

Robert S Paton

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2444369/publications.pdf>

Version: 2024-02-01

162
papers

8,351
citations

50566

48
h-index

68831

81
g-index

223
all docs

223
docs citations

223
times ranked

9911
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|---|------|-----------|
| 1 | Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins. <i>Communications Chemistry</i> , 2022, 5, . | 2.0 | 5 |
| 2 | [¹⁸ F]Difluorocarbene for positron emission tomography. <i>Nature</i> , 2022, 606, 102-108. | 13.7 | 30 |
| 3 | Asymmetric Azidation under Hydrogen Bonding Phase-Transfer Catalysis: A Combined Experimental and Computational Study. <i>Journal of the American Chemical Society</i> , 2022, 144, 4572-4584. | 6.6 | 13 |
| 4 | Homologation of Electron-Rich Benzyl Bromide Derivatives via Diazo C=C Bond Insertion. <i>Journal of the American Chemical Society</i> , 2022, 144, 86-92. | 6.6 | 13 |
| 5 | Mechanistic Studies Yield Improved Protocols for Base-Catalyzed Anti-Markovnikov Alcohol Addition Reactions. <i>Journal of the American Chemical Society</i> , 2022, 144, 9586-9596. | 6.6 | 6 |
| 6 | Expanding chemical space by para-H arylation of arenes. <i>Nature Communications</i> , 2022, 13, . | 5.8 | 17 |
| 7 | Elucidating the chemical pathways responsible for the sooting tendency of 1 and 2-phenylethanol. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 1327-1334. | 2.4 | 7 |
| 8 | Real-time prediction of ¹ H and ¹³ C chemical shifts with DFT accuracy using a 3D graph neural network. <i>Chemical Science</i> , 2021, 12, 12012-12026. | 3.7 | 50 |
| 9 | Asymmetric Total Synthesis and Determination of the Absolute Configuration of (+)-Srilankenyne via Sequence-Sensitive Halogenations Guided by Conformational Analysis. <i>Organic Letters</i> , 2021, 23, 1321-1326. | 2.4 | 5 |
| 10 | Importance of Engineered and Learned Molecular Representations in Predicting Organic Reactivity, Selectivity, and Chemical Properties. <i>Accounts of Chemical Research</i> , 2021, 54, 827-836. | 7.6 | 47 |
| 11 | Mechanistic investigation of Rh(I)-catalysed asymmetric Suzuki-Miyaura coupling with racemic allyl halides. <i>Nature Catalysis</i> , 2021, 4, 284-292. | 16.1 | 18 |
| 12 | Phosphorus-mediated sp ² -sp ³ couplings for C-H fluoroalkylation of azines. <i>Nature</i> , 2021, 594, 217-222. | 13.7 | 84 |
| 13 | Controlling Intramolecular Interactions in the Design of Selective, High-Affinity Ligands for the CREBBP Bromodomain. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 10102-10123. | 2.9 | 17 |
| 14 | Reactions of NO ₃ with aromatic aldehydes: gas-phase kinetics and insights into the mechanism of the reaction. <i>Atmospheric Chemistry and Physics</i> , 2021, 21, 13537-13551. | 1.9 | 7 |
| 15 | A quantitative metric for organic radical stability and persistence using thermodynamic and kinetic features. <i>Chemical Science</i> , 2021, 12, 13158-13166. | 3.7 | 30 |
| 16 | Unconventional Reactivity of Ethynylbenziodoxolone Reagents and Thiols: Scope and Mechanism. <i>Chemistry - A European Journal</i> , 2020, 26, 2386-2394. | 1.7 | 28 |
| 17 | Alkyne Linchpin Strategy for Drug:Pharmacophore Conjugation: Experimental and Computational Realization of a <i>Meta</i> -Selective Inverse Sonogashira Coupling. <i>Journal of the American Chemical Society</i> , 2020, 142, 3762-3774. | 6.6 | 111 |
| 18 | Effects of substituents X and Y on the NMR chemical shifts of 2-(4-X phenyl)-5-Y pyrimidines. <i>Journal of Molecular Structure</i> , 2020, 1204, 127489. | 1.8 | 6 |

