

Kendall Houk

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730 papers	40,336 citations	100 h-index	169 g-index
779 ext. papers	45,982 ext. citations	12.3 avg, IF	7.93 L-index

#	Paper	IF	Citations
730	Benchmarking the Conductor-like Polarizable Continuum Model (CPCM) for Aqueous Solvation Free Energies of Neutral and Ionic Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2005 , 1, 70-7	6.4	833
729	Distortion/interaction energy control of 1,3-dipolar cycloaddition reactivity. <i>Journal of the American Chemical Society</i> , 2007 , 129, 10646-7	16.4	674
728	Computational design of an enzyme catalyst for a stereoselective bimolecular Diels-Alder reaction. <i>Science</i> , 2010 , 329, 309-13	33.3	652
727	Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 10070-10086	16.4	649
726	Origin of reactivity, regioselectivity, and periselectivity in 1,3-dipolar cycloadditions. <i>Journal of the American Chemical Society</i> , 1973 , 95, 7301-7315	16.4	632
725	Theory of 1,3-dipolar cycloadditions: distortion/interaction and frontier molecular orbital models. <i>Journal of the American Chemical Society</i> , 2008 , 130, 10187-98	16.4	627
724	Frontier molecular orbital theory of cycloaddition reactions. <i>Accounts of Chemical Research</i> , 1975 , 8, 361-369	16.4	619
723	Pericyclic Reaction Transition States: Passions and Punctilios, 1935-1995. <i>Accounts of Chemical Research</i> , 1995 , 28, 81-90	24.3	558
722	Transition Structures of Hydrocarbon Pericyclic Reactions. <i>Angewandte Chemie International Edition in English</i> , 1992 , 31, 682-708		512
721	Frontier molecular orbitals of 1,3 dipoles and dipolarophiles. <i>Journal of the American Chemical Society</i> , 1973 , 95, 7287-7301	16.4	507
720	Quantum mechanical predictions of the stereoselectivities of proline-catalyzed asymmetric intermolecular aldol reactions. <i>Journal of the American Chemical Society</i> , 2003 , 125, 2475-9	16.4	497
719	Density Functional Theory Prediction of the Relative Energies and Isotope Effects for the Concerted and Stepwise Mechanisms of the Diels-Alder Reaction of Butadiene and Ethylene. <i>Journal of the American Chemical Society</i> , 1996 , 118, 6036-6043	16.4	470
718	Binding affinities of host-guest, protein-ligand, and protein-transition-state complexes. <i>Angewandte Chemie - International Edition</i> , 2003 , 42, 4872-97	16.4	442
717	Constructive molecular configurations for surface-defect passivation of perovskite photovoltaics. <i>Science</i> , 2019 , 366, 1509-1513	33.3	434
716	A hierarchy of homodesmotic reactions for thermochemistry. <i>Journal of the American Chemical Society</i> , 2009 , 131, 2547-60	16.4	418
715	Substituent effects in the benzene dimer are due to direct interactions of the substituents with the unsubstituted benzene. <i>Journal of the American Chemical Society</i> , 2008 , 130, 10854-5	16.4	385
714	Conversion of amides to esters by the nickel-catalysed activation of amide C-N bonds. <i>Nature</i> , 2015 , 524, 79-83	50.4	377

713	Computational enzyme design. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 5700-25	16.4	351
712	Polyacene and cyclacene geometries and electronic structures: bond equalization, vanishing band gaps, and triplet ground states contrast with polyacetylene. <i>Journal of Organic Chemistry</i> , 2001 , 66, 5517-21	16.4	275
711	Generalized frontier orbitals of alkenes and dienes. Regioselectivity in Diels-Alder reactions. <i>Journal of the American Chemical Society</i> , 1973 , 95, 4092-4094	16.4	275
710	Palladium-catalyzed meta-selective C-H bond activation with a nitrile-containing template: computational study on mechanism and origins of selectivity. <i>Journal of the American Chemical Society</i> , 2014 , 136, 344-55	16.4	270
