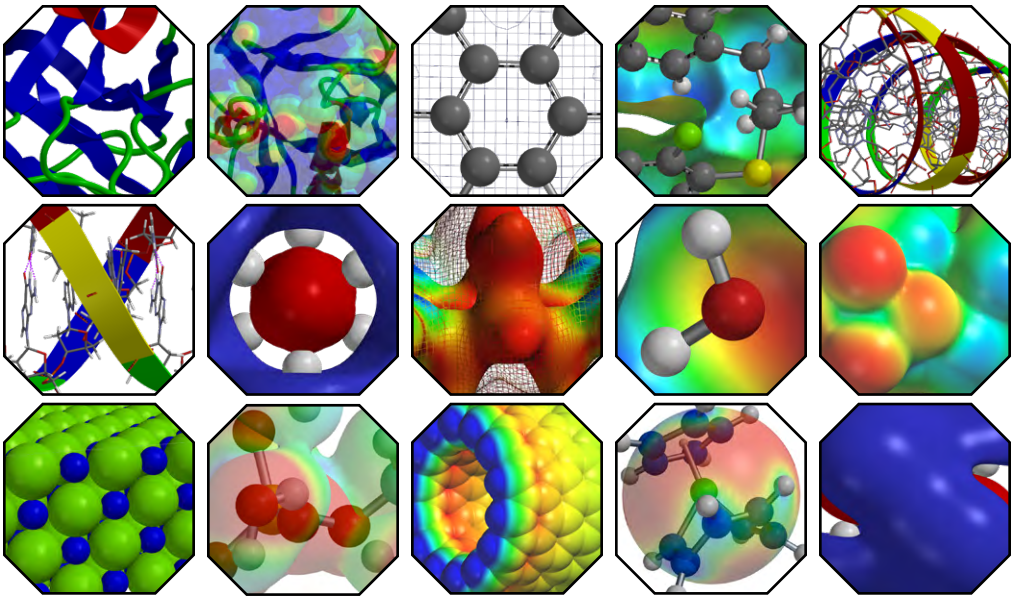
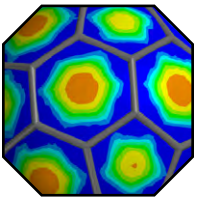
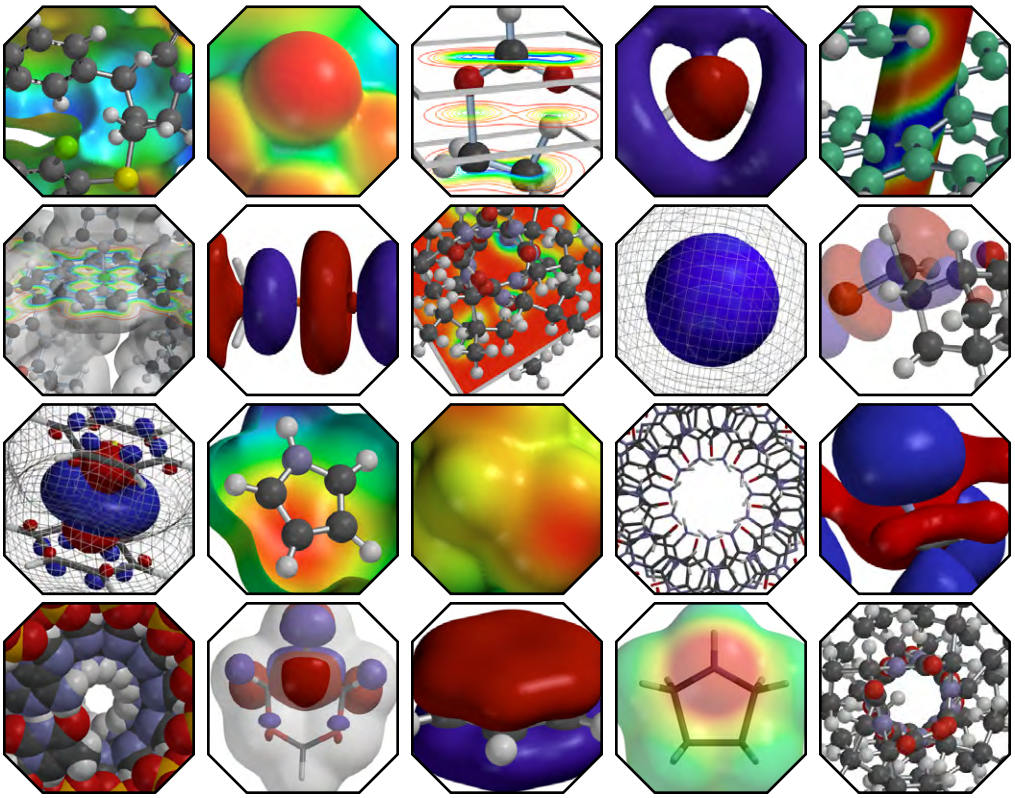


Spartan'26

for Windows, Macintosh and Linux





Spartan'26 is the latest release of the ***Spartan*** molecular modeling application and is a culmination of visualization, computational capabilities, and data interpretation tools, developed and refined since **1991**. New and improved features in ***Spartan'26*** include: An expanded 2D environment allowing access to the vast majority of functionality previously available from 3D only. This release introduces the **NMR Protocol** task (for flexible organic molecules), enabling pre-configured access to two QM and two ML-based predicted NMR workflows. This release builds on the number of tasks supported with ML (neural network models) the present ***Spartan'26*** includes a growing family of 8 unique neural network models, supporting and supplementing a growing set of applications, including:

NMR PROTOCOLS (MULTI-STEP WORKFLOWS)

The multi-step **2019 QM-NMR ("Hehre") protocol**[1] provides high quality predicted ^{13}C shifts for flexible organic molecules. An analogous **MLHF-NMR**[2] machine-learning workflow is now available. The integrated **P2O** (predicted-to-observed) network provides ^{13}C shifts with average MAE of **1.24 ppm** and average RMSE of **1.66 ppm** (based on 420 structures[2] from the natural products literature). ***Spartan*** **MLNMR** results confirm or favor the correct diastereomer **94-100%** of the time (based on analysis of 100 X-ray crystal confirmed structures with 2-11 chiral centers). Average computational times are **under two minutes** per structure.

IMPROVED CONFORMER ENERGY CALCULATIONS: CORRECTED MMFF[3]

Assessment of the widely used MMFF molecular-mechanics approach indicates that while geometries are generally reasonable, the resulting conformer energy differences are often inaccurate. ***Spartan'26*** employs a neural network trained on ωB97X-V/6-311+G(2df,2p)[6-311G*] energy calculations derived from underlying MMFF geometries. This significantly improves the accuracy of underlying conformer energy differences. This saves considerable time by reducing the number of conformers required to obtain reliable Boltzmann distributions.

ESTIMATED DENSITY FUNCTIONAL GEOMETRIES[4]

Spartan'26 provides a neural network routine trained to more than 6 million energy and force calculation from ωB97X-D/6-31G* for molecules ranging from 200-600 AMU. Results return several orders of magnitude faster than the underlying quantum chemical model and assessment suggests a high level of agreement. This routine is also available for use within the multistep NMR Spectrum task and utilized in conformational searching.

IMPROVED CONFORMER ENERGY CALCULATIONS: BOLTZMANN WEIGHTS[5]

Spartan's multi-step protocols for conformation and predicting NMR shifts for flexible organic molecules require accurate Boltzmann weights. In QM workflows these originate from ωB97X-V/6-311+G(2df,2p)//ωB97X-D/6-31G* (or the ωB97M-V or ωB97M(2) models). As even simple organic molecules may access hundreds or thousands of conformers, practical time concerns discourage and limit application. ***Spartan'26*** allows replacement of this step with a neural net trained on the same underlying functionals, substantially reducing the overall computation cost for an NMR calculation.

NMR CALCULATIONS FROM NEURAL NETWORKS[6]

^{1}H and ^{13}C shifts are available from neural networks as well. These were trained from underlying corrected ωB97X-D/6-31G* GIAO results (>33M carbon and 44M proton shifts), and largely reproduce the corrected density functional results, but do so in seconds. An additional P2O neural network further corrects the predicted 13C shifts to experiment, routinely yielding results of 1.6 ppm RMSE, 1.2 ppm MAE).

TRAINING DATA

neural network	# training molecules	# layers	description
DLFF03	≈140 thousand	3 (L+NL)	Corrected MMFF energies
DLFFG1	≈6.0 million	3 (L)	Est. ωB97X-D/6-31G* geometries
DLHF2XD	≈11.0 million	3 (L)	Est. ωB97X-D/6-31G* energies
DLXD2XV	≈310 thousand	3 (L+NL)	Est. ωB97X-V/6-311+G(2df,2p) energies
DLXD2MV	≈300 thousand	3 (L+NL)	Est. ωB97M-V/6-311+G(2df,2p) energies
DLXD2M2	≈280 thousand	3 (L+NL)	Est. ωB97M(2)/6-311+G(2df,2p) energies
DLNMR1	≈2.7 million*	6 (L)	Est. ωB97X-D/6-31G* GIAO NMR shifts

All current neural networks in ***Spartan'26*** were developed with the SpookyNet Learning Forcefield framework and represent hundreds of years of computer time (in training set development).

1. *J. Nat. Prod*. **2019**, 82 (8), 2299–2306. doi: 10.1021/acs.jnatprod.9b00603
2. *ChemRxiv* **2026**. doi: 10.26434/chemrxiv.15001441/v2
3. *J. Comp. Chem*. **2025**, 46 (1), 70016. doi: 10.1002/jcc.70016
4. *J. Chem. Info. Mod*. **2025**, 65 (5), 2314–2321. doi: 10.1021/acs.jcim.4c01898
5. *J. Comp. Chem*. **2025**, 46 (13), 70129. doi: 10.1002/jcc.70129
6. *J. Org. Chem*. **2025**, 90 (32), 11478–11485. doi: 10.1021/acs.joc.5c00927

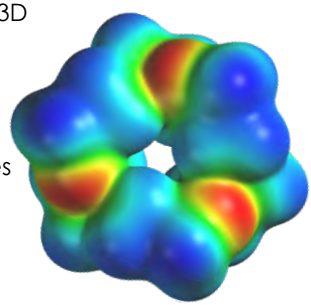
SPARTAN'26 FEATURE SET

GRAPHICAL INTERFACE



Sketch organic, inorganic, organometallic molecules in 2D and automatically convert to 3D structures. Groups, rings and ligands templates are available

Build organic, inorganic and organometallic molecules, peptides and nucleotides, and systematically substituted molecules in 3D



Auto-convert 3D structures to 2D sketches

Link seamlessly to ChemDraw® (Win Only)

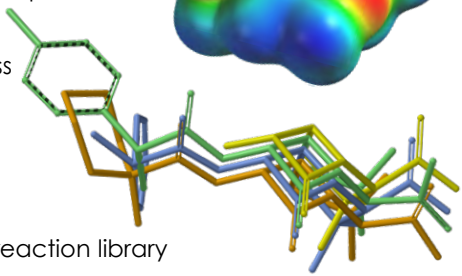
Display/query molecules in a variety of model styles

Display dipole vector, hydrogen bonds, points and planes

Display and customize chemical function descriptors

Display user-defined annotations

New dual (2D/3D) visualization/feature access



Align molecules using structure, chemical function descriptors, or atom labels

Align molecules to pharmacophores

Build transition states using reaction arrows

Generate transition states from an extensive reaction library

Generate lists of regio and stereoisomers and lists of tautomers

Generate and display molecular orbitals, electron densities, spin densities electrostatic potentials, electrostatic potential maps, orbital maps, and local ionization potential maps

Optionally silhouette mesh and transparent surfaces for improved visualization

Generate and display orbital energy diagrams on-the-fly

Input experimental proton and ^{13}C chemical shifts

Toggle between default and absolute property ranges for property maps

Display electron density based on % of enclosed electrons

Highlight solvent accessible regions on surfaces and property maps

Display R/S chirality markers, invert chiral centers and absolute chirality

Automated estimated energies from machine learning routines

Integrated reaction energy calculator

Organize data in spreadsheets

Confirm structure and stereochemistry assignments

Print and save calculated spectra tables as PDF files

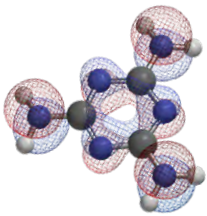
Perform regression analysis and make, save and print 2D or 3D plots

Plot, print, and save calculated and experimental IR, Raman, VCD and UV/vis spectra

Display calculated 1D (proton, ^{13}C, DEPT) and 2D (COSY, HSQC, HMBC) and experimental 1D proton and ^{13}C NMR shifts/spectra (and NICS)

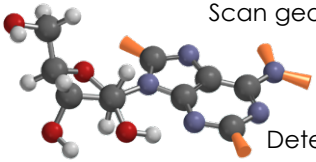
Overlay experimental HMBC and COSY 2D NMR spectra with calculated results

Automatically check and optionally install updates



TASKS

Calculate strain energy, total energy and heat of formation
Determine gas-phase equilibrium and transition-state geometries
Determine geometries and IR spectra in the presence of solvent
Identify global minimum; calculate Boltzmann weights to obtain conformer energy distributions
Build libraries of diverse conformers for use in similarity analysis
Perform similarity analysis on the basis of structure or chemical functionality
Scan geometrical coordinates and generate reaction sequences
Calculate reaction and activation energies
Calculate IR, Raman, UV/vis, VCD, and NMR spectra
Calculate NICS (nucleus-independent chemical shifts)
Determine ^{1}H and ^{13}C shifts with NMR protocols (QM and ML)
Compare calculated and experimental spectra
Search SSPD and NIST experimental database for match to calculated IR spectra
Mine databases of calculated molecular, atomic, and reaction properties



COMPUTATIONAL METHODS

Molecular Mechanics. SYBYL, MMFF94, MMFF(aq)
Corrected MMFF (neural network energy)
Semi-Empirical. MNDO, AM1, RM1, PM3 (with transition metal parameters), PM6
Hartree-Fock molecular orbital theory
Density Functional Theory (functionals available from menus):
GGA functionals: B86PW91, BLYP, BPW91, B97-D2, SOGGA11, PBE-D3, VV10
GH-GGA functionals: B3LYP, B3LYP-D3, EDF2, B3PW91, B97-3, SOGGA11-X
RSH-GGA functionals: ωB97X-D, ωB97X-V, ωB97X, CAM-B3LYP, N12-SX, LC-VV10
mGGA functionals: B97M-V, M06-L, BMK, M11-L, TPSS-D3
GH-mGGA functionals: M06-2X, M06, M08-HX, M08-SO, MPW1B95
RSH-mGGA functionals: M11, ωB97M-V, MN12-SX
DH-RSH-mGGA functionals: ωB97M(2)
Estimated ωB97X-D/6-31G* geometries (neural network structure)
Energies from neural networks trained to ωB97X-D, ωB97M-V, ωB97M(2)
Møller Plesset. MP2, MP3, MP4, and RI-MP2
Wave function based advanced correlated models:
G3(MP2)elect, G3elect, G4elect, QCISD, QCISD(T), CCSD, CCSD(T)
Wave function based advanced correlated methods include CCSD, CCSD(T), OD, OD(T), QCCD, VOD, and VQCCD
Excited-state methods. CIS, CIS(D), RI-CIS(D), QCIS(D), QCISD(T) and TDDFT
Gradients available for CIS, CIS(D) and TDDFT
Thermochemical Recipes. T1, G3(MP2), G3, G4
Basis Sets (available from menus):
Pople: STO-3G, 3-21G, 6-31G*, 6-31G**, 6-31+G**, 6-311G**, 6-311+G**, 6-311G(2d,p), 6-311+G(2d,p), 6-311+G(2df,2p); other variations on 6-31G and 6-311G may be specified. Automatic use of pseudopotentials for elements >Kr
Dunning: cc-pVDZ, aug-cc-pVDZ, cc-pVTZ, aug-cc-pVTZ, cc-pVQZ, aug-cc-pVQZ
Ahlrichs/Weigend: def2-SV(P), def2-SVPD, def2-TZVP, def2-TZVPPD, def2-QZVP, def2-QZVPPD
Dual basis set approximation available