| # | ARTICLE | IF | CITATIONS |
|----|--|------|-----------|
| 19 | Quantum chemical calculations for over 200,000 organic radical species and 40,000 associated closed-shell molecules. <i>Scientific Data</i> , 2020, 7, 244. | 2.4 | 49 |
| 20 | BIMPâ€Catalyzed 1,3â€Prototropic Shift for the Highly Enantioselective Synthesis of Conjugated Cyclohexenones. <i>Angewandte Chemie</i> , 2020, 132, 17570-17575. | 1.6 | 6 |
| 21 | Visibleâ€Lightâ€Mediated Heterocycle Functionalization via Geometrically Interrupted [2+2] Cycloaddition. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 23020-23024. | 7.2 | 29 |
| 22 | Visibleâ€Lightâ€Mediated Heterocycle Functionalization via Geometrically Interrupted [2+2] Cycloaddition. <i>Angewandte Chemie</i> , 2020, 132, 23220-23224. | 1.6 | 5 |
| 23 | Stereoretention in styrene heterodimerisation promoted by one-electron oxidants. <i>Chemical Science</i> , 2020, 11, 9309-9324. | 3.7 | 8 |
| 24 | Fungal-derived brevianamide assembly by a stereoselective semipinacolase. <i>Nature Catalysis</i> , 2020, 3, 497-506. | 16.1 | 47 |
| 25 | Prediction of organic homolytic bond dissociation enthalpies at near chemical accuracy with sub-second computational cost. <i>Nature Communications</i> , 2020, 11, 2328. | 5.8 | 128 |
| 26 | Selective Halogenation of Pyridines Using Designed Phosphine Reagents. <i>Journal of the American Chemical Society</i> , 2020, 142, 11295-11305. | 6.6 | 39 |
| 27 | Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. <i>Communications Chemistry</i> , 2020, 3, . | 2.0 | 13 |
| 28 | BIMPâ€Catalyzed 1,3â€Prototropic Shift for the Highly Enantioselective Synthesis of Conjugated Cyclohexenones. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 17417-17422. | 7.2 | 24 |
| 29 | Hydrogen Bonding Phase-Transfer Catalysis with Ionic Reactants: Enantioselective Synthesis of Î³-Fluoroamines. <i>Journal of the American Chemical Society</i> , 2020, 142, 14045-14051. | 6.6 | 53 |
| 30 | Ligand Design for Asymmetric Catalysis: Combining Mechanistic and Chemoinformatics Approaches. <i>Topics in Organometallic Chemistry</i> , 2020, , 153-189. | 0.7 | 1 |
| 31 | Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins. <i>Molecules</i> , 2020, 25, 1918. | 1.7 | 8 |
| 32 | Enantiomerically enriched tetrahydropyridine allyl chlorides. <i>Chemical Science</i> , 2020, 11, 4125-4130. | 3.7 | 8 |
| 33 | Experimental and theoretical insight into the soot tendencies of the methylcyclohexene isomers. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 1083-1090. | 2.4 | 13 |
| 34 | A Pyridineâ€Pyridine Crossâ€Coupling Reaction via Dearomatized Radical Intermediates. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 14882-14886. | 7.2 | 61 |
| 35 | Retooling Asymmetric Conjugate Additions for Sterically Demanding Substrates with an Iterative Data-Driven Approach. <i>ACS Catalysis</i> , 2019, 9, 7179-7187. | 5.5 | 26 |
| 36 | A Pyridineâ€Pyridine Crossâ€Coupling Reaction via Dearomatized Radical Intermediates. <i>Angewandte Chemie</i> , 2019, 131, 15024-15028. | 1.6 | 10 |

