

Selection of research articles utilizing *Spartan* software:

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://www.science.org/doi/10.1126/science.adl6163>

Hugo A. Sanchez-Martinez, Juan A. Moran-Pinzon, Esther del Olmo Fernandez, David Lopez Eguiluz, Jose F. Adserias Vistue, Jose L. Lopez-Perez,* and Estela Guerrero De Leon*. Synergistic Combination of NAPROC-13 and NMR ¹³C DFT Calculations: A Powerful Approach for Revising the Structure of Natural Products. *J. Nat. Prod.* **2023**, 86, 2252–2261. <https://pubs.acs.org/doi/10.1021/acs.jnatprod.3c00437>

Otso Peräkylä,*Torsten Berndt, Lauri Franzon, Galib Hasan, Melissa Meder, Rashid R. Valiev, Christopher David Daub, Jonathan G. Varelas, Franz M. Geiger, Regan J. Thomson, Matti Rissanen, Theo Kurtén, and Mikael Ehn*. Large Gas-Phase Source of Esters and Other Accretion Products in the Atmosphere. *J. Am. Chem. Soc.* **2023**, 145, 7780–7790. <https://pubs.acs.org/doi/10.1021/jacs.2c10398>

Maja Lopandic, Fatima Merza, and John F. Honek*. Thermodynamic Overview of Bioconjugation Reactions Pertinent to Lysine and Cysteine Peptide and Protein Residues. *Compounds* **2023**, 3, 464–503. <https://www.mdpi.com/2673-6918/3/3/35>

Monika Warzecha, Graeme Morris, Andrew J. McLean, Jesus Calvo-Castro*, and Callum J. McHugh*. Detection of Nitroaromatic and Peroxide-Based Explosives with Amine- and Phosphine-Functionalized Diketopyrrolopyrroles. *ACS Appl. Mater. Interfaces* **2023**, 15, 23, 27915–27927. <https://pubs.acs.org/doi/10.1021/acsami.3c02714>

Maria Karlsson, Joakim Romson, Thomas Elder, Åsa Emmer*, and Martin Lawoko*. Lignin Structure and Reactivity in the Organosolv Process Studied by NMR Spectroscopy, Mass Spectrometry, and Density Functional Theory. *Biomacromolecules* **2023**, 24, 5, 2314–2326. <https://pubs.acs.org/doi/10.1021/acs.biomac.3c00186>

Estela Guerrero De Leon, Hugo Sanchez-Martinez, Juan A. Moran-Pinzon, Esther del Olmo Fernandez, and Jose L. Lopez-Perez*. Computational Structural Revision of Elaeophorbate and Other Triterpenoids with the Help of NAPROC-13. A New Strategy for Structural Revision of Natural Products. *J. Nat. Prod.* **2023**, 86, 897–908. <https://pubs.acs.org/doi/abs/10.1021/acs.jnatprod.2c01135>

K. J. Winchell, Patrick Y. Yee, Yolanda L. Li, Alexander F. Simafranca, Julia Chang, Christian Beren, Xinyu Liu, Diego Garcia Vidales, Robert J. Thompson, Charlene Z. Salamat, Quynh M. Duong, Robert S. Jordan, Benjamin J. Schwartz, William M. Gelbart, Yves Rubin*, and Sarah H. Tolbert*. Designing Amphiphilic Conjugated Polyelectrolytes for Self-Assembly into Straight-Chain Rod-like Micelles. *Macromolecules* **2023**, 56, 8, 3160–3170. <https://pubs.acs.org/doi/10.1021/acs.macromol.2c02057>

Shahzaib Ahamad*, Kanipakam Hema, and Dinesh Gupta*. Identification of Novel Tau-Tubulin Kinase 2 Inhibitors Using Computational Approaches. *ACS Omega* **2023**, 8, 14, 13026–13037. <https://pubs.acs.org/doi/10.1021/acsomega.3c00225>

Kiran K. Yalamanchi*, Yang Li, Tairan Wang, M. Monge-Palacios, S. Mani Sarathy. Large-scale thermochemistry calculations for combustion models. *Applications in Energy and Combustion Science*. **2022**, 12, 100084. <https://doi.org/10.1016/j.jaecs.2022.100084>

McGeoch*, J.E.M., McGeoch, M.W. Chiral 480 nm absorption in the hemoglycin space polymer: a possible link to replication. *Sci Rep* **2022**, 12, 16198. <https://doi.org/10.1038/s41598-022-21043-4>

Tsuyoshi Wauke, Novriyandi Hanif, Sean Ohlinger, Nicole Joy de Voogd, Viqqi Kurnianda, Takahiro Jomori, and Junichi Tanaka*. Amitorin, a Cytotoxic Diterpenoid from a Sponge Halichondria sp. *Chem. Lett.* **2022**, 51, 11, 1080-1082. <https://www.journal.csj.jp/doi/10.1246/cl.220371>

Jia-Meng Jiang, Ze-Hui Shi, Xue-Wen Yang, Dan Zhu, Bao-Jun Zhao, Yue Gao, Dan Xia, Zhi-Qi Yin*, and Ke Pan*. Structural Revision of the *Stemona* Alkaloids Tuberostemonine O, Dehydrocroomines A and B, and Dehydrocroomine. *J. Nat. Prod.* **2022** 85 (8), 2110-2115. <https://pubs.acs.org/doi/abs/10.1021/acs.jnatprod.2c00332>

Chiara Borsari, Erhan Keles, Jacob A. McPhail, Alexander Schaefer, Rohitha Sriramaratnam, Wojciech Goch, Thorsten Schaefer, Martina De Pascale, Wojciech Bal, Matthias Gstaiger, John E. Burke, and Matthias P. Wymann*. Covalent Proximity Scanning of a Distal Cysteine to Target PI3K α . *J. Am. Chem. Soc.* **2022**, 144, 14, 6326–6342. <https://pubs.acs.org/doi/10.1021/jacs.1c13568>

Murray G. Rosenberg and Udo H. Brinker*. Carbene Routes to Cyclopropanetetrahedrane. *J. Org. Chem.* **2022**, 87, 24, 16902–16906. <https://pubs.acs.org/doi/10.1021/acs.joc.2c02217>

