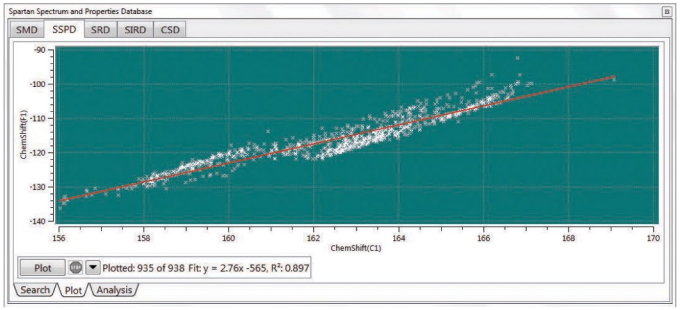
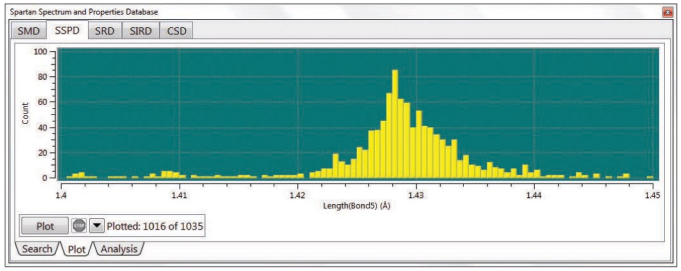
## DATA MINING

The information contained in ***SSPD*** may be "mined", allowing trends in calculated properties to be examined and relationships among different properties established. ***Spartan*** provides for x/y and histogram plots from mined data as well as multi variable regression analyses.




*Above: Relationship between $^{19}F$ chemical shift and $^{13}C$ shift on the carbon to which it is bonded in p-substituted fluorobenzenes.*




*Above: Variation in fused-ring bond length in substituted naphthalenes.*

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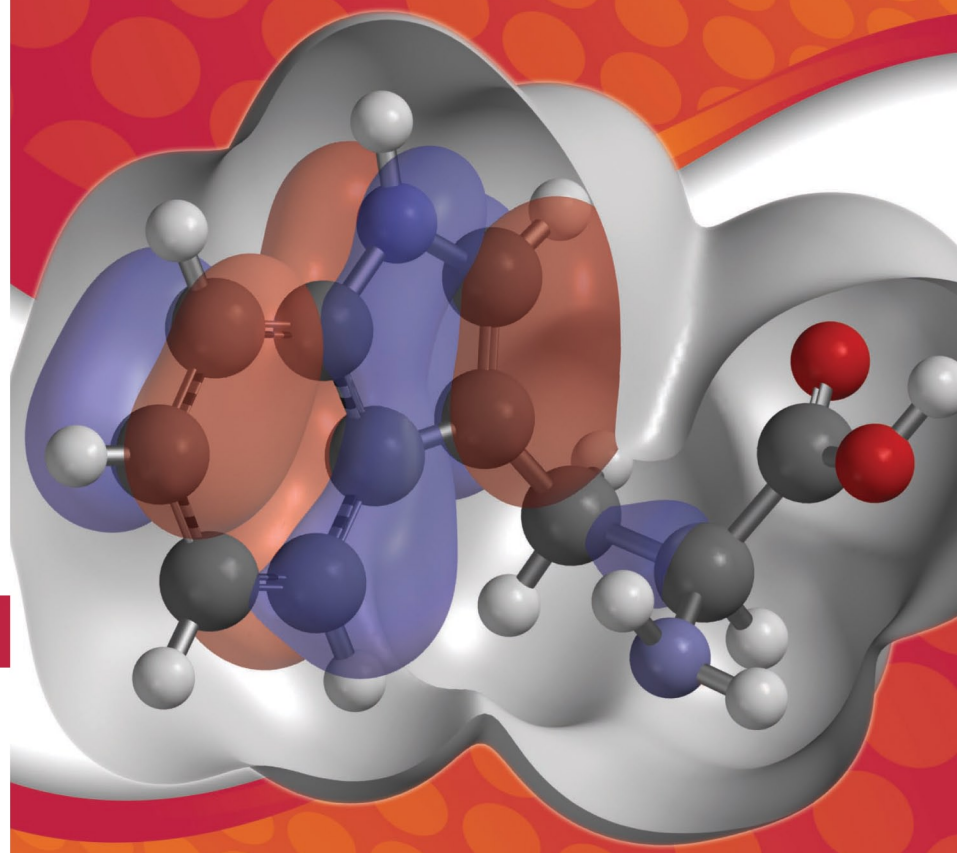
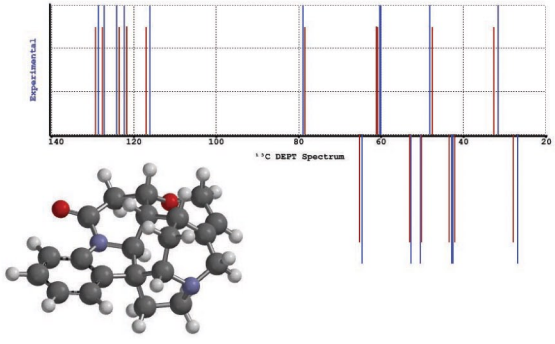
# Spartan Spectra and Properties Database



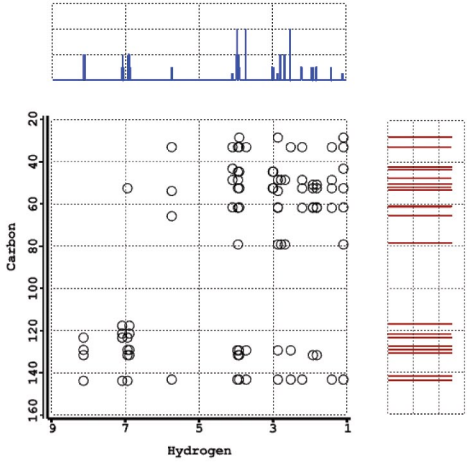
WHAT IS THE

# Spartan Spectra and Properties Database

The ***Spartan Spectra and Properties Database*** (***SSPD***) is a collection of infrared and NMR spectra, together with a wide variety of atomic and molecular properties and QSAR descriptors for ~300,000 molecules with molecular and ωB97X-D/6-31G* weights up to 500 amu. These have been obtained from the EDF2/6-31G* density functional models based on the lowest-energy conformation assigned from the T1 thermochemical recipe. The wavefunction is included in each database entry, allowing on-the-fly calculations of graphical surfaces and property maps. ***SSPD*** is accessed from ***Spartan*** by substructure, name, formula or by best match to and unknown (experimental) infrared spectrum. In addition, results are instantly available for any molecule that has been built by or imported into ***Spartan*** for which a database entry exists.



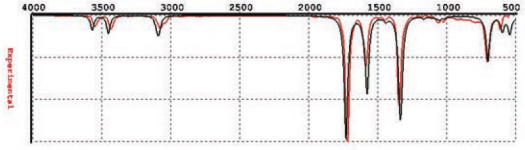

## NMR SPECTRA




Chemical shifts are calculated while HH coupling constants are estimated based on the 3D geometry. Proton, $^{13}$C and $^{13}$C DEPT spectra as well as COSY, HSQC and HMBC spectra may be displayed. Chemical shifts for other nuclei, for example, $^{19}$F, are available. Directly calculated $^{13}$C chemical shifts, which over a large selection of organic molecules show an RMS error of 5.5 ppm relative to experimental values, have been empirically corrected based on bond counts and bond orders. The resulting data show an RMS error of 1.8 ppm for EDF2 and 1.5 for ωB97X-D.

## INFRARED SPECTRA

Infrared frequencies calculated from the EDF2/6-31G* density functional model are systematically 4-6% larger than experimental frequencies, due primarily to the harmonic approximation. Also, the lines in an infrared spectrum at finite temperature are broadened due in part to rotational structure. Calculated infrared spectra that have been uniformly scaled and fit to a Lorentzian function with the peak width at half height as a second parameter are typically in good accord with experimental spectra. This allows ***SSPD*** to be searched for best fit to an unknown (experimental) infrared spectrum.

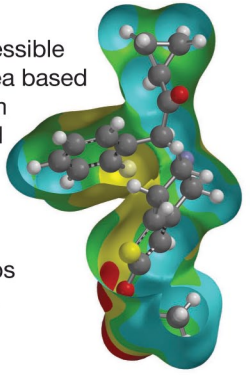



## ATOMIC AND MOLECULAR PROPERTIES, QSAR DESCRIPTORS AND THERMODYNAMIC QUANTITIES

Molecular properties include the ωB97X-D/6-31G* or EDF2/6-31G* geometry, area, accessible area volume and ovality, energy, heat of formation from the T1 thermochemical recipe, zero-point energy, HOMO and LUMO energies, aqueous solvation energy estimated from the SM5.4 model and dipole moment. Also available are the estimated numbers of conformers and tautomers.

Atomic properties include exposed surface areas, Mulliken and natural charges as well as charges based on fits to the electrostatic potential. R/S chirality assignments are also provided.

QSAR descriptors include the polar surface area and accessible polar surface area, the polar area and accessible polar area based on different values of the electrostatic potential, LogP from the Ghose-Crippen model, polarizability, the minimum and maximum of the electrostatic potential and the minimum of the local ionization potential. Also available are the number of hydrogen-bond donors and acceptors.



Thermodynamic quantities include enthalpy, entropy, Gibbs energy and heat capacity, all as a function of temperature.

## GRAPHICAL DISPLAYS

Graphical surfaces and property maps are generated “on-the-fly”. In addition to the ***molecular orbitals***, these include the ***electron density***, providing overall molecular size and shape, the ***electrostatic potential map***, indicating molecular charge distribution and revealing hydrophilic or hydrophobic character, the ***local ionization potential map***, designating electron-rich regions where electrophilic attack is likely to occur, and the ***LUMO map***, designating electron-poor regions where nucleophilic attack is likely to occur.