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Modeling of rabies viral proteins**A Rai, N Rai*, Soni Gangwar, P K Gupta**

Division of Animal Biotechnology, Indian Veterinary Research Institute, Izatnagar, Bareilly-243122, UP, India, *Gayatri College of Biomedical Science, Ballapur Chowk, GMS Road, Dehradun-248001, Uttarakhand.

Abstract

The amino acid sequence of rabies virus ERA and CVS strains glycoprotein, phosphoprotein and nucleoprotein were submitted to SWISS-MODEL website online for modeling and the results obtained were visualized using spdbv and Rasmol softwares. It is evident that the proteins have different groups, which show the reactive sites on the proteins. 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.

Key words: Protein modeling, rabies virus, glycoprotein, phosphoprotein, nucleoprotein.

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.

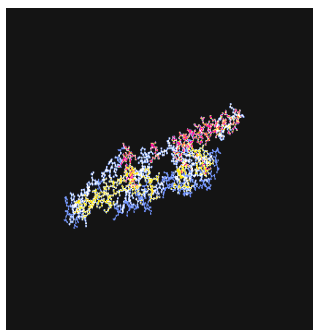
Among all current computational approaches, homology modeling is the only method that can reliably generate a three-dimensional model for a protein (Tramontano et al., 2001). If a target protein shares significant amino acid sequence similarity to at least one experimentally solved three-dimensional 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 amino acid sequence of rabies virus glycoprotein, phosphoprotein and nucleoprotein were 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).

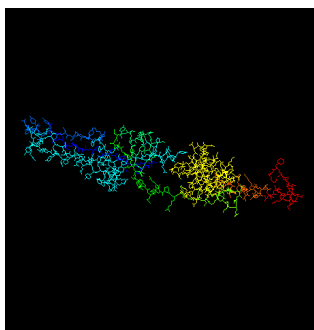
The modeling results of proteins of rabies virus obtained from the SWISS-MODEL server are shown (Fig.1-12). It is evident that the proteins have different groups, which show the reactive sites on the proteins. When various parameters were applied in the Swiss-model software, different groups like strand 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 rabies glycoprotein 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. The amino acid sequences are 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).

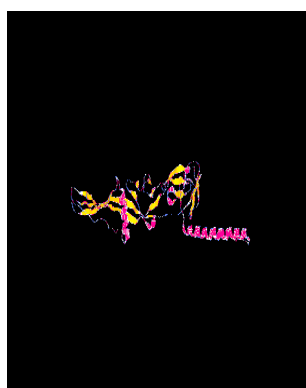
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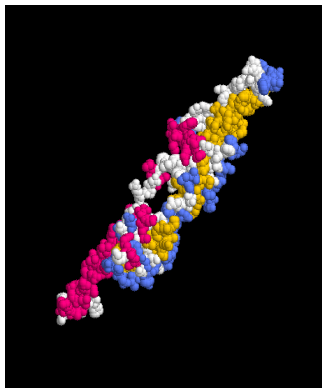
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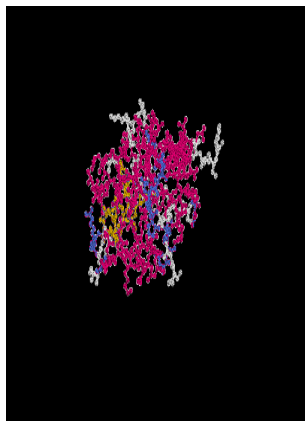
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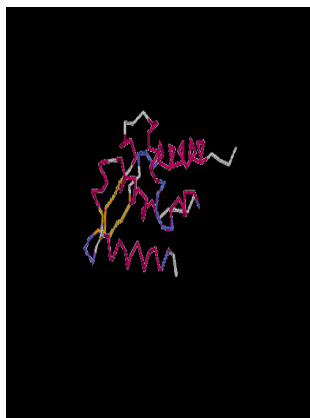
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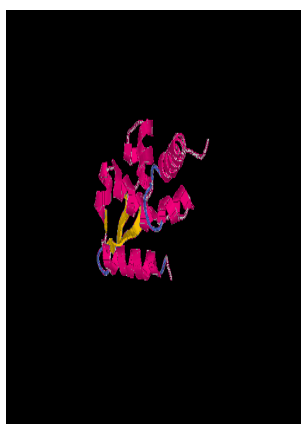
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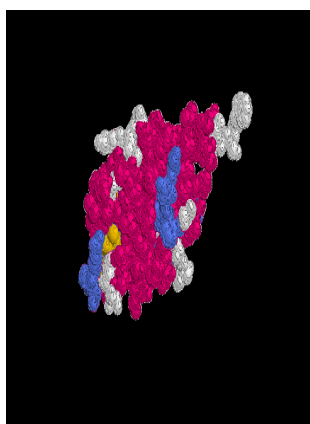
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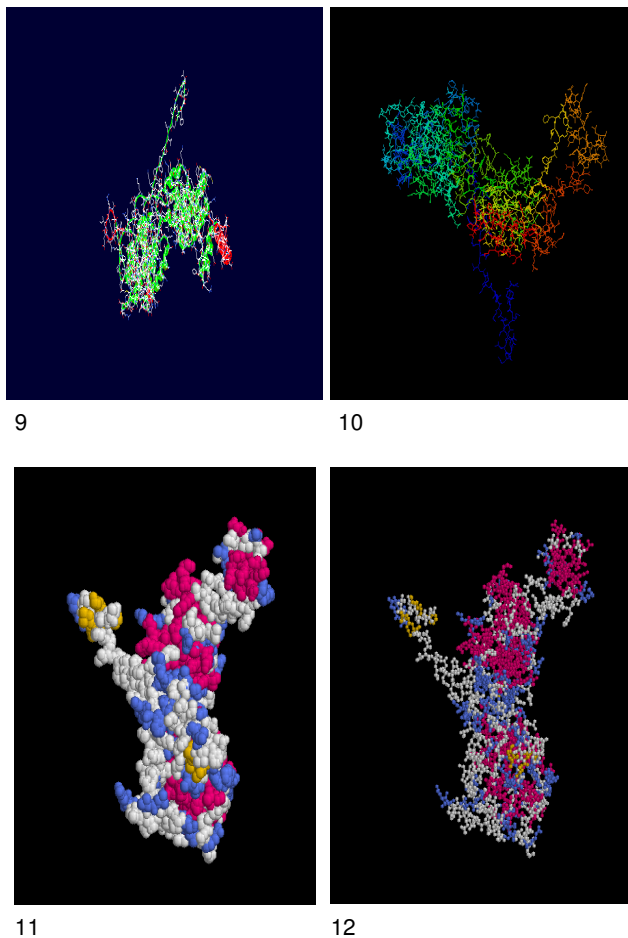


Fig. Rabies virus ERA strain glycoprotein, 1. Rasmol 2.7.3, color group, 2. Rasmol colour structure, 3., Rasmol colour ribbon, 4. Rasmol colour structure, space fill, 5., Rabies virus CVS colour structure phosphoprotein, Rasmol colour structure, ball and stick, 6. Rabies CVS phosphoprotein Rasmol colour structure, ball and stick, 7. Rabies CVS color structure phosphoprotein, Rasmol colour, 8., Rabies CVS colour structure phosphoprotein, Rasmol colour spacefill, 9. Rabies CVS nucleoprotein spdbv, 10. Rabies CVS nucleoprotein rasmol colour group, 11. Rabies CVS nucleoprotein rasmol colour structure, spacefill, 12. Rabies CVS nucleoprotein rasmol colour structure, ball and stick.

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