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Molecular modeling studies for virtual screening of new TAK-1 inhibitors-ChemBridge library (Part 1)

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The mitogen activated protein kinase "Transforming growth factor β receptor-associated kinase 1 or TAK-1" has emerged as an interesting therapeutic target for inflammatory diseases and cancer. TAK-1 is a member of the mitogen-activated protein kinase (MAPK) family and has been implicated in various signaling pathways. Identification of small molecule inhibitors of TAK1 may represent an exciting therapeutic approach for both inflammatory disease and cancer. In this study, the main focus was to use Multiple Linear Regression (MLR) analysis was employed to search for optimal 2D-QSAR model for activity prediction as well as valid 3D pharmacophore models for TAK-1 antagonists, using it in virtual screening of 50,000 compounds from ChemBridge for new lead compounds and find their interactions with catalytic residues of TAK-1 by molecular docking.

Biography

Doaa B.Farag completed her PhD in Medicinal Chemistry in November 2014 from Faculty of Pharmacy, Ain Shams University, Cairo, Egypt. Her primary research goals are directed towards application of organic synthetic chemistry and computational techniques towards the broad goals of drug discovery and optimization. Her previous research projects started in University of South Carolina, USA in 2008, Department of Pharmaceutical and Biomedical Sciences. Another research project for the PhD was held in Egypt, which involved multistep synthetic procedures, purification and characterization steps for small novel molecules as promising anti-inflammatory activities. Several molecular modeling techniques were employed as docking, 3D pharmacophore and QSAR.

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