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In silico modeling and simulation of a proteasome subunit as molecular target for multiple myeloma

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Multiple myeloma like other forms of cancer is a incurable malignancy of antibody producing plasma cells.Interference with the Ubiquitin-Proteasome pathway has immense potential to evolve as an efficient strategy for the treatment of cancer.

Proteasome is a multicatalytic protease that regulates cell cycle and apoptosis via NF-κB mediated pathway. So,**Targeting the proteasome pathway using proteasome inhibitors represents an effective and novel approach for cancer treatment.**

Till date the only proteasomal inhibitor approved by FDA is Bortezomib, which binds with the beta subunit of 20s proteasome,thus targeting its chymotryptic activity.

But Bortezomib has been reported to show certain side-effects. This problem can be well solved by developing safe and effective inhibitors against β5 subunit by means of computational approaches.

With the aim of designing efficient and safe inhibitor, our team targeted β5 subunit of 20s proteasome for constructing its 3D protein model. Among the various modeling softwares used,that included Modeller9v8, I-Tasser, ModBase, Swiss Model, **Modeller9v8** gave the best model of the β5 subunit having scores of 91%, 73%, 69% respectively in terms of Ramachandran score,Verify3D & Quality factor.

The model was further refined using Molprobity and Coot which increased the quality factor by 2%.Refined model was simulated for 1.2 ns in aqueous medium using Desmond and OPLS force field and 25 structural frames were recorded at uniform time intervals with improved overall quality factor of 95%.

High quality and accuracy of the modeled protein will help in efficient designing of ligands via docking simulation and de-novo ligand Designing in the next step of the study. So there is a lot of scope for the new inhibitors which can be tested for their efficacy and safety.

Biography

Nisha k.chauhan completed her M.sc in Biotechnology from Kurukshetra University and is currently pursuing M.Tech in Bioinformatics from Indian Institute of Information Technology Allahabad.She has worked as a summer trainee in Ranbaxy laboratories for a period of six months.Her abstract was selected for oral presentation in the **National Conference on Emerging Trends in Biopharmaceuticals** held at Thapar University, Patiala on 12 Nov 2010.

She participated and presented a Poster in the **International Conference on Recent Advances in Cancer Research** held at CUG, Gandhinagar on 20th Feb 2011.