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SENSITIVE QUANTITATIVE PREDICTIONS OF MHC BINDING PEPTIDE FROM *TAENIA CRASSICEPS:* NEW DRUG TARGETS

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Abstract- *Taenia crassiceps is a tapeworm member of the Taenia genus. It is related to pork tapeworm Taenia solium, and the beef tapeworm Taenia saginata. Its larvae eat tiny holes in the human retina, eventually detaching it. The life cycle is when an adult lays eggs inside a wild canine.* Peptide fragments of antigen protein can be used to select nonamers for use in rational vaccine design and to increase the understanding of roles of the immune system in infectious diseases. Analysis shows MHC class II binding peptides of antigen protein from *Taenia crassiceps* are important determinant for protection of host form parasitic infection. In this approach, we used SVM and PSSM algorithms for antigen design and predicted the binding affinity of antigen protein having 194 amino acids, which shows 186 nonamers. Binding ability prediction of antigen peptides to major histocompatibility complex (MHC) class I & II molecules is important in vaccine development from *Taenia crassiceps*.

Keywords- antigen protein, epitope, PSSM, SVM, MHC, peptide vaccine

Abbreviations: *Goldman, Engelberg and Steitz, (GES); major histocompatibility complex, (MHC); Position Specific Scoring Matrices, (PSSMs); Support Vector Machine, (SVM)*

I. Introduction

Taenia crassiceps antigen peptides are most suitable for subunit vaccine development because with single epitope, the immune response can be generated in large population [1,2]. This approach is based on the phenomenon of cross-protection, whereby infected with a mild strain and is protected against a more severe strain of the same. The phenotype of the resistant transgenic hosts includes fewer centers of initial infection, a delay in symptom development, and low accumulation. Antigen protein from *Taenia crassiceps* is necessary for new paradigm of synthetic vaccine development and target validation [3-5].

II. Methodology

In this research work antigenic epitopes of antigen protein from *Taenia crassiceps* is determined using the Gomase method in 2007, Hopp & Woods, Roseman, Wolfenden Hydrophobicity and Chou & Fasman and Deleage & Roux antigenicity [6-8]. The major histocompatibility complex (MHC) peptide binding of antigen protein is predicted using neural networks trained on C terminals of known epitopes. In analysis predicted MHC/peptide binding of antigen protein is a log-transformed value related to the IC50 values in nM units. MHC2Pred predicts peptide binders to MHCI and MHCII molecules from protein sequences or sequence alignments using Position Specific Scoring Matrices (PSSMs). Support Vector Machine (SVM) based method for prediction of promiscuous MHC class II binding peptides. SVM has been trained on the binary input of single amino acid sequence [9-14]. In addition, we predict those MHC ligands from whose C-terminal end is likely to be the result of proteosomal cleavage [15-18].

III. Results and Interpretations

We found binding of peptides to a number of different alleles using Position Specific Scoring Matrix. An antigen protein sequence is 194 residues long, having antigenic MHC binding peptides. MHC molecules are cell surface glycoproteins, which take active part in host immune reactions and involvement of MHC class-I and MHC II in response to almost all antigens. PSSM based server predict the peptide binders to MHCI molecules of antigen protein sequence are as 11mer_H2_Db, 10mer_H2_Db, 9mer_H2_Db, 8mer_H2_Db and also peptide binders to MHCII molecules of antigen protein sequence as I_Ab.p, I_Ad.p, analysis found antigenic epitopes region in putative antigen protein (Table 1). We also found the MHCII-IAb peptide regions; MHCII-IAd peptide regions; and MHCII-IAg7 peptide regions which represented predicted binders from bacterial antigen protein (Table 2). The predicted binding affinity is normalized by the 1% fractil. We describe an improved method for predicting linear epitopes (Table 2). The region of maximal hydrophilicity is likely to be an antigenic site, having hydrophobic characteristics, because terminal regions of antigen protein is solvent accessible and unstructured, antibodies against those regions are also likely to recognize the native protein (Fig. 1, 2, 3). It was shown that an antigen protein is hydrophobic in nature and contains segments of low complexity and high-predicted flexibility (Fig. 4, 5). Predicted antigenic fragments can bind to MHC molecule is the first bottlenecks in vaccine design.

