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Modeling of infectious bursal disease virus VP2 capsid protein

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Abstract

The VP2 capsid protein of infectious bursal disease virus has different groups, which show the reactive sites on the protein. When various parameters were applied in the Swiss-model software, different groups like strand color group, ball and stick color group, ribbon color group, space-fill color group, wire frame color group could be seen. These model features showed clearly the reactive sites as well as grooves on the protein. The three dimensional protein structures are essential for the proper understanding of the molecular basis of protein function. Since VP2 is responsible for neutralizing antibody which gives protection, the epitopes groups seen in the model structure could be the antigenic sites for neutralising antibody.

Key words: **IBD virus, VP2 capsid protein, modeling**

The capsid protein VP2 of IBDV (Chauhan et al ., 2004) was used for modeling using SWISS-MODEL software online and viewed using Rasmol V2.7.2.1.1 and Swiss PDB viewer (SPDV V3.7) (Schwede et al., 2003; Guex and Peitsh, 1997; Peitsch, 1995, 1996, 1997; Peitsch et al., 2000; Kopp and Schwede, 2004; Gasteiger et al., 2001;Boeckmann et al., 2003; Westbrook et al., 2003; Sayle and Milner-White, 1995). The amino acid sequence of VP2 was submitted to SWISS-MODEL website online for modeling and the results obtained

were visualized using spdbv and Rasmol softwares (Kopp and Schwede, 2004; Schwede et al, 2003; Guex Peitsch, 1997; Peitsch, 1995).

Among all current computational approaches, homology modeling is the only method that can reliably generate a three-dimensional model for a protein (Tramontano et al., 2001). If a target protein shares significant amino acid sequence similarity to at least one experimentally solved three-dimensional structure (template), homology or comparative modeling can be applied to construct a three-dimensional model for the new protein (Kopp and Schwede, 2004). Protein structure determination and comparative modeling complement one another in the exploration of the protein structure space (Sanchez et al., 2000).

The modeling results of capsid protein VP2 of IBDV obtained from the SWISS-MODEL server are shown (Fig.1-6). It is evident that the VP2 capsid protein has different groups, which show the reactive sites on the protein. When various parameters were applied in the Swiss-model software, different groups like strand color group, ball and stick color group, ribbon color group, space-fill color group, wire frame color group could be seen. These model features showed clearly the reactive sites as well as grooves on the protein. The three dimensional protein structures are essential for the proper understanding of the molecular basis of protein function (Kopp and Schwede, 2004). Since VP2 is responsible for neutralizing antibody which gives protection (Turiso et al., 1991), the epitope groups seen in the model structure could be the antigenic sites for neutralising antibody.

Application for high quality models are manifold and include planning site-directed mutagenesis experiments and rationalizing the effects of mutation characterization of molecular functions and structure based drug design (Kopp and Schwede, 2004; Vaidehi et al., 2002; Murray and Honig, 2002; Schafferhans and Klebe, 2001; Schapira et al., 2003). Sanchez et al., (2000) proposed that the availability of structural information for the whole protein families, organisms or metabolic pathways will encourage newer applications like development of drugs with higher selectivity for a given target protein would be facilitated by the availability of structural models for all proteins sharing similar ligand binding sites. Structural comparisons would allow screening for drug candidates with better specificity at earlier stages of drug development.

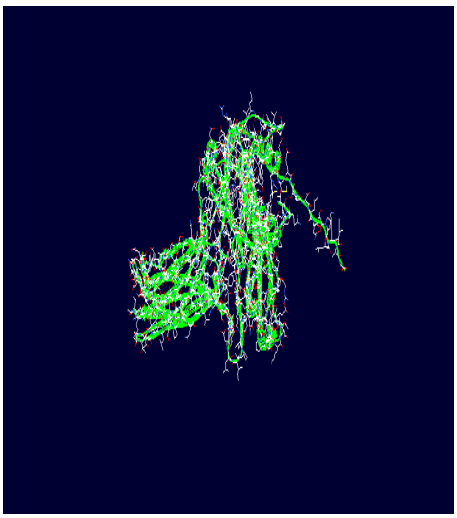

Fig.1 IBDvp2 protein, spdbv 3.7

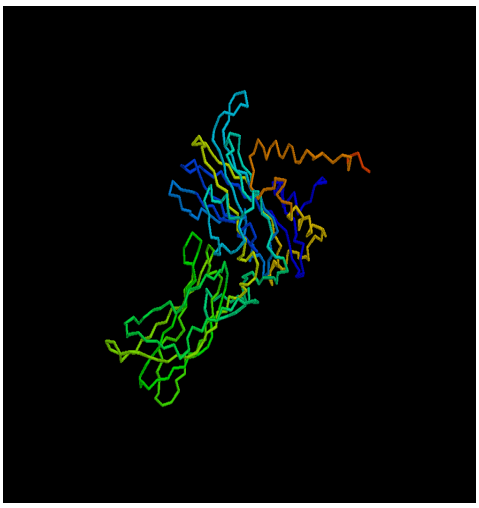

Fig.2.IBDvp2 color group backbone

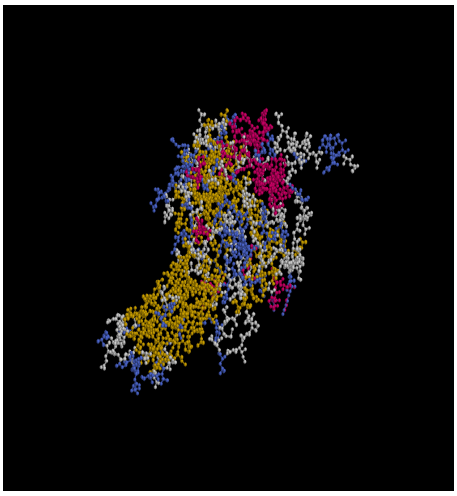

Fig3. IBDvp2 color group ball & stick

Fig.4.IBDvp2 color group ribbon

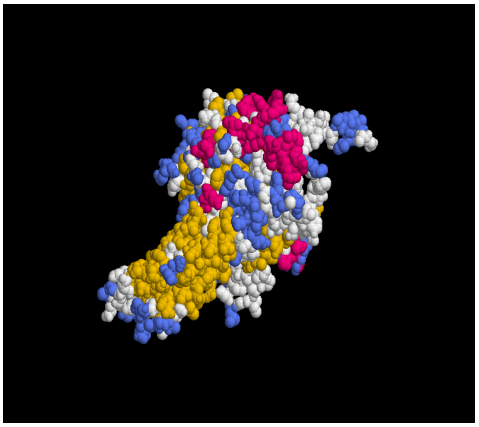

Fig.5.IBDvp2 color group spacefill

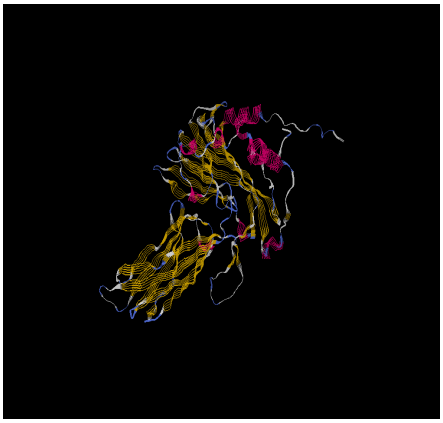

Fig.6.IBDvp2 color group strand

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