Hang-Fei Tu, Aliénor Jeandin, and Marcos G. Suero*. Catalytic Synthesis of Cyclopropenium Cations with Rh-Carbynoids. *J. Am. Chem. Soc.* **2022**, 144, 37, 16737–16743. <https://pubs.acs.org/doi/10.1021/jacs.2c07769>

Anna M. Costa*, Víctor Cascales, Alejandro Castro-Alvarez, and Jaume Vilarrasa*. Computational Study of the Stability of Pyrrolidine-Derived Iminium Ions: Exchange Equilibria between Iminium Ions and Carbonyl Compounds. *ACS Omega* **2022**, 7, 22, 18247–18258. <https://pubs.acs.org/doi/10.1021/acsomega.1c07020>

Dan Xia, Zi-Han Wang, Jia-Meng Jiang, Xue-Wen Yang, Yue Gao, Yin-Ying Xu, Lin-Yue Chang, Dan Zhu, Bao-Jun Zhao, Xin-Liu Zhu, Jian Zhang, Zhi-Qi Yin,* and Ke Pan*. Lycojapomines A–E: Lycopodium Alkaloids with Anti-Renal Fibrosis Potential from *Lycopodium japonicum*. *Org. Lett.* **2022**, 24, 25, 4684–4688. <https://pubs.acs.org/doi/abs/10.1021/acs.orglett.2c01877>

Naoaki Kurisawa, Arihiro Iwasaki*, Kazuya Teranuma, Shingo Dan, Chikashi Toyoshima, Masaru Hashimoto, and Kiyotake Suenaga*. Structural Determination, Total Synthesis, and Biological Activity of lezoside, a Highly Potent Ca²⁺-ATPase Inhibitor from the Marine Cyanobacterium *Leptochromothrix valpauliae*. *J. Am. Chem. Soc.* **2022**, 144, 24, 11019–11032. <https://pubs.acs.org/doi/pdf/10.1021/jacs.2c04459>

Marco Masi, Stefany Castaldi, Francisco Sautua, Gennaro Pescitelli*, Marcelo Anibal Carmona, and Antonio Evidente*. Truncatenolide, a Bioactive Disubstituted Nonenolide Produced by *Colletotrichum truncatum*, the Causal Agent of Anthracnose of Soybean in Argentina: Fungal Antagonism and SAR Studies. *J. Agric. Food Chem.* **2022**, 70, 32, 9834–9844. <https://pubs.acs.org/doi/10.1021/acs.jafc.2c02502>

Tappey H. Jones*, Daniel P. Harrison, Carla Menegatti, Emily Mevers, Kenneth Knott, Paul Marek, Derek A. Hennen, Matt T. Kason, Angie M. Macias, Brian Lovett, and Ralph A. Saporito. Deoxybuzonamine Isomers from the Millipede *Brachycybe lecontii* (Platydesmida: Andrognathidae). *J. Nat. Prod.* **2022**, 85, 4, 1134–1140. <https://pubs.acs.org/doi/10.1021/acs.jnatprod.2c00077>

Tayeb Kakeshpour and Ad Bax*. Simultaneous Quantification of H₂O₂ and Organic Hydroperoxides by ¹H NMR Spectroscopy. *Anal. Chem.* **2022**, 94, 15, 5729–5733. <https://pubs.acs.org/doi/10.1021/acs.analchem.2c00264>

J. Grant Hill and Anthony C. Legon*. Radial Potential Energy Functions of Linear Halogen-Bonded Complexes YX...CIF (YX = FB, OC, SC, N2) and the Effects of Substituting X by Second-Row Analogues: Mulliken Inner and Outer Complexes. *J. Phys. Chem. A* **2022**, 126, 16, 2511–2521. <https://pubs.acs.org/doi/10.1021/acs.jpca.2c01205>

Leiyang Lv*, Huijun Qian, Anna B. Crowell, Shuming Chen*, and Zhiping Li*. Pd/NHC-Controlled Regiodivergent Defluorinative Allylation of gem-Difluorocyclopropanes with Allylboronates. *ACS Catal.* **2022**, 12, 11, 6495–6505. <https://pubs.acs.org/doi/10.1021/acscatal.2c01391>

Zeynep Mine Senol, Serap Çetinkaya, Ali Fazıl Yenidünya, Faika Basoglu-Ünal, Abdulillah Ece*. Epichlorohydrin and tripolyphosphate-crosslinked chitosan–kaolin composite for Auramine O dye removal from aqueous solutions: Experimental study and DFT calculations. *Int. J. Biol.* **2022**, 119, 318–330. <https://www.sciencedirect.com/science/article/abs/pii/S0141813022000095>

Danielle T. Webb, Matthew R. Nagorzanski, David M. Cwiertny, and Gregory H. LeFevre*. Combining Experimental Sorption Parameters with QSAR to Predict Neonicotinoid and Transformation Product Sorption to Carbon Nanotubes and Granular Activated Carbon. *ACS EST Water* **2022**, 2, 1, 247–258. <https://pubs.acs.org/doi/10.1021/acsestwater.1c00492>

Aidan W. McFord, Craig P. Butts*, Natalie Fey*, and Roger W. Alder*. 3× Axial vs 3× Equatorial: The Δ GGA Value Is a Robust Computational Measure of Substituent Steric Effects. *J. Am. Chem. Soc.* **2021**, 143, 34, 13573–13578. <https://pubs.acs.org/doi/10.1021/jacs.1c04247>

Sekiha Ishikawa, Yoshikazu Masuyama, Takeshi Adachi, Takeshi Shimonishi, Shotaro Morimoto, and Yoo Tanabe*. Synthesis of Naphthaleman Family Utilizing Regiocontrolled Benzannulation: Unique Molecules Composed of Multisubstituted Naphthalenes. *ACS Omega* **2021**, 6, 48, 32682–32694. <https://pubs.acs.org/doi/10.1021/acsomega.1c04413>

Corey A. Baldasare and Paul G. Seybold*. Computational Estimation of the Aqueous Acidities of Alcohols, Hydrates, and Enols. *J. Phys. Chem. A* **2021**, 125, 17, 3600–3605. <https://pubs.acs.org/doi/10.1021/acs.jpca.1c01330>

