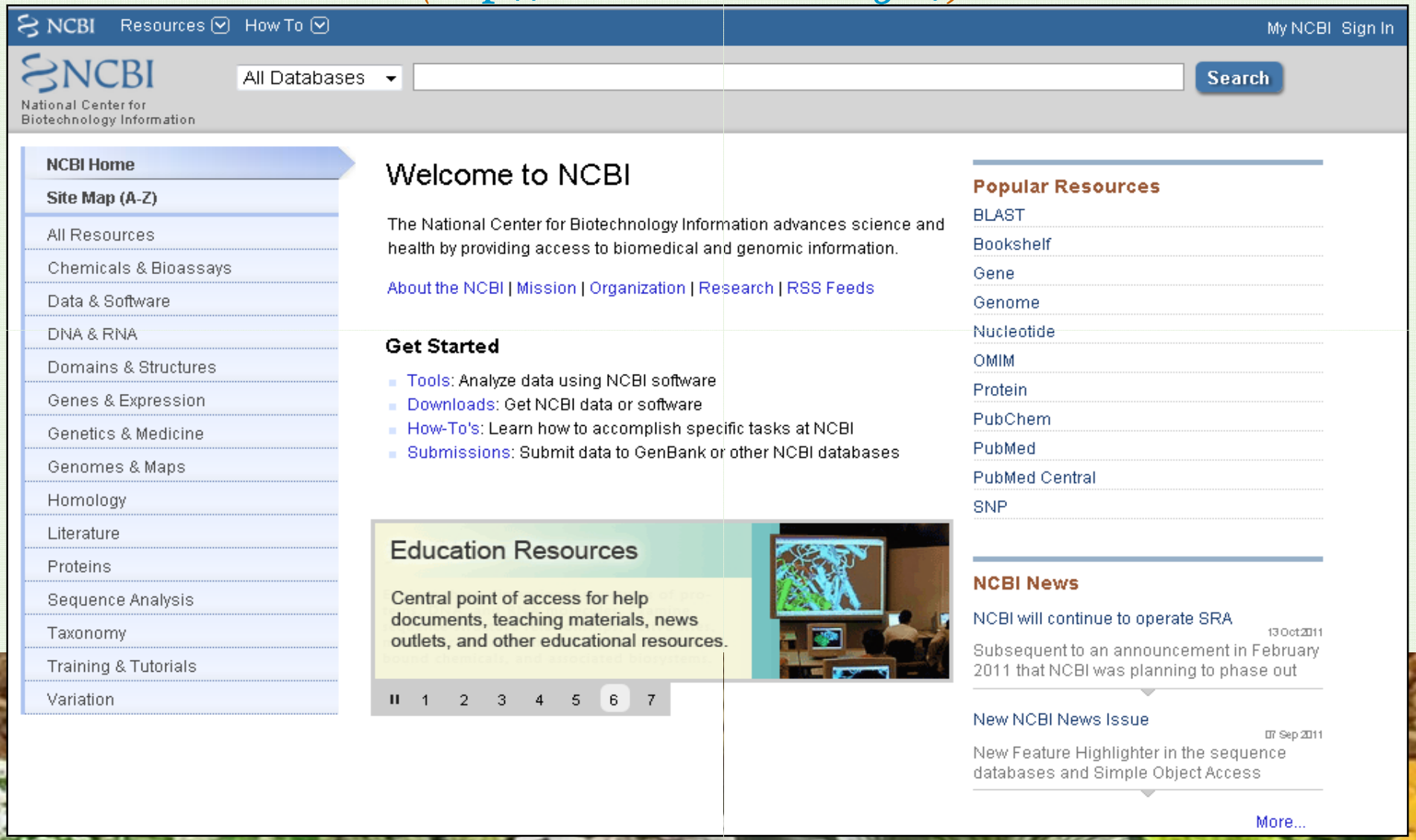
- The raw data was collected from NCBI a public domain for structural analysis.

- It is a comprehensive website for biologists including:
  - biology-related databases,
  - tools for viewing and analyzing
  - automated systems for storing and retrieval



NCBI - Home Page

(http://www.ncbi.nlm.nih.gov/)



Calculation of Physicochemical properties

rotParam : A tool which allows the computation of various physical ar
hemical parameters for a given protein .

http://www.expasy.org/tools/Protparam)