IV. Conclusion

An antigen protein from *Taenia crassiceps* peptide nonamers are from a set of aligned peptides known to bind

to a given MHC molecule as the predictor of MHC-peptide binding. MHCII molecules bind peptides in similar yet different modes and alignments of MHCII-ligands were obtained to be consistent with the binding mode of the peptides to their MHC class, this means the increase in affinity of MHC binding peptides may result in enhancement of immunogenicity of antigen protein. These predicted of antigen protein antigenic peptides to MHC class molecules are important in vaccine development from *Taenia crassiceps.*

V. References

[1] Reyes J.L., Espinoza-Jiménez A.F., González M.I., Verdin L., Terrazas L.I. (2011) *Cell Immunol.,* 267(2):77-87.

[2] Sciutto E., Fragoso G., Larralde C. (2011) *Parasite Immunol.,*33(1):79-80.

[3] Lightowlers M.W. (2010) *Parasite Immunol*., 32(11-12):701-9.

[4] McDonald D., Stockwin L., Matzow T., Blair Zajdel M.E., Blair G.E. (1999) *Gene Ther.*, 6(9),1512-9.

[5] Gomase V.S., Kale K.V. and Shyamkumar K. (2008) *J. of Proteomics & Bioinformatics*, 1 (4), 188- 205.

[6] Gomase V.S., Kale K.V., Chikhale N.J., Changbhale S.S. (2007) *Curr. Drug Discov. Technol*., 4(2),117-1215.

[7] Gomase V.S. and Kale K.V. (2008) *Int. J. of Applied Computing*, 1(1), 39-46.

[8] Gomase V.S. and Kale K.V. (2008) *Int. J. of Applied Computin*g, 1(1), 33-38.

[9] Gomase V.S. and Kale K.V. (2008) Int. *J. of Information Retrieval*, 1(1), 11-15.

[10] Gomase V.S., Kale K.V., Shyamkumar K. and Shankar S. (2008) *ICETET 2008, IEEE Computer Society in IEEE Xplore, Los Alamitos, California*, 629-634.

[11] Gomase V.S., Tandale J.P., Patil S.A., Kale K.V. (2006) *14th International Conference on Advance Computing & Communication, Published by IEEE Computer Society in IEEE Xplore USA* 614-615.

[12] Reche P.A., Glutting J.P., Reinherz E.L. (2002) *Hum Immun*., 63, 701-709.

[13] Buus S., et al. (2003) *Tissue Antigens*, 62, 378-384.

[14] Nielsen M., et al. (2003) *Protein Sci*., 12, 1007-1017.

[15] Bhasin M. and Raghava G.P. (2005) *Nucleic Acids Research*, 33, W202-207.

[16] Gomase V.S., Kapoor R.A., Ladak S.S. (2010) *Journal of Infectious Diseases Letters*, 1(1), 01-06.

[17] Gomase V.S. and Shyamkumar K. (2009) *African Journal of Biotechnology*, 8 (23), 6658-6676.

[18] Gomase V.S., Kapoor R.A., Ladak S.S. (2010) *Software and Computing Technology, ICSCT 2010, IEEE Computer Society in IEEE Xplore, USA*.

Table 1- PSSM based prediction of MHC ligands, from whose C-terminal end are proteosomal cleavage sites

