Jan 25, 2023 Version 1

Protocol 1: Protein-ligand docking V.1

DOI
dx.doi.org/10.17504/protocols.io.3byl4j362lo5/v1

Phaniendra Alugoju[1,2], Vishwambhar Vishnu Bhandare[3], Vishal S Patil[4,5], Krishna Swamy V K D[6], Prem Kumar Borugadda[7], Tewin Tencomnao[1,2]

[1]Department of Clinical Chemistry, Faculty of Allied Health Sciences, Chulalongkorn University, Bangkok, 10330, Thailand;
[2]Natural Products for Neuroprotection and Anti-Ageing Research Unit, Chulalongkorn University, Bangkok, 10330, Thailand;
[3]Department of Microbiology, Shivaji University, Kolhapur, Maharashtra, 416004, India;
[4]Department of Pharmacology and Toxicology, KLE College of Pharmacy Belagavi, KLE Academy of Higher Education and Research (KAHER), Belagavi, Karnataka, 590010, India;
[5]ICMR-National Institute of Traditional Medicine, Belagavi, Karnataka, 590010, India;
[6]Phytomedicine and Ageing laboratory, Department of Biochemistry and Molecular Biology, Pondicherry University (A Central University), Puducherry, 605 014, India;
[7]Department of Computer Science, School of Engineering and Technology, Pondicherry University (A Central University), Karaikal Campus, Karaikal 609605, India

tewin.t

OPEN ACCESS

DOI: https://dx.doi.org/10.17504/protocols.io.3byl4j362lo5/v1

Document Citation: Phaniendra Alugoju, Vishwambhar Vishnu Bhandare, Vishal S Patil, Krishna Swamy V K D, Prem Kumar Borugadda, Tewin Tencomnao 2023. Protocol 1: Protein-ligand docking. **protocols.io** https://dx.doi.org/10.17504/protocols.io.3byl4j362lo5/v1

Created: January 25, 2023

Last Modified: January 25, 2023

Document Integer ID: 75841

Keywords: docking, ligand, binding energy, bonded interaction, binding mode

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.

Troubleshooting

Protocol 1 Protein-Ligand Docking....