W. Buijs*. Molecular Modeling Study to the Relation between Structure of LPEI, Including Water-Induced Phase Transitions and CO₂ Capturing Reactions. *Ind. Eng. Chem. Res.* **2021**, 60 (30), 11309–11316. <https://pubs.acs.org/doi/pdf/10.1021/acs.iecr.1c00846>

Carl Jacky Saint-Louis, David J. Warner, Katie S. Keane, Melody D. Kelley, Connor M. Meyers, and Silas C. Blackstock*. Photo-Electroswitchable Arylaminoazobenzenes. *J. Org. Chem.* **2021**, 86, 17, 11341–11353. <https://pubs.acs.org/doi/10.1021/acs.joc.1c00763?ref=PDF>

Siddharth Iyer, Matti P. Rissanen, Rashid Valiev, Shawon Barua, Jordan E. Krechmer, Joel Thornton, Mikael Ehn & Theo Kurtén. Molecular mechanism for rapid autoxidation in α -pinene ozonolysis. *Nat. Commun.* **2021**, 12, 878. <https://doi.org/10.1038/s41467-021-21172-w>

Priyanka Venkatachalam, Savithiri Ganesan, Subadevi Rengapillai*, and Sivakumar Marimuthu*. Gradual Development of Maricite NaMnPO₄ with the Influence of Diol Chain Length on the Polyol Process of Surpassed Sodium Intercalation. *Ind. Eng. Chem. Res.* **2021**, 60, 16, 5861–5868. <https://pubs.acs.org/doi/10.1021/acs.iecr.1c00102>

Anna Joselle V. Lomboy and Robert Q. Topper*. Nonuniform Proton Transfer and Strong Hydrogen Bonding within Cation, Anion, and Neutral Clusters of Ammonia and Hydrogen Fluoride. *J. Phys. Chem. A*. **2021**, 125, 12, 2546-2557. <https://pubs.acs.org/doi/10.1021/acs.jpca.1c00732>

Duane D. Miller*, Jie Yu, and Steven S.C. Chuang*. Unraveling the Structure and Binding Energy of CO₂/H₂O on Amine Sorbents. *J. Phys. Chem. C*. **2020**, 124, 45, 24677-24689. <https://pubs.acs.org/doi/10.1021/acs.jpcc.0c04942>

Wim Buijs*. Molecular Modeling Study of the SO₂ Deactivation of an Amine Resin and a Procedure to Avoid SO₂ Deactivation Using Polyethylene Glycol/Tertiary Amine System. *Ind. Eng. Chem. Res.* **2020**, 59, 30, 13388–13395. <https://pubs.acs.org/doi/10.1021/acs.iecr.0c01800>

Dong-Dong Zhang, Jin-Biao Xu, Yao-Yue Fan, Li-She Gan, Hua Zhang, and Jian-min Yue. Daphnillonins A and B: Alkaloids Representing Two Unknown Carbon Skeletons from *Daphniphyllum longeracemosum*. *J. Org. Chem.* **2020**, 85, 5, 3742-3747, <https://doi.org/10.1021/acs.joc.9b03310>

Shuming Chen, Jonathan Wong, and K. N. Houk. Mechanism of the Manolikakes Enamide-Based Domino Reaction for the Stereospecific Construction of Tetrahydropyrans. *J. Org. Chem.* **2020**, 85, 5, 3806-3811. <https://pubs.acs.org/doi/10.1021/acs.joc.9b03440>

Isabel M. Klein, Corey C. Husic, Dávid P. Kovács, Nicolas J. Choquette, and Maxwell J. Robb*. Validation of the CoGEF Method as a Predictive Tool for Polymer Mechanochemistry. *J. Am. Chem. Soc.* **2020**, 142, 38, 16364–16381. <https://pubs.acs.org/doi/10.1021/jacs.0c06868>

Hatsumi Wakamatsu, Yosuke Matsuo, Mohamed Omar, Yoshinori Saito, Koyo Mishida, and Takahashi Tanaka*. Oxidation of the Oak Ellagitannin, Vescalagin. *J. Nat. Prod.* **2020**, 83, 2, 413-421. <https://pubs.acs.org/doi/10.1021/acs.jnatprod.9b00917>

Zahra A. Tabasi, Joshua C. Walsh, Graham J. Bodwell, David W. Thompson, and Yuming Zhao. Crystal Engineering and Photophysical Properties of Phenyl-Pyrenimidazole Systems. *Cryst. Growth Des.* **2020**, 20, 3, 1681-1693. <https://pubs.acs.org/doi/10.1021/acs.cgd.9b01443>

Kleoniki Giannousi, George Dimitrios Geromichalos, Dionysia Kakolyri, Stefanos Mourdikoudis, Catherine Dendrinou-Samara. The interaction of ZnO nanostructures with proteins: In vitro fibrillation/antifibrillations studies and in silico molecular docking simulations. *ACS Chem. Neurosci.* **2020**, 11, 3, 436-444. <https://pubs.acs.org/doi/10.1021/acschemneuro.9b00642>

Keisuke Fukaya, Daisuke Urabe*, Masato Hiraizumi, Keiichi Noguchi, Takashi Matsumoto, Kaori Sakurai*. Computational and Experimental Analysis on the Conformational Preferences of Anticancer Saponin OSW-1. *J. Org. Chem.* **2020**, 85, 2, 339-344. <https://pubs.acs.org/doi/10.1021/acs.joc.9b02085>

Hans Choi, Harry J. Shirley, Harry R. M. Aitken, Tim Schulte, Tilo Söhnel, Paul A. Hume, Margaret A. Brimble* and Daniel P. Furkert*. Intermolecular Diels-Alder Cycloaddition/Cross-Coupling Sequences of 2-Bromo-1,3-butadienes. *Organic Letters*, **2020**, 22, 3, 1022-1027. <https://pubs.acs.org/doi/10.1021/acs.orglett.9b04567>

