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Research article: In silico investigation of potent inhibitors of TRABID, a putative target of cancer

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Background: TRABID is an enzyme which is associated with different types of cancers by up-regulating the Wnt signaling pathway. TRABID also acts as a Deubiquitinating enzyme which cleaves Lys63 and Lys29-linked diubiquitin through its OTU domain. This prompts direct participation in regulating the metabolic reprogramming in oncogenic cells, therefore, targeting TRABID holds a huge potential to develop anti-cancer drugs. Objective: The current study was aimed to identify some bioactive compounds phytochemicals that could bind and inhibits the active site of TRABID. Methodology: 1051 therapeutically important compounds from otava chemicals library were docked against the active sites of TRABID protein by using Molecular Operating Environment (MOE v. 2009) software. The interactions between the ligands and the binding site of the top five docked complexes, based on the docking scores, were further elucidated by 2D and 3D interactions via discovery studio and pymol software, respectively. The top ten compounds were further screened for drug-like properties by SwissADME online tool. Results: Findings of molecular docking suggested that compounds with catalogue numbers P1686150, P7016750052, P1676209, P7020533379, P7020618953, P1684972, P7216540213, P7566563, P1106282, and P7119831633, with district chemical scaffolds are best docked in the binding site of TRABID, with docking scores ranging from -11.4 to -9.8 kcal/mol. However, among them, compounds P7020533379, P7566563, and P7119831633 depicted acceptable pharmacokinetics and other drug-like properties with stable hydrogen bonds with the active site residues of TRABID. Conclusion: Identified lead compounds can be considered as the strong inhibitors of TRABID, however, further in-vitro and in-vivo experiments are required to validate these results.