Chem Office / Chem Draw ultra: It is used to draw the structures of drug molecules in 2D and then to convert them in 3D, to find the IUPAC name of the unknown compound, to find the structure of the drug from its IUPAC name, to give NMR spectrum (approx) of unknown drug.

Software used to visualize the protein/ peptide 3D structure: Pymol, Rasmol, Jmol, Molmol, and VMD.

Structure Activity Relationship 2D QSAR, 3D QSAR: CoMFA,CoMSIA

Sequence alignment of proteins & nucleic acids: BLAST, FASTA, PROSPECTUS, COPIA

Gene finding and sequence analysis: Genscan, Glimmer

For sequence alignment of proteins: CLUSTAL W, CLUSTAL X

3D structure visualization, molecular dynamics, energy minimization: AMBER, CHARMM, HyperChem, chem2pac, GROMOS, GROMACS, MOE, SCHRODINGER

Molecular dynamics: MM2, MOPAC, AM1, PM

For quantum chemistry calculations: Gaussian

For statistical calculations: Sigmastat, Graphpad Prism, Sigma plot

For molecular design and drug design: Tripose, VLife

Structure drawing, 3D visualization of drugs and proteins: Alchemi, Cache, SYBYL

Cluster of many software used mainly for homology modeling: EMBOSS, GCG, Sybyl, Schrodinger.

For Docking (checking drug molecular fitting into receptor): Autodock, GOLD.

Toxicity prediction: Topkat