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 37 | Synthesis, Characterization, and Reactivity of Complex Tricyclic Oxonium Ions, Proposed Intermediates in Natural Product Biosynthesis. <i>Journal of the American Chemical Society</i> , 2019, 141, 15951-15962. | 6.6 | 10 |
| 38 | Fungal indole alkaloid biogenesis through evolution of a bifunctional reductase/Diels-Alderase. <i>Nature Chemistry</i> , 2019, 11, 972-980. | 6.6 | 52 |
| 39 | Frontier molecular orbital effects control the hole-catalyzed racemization of atropisomeric biaryls. <i>Chemical Science</i> , 2019, 10, 2285-2289. | 3.7 | 19 |
| 40 | Conformational Effects on Physical-Organic Descriptors: The Case of Sterimol Steric Parameters. <i>ACS Catalysis</i> , 2019, 9, 2313-2323. | 5.5 | 96 |
| 41 | Hydrogen Bonding Phase-Transfer Catalysis with Potassium Fluoride: Enantioselective Synthesis of β^2 -Fluoroamines. <i>Journal of the American Chemical Society</i> , 2019, 141, 2878-2883. | 6.6 | 94 |
| 42 | Palladium-Catalyzed Directed <i>meta</i> -Selective $C^{\alpha}H$ Allylation of Arenes: Unactivated Internal Olefins as Allyl Surrogates. <i>Angewandte Chemie</i> , 2019, 131, 10461-10468. | 1.6 | 24 |
| 43 | Palladium-Catalyzed Directed <i>meta</i> -Selective $C^{\alpha}H$ Allylation of Arenes: Unactivated Internal Olefins as Allyl Surrogates. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 10353-10360. | 7.2 | 76 |
| 44 | Iterative Arylation of Amino Acids and Aliphatic Amines via γ -C(sp ³) α H Activation: Experimental and Computational Exploration. <i>Angewandte Chemie</i> , 2019, 131, 5689-5694. | 1.6 | 26 |
| 45 | Structure Determination of a Chloroenyne from <i>Laurencia majuscula</i> Using Computational Methods and Total Synthesis. <i>Journal of Organic Chemistry</i> , 2019, 84, 4971-4991. | 1.7 | 18 |
| 46 | Iterative Arylation of Amino Acids and Aliphatic Amines via γ -C(sp ³) α H Activation: Experimental and Computational Exploration. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 5633-5638. | 7.2 | 90 |
| 47 | Biosynthesis of Providencin: Understanding Photochemical Cyclobutane Formation with Density Functional Theory. <i>Organic Letters</i> , 2019, 21, 1243-1247. | 2.4 | 14 |
| 48 | Data-mining the diaryl(thio)urea conformational landscape: Understanding the contrasting behavior of ureas and thioureas with quantum chemistry. <i>Tetrahedron</i> , 2019, 75, 697-702. | 1.0 | 20 |
| 49 | Non-Hydrolytic β -Lactam Antibiotic Fragmentation by β -Transpeptidases and Serine β -Lactamase Cysteine Variants. <i>Angewandte Chemie</i> , 2019, 131, 2012-2016. | 1.6 | 4 |
| 50 | Hydrogen-Bond-Dependent Conformational Switching: A Computational Challenge from Experimental Thermochemistry. <i>Journal of Organic Chemistry</i> , 2019, 84, 613-621. | 1.7 | 5 |
| 51 | Non-Hydrolytic β -Lactam Antibiotic Fragmentation by β -Transpeptidases and Serine β -Lactamase Cysteine Variants. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1990-1994. | 7.2 | 27 |
| 52 | Enantioselective rhodium-catalysed insertion of trifluorodiaoethanes into tin hydrides. <i>Tetrahedron</i> , 2019, 75, 17-25. | 1.0 | 12 |
| 53 | Hydrogen-Bond-Enabled Dynamic Kinetic Resolution of Axially Chiral Amides Mediated by a Chiral Counterion. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 2795-2798. | 7.2 | 48 |
| 54 | Evolution of a bifunctional reductase/Diels-Alderase for fungal indole alkaloid biosynthesis. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, a244-a245. | 0.0 | 0 |