MHC-I ALLELE	POS.	N	SEQUENCE	C	MW (Da)	SCORE	% OPT.
8mer_H2_Db	121	EQG	VALRGLFI	IDD	870.11	17.335	33.02 %
8mer_H2_Db	133	DDK	GVLRQITI	NDL	881.08	16.347	31.14 %
8mer_H2_Db	40	LFF	YPMDFTFV	CPT	1001.17	11.13	21.20 %
8mer_H2_Db	62	ADE	FHQRGCQL	LAC	970.12	10.904	20.77 %
8mer_H2_Db	91	RKD	GGVQGMRI	PML	798.95	6.114	11.65 %
8mer_H2_Db	10	RPA	PGFTCKAL	VDG	818.0	5.96	11.35 %
8mer_H2_Db	63	DEF	HQRGCQLL	ACS	936.1	4.123	7.85 %
8mer_H2_Db	94	GGV	QGMRIPML	ADT	927.19	2.972	5.66 %
8mer_H2_Db	46	DFT	FVCPTEII	AFN	903.11	2.621	4.99 %
8mer_H2_Db	109	HRI	SRDYGVLI	EEQ	904.04	2.567	4.89 %
8mer_H2_Db	18	KAL	VDGELKDI	SLS	869.97	1.745	3.32 %
8mer_H2_Db	33	YKG	KYVILFFY	PMD	1074.34	0.974	1.86 %
8mer_H2_Db	45	MDF	TFVCPTEI	IAF	891.05	0.298	0.57 %
9mer_H2_Db	62	ADE	FHQRGCQLL	ACS	1083.28	13.56	26.92 %
9mer_H2_Db	180	SDA	FKPNAGDLK	SFM	971.12	12.17	24.16 %
9mer_H2_Db	44	PMD	FTFVCPTEI	IAF	1038.23	9.956	19.77 %
9mer_H2_Db	121	EQG	VALRGLFII	DDK	983.27	8.437	16.75 %
9mer_H2_Db	38	VIL	FFYPMDFTF	VCP	1196.4	6.77	13.44 %
9mer_H2_Db	148	VGR	CVDEALRLL	DAF	1013.23	5.726	11.37 %
9mer_H2_Db	73	LAC	STDSAYCHL	AWS	978.05	5.232	10.39 %
9mer_H2_Db	88	NVS	RKDGGVQGM	RIP	929.05	4.824	9.58 %
9mer_H2_Db	78	DSA	YCHLAWSNV	SRK	1051.22	4.461	8.86 %
9mer_H2_Db	39	ILF	FYPMDFTFV	CPT	1148.35	1.633	3.24 %
9mer_H2_Db	137	VLR	QITINDLPV	GRC	994.15	1.597	3.17 %
9mer_H2_Db	151	CVD	EALRLLDAF	QFT	1029.22	1.21	2.40 %
9mer_H2_Db	7	VIG	RPAPGFTCK	ALV	958.15	1.209	2.40 %
9mer_H2_Db	127	RGL	FIIDDKGVL	RQI	1001.19	0.827	1.64 %
10mer_H2_Db	6	AVI	GRPAPGFTCK	ALV	1015.2	19.537	33.19 %
10mer_H2_Db	53	TEI	IAFNDRADEF	HQR	1179.27	6.056	10.29 %
10mer_H2_Db	178	PGS	DAFKPNAGDL	KSF	1029.12	5.116	8.69 %
10mer_H2_Db	171	VCP	ANWRPGSDAF	KPN	1079.18	3.091	5.25 %
10mer_H2_Db	25	LKD	ISLSDYKGKY	VIL	1155.32	1.482	2.52 %

Table 2- PSSM based prediction of promiscuous MHC class II binding peptides from antigen protein

MHC-II ALLELE	RANK	POS.	N	SEQUENCE	C	MW (Da)	SCORE	% OPT.
I_Ab	1	46	DFT	FVCPTEIIA	FND	974.19	17.046	47.84 %
I_Ab	2	74	ACS	TDSAYCHLA	WSN	962.05	12.52	35.14 %
I_Ab	3	135	KGV	LRQITINDL	PVG	1067.25	10.241	28.74 %
I_Ab	4	79	SAY	CHLAWSNVS	RKD	975.12	9.756	27.38 %
I_Ad	1	76	STD	SAYCHLAWS	NVS	996.15	18.979	35.71 %
I_Ad	2	151	CVD	EALRLLDAF	QFT	1029.22	9.325	17.55 %
I_Ad	3	157	RLL	DAFQFTDKH	GEV	1090.16	8.695	16.36 %
I_Ad	4	159	LDA	FQFTDKHGE	VCP	1090.16	8.059	15.16 %
I_Ag7	1	148	VGR	CVDEALRLL	DAF	1013.23	13.368	32.71 %
I_Ag7	2	172	CPA	NWRPGSDAF	KPN	1008.1	11.697	28.62 %
I_Ag7	3	154	EAL	RLLDAFQFT	DKH	1092.27	9.236	22.60 %
I_Ag7	4	182	AFK	PNAGDLKSF	MSS	930.03	8.728	21.35 %

