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Analytical Study of Plasmodium Vivax

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Abstract: Protein sequence of plasmodium vivax was found from genpept data base (ACCESSION NO.-P22290) .We use P2290 to predict its amino acid, atomic, PEAST region, solvent accessibility, molecular mass, theoretical PI and catalytic site, P22290 structure identification by its three dimensional structure using bioinformatics tool. We study P22290 solvent accessibility threw protein predict online server and secondary structure was studied by HNN bioinformatics tool to find its physical and chemical properties. PEST find tools help us to determine hydrophobicity index value. Hydrophobicity and catalytic site was checked using protscale tool (1). We also studied formation of disulphide bond, point mutation effect using heat map and catalytic site of P22290 resulting thirteen identified region with maximum score of 0.005 and minimum score was 0.004. Amino acid composition and Atomic composition of P22290 can accelerate by PROTPARM tool by using amino acid sequence. ProtParam is a tool which allows the computation of various physical and chemical parameters for a given protein stored in Swiss-Prot for a user entered protein sequence. The computed parameters include the molecular weight, theoretical pI, amino acid composition, atomic composition, extinction coefficient, estimated half-life, instability index, aliphatic index and grand average of hydropath city (GRAVY).The total number of atoms 16513 was presented where 5112 carbon, 8125 hydrogen, 1495 nitrogen, 1740 oxygen and 41 atom of sulphur were presented. The atomic formula of given protein was c5112h8125n1495 s41. The instability index (II) is computed to be 36.42. This classifies the protein as stable.

I. INTRODUCTION

Plasmodium vivax is a causative agent of malaria. Malaria is a most important topical disease in Asia and South Africa. At least 80 million individuals world wide suffer from vivax malaria. Duffy binding protein (DBP) is most critical ligand for Plasmodium vivax merozoite invasion of hymen erythrocyte surface (1, 2). DBP belongs to a family of homologous Duffy binding-like erythrocyte binding proteins (DBL–EBP) located within the micronemes of P.vivax and P.knowlesi merozoites [3].The Plasmodium vivax vaccineisa protein necessary for P.vivax invasion of reticulocytes(4). The polymorphic nature of DBP induces strain specific immune responses that pose unique challenge for vaccine development. (5). Plasmodium vivax DBP is a 140KDa protein secreted by micronemes of a parasite organelles at the apical end of the merozoite as it's invades erythrocytes (6).DBP is a most leading vaccine candidate against Plasmodium vivax malaria (7). P22290 represents the N terminus of the Duffy-antigen binding protein and is thought to bind to the human erythrocytes Duffy blood group determinant. These domains are found in eukaryotic proteins and are approximately 70 amino acids in length (8). Duffy receptor P22290 has great role in invasion in erythrocyte (9)

II. METHODOLOGY

The protein sequence was received from GenePept database whose source accession no was P22290 available at NCBI website (10).The retrieved protein sequence was checked for its several chemical and physical properties such as molecular weight, sulphide, theoreandtical Pi, instability index ,aliphatic index and percentage of amino acid using Protparm tool from whence chemical structure and formula were deduced. The amino acid sequence was first used to predict 2D structure using HNN. Hydrophobicity was checked out by analyzing data of protein in protscale tool. (11). Then protein sequence was used to check its several other properties like disulphide bond, solvent accessibility, effect of point mutation, heat map prediction using online server predict protein (12). Based on hydrophobicity value, theoretical pi, molecular weight and some other values checked for putative protein family using propsearch tool (13). Sulfated tyrosine detected Expasy tool (14). Catalytic site of P22290 is determined by online web server http:// www.catsid.llnl.gov (15).

III. RESULT AND DISCUSSION

The amino acid sequence of plasmodium vivax (ACCESSION NO- P22290) 1070 was found from genpept data base available at NCBI website. This protein sequences was submitted to predictprotein.org online server to get solvent accessibility, amino acid composition, Disulphide Bridge, secondary structure composition, heat map. we got secondary structure of given protein sequence by using bioinformatics tool hierarchical neural network(HNN).

