Proceedings
International Journal of Nanomaterials, Nanotechnology and Nanomedicine

Special Issue: NCNN-2014
(National Conference on Nanoscience and Nanotechnology - 2014)

Pharmacophore Modeling, Atom Based 3D-QSAR and Docking Studies of Azetidin-2-Ones Derivatives as Tubulin Inhibitors

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Azetidin-2-ones have been recognized as effective tubulin polymerization inhibitors that bind to the colchicine site on β-tubulin. Energetic based pharmacophore mapping (hybrid structure and ligand based method) explain how the energy parameter from the Glide XP scoring function are plotted onto pharmacophore sites from the docked fragments so as to rank their implication for binding. Pharmacophore and atom based 3D QSAR modeling (ligand based method) were performed on 71 compounds of azetidin-2-ones derivatives as tubulin-binding agents for antitumor activity. Five-point common pharmacophore hypothesis were selected for alignment of all compounds. The 3D-QSAR models developed using training set of 51 compounds and test set of 20 compounds. The generated common pharmacophore hypothesis (CPHs) and 3D-QSAR models were confirmed further externally by estimating the activity of database of compounds and comparing it with actual activity. Molecular docking (structure based method) were performed on a series of azetidin-2-ones using colchicines binding site of β tubulin. The docking studies indicate important interactions of trimethoxy benzene with Cys241 and Val318 for anticancer activity. We have established structure activity correlation by using Pharmacophore Modeling, Atom based 3D-QSAR and Docking Studies. The results of these studies would be beneficial to refine the pharmacophore for design of novel potential compounds for antitumor activity.

Citation: *Patel VK, Rajak H (2015) Pharmacophore Modeling, Atom Based 3D-QSAR and Docking Studies of Azetidin-2-Ones Derivatives as Tubulin Inhibitors. Int J Nanomater Nanotechnol Nanomed S: 169.*