Kalpana C Maheria et al., Med Chem 2014, 4:12
http://dx.doi.org/10.4172/2161-0444.S1.013

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
December 08-10, 2014 DoubleTree by Hilton Hotel San Francisco Airport, USA

Green synthesis of medicinally important novel DHPMS derivatives and their related DFT, docking, antimicrobial and SAR studies

Kalpana C Maheria, Manojkumar K Rathod and **Suban K Sahoo**
S V National Institute of Technology, India

A facile green synthetic approach was utilized to synthesize medicinally important heterocyclic novel dihydropyrimidinones (DHPMs) derivatives using zeolite H-BEA as solid acid catalyst, through Biginelli three component reaction (MCRs). This green approach offer high yields within short reaction time. Further, *in silico* proficiency of Lipinski's, DFT, docking and SAR study have been carried out in order to get target drug like novel DHPMs molecules with desired activity. Computer aided drug designing (CADD), Mol Soft and Osiris tool were used to predict DHPMs structural parameters of "Lipinski rule" which meant to find molecular membrane permeability, oral bioavailability, drug-likeness and drug score. In addition, DFT method was employed to calculate DHPMs structural geometries, molecular stability and electronics structures using Schrodinger Jaguar tool. Moreover, the grid-based flexible docking (using Glide tool) method was utilized to determine voltage-dependent calcium channel blockers receptor-DHPMs ligand interactions and molecular surface bonding. The synthesized products were characterized by FT-IR and 1H NMR spectral analysis and then evaluated for their bioassay against bacterial and fungal strains. SAR study correlates DHPMs structure to a property, effect and biological activity. In this paper, theoretical (CADD) and experimental (MCRs and Catalysis) approaches were brought together in order to synthesize target DHPMs molecules with desired activity which in turn will serve as vital aid for future researchers working in the area of medicinal chemistry.

maheria@gmail.com