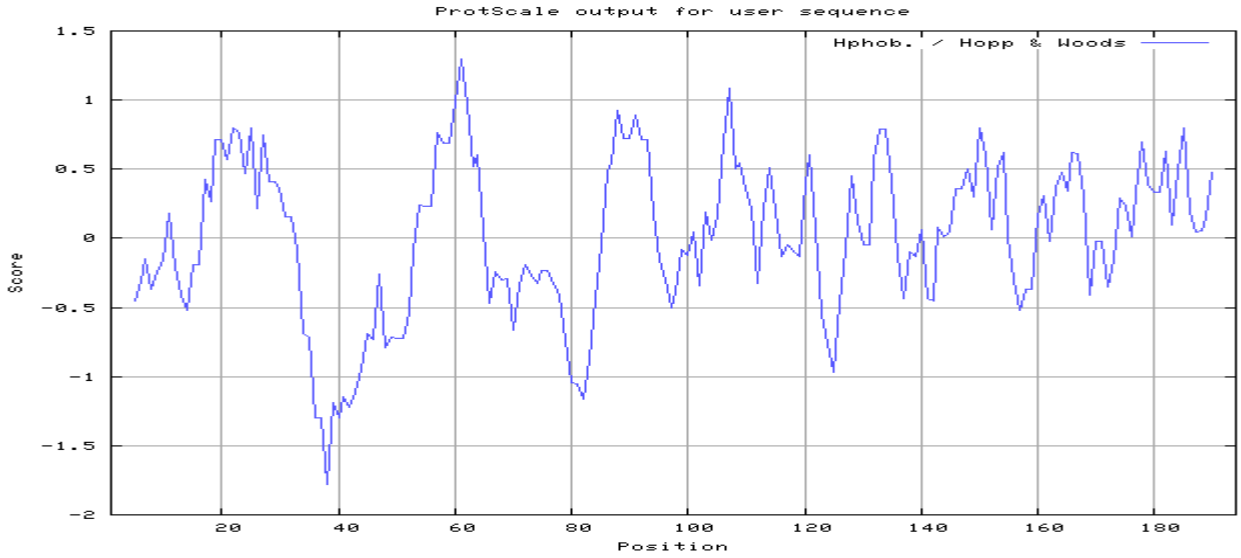

Fig. 1- Hydrophobicity plot of antigen protein by Hphob / Hopp & Woods, scale

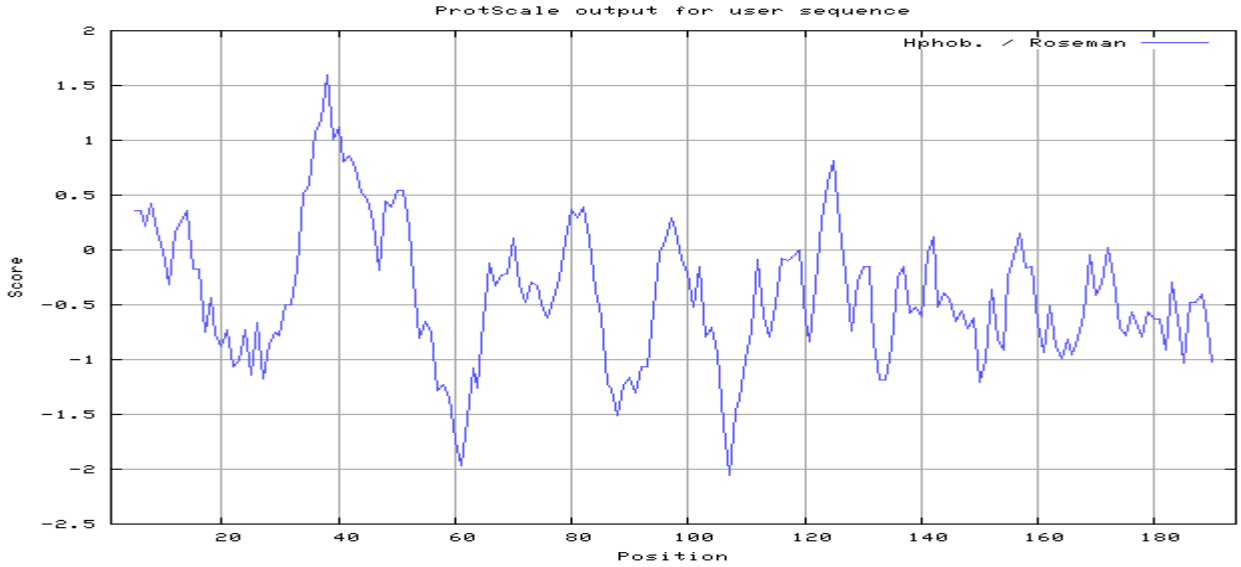

