Drug Design Methodology

1.Target Identification (Protein & Ligand/Structures)

1.1. Literature Review (Google Scholar, PubMed)

1.2. Protein Download (Protein Data Bank ,Uniport)

1.3. Compounds Searching & Download (PubChem, Ambinter, ChEMBL, IMPPAT, MPDB 2.0, etc…)

2.Proteins Preparation

2.1. View and delete unnecessary elements (BIOVIA Discovery Studio Visualizer)

2.2. Protein Active Site identification (BIOVIA Discovery Studio Visualizer)

2.3. Solve formatting issues for docking (Swiss PDB Viewer)

3.Ligand preparation

3.1. Merge All ligand in one SDF file (Open Babel)

4. Virtual Screening & Molecular docking

4.1. Single Docking (PyRx)

4.2. Multiple Docking (PyRx)

5.ADME Analysis

5.1. ADME - absorption, distribution, metabolism, excretion (SwissADME)

6.Toxicological Properties

6.1. Toxicity Prediction (Protox2, admetSAR)

7.Molecular Dynamic Simulation

7.1. Windows Based (Yasara)

7.2. Linux Based (Gromace)

7.3. Web server Based (Simlab)

8.MM/PBSA Analysis

8.1. Free Binding Energy calculation (Yasara)

9.PCA Analysis

9.1. Software based (minitab 18)

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