

Recent Research applications utilizing **Spartan** in:

- Geometry optimization
- Energy calculation/comparison
- QSAR applications

● ● ● Muhammad Qasid, Maleah A. Pfeiffer, Cameron J. Jeffries, Lauren F. Hornbrook, Gordon H. Purser, and Angus A. Lamar*, Organocatalytic Halogenation of Indazoles and Pyrazoles with N-Halosuccinimides Enhanced by Gallocyanine as Halogen-Transfer Agent. *J. Org. Chem.* **2025**, Articles ASAP, <https://doi.org/10.1021/acs.joc.5c01711>

● ● ● 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]

● ● ● Tevhide Ayça Yıldız, İbrahim Deneme, Hakan Usta*, Achieving Extreme Solubility and Green Solvent-Processed Organic Field-Effect Transistors: A Viable Asymmetric Functionalization of [1]Benzothieno[3,2-b][1] benzothiophenes. *ACS Appl. Mater. Interfaces* **2025**, 17, 35, 49720–49736. <https://doi.org/10.1021/acsami.5c12618> [open access]

● ● ● Muhammadiqbolı Musozoda, Richard A. O'Brien, Zachary J. Metott, Raychell A. Jerdo, Christopher M. Butch, Matthias Zeller, Gregory R. Boyce*, Patrick C. Hillesheim*, and Arsalan Mirjafari*, Lipid-Inspired Low Melting Ionic Liquids via Synergistic Cyclopropanation and Branching of Terpenoids. *ACS Mater. Au* **2025**, 5, 5, 878–885. <https://doi.org/10.1021/acsmaterialsau.5c00089> [open access]

● ● Samantha J. Kruse, Tori Z. Forbes, and Leonard R. MacGillivray*, Effects of Ionizing Radiation on Halogen-Bonded Dipyrıdyl-Naphthalenediimide Cocrystals. *Cryst. Growth Des.* **2025**, 25, 13, 4968–4973. <https://doi.org/10.1021/acs.cgd.5c00441> [open access]

● ● 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]

Philip Klunzinger, Thomas Hehre, Bernard Deppmeier, William Ohlinger, Warren Hehre*, Practical Machine Learning Strategies. 2. Accurate Prediction of ω B97X-V/6-311+G(2df,2p), ω B97M-V/6-311+G(2df,2p) and ω B97M(2)/6-311+G(2df,2p) Energies From Neural Networks Trained From ω B97X-D/6-31G* Equilibrium Geometries and Energies. *J. Comp. Chem.* **2025**, 46(13), 70129. <https://doi.org/10.1002/jcc.70129> [wavefunction article]

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