Molecular weight

Theoretical PI

Amino acid composition

Atomic composition

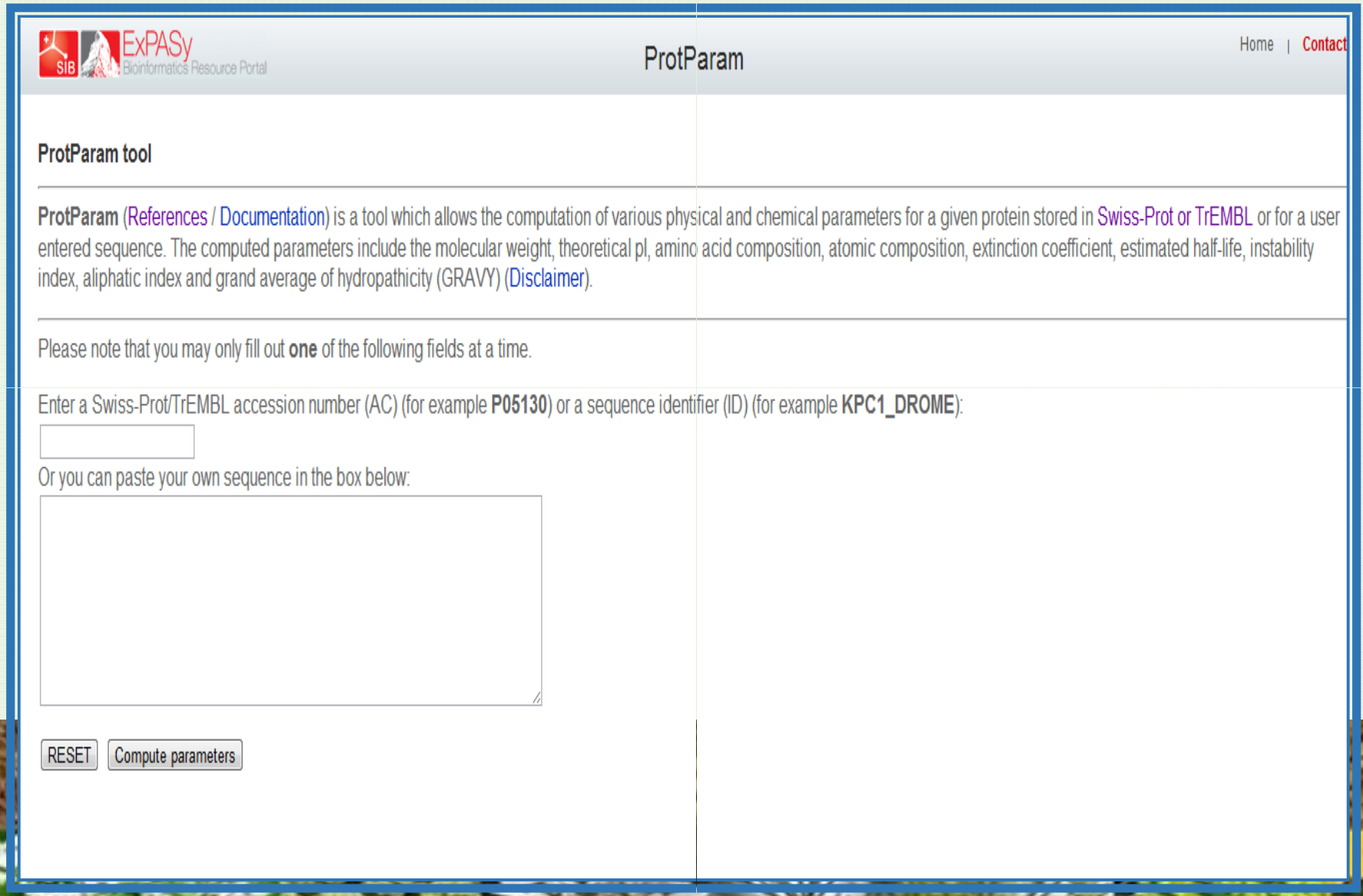
nstability index

Aliphatic index and

Grand average of hydropathicity (GRAVY)



The Homepage of ProtParam



Secondary Structure Prediction

- **GORIV**
- **PSIPRED**



GOR IV

OR is information ory based method and gives the information ut Alpha helix, ended strand, and beta n in the form of pensities.



