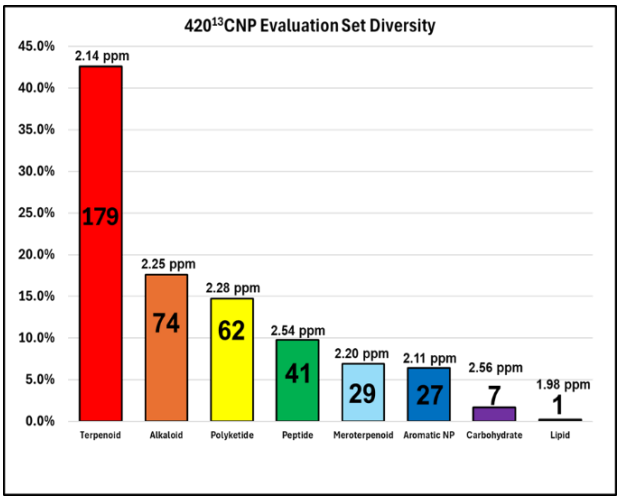
New in *Spartan'26*. Highlighted new items in the ***Spartan'26 v.1***[1] release:

Fast, accurate ^{13}C NMR shift prediction for flexible organic molecules.

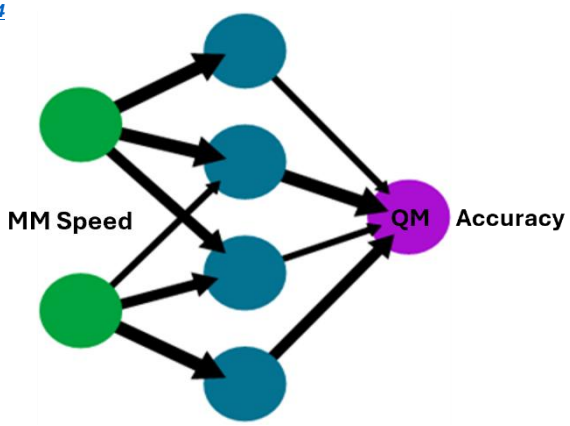
MLHF-NMR (and MLXD-NMR) protocols are defined and assessed in the latest Machine Learning publication[2] ***(preprint available).*** The application of machine learning models defines next generation in flexible molecule NMR prediction. Providing the same quality as the best quantum-chemical ^{13}C NMR shift predictions, MLHF-NMR was validated against the DELTA50 benchmark of high accuracy rigid molecules and provides **^{13}C shifts** at **1.7 ppm** and **^{1}H shifts** at **0.15 ppm** level **RMS error**.



Validated against a challenging, diverse set of 420 predominantly flexible structures (in multiple solvent environments) from the natural products literature, MLHF-NMR provides accuracy with average per molecule **^{13}C shift** performance of **1.7 ppm MAE** and **2.2 ppm RMS error**. On a larger validation set of 855 natural products including X-ray crystal verification from the Cambridge Structural Database[2], MLHF-NMR provided **^{13}C shift** performance of **1.5 ppm MAE** and **2.0 ppm RMS error**. The average per molecular calculation time for both flexible molecule validation sets was **1 minute 35 seconds** on a consumer-grade laptop.

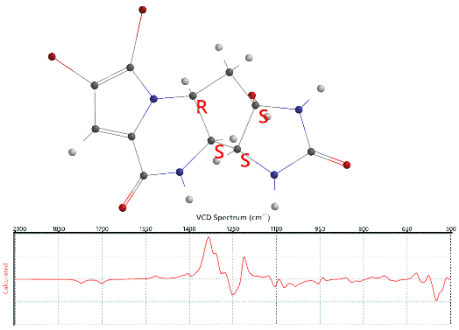
Available *Machine Learning* Model Tasks.

Instantaneous conformational-energy refinement[3,4]
From DFT and ML-Est. DFT geometries
From MMFF geometries
Fast est. DFT geometry optimizations[5]
From MMFF geometries
Instantaneous Boltzmann distribution energies[6]
From DFT(ωB97X-D) and ML-Est. DFT (ωB97X-D)
Instantaneous ^{1}H and ^{13}C Chemical shifts[7]
From DFT(ωB97X-D) and ML-Est. DFT (ωB97X-D)
Available for neutral closed-shell molecules containing **H**, **C**, **N**, **O**, **F**, **S**, **Cl** and **Br**.



