Sana Gul et al., Med chem 2013, 3:4
http://dx.doi.org/10.4172/2161-0444.S1.009

OMICS Group Conferences
Accelerating Scientific Discovery

2nd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
October 15-17, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

Structure and dynamics of water molecules in the inhibitor bound human pim-3 kinase

Sana Gul and Zaheer-ul-Haq
University of Karachi, Pakistan

Kinases occupy ~2% of the whole human genome and are primarily regarded as human kinome which contains more than 500 different protein kinases for instance, serine/threonine kinases and tyrosine kinases (in the ratio of 8:2). One of the serine/threonine kinases is PIM kinases recognized as oncogenes and responsible for cancer cell growth. To inhibit the growth of cancer cells, PIM-kinases are being considered as a potential target. To understand the role of human PIM-kinase its structure needs to be characterized, chiefly via experimental techniques that are not exlore completely so far. Therefore, this can be overcome via modeling approach as an alternative or a complement to the experiment. Availability of the 3-D structures of the protein establishes a rational with its function, therefore, *in silico* approaches were adopted to model and characterize 3-D structure of PIM-3 kinase, since, no experimental structure is solved yet. Molecular docking study helps in exploring the role of water molecules; it was carried out to understand the binding pattern of the inhibitor (BI1) in the active site of the protein. .Furthermore, role of water molecules in the active site was explored via radial distribution function (RDF) obtained from molecular dynamics (MD) simulations of the PIM-3 kinase. RDF plots yielded water mediated interactions of inhibitor with the binding site. Distance dynamics of the binding partners were also evaluated to understand the stability of the protein-inhibitor complex. Hydrogen bond analysis showed that the inhibitor forms strong H-bond in the hinge region facilitated by the GLU-90. The study suggested that incorporation of water molecules in the molecular docking helps to predict correct binding pose of the ligand that was further validated by a long run MD simulation study.

Biography

Born in Pakistan on August 09, 1986, I began my journey of life. When I was a child my parents teach me about punctuality. At 17 years, I completed my college education. I enrolled at the University of Karachi, Karachi. From there I did Masters in Chemistry and stood 1st, achieve two Gold Medals. Soon I decided to take admission for PhD in Research Institute of Chemistry. I have keen interest in research and always enjoy while doing. During research phase I feel how beneficial my work is. So, I applied for job in the field of Genomics in our Institute and I got appointment. Still I am working in my field "Computational Chemistry".

sana_aslam_100@yahoo.com