

Research applications utilizing **Spartan** in:

- **Machine Learning / Neural Network model development**
- **Machine Learning model Assessment/Application**

● ● ● Bo Qin, Alex Szypererek, Martin Tomanik*, Total Synthesis of the Nominal Structure of (+)-Talaromyolide D. *J. Am. Chem. Soc.* **2025**, 147, 34, 31221–31227.
<https://doi.org/10.1021/jacs.5c10325> [open access]

● ● ● Wim Buijs*, A Molecular Modeling Case Study on the Thermodynamic Partition of DIPNs Derived from Naphthalene and C3-Sources Using Non-Shape-Selective Acid Catalysts. *Molecules*. **2025**, 30 3606. <https://doi.org/10.3390/molecules30173606> [open access]

● ● Thomas Hehre, Philip E. Klunzinger, Bernard J. Deppmeier, William Sean Ohlinger, Warren J Hehre*, Practical Machine Learning Strategies 4: Using Neural Networks to Replicate Proton and ¹³C NMR Chemical Shifts Obtained from ωB97X-D/6-31G* Density Functional Calculations. *J. Org. Chem.* **2025**, 90, 32, 11478-11485. <https://pubs.acs.org/doi/10.1021/acs.joc.5c00927>
[wavefunction article]

● ● Philip Klunzinger, Thomas Hehre, Bernard Deppmeier, William Ohlinger, Warren Hehre*, Practical Machine Learning Strategies. 2. Accurate Prediction of ωB97X-V/6-311+G(2df,2p), ωB97M-V/6-311+G(2df,2p) and ωB97M(2)/6-311+G(2df,2p) Energies From Neural Networks Trained From ωB97X-D/6-31G* Equilibrium Geometries and Energies. *J. Comp. Chem.* **2025**, 46(13), 70129.
<https://doi.org/10.1002/jcc.70129> [wavefunction article]

● ● ● Thomas Hehre, Philip Klunzinger, Bernard Deppmeier, William Ohlinger, and Warren Hehre*, Accurate Prediction of ωB97X-D/6-31G* Equilibrium Geometries from a Neural Net Starting from Merck Molecular Force Field (MMFF) Molecular Mechanics Geometries. *J. Chem. Info. Mod.*, **2025**, 65, 5, 2314-2321. <https://doi.org/10.1021/acs.jcim.4c01898> [wavefunction article]

● ● Derek T. Ahneman, Jesus G. Estrada, Shishi Lin, Spencer D. Dreher*, Abigail G. Doyle*, Predicting reaction performance in C-N cross-coupling using machine learning. *Science*, **2018**, 6385(360), 186-190. <https://doi.org/10.1126/science.aar5169>