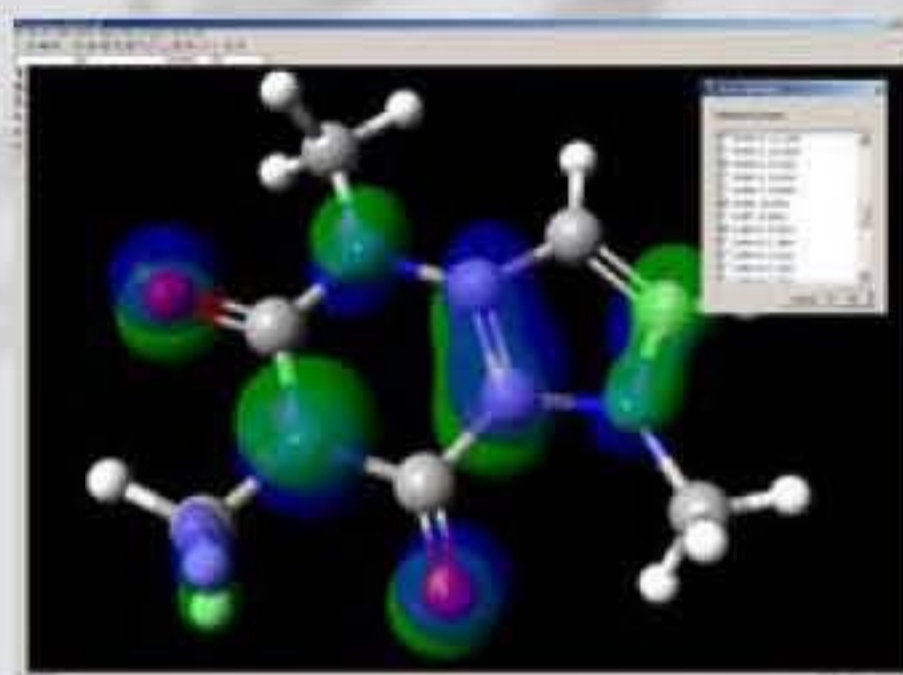




Scigress Explorer is a leading computer-aided chemistry modeling package designed for computational chemists as well as experimental chemists conducting research in life sciences, materials and chemicals and undergraduate and graduate educators. Scigress Explorer lets every chemist visualize molecules in 3D, search for conformations, analyze chemical reactivity, and predict properties of compounds with an easy-to-use interface on desktop computers.

#### Scigress Explorer User Interfaces

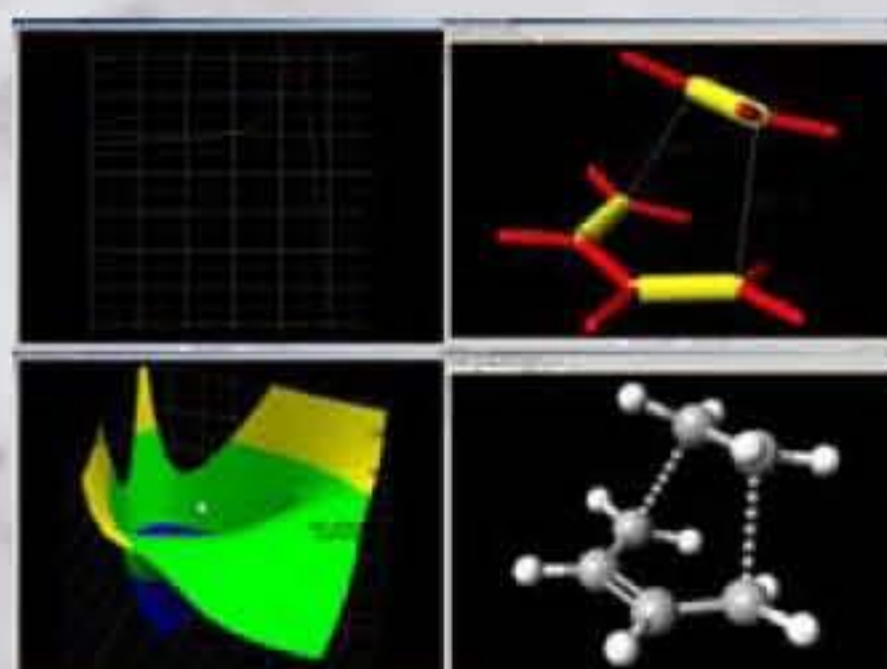
**Workspace** - Create molecules; clean up valences; correct geometry; display atomic charges, bond orders, bond strain; view energy maps, IR spectra, UV-visible spectra, orbitals, and reactivity surfaces; surfaces, and orbitals; superimpose molecules; link spectra and energy maps to structures. Fragment Library contains amino acids, nucleic acids, transition states, organometallics, organics, inorganics, drugs, and others. Display PDB files; build peptides from sequence; edit protein structures; automatic sequence alignment (Needleman-Wunsch algorithm); solvent accessible surface; ligand pocket surface; and automatic ligand docking. Interface to Gaussian\*.