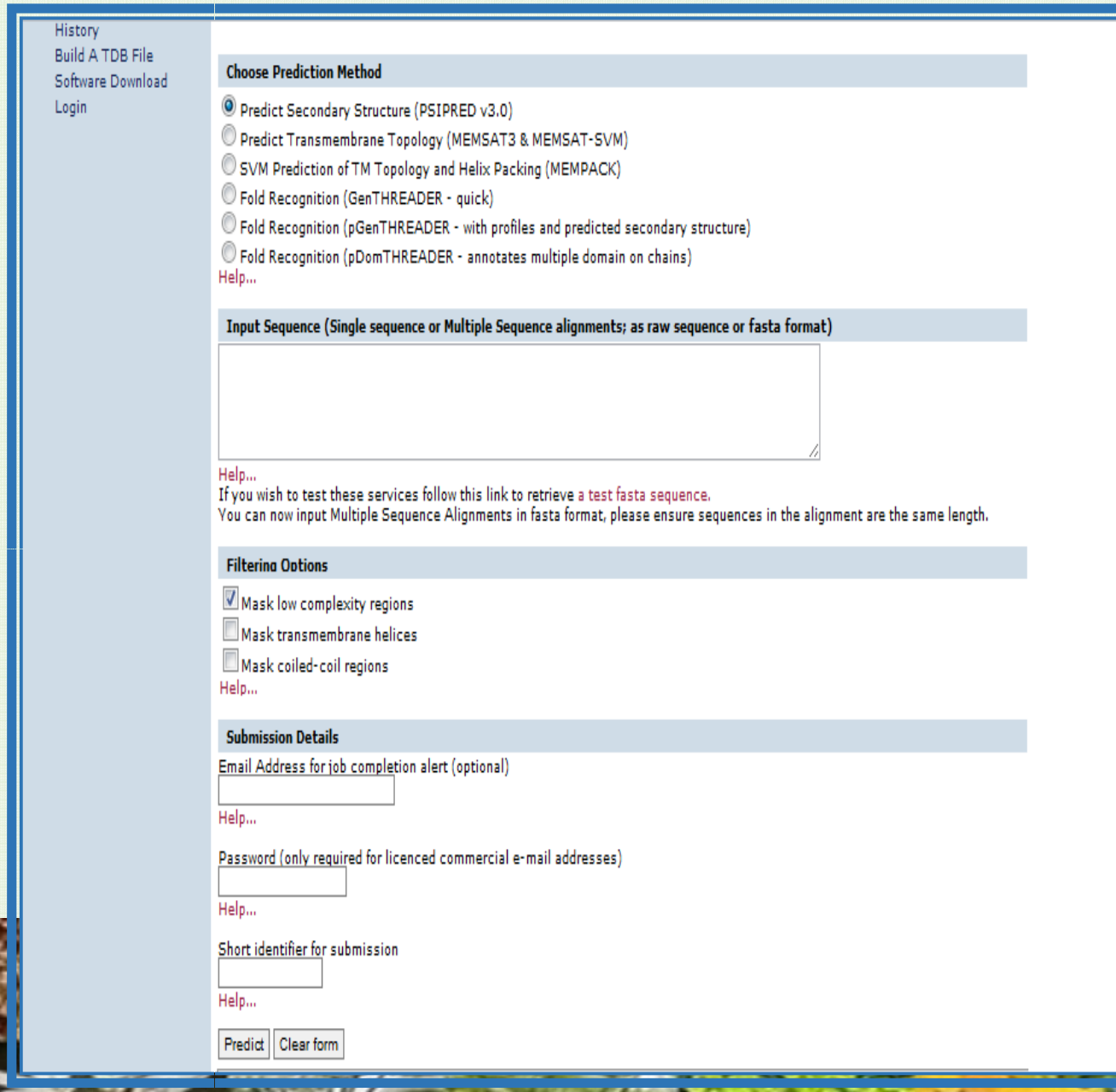
PSIpred

IPRED
oinf.cs.ucl.ac.uk/psipred)

GORITHM

t incorporates two feed-orward neural networks vhich perform an analysis n output obtained rom *PSI-BLAST*

Position Specific Iterated BLAST)