709	Bifurcations on potential energy surfaces of organic reactions. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 7592-601	16.4	262
708	Suzuki-Miyaura cross-coupling of aryl carbamates and sulfamates: experimental and computational studies. <i>Journal of the American Chemical Society</i> , 2011 , 133, 6352-63	16.4	260
707	Electronic Control of Stereoselectivities of Electrocyclic Reactions of Cyclobutenes: A Triumph of Theory in the Prediction of Organic Reactions. <i>Accounts of Chemical Research</i> , 1996 , 29, 471-477	24.3	259
706	Ligand-accelerated enantioselective methylene C(sp ³)-H bond activation. <i>Science</i> , 2016 , 353, 1023-1027	33.3	248
705	Stereoselective nitrile oxide cycloadditions to chiral allyl ethers and alcohols. The inside alkoxy effect. <i>Journal of the American Chemical Society</i> , 1984 , 106, 3880-3882	16.4	247
704	Computational prediction of small-molecule catalysts. <i>Nature</i> , 2008 , 455, 309-13	50.4	244
703	The origin of stereoselectivity in proline-catalyzed intramolecular aldol reactions. <i>Journal of the American Chemical Society</i> , 2001 , 123, 12911-2	16.4	236
702	Role of N-acyl amino acid ligands in Pd(II)-catalyzed remote C-H activation of tethered arenes. <i>Journal of the American Chemical Society</i> , 2014 , 136, 894-7	16.4	233
701	Origin of regioselectivity in palladium-catalyzed cross-coupling reactions of polyhalogenated heterocycles. <i>Journal of the American Chemical Society</i> , 2007 , 129, 12664-5	16.4	225
700	Stereoselective substituent effects on conrotatory electrocyclic reactions of cyclobutenes. <i>Journal of the American Chemical Society</i> , 1984 , 106, 7989-7991	16.4	225
699	Mechanism of ene reactions of singlet oxygen. A two-step no-intermediate mechanism. <i>Journal of the American Chemical Society</i> , 2003 , 125, 1319-28	16.4	224
698	Lewis acid catalysis of Diels-Alder reactions. <i>Journal of the American Chemical Society</i> , 1973 , 95, 4094-4096	16.4	224
697	The role of aryne distortions, steric effects, and charges in regioselectivities of aryne reactions. <i>Journal of the American Chemical Society</i> , 2014 , 136, 15798-805	16.4	207
696	Indolyne and aryne distortions and nucleophilic regioselectivities. <i>Journal of the American Chemical Society</i> , 2010 , 132, 1267-9	16.4	204

695	Experimental and Theoretical Kinetic Isotope Effects for Asymmetric Dihydroxylation. Evidence Supporting a Rate-Limiting (3 + 2) Cycloaddition. <i>Journal of the American Chemical Society</i> , 1997 , 119, 9907-9908	16.4	204
694	Ligand-controlled regioselectivity in palladium-catalyzed cross coupling reactions. <i>Journal of the American Chemical Society</i> , 2010 , 132, 2496-7	16.4	201
693	Control of the exo and endo pathways of the Diels-Alder reaction by antibody catalysis. <i>Science</i> , 1993 , 262, 204-8	33.3	201
692	Reactivity of biarylazacyclooctynones in copper-free click chemistry. <i>Journal of the American Chemical Society</i> , 2012 , 134, 9199-208	16.4	200
691	Computational evidence for the enamine mechanism of intramolecular aldol reactions catalyzed by proline. <i>Angewandte Chemie - International Edition</i> , 2004 , 43, 5765-8	16.4	197
690	Theozymes and compuzymes: theoretical models for biological catalysis. <i>Current Opinion in Chemical Biology</i> , 1998 , 2, 743-50	9.7	196
689	The magnitude of [C-H...O] hydrogen bonding in molecular and supramolecular assemblies. <i>Journal of the American Chemical Society</i> , 2001 , 123, 9264-7	16.4	194
688	Mechanisms and origins of switchable chemoselectivity of Ni-catalyzed C(aryl)-O and C(acyl)-O activation of aryl esters with phosphine ligands. <i>Journal of the American Chemical Society</i> , 2014 , 136, 2017-25	16.4	191
687	Reactivity and regioselectivity in 1,3-dipolar cycloadditions of azides to strained alkynes and alkenes: a computational study. <i>Journal of the American Chemical Society</i> , 2009 , 131, 8121-33	16.4	185