Rong Fan, Ryo Sumitani, and Tomoyuki Mochida*. Synthesis and Reactivity of Cyclopentadienyl Ruthenium(II) Complexes with Tris(alkylthio)benzenes: Transformation between Dinuclear and Sandwich-Type Complexes. *ACS Omega* **2020**, 5, 4, 2034-2040. <https://pubs.acs.org/doi/10.1021/acsomega.9b04272>

Qiuying Wang, Kaijin Zhang, Wei Wang, Guojian Zhang, Tianjiao Zhu, Qian Che, Qianqun Gu, and Dehai Li*. Amphiepicrocins A–J: Epipolythiodioxopiperazines from the Fish-Gill-Derived Fungus *Epicoccum nigrum* HDN17-88. *J. Nat. Prod.* **2020**, 83, 2, 524–531. <https://pubs.acs.org/doi/10.1021/acs.jnatprod.9b01242>

Samaneh Bashiri, Jafar Abdollahzadeh, Roberta Di Lecce, Daniela Alioto, Marcin Górecki, Gennaro Pescitelli, Marco Masi*, and Antonio Evidente. Rabenchromenone and Rabenzophenone, Phytotoxic Tetrasubstituted Chromenone and Hexasubstituted Benzophenone Constituents Produced by the Oak-Dieback-Associated Fungus *Fimmetariella rabenhorstii*. *J. Nat. Prod.* **2020**, 83, 2, 447–452. <https://pubs.acs.org/doi/10.1021/acs.jnatprod.9b01017>

Karolina Tiara, Mykhaylo A. Potopnyk, Pawel Swider, and Slawomir Jarosz*. Stereocontrolled Debenzylative Cycloetherification Reaction as a Route to Enantiopure C-Furanosides with Amino Substituents in the Side Chain. *J. Org. Chem.* **2020**, 85, 5, 3517–3526. <https://pubs.acs.org/doi/10.1021/acs.joc.9b03247>

Cyndi Qixin He, Ching Ching Lam, Peiyuan Yu, Zhihui Song, Maggie Chen, Yu-hong Lam, Shuming Chen, and K. N. Houk. Catalytic Effects of Ammonium and Sulfonium Salts and External Electric Fields on Aza-Diels–Alder Reactions. *J. Org. Chem.*, **2020**, 84, 4, 2618–2625. <https://doi.org/10.1021/acs.joc.9b03446>

Samuele Sala, Gareth L. Nealon, Alexandre N. Sobolev, Jane Fromont, Oliver Gomez, and Gavin R. Flematti*. Structure Reassignment of Echin sulfone A and the Echin sulfonic Acids A–D Supported by Single-Crystal X-ray Diffraction and Density Functional Theory Analysis. *J. Nat. Prod.* **2020**, 83, 1, 205–110. <https://pubs.acs.org/doi/10.1021/acs.jnatprod.9b00902>

Miguel A. González, Albert Gallen, Montserrat Ferrer,* and Manuel Martínez*. Self-Assembly and Properties of a Discrete Water-Soluble Prussian Blue Analogue Fe^{II}/Co^{III} Cube: Confinement of a Water Molecule in Aqueous Solution. *Inorg. Chem.* **2020**, 59, 3, 1582–1587. <https://pubs.acs.org/doi/10.1021/acs.inorgchem.9b03274>

Braden D. Kelly* and William R. Smith*. Alchemical Hydration Free-Energy Calculations Using Molecular Dynamics with Explicit Polarization and Induced Polarity Decoupling: An On-the-Fly Polarization Approach. *J. Chem. Theory Comput.* **2020**, 16, 2, 1146–1161. <https://pubs.acs.org/doi/10.1021/acs.jctc.9b01139>

Bun Chan*. Aqueous-Phase Conformations of Lactose, Maltose, and Sucrose and the Assessment of Low-Cost DFT Methods with the DSCONF Set of Conformers for the Three Disaccharides. *J. Phys. Chem. A.* **2020**, 124, 3, 582–590. <https://pubs.acs.org/doi/10.1021/acs.jpca.9b10932>

Yuji Shinohara and Naoto Tsubouchi*. Electronic State of Low-Rank Coals with Exchanged Sodium Cations. *ACS Omega* **2020**, 5, 3, 1688–1697. <https://pubs.acs.org/doi/10.1021/acsomega.9b03780>

Warren Hehre*, Phillip Klunzinger, Bernard Deppmeier, Andy Driessen, Noritaka Uchida, Masaru Hashimoto, Eri Fukushi, Yusuke Takata. Efficient Protocol for Accurately Calculating ¹³C Chemical Shifts of Conformationally Flexible Natural Products: Scope, Assessment, and Limitations. *J. Nat. Prod.* **2019**, 82(8), 2299–2306. <https://pubs.acs.org/doi/pdf/10.1021/acs.jnatprod.9b00603?rand=m59lzdpe>

Kristian H. Møller, Theo Kurtén, Kelvin H. Bates, Joel A. Thornton, and Henrik G. Kjaergaard*. Thermalized Epoxide Formation in the Atmosphere. *J. Phys. Chem. A* **2019**, 123, 49, 10620–10630. <https://pubs.acs.org/doi/10.1021/acs.jpca.9b09364>

Wim Buijs. Direct Air Capture of CO₂ with an Amine Resin: a Molecular Modelling Study of the Deactivation Mechanism by CO₂. *Ind. Eng. Chem. Res.* **2019**, 58, 32, 14705-14708.
<https://pubs.acs.org/doi/10.1021/acs.iecr.9b02637>

Hsin-Kai Kao, Xin-Jie Lin, Bor-Cherng Hong,* Van-Wei Yang, and Gene-Hsiang Lee. Enantioselective Synthesis of Yohimbine Analogues by an Organocatalytic and Pot-Economic Strategy. *J. Org. Chem.* **2019**, 84, 12138-12147. <https://pubs.acs.org/doi/abs/10.1021/acs.joc.9b01193>

David J. Bergman, Edward M. Kosower. Theory of new states, FEXs, Fast-formed Excited states by the combination of an IR photon and water. *Spectrochimica Acta Part A*, **2019**, 215, 303-306.
<https://www.sciencedirect.com/science/article/pii/S1386142519302173>