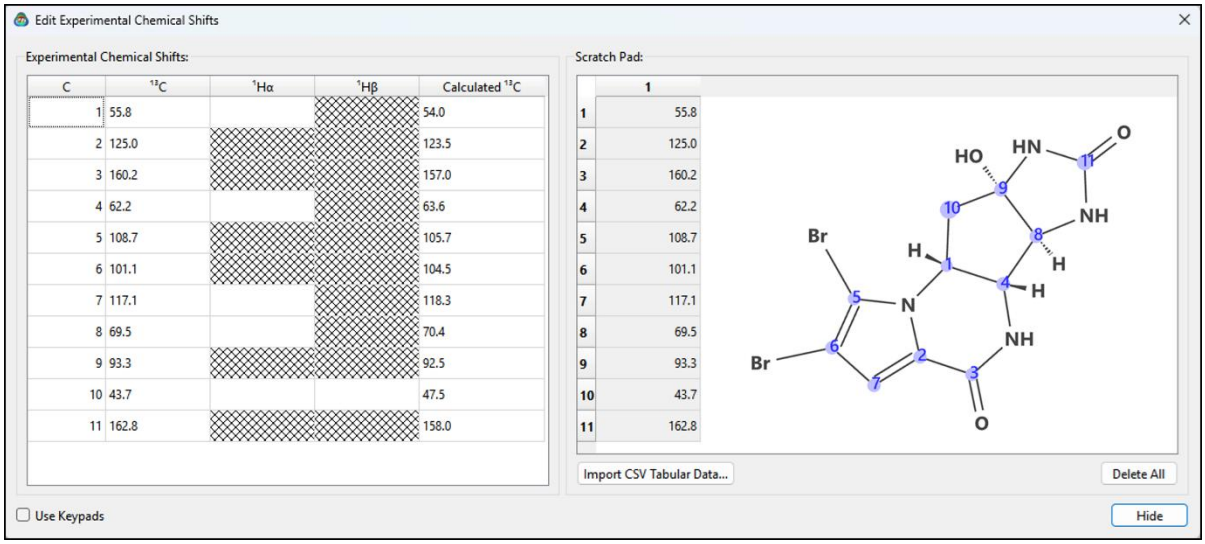
VCD Spectra.

Calculated spectra from QM models (Hartree-Fock and Density Functional) now include Vibrational Circular Dichroism (VCD) spectra. Used to determine the absolute configuration, chirality, and three-dimensional stereochemical structure of chiral molecules, in conjunction with NMR diastereomer analysis facilitated assignment of the correct enantiomer.

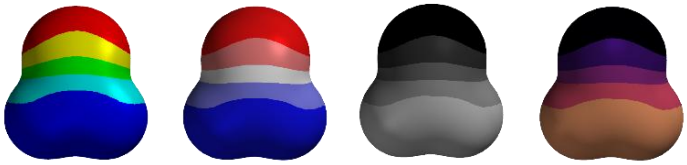


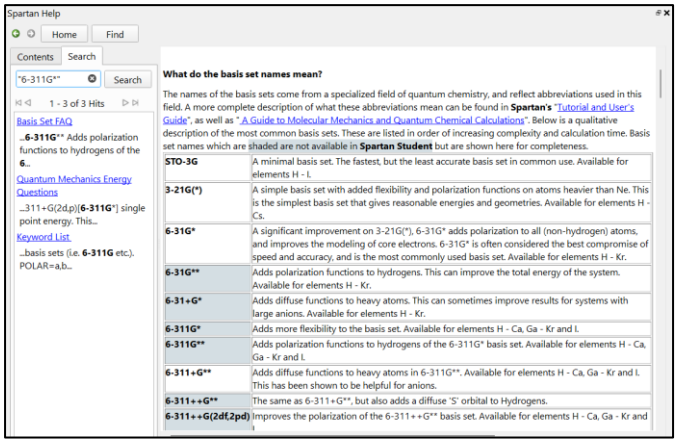
Infrastructure.