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 55 | Recognition of shorter and longer trimethyllysine analogues by epigenetic reader proteins. <i>Chemical Communications</i> , 2018, 54, 2409-2412. | 2.2 | 15 |
| 56 | A New Mechanism for β -Lactamases: Class D Enzymes Degrade β -Methyl Carbapenems through Lactone Formation. <i>Angewandte Chemie</i> , 2018, 130, 1296-1299. | 1.6 | 4 |
| 57 | Formation of quaternary centres by copper catalysed asymmetric conjugate addition to β -substituted cyclopentenones with the aid of a quantitative structure-selectivity relationship. <i>Chemical Science</i> , 2018, 9, 2628-2632. | 3.7 | 29 |
| 58 | Cation- π interactions in protein-ligand binding: theory and data-mining reveal different roles for lysine and arginine. <i>Chemical Science</i> , 2018, 9, 2655-2665. | 3.7 | 184 |
| 59 | NMR Prediction. , 2018, , 165-189. | | 2 |
| 60 | The True Catalyst Revealed: The Intervention of Chiral Ca and Mg Phosphates in Brønsted Acid Promoted Asymmetric Mannich Reactions. <i>Journal of the American Chemical Society</i> , 2018, 140, 5412-5420. | 6.6 | 21 |
| 61 | Experimental and theoretical study of oxidative stability of alkylated furans used as gasoline blend components. <i>Fuel</i> , 2018, 212, 576-585. | 3.4 | 31 |
| 62 | A New Mechanism for β -Lactamases: Class D Enzymes Degrade β -Methyl Carbapenems through Lactone Formation. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 1282-1285. | 7.2 | 27 |
| 63 | Asymmetric Total Syntheses and Structure Confirmation of Chlorofucins and Bromofucins. <i>Chemistry - A European Journal</i> , 2018, 24, 2634-2642. | 1.7 | 12 |
| 64 | Direct sulfonylation of anilines mediated by visible light. <i>Chemical Science</i> , 2018, 9, 629-633. | 3.7 | 61 |
| 65 | Selectivity in Transition Metal-catalyzed Cyclizations: Insights from Experiment and Theory. <i>Chimia</i> , 2018, 72, 614. | 0.3 | 0 |
| 66 | Heterobiaryl synthesis by contractive C-C coupling via P(V) intermediates. <i>Science</i> , 2018, 362, 799-804. | 6.0 | 145 |
| 67 | Catalytic Enantio- and Diastereoselective Mannich Addition of TosMIC to Ketimines. <i>Chemistry - A European Journal</i> , 2018, 24, 17660-17664. | 1.7 | 17 |
| 68 | Stereospecific 1,3-H Transfer of Indenols Proceeds via Persistent Ion-Pairs Anchored by NH \cdots π Interactions. <i>Journal of the American Chemical Society</i> , 2018, 140, 16740-16748. | 6.6 | 29 |
| 69 | Post-translational site-selective protein backbone α -deuteration. <i>Nature Chemical Biology</i> , 2018, 14, 955-963. | 3.9 | 27 |
| 70 | Bifunctional iminophosphorane catalysed enantioselective sulfa-Michael addition of alkyl thiols to alkenyl benzimidazoles. <i>Chemical Science</i> , 2018, 9, 6969-6974. | 3.7 | 66 |
| 71 | Asymmetric nucleophilic fluorination under hydrogen bonding phase-transfer catalysis. <i>Science</i> , 2018, 360, 638-642. | 6.0 | 137 |
| 72 | Dynamic Intermediates in the Radical Cation Diels-Alder Cycloaddition: Lifetime and Suprafacial Stereoselectivity. <i>Organic Letters</i> , 2018, 20, 2821-2825. | 2.4 | 20 |