Tertiary structure Prediction

- **Swiss model**
- **Phyre2**
- **I-TASSER.**

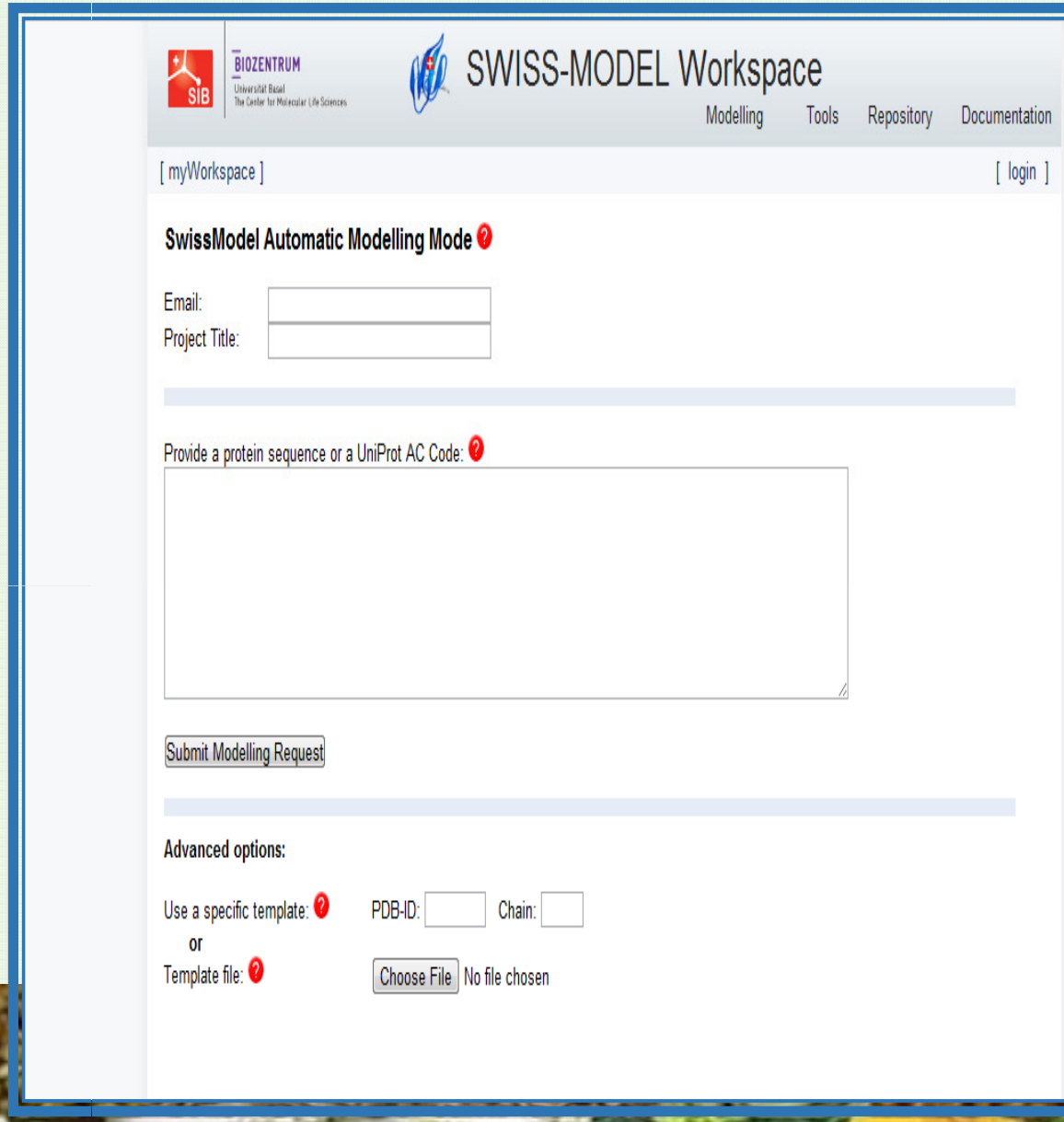


wiss model

VISS MODEL

p://swissmodel.expasy.org) A
ly automated protein structure
mology-modeling server,
essible via the ExPASy.

is a server used for automated
mparative modeling of three-
nensional (3D) protein