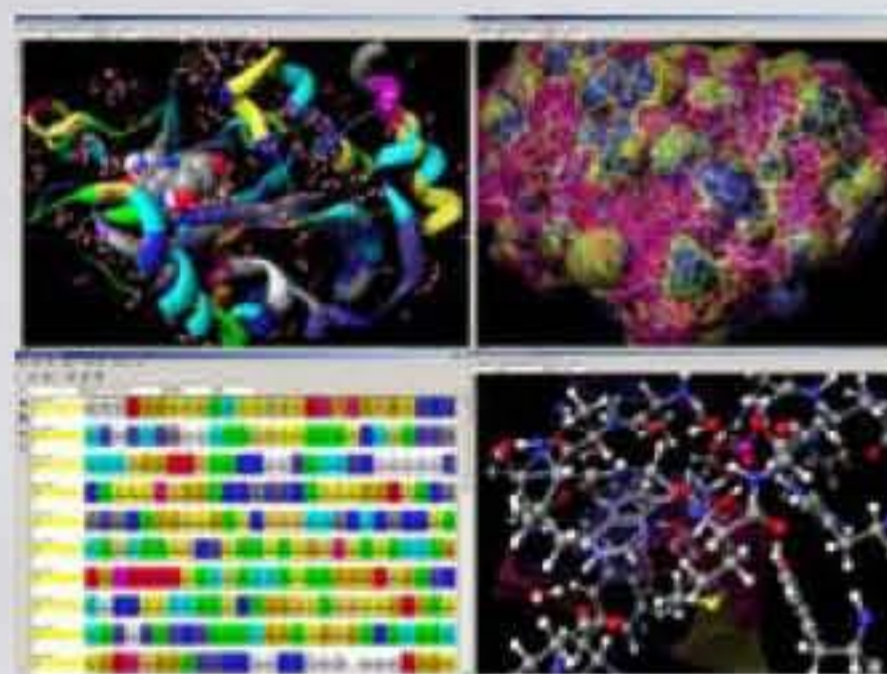
**ProjectLeader** - Automated batch processing; research project management; property driven spreadsheet interface; tracking and annotation; automatic 2D-3D conversion; scatter graphs; simple, multiple and step-wise regressions; QSAR & QSPR for ADME, logP, Rule-of-5. Handles thousands of molecules. Auto-docking module.

#### Scigress Explorer Computational Tools

**Molecular Mechanics and Dynamics** - All elements; organics and inorganics; MM2, MM3, and AMBER; adjustable mechanics parameters; conformational searching; energy maps; geometry optimization; molecular dynamics calculations.



**MOPAC** - Main group elements; organics and inorganics; AM1, PM3, PM5, MINDO/3, MNDO; d-orbitals for transition metals; COSMO solvent model; MOZYME for up to 20,000 atoms; ESR; IR spectra; heat of formation; free energy; transition state searching; intrinsic reaction coordinates; dynamic reaction coordinates; activation energy; polarizabilities; reactivity surfaces; dipole moments; partial charges; bond orders; potential energy surfaces; geometry optimization; excited states, open shell systems; intersystem crossing.



**ZINDO** - d-orbitals, INDO and CNDO, organics and inorganics; atom partial charges, bond orders, UV-visible spectra; SCRF solvent modeling, reactivity surfaces.

**MOS-F** - Predicts spectroscopic properties of both open and closed-shell molecules. Extends the capabilities of Scigress Explorer beyond

those provided by MOPAC and ZINDO: Semi-empirical methods: AM1, PM3, PM5, INDO/S, CNDO/S, CNDO/S2, CNDO/S3. RPA/CIS methods. Onsager solvation model.

**DGauss** - Higher accuracy models based on Density Functional Theory; NMR and vibrational spectra; transition metals, pseudo potentials. DGauss has been highly optimized to take maximum advantage of multiprocessor systems.

**CONFLEX** - Automated global minimum search, systematic and exhaustive generation of low energy conformers of a molecule of any shape, including rings; automatic and full characterization of optimum geometries, eliminating duplicates and stationary structures that are not minima.

**LocalSCF** - A novel linear scaling quantum mechanics method able to calculate more than 100 000 atoms. The algorithm has been designed for very fast calculations of electronic structure of proteins.

#### Hardware and software requirements

Suggested hardware configuration for Windows version: Intel Pentium 4 2.0 GHz or higher; 512 MB RAM or more; 500 MB HDD space or more.

Operating Systems: Windows 98/ME/2000/XP  
Scigress Explorer is also available as a GroupServer for Linux

\* Gaussian is not included in the package. Scigress Explorer works with Gaussian 03W revision B.03 or higher.