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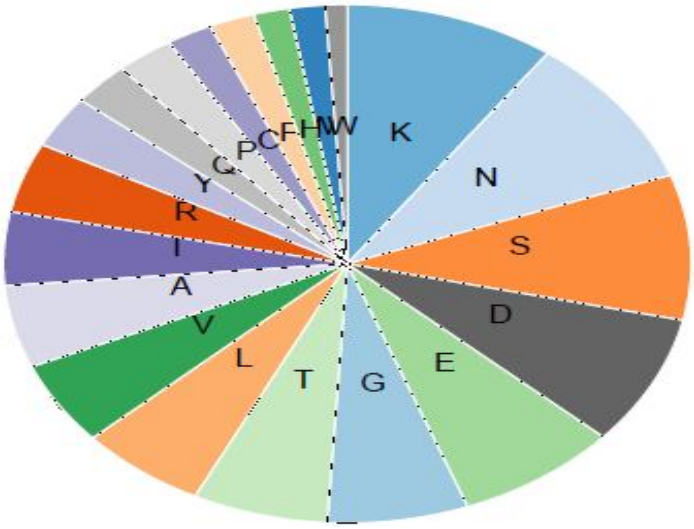
PEAST finding bioinformatics tool show many regions with poor and potential amino acid sequences.
HEATMAP show each substitution independently for each position of a given sequence. Dark red indicate high score and green show low score.
After that we study catalytic site of p22290 protein. Here we mention detail of first 5 catalytic site found in protein.
Atomic composition of P22290 was found by using protparm tool. The total number of atoms 16513 was presented where 5112 carbon, 8125 hydrogen, 1495 nitrogen, 1740 oxygen and 41 atom of sulphur were presented. The atomic formula of given protein was c5112h8125n1495 s41.

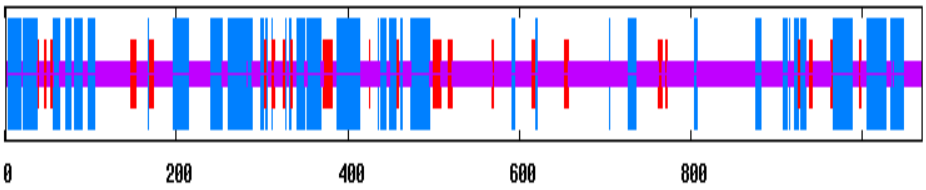
Figure -1 Amino acid composition



(Figure-1)

Amino acid composition details showed us that lysine was highest (9.9%) presented. The N terminal of the sequence considered was methionine (MET). The total number of negatively charged residues (asp+glu) was 169 and positively charged residues (arg+lys) was 153. The molecular mass of this protein was 11968.1. Theoretical Pi value was 5.79 and instability index was computed 36.42. This classified the protein as stable. The aliphatic index was 61.50and grand average of hydrophaticity (GRAVY) WAS -0.966.

Figure-2 Protein secondary structure



(Figure:2)

HNN

Alpha helix	(Hh):	345	is	32.24%	
3_{10} helix	(Gg):	0	is	0.00%	
Pi helix	(Ii):	0	is	0.00%	
Beta bridge	(Bb):	0	is	0.00%	
Extended strand	(Ee) :	85	is	7.94%	
Beta turn	(Tt):	0	is	0.00%	
Bend region	(Ss):	0	is	0.00%	
Random coil	(Cc):	640	is	59.81%	
Ambiguous states	(?):	0	is	0.00%	
Other states	:	0	is	0.00%	

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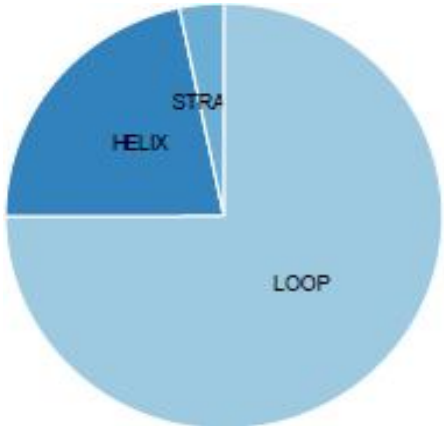
Figure -3 Secondary structure composition



