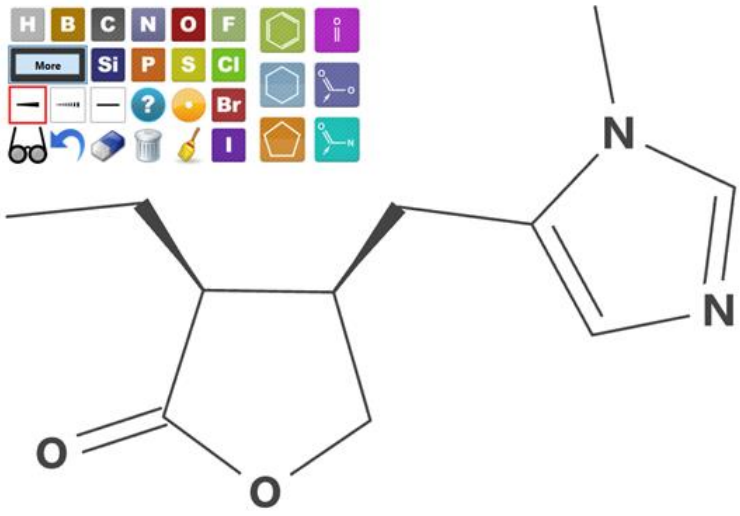
**New in *Spartan Student Edition v.9:***

## Graphical Interface.

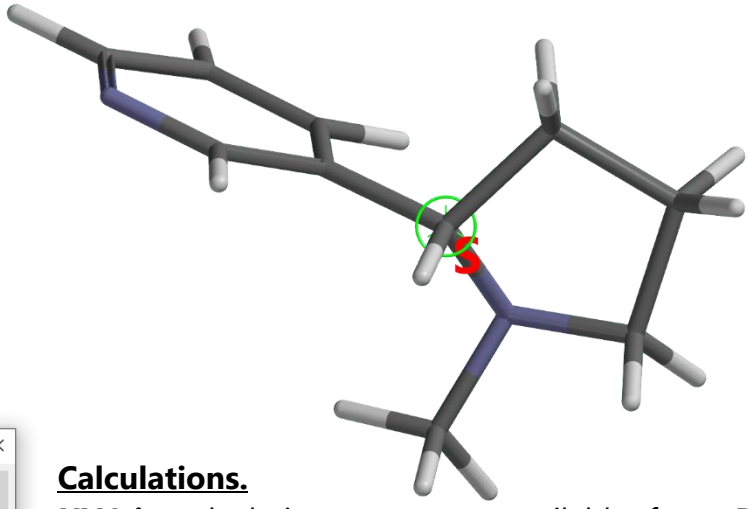


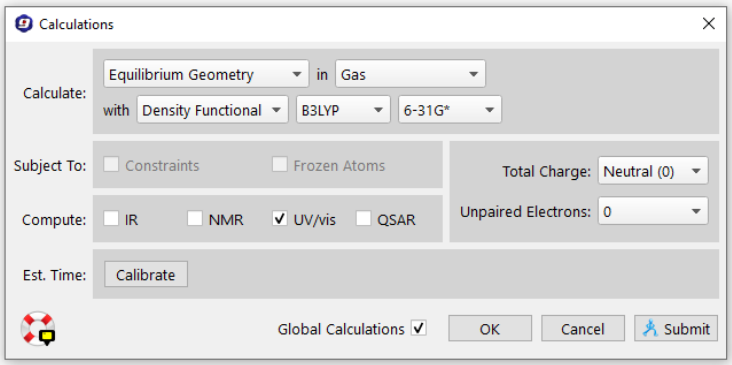

***2D Drawings***. Spartan derived 2D drawings (from the Sketch builder) have been improved to allow for a more user-friendly option for increasing bond count (single to double, double to triple). Improvements to designation of stereochemistry via wedges are implemented. Users can instantly build with wedges, rather than having to modify an existing bond with stereochemical markers. User input of experimental shifts in 2D has also been implemented.

Transition state construction using arrow-pushing nomenclature is available from both the 2D Sketch builder and the original 3D builders (Model Kit).

***Output Summary***. This HTML presentation format has been improved resulting in an order or magnitude (or more) speed increase as some data tables are calculated on-the-fly upon opening. Most data, including NMR Summary tables $^{n}$J coupling, IR and thermodynamic data, UV/vis output, Orbital Energies, and Atomic Charges and Bond Orders are available in HTML tables that can be hidden or exposed as needed and optionally copied/pasted. The entire output summary is available to save in PDF format.

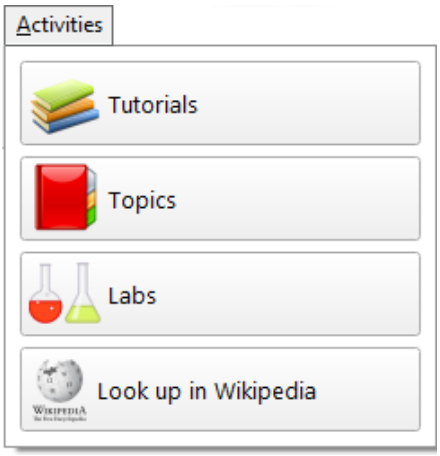
***Generate Isomers***. A new tool provides automatic stereoisomer/regioisomer elaboration. The input consists of a single molecule (isomer) with appropriate markers to indicate centers to be inverted (leading to stereoisomers), or adds bonds to be modified (leading to regioisomers).




## Calculations.

**UV/vis** calculations are now available from DFT models (using the corresponding TDDFT approaches for the excited state calculations. **Mulliken** and **Natural** charges are now available in the Output Summary. Empirical **coupling constants** are also accessible from via data table in the Output Summary.




