New in *Spartan'20 Parallel Suite*. Below is a list of new features in the 2020-21 release of ***Spartan***.

NMR.

Boltzmann Averaged NMR. A new, simplified (and order of magnitude faster) protocol for calculating NMR chemical shifts for conformationally-flexible molecules, has been implemented. This replaces the accurate calculation of Boltzmann weights (the slow step in the protocol released in Spartan'18) by choosing from among "reasonable" low-energy conformers providing proton and ^{13}C chemical shifts that best match experimental values.

An important if not the most important use of NMR spectroscopy by synthetic chemists is to establish stereochemistry for a "known" reaction. By combining automatic isomer generation with previous or new protocols for dealing with conformationally-flexible molecules, ***Spartan'20*** can do this in a single step, starting with a single conformer of one isomer and resulting in proton and ^{13}C chemical shifts that have been properly conformationally averaged (or, in the case of the new protocol, best fit the experimental data) for each of the isomers. The **DP4** score can then be examined to decide which isomer best fits the experimental proton and/or ^{13}C chemical shifts.

Coupling Constants. Empirical relationship for 2 and 3-bond CH coupling constants based on comparisons of calculated coupling constants (previously available in *Spartan'18*), with experimental data. Whereas, empirical (Karplus-like) relationships for 3-bond HH coupling constants have long been available (including in Spartan), this provides (to our knowledge) previously unavailable and analogous but much more complicated relationships for CH coupling constants.

2D NMR Spectra. 2D NMR spectra, COSY (proton vs. proton) and (more importantly) HMBC (^{13}C vs. proton), based on calculated chemical shifts and either calculated or empirical estimated HH and CH coupling constants. 2D displays with or without experimental couplings.

Databases.

Natural Products Database. A Database of natural products with conformationally averaged calculated NMR spectra and experimental spectra. Now about 3,500 compounds (and growing. This is being updated with new literature, so it will grow modestly in the coming years.

Spartan Spectra & Properties Database (SSPD). The *Spartan Spectra & Properties Database* (SSPD) subset (installed automatically with the program) has been expanded to include IR frequencies from the ωB97X-D/6-31G* model structures. The full 300,000+ database (separate installation) now includes energies from the ωB97X-V/6-311+G(2df,2p) energies (as a property). These energies are accessible from the Molecule Properties and the Reactions dialogues.

Infrastructure.

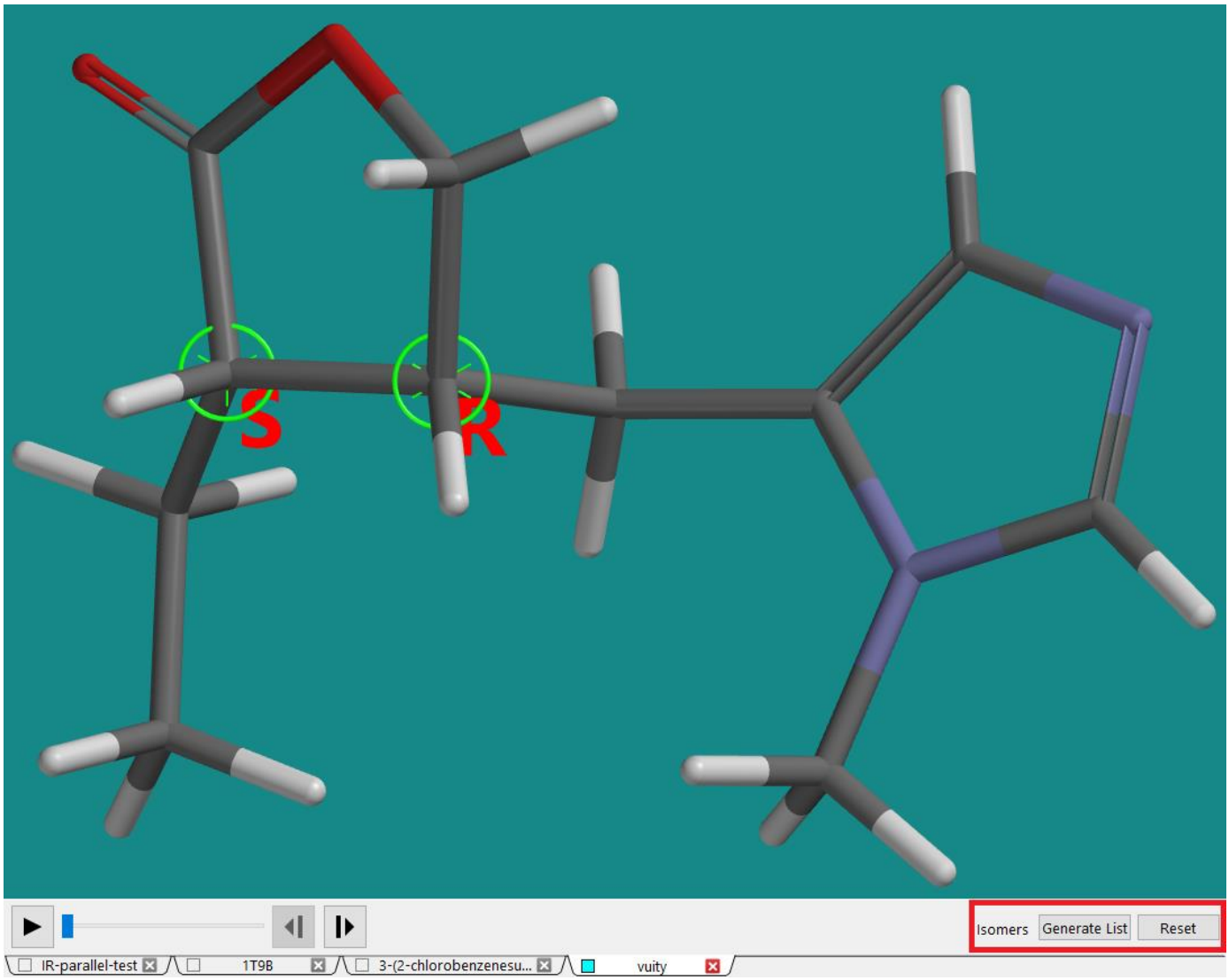
The additional capabilities related to input of experimental coupling constants and comparison / confirmation associated with calculated values have resulted in a new menu called Experimental Data. Future development plans also include the ability to input IR, Raman, and UV/vis data. Additionally, Spartan now also now reads/writes additional formats:

