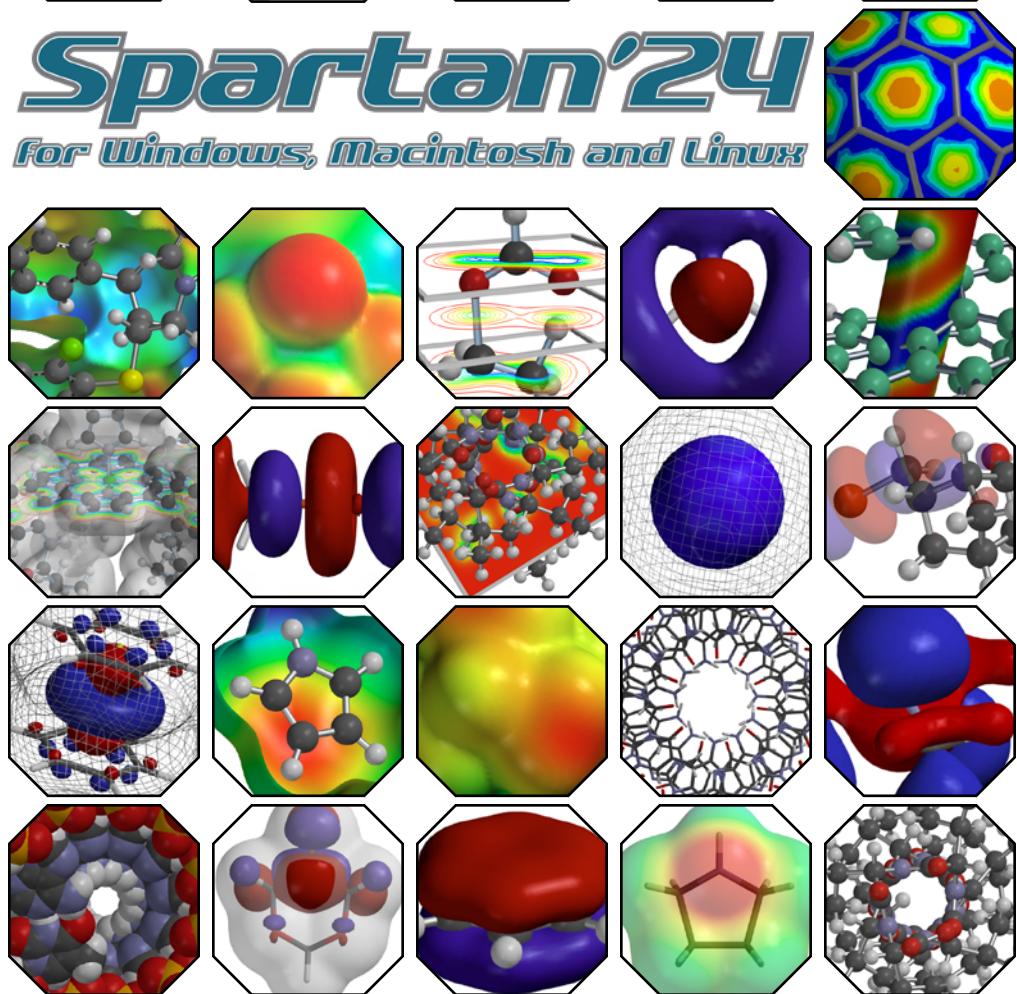


Spartan'24

for Windows, Macintosh and Linux



Spartan'24 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'24** include: databasing tools to allow users to easily construct their own data collection with compatibility to the (>317k entry) Spartan Spectra & Properties Database. This release is also the first to incorporate computational models developed using Machine Learning technology. **Spartan'24** introduces a set of 7 unique neural network models, supporting a growing set of applications, including:



IMPROVED CONFORMER ENERGY CALCULATIONS: CORRECTED MMFF¹

Assessment of the widely used MMFF molecular mechanics approach in conformational searching suggests that resulting conformer energy differences are not very accurate. **Spartan'24** employs a neural network model that has been trained on ω B97X-V/6-311+G(2df,2p)[6-311G*] energy calculations from underlying MMFF geometries. In practice, as each MMFF conformer is generated its energy is corrected with a neural network to obtain a "better" energy. This significantly improves accuracy and reduces the number of conformers that need to be considered with better approaches (in **Spartan's** multi-step protocols for conformer distribution and the NMR spectra task).