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 73 | Asymmetric Total Synthesis and Structure Confirmation of (+)-(3E)-Isolaurefucin Methyl Ether. <i>Heterocycles</i> , 2018, 97, 179. | 0.4 | 4 |
| 74 | Correlating Reactivity and Selectivity to Cyclopentadienyl Ligand Properties in Rh(III)-Catalyzed C-H Activation Reactions: An Experimental and Computational Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 1296-1310. | 6.6 | 169 |
| 75 | Divergent Photocyclization/1,4-Sigmatropic Rearrangements for the Synthesis of Sesquiterpenoid Derivatives. <i>Organic Letters</i> , 2017, 19, 484-487. | 2.4 | 7 |
| 76 | Enantioselective Silver and Amine Co-catalyzed Desymmetrizing Cycloisomerization of Alkyne-Linked Cyclohexanones. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 5834-5838. | 7.2 | 47 |
| 77 | Enantioselective Silver and Amine Co-catalyzed Desymmetrizing Cycloisomerization of Alkyne-Linked Cyclohexanones. <i>Angewandte Chemie</i> , 2017, 129, 5928-5932. | 1.6 | 18 |
| 78 | Structural and stereoelectronic insights into oxygenase-catalyzed formation of ethylene from 2-oxoglutarate. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 4667-4672. | 3.3 | 45 |
| 79 | Visible Light Photocatalysis of 6-Heterocyclization. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9468-9472. | 7.2 | 79 |
| 80 | Dual Gold-Catalyzed Three-Component Reaction: Efficient Synthesis of Indene-Fused Esters, Acids, and Lactones through Gold Vinylidene Intermediates. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 1561-1565. | 1.2 | 7 |
| 81 | Phosphazene Catalyzed Addition to Electron-Deficient Alkynes: The Importance of Nonlinear Allenyl Intermediates upon Stereoselectivity. <i>Journal of Organic Chemistry</i> , 2017, 82, 3855-3863. | 1.7 | 24 |
| 82 | Detailed Mechanistic Studies on Palladium-Catalyzed Selective C-H Olefination with Aliphatic Alkenes: A Significant Influence of Proton Shuttling. <i>Journal of the American Chemical Society</i> , 2017, 139, 763-775. | 6.6 | 99 |
| 83 | Asymmetric Induction in C-Alkylation of Tropane-Derived Enamines: Congruence Between Computation and Experiment. <i>Journal of Organic Chemistry</i> , 2017, 82, 10479-10488. | 1.7 | 9 |
| 84 | C-H Cyanation of 6-Ring N-Containing Heteroaromatics. <i>Chemistry - A European Journal</i> , 2017, 23, 14733-14737. | 1.7 | 31 |
| 85 | Enantioselective Conjugate Addition Catalyzed by a Copper Phosphoramidite Complex: Computational and Experimental Exploration of Asymmetric Induction. <i>ACS Catalysis</i> , 2017, 7, 6729-6737. | 5.5 | 31 |
| 86 | Investigating lysine stereochemistry for epigenetic methylation, demethylation and recognition. <i>Chemical Communications</i> , 2017, 53, 13264-13267. | 2.2 | 29 |
| 87 | Construction of 6,10-syn- and -anti-2,5-Dioxabicyclo[2.2.1]heptane Skeletons via Oxonium Ion Formation/Fragmentation: Prediction of Structure of (<i>E</i>)-Ocellenyne by NMR Calculation. <i>Organic Letters</i> , 2017, 19, 6252-6255. | 2.4 | 5 |
| 88 | Total Synthesis of ($\hat{\alpha}$)-Himalensine A. <i>Journal of the American Chemical Society</i> , 2017, 139, 17755-17758. | 6.6 | 146 |
| 89 | Visible Light Photocatalysis of 6-Heterocyclization. <i>Angewandte Chemie</i> , 2017, 129, 9596-9600. | 1.6 | 17 |
| 90 | Mechanistic Insight into Palladium-Catalyzed Cycloisomerization: A Combined Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 10104-10114. | 6.6 | 58 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|------|-----------|
| 91 | Molecular Recognition in Asymmetric Counteranion Catalysis: Understanding Chiral Phosphate-Mediated Desymmetrization. <i>Journal of the American Chemical Society</i> , 2017, 139, 8886-8896. | 6.6 | 47 |
| 92 | Adenosine Monophosphate Binding Stabilizes the KTN Domain of the <i>Shewanella denitrificans</i> Kef Potassium Efflux System. <i>Biochemistry</i> , 2017, 56, 4219-4234. | 1.2 | 9 |
| 93 | Heptamethylindenyl (Ind*) enables diastereoselective benzamidation of cyclopropenes via Rh-catalyzed C-H activation. <i>Chemical Science</i> , 2017, 8, 1015-1020. | 3.7 | 95 |
| 94 | Furan Production from Glycoaldehyde over HZSM-5. <i>ACS Sustainable Chemistry and Engineering</i> , 2016, 4, 2615-2623. | 3.2 | 19 |
| 95 | Development of a True Transition State Force Field from Quantum Mechanical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1833-1844. | 2.3 | 27 |
