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Abstract

Identification of cryptic binding site for anti diabetic GLP-1 small molecular agonist using in silico approaches

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Abstract:

Incretin based therapy is a well known strategy, which is used by many , a researcher to develop potential anti diabetic agents. Among the incretins viz., DDP4, GIP and GLP, the drugs targeting GLP-1 receptor are very well known owing to their pleiotropic effect. The activation of GLP-1 receptor by its agonist is a very vital step in treating Type 2 diabetes and curing its macro as well as microvascular complications. However, till date, the marketed agonists are peptide based, hence developing small molecular agonists has become a challenge thus attracting many researchers. In the present study, we attempt to design small molecular GLP-1 agonists that will play the identical role as the marketed Liraglutide or Semaglutide. In the present study, using various computational approaches, we identified the most probable binding site for a small molecule which is reported. Subsequently, we subjected both the modelled agonist-GLP1R and the known antagonist-GLP1R complexes to Molecular Dynamics Simulations (MDS). The analyses of the conformational changes the receptor undergoes in both complexes shed light on the cryptic binding site of small agonists and gives us insight into their probable mechanism. This may leadto the solving of the unsolved mystery of small molecule GLP-1 agonists.

Biography:

Ketan Ghosh has completed his Masters degree from NIPER, Kolkata in the year 2016.He is pursuing his research work from NIPER,S.A.S. Nagar and currently enrolled in the 3rd year of PhD. He has expertise in computer aided drug design (CADD) and molecular modeling.

Recent Publications:

1. Ketan Ghosh,Computational Studies to Identify Potential Main Protease Inhibitors for SARS-CoV-19,2020
2. Ketan Ghosh, A Multi-Perspective Review on Dengue Research,2019

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