(Figure-3)

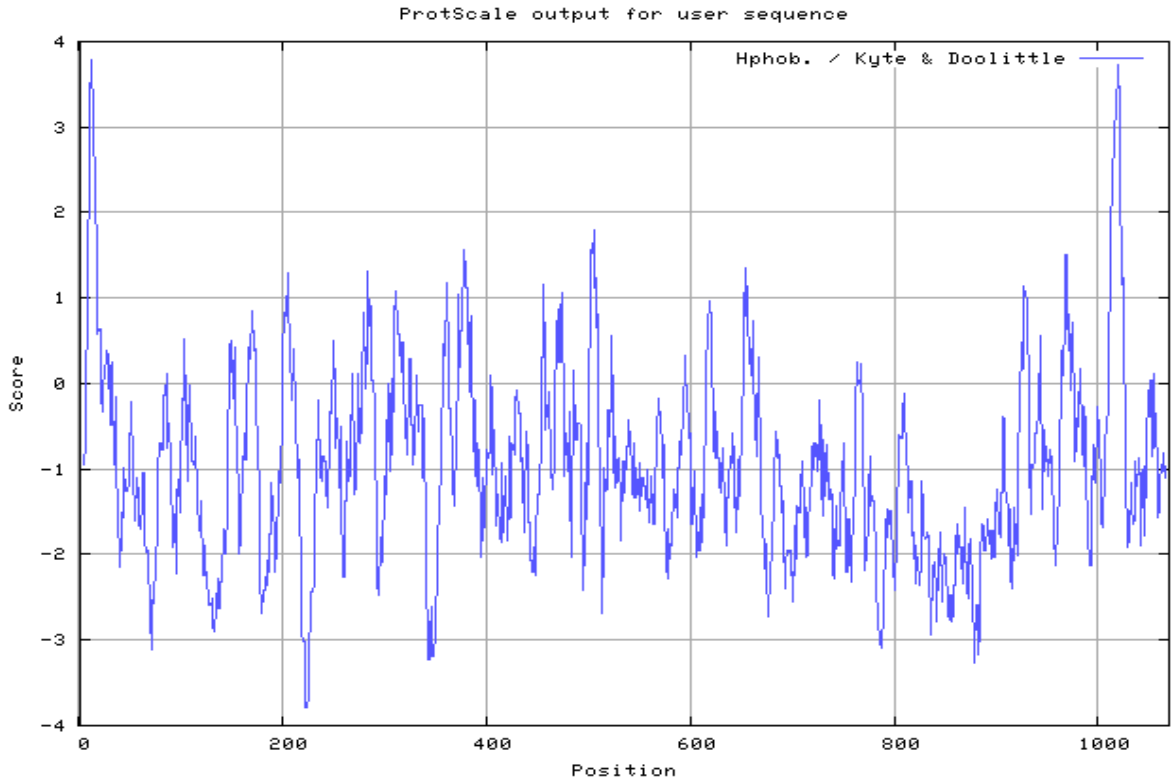
Predicting secondary structure by HNN showed that 59.81% is random coil, alpha helix is 32.85% and extended strains are only 13.14%.

Figure- 4 The individual values for the 20 amino Using the scale Hphob. / Kyte & Doolittle acids are:

Ala:	1.800	Arg:	-4.500	Asn:	-3.500	Asp:	-3.500	Cys:	2.500	Gln:	-3.500
Glu:	-3.500	Gly:	-0.400	His:	-3.200	Ile:	4.500	Leu:	3.800	Lys:	-3.900
Met:	1.900	Phe:	2.800	Pro:	-1.600	Ser:	-0.800	Thr:	-0.700	Trp:	-0.900
Tyr: -1.300		Val:	4.200	: -3.500		: -3.500		: -0.490			

(Figure- 4)

(Figure:-5) protscale output for hydrophobicity of p22290



(Figure:-5)