Import: New imports include .FChk (formatted checkpoint file), .wfx (AIMExtended 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 exports include .FChk (formatted checkpoint file) and .jxyz (Jmol xyz list file).

Graphical Interface.

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) and bonds to be modified (leading to regioisomers).

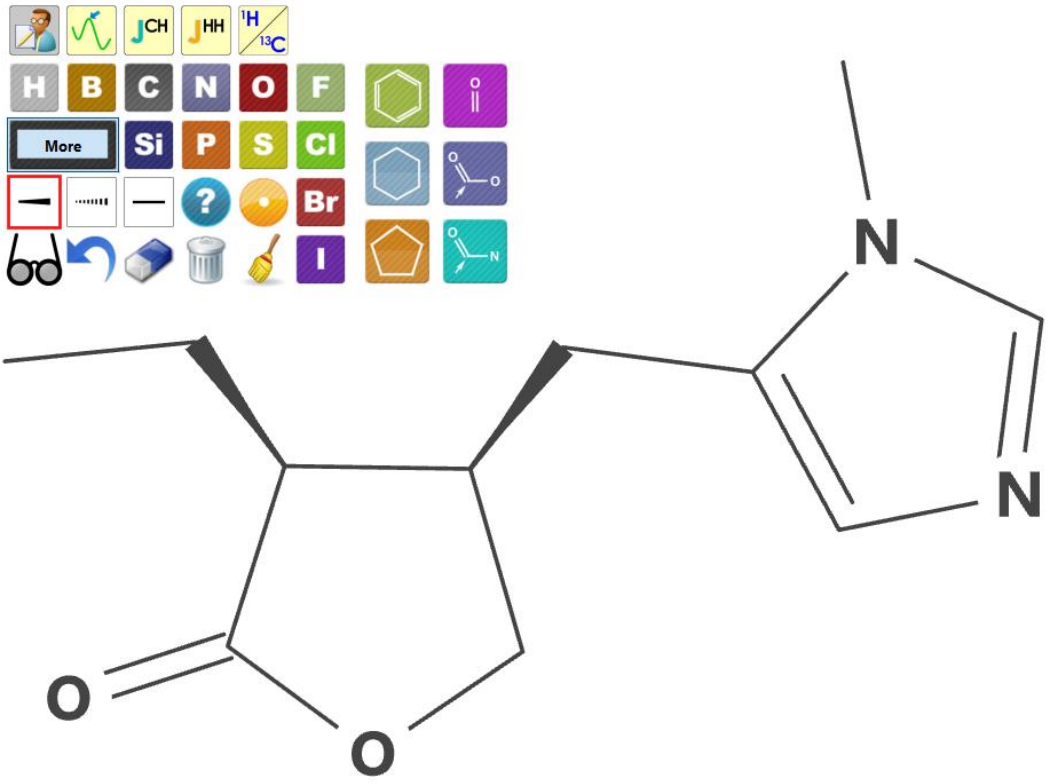


The result is a list of isomers. This list can then be submitted as a/an:

Equilibrium Geometry calculation - optionally with NMR leading to DP4 scores for each isomer
Equilibrium Conformer calculation leading to a list of the best conformer of each isomer
Conformer Distribution calculation leading to Boltzmann weighted conformer lists for each isomer
NMR Spectrum a multi-step conformer distribution/NMR task that leads to a Boltzmann weighted NMR shifts

Future developments will extend isomer generation to include regio-isomers and will apply this to reactions, automatically generating guesses at transition states that lead to isomeric products.

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). We have also made improvements to designation of stereochemistry via wedges, users can instantly build with wedges, rather than having to modify an existing bond. Visualization of calculated HH and CH couplings have been implemented in 2D and 3D. User input of experimental shifts in 2D has also been implemented.



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.

Computational Enhancements.

Parallel Processing.

Aside from NMR and frequencies, we have made improvements to parallel performance which previously saw a performance plateau at around 10 cores. This now begins to plateau at around 15 cores (energy and geometry calculations). The plateau will become more and more relevant as the number of cores in chips that are readily available continues to increase (one can now access 32 and 64 core chips and this may extend to t 128 and 256 core chips in the not too distant future. Modest improvements to parallel performance of the frequency code have been implemented. Future development efforts include a parallelization of the NMR code.

Spartan'20 Parallel Suite will take advantage of up to 16 cores for parallel jobs, with the option to license >16 cores as well (for high performance multicore systems), and will include our implementation of the latest ***Q-Chem*** version (5.1 at the time this list was compiled) and is the result of continued collaboration (begun with the release of *Spartan'02* in 2002). Through this collaboration our customers benefit from both GUI and computational enhancements in the ***Spartan*** code-base, as well as a growing range of computational approaches and modern computational methods included in ***Q-Chem***.

Last updated Dec 2021