uctures using its sequence.



PHYRE2

Protein **H**omology/**A**nalog**Y** **R**ecognition **E**ngine

(http://www.sbg.bio.ic.ac.uk/Phyre2/html/page.cgi?id=index)

Web-based services for protein structure prediction.

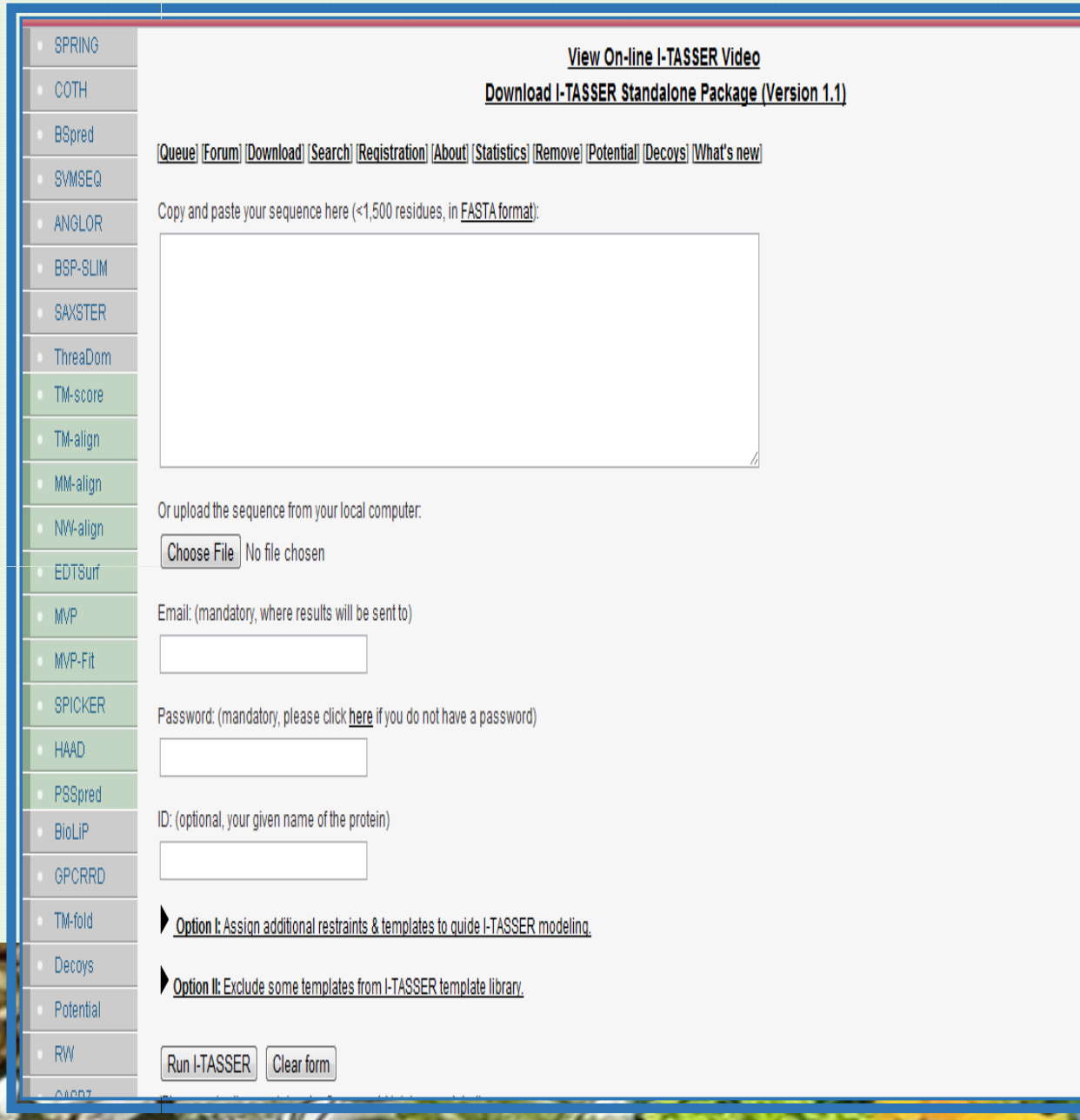
Generates reliable protein models when other widely us
methods such as PSI-BLAST cannot.