Fig. 2- Hydrophobicity plot of antigen protein by Hphob/ Roseman, scale

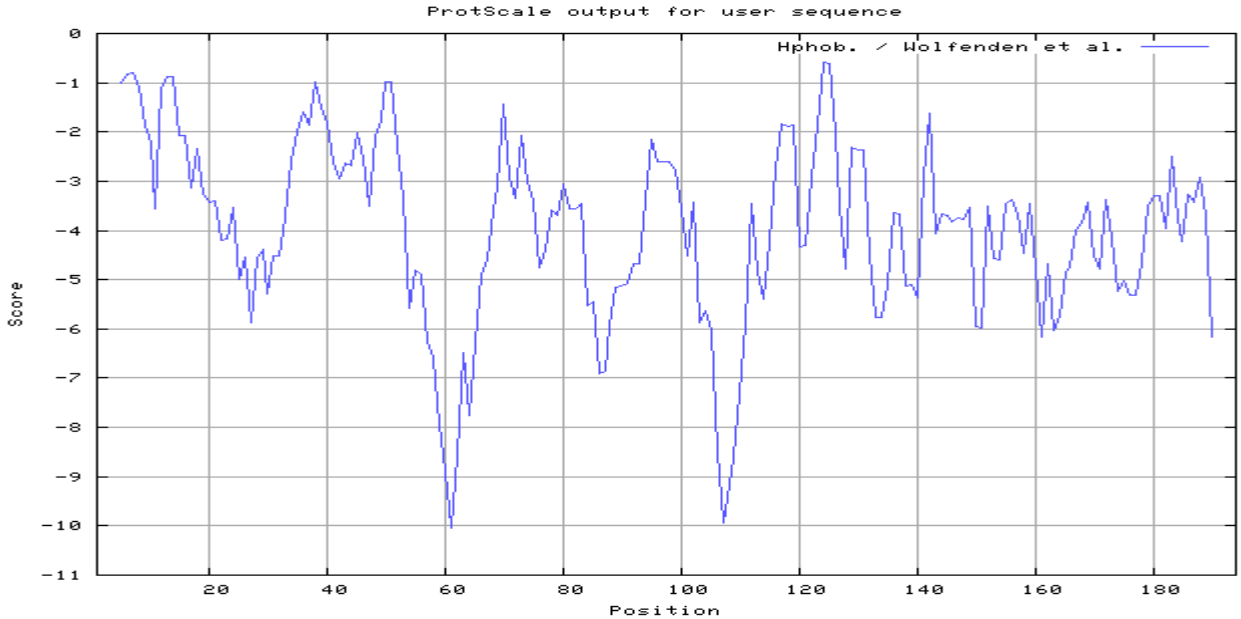

Fig. 3-Hydrophobicity plot of antigen protein by Hphob. / Wolfenden & et al., scale