PROPERTIES AND QSAR DESCRIPTORS

Mulliken, natural, and electrostatic-fit charges
Dipole and higher moments, polarizabilities and hyperpolarizabilities
Enthalpies, entropies and free energies
Solvation energies from C-PCM and a number of Truhlar models
Statistical tools for comparing calculated and experimental ^{1}H and ^{13}C NMR shifts
NICS (nucleus-independent chemical shifts)
HOMO, LUMO and SOMO energies
Areas, polar surface areas and volumes based on space-filling models
Areas, accessible areas, polar areas, and volumes based on the electron density
Min/Max of electrostatic potential and Min of local ionization potential
Number of conformers and tautomers
Number of hydrogen bond acceptors and donors

SPECTRA

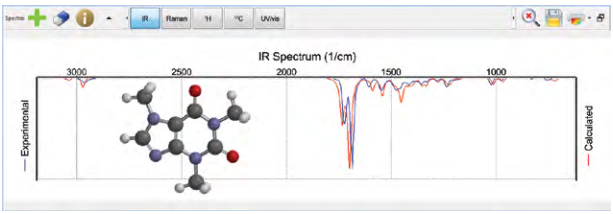
NMR, IR, Raman, VCD and UV/visible spectra are available from a variety of theoretical models including Hartree-Fock and density functional models. Spectra search of experimental IR against calculated IR from the SSPD is supported.

NMR

Corrected, Boltzmann-weighted NMR shifts are available for flexible molecules. ***Spartan'26*** provides neural network routines that *significantly reduce* computational time with high-level accuracy (sub 1.3 MAE ppm for ^{13}C shifts of challenging natural products).

Both empirical and calculated couplings are supported. COSY and NOSY plots are available. NICS may be calculated.

IR AND RAMAN



Infrared (and Raman) frequencies calculated from density functional models are scaled to account for systematic errors associated with the harmonic approximation. Frequencies and intensities are fit to a Lorentzian function with a line width parameter. Alternatively, scale and line width may be adjusted to best fit a spectrum calculated using any theoretical model to an experimental spectrum.

UV/VISIBLE

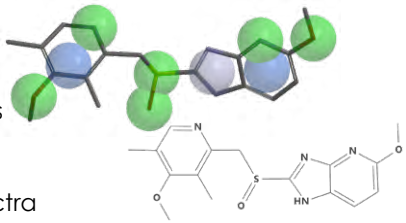
UV/visible spectra are obtained by explicit calculation of the ground state energies and the low-lying excited states. CIS models are paired with Hartree-Fock models. TDDFT (time dependent density functional) models are paired with density functional models.

VCD

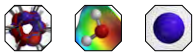
Calculated spectra from QM models (Hartree-Fock and Density Functional) now include Vibrational Circular Dichroism (VCD) spectra. Used to determine the absolute configuration (enantiomer differentiation) of chiral molecules, in conjunction with NMR diastereomer analysis VCD (and upcoming ECD) spectra facilitate assignment of the correct enantiomer.

ADDITIONAL FEATURES

Multi-core parallel processing for HF, DFT, RI-MP2, and thermochemical recipes.
Automatic processing of groups of molecules
Automatic use of molecular symmetry
View recent documents from File menu
Optimize using constraints and/or frozen atoms
NOEs for conformational searching
Identify tautomers and generate tautomer lists
Import experimental IR, Raman, and NMR spectra



Import InChI, SMILES, CDX, CDXML, CIF, SKC, SDF, TGF, XYZ, Macromodel, PDB, SYBYL MOL and MOL2 format
Retrieve structures from Cambridge Structural Database and Protein Data Bank
Extract ligands and binding sites from proteins (PDB files)



DATABASES

Spartan Spectra and Properties Database *(SSPD)*® comprises a collection of 317,000 entries, primarily obtained from the ωB97X-D/6-31G* model. Included are the optimized geometry, the energy and a selection of molecular properties, the wave function (allowing on-the-fly generation of graphical surfaces), and the NMR spectrum. The infrared spectrum is provided from EDF2/6-31G*. SSPD entries can replace user-built structures, both collections are searchable by substructure, name, formula, and isomer.

Spartan Reaction Database *(SRD)*® will comprise transition states for ≈8,000 reactions searchable by combination of substructure and "reaction arrows" from either 2D sketches or 3D models.