-TASSER

ver is an Internal service tem for protein structure and ction predictions.

models was built based on ltiple-threading alignments formed by iterative TASSER embly simulation; functional ghts are then derived by tching the predicted models n protein function database ibed in it .



Result and Discussion



Physicochemical-properties

otParam computes various physicochemical properties fro
he protein sequence. The parameters computed by the Serv
nclude the molecular weight, theoretical pI, amino ac
composition, atomic composition, extinction coefficien
stimated half life, instability index, aliphatic index, and gra
verage of hydropathicity (GRAVY).



Properties	Fenugreek Protein
of Amino Acid:	102
ecular weight:	11372.8
oretical Pi:	10.38
l no. of (-)charged residues (Asp + Glu):	8
l no. of (+) charged residue:	15
l number of atoms:	1583
coefficient (assuming all pairs of Cys residues form cystines)	3105 M-1 cm-1
ability index (II):	34.26
natic index:	68.82
nd average of hydropathicity (GRAVY):	-0.653

Secondary structure

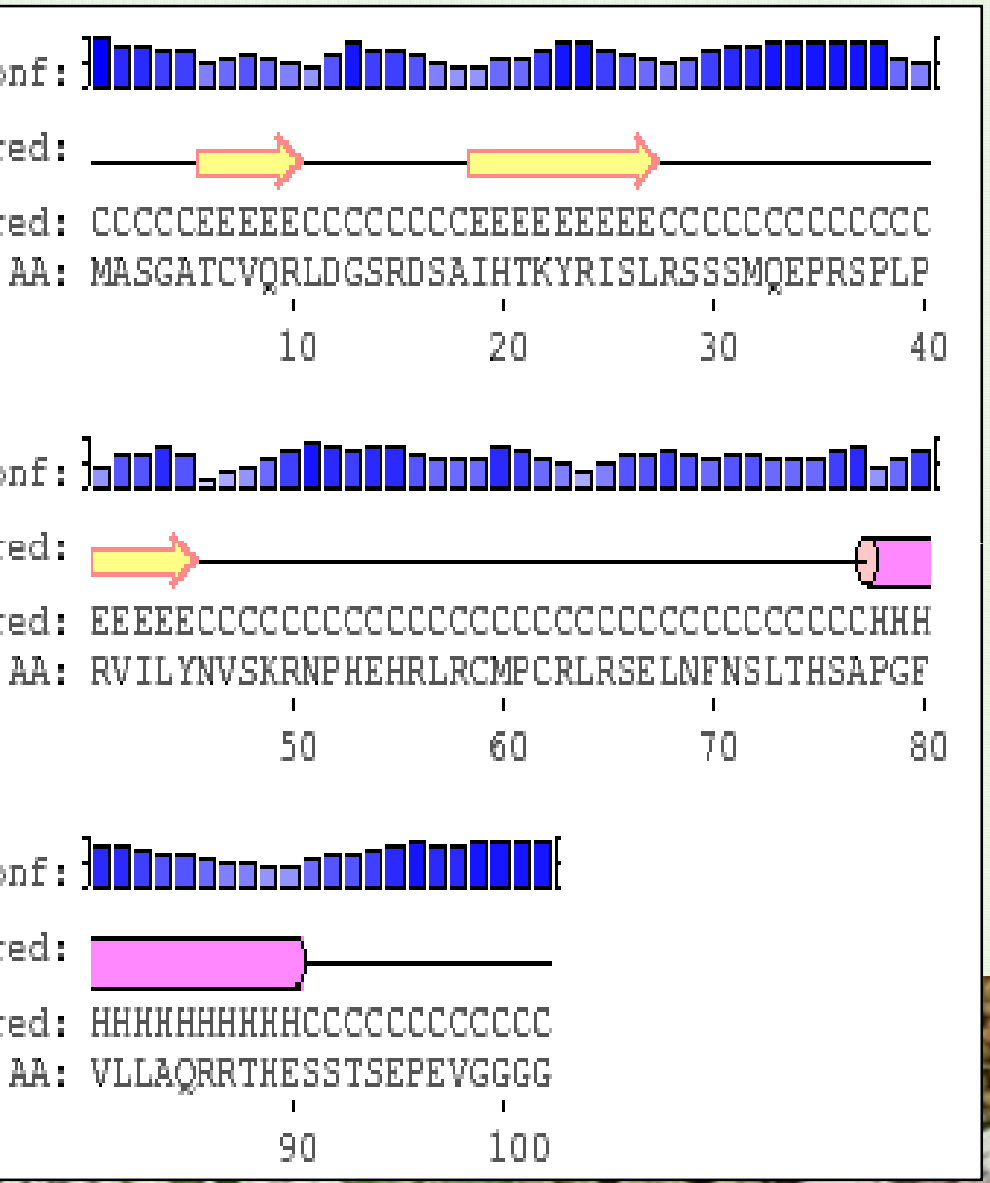
- **GOR IV**
- **PSIPRED**

Secondary structure of protein was predicted by the formation of alpha helix and ß-sheets.

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



2D visualization by PSIPred



Statistics of Secondary Structure

Sequence length : 102

GOR4 :

Alpha helix	(Hh)	:	5 is	4.90
3_{10} helix	(Gg)	:	0 is	0.0
Pi helix	(Ii)	:	0 is	0.00
Beta bridge	(Bb)	:	0 is	0.00
Extended strand	(Ee)	:	26 is	25.49
Beta turn	(Tt)	:	0 is	0.00
Bend region	(Ss)	:	0 is	0.00
Random coil	(Cc)	:	71 is	69.61
Ambigous states	(?)	:	0 is	0.00
Other states		:	0 is	0.00