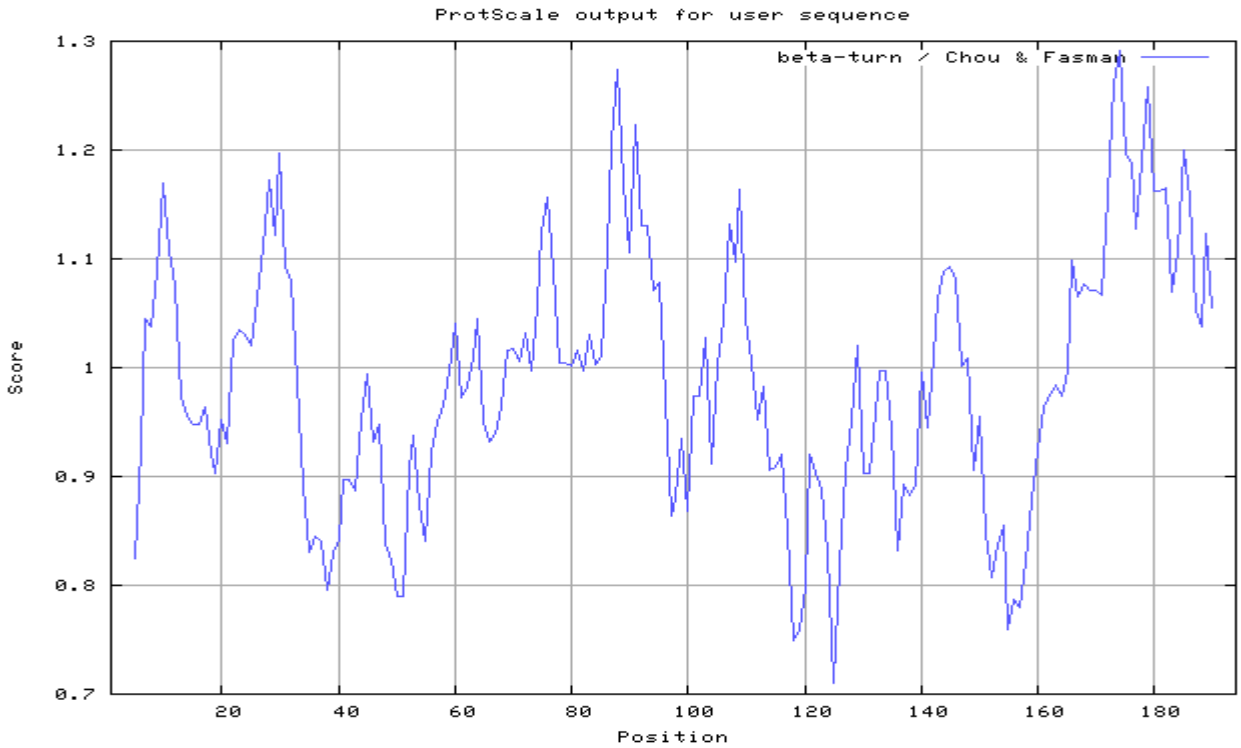

Fig. 4- Antigenicity plot of antigen protein by Beta turn / Chou & Fasman, scale

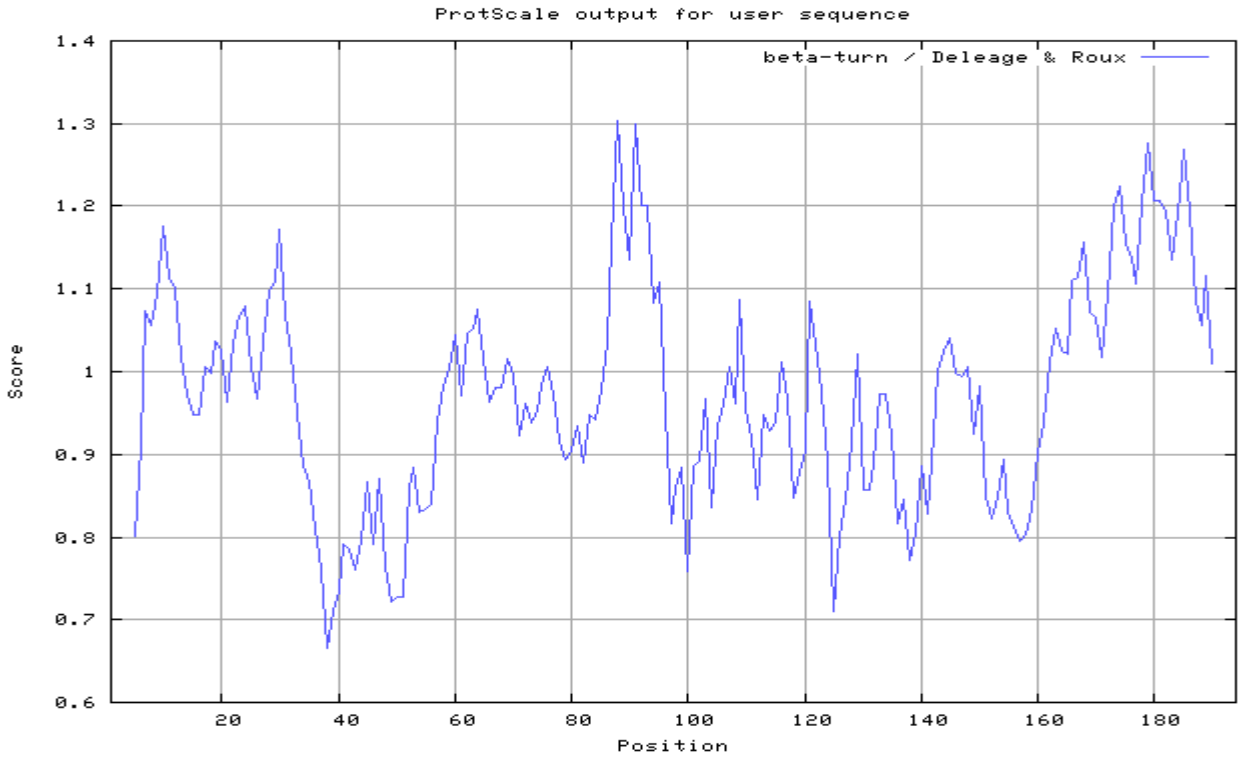

Fig. 5- Antigenicity plot of antigen protein by Beta turn. / Deleage & Roux, scale