ESTIMATED DENSITY FUNCTIONAL GEOMETRIES²

Spartan'24 provides a neural network routine trained to more than 6 million energy and force calculation from ω B97X-D/6-31G* for molecules ranging from 200-600 AMU. Results return several orders of magnitudes faster than the underlying quantum chemical model and assessment suggests a high level of agreement. This routine is *also* available for use within the multi-step NMR Spectrum task and utilized in conformational searching.



IMPROVED CONFORMER ENERGY CALCULATIONS: BOLTZMANN WEIGHTS

The penultimate and most costly step in the **Spartan's** multi-step protocols for conformer searching and for calculating the NMR spectrum of a flexible molecule involve determining Boltzmann weights for all accessible conformers using the ω B97X-V/6-311+G(2df,2p)// ω B97X-D/6-31G* model. As even simple organic molecules may access hundreds or thousands of conformers, practical time concerns discourage and limit application. **Spartan'24** allows replacement of this step with a neural net trained on ω B97X-V/6-311+G(2df,2p) energy calculations from underlying ω B97X-D/6-31G* structures, cutting the overall computation cost for an NMR calculation by more than half.

IMPROVED ENERGY CALCULATIONS



It is generally accepted that better (more complicated) functionals and larger (more flexible) basis sets will lead to significantly improved reaction energies, but at a significant increase in computation cost. Three functionals ω B97X-V, ω B97M-V and ω B97M(2) with 6-311+G(2df,2p) using ω B97X-D/6-31G* geometries, closely approach the results of CCSD(T) calculations, the “gold standard”. **Spartan’24** incorporates three neural nets that estimate total energies from the above models starting from ω B97X-D/6-31G* geometries with rms errors of only a few kJ/mol. Practically speaking, this extends the size of systems that can be routinely submitted from a few hundred to well over molecular weight 1000 amu.

MULTI-STEP WORKFLOWS



Collectively, the machine learning models are available in most of **Spartan’24**’s available computational tasks, including: **Energy**, **Equilibrium Geometry**, **Equilibrium Conformer**, **Conformer Distribution**, and the Boltzmann Weighted **NMR Spectrum** task³. In particular, the multi-step conformational searching components are available at orders of magnitude faster than the same tasks run with pure quantum chemical models.

TRAINING DATA

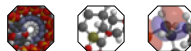


SpookyNet⁴ has been used to generate the initial five neural networks. Data sets comprise ≈ 150 k molecules with ≈ 1.8 million conformers obtained from ω **B97X-V/6-311+G(2df,2p)[6-311G*]**//**MMFF** calculations for the MMFF correction neural net. Collections of $\approx 120,000$ molecules each with equilibrium geometries and 50 distorted geometries (a total of ≈ 6.1 million structures) obtained from ω **B97X-D/6-31G*** calculations for the estimated ω **B97X-D/6-31G*** geometry neural net, $\approx 250,000$ molecules obtained from ω **B97X-V/6-311+G(2df,2p)**// ω **B97X-D/6-31G*** calculations for the estimated ω **B97X-V/6-311+G(2df,2p)** energy neural net, $\approx 250,000$ molecules obtained from ω **B97M-V/6-311+G(2df,2p)**// ω **B97X-D/6-31G*** calculations for the estimated ω **B97M-V/6-311+G(2df,2p)** energy neural net, and $\approx 200,000$ molecules obtained from ω **B97M(2)/6-311+G(2df,2p)**// ω **B97X-D/6-31G*** calculations for the estimated ω **B97M(2)/6-311+G(2df,2p)** energy neural net. Training sets for all three of the final energy neural networks ω **B97X-V/6-311+G(2df,2p)**, ω **B97M-V/6-311+G(2df,2p)**, ω **B97M(2)/6-311+G(2df,2p)** will soon be searchable from within **Spartan** from the **Databases** dialog (searches available via substructure, formula, isomer, molecular weight, and name).

1. *J. Comp. Chem.* **2025**, 46, 1, 70016.
2. *J. Chem. Inf. Model.* **2025**, 65(5), 2314-2321.
3. *J. Nat. Prod.* **2019**, 82 8, 2299-2306.
4. *Nat. Commun.* **2021**, 12(1), 1-14.