NMR menu. Replaces the previously named Expt. Data menu and enables easy Copy/Paste tools supporting instant import and easy formatting of experimental ^{13}C and ^{1}H shifts. Data can be imported via CSV or pasted directly into a spreadsheet utility supporting assignment.



Additional color options. For users with color-blindness, additional gradient options (for surface maps) including black-violet-sand, gray scale, and the option of importing custom configured gradients.





Search enabled Help Content.

Help menu content available in the form of >200 pages of topic-based HTML content is accessible to browse. **Spartan'26** enables text searching across the multi-file content, making accessing specific content of interest both easier and more efficient. The Calculations dialogue includes contextual-based links in the case of common challenges and/or error messages (for example, help with geometry convergence).

Databases.

Spartan Spectra & Properties Database (SSPD). The *Spartan Spectra & Properties Database* (SSPD) has added several thousand primarily drug, natural product, and pesticide molecules. The collection of ≈325k molecules and nearly 10,000 transition states has reduced the memory footprint down to less than 15 GB. Most **SSPD** entries contain **ωB97X-D/6-31G* geometry, frequencies,** and **NMR chemical shifts**, energies are available from the geometry model as well as up to three different DFT/large basis set and/or ***machine learning*** models, also available is the **T1**[8] **heat of formation**. **IR spectra** (based on ωB97X-D/6-31G* geometries/frequencies) can be displayed and vibrational motions can be animated. Additional data available includes:

DFT Energy Databases. Energies from three *good* energy models are available for most of the SSPD collection, from: ***ωB97X-V***[9]***/6-311+G(2df,2p)*** (≈309k), ***ωB97M-V***[10]***/6-311+G(2df,2p)*** (≈287k), ***ωB97M(2)***[11]***/6-311+G(2df,2p)*** (≈249k).

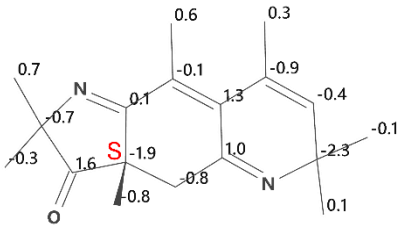
Natural Products Database. The collection included in the previous SSPD has been extended and refined, and may be searched separately from the full collection. The collection has grown to >3000 published natural products and includes information for the lowest energy conformer (based on ωB97X-V/6-311+G(2df,2p)[6-311G*]//ωB97X-D/6-31G* calculations). Also provided are ***calculated*** proton and ^{13}C chemical shifts and ***experimental*** ^{13}C shifts for this growing collection of published natural products molecules.

SDSD. The **Synthetic Drug Spartan Dataset**[3] is a collection of >1900 drug and drug-like molecules (name and InChI[12]-validated from PubChem[13]) that have been conformationally searched, geometry optimized and provided with Boltzmann weighted ^{1}H and ^{13}C NMR shifts from the MLHF-NMR protocol. In general, the **SDSD** is less conformationally flexible than the two validation sets used to evaluate MLHF-NMR performance (of 420 and 855 natural products structures respectively). Average ^{13}C shift performance on the combined 1275 validation structures, below. Spartan Machine Learning[14] model performance against the SDSD is anticipated comparable or better.

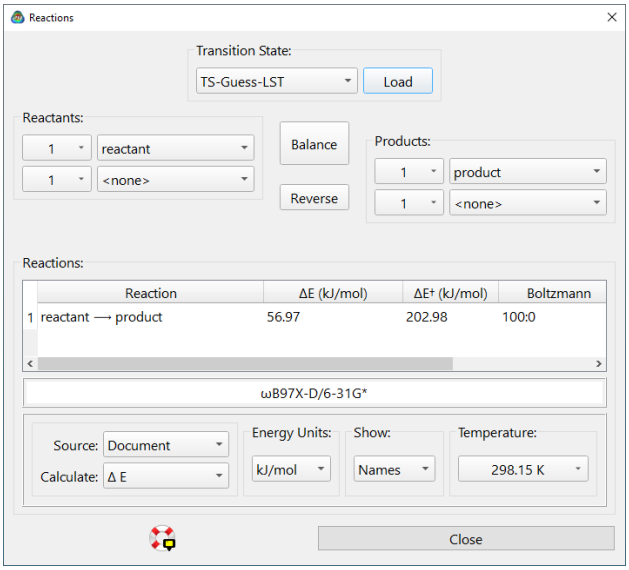
Average **flexible** performance:

RMS error:	**2.06 ppm**
median error:	**1.20 ppm**
mean error:	**1.58 ppm**
max error:	**5.04 ppm**

Sample **rigid** performance:



Check for Updates. The Help menu includes a user-friendly *version update* procedure. Clicking on the recently implemented **Check for Updates**… results in ***Spartan*** comparing the version number of 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 this. Minor point releases are ***always*** available at ***no additional charge***; the latest versions are also ***always accessible*** from the ***Downloads*** page on the ***Wavefunction*** website: https://www.wavefun.com/downloads. If ***Spartan*** is online, license updates can be managed via online server query, *no longer* requiring access to the key_update.V2C file in order to apply updated license features and maintenance dates.



Reactions Dialogue. Spartan'26 allows for both the included SSPD (as well as custom, user-generated databases) to be accessed to report ***activation energies*** (enthalpy, Gibbs energy) as well as overall reaction energies (enthalpies, Gibbs energies). Data from the SSPD can be combined with entries in a .spartan document (or the document can be used independently. Integrated Transition State isolation is supported via familiar arrow pushing display mode and facilitates a search of known transition states. If a similar transition state is not available, the fallback is a linear synchronous transit approach, attempting to average the structural data from reactants and products.

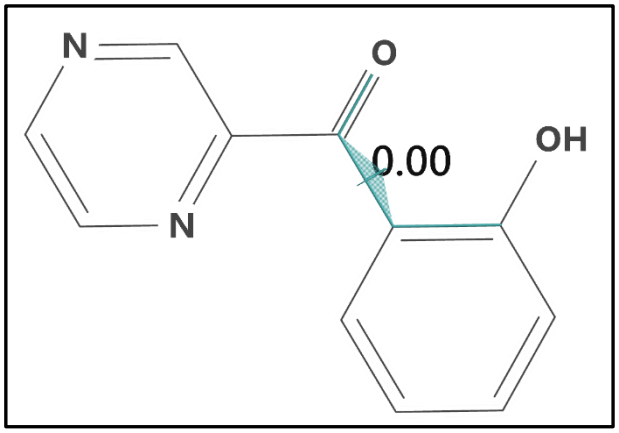
Properties Dialogue. The **Molecule** tab has been updated to allow for InChI string search of the NIH PubChem collection[13] of >119M compounds (https://pubchem.ncbi.nlm.nih.gov/). Molecules from PubChem may be imported into ***Spartan*** via Save As and Import of 2D or 3D SDF, or via Copy/Paste of InChI string into the InChI field in the Model Kit (3D build/edit mode).

Output Summary. The 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. All data from the Output Summary is available for export in single or multi-molecule format.

Activities menu. In addition to accessing step-by-step topic-based tutorials and a collection of essays, a wide range of computational topics, this menu also links to Wavefunction's *YouTube channel*, providing videos for a collection of basic tutorials and a selection of advanced tutorials and workflows.

Graphical Interface.

2D Extensions. A new 2D view mode enables a neutral environment allowing for assignment of NMR shifts and H-H and C-H couplings, as well as a host of standard tasks previously only available in 3D: measuring and constraining distances, angles, and dihedrals, enumerating tautomers and isomers (including diastereomers), as well as general access to atomic and molecular properties dialogues and ***Spartan*** spreadsheet.



