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## Ligand-based pharmacophore mapping and virtual screening for identification of potential DDR1 inhibitors

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Discoidin domain receptors are novel class of receptor tryosine kinase which is known to be key regulators of various physiological process including cellular morphogenesis, differentiation and proliferation. Discoidin domain receptor 1 (DDR1) is involved in cancer invasion and it's over expression, stimulate the lung cancer migration. Hence, DDR1 is an emerging potential molecular target for new anticancer drug Discovery. In order to identify the potential lead molecules to inhibit the DDR1, five featured pharmacophore model was developed using set of 38 compounds. The model was subjected to virtual screening against binding database. The hit compounds were filtered with Lipinski's rule of five, ADME and docking protocols, which results in nine lead molecules. For further validation induced fit docking, Prime MMGB-SA and molecular dynamics simulation studies were carried out with virtually screened compounds. All the nine compounds have favorable G-score, G-energy, hydrogen bond interaction, binding free energy and ADME/T properties. From the results, we have concluded that these compounds may act as potential inhibitors DDR1 receptor as anticancer agent.