

# Desmodin

Cyclin-dependent kinase 5 ([CDK5](#)) is a proline-directed serine-threonine protein kinase vital for neuronal cell cycle arrest and differentiation. It activates by binding with p35 and p39 and is important for the functioning of the nervous system. A growing body of evidence suggests that CDK5 contributes to the onset and progression of neurodegeneration and tumorigenesis and represents itself as a potential therapeutic target. Our research illustrates virtual screening of phytochemicals from the IMPPAT (Indian Medicinal Plants, Phytochemistry and Therapeutics) library to search for potential inhibitors of CDK5. Initially, the compounds from the parent library were filtered out via their physicochemical properties following the Lipinski rule of five. Then sequentially, molecular docking-based virtual screening, PAINS filter, ADMET, PASS analysis, and molecular dynamics (MD) simulation were done using various computational tools to rule out adversities that can cause hindrances in the identification of potential inhibitors of CDK5. Finally, two compounds were selected via the extensive screening showing significant binding with CDK5 ATP-binding pocket and ultimately were selected as potent ATP-competitive inhibitors of CDK5. Finally, we propose that the elucidated compounds Desmodin and Isopongachromene can be used further in the drug discovery process and act as therapeutics in the medical industry to treat certain complex diseases, including cancer and neurodegeneration <sup>1)</sup>.

<sup>1)</sup>

Atiya A, Batra S, Mohammad T, Alorfi NM, Abdulmonem WA, Alhumaydhi FA, Ashraf GM, Baeesa SS, Elasbali AM, Shahwan M. Desmodin and isopongachromene as potential inhibitors of cyclin-dependent kinase 5: phytoconstituents targeting anticancer and neurological therapy. J Biomol Struct Dyn. 2022 Oct 2:1-11. doi: 10.1080/07391102.2022.2128877. Epub ahead of print. PMID: 36184739.

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