**Integrated Lab Activities.** In addition to the Topics and Tutorials sections, the Activities menu now includes a growing collection of molecular modeling lab activities supporting general, organic, physical, organometallic and biochemical pedagogies. Want to see your school's lab content here? Contact support@wavefun.com for additional information.

**Computational Models.**

***Molecular Mechanics (MMFF)*** no atom limits.
***Semi-empirical (PM3)*** up to 75 atoms.
***Hartree-Fock molecular orbital*** up to 30 atoms.
***Density functional theory (ωB97X-D, B3LYP and EDF2)*** up to 30 atoms.
***Møller-Plesset (MP2)*** up to 20 atoms.
***T1 thermochemical recipe*** up to 20 atoms.
***Solvation Models.*** Hartree-Fock and density functional models include the option of using the **C-PCM** solvent model (polar, non-polar, and water) for energy calculations and for geometry or transition state geometry optimizations. Aqueous Solvent models are also available for MMFF (SM5.0R) and PM3 (SM5.4).

**Spectroscopy.**

***NMR.*** Empirical corrections to $^{13}$C chemical shifts are available for the ωB97X-D/6-31G*, B3LYP/6-31G* and EDF2/6-31G* models, offering increased accuracy (over raw calculated shifts).
***IR.*** ωB97X-D/6-31G*, B3LYP/6-31G* and EDF2/6-31G* frequencies are automatically scaled to account for systematic errors associated with the underlying harmonic approximation.
***UV/vis.*** New to Spartan Student v.9, UV/vis spectra plots are available based on ground state geometries (DFT only) and excited state energies (full TD-DFT), a variant of the 6-31G* basis set including diffuse functions for heavy atoms is utilized for both ground and excited state calculations. While in most cases, the resulting λmax is not sufficient to confirm or identify color, it is often sufficient to indicate if atom or functional group substitutions shift the overall color toward red or blue.

**Parallel Processing.**

Like the previous version, ***Spartan Student 9*** takes advantage of up to 16 cores in parallel, ***significantly*** improving performance (speed) of energies, geometry optimizations and transition state optimizations from Hartree-Fock, density functional, and Møller-Plesset models. The individual steps of the T1 thermochemical recipe have also been parallelized.

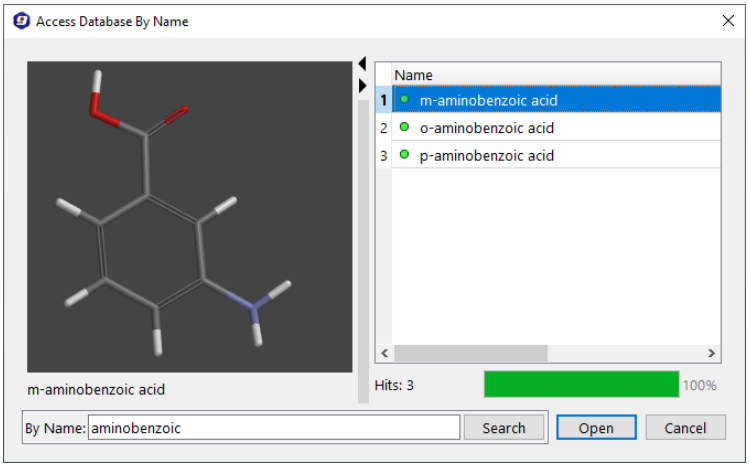
**Infrastructure.**

Spartan Student now also now reads/writes additional file formats:

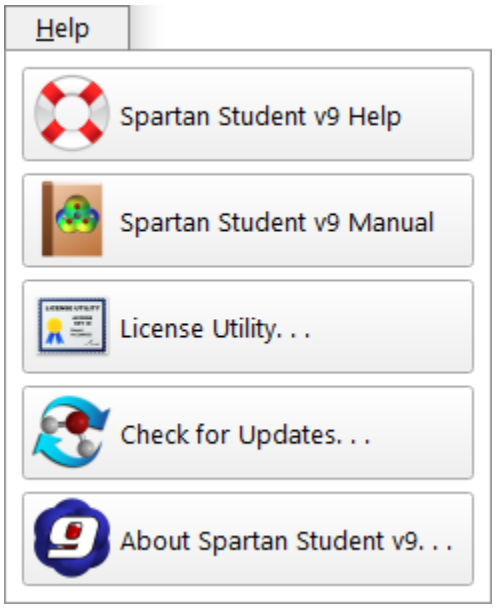
**Import**: New import types: .FChk (formatted checkpoint file), .wfx (AIM Extended file), .q, .in (Q-Chem input files), .mmx, .mm2, .mm3, .mmf (molecular mechanics formats), and .amsol, .ampac, and .mop (AMSOL/AMPAC and MOPAC formats).

**Export**: New export types: .FChk (formatted checkpoint file) and .jxyz (Jmol xyz list file).

**Access Database by name:** The file menu includes an entry allowing for search/retrieval of one or more hits from the included SSPD subset of >6k molecules. A 3D window allowing for preview of the molecule has been updated for improved visibility of the molecular structure.




**Help menu:**




The Help menu has been extended to include a non-invasive version update procedure. Clicking on the Check for Updates… entry compares the version number the user's license against the latest version available. If a newer version is available, the user has the option to visit Wavefunction's website and install the latest version available. As a reminder, minor point releases are ***always*** available at no additional charge, and it is *always* a good idea to download the very latest version of ***Spartan*** as any bug fixes and feature updates released are always bundled with minor point releases. The latest versions are also always accessible from the direct link: https://www.wavefun.com/downloads.

Our thanks to the user community for consistent feedback and suggestions for development directions in the ***Spartan Student Edition*** program, and stay tuned for the release of ***Spartan'22*** planned for late this year to early 2023…

Last Updated Oct 2022