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3D-QSAR studies and molecular docking in order to find the relationship between the molecular properties and biological activity have been carried out on a series of GSK-3 on maleimide-based inhibitors as mood stabilizer. An alignment rule for the compounds based on maximum common substructure was defined using Distill in SYBYL 7.3. Internal and external validation for robustness and predictive ability of models were done. The statistical parameters from the models indicate that the CoMFA-RF had high predictive ability. Molecular docking analysis was performed to define key structural features of binding of the inhibitors into the receptor and predicting bioactive conformers. Moreover, the resulting 3D CoMFA contour maps provide useful guidance for designing highly active inhibitors. Finally, *in silico* ADMET studies was performed on new design compounds to compare the computed ADMET descriptor values with the accepted ranges.

Keywords: 3D-QSAR, GSK-3, CoMFA-RF, CoMSIA, Molecular docking and ADMET.

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Molecular docking and CoMFA and CoMSIA 3D-QSAR studies on Maleimide-based glycogen synthase kinase 3(GSK-3) inhibitors

Supervisors:
Dr. Fereshteh Shiri
Dr. Massoud Nejati-Yazdinejad

By:
Ali Reza Shahraki

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