Jignasa K. Savjani, J Vaccines Vaccin 2011, 2:5
doi: http://dx.doi.org/10.4172/2157-7560.S1.02

International Conference & Exhibition on
Vaccines & Vaccination

22-24 Nov 2011 Philadelphia Airport Marriott, USA

Computer aided docking studies of some antimicrobial agents

Jignasa K. Savjani and Anuradha K. Gajjar

Nirma University, India

Docking analysis is an operation in which one molecule is brought into the vicinity of another while calculating the interaction energies of the many mutual orientations and conformations of the two interacting species. Docking studies on thirty six imidazolidine-2-thione molecules were performed using software like Autodock 4.0, Autodock Vina and Accelrys DS visualizer 2.0. Dihydrofolate reductase (DHFR), Topoisomerase IV and DNA gyrase enzymes were used as targets for the docking studies; the structures of which were taken from the Protein Data Bank (PDB). Docking simulations were carried out using the Lamarckian Genetic Algorithm. Best conformation of the ligand was analyzed based on energies like docked energy, binding energy, and possibly per atom electrostatic and van der Waals energies. The 'best' docking result was considered to be the conformation with the lowest (docked) energy. From the docking studies it was found that ligand interaction with Dihydrofolate Reductase (3FRB) and DNA gyrase (3G7E) involves less binding energy as well as appreciable KI value when compared with the standard. Interaction of ligand with Topoisomerase-IV did not show good result as compared to standard because of large binding energy differences hence, it can be postulated that Dihydrofolate reductase and DNA gyrase enzymes are the probable targets for the type of imidazolidine-2-thione derivatives studied as antibacterial agents.

Biography

Jignasa K. savjani, has completed her Ph.D at the age of 32 years from Nirma University in 2011. She is working with Institute of Pharmacy, Nirma University, as an Assistant Professor from 2007 to till date. She has more than 8 years of teaching as well as 4 years of research experience. She has number of publications and presentations to her credit. She delivered various guest lectures on topics related to medicinal chemistry. She is also a reviewer of internationally repute journal. In recent year she focused on the Computational drug design of antimicrobial agents. She filed a patent on the methods of synthesis and some novel derivatives acting as antimicrobial agents.