| 96 | Mechanisms of histone lysine-modifying enzymes: A computational perspective on the role of the protein environment. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 67, 69-84. | 1.3 | 12 |
| 97 | Catalytic Control in Cyclizations: From Computational Mechanistic Understanding to Selectivity Prediction. <i>Accounts of Chemical Research</i> , 2016, 49, 1042-1051. | 7.6 | 71 |
| 98 | A Counterion-Directed Approach to the Diels-Alder Paradigm: Cascade Synthesis of Tricyclic Fused Cyclopropanes. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 13813-13817. | 7.2 | 9 |
| 99 | Synthesis of malhamensilipin A exploiting iterative epoxidation/chlorination: experimental and computational analysis of epoxide-derived chloronium ions. <i>Chemical Science</i> , 2016, 7, 7040-7049. | 3.7 | 13 |
| 100 | Computing organic stereoselectivity from concepts to quantitative calculations and predictions. <i>Chemical Society Reviews</i> , 2016, 45, 6093-6107. | 18.7 | 175 |
| 101 | A Counterion-Directed Approach to the Diels-Alder Paradigm: Cascade Synthesis of Tricyclic Fused Cyclopropanes. <i>Angewandte Chemie</i> , 2016, 128, 14017-14021. | 1.6 | 3 |
| 102 | Cation interactions in CREBBP bromodomain inhibition: an electrostatic model for small-molecule binding affinity and selectivity. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 10926-10938. | 1.5 | 27 |
| 103 | Investigations on recyclisation and hydrolysis in avibactam mediated serine β -lactamase inhibition. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 4116-4128. | 1.5 | 23 |
| 104 | Computational ligand design in enantio- and diastereoselective ynamide [5+2] cycloisomerization. <i>Nature Communications</i> , 2016, 7, 10109. | 5.8 | 110 |
| 105 | QM/MM study on the enantioselectivity of spiroacetalization catalysed by an imidodiphosphoric acid catalyst: how confinement works. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3031-3039. | 1.5 | 24 |
| 106 | Unraveling innate substrate control in site-selective palladium-catalyzed C-H heterocycle functionalization. <i>Chemical Science</i> , 2016, 7, 3900-3909. | 3.7 | 58 |
| 107 | Dioxygen Binding in the Active Site of Histone Demethylase JMJD2A and the Role of the Protein Environment. <i>Chemistry - A European Journal</i> , 2015, 21, 18869-18869. | 1.7 | 1 |
| 108 | Dioxygen Binding in the Active Site of Histone Demethylase JMJD2A and the Role of the Protein Environment. <i>Chemistry - A European Journal</i> , 2015, 21, 18983-18992. | 1.7 | 17 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 109 | Substrate-Controlled Asymmetric Total Syntheses of Microcladallenesâ€¦A, B, and C Based on the Proposed Structures. <i>Chemistry - A European Journal</i> , 2015, 21, 15988-15997. | 1.7 | 22 |
| 110 | Role of Hydrogenâ€¦Bonding Acceptors in Organoâ€¦Enamine Catalysis. <i>Chemistry - A European Journal</i> , 2015, 21, 11687-11691. | 1.7 | 15 |
| 111 | Origins of Asymmetric Phosphazene Organocatalysis: Computations Reveal a Common Mechanism for Nitro- and Phospho-Aldol Additions. <i>Journal of Organic Chemistry</i> , 2015, 80, 2756-2766. | 1.7 | 30 |
| 112 | Small Molecule Inhibitors of Bromodomainâ€¦Acetyl-lysine Interactions. <i>ACS Chemical Biology</i> , 2015, 10, 22-39. | 1.6 | 156 |
| 113 | Catalytic enantioselective synthesis of indanes by a cation-directed 5-endo-trig cyclization. <i>Nature Chemistry</i> , 2015, 7, 171-177. | 6.6 | 87 |
| 114 | Enantioselective Desymmetrization of Prochiral Cyclohexanones by Organocatalytic Intramolecular Michael Additions to Î±,Î²â€¦Unsaturated Esters. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 4899-4903. | 7.2 | 73 |
| 115 | Coordination diversity in hydrogen-bonded homoleptic fluorideâ€¦alcohol complexes modulates reactivity. <i>Chemical Science</i> , 2015, 6, 5293-5302. | 3.7 | 74 |
| 116 | Thermal and Photochemical Mechanisms for Cyclobutane Formation in Bielschowskysin Biosynthesis. <i>Synlett</i> , 2015, 26, 501-507. | 1.0 | 9 |
| 117 | Ethanol Dehydration in HZSM-5 Studied by Density Functional Theory: Evidence for a Concerted Process. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3604-3614. | 1.1 | 44 |