Muhammad Zeeshan, Vahid Nozari, Seda Keskin*, and Alper Uzun*. Structural Factors Determining Thermal Stability of Ionic Liquids/MOF Composites: Imidazolium Ionic Liquids Combined with CuBTC and ZIF-8. *Ind. Eng. Chem. Res.* **2019**, 58, 31, 14124–14138. <https://pubs.acs.org/doi/10.1021/acs.iecr.9b02415>

Rashid R. Valiev*, Galib Hasan, Vili-Taneli Salo, Jakub Kubečka, and Theo Kurtén*. Intersystem Crossings Drive Atmospheric Gas-Phase Dimer Formation. *J. Phys. Chem. A* **2019**, 123, 30, 6596–6604.
<https://pubs.acs.org/doi/10.1021/acs.jpca.9b02559>

Armelle Tontsa Tsamo*, Julio Issah Mawouma Pagna, Pamela Kemda Nangmo, Pierre Mkounga, Hartmut Laatsch and Augustin Ephrem Nkengfack. Rubescins F–H, new vilasinin-type limonoids from the leaves of *Trichilia rubescens* (Meliaceae). *Z. Naturforsch.*, **2019**, 74(7-8), 175-182.
<https://doi.org/10.1515/znc-2018-0187>

Yanpeng Zhu, Xiaoyu Guo, Yang Li, and Jiaobing Wang*. Fusing of Seven HBCs toward a Green Nanographene Propeller. *J. Am. Chem. Soc.* **2019**, 141, 5511-5517. <https://pubs.acs.org/doi/10.1021/jacs.9b01266>

Wim Buijs*, Ibelwaleed A. Hussein, Mohamed Mahmoud, Abdulmujeeb T. Onawole, Mohammed A. Saad, Golibjon R. Berdiyrov. Molecular Modeling Study toward Development of H₂S-Free Removal of Iron Sulfide Scale from and Gas Wells. *Ind. Eng. Chem. Res.*, **2018**, 57(31), 10095–10104.
<https://pubs.acs.org/doi/10.1021/acs.iecr.8b01928>

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://science.sciencemag.org/content/early/2018/02/14/science.aar5169>

Joel A. Olson, Raymond J. Terryn III, Elizabeth L. Stewart, J. Clayton Baum, Mark J. Novak. New insight into the action of tryptanthins against *Plasmodium falciparum*: Pharmacophore identification via a novel submolecular QSAR descriptor. *J. Mol. Graph. Model.*, **2018**, 80, 138-146.
<https://www.sciencedirect.com/science/article/pii/S1093326317307210>

Anne-Frances Miller*, Jonathan T. Park, Kyle L. Ferguson, Warintra Pitsawong, Andreas S. Bommarius. Informing Efforts to Develop Nitroreductase for Amine Production. *Molecules*, **2018**, 23(2), 211.
<https://www.mdpi.com/1420-3049/23/2/211>

Yunlong Zhou, Pablo F. Damasceno, Bagganahalli S. Somashekar, Michael Engel, Falin Tian, Jian Zhu, Rui Huang, Kyle Johnson, Carl McIntyre, Kai Sun, Ming Yang, Peter F. Green, Ayyalusamy Ramamoorthy, Sharon C. Glotzer & Nicholas A. Kotov. Unusual multiscale mechanics of biomimetic nanoparticle hydrogels. *Nat. Commun.*, **2018**, 181. <https://www.nature.com/articles/s41467-017-02579-w>

Robert W. Baker*. Asymmetric Induction via the Structural Indenyl Effect. *Organometallics*, **2018**, 37(3), 433-440. <https://pubs.acs.org/doi/10.1021/acs.organomet.7b00841>

Adeboye Omolara*. Computational modelling Procedures for Geometry Optimization, Kinetic and Thermodynamic Calculations using Spartan Software - A Review. *Arc Org Inorg Chem Sci* **2018**, 1(5) 122-125. <https://www.sciencegate.app/document/10.32474/aoics.2018.01.000123>

Nianqiang Jiang, Ziyong Yuan, Tao Li, Yanpeng Zhu, Yu-Sheng Chen, Liqiong Lin, Jingrui Zhang, Yi-Tsu Chan, Jiabing Wang*. Synthesis and Characterization of Ferrocene Based Hemicages. *J. Org. Chem.*, **2018**, 83,8, 4824-4830. <https://pubs.acs.org/doi/10.1021/acs.joc.8b00146>

Edward M. Kosower* and Galina Borz. Neutral dipole-dipole dimers: A new field in science. *Spectrochimica Acta Part A.*, **2017**, 192, 291-296. <https://doi.org/10.1016/j.saa.2017.11.026>

Mark P. Heitz, Kristina L. Fuller, and Kaitlin A Ordiway. Dissolution of Trihexyltetradecylphosphonium Chloride in Supercritical CO₂ *ChemEngineering*, **2017**, 1(2), 12. <https://www.mdpi.com/2305-7084/1/2/12>

D. R. Eichler, G. A. Papadantonakis. Methylation of DNA Bases by Dimethyl Sulfate. *Chemical Physics Letters*, **2017** 689, 8-14. <https://www.sciencedirect.com/science/article/abs/pii/S0009261417309193>

Eva Schütznerová, Allen G. Oliver, Greg A. Slough, and Viktor Krchňák*, Traceless Solid-Phase Synthesis of Fused Chiral Macrocycles via Conformational-Assisted Cyclic Iminium Formation. *Chem. Eur. J.*, **2017**, 23, 12876-12885. <https://onlinelibrary.wiley.com/doi/abs/10.1002/chem.201702461>

Wim Buijs* and Stijn de Flart, Direct Air Capture of CO₂ with Amine Resin: A Molecular Modeling Study of the CO₂ Capturing Process. *Ind. Eng. Chem. Res.*, **2017**, 56(43), 12297–12304. <https://pubs.acs.org/doi/abs/10.1021/acs.iecr.7b02613>

Mary J. Garson*, Warren Hehre, Gregory K. Pierens, and Suciati, Revision of the Structure of Acremine P from a Marine-Derived Strain of *Acremonium persicinum*. *Molecules*, **2017**, 22(4), 521-526. <https://www.mdpi.com/1420-3049/22/4/521>

Anuradha Balasubramanian, Tadahisa Teramoto, Amol A. Kulkarni, Apurba K. Bhattacharjee, Radhakrishnan Padmanabhan*. Antiviral activities of selected antimalarials against dengue virus type 2 and Zika virus. *Antivir. Res.*, **2017**, 137, 141-150. <https://doi.org/10.1016/j.antiviral.2016.11.015>

Izar Capel Berdiell, Rafal Kulmaczewski, and Malcolm A. Halcrow*, Iron(II) Complexes of 2,4-Dipyrazolyl-1,3,5-triazine Derivatives—The Influence of Ligand Geometry on Metal Ion Spin State. *Inorg. Chem.*, **2017**, 56(15), 8817-8828. <https://pubs.acs.org/doi/abs/10.1021/acs.inorgchem.7b00699>

Thomas Elder*, Laura Berstis, Gregg T. Beckham, and Michael F. Crowley, Density Function Theory Study of Spirodienone Stereoisomers in Lignin. *Sustainable Chem. Eng.*, **2017**, 5(8) 7188-7194. <https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.7b01373>

Henrik G. Bohr*, Irene Shim, Cy Stein, Henrik Orum, Henrick F. Hansen, and Troel Koch, Electronic Structures of LNA Phosphorothioate Oligonucleotides. *Molecular Therapy – Nucleic Acids*, **2017**, 8, 428-441.
<http://dx.doi.org/10.1016/j.omtn.2017.05.011>

Daniel R. Eichler, Haley A. Hamann, Katherine A. Harte, George A. Papadantonakis*, Hydration effects on the photoionization energy of 2'-deoxyguanosine 5'-phosphate and activation barriers for guanine methylation by carcinogenic methane diazonium ions. *Chem. Phys. Lett.*, **2017**, 680, 83-89.
<https://doi.org/10.1016/j.cplett.2017.05.025>

Xavier Garcia-LLinas, Antonio Bauza, Saikat K. Seth, and Antonio Frontera, Importance of R—CF₃---O Tetrel Bonding Interactions in Biological Systems. *J. Phys. Chem. A*, **2017**, 121(28), 5371-5376.
<https://pubs.acs.org/doi/abs/10.1021/acs.jpca.7b06052>

Serli Onlu* and Melek Turker Sacan, Impact of geometry optimization methods on QSAR modeling: A case study for predicting human serum albumin binding affinity. *SAR QSAR Environ. Res.*, **2017**, 28(6), 491-509.
<https://www.tandfonline.com/doi/full/10.1080/1062936X.2017.1343253>

Laetitia Schoepff, Lucas Kocher, Stephanie Durot*, and Valerie Heitz*, Chemically Induced Breathing of Flexible Porphyrinic Covalent Cages. *J. Org. Chem.*, **2017**, 82(11), 5845-5851.
<https://pubs.acs.org/doi/abs/10.1021/acs.joc.7b00698>

Shizuya Tanaka, Yuna Honmura, Shota Uesugi, Eri Fukushi, Kazuaki Tanaka, Hayato Maeda, Ken-ichi Kimura, Tatsuo Nehira, and Masaru Hashimoto*, Cyclohelminthol X, a Hexa-substituted Spirocyclopropane from *Helminthosporium velutinum* yone96: Structural Elucidation, Electronic Circular Dichroism Analysis, and Biological Properties. *J. Org. Chem.*, **2017**, 82(11), 5574-5582.
<https://pubs.acs.org/doi/abs/10.1021/acs.joc.7b00393>

Kenneth M. Doll*, Grigor B. Bantchev, Ering L. Walter, Rex E. Murray, Michael Appell, James C. Lansing, Bryan R. Moser, Parameters Governing Ruthenium Sawhorse-Based Decarboxylation of Oleic Acid. *Ind. Eng. Chem. Res.*, **2017**, 56(4), 864-871. <https://pubs.acs.org/doi/abs/10.1021/acs.iecr.6b04555>

Kazuaki Kusakabe, Yuna Honmura, Shota Uesugi, Akio Tonouchi, Hayato Maeda, Ken-ichi Kimura, Hiroyuki Koshino, and Masaru Hashimoto*, Neomacrophorin X, a [4.4.3]Propellane-Type Meroterpenoid from *Trichoderma* sp. 1212-03. *J. Nat. Prod.*, **2017**, 80(5), 1484-1492.
<https://pubs.acs.org/doi/abs/10.1021/acs.jnatprod.6b01177>

Serli Onlu* and Melek Turker Sacan, An *in silico* algal toxicity model with a wide applicability potential for industrial chemicals and pharmaceuticals. *Environ. Toxicol. Chem.*, **2017**, 36(4), 1012-1019.
<https://onlinelibrary.wiley.com/doi/10.1002/etc.3620/abstract>

Olga E. Eremina, Alexander V. Sidorov, Tatyana N. Shekhovstova, Eugene A. Goodilin*, and Irina A. Veselova, Novel Multilayer Nanostructured Materials for Recognition of Polycyclic Aromatic Sulfur Pollutants and Express Analysis of Fuel Quality and Environmental Health by Surface Enhanced Raman Spectroscopy. *Appl. Mater. Interfaces*, **2017**, 9(17), 15058-15067. <https://pubs.acs.org/doi/abs/10.1021/acsami.7b02018>

Mark D. Ellison*, Samuel Menges, Laura Nebel, Gabrielle D'Arcangelo, Anna Kramer, Lee Drahushuk, Steven Shimizu, and Michael S. Strano, Electrokinetic Transport of Methanol and Lithium Ions Through a 2.25-nm-Diameter Carbon Nanotube Nanopore. *J. Phys. Chem. C*, **2017**, 121(3), 2205-2013.
<https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b12104>

Serli Onlu* and Melek Turker Sacan, An *in silico* approach to cytotoxicity of pharmaceuticals and personal care products on the rainbow trout liver cell line RTL-W1. *Environ. Toxicol. Chem.*, **2017**, 36(5), 1162-1169. <https://onlinelibrary.wiley.com/doi/10.1002/etc.3663/abstract>

