Protein Modeling Studies for antibacterial Drug Target

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Toxin production is auto-induced by the protein RNAIII-activating protein (RAP).RAP specifically induces the phosphorylation of a novel 21-kDa protein, whereas RIP inhibits its phosphorylation. This protein was termed target of RAP (TRAP). TRAP protein of *Staphylococcus aureus* (strain MRSA252) was modeled with Discovery studio model and on line web serve of SWISS-MODEL, MODBASE, GENO3D,CPH models and I-TASSER. Six different protein structures were generated by using different protein template having sequential similarity and similar protein super family. Secondary structure confirmations of Discovery studio and I-TASSER modeled protein were found resembling to the experimentally observed NMR results of literature. In the Comparative analysis of Ramachandran Plot all the 167 residue found to be included with model of Discovery Studio and I –TASSER. Respectively 93.3% and92.2% residues were found in favored region. In the Comparative Verify Protein (Profiles-3D) analysis by Discovery Studio utility maximum score was observed with I -TASSER and Discovery Studio 60.56and 61.15 respectively. In the Discovery Studio Protein Health Report comparative analysis overall result indicated variable but acceptable violation for all the modeled structure. The VADAR 3 D profile index was good for Discovery studio, MODBASE, SWISSMODEL and I-TASSER compared to GENO3D and CPH models. In the 3-D Superimposition and Alignment of Predicted Structure GENO3D, CPH models, SWISS-MODEL fail to align. While, Discovery Studio, MODBASE and I-TASSER model was align with each other. Best alignment with Lowest RMSD of0.837 A0 was observed between I-TASSER – Discovery Studio. Biological role of predicted protein was inspected with Molecular docking study with inhibitor RIP (RNA III Inhibiting Peptide) using GOLD. Maximum of 53.4617 score was obtained for the Discovery Studio generated model. Discovery studio base model was found to be best among all, which can be further explored for examining functional behavior of TRAP and anti MRSA drug discovery.