

Title: Exploration of the Binding Properties of the Human Serum Albumin Sites with neurology Drugs byDocking and Molecular Dynamics Simulation

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The binding properties of a set of neurology drugs to human serum albumin (HSA) were studied by docking and MD. At first, docking analysis has been done; then MD simulations have been done for each ligand-protein complex to investigate the stability of the complex. The RMSD values for the simulation period showed that the complexes are stable and the MD simulations showed that the interactions within ligand-protein complexes are changed during the simulation process. In some case such as Nordazepam in final structure no interaction between ligand and protein are observed and as a result the complex is not stable enough, but based on the MD simulation, diazepam has the best affinity to the protein structure, considering binding energy, hydrogen bonding and Gibbs energy among the selected ligand.

Studies indicated that site II of HSA has shown a high affinity toward these drugs and the amino acids such as Lys414, Tyr411, Arg410 and 485, Leu387, Asn391 have the most important contributions in the attachment of the drugs. Different kinds of interactions, including hydrogen bonding, π-cation interactions, and π-π interactions are observable between ligand and protein during the MD simulation process.Finally, The MMGBSA calculations have been done to evaluate the binding energy of the ligands and protein. The calculated energies are in good agreement with the previously reported experimental results. In some cases there is a direct relation between the calculated binding energy with the half-life of the drugs, as it was expected. The results of MMGBSA studies imply that the Cloxazolam has the most and the Flunitrazepamhas the least binding energies. And we choose the better Drug according to binding energy, hydrogen bonding, and interaction toward the HSA and Gibbs energy. This finding could be used to design drugs which they have more affinity toward the HSA. Because there is a connection between

the binding energies and the drug half-life, it means that the drug will be available for more time in the body and therefore lesser dosage of it can be prescribed.

Biography

I am a final Term of P.h.D. candidate in computational chemistry in Iran and will receive my degree soon(maybe two months later). I have been doing my project under Prof. Ulf Ryde and Prof. Mansour Zahedi , I spent some months at Lund city.My thesis is about "QM/MM study of the conversion of iron (III) superoxo oxophlorin into verdoheme and biliverdin" in Lund University in conjunction with Shahid Beheshti University. I am very interested in molecular dynamics simulation, so I decided to study in this field, too. I have done some studies about binding properties of the human serum albumin sites with neurology drugs and Evaluation of the effect of the chiral centers ofTaxol on binding to β-tubulinby.

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