Indian Journal of Chemistry
Vol. 64, January 2025, pp. 22-37
DOI: 10.56042/ijc.v64i1.13952

Ligand based pharmacophoric discovery of new CLK1 inhibitors

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Received 25 September 2024; accepted(revised) 27 December 2024

CLK1 has been recognized as an optimistic target against an array of diseases, including cancer due to their pre-mRNA splicing function. In this study, ligand-based pharmacophore approach has been employed to identify new CLK1 inhibitors from kinase and FDA approved drug libraries. Two ligands, **K6** and **D1** have been extracted, which established consistent interactions with hinge residues while maintaining a web of interactions in DFG region. Additionally, their stable protein dynamics comparable with reference CLK1 inhibitor (**T24**) and Apo ratify them as aspiring CLK1 inhibitors. Further, **D1** has been identified as a CLK1 binder and **K6** as a potential kinase inhibitor by Swiss Target Prediction server. Moreover, their adequate pharmacokinetic and toxicity profiles make them worth future investigations.

Keywords: CLK kinase, Dynamics, *In silico* ADMET study, *In silico* target prediction, Pharmacophore, Rosiglitazone