

BIOPHARMACEUTICS AND BIOLOGIC DRUGS & 5th INTERNATIONAL PHARMACY CONFERENCE

August 31-September 01, 2017 Philadelphia, USA

Identification, optimization, designing and synthesis of drug-like heterocyclic templates for the treatment of Type II diabetes mellitus

Gajjar Krishna¹ and Gajjar Anuradha²

¹Nirma University, India

²RPCP Charusat, India

Free fatty-acid receptor 1, is a G-protein-coupled receptor that binds long chain free fatty acids to enhance glucose-dependent insulin secretion and are therefore viable targets for diabetes and metabolic disorders. In the course of the research work, QSAR study, Pharmacophore generation, Molecular Docking, *in-silico* ADME studies and synthesis was performed to explore the molecular determinants responsible for the agonist action at GPR40. The generation of ligand & structure based pharmacophore using the standard tools within Catalyst from different training sets consisted of Hydrophobic, Hydrogen Bond Acceptor and Aromatic ring features as essential aspects. The most representative features were selected and included in the pharmacophore model which was further validated and utilized as a query tool to search 3D databases. CoMFA, CoMSIA and HQSAR were performed on series of 3-aryl-3-ethoxypropanoic acid derivatives to build 3D-QSAR models. Contour maps provided significant insights which gave hints for the modification required to design new molecules with improved biological activity. Molecular docking studies were carried out on designed molecules using Sybyl-X software. Out of these the best Heteroaryl systems, specifically the five membered pyrazole ring system was being explored and some of the virtual structures were synthetically explored, and 3-[3-(4-methoxyphenyl)-4-(phenoxyethyl)-1H-pyrazol-1-yl] acetic acid derivative class of compounds were synthesized taking into the account of sustainability and feasibility of the chemistry, which may act as a starting point for the in-house discovery program.

Biography

Krishna Gajjar is a Pharma Student, having Bachelors and Master degree in Pharmacy and currently pursuing PhD as Research Fellow (in Pharmaceutical Sciences- specialization in Medicinal Chemistry) from Nirma University, Ahmedabad, (Gujarat) India, under the guidance of Prof. Anuradha K. Gajjar.

12ftphdp12@nirmauni.ac.in

Notes: