

Recent Research applications utilizing **Spartan** in:

● **NMR Chemical Shifts**

● **Structure Assignment/Reassignment**

● ● 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]

● ● Noah M. Bartfield, Brandon W. Alexander, Seth B. Herzon. Total Synthesis of Chartelline C. *J. Am. Chem. Soc.* **2025**, 147 (28) , 24921-24931. <https://doi.org/10.1021/jacs.5c07148>

● ● Kanji Niwa, David A. Delgadillo, Danielle A. Yee, Chuhang Luo, Flora Fan, Kunal K. Jha, Hosea M. Nelson, and Yi Tang*. Genome Mining of Fungal Aza-Polycyclic Natural Products Derived from Arginine-Containing Cyclodipeptides. *J. Nat. Prod.* **2025**, 88, 1506–1513.

<https://pubs.acs.org/doi/10.1021/acs.jnatprod.5c00455> [available online]

● ● Fatemeh Haghighi, Luke T. Jesikiewicz, Corrinne E. Stahl, Jordan Nafie, Amanda Ortega-Vega, Peng Liu*, Kay M. Brummond*, Stereo-Differentiating Asymmetric Rh(I)-Catalyzed Pauson–Khand Reaction: A DFT-Informed Approach to Thapsigargin Stereoisomers. *J. Am Chem. Soc.* **2025**, 147, 498-509. <https://doi.org/10.1021/jacs.4c11661>

[open access]

● Shu-Rong Chen, Yang-Chen Chang, Yi Chen, Yih-Fung Chen, Yu-Chi Lin, Cheng-chau Chiu, Yuan-Bin Cheng*, Discovery of Zoanthamine Alkaloids from *Zoanthus vietnamensis* with Antioxidant and Neuroprotective Activities. *J. Org. Chem.* **2025**, 90, 14, 5019-5035.

<https://doi.org/10.1021/acs.joc.5c00280> [open access]

● Dan Chen, Florent Rouvier, Robert Keyzers, Marie-Lise Bourguet-Kondracki, Jean Michel Brunel, Melissa M. Cadelis, and Brent R. Copp*, Ohauamines A–D, Structurally Unprecedented Tricyclic Depsi-tripeptides from the New Zealand Ascidian *Pycnoclavella kottae*. *J. Nat. Prod.* **2025**, 88, 3, 871-876. <https://doi.org/10.1021/acs.jnatprod.5c00033>



Thomas Hehre, Philip E. Klunzinger, Bernard Deppmeier, William Ohlinger, Warren Hehre*, Practical Machine Learning Strategies I. Correcting MMFF Molecular Mechanics Model to More Accurately Provide Conformational Energy Differences in Flexible Organic Molecules. *J. Comp. Chem.* **2025**, 46(1), 70016. <https://doi.org/10.1002/jcc.70016> [wavefunction article]



Brandon W. Alexander, Noah M. Bartfield, Vaani Gupta, Brandon Q. Mercado, Mark Del Campo, Seth B. Herzon*, An oxidative photocyclization approach to the synthesis of Securiflustra *securifrons* alkaloids. *Science*. **2024**, 383, 849-854. <https://doi.org/10.1126/science.adl6163>



Fatemeh Haghighi, Luke T. Jesikiewicz, Corrinne E. Stahl, Jordan Nafie, Amanda Ortega-Vega, Peng Liu*, Kay M. Brummond*, Stereo-Differentiating Asymmetric Rh(I)-Catalyzed Pauson–Khand Reaction: A DFT-Informed Approach to Thapsigargin Stereoisomers. *J. Am Chem. Soc.* **2025**, 147, 498-509. <https://doi.org/10.1021/jacs.4c11661> [open access]



Benita Barton*, Cedric W McClelland*, Mino R Caira*, Muhammad-Ameen Adam, and Eric C Hosten. Host-Guest Complexations of a Diastereoisomeric Mixture of cis-and trans-1,4-Bis (diphenylhydroxymethyl) cyclohexane in Pyridine and Methylpyridine Solutions: Significant Inclusion Selectivities and an Uncommon Host Conformation. *Cryst. Growth Des.* **2024**, 24, 8528-8543. <https://doi.org/10.1021/acs.cgd.4c01041> [open access]



Manuel Rangel-Grimaldo, Cody E. Earp, Huzefa A. Raja, Jared S. Wood, Lina Mardiana, Kin Lok Ho, Alexandra Longcake, R. Thomas Williamson, Lukáš Palatinus, Michael J. Hall, Michael R. Probert, and Nicholas H. Oberlies*, Wheldone Revisited: Structure Revision Via DFT-GIAO Chemical Shift Calculations, 1,1-HD-ADEQUATE NMR Spectroscopy, and X-ray Crystallography Studies. *J. Nat. Prod.* **2024**, 87, 2095-2100. <https://doi.org/10.1021/acs.jnatprod.4c00649> [open access]



Novriyandi Hanif*, Berlian Safriana Nuraulia, William Sean Ohlinger, Trianda Ayuning Tyas, Henny Dwi Yanti, Fabians Faisal Dinelsa, Dudi Tohir, Andi Setiawan, Anggia Murni, Junichi Tanaka. Stereochemical assignment of varicosenone, a merosteroid flexible side chain, from the Indonesian sea slug *Phyllidia varicosa* using NMR and DFT-based NMR calculations. *J. Appl. Pharm. Sci.* **2024**, 14(05), 240-244. <https://dx.doi.org/10.7324/JAPS.2024.172377> [open access] [wavefunction authors]



Brandon W. Alexander, Noah M. Bartfield, Vaani Gupta, Brandon Q. Mercado, Mark Del Campo, Seth B. Herzon*, An oxidative photocyclization approach to the synthesis of Securiflustra *securifrons* alkaloids. *Science*. **2024**, 383, 849-854. <https://doi.org/10.1126/science.adl6163>