INTRODUCTION TO SPARTAN:

- ***Computational Capabilities*:**

1. Molecular mechanics.:- MMFF, (for validation test suite), MMFF with extensions, and SYBYL force fields
2. Semi-empirical calculations.
3. Hartree-Fock / SCF methods,

- Density Functional Theory (DFT) methods, available with implicit solvent(SM8).

Standard Functionals: BP, BLYP, B3LYP, EDF1, EDF2, M06, ωB97X-D

– Exchange functionals: HF, Slater-Dirac,Becke88,Gill96,GG99,B(EDF1), PW91

– Correlation functionals: VWN,LYP,PW91,P86,PZ81,PBE.

– Hybrid or Combination functionals: B3PW9,B3LYP,B3LYP5, EDF,EDF2,BMK

– Truhlar Group Functionals: M05, M05-2X, M06, M06-L M06-2X,M06-HF

– Head-Gordon Group Functionals: ωB97, ωB97X, ωB97X-D

4. Coupled cluster methods.
5. Møller-Plesset methods.
6. Excited State methods.
7. Quantum chemistry composite methods / thermochemical recipes.

- ***Task Performed:*-**Available computational models provide molecular, thermodynamic, QSAR, atomic, graphical and spectral properties. A calculation dialogue provides access to the following computational tasks:

1. Energy - For a given geometry, provides energy and associated properties of a molecule or system. If quantum chemical models are employed, the wavefunction is calculated.
2. Equilibrium Geometry- Locates the nearest local minimum and provides energy and associated properties.
3. Transition State Geometry- Locates the nearest first-order saddle point (a maximum in a single dimension and minima in all others) and provides energy and associated properties.
4. Equilibrium Conformer- Replaces the submitted molecule with its lowest-energy conformation. Often performed prior to calculating structure using a quantum chemical model.
5. Conformer Distribution - Creates a new file consisting of a selection of low-energy conformers. Commonly used to identify the shapes a specific molecule is

likely to adopt and to determine a Boltzmann distribution for calculating average molecular properties.

6. Conformer Library- Replaces the submitted molecule with its lowest-energy conformer and attaches the coordinates of a set of conformers spanning all shapes accessible to the molecule without regard to energy. Used to build libraries for similarity analysis.
7. Energy Profile - Steps a molecule or system through a user defined coordinate set, providing equilibrium geometries for each step (subject to user-specified constraints).
8. Similarity Analysis - quantifies the likeness of molecules (and optionally their conformers) based on either structure or chemical function (Hydrogen Bond Acceptors/Donors,Positive/Negative Ionizables, Hydrophobes, Aromatics). Quantifies likeness of a molecule (and optionally its conformers) to a pharmacophore.

- ***Available spectra data and plots for:***

1. IR Spectra (FT-IR,Raman IR)
2. NMR Spectra(^{1}H,^{13}C Chemical Shifts,Coupling Constants,Boltzmann averaged shifts,COSY plots,HSQC spectra,HMBC spectra)
3. UV/vis Spectra

Experimental spectra may be imported for comparison with calculated spectra: IR and UV/vis spectra in JCAMP (.dx) format and NMR spectra in Chemical Markup Language (.cml) format. Access to public domain spectral databases is available for (FT-IR Spectra,^{1}H and ^{13}C NMR spectra,UV/vis spectra).

- ***Graphical Models***:- Graphical models, especially molecular orbitals, electron density, and electrostatic potential maps, are a routine means of molecular visualization in chemistry education.Molecular Orbitals (homo,lumo), Electron Density, Van der Waals surface, Electrostatic Potential, Solvent Accessible surface, Polarization Potential

Composite Surfaces (Maps):- Electrostatic Potential Map, Local Ionization Potential Map, LUMO Map (Nucleophilic indicator)

We look forward for an opportunity to have an online demonstration of the product so that you can experience various features of the software