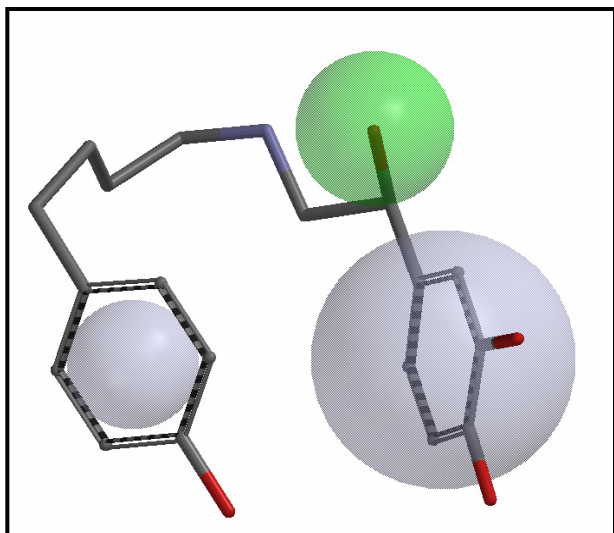




Trident

Molecular Modeling for Medicinal Chemists



Molecular Modeling Tools for Medicinal Chemists

Trident provides medicinal chemists with desktop access to state-of-the-art molecular modeling tools. Build or import and display molecules. Determine preferred conformations and calculate conformer energies. Calculate and analyze molecular structures, energies, and properties. Quantify 3D molecular similarity based on structure, chemical function descriptors of pharmacophore models. The easy to use graphical interface is fully compatible with Wavefunction's Spartan software.

F E A T U R E S

Build and Import, Display and Query

- Build and edit organic molecules
- Generate substituted molecules
- Import 1D, 2D, or 3D files
- View and manipulate molecular models
- Query structural properties
- Tabulate data in spreadsheets
- Perform linear regression analysis
- Construct Plots

Structure/Property Calculations

- Calculate geometry, energy, and properties with Semi Empirical or Hartree-Fock molecular orbital models
- Evaluate conformer energies and Boltzmann distributions
- Identify 'best' tautomer and evaluate tautomer energies
- Calculate dipole moments, atomic charges, and other QSAR properties

Conformational Analysis

- Locate the 'best' conformer
- Establish distributions of 'good' conformers
- Systematic or Monte Carlo search
- Energy correction for aqueous solvent
- Build libraries of diverse conformers

Similarity Analysis

- Quantify similarity using diverse conformers
- Locate 'similar' molecules and quantify molecular similarity based on structure or chemical function
- Quantify similarity of molecules to pharmacophores

Graphical Surfaces

- Display of calculated electronic structure graphics
- Including electron density, HOMO/LUMO orbitals
- electrostatic potential, Local ionization potential, with option to highlight 'accessible regions'

Databases

- Spartan Molecular Database contains:
 - ~120K molecular structures and properties obtained from Hartree-Fock calculations
 - ~70K compounds represented with diverse conformers from Maybridge's 'Compounds for Drug Discovery'
 - ~5K collection of common drug and drug candidates represented with diverse conformers
 - ~2K collection of ligands bound to proteins from PDB
- Cambridge Structural Database (CSD) from CCDC with over 350K x-ray crystal structures (additional licensing required)