Duane D. Miller* and Steven S.C. Chuang*, Control of CO₂ Absorption and Desorption Using Polyethylene Glycol in a Tetraethylenepentamine Thin Film: An In Situ ATR and Theoretical Study. *J. Phys. Chem. C*, **2016**, 120(44), 25489-25504. <https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b09506>

Krishnan Sriraman, Raymond J. Terryn, III, Xixuan Guo, Mark J. Novak, J. Clayton Baum, and Joel A. Olson*, Semiquantitative Submolecular Barrier Height Measurements of 4-Aza-8-fluorotryptanthrin Monolayers on HOPG: Orbital-Mediated Tunneling. *J. Phys. Chem. C*, **2016**, 120(6), 3420-3427. <https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.5b11959>

A. Ozalp, S.C. Yavuz, N. Sabanci, F. Copur, Z. Kokbudak, and E. Saripinar*, 4D-QSAR investigation and pharmacophore identification of pyrrolo[2,1-c][1,4]benzodiazepines using electron conformational-genetic algorithm method. *SAR QSAR Environ. Res.*, **2016**, 27(4), 317-342. <https://www.tandfonline.com/doi/full/10.1080/1062936X.2016.1174152>

Duane D. Miller* and Steven S.C. Chuang*, The Effect of Electron-Donating Groups and Hydrogen Bonding on H₂S Capture over Polyethylene Glycol/Amine Sites *J. Phys. Chem. C*, **2016**, 120(2), 1147-1162. <https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.5b11796>

Edward M. Kosower* and Galina Borz, Low polarity water, a novel transition species at the polyethylene-water interface.† *Phys. Chem. Chem. Phys.* **2015**, 17, 24895-24900. <https://pubs.rsc.org/en/Content/ArticleLanding/2015/CP/C5CP04439A#!divAbstract>

P. Erzincan, M. Turker Sacan*, B. Yuce-Dursun, O. Danis, S. Demir, S.S. Erdem, A. Ogan, QSAR models for antioxidant activity of new coumarin derivatives. *SAR QSAR Environ. Res.*, **2015**, 26(7-9), 721-737. <https://www.tandfonline.com/doi/full/10.1080/1062936X.2015.1088571>

Marcus Baumann, André P. Dieskau, Brad M. Loertscher, Mary C. Walton, Sangkil Nam, Jun Xie, David Horne* and Larry E. Overman*, Tricyclic analogues of epidithiodioxopiperazine alkaloids with promising in vitro and in vivo antitumor activity.† *Chem. Sci.* **2015**, 6, 4451-4457. <https://pubs.rsc.org/en/Content/ArticleLanding/2015/SC/C5SC01536G#!divAbstract>

Yuna Honmura, Hiroto Takekawa, Kazuaki Tanaka, Hayato Maeda, Tatsuo Nehira*, Warren Hehre, and Masaru Hashimoto*. Computation-Assisted Structural Elucidation of Epoxyroussoeone and Epoxyroussoedione Isolated from *Roussoella japonensis* KT1651. *J. Nat. Prod.* **2015**, 78, 7, 1505-1510. <https://pubs.acs.org/doi/10.1021/np500924n>

Roberta Galdani*, Francesco Tadini-Buoninsegni, Mariagrazia Roselli, Ivana Defrenza, Marialessandra Contino, Nicola Antonio Colabugy, and Giovanni Lentini, Inhibition of hERG potassium channel by the antiarrhythmic agent mexiletine and its metabolite m-hydroxymexiletine. *Pharmacol. Res. Perspect.* **2015**, 3 (5): e00160. <https://onlinelibrary.wiley.com/doi/10.1002/prp2.160/abstract>

Duane D. Miller* and Steven S.C. Chuang*, Experimental and Theoretical Investigation of SO₂ Adsorption over the 1,3-Phenylenediamine/SiO₂ System. *J. Phys. Chem. C*, **2015**, 119(12), 6713-6727. <https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.5b01131>

E. Orucu, G. Tugcu, and M.T. Sacan*, Molecular structure-absorptions study on current textile dyes. *SAR QSAR Environ. Res.*, **2014**, 25(12), 983-998. <https://www.tandfonline.com/doi/abs/10.1080/1062936X.2014.976266>

Daniel Fankhauser, Dušan Kolarski, Wolfram R. Grüning, and François Diederich*, Resorcin[4]arene-Based Molecular Baskets and Water-Soluble Container Molecules: Synthesis and ¹H NMR Host–Guest Complexation Studies. *Eur. J. Org. Chem.*, **2014**, 17, 3575–3583. <https://onlinelibrary.wiley.com/doi/10.1002/ejoc.201402140/abstract>

Troels Koch*, Irene Shim, Morten Lindow, Henrik Ørum, and Henrik G. Bohr, Quantum Mechanical Studies of DNA and LNA. *Nucleic Acid Therapeutics*, **2014**, 2(24), 139-148. <https://www.liebertpub.com/doi/full/10.1089/nat.2013.0465>

P. Ganga Raju Achary, Simplified molecular input line entry system-based optimal descriptors: QSAR modelling for voltage gated potassium channel subunit Kv7.2. *SAR QSAR Environ. Res.*, **2014**, 25(1), 73-90. <https://www.tandfonline.com/doi/abs/10.1080/1062936X.2013.842930>

Changming Fang, Xiaoqian Lu, Wim Buijs, Zhaochuan Fan, Fatma Elif Genceli Güner, Marijn A .van Huis, Geert-Jan Witkamp, Thijs J. H. Vlugt*, Crystal structure, stability, and electronic properties of hydrated metal sulfates MSO₄(H₂O)_n (M=Ni, Mg; n=6, 7) and their mixed phases: A first principles study. *Chemical Engineering Science*. **2014**, 121, 77–86. <https://www.sciencedirect.com/science/article/pii/S0009250914003716>

Julie E. M. McGeoch*, Malcolm W. McGeoch, Polymer Amide as an Early Topology. *PLoS ONE*, **2014**, 9(7) e103036. <https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0103036>