SPARTAN'24 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

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

Input observed 3-bond HH couplings and 2 and 3-bond CH couplings for superposition onto calculated COSY and HMBC plots

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

Print and save calculated spectra tables as PDF files

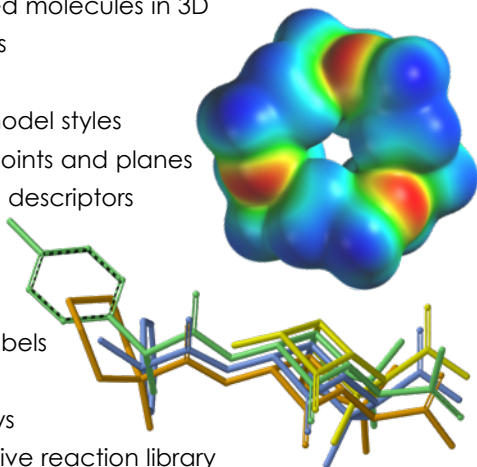
Perform regression analysis and make, save and print 2D or 3D plots

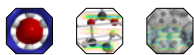
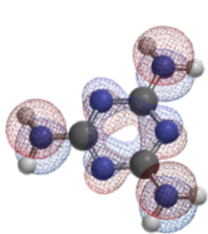
Plot, print, and save calculated and experimental IR, Raman, and UV/vis spectra

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

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

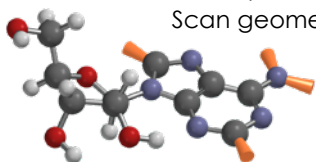
Calculate IR, Raman, UV/vis, and NMR spectra

Determine NMR spectra for flexible molecules

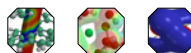
Compare calculated and experimental spectra

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: ω B97X-D, ω B97X-V, ω B97X, 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, ω B97M-V, MN12-SX

DH-RSH-mGGA functionals: ω B97M(2)

Estimated ω B97X-D/6-31G* geometries (neural network structure)

Energies from neural networks trained to ω B97X-D, ω B97M-V, ω B97M(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):

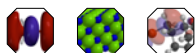
Pople: STO-3G, 3-21G, 6-31G*, 6-31G**, 6-31+G**, 6-311G**, 6-311+G**, 6-311G(2d,p), 6-311+G(2d,p), 6-311+G(2df,2p), 6-311+G(3df,2p); other variations on 6-31G and 6-311G may be specified

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

Automatic use of pseudopotentials for elements >Kr

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 ^1H and ^{13}C NMR 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 and UV/visible spectra may be calculated using a variety of theoretical models including Hartree-Fock and density functional models. IR spectra of an unknown molecule may be searched against the SSPD entries for best match.

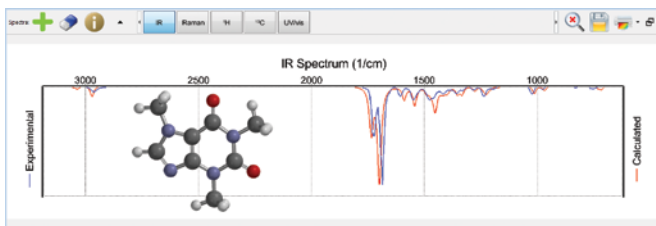
NMR

Corrected, Boltzmann-weighted NMR shifts are available for flexible molecules. **Spartan'24** provides neural network routines that *significantly reduce* computational time.

Three-bond HH, CH, and CC coupling constants [using the B3LYP functional with PCJ-0 (PCJ-1 and PCJ-2 basis sets are also available)] allow for ^1H , ^{13}C and DEPT 1D spectra and COSY, HSQC and HMBC 2D spectra. Proton spectra may be displayed with or without HH coupling. Observed HH and CH couplings may be inputted to construct "experimental" COSY and HMBC plots which can then be superimposed onto calculated plots.

IR AND RAMAN

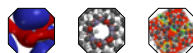
Infrared (and Raman) frequencies calculated from $\omega\text{B97X-D/6-31G}^*$, B3LYP/6-31G* and EDF2/6-31G* density functional models are scaled to account for systematic errors associated with the harmonic approximation. Frequencies and intensities are fit to a Lorentzian function with a line width 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.

ADDITIONAL FEATURES



Multi-core parallel processing for Hartree-Fock, density functional, 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

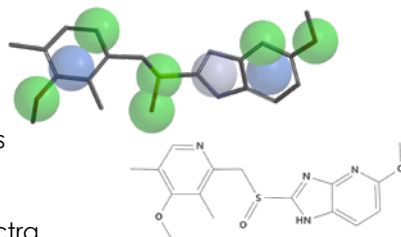
Identify tautomers and generate tautomer lists

Import experimental IR, Raman, and NMR spectra

Import structures in InChI, SMILES, CDX, 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)

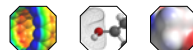


DATABASES

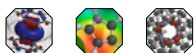
Spartan Spectra and Properties Database (SSPD)[®] comprises a collection of 317,000 entries, primarily obtained from the ω B97X-D/6-31G* model. Included are the optimized geometry, the energy and a selection of molecular properties, the wave function (allowing on-the-fly generation of graphical surfaces), 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 $\approx 8,000$ reactions searchable by combination of substructure and "reaction arrows" from either 2D sketches or 3D models.

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



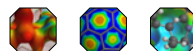
SSPD entries now include three highly accurate density functional databases, comprised of $\approx 250,000$ ω B97X-V/6-311+G(2df,2p) and ω B97M-V/6-311+G(2df,2p), and $\approx 200,000$ ω B97M(2)/6-31+G(2df,2p) energies, from underlying ω B97X-D/6-31G* geometries.



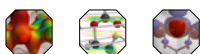
CORRECTED MMFF ENERGIES

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 ω B97X-D/6-31G* structures and instantly provides 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.

	Academic	Government	Commercial
Spartan'24 (up to 16 cores)**	\$ 1,800	\$ 3,600	\$ 5,400
Spartan'24 (greater than 16 cores)**	\$ 2,700	\$ 5,400	\$ 8,100

Academic Lab Pricing

- 5 Seat Lab License**
10 Seat Lab License
20 Seat Lab License

Spartan'24 Parallel Suite

- \$ 7,650
 \$ 13,500
 \$ 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 site license available, contact sales@wavefun.com for pricing.

** **Spartan'24** provides parallel processing for select methods and tasks and is available for up to 16 cores (standard), or as a greater than 16 core license (for HPC systems). **Spartan** also includes access to the **Spartan Spectra and Properties Database (SSPD)**, and the ability to act as a computation server for other **Spartan** licenses or the **iSpartan** app.

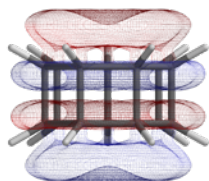
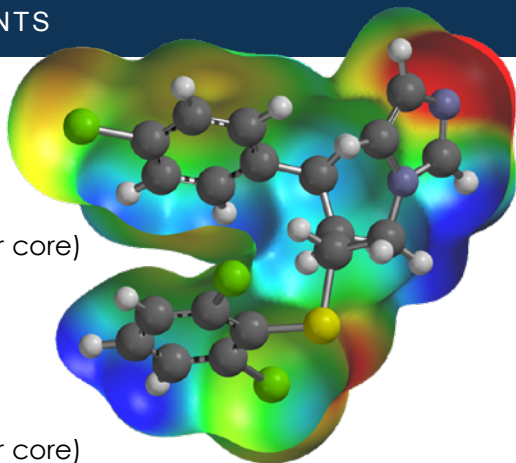
MINIMUM SYSTEM REQUIREMENTS

WINDOWS

- Intel or AMD (64-bit only)
- Windows 10 or 11
- 128 GB disk space or higher (SSD recommended)
- 4 GB of RAM (at least 2GB RAM per core)

MACINTOSH

- Intel or M1 chips (only)
- OS X 11 (Big Sur) - 15.X (Sequoia)
- 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)
- Linux RHEL 8, CentOS 8, Ubuntu 20.04 LTS
- 128 GB disk space or higher (SSD recommended)
- 4 GB RAM (at least 2GB of RAM per core)

Spartan'24
 for Windows, Macintosh and Linux

is a collaboration with **Q-CHEM**
a Quantum Theory 900, Inc. Company

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