Acharya & BM Reddy College of Pharmacy

Soladevanahalli, Bengaluru

Preincubation Unit

CADD Center

In-Charge:

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Cheminformatics, another branch of computer aided drug design, we provide in silico evidence for the drug pharmacological actions. Equipped with advanced computing instruments and software, our scientists can provide cheminformatics for medicinal chemists, pharmacologists, formulation chemists, natural product chemist, etc. Bioinformatics, as a powerful tool, has become increasingly important in mining and interpreting the tremendous biological data for high-throughput research.

Software's available	Experiments conducted
1. Biovia Discovery Studio workstation 2. Autodock 3. Autodock Vina 4. ACS Chemdraw 5. Gromacs 6. Pymol	1. Structure based drug design: ✓ Docking ✓ Virtual screening ✓ Molecular dynamics ✓ De novo drug design ✓ Pharmacophore screening ✓ Binding site mapping ✓ Protein-protein interactions ✓ Homology modeling, etc 2. Ligand based drug design: ✓ QSAR ✓ COMFA ✓ COMSIA ✓ Similarity search ✓ ADMET prediction ✓ Penetration into BBB ✓ PKPD, studies, etc