Jianrong Li, Wim Buijs, Rob J. Berger, Jacob A. Mouligna and Michiel Makkee*, Sorbitol dehydration in a ZnCl₂ molten salt hydrate medium: molecular modeling. *Catal. Sci. Technol.*, **2014**, 4, 152-163. <https://pubs.rsc.org/en/Content/ArticleLanding/2014/CY/c3cy00686g#!divAbstract>

Patricia Wright*, Alexander Alex, Frank Pullen, Predicting collision-induced dissociation spectra: Semi-empirical calculations as a rapid and effective tool in software-aided mass spectral interpretation. *Mass Spectrom.* **2014**, 28, 1127-1143. <https://onlinelibrary.wiley.com/doi/10.1002/rcm.6870/abstract>

S. Eric*, M. Kalinic, K. Ilic, and M. Zloh, Computational classification models for predicting the interaction of drugs with P-glycoprotein and breast cancer resistance protein. *SAR QSAR Environ. Res.*, **2014**, 25(12), 939-966. <https://www.tandfonline.com/doi/abs/10.1080/1062936X.2014.976265>

T.S. Garcia, D.C. Silva, J.C. Gertrudes, V.G. Maltarollo, and K.M. Honorio*, Molecular features related to the binding of PPAR δ agonists from QSAR and docking analyses. *SAR QSAR Environ. Res.*, **2013**, 2(24), 157-173. <https://www.tandfonline.com/doi/abs/10.1080/1062936X.2012.751453>

Krishnan Sriraman, Mark J. Novak, J. Clayton Baum, Andrew Herron, Joel A. Olson*, Surface behavior and imaging of the lowest unoccupied molecular orbital of indolo[2,1-b]quinazoline-6,12-dione (tryptanthrin) via scanning tunneling microscopy. *Surface Science*. **2013**, 616 110–114. <https://www.sciencedirect.com/science/article/pii/S0039602813001829>

Katharine J. Cahill and Richard P. Johnson*, Beyond Frontier Molecular Orbital Theory: A Systematic Electron Transfer Model (ETM) for Polar Bimolecular Organic Reactions. *J. Org. Chem.* **2013**, 78, 1864–1873. <https://pubs.acs.org/doi/abs/10.1021/jo301731v>

Ekaterina V. Filippova, Leigh A. Weston, Misty L. Kuhn, Brett Geissler, Alexandra M. Gehring, Nicola Armoush, Chinessa T. Adkins, George Minasov, Ievgeniia Dubrovskaya, Ludmilla Shuvalova, James R. Winsor, Luke D. Lavis, Karla J. F. Satchell, Daniel P. Becker, Wayne F. Anderson, and R. Jeremy Johnson, Large Scale Structural Rearrangement of a Serine Hydrolase from *Francisella tularensis* Facilitates Catalysis. *J. Biol. Chem.* **2013**, 288 10522-10535. <https://www.jbc.org/content/288/15/10522.full>

G. Tugcu, M. Turker Sacan*, M. Vracko, M. Novic, and N. Minovski, QSTR modelling of the acute toxicity of pharmaceuticals to fish. *SAR QSAR Environ. Res.*, **2012**, 23(3-4), 297-310. <https://www.tandfonline.com/doi/full/10.1080/1062936X.2017.1352621?src=recsys>

Gerald Kagan, Weibin Li, Deyu Li, Russell Hopson, and Paul G. Williard*, Characterization of Dimeric Chiral Lithium Amide Structure Derived from N-isopropylsilyl Valinol. *J. Am. Chem. Soc.*, **2011**, 133(17), 6596-6602. <https://pubs.acs.org/doi/10.1021/ja109041z>

Duane D. Miller*, Ranjani Siriwardane, and Thomas Simonyi, Theoretical and Experimental Analysis of Oxygen Separation from Air over Ni-Transition Metal Complexes *Energy Fuels*, **2011**, 25(10), 4261-4270. <https://pubs.acs.org/doi/10.1021/ef200779m>

Helene Perrotin-Brunel*, Wim Buijs, Jaap van Spronsen, Maaike J.E. van Roosmalen, Cor J. Peters, Rob Verpoorte, Geert-Jan Witkamp, Decarboxylation of Δ^9 -tetrahydrocannabinol: Kinetics and molecular modeling. *J. Mol. Struct.* **2011**, 987(1), 67-73. <https://www.sciencedirect.com/science/article/pii/S0022286010009270>

Prakash C. Joshi, Michael F. Aldersley, James P. Ferris. Homochiral Selectivity in RNA Synthesis: Montmorillonite-catalyzed Quaternary Reactions of D, L-Purine with D, L- Pyrimidine Nucleotides. *Origins Life Evol. B.* **2011**, 41(3), 213-236. <https://www.springer.com/journal/11084>

N. Schultheiss, K. Lorimer, S. Wolf, and J. Desper, Attempted construction of minoxidil: carboxylic acid cocrystals; 7 salts and 1 cocrystal resulted. *Cryst. Eng. Comm.* **2010**, 12, 742-749. <https://pubs.rsc.org/en/content/articlelanding/2010/ce/b910136e/unauth#!divAbstract>

Salvatore Profeta Jr. *, V.S. Senthil Kumar, Richard Austin, S. Stanley Young, Differential reactivity of thiophene-2-carboxylic and thiophene-3-carboxylic acids: Results from DFT and Hartree-Fock theory. *J. Mol. Graph. Mod.* **2010**, 28, 540-547. <https://www.sciencedirect.com/science/article/pii/S1093326309001661>

W. S. Ohlinger, P. E. Klunzinger, B. J. Deppmeier, W. J. Hehre*. Efficient Calculation of Heats of Formation. *J. Phys. Chem. A.* **2009**, 113, 10, 2165-2175. <https://pubs.acs.org/doi/10.1021/jp810144q>

Ning Shangguan, Warren J. Hehre, William S. Ohlinger, Mary Pat Beavers, and Madeleine M. Joullié*. The Total Synthesis of Roquefortine C and a Rationale for the Thermodynamic Stability of Iso-roquefortine C over Roquefortine C. *J. Am. Chem. Soc.* **2008**, 130, 19, 6281-6287. <https://pubs.acs.org/doi/10.1021/ja800067q>

Last Update Feb 2024
support@wavefu.com