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Prediction of antigenic peptides of LTx5 toxin from *Lasiodora sp. IBSP8539*

Gomase V.S.*, Shankar S., Gangawane A.K. and Sherkhane A.S.[1]

[*]Proteomics Unit, Department of Bioinformatics, Padmashree Dr. D. Y. Patil University, Plot No-50, Sector-15, CBD Belapur, Navi Mumbai, 400614, MS, India, Mobile- +91-9987770696, Mail- virusgene1@yahoo.co.in

[1]Department of Biotechnology, College of computer Science and information Technology, Latur, 413531, MS, India

Abstract- The toxin LTx5 toxin is an 116aa residue peptide is isolated from the venom of Lasiodora sp. IBSP8539.In this assay we have predicted the binding affinity of toxin LTx5 toxin having 116 amino acids, which shows 109 nonamers. Peptide fragments of the neurotoxin can be used to select nonamers for use in rational vaccine design and to increase the understanding of roles of the immune system in neurotoxin studies. Small segment '3- STFIIMISLAVALATWPSEH-22' of toxin protein called the antigenic epitopes is sufficient for eliciting the desired immune response. Immunization cassettes should be capable of immunizing of broad immunity against both humoral and cellular epitope thus giving vaccines the maximum ability to deal with neurotoxin protein of Eurypelma californicum. Binding ability prediction of antigen peptides to MHC class molecules is important in vaccine development, We also found the SVM based MHCII-IAb peptide regions, 40- YALADRAEK, 10- ISLAVALAT, 99- MYQAERALE, 14- VALATWPSE, (optimal score is 1.494); MHCII-IAd peptide regions, 96- LDIMYQAER, 29- SETKLNVEL, 68- GASVLCEAV, 4- STFIIMISL, (optimal score is 0.604); MHCII-IAg7 peptide regions , 38- GPYALADRA, 98- IMYQAERAL, 9- MISLAVALA, 99- MYQAERALE, (optimal score is 1.904); and MHCII- RT1.B peptide regions, 17- ATWPSEHIE, 101- QAERALEKL, 98- IMYQAERAL, 108- KLASSFRCE, (optimal score is 0.601) which represented predicted binders from neurotoxin protein. We have predicted a successful immunization.

Key words: Antigen, 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

Lasiodora sp. IBSP8539

Lasiodora spider venom is a complex mixture comprising low-molecular weight components and polypeptides toxins, which are used to paralyze and/or kill their prey. The spider toxins characterized to date have been found to target neuronal receptors, neuronal ion channels or presynaptic membrane proteins involved in neurotransmitter release. The venom has been shown to contain components that inhibit L-type Calcium channels and modulate the activity of Sodium channel [1].

Molecular Aspect

The Lasiodora sp. IBSP8539 species secretes various types of proteins which develop body structure and body mechanism, internally or externally. In the NCBI entrez record, there are five types of proteins secreted by this species and one taxonomic link. LTx5 toxin has been taken in analysis because only this is the one toxin in five others which has high level of expression [2, 3].

II. Methodology

MHC molecules are cell surface glycoproteins, which take active part in host immune reactions. The involvement of MHC class molecules in response to almost all antigens and the variable length of interacting peptides make the study of MHC Class molecules very interesting. MHC molecules have been well characterized in terms of their role in immune reactions [4-6]. They bind to some of the peptide fragments generated after proteolytic cleavage of antigen [7]. This binding acts like red flags for antigen specific and to generate immune response against the parent antigen. So a small fragment of antigen can induce immune response against whole antigen. LTx5 toxin peptides are most suitable for subunit vaccine development because with single epitope, the immune response can be generated in large population. TAP is a transporter associated with MHC class I restricted antigen processing. The TAP is heterodimeric transporter belong to the family of ABC transporter, that uses the energy provided by ATP to translocate the peptides across the membrane [8]. The subset of this transported peptide will bind MHC class I molecules and stabilize them. These MHC-peptide complexes will be translocated on the surface of antigen presenting cells (APCs). This theme is implemented in designing subunit and synthetic peptide vaccines [9]. One of the important problems in subunit vaccine design is to search antigenic regions in an antigen [10] that can stimulate T cells called T-cell epitopes. T-cell immune responses are triggered by the recognition of foreign peptide antigens bound to cell membrane-expressed major histocompatibility complex (MHC) molecules [11].

