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E-PPARM-Exploring pharmacophore, 3D-finger print and de novo design of selective PPARγ modulator

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Inspite of significant scientific progress and growth of modern drugs, at least 30 million people throughout the world still suffer from the diseases related to metabolic syndrome. Peroxisome proliferator-activated receptors (PPARα, δ, and γ) play important roles in the regulation of metabolism, inflammation, and cell differentiation. Considering the importance of the regulating receptor, most studies have been focused on developing PPARγ modulators for reducing the complications associated with type-2 diabetes mellitus (T2DM). But only few studies were performed to explore the role of γ-receptor subtype. In present work, multi-chemometric techniques, such as ligand-based pharmacophore, e-pharmacophore, hologram based quantitative structural activity relationship (HQSAR), de novo design and stepwise virtual screening with MM-GBSA analysis have been performed for exploring potent and selective PPARγ modulators. The two different types of pharmacophore models infer that compounds bearing three aromatic rings are crucial for PPARγ agonistic activity. The HQSAR model adjudged the importance of the aromatic rings, benzene and substituted indole nucleus along with carbonyl functional group for the optimal activity of the molecules. After drug-likeness screening by Lipinski filter, traditional Chinese medicine database and de novo designed molecules were mapped for hits identification. From the docking and MMGB-SA study of the hit molecules, it is observed that 14 molecules, having dockscore <5, showed similar interactions with the amino acid residues at the active site of PPARγ as that of the co-crystallized ligands rosiglitazone. The chemometric studies provide key information on activity pattern for development of potent and selective PPARγ modulators is schematically represented.

Biography

Ashis Nandy has completed Master in Pharmacy from Jadavpur University in 2013, and now pursuing PhD program in University of Calcutta as a Junior Research Fellow under the project funded by Science and Engineering Research Board, Govt. of India.

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