Swati Singh, Pharm Anal Acta 3:1
doi: http://dx.doi.org/10.4172/2153-2435.S1.09

OMICS Group Conferences
Accelerating Scientific Discovery

2nd International Conference on
Pharmaceutics & Novel Drug Delivery Systems

20-22 February 2012 San Francisco Airport Marriott Waterfront, USA

TITLE

Structural Modeling and Simulation Studies of Human Cyclooxygenase1 (HsCOX1) with Anti-inflammatory Terpenoids: Implications in Drug Targeting and Designing

Swati Singh
University of Lucknow, India

The terpenoids have been reported to be naturally occurring anti inflammatory substances. One of the mode of action of these anti-inflammatory substances is through inhibition of cyclooxygenase (COX), thereby lowering the production of prostaglandins (PGs). Thus, for identification and determination of efficacy of anti inflammatory drugs, COX, a key enzyme in PG synthesis, has been used as a target. Ten naturally occurring terpenoids, namely β-bisabolene, curcumin, zingiberene, β-carotene, β-phellandrene, oleanol, farnesene, α-Pinene, sabinene, and α-humulene have been analyzed for their anti-inflammatory properties based on molecular docking studies using a modeled human cyclooxygenase1 (HsCOX1) as target. Based on the parameters namely, binding energy, intermolecular energy, RMSD value and the inhibitor constant (K_i), among all the terpenoids analyzed, the triterpene oleanol was found to be the most potent inhibitor of HsCOX1 (K_i = 5.57 x 10^{-8} μM with binding energy of -18.08 Kcal/mol). A nitro derivatives of oleanol, exhibited about 20 folds enhancement of inhibitory potential, as compare to that of oleanol against the HsCOX1. Furthermore, when oleanol and its nitro derivative were compared for their anti-inflammatory potentials with those of commonly used drugs such as alverine, aspirin and ibuprofen, through molecular docking analysis using HsCOX1 as target, both oleanol and its nitro derivative exhibited many thousand folds higher inhibitory potential as compared to the best docked drug alverine. Thus, the present work makes a solid foundation for further clinical studies using oleanol and its derivatives as highly potential anti-inflammatory terpenoids, targeted against HsCOX1.

Biography

Swati singh: M.Sc. Bioinformatics, Research Fellow, Centre of excellence in bioinformatics, Department of Biochemistry, University of Lucknow, Lucknow-226007, U.P., India Email: swtsingh0@gmail.com