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## Molecular docking study of selected natural compounds for cancer stem cells targeted anti-cancer activity

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Cancer Stem Cells (CSCs) play significant roles in tumor initiation, relapse, angiogenesis, metastasis and therapy. Collectively Wnt, notch and hedgehog are major pathways that have been linked to the resistance of CSCs to conventional therapy. Most conventional therapies are directed at the rapidly growing tumor mass but not at the slow dividing CSCs. Eliminating CSCs has been suggested as a promising approach to cure cancer. *In silico*, molecular docking simulations were carried out for the binding of 35 selected natural compounds with receptor proteins which are involved in the main signalling pathways of CSCs, such as  $\beta$ -catenin chain A and Smo receptor from the Wnt and hedgehog pathways respectively, using Hex 8.0.0, DOCK6 and AutoDock Vina software. Additionally docking interaction residue analysis, score functions such as Drug score, X score, Per Contact Score (PCS) and Average affinity PCS and drug-likeness study were carried out for the selected compounds. Overall 11 compounds were identified with good binding energy, interaction, binding affinity and better drug likeness for  $\beta$ -catenin chain A involved in Wnt inhibition. There was no considerable overall binding ability for Smo inhibition. Energy values for Wnt inhibition obtained using AutoDock Vina were as follows. Gedunin (-7.3 kcal/mol), Kaempferol (-6.1 kcal/mol), Methylripariochromene A (-5.3 kcal/mol), Myrigalone G (-5.1 kcal/mol), Catechin (-6.5 kcal/mol), Myricetin (-6.5 kcal/mol), Discretine (-5.6 kcal/mol), Lauroilsine (-5.9 kcal/mol), Myricitrin (-6.3 kcal/mol), Nordicentrine (-6.0 kcal/mol) and Phloretin (-5.4 kcal/mol). These novel Wnt inhibitors need further attention to assess their potential application in CSC targeted therapy.

### Biography

Karthika Mayan is currently employed as a Research Assistant, in the study titled "An Exploratory Study on Environmental, Medicinal, Genetic and Dietary Determinants of Chronic Kidney Disease of Uncertain Aetiology Based on Postmortem Tissue Analysis" at Faculty of Forensic medicine, University of Colombo, Sri Lanka. Having completed Master degree in Bioinformatics with a merit pass and Bachelor's degree in Biochemistry and Molecular biology at University of Colombo. During the MSc degree she investigated that 11 natural compounds can be used as cancer stem cells targeted potential anti-cancer compounds. In between she got the opportunity to work on a research project titled "In silico characterization of a RNA binding protein of cattle filarial parasite *Setaria digitata*" and published. Last year she has worked as a Research assistant at Bioinformatics and Computational Biology research group in UCSC, University of Colombo, and research topic on Co-evolution of Dengue virus and human. Since her long term goal was to be actively involved research. In the future she hopes that her research experience gained so far will be helpful that she can carry out valuable outcomes from her novel findings.

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