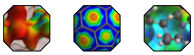
6-311+G(2df,2p) ENERGY DATABASES

SSPD entries now include three highly accurate density functional databases, comprised of ≈250,000 ωB97X-V/6-311+G(2df,2p) and ωB97M-V/6-311+G(2df,2p), and ≈200,000 ωB97M(2)/6-31+G(2df,2p) energies, from underlying ωB97X-D/6-31G* geometries.

CORRECTED MMFF ENERGIES

Access extremely fast ω**B97X-D/6-311+G(2df,2p)[6-311G*]//MMFF** energy approximation for use in conformational energy comparisons from a new machine learning routine.

ESTIMATED DENSITY FUNCTIONAL STRUCTURES



Machine learning routine provides estimated ω**B97X-D/6-31G*** structures from MMFF geometries, at something like 1-2 orders of magnitude faster than structures derived from quantum mechanics.

ESTIMATED QM ENERGIES

Machine learning routines start from ωB97X-D/6-31G* structures and instantly provide estimated ω**B97X-V**, ω**B97M-V**, and ω**B97M(2)** [all trained with the **6-311+G(2df,2p)** basis set] for improved energies at several orders of magnitude faster than they can be calculated from quantum mechanics.

SPARTAN'26 LICENSING*

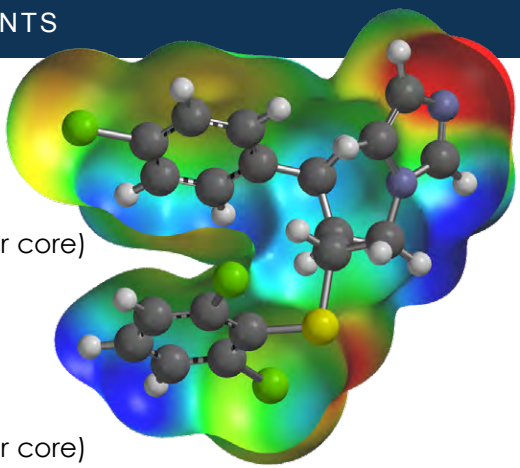
	Academic	Government	Commercial
Spartan'26* (up to 16 cores)*	$ 1,800	$ 3,600	$ 5,400
Spartan'26* (greater than 16 cores)*	$ 2,700	$ 5,400	$ 8,100

Academic Lab Pricing	***Spartan'26 Parallel Suite***
5 Seat Lab License	$ 7,650
10 Seat Lab License	$ 13,500
20 Seat Lab License	$ 18,000

New licensing includes one year of maintenance, providing for the full SSPD, all minor and major version updates, any necessary license transfers, and priority technical support.

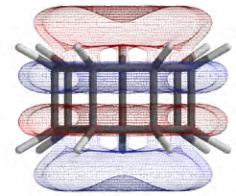
* *Annual campus-wide licensing available, contact* ***sales@wavefun.com*** *for pricing.*
** ***Spartan'26*** *parallel processing is available for up to 16 cores (standard), or as a greater than 16 core license for HPC systems (license covers unlimited cores per workstation/server).*

MINIMUM SYSTEM REQUIREMENTS



WINDOWS
- Intel or AMD (64-bit only)
- Windows 11
- 128 GB disk space or higher (SSD recommended)
- 4 GB of RAM (at least 2GB RAM per core)

MACINTOSH
- Mx chip (only)
- MacOS Monterey 12.7 – Tahoe 26
- 128 GB disk space or higher (SSD recommended)
- 4 GB RAM (at least 2GB of RAM per core)



LINUX
- Modern Intel or AMD Processors (64-bit only)
- RHEL 8/9/10, Rocky Linux 9/10, AlmaLinux 9/10, Ubuntu LTS (22.04, 24.04, 26.04)
- 128 GB disk space or higher (SSD recommended)
- 4 GB RAM (at least 2GB of RAM per core)

Spartan'26
for Windows, Macintosh and Linux
is a collaboration with Q-CHEM

WAVEFUNCTION, INC.
18401 Von Karman Ave., Suite 435
Irvine, CA 92612 U.S.A.
(949) 955-2118 fax
sales@wavefun.com
www.wavefun.com

WAVEFUNCTION, INC.,
JAPAN BRANCH OFFICE
3-5-2, Kouji-machi, Suite 608
Chiyoda-ku, Tokyo, Japan 102-0083
japan@wavefun.com
www.wavefun.com/japan