| 118 | Î±- and Î±â€¦2-Lithiationâ€¦Electrophile Trapping of <i>N</i>-Thiopivaloyl and <i>N</i>-<i>tert</i>-<i>Butoxythiocarbonyl</i>-Substituted Azetidines: Rationalization of the Regiodivergence Using NMR and Computation. <i>Journal of Organic Chemistry</i> , 2015, 80, 9838-9846. | 1.7 | 21 |
| 119 | Quantum mechanical calculations suggest that lytic polysaccharide monooxygenases use a copper-oxyl, oxygen-rebound mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 149-154. | 3.3 | 210 |
| 120 | Asymmetric Total Synthesis of (+)â€¦Bermudenynol, a C₁₅<i>Laurencia</i> Metabolite with a Vinyl Chloride Containing Oxocene Skeleton, through Intramolecular Amide Enolate Alkylation. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 272-276. | 7.2 | 36 |
| 121 | Ligand Bite Angleâ€¦Dependent Palladiumâ€¦Catalyzed Cyclization of Propargylic Carbonates to 2â€¦Alkynyl Azacycles or Cyclic Dienamides. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 1915-1920. | 7.2 | 48 |
| 122 | Intramolecular Dielsâ€¦Alder Reactions of Cycloalkenones: Stereoselectivity, Lewis Acid Acceleration, and Halogen Substituent Effects. <i>Journal of the American Chemical Society</i> , 2014, 136, 2397-2403. | 6.6 | 46 |
| 123 | Phaseâ€¦Transferâ€¦Catalysed Synthesis of Pyrroloindolines and Pyridoindolines by a Hydrogenâ€¦Bondâ€¦Assisted Isocyanide Cyclization Cascade. <i>Chemistry - A European Journal</i> , 2014, 20, 3005-3009. | 1.7 | 18 |
| 124 | It's all downhill from here. <i>Nature Chemistry</i> , 2014, 6, 88-89. | 6.6 | 15 |
| 125 | A Series of Potent CREBBP Bromodomain Ligands Reveals an Inducedâ€¦Fit Pocket Stabilized by a Cationâ€¦Î¶ Interaction. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 6126-6130. | 7.2 | 108 |
| 126 | A Mechanistic Investigation of Acid-Catalyzed Cleavage of Aryl-Ether Linkages: Implications for Lignin Depolymerization in Acidic Environments. <i>ACS Sustainable Chemistry and Engineering</i> , 2014, 2, 472-485. | 3.2 | 317 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|------|-----------|
| 127 | Dissecting non-covalent interactions in oxazaborolidinium catalyzed cycloadditions of maleimides. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 1717. | 1.5 | 29 |
| 128 | Rapid Cross-Metathesis for Reversible Protein Modifications via Chemical Access to α -Se-Allyl-selenocysteine in Proteins. <i>Journal of the American Chemical Society</i> , 2013, 135, 12156-12159. | 6.6 | 109 |
| 129 | Structure Reassignment of Laurefurenynes A and B by Computation and Total Synthesis. <i>Chemistry - A European Journal</i> , 2013, 19, 12644-12648. | 1.7 | 31 |
| 130 | Mechanistic Investigations into the Enantioselective Conia-Ene Reaction Catalyzed by Cinchona-Derived Amino Urea Pre-Catalysts and Cu(I). <i>Chemistry - A European Journal</i> , 2013, 19, 14286-14295. | 1.7 | 30 |
| 131 | Enhanced Reactivity in Dioxirane C-H Oxidations via Strain Release: A Computational and Experimental Study. <i>Journal of Organic Chemistry</i> , 2013, 78, 4037-4048. | 1.7 | 74 |
| 132 | Mechanistic Study of a Ru-Xantphos Catalyst for Tandem Alcohol Dehydrogenation and Reductive Aryl-Ether Cleavage. <i>ACS Catalysis</i> , 2013, 3, 963-974. | 5.5 | 42 |
| 133 | α -Alkylation of Chiral Tropane- and Homotropane-Derived Enamines. <i>Journal of Organic Chemistry</i> , 2013, 78, 1508-1518. | 1.7 | 12 |
| 134 | Computational organic chemistry. <i>Annual Reports on the Progress of Chemistry Section B</i> , 2013, 109, 235. | 0.8 | 15 |
| 135 | Diels-Alder Reactivities of Strained and Unstrained Cycloalkenes with Normal and Inverse-Electron-Demand Dienes: Activation Barriers and Distortion/Interaction Analysis. <i>Journal of the American Chemical Society</i> , 2013, 135, 15642-15649. | 6.6 | 165 |
| 136 | Synthesis of Cyclic β -Aminophosphonates through Copper-Catalyzed Enamine Activation. <i>Synthesis</i> , 2013, 45, 463-470. | 1.2 | 10 |
| 137 | Concise Substrate-Controlled Asymmetric Total Syntheses of Dioxabicyclic Marine Natural Products with 2,10-Dioxabicyclo-[7.3.0]dodecene and 2,9-Dioxabicyclo[6.3.0]undecene Skeletons. <i>Journal of the American Chemical Society</i> , 2012, 134, 20178-20188. | 6.6 | 35 |
| 138 | Enzymatic catalysis of anti-Baldwin ring closure in polyether biosynthesis. <i>Nature</i> , 2012, 483, 355-358. | 13.7 | 117 |