686	Extended Hartree-Fock (EHF) theory of chemical reactions. <i>Theoretica Chimica Acta</i> , 1988 , 73, 337-364		185
685	Aromatic interactions as control elements in stereoselective organic reactions. <i>Accounts of Chemical Research</i> , 2013 , 46, 979-89	24.3	183
684	Indolyne experimental and computational studies: synthetic applications and origins of selectivities of nucleophilic additions. <i>Journal of the American Chemical Society</i> , 2010 , 132, 17933-44	16.4	182
683	Distortion/Interaction analysis reveals the origins of selectivities in iridium-catalyzed C-H borylation of substituted arenes and 5-membered heterocycles. <i>Journal of the American Chemical Society</i> , 2014 , 136, 4575-83	16.4	179
682	Magnitudes and chemical consequences of R(3)N(+)-C-H...O[double bond]C hydrogen bonding. <i>Journal of the American Chemical Society</i> , 2002 , 124, 7163-9	16.4	175
681	Through-Space Effects of Substituents Dominate Molecular Electrostatic Potentials of Substituted Arenes. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 2301-2312	6.4	171
680	Substituent effects in cation/pi interactions and electrostatic potentials above the centers of substituted benzenes are due primarily to through-space effects of the substituents. <i>Journal of the American Chemical Society</i> , 2009 , 131, 3126-7	16.4	170
679	Transition states of strain-promoted metal-free click chemistry: 1,3-dipolar cycloadditions of phenyl azide and cyclooctynes. <i>Organic Letters</i> , 2008 , 10, 1633-6	6.2	167
678	Palladium-Catalyzed Suzuki-Miyaura Coupling of Aryl Esters. <i>Journal of the American Chemical Society</i> , 2017 , 139, 1311-1318	16.4	165

- 677 Transition States of Epoxidations: π -Diradical Character, Spiro Geometries, Transition State Flexibility, and the Origins of Stereoselectivity. *Journal of the American Chemical Society*, **1997**, 119, 10147-10152 ^{16.4} ¹⁶⁴
- 676 Hetero-Diels-Alder reaction transition structures: reactivity, stereoselectivity, catalysis, solvent effects, and the exo-lone-pair effect. *Journal of Organic Chemistry*, **1993**, 58, 3330-3343 ^{4.2} ¹⁶³
- 675 Probing substituent effects in aryl-aryl interactions using stereoselective Diels-Alder cycloadditions. *Journal of the American Chemical Society*, **2010**, 132, 3304-11 ^{16.4} ¹⁵⁹
- 674 Z-Selectivity in olefin metathesis with chelated Ru catalysts: computational studies of mechanism and selectivity. *Journal of the American Chemical Society*, **2012**, 134, 1464-7 ^{16.4} ¹⁵⁷
- 673 Experimental-Computational Synergy for Selective Pd(II)-Catalyzed C-H Activation of Aryl and Alkyl Groups. *Accounts of Chemical Research*, **2017**, 50, 2853-2860 ^{24.3} ¹⁵⁰
- 672 Sources of error in DFT computations of C-C bond formation thermochemistries: $\pi \rightarrow \sigma$ transformations and error cancellation by DFT methods. *Angewandte Chemie - International Edition*, **2008**, 47, 7746-9 ^{16.4} ¹⁴⁸
- 671 Diels-Alder reactivities of strained and unstrained cycloalkenes with normal and inverse-electron-demand dienes: activation barriers and distortion/interaction analysis. *Journal of the American Chemical Society*, **2013**, 135, 15642-9 ^{16.4} ¹⁴⁶
- 670 Dynamics, transition states, and timing of bond formation in Diels-Alder reactions. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 12860-5 ^{11.5} ¹⁴⁴
- 669 From Porphyrin Isomers to Octapyrrolic Figure Eight π -Macrocycles. *Angewandte Chemie International Edition in English*, **1995**, 34, 2511-2514 ¹⁴³
- 668 Das Distortion/Interaction-Activation-Strain-Modell zur Analyse von Reaktionsgeschwindigkeiten. *Angewandte Chemie*, **2017**, 129, 10204-10221 ^{3.6} ¹³⁶
- 667 Theoretical study of the molecular ordering, paracrystallinity, and charge mobilities of oligomers in different crystalline phases. *Journal of the American Chemical Society*, **2015**, 137, 2856-66 ^{16.4} ¹³⁶
- 666 The role of distant mutations and allosteric regulation on LovD active site dynamics. *Nature Chemical Biology*, **2014**, 10, 431-6 ^{11.7} ¹³²
- 665 Why delta-valerolactone polymerizes and gamma-butyrolactone does not. *Journal of Organic Chemistry*, **2008**, 73, 2674-8 ^{4.2} ¹³⁰
- 664 Diels-Alder and ene reactions of singlet oxygen, nitroso compounds and triazolinediones: transition states and mechanisms from contemporary theory. *Chemical Communications*, **2002**, 1243-55 ^{5.8} ¹²⁹
- 663 Transition state distortion energies correlate with activation energies of 1,4-dihydrogenations and Diels-Alder cycloadditions of aromatic molecules. *Journal of the American Chemical Society*, **2009**, 131, 4084-9 ^{16.4} ¹²⁸
- 662 The Mechanism of the Slippage Approach to Rotaxanes. Origin of the π -All-or-Nothing π -Substituent Effect π . *Journal of the American Chemical Society*, **1998**, 120, 9318-9322 ^{16.4} ¹²⁸
- 661 Synchronous or Asynchronous? An Experimental π -Transition State from a Direct Comparison of Experimental and Theoretical Kinetic Isotope Effects for a Diels-Alder Reaction. *Journal of the American Chemical Society*, **1996**, 118, 9984-9985 ^{16.4} ¹²⁸
- 660 Short, Strong Hydrogen Bonds in the Gas Phase and in Solution: Theoretical Exploration of pKa Matching and Environmental Effects on the Strengths of Hydrogen Bonds and Their Potential Roles in Enzymatic Catalysis. *Journal of Organic Chemistry*, **1998**, 63, 4611-4619 ^{4.2} ¹²⁷

- 659 An antibody exo Diels-Alderase inhibitor complex at 1.95 angstrom resolution. *Science*, **1998**, 279, 1934-1939, 127
- 658 Isomeric cyclopropenes exhibit unique bioorthogonal reactivities. *Journal of the American Chemical Society*, **2013**, 135, 13680-3 16.4 125
- 657 Control and design of mutual orthogonality in bioorthogonal cycloadditions. *Journal of the American Chemical Society*, **2012**, 134, 17904-7 16.4 125
- 656 Nonplanar alkenes and carbonyls: a molecular distortion which parallels addition stereoselectivity. *Journal of the American Chemical Society*, **1981**, 103, 2436-2438 16.4 123
- 655 Potassium tert-Butoxide-Catalyzed Dehydrogenative C-H Silylation of Heteroaromatics: A Combined Experimental and Computational Mechanistic Study. *Journal of the American Chemical Society*, **2017**, 139, 6867-6879 16.4 122
- 654 Evidence for the concerted mechanism of the Diels-Alder reaction of butadiene with ethylene. *Journal of the American Chemical Society*, **1986**, 108, 554-6 16.4 122
- 653 Torquoselectivity in the electrocyclic conversion of benzocyclobutenes to o-xylylenes. *Journal of the American Chemical Society*, **1992**, 114, 1157-1165 16.4 121
- 652 Steric effects compete with aryne distortion to control regioselectivities of nucleophilic additions to 3-silylarynes. *Journal of the American Chemical Society*, **2012**, 134, 13966-9 16.4 117
- 651 Dynamics of 1,3-dipolar cycloadditions: energy partitioning of reactants and quantitation of synchronicity. *Journal of the American Chemical Society*, **2010**, 132, 3029-37 16.4 115
- 650 Nickel-Catalyzed Activation of Acyl C-O Bonds of Methyl Esters. *Angewandte Chemie - International Edition*, **2016**, 55, 2810-4 16.4 115
- 649 Theoretical elucidation of the origins of substituent and strain effects on the rates of Diels-Alder reactions of 1,2,4,5-tetrazines. *Journal of the American Chemical Society*, **2014**, 136, 11483-93 16.4 113
- 648 Theory and Modeling of Asymmetric Catalytic Reactions. *Accounts of Chemical Research*, **2016**, 49, 750-624.3 16.4 111
- 647 Iodoarene-Catalyzed Stereospecific Intramolecular sp(3) C-H Amination: Reaction Development and Mechanistic Insights. *Journal of the American Chemical Society*, **2015**, 137, 7564-7 16.4 111