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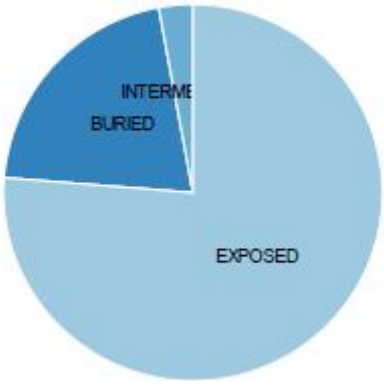
Figure:-6 diagrammatic representation of solvent accessibility



Solvent Accessibility
(Figure:-6)

Figure:-8 PEAST region detail

PEAST- FIND tool is used to find potential and poor motif in given protein sequence. Here we use P22290 which has 1070 amino acid chain to find out result.

Sequence was checked for PEAST motif where one PEAST motif with 19 amino acids was identified potential with PEAST score 19.02.and motif with 31 amino acids was very poor found in between position 848-868 with PEAST score -9.38.

Figure:-9 heat map representation of p22290

We show each substitution independently for each position of a protein in a heat map representation. Dark red indicates a high score (score > 50, strong signal for effect), white indicates weak signals (-50 < score < 50), and green a low score (score < -50, strong signal for neutral/no effect

Figure:-10 first five catalytic site of P22290

	1ok4-9	4nuv	0.005	4.01.02.0013	Fructose-bisphosphate aldolase class i	asp.498.b-asp.24.j, lys.446.b-lys.177.j, tyr.400.b-tyr.146.j,
	1ptd-1	4nuv	0.005	4.06.01.0013	Phosphatidylinositol-specific phospholipase c	arg.394.a-arg.69.a, asp.451.a-asp.274.a, leu.453.a-his.32.a, leu.478.a-his.82.a,
	1qb4-1	4nuv	0.005	4.01.01.0031	Phosphoenolpyruvate carboxylase	arg.304.b-arg.396.a, arg.398.b-arg.581.a, arg.223.b-arg.713.a,
	1qpr-0A	4nuv	0.005	2.04.02.0019	Quinolinic acid phosphoribosyltransferase	asp.399.b-asp.222.a, glu.395.b-glu.201.a, lys.220.b-lys.140.a,
	1qpr-1B	4nuv	0.005	2.04.02.0019	Quinolinic acid phosphoribosyltransferase	asp.399.a-asp.222.b, glu.395.a-glu.201.b, lys.220.a-lys.140.b,

Figure -11 is a software tool able to predict tyrosine sulfation sites in protein sequences

The Sulfinator is a software tool able to predict tyrosine sulfation sites in protein sequences. It employs four different Hidden Markov Models that were built to recognize sulfated tyrosine residues located N-terminally, within sequence windows of more than 25 amino acids and C-terminally, as well as sulfated tyrosine clustered within 25 amino acid. sulphated tyrosines also participate in the association of DARC with each of its four known chemokine

E-cutoff value is 55

Protein / sequence name Position E-value Sequence sequence

PVDR_PLAVS P22290 943 [44] NISLEYCNSVED----K

+++ +Y+ ++ k

[1.1] NEFEEYCDNIHRIPL-M

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+e+++Y+++ +++ +

1069 [31] EHMQPSTPLDY

++ ++ ++ dY

Sequence(s) processed: 1
Sulfated tyrosine detected: 3 (of 35)
Number of proteins with at least one hit: 1

IV. CONCULISION

It is very critical task for searching sequence from large data base and analyzing them in various aspects like physical and chemical properties, amino acid composition, solvent accessibility, Disulphide Bridge, secondary structure composition and heat map
Its chemical structure is C5112H8125 N1495S41 which shows 5112 atoms of carbon, 8125 atoms of hydrogen, 1495 atoms of nitrogen and 41 atoms of sulphur. Amino acid composition details showed us that lysine was highest (9.9%) presented. The N terminal of the sequence considered was methionine (MET). The total number of negatively charged residues (asp+glu) was 169 and positively charged rise use (rg+lys) was 153. The molecular mass of this protein was 11968.1. Theoretical Pi value was 5.79 and instability index was computed 36.42. This classified the protein as stable. The aliphatic index was 61.50and grand average of hydrophaticity (GRAVY) WAS -0.966.