III. Results and Interpretations

The sequence of protein is 116 amino acids in which include some hydrophilic, some hydrophobic, some are MHC binder protein and some are epitope binding proteins. If we predict the all data of hydrophilic, hydrophobic, epitope binding and MHC class I and II binding proteins, then we easily predict the antigenicity of protein LTx5 toxin from Lasiodora sp. IBSP8539. The high score of LTx5 toxin is the 1.9, 1.6 and 1.4 of the I- Ag7 allele and residue number is 38, 98, 9 and 99, which bind the sequence is GPYALADRA, IMYQAERAL, MISLAVALA and MYQAERALE **(Table-1)**. The TAP pred prediction tool is useful for the prediction of

MHC class I. This tool function is same as the MHC2pred. This result for LTx5 toxin is the start position at 79, sequence is TRSPMYKCM, score is 8.606 and prediction affinity is high also start position 4, sequence STFIIMISL, score is 7.803 and prediction affinity is high **(Table-2)**. It was shown that the toxin protein is hydrophobic in nature and contains segments of low complexity and high-predicted flexibility. Predicted antigenic fragments can bind to MHC molecule is the first bottlenecks in vaccine design.

IV. Conclusion

Lasiodora sp. IBSP8539 involved multiple antigenic components to direct and empower the immune system to protect the host from infection. MHC molecules are cell surface proteins, which take active part in host immune reactions and involvement of MHC class in response to almost all antigens and it give effects on specific sites. Predicted MHC binding regions acts like red flags for antigen specific and generate immune response against the parent antigen. So a small fragment of antigen can induce immune response against whole antigen. This theme is implemented in designing subunit and synthetic peptide vaccines. The sequence analysis method is allows potential drug targets to identify active sites, which form antibodies against or spider venom infection. The method integrates prediction of peptide MHC class binding; proteosomal C terminal cleavage and TAP transport efficiency. Antigenic epitopes of LTx5 toxin protein are important antigenic determinants against the various toxic reactions and spider venom infections.

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TABLE 1: MHC class II binding peptide nonamers from LTx5 toxin Protein

MHC ALLELE	Rank	Sequence	Residue No.	Peptide Score
I-Ab	1	YALADRAEK	40	1.494
I-Ab	2	ISLAVALAT	10	0.914
I-Ab	3	MYQAERALE	99	0.763
I-Ab	4	VALATWPSE	14	0.727
I-Ad	1	LDIMYQAER	96	0.604
I-Ad	2	SETKLNVEL	29	0.580
I-Ad	3	GASVLCEAV	68	0.529
I-Ad	4	STFIIMISL	4	0.479
I-Ag7	1	GPYALADRA	38	1.901
I-Ag7	2	IMYQAERAL	98	1.624
I-Ag7	3	MISLAVALA	9	1.543
I-Ag7	4	MYQAERALE	99	1.431
RT1.B	1	ATWPSEHIE	17	0.601
RT1.B	2	QAERALEKL	101	0.540
RT1.B	3	IMYQAERAL	98	0.482
RT1.B	4	KLASSFRCE	108	0.473

TABLE 2 : TAP Peptide binder of LTx5 toxin Protein

Peptide Rank	Start Position	Sequence	Score	Predicted Affinity
1	79	TRSPMYKCM	8.606	High
2	4	STFIIMISL	7.803	High
3	75	AVYGTRSPM	6.875	High
4	85	KCMIKRLPI	6.069	High
5	46	AEKGKDDSL	6.060	High
6	59	PCQFHCECR	5.902	Intermediate
7	12	LAVALATWP	5.728	Intermediate
8	88	IKRLPISVL	5.653	Intermediate
9	83	MYKCMIKRL	5.523	Intermediate
10	5	TFIIMISLA	5.478	Intermediate
11	105	ALEKLASSF	5.303	Intermediate
12	76	VYGTRSPMY	5.303	Intermediate
13	94	SVLDIMYQA	5.060	Intermediate
14	78	GTRSPMYKC	5.048	Intermediate