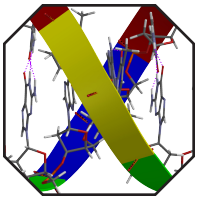
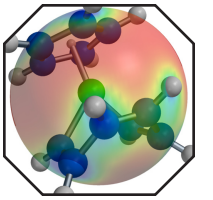
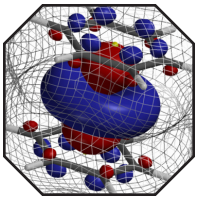


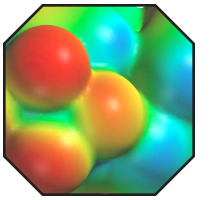
Spartan'24

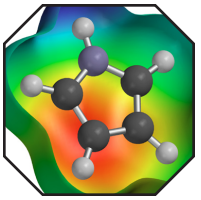
for Windows, Macintosh and Linux

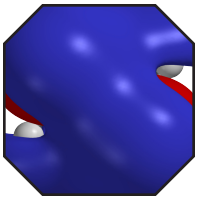


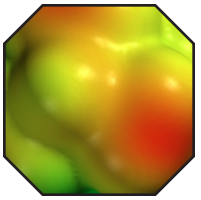


Spartan'24 is the latest release of the ***Spartan*** molecular modeling application and is a culmination of visualization, computational capabilities, and data interpretation tools, developed and refined since **1991**. New and improved features in ***Spartan'24*** include: extension to the Spartan Spectra & Properties Database (>313,000 molecules and growing), as well as a new SSPD compatibility task, enabling a single submitted task so users can easily expand their local SSPD to include molecules of specific interest. The underlying Q-Chem computation code will be updated to the latest (v.6.1). This release is also the first (but we suspect not the last) to incorporate AI in the form of neural network models for four initial applications.

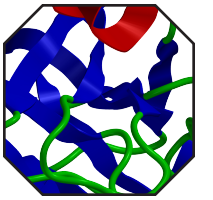




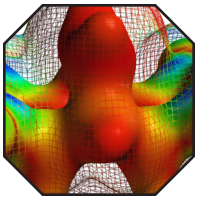


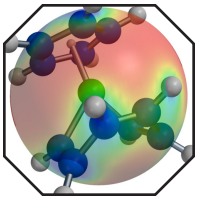


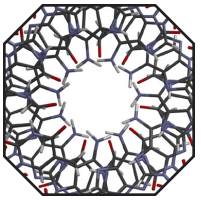
IMPROVED CONFORMER ENERGY CALCULATIONS: MOLECULAR MECHANICS

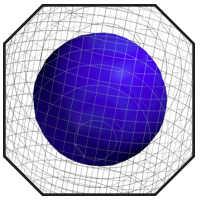


Assessment of the widely used MMFF molecular mechanics approach in conformational searching suggests that resulting conformer energy differences are not very accurate. ***Spartan'24*** employs a neural network model that has been trained on ωB97X-V/6-311+G(2df,2p) energy calculations from underlying MMFF geometries. In practice, as each MMFF conformer is generated its energy is corrected with a neural net to obtain a "better" energy. The procedure is only slightly more costly than the underlying MMFF calculation itself, but greatly 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).