Tertiary Structure Prediction

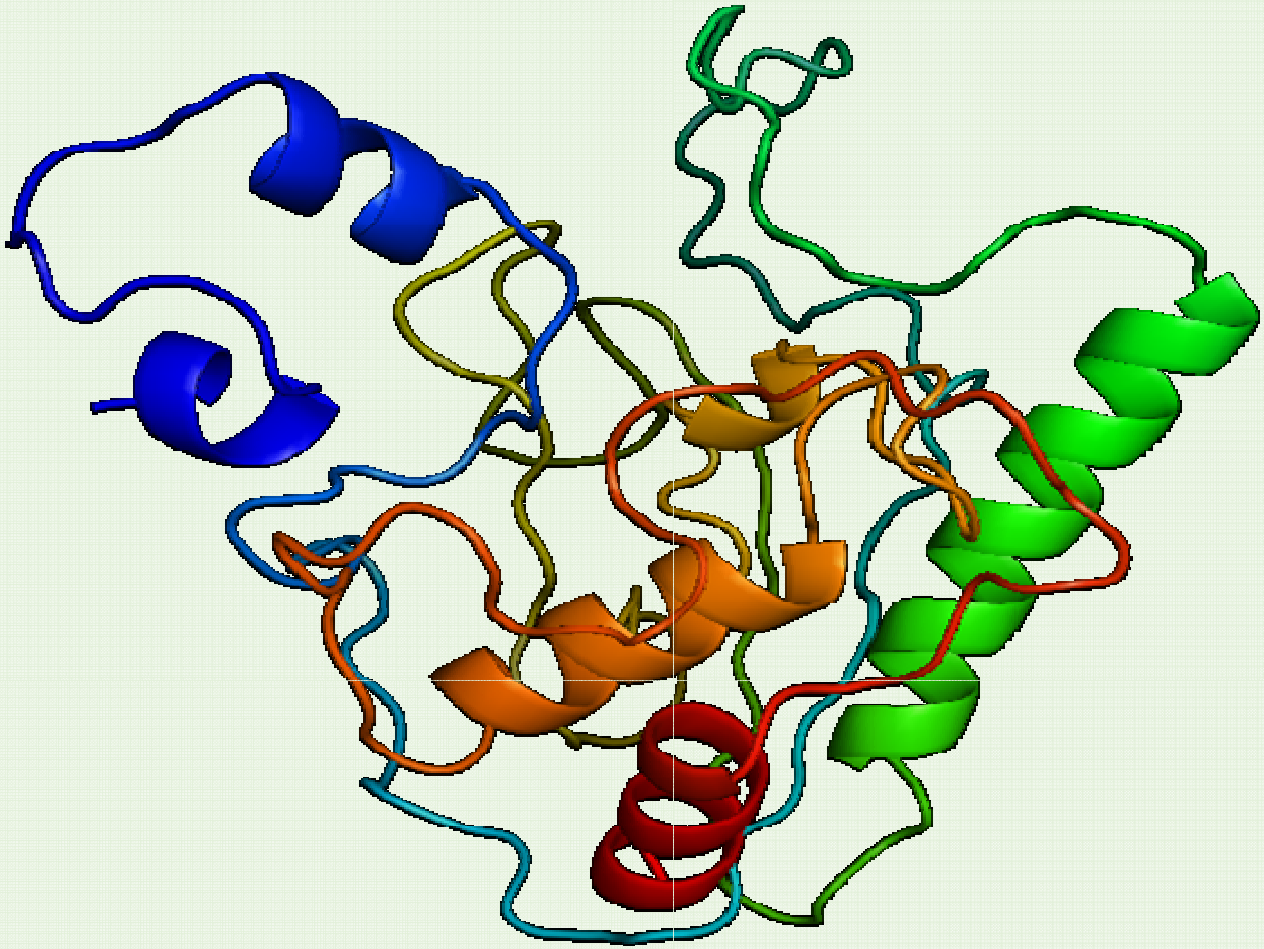
Swiss model is homology based method

Automated mode was used to get tertiary structure. But on the b
of structure validation the structure was found to be inappropriate
Next **Phyre2, I-TASSER** were used for 3D structure generat
These are threading based software.

Verification :

Through the Structural Analysis and Verification Server (SAVS)
tructure by Phyre2 was found to be better as compared to others



