19th International Conference on
Medicinal Chemistry & Multi Targeted Drug Delivery
&
International Conference on Catalysis and Pyrolysis
November 05-06, 2018 | San Francisco, USA

Interaction analysis of DPP4 inhibitor by fragment molecular orbital method

Natsumi Mori[1], **Tatsuya Takagi**[2], **Tian Yu-shi**[1], **Hirotomo Moriwaki**[2] and **Norihito Kawashita**[3]
[1]School of Pharmaceutical Sciences, Osaka University, Japan
[2]Graduate School of Pharmaceutical Science, Osaka University, Japan
[3]Kindai University, Japan

Dipeptidyl Peptidase-4 (DPP4) is responsible for the degradation of incretins that accelerate secretion of insulin. DPP4 inhibitor prevents the degradation of incretin by inactivating DPP4 and shows a hypoglycemic effect. The DPP4 protein is composed of 766 amino acid residues, a large number of co-crystal structures of DPP4 and inhibitors have been reported in PDB. In this study, we calculated Inter-Fragment Interaction Energies (IFIE) of co-crystal structure of DPP4 with inhibitors by Fragment Molecular Orbital (FMO) method and analyzed the linearity between sum of IFIEs and pIC50s. All calculations were conducted using the structures after minimizing the energies by optimizing the coordinates of hydrogens using MOE2018. We used ABINIT-MP6.0 + for FMO calculations. MP2 method and 6-31G * basis set were used. We computed structures and obtained a good correlation (R2 = 0.) Between pIC50s. In addition, we found some significant fragments for DPP4-inhibitor interactions. Thus, we concluded that FMO method is effective for in Silico drug design.

Biography

Natsumi Mori is a 6th year undergraduate student of School of Pharmaceutical Sciences, Osaka University. She already finished the clinical training and is going to take a national examination for Pharmacist in this school year. She was supposed to give a presentation at a conference which was cancelled due to a natural disaster.

4.4.natsumi@gmail.com

Notes: