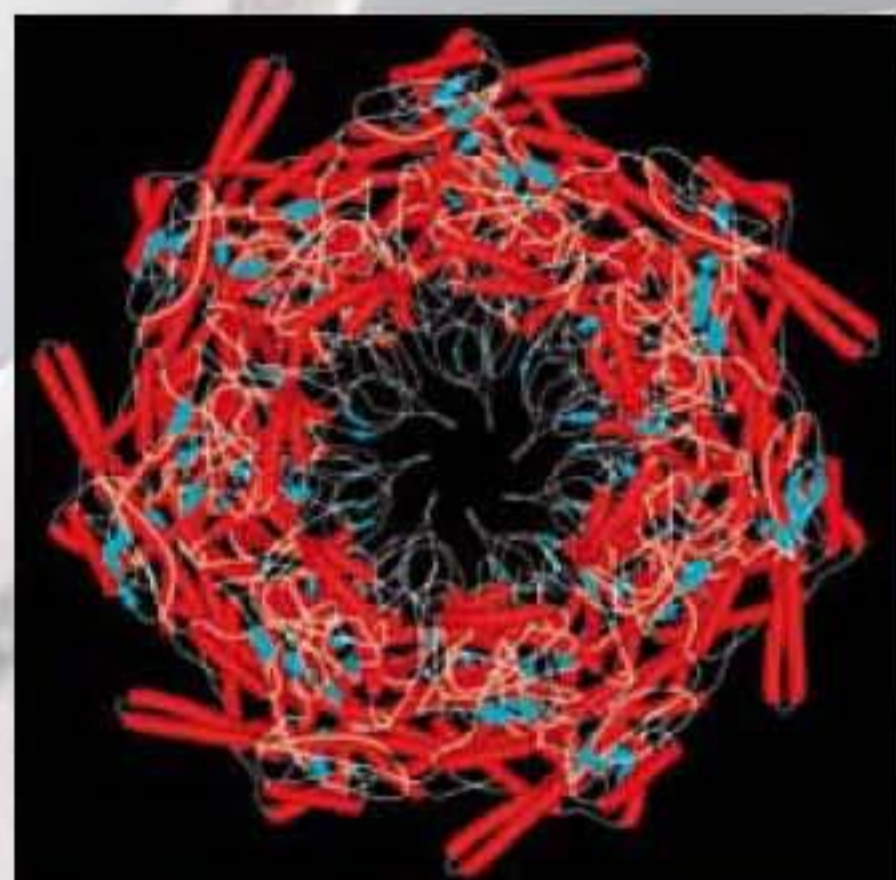


LocalSCF - the only commercially supported semi-empirical code capable of optimizations on molecules and ensembles of up to 120 000 atoms on a desktop PC. This giant molecule capability opens up whole new areas of chemistry and biochemistry for study, such as protein-ligand interactions, polymers, and materials chemistry.

The program utilizes standard NDDO approach and supports MNDO, AM1, PM3, and PM5 semiempirical Hamiltonians. Closed shell RHF energy calculations in frozen geometry and geometry optimization calculations in gas phase and those using COSMO continuum solvent models are supported by calculation modes.

Area of application

The program has been designed for very fast calculations of electronic structure of proteins. Although the program application is not limited to proteins, its numerous default settings were optimized especially for the efficient treatment of proteins, hence the program may show different performance on other classes of chemical compounds.

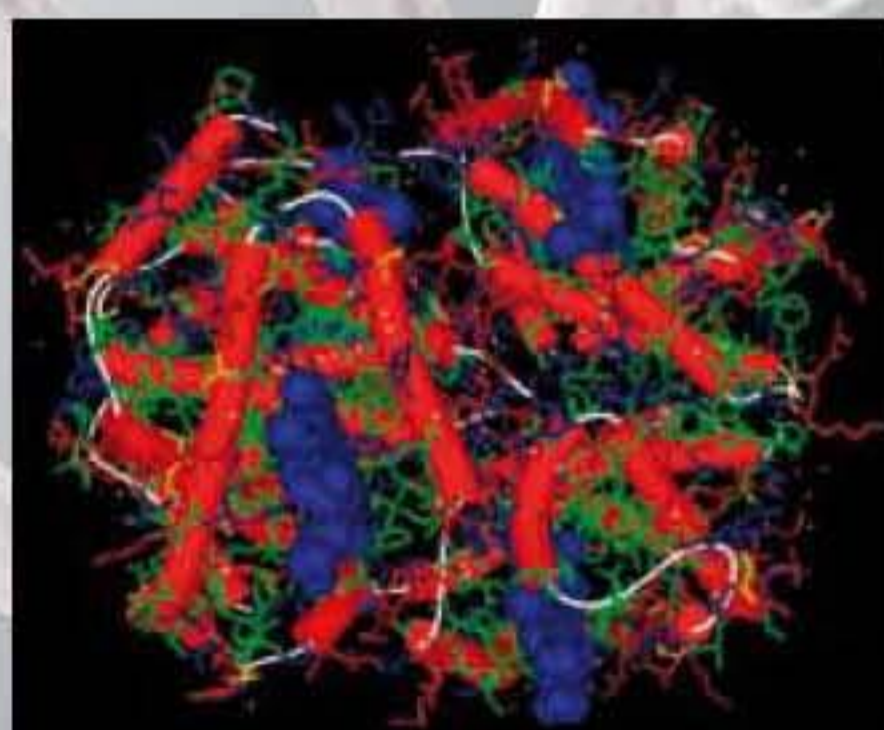


Program capabilities

- Ultra large 100,000+ atoms' protein systems.
- Very fast advanced geometry optimization specially tuned for proteins.
- Powerful control options for balancing between speed and accuracy.
- Linear scaling COSMO solvation model.
- Fast Multipole Method for evaluation of Coulomb integrals.
- True variational linear scalability.
- Semi-empirical Hamiltonians: MNDO, AM1,

PM3, and PM5 (d-orbitals for transition metals).

- Langevin and NTV Molecular Dynamics of proteins in gas-phase and COSMO.
- Lennard-Jones energy correction.
- Ligand optimization in QM/QM mode in gas-phase and COSMO.
- Flexible-ligand high throughput docking in gas-phase and COSMO.
- CM2 and CM3 charges.
- Ligand conformation generator for ligand bound to protein.



Advanced geometry optimization options

- Recognition of protein structure from Cartesian coordinates.
- Structure quality checking and verification.



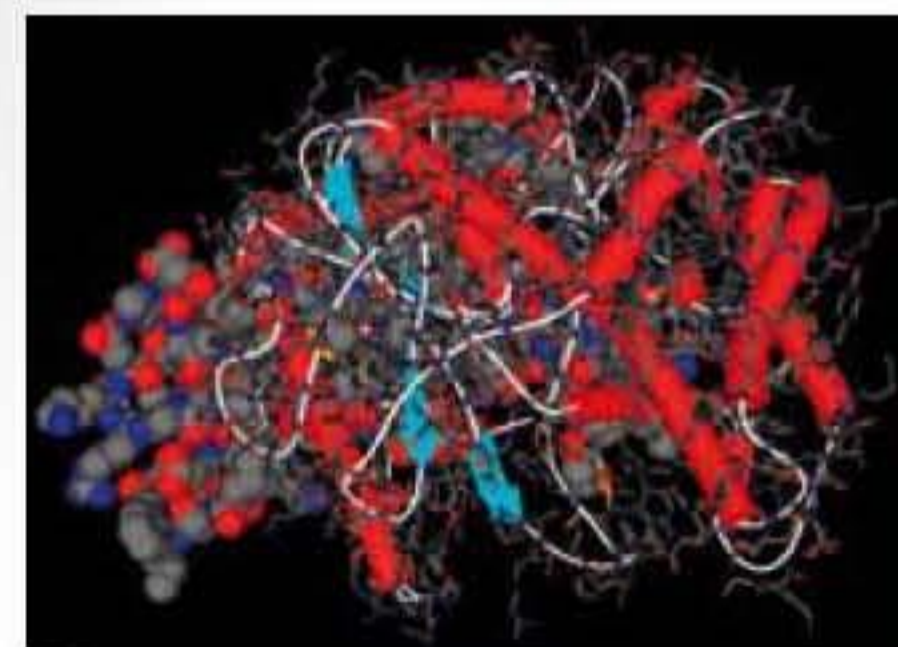
- Identification of various molecular fragments: amino acid backbone, side-chain, terminal atoms, water molecules, and counterions.
- Intuitive and easy to use interface for specification of geometry optimization modes through definition of particular fragments or amino acid numbers.
- Keyword based recognition and on-fly optimization of drug molecules in the enzyme cavity.

Fast Multipole Method

- Assures very low memory requirement, extremely fast calculation of large systems and high accuracy of evaluation of Coulomb interactions.
- Provides flexible control over resource consumption.

True variational linear scaling method

- Retains high accuracy for short localized molecular orbitals (the shorter the LMOs the less RAM is consumed).
- Provides an optimal user-controllable balance between speed and accuracy.
- The built-in mechanism for accuracy validation allows comparison of molecular properties in connection with particular keyword options.



Hardware and software requirements

- Suggested hardware configuration for Windows version: Intel Pentium 4 2.0 GHz or higher; 1.0 GB RAM or more*; 500MB HDD space or more.
- Operating Systems: Windows 2000/XP, and Linux (64-bit support on Linux platform). LocalSCF has also been ported to Linux and Windows parallel computers.

* There is no hard-coded limit on the number of atoms. However, 2GB memory allocation limit on the 32-bit platforms will restrict the molecule size to approximately 150 000 atoms.