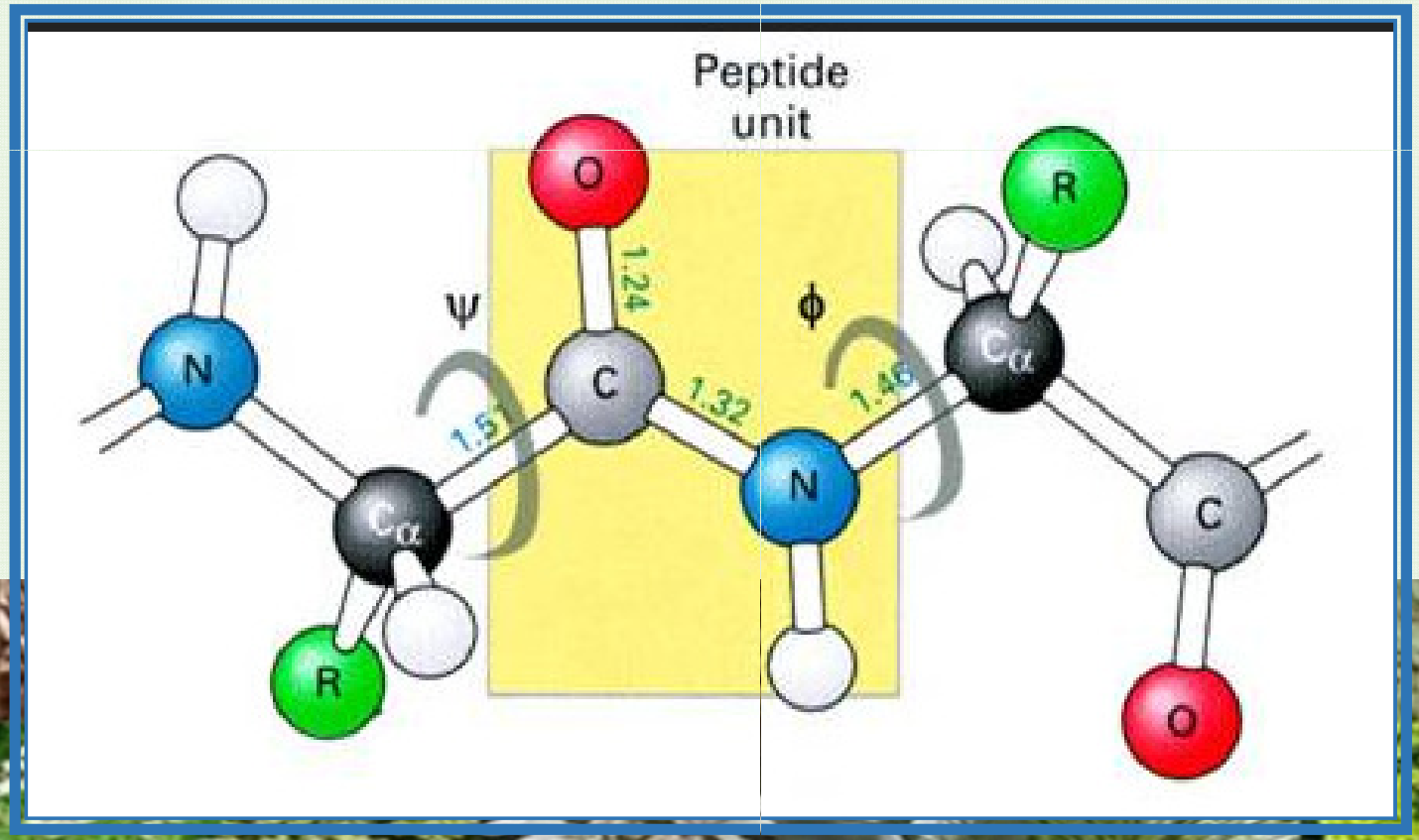


3D Structure for fenugreek protein

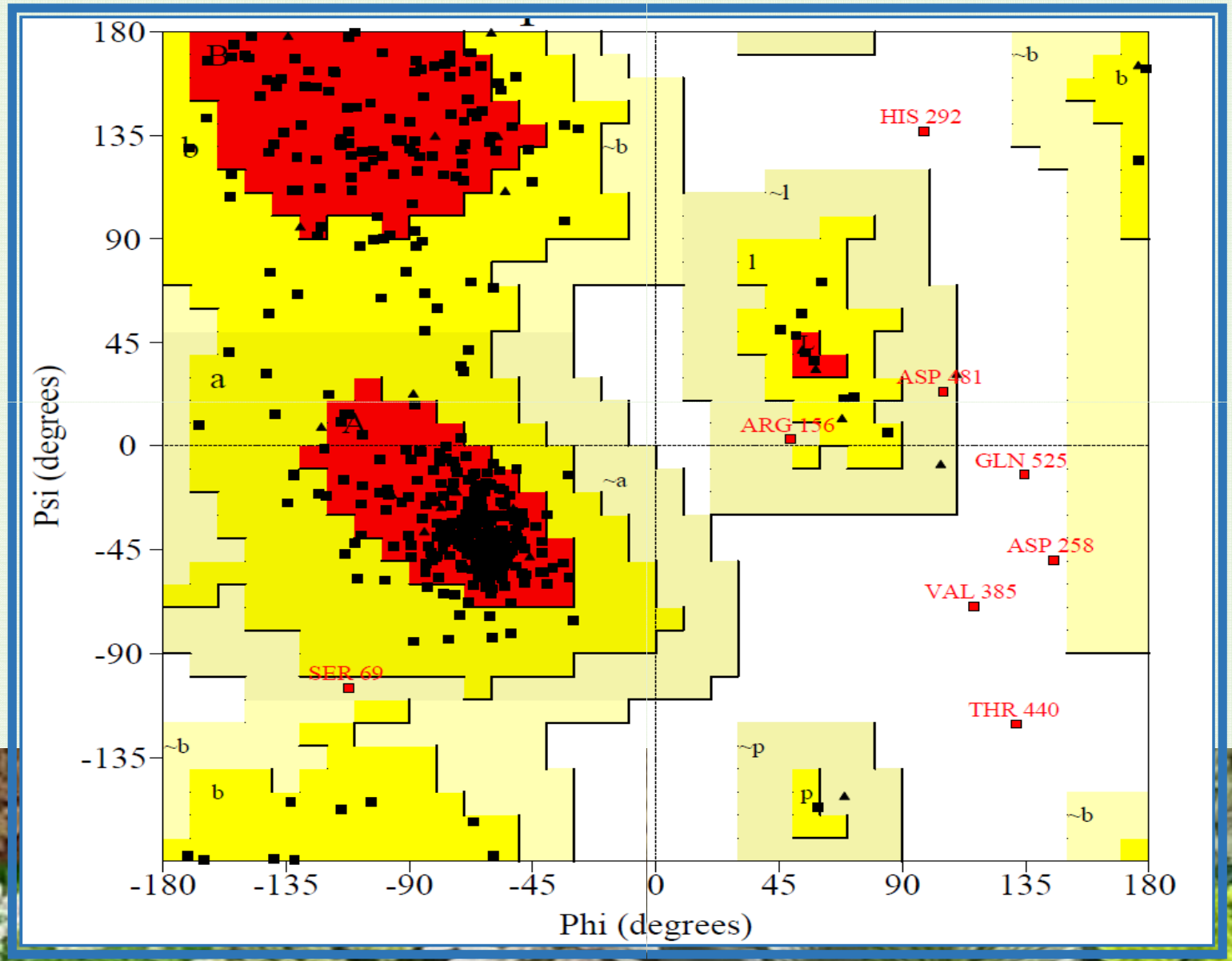


Ramachandran Plot

he Ramachandran plot is a plot of the torsional angles phi and psi of esidue (amino acids) contained in a peptide. By making a Ramachan lot of the protein structure one can determine which torsion angles ying in allowed region of the plot.



Ramachandran plot by SAVES Serve



Conclusion

The predicted protein is stable, globular and basic in nature having lining, depicting it as transmembrane protein

The identified protein of fenugreek showed homology with the pro domain of humans and E-coli illustrating that the database available *Apicaeae and Fabaceae* family are sparsely populated with sequences.

FFPred predicted its functions in 2 categories: 1) Biological Proc phosphate-containing compound metabolic process with a probabilit 95.9% and 2) Molecular function: ATP binding with 98.1% probability



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