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Protocol 1: Protein-ligand docking V.1

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ABSTRACT

Autodock Vina version 1.1.2 (RRID:SCR_011958) for docking. The grid box's dimensions were fixed at XYZ=30Å × 30Å × 30Å which was found to be the best size for the default exhaustiveness (=8), and the ligand binding site was positioned in the middle of the grid box. The details of spatial dimensions (along XYZ axis) and the grid box's size which were specified in a configuration file. Using AutoDock vina version 1.1.2's (RRID:SCR_011958) command line interface, docking was accomplished. The log file created listed the binding modes along with their corresponding binding energies. With the help of BIOVIA Discovery studio visualizer 2021, the binding modes were created as a single file in '*pdbqt*' format, and all non-bonded interactions were recorded.

Protocol 1 Protein-Ligand Docking.docx