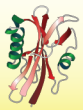
Preparation of ligand library

- 14011 phytochemicals from Indian Medicinal Plants
- 10510 drug-like phytochemicals
- 3D structure from PubChem - energy minimized

SARS-CoV-2 helicase Nsp13

- Nsp13 crystal structure from PDB (6ZSL) - energy minimized
- 100 ns MD simulation of prepared crystal structure of Nsp13
- 10 Nsp13 structures from geometric clustring of the MD simulation trajectory

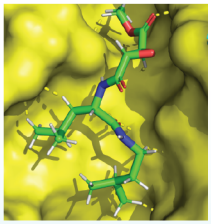
RCSB PDB



Virtual screening

- Molecular docking
- Binding energy cut-off from co-crystalized structures of Nsp13
- Binding energy cut-off based filtering of phytochemicals
- Filtering of phytochemicals based on ligand binding and non-covalent interactions with ATP-binding site residues of Nsp13
- 368 potential phytochemical inhibitors of helicase Nsp13
- Plant source, physicochemical and ADMET properties of potential inhibitors

AutoDock Vina



MD simulation of protein-ligand complex

- 50 ns MD simulation of protein-ligand complex of top 5 potential phytochemical inhibitors
- Binding energy using MM-PBSA method