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Revealing Potential Drug Targets against Proto-Oncogene Wnt10B by Comparative Molecular Docking

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Abstract : Wingless type Mouse mammary tumor virus (MMTV) Integration site-10B (Wnt10B) is an important member of the Wnt protein family that functions as cellular messenger in paracrine manner. Aberrant Wnt10B activity is the cause of several abnormalities including cancers of breast, cervix, liver, gastric tract, esophagus, pancreas as well as physiological problems like obesity, and osteoporosis. The objective of this study was to determine the possible inhibitors against aberrant expression of Wnt10B in order to prevent and treat the physiological disorders associated with it. Wnt10B3D structure was predicted by using comparative modeling and then analyzed by PROCHECK, Verify3D, and Errat. The model having 84.54% quality value was selected and acylated to satisfy the hydrophobic nature of Wnt10B. For search of inhibitors, virtual screening was performed on Natural Products (NP) database. The compounds were filtered and ligand-based screening was performed using the antagonist for mouse Wnt-3A. This resulted in a library of 272 unique compounds having most potent drug like activities for Wnt-4. Out of the 271 molecules analyzed three small molecules ZINC35442871, ZINC85876388, and ZINC00754234 having activity against Wnt4 abbarent expression were found common through docking experiment of Wnt10B. It is concluded that the three molecules ZINC35442871, ZINC85876388, and ZINC00754234 can be considered as lead compounds for performing further drug designing experiments against aberrant Wnt expressions.

Keywords : Wnt10B inhibitors, comparative computational studies, proto-oncogene, molecular docking
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