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Research Article

MODELING OF HEPATITIS B VIRUS SURFACE ANTIGEN PROTEIN

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ABSTRACT

The modelling of hepatitis B virus surface antigen protein was done using Swiss-Model software online which yielded two models. The structural details were obtained.

Keywords: Hepatitis B, surface antigen, protein modelling.

INTRODUCTION

Hepatitis B virus (HBV) is an important pathogen causing severe disease conditions in human. It mainly affects the liver and is widely prevalent globally. It is widely prevalent in India also. The surface antigen protein induces immune response which plays important role in protection against the disease. Hence it was considered useful to study the structural properties of this protein.

MATERIALS AND METHODS

The HBsAg gene sequence of an Indian isolate was downloaded from Pub Med of NCBI website, hepatitis B virus isolate Ind 1992 S protein gene, complete cds GenBank: JN107758.1, 684 bp DNA. The amino acid sequence is given in Table 1.

Table 1. **Primary amino acid sequence used for modeling.**

MENITSGFLGPLLVLQAGFFLLTRILTIPQSLDSWWTSLNFLGG

SPVCLGQNSQSPTSNHSPTSCPPICPGYRWMCLRRFIIFLFILLLCLIFLLVLLDYQG

MLPVCSLIPGSTTTSTGPCKTCTTPAQGNSMFPSCCCTKPTDGNCTCIPIPSSWAFAK

YLWEWASVRFSWLSLLVPFVQWFVGLSPTVWLSAIWMMWYWGPSLYSIVSPFIPLLPIFLCL
WVYI

Model Building

Template search with BLAST and HHBlits has been performed against the SWISS-MODEL template library (SMTL, last update: 2018-06-01, last included PDB release: 2018-05-25).The target sequence was searched with BLAST against the primary amino acid sequence contained in the SMTL. For each identified template, the template's quality has been predicted from features of the target-template alignment. The templates with the highest quality have then been selected for model building. Models are built based on the target-template alignment using ProMod3. Coordinates which are conserved between the target and the template are copied from the template to the model. Insertions and deletions are remodelled using a fragment library. Side chains are then rebuilt. Finally, the geometry of the resulting model is regularized by using a force field. In case loop modelling with ProMod3 fails, an alternative model is built with PROMOD-II (Guex *et al.*, 2009; Camacho *et al.*, 2009; Benkert *et al.*, 2011; Remmert *et al.*, 2012; Bertoni *et al.*, 2017; Bienert *et al.*, 2017; Waterhouse *et al.*, 2018).

RESULTS AND DISCUSSION

The modelling yielded one model as shown in Fig. 1.1. This model was then visualised in spdbv 4.10 and different forms were seen (Fig. 1.2, 1.3, 1.4). The modelling parameters obtained are shown in Table 2.

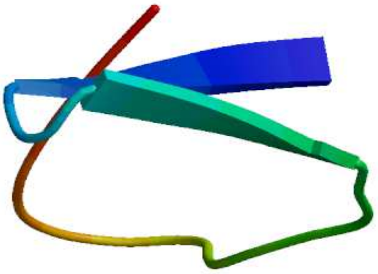

Fig. 1.1. Model 1 of HBsAg protein constructed using Swiss-Model.

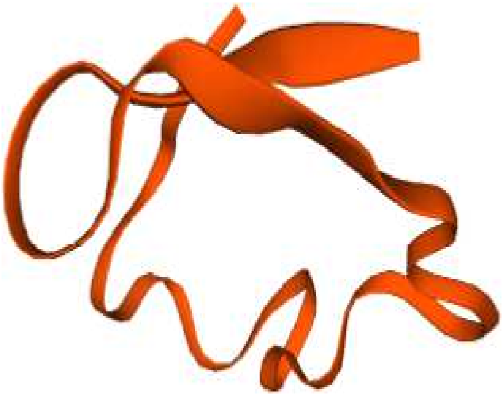

Fig. 1.2. Model in fig 1 seen as ribbon.

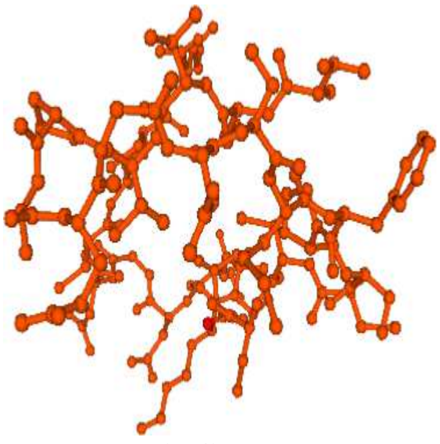

Fig.1.3. Model in fig 1 seen as Ball and stick.

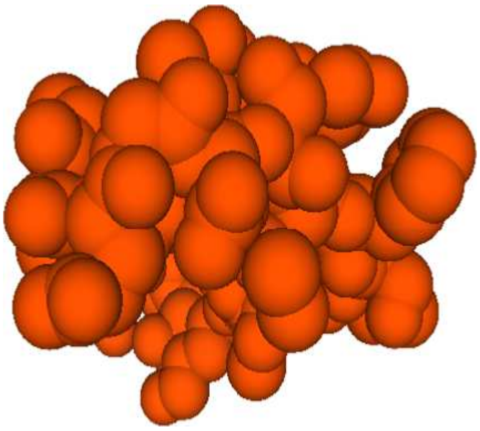

Fig. 1.4. Model in fig 1 seen as space-fill model

Table 2. Model-Template Alignment and results obtained thereof.

Model_01	MENITSGFLGPLLVLQAGFFLLTRILTIPQSLDSWWTSLNFLGGSPVCLGQNSQSPTSNHSPTSCPPICPGYRWMCLRRF	80
3sjl.1.C	--	
Model_01		
3sjl.1.C	IIFLFILLLCLIFLLVLLDYQGMLPVCSLIPGSTTTSTGPCK**TCTTPAQGNSMFPS**–**CCCTKPTDGNCTCI**PIPSSWAF	158
Model_01	--	
	SCYNPTDGQSYLIAYRDCCGYNVSGRCPCL--------	89
3sjl.1.C		
	AKYLWEWASVRFSWLSLLVPFVQWFVGLSPTVWLSAIWMMWYWGPSLYSIVSPFIPLLPIFLCLWVYI	226
	--	

State Oligo-	Ligands	GMQE	QMEAN
Monomer	None	0.04	-3.63

Global Quality Estimate		Local Quality Estimate	Comparison
QMEAN	-3.63		
Cβ	-3.02	Residue Number	
All Atom	-1.86		
solvation	-4.76	★Protein Size (Residues)	
torsion	-1.29		

Template	Seq Identity	Coverage	Description
3sjl.1.C	32.14%		Methylamine dehydrogenase light chain

CONCLUSION

The modelling of HBsAg protein using Swiss-Model revealed valuable structural details of the protein and its reacting sites.

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