

Hardware:

Extensive Computer facilities are available for the students at the laboratory and have been greatly expanded. The newly updated computer facility contains over twenty desktop computers running a variety of scientific and chemistry related software. SuSE is our main operating system to perform computational chemistry related projects.

Additionally a LINUX cluster system has recently been installed to facilitate the long computational Chemistry calculations with 5 nodes, each having the 4 Intel® Xeon T processors of 2.66 GHz

Software:

Following Software are in used for research in the laboratory

Molvision is the most flexible tool to visualise chemical systems, from simple molecules to large biopolymers and dynamics of liquids and multi-component solutions.

MOE is a comprehensive system that addresses the needs of the variety of research displines. These include: Molecular Modelling and simulation, protein Modeling, bioinformatics, structure based design, High Throughput Discovery, and chemoinformatics.

Gaussian View is used to predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types. Further, it can be used to study molecules and reactions under a wide range of conditions.

AutoDock is a suite of programs designed to predict the bound conformation(s) of a flexible ligand to a macromolecular target of known structure, like an enzyme or DNA.

AutoDoct Tool AutoDockTools, or ADT, can use it to set up, run and analyze AutoDock dockings and isocontour AutoGrid affinity maps, as well as compute molecular surfaces, display secondary structure ribbons, compute hydrogen-bonds, and do many more useful things.

Flex FlexX is a first, flexible docking method that uses on incremental construction algorithm to place ligand into an active site. It predicts geometry of protein-ligand complex and estimate binding affinity in less than 15 seconds.

[Ligplot](#) automatically generates schematic diagrams of protein-ligand interactions for a given PDB file. The interactions shown are those mediated by hydrogen bonds and by hydrophobic contacts.

[VMD](#) (Visual Molecular Dynamics) is a molecular graphics program designed for the interactive visualization and analysis of biopolymers such as proteins, nucleic acids, lipids and membranes.

Amber7.0

Rasmol

Pymol

Babel

Molden

Dock4.0

Gold

DS Viewer