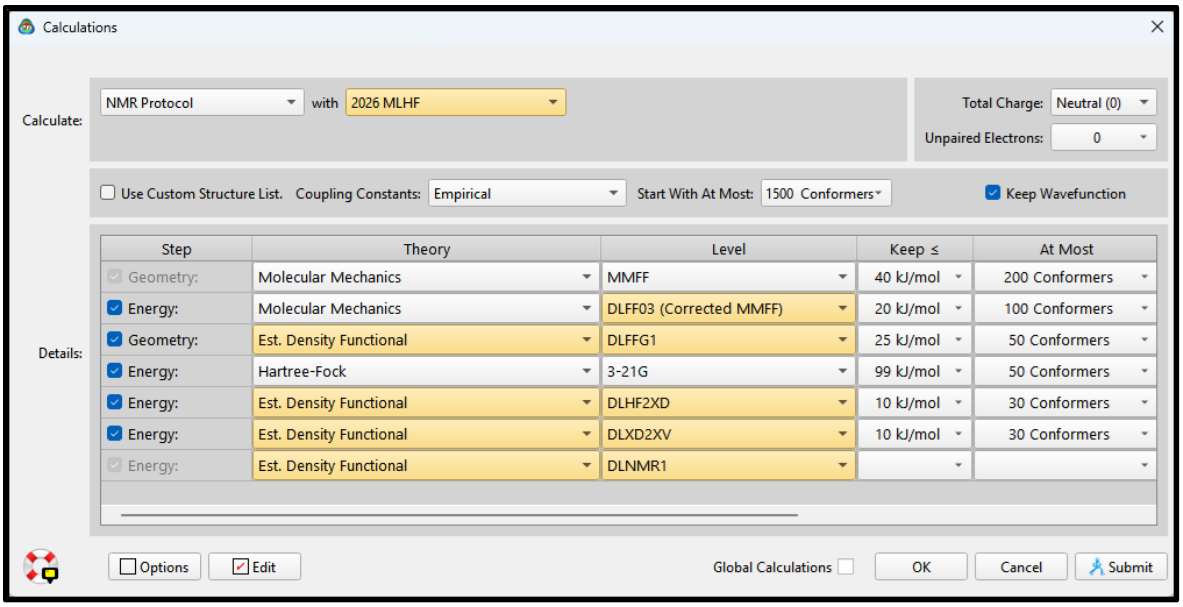
2D/3D Toggles. User-interface icons facilitate seamless conversion of molecular structures between two and three-dimensional views, A **Dual Display** option is available from either mode (a 2D dialogue 3D mode or a 3D dialogue in 2D mode).

Calculations Dialogue. A new entry, "NMR Protocol" provides access to four published computational workflows for predicting ^{1}H and ^{13}C shifts for flexible organic molecules:

1. 2019 QM-NMR protocol[15]
2. 2024 QM-NMR protocol[3]
3. 2025 MLXD-NMR protocol[3]
4. 2026 MLHF-NMR protocol[3]

Includes customization of NMR workflows via ☑ **Edit** of protocol details. The previous interface option: "NMR Spectra" remains available for full backward compatibility, although it can be effectively replaced by the new NMR Protocol task.

Machine Learning (Neural Network) options. To enable clear distinction between traditional molecular mechanics and quantum chemical approaches, and the growing library of published neural networks, any time the method is based on ***ML***, the Calculations dialogue uses a golden background color:



Standard ***Spartan'26*** licensing will take advantage of ***up to 16 cores/threads*** for parallel jobs, with the option to license a ***>16 core/thread*** version for use on high performance multi-core servers and workstations (note: by default, our enterprise licensing which can be local or cloud-based, includes the greater than 16 core functionality).

Spartan'26 includes significant computational capabilities from the ***Q-Chem***[16] package. This release includes both new neural networks and a new QM module based on the latest version of ***Q-Chem*** (v.6.3–6.4 at the time this list was prepared). Continuing our collaboration begun with *Spartan'02* in the early 2000's. Customers benefit from both from our GUI and computational enhancements in ***Spartan*** (like the T1 thermochemical recipe, the 2019 QM-NMR protocols for flexible molecule shifts, and the *new* ***ML*** models trained to approximate QM results in specific task-based workflows, *and* the broad spectrum of modern computational approaches and methodology included in the ***Q-Chem***[16] application. Got feedback? We'd love to hear your input, reach out to us via ***info@wavefun.com***.

References:

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Last updated April 2026