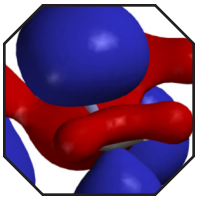




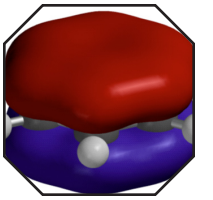


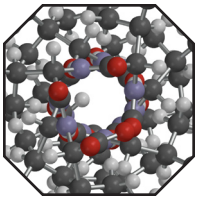


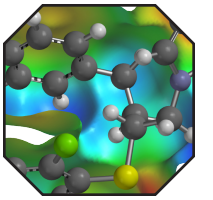
IMPROVED CONFORMER ENERGY CALCULATIONS: BOLTZMANN WEIGHTS

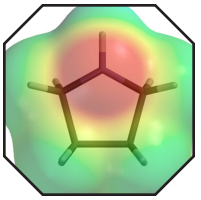


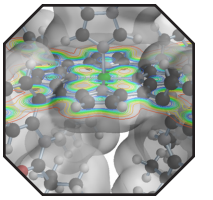
The penultimate and most costly step in the ***Spartan's*** multi-step protocols for conformer searching and for calculating the NMR spectrum of a flexible molecule involve determining Boltzmann weights for all accessible conformers using the ωB97X-V/6-311+G(2df,2p)//ωB97X-D/6-31G* model. As even simple 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 ωB97X-V/6-311+G(2df,2p) energy calculations from underlying ωB97X-D/6-31G* structures, cutting the overall computation cost for an NMR calculation by more than half.



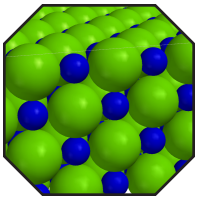




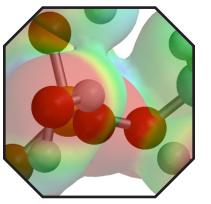




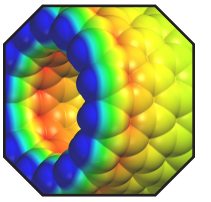
IMPROVED ENERGY CALCULATIONS



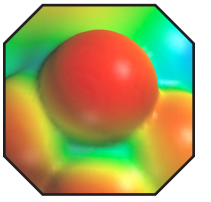
It is generally accepted that better (more complicated) functionals and larger (more flexible) basis sets will lead to significantly improved reaction energies, but at a significant increase in computation cost. Two models ωB97X-V/6-311+G(2df,2p) and ωB97M-V/6-311+G(2df,2p) using ωB97X-D/6-31G* geometries have been shown to closely approach the results of CCSD(T) calculations, the "gold standard". ***Spartan'24*** incorporates two neural nets that predict total energies for ωB97X-V/6-311+G(2df,2p) and ωB97M-V/6-311+G(2df,2p) models starting from ωB97X-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.

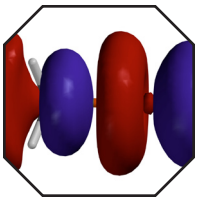


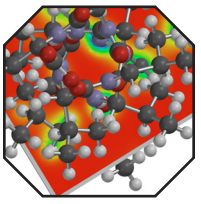
POLARIZATION ENERGIES FROM SOLVENT

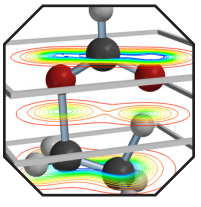


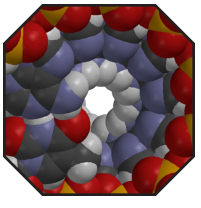
Spartan'24 also includes neural network models trained to reproduce energies obtained from the CPCM solvent model (the current default solvent model) for chloroform, THF, DMSO and methanol.











MINIMUM SYSTEM REQUIREMENTS

Initial Release - Fall 2023

WINDOWS

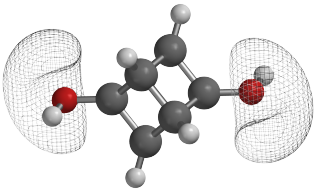
Intel or AMD (64-bit only)
Windows 10 and 11
256 GB disk space or higher
(SSD recommended)
8 GB of RAM
2GB per core
(up to 16 GB recommended)

MACINTOSH

Intel or Apple Silicon chips (only)
OS X 10.14.6 (Mojave) - 13.X (Ventura)
256 GB disk space or higher
(SSD recommended)
8 GB RAM - Apple Silicon
2GB per core
(up to 16GB - Intel)

LINUX

Intel or AMD Processors (64-bit only)
Linux RHEL 8, CentOS 8, Ubuntu 20.04 and 22.04 LTS
256 GB disk space or higher (SSD recommended)
8 GB per core (up to 16 recommended)



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Spartan'24
for Windows, Macintosh and Linux

is a collaboration with Q-CHEM

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