- 646 Experimental Diels-Alder reactivities of cycloalkenones and cyclic dienes explained through transition-state distortion energies. *Angewandte Chemie - International Edition*, **2011**, 50, 10366-8 16.4 110
- 645 Computational predictions of stereochemistry in asymmetric thiazolium- and triazolium-catalyzed benzoin condensations. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 5770-5 11.5 109
- 644 Brønsted acid catalyzed asymmetric propargylation of aldehydes. *Angewandte Chemie - International Edition*, **2012**, 51, 1391-4 16.4 108
- 643 SAM-dependent enzyme-catalysed pericyclic reactions in natural product biosynthesis. *Nature*, **2017**, 549, 502-506 50.4 108
- 642 Understanding reactivity and stereoselectivity in palladium-catalyzed diastereoselective sp³ C-H bond activation: intermediate characterization and computational studies. *Journal of the American Chemical Society*, **2012**, 134, 14118-26 16.4 106

- 641 Covalently patterned graphene surfaces by a force-accelerated Diels-Alder reaction. *Journal of the American Chemical Society*, **2013**, 135, 9240-3 16.4 106
- 640 Theoretical studies of stereoselectivities of intramolecular aldol cyclizations catalyzed by amino acids. *Journal of the American Chemical Society*, **2005**, 127, 11294-302 16.4 106
- 639 Evolution of shape complementarity and catalytic efficiency from a primordial antibody template. *Science*, **1999**, 286, 2345-8 33.3 106
- 638 Computational methods to calculate accurate activation and reaction energies of 1,3-dipolar cycloadditions of 24 1,3-dipoles. *Journal of Physical Chemistry A*, **2011**, 115, 13906-20 2.8 104
- 637 Dynamics of the degenerate rearrangement of bicyclo[3.1.0]hex-2-ene. *Journal of the American Chemical Society*, **2006**, 128, 90-4 16.4 104
- 636 Influence of molecular distortions upon reactivity and stereochemistry in nucleophilic additions to acetylenes. *Journal of the American Chemical Society*, **1979**, 101, 1340-1343 16.4 103
- 635 1,2,4-Triazines Are Versatile Bioorthogonal Reagents. *Journal of the American Chemical Society*, **2015**, 137, 8388-91 16.4 101
- 634 Bioorthogonal Cycloadditions: Computational Analysis with the Distortion/Interaction Model and Predictions of Reactivities. *Accounts of Chemical Research*, **2017**, 50, 2297-2308 24.3 101
- 633 Computational Exploration of Rh(III)/Rh(V) and Rh(III)/Rh(I) Catalysis in Rhodium(III)-Catalyzed C-H Activation Reactions of N-Phenoxyacetamides with Alkynes. *Journal of the American Chemical Society*, **2016**, 138, 6861-8 16.4 101
- 632 Holy Grails for Computational Organic Chemistry and Biochemistry. *Accounts of Chemical Research*, **2017**, 50, 539-543 24.3 100
- 631 Asymmetric phosphoric acid-catalyzed four-component Ugi reaction. *Science*, **2018**, 361, 33.3 100
- 630 Theoretical secondary kinetic isotope effects and the interpretation of transition state geometries. 1. The Cope rearrangement. *Journal of the American Chemical Society*, **1992**, 114, 8565-8572 16.4 98
- 629 exo-Lone-pair effect on hetero-Diels-Alder cycloaddition stereochemistry. *Journal of the American Chemical Society*, **1992**, 114, 1499-1500 16.4 98
- 628 Ligand steric contours to understand the effects of N-heterocyclic carbene ligands on the reversal of regioselectivity in Ni-catalyzed reductive couplings of alkynes and aldehydes. *Journal of the American Chemical Society*, **2011**, 133, 6956-9 16.4 97
- 627 Gating as a control element in constrictive binding and guest release by hemicarcerands. *Science*, **1996**, 273, 627-9 33.3 97
- 626 Transition structures for hydrogen atom transfers to oxygen. Comparisons of intermolecular and intramolecular processes, and open- and closed-shell systems. *Journal of the American Chemical Society