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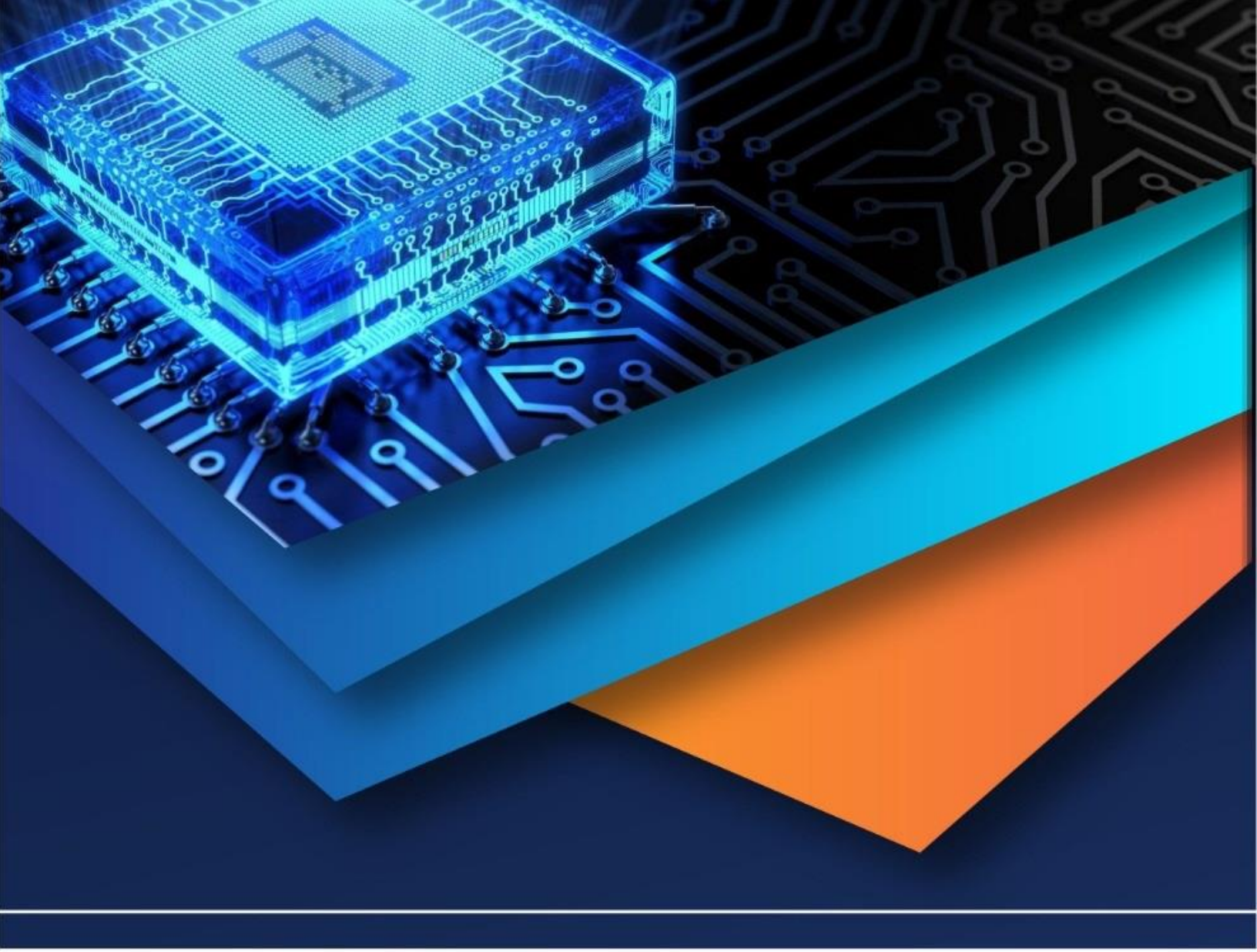

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