| 139 | Unusual Base-Induced Rearrangement of exo-9-Oxabicyclo[4.2.1]non-7-ene Oxide to exo-8-Hydroxybicyclo[3.3.0]octan-2-one. <i>Heterocycles</i> , 2012, 84, 625. | 0.4 | 6 |
| 140 | Dinuclear Palladium Complexes as Precursors or Catalysts?. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 10448-10450. | 7.2 | 50 |
| 141 | An Efficient Computational Model to Predict the Synthetic Utility of Heterocyclic Arynes. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 2758-2762. | 7.2 | 96 |
| 142 | Unraveling the Mechanism of Cascade Reactions of Zincke Aldehydes. <i>Journal of the American Chemical Society</i> , 2011, 133, 3895-3905. | 6.6 | 88 |
| 143 | Computational Study of Bond Dissociation Enthalpies for a Large Range of Native and Modified Lignins. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2846-2852. | 2.1 | 318 |
| 144 | A stereoselective total synthesis of (β)-tormesol. <i>Tetrahedron</i> , 2011, 67, 10017-10025. | 1.0 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 145 | Experimental Diels-Alder Reactivities of Cycloalkenones and Cyclic Dienes Explained through Transition-State Distortion Energies. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 10366-10368. | 7.2 | 125 |
| 146 | Gold-Catalyzed, Intramolecular, Oxygen-Transfer Reactions of 2-Alkynyl-1,5-diketones or 2-Alkynyl-5-ketoesters: Scope, Expansion, and Mechanistic Investigations on a New [4+2] Cycloaddition. <i>Chemistry - A European Journal</i> , 2011, 17, 10690-10699. | 1.7 | 17 |
| 147 | Indolyne and Aryne Distortions and Nucleophilic Regioselectivities. <i>Journal of the American Chemical Society</i> , 2010, 132, 1267-1269. | 6.6 | 225 |
| 148 | The [4+2], not [2+2], Mechanism Occurs in the Gold-Catalyzed Intramolecular Oxygen Transfer Reaction of 2-Alkynyl-1,5-Diketones. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 9132-9135. | 7.2 | 35 |
| 149 | Origins of Regioselectivity of Diels-Alder Reactions for the Synthesis of Bisanthraquinone Antibiotic BE-43472B. <i>Journal of Organic Chemistry</i> , 2010, 75, 922-928. | 1.7 | 18 |
| 150 | Indolyne Experimental and Computational Studies: Synthetic Applications and Origins of Selectivities of Nucleophilic Additions. <i>Journal of the American Chemical Society</i> , 2010, 132, 17933-17944. | 6.6 | 215 |
| 151 | Origins of Stereoselectivity in the <i>trans</i> Diels-Alder Paradigm. <i>Journal of the American Chemical Society</i> , 2010, 132, 9335-9340. | 6.6 | 101 |
| 152 | Mechanistic Insights into the Catalytic Asymmetric Allylboration of Ketones: Brønsted or Lewis Acid Activation?. <i>Organic Letters</i> , 2009, 11, 37-40. | 2.4 | 41 |
| 153 | Gold(I)-Catalyzed Intermolecular Hydroalkoxylation of Allenes: A DFT study. <i>Organic Letters</i> , 2009, 11, 2237-2240. | 2.4 | 118 |
| 154 | Hydrogen Bonding and π -Stacking: How Reliable are Force Fields? A Critical Evaluation of Force Field Descriptions of Nonbonded Interactions. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 944-955. | 2.5 | 161 |
| 155 | Stereostructure Assignment of Flexible Five-Membered Rings by GIAO ^{13}C NMR Calculations: Prediction of the Stereochemistry of Elatenyne. <i>Journal of Organic Chemistry</i> , 2008, 73, 4053-4062. | 1.7 | 82 |
| 156 | Theoretical Study of the Asymmetric Conjugate Alkenylation of Enones Catalyzed by Binaphthols. <i>Journal of Organic Chemistry</i> , 2008, 73, 5078-5089. | 1.7 | 54 |
| 157 | 1,5-Anti Stereocontrol in the Boron-Mediated Aldol Reactions of β^2 -Alkoxy Methyl Ketones: The Role of the Formyl Hydrogen Bond. <i>Journal of Organic Chemistry</i> , 2008, 73, 1253-1263. | 1.7 | 65 |
| 158 | Enantioselectivity in the boron aldol reactions of methyl ketones. <i>Chemical Communications</i> , 2007, , 2124. | 2.2 | 28 |
| 159 | Exploration of the Accessible Chemical Space of Acyclic Alkanes. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 2124-2132. | 2.5 | 15 |
| 160 | Understanding the Origins of Remote Asymmetric Induction in the Boron Aldol Reactions of β^2 -Alkoxy Methyl Ketones. <i>Organic Letters</i> , 2006, 8, 4299-4302. | 2.4 | 67 |
| 161 | GoodVibes: automated thermochemistry for heterogeneous computational chemistry data. <i>F1000Research</i> , 0, 9, 291. | 0.8 | 212 |
| 162 | Modeling Catalysis in Allosteric Enzymes: Capturing Conformational Consequences. <i>Topics in Catalysis</i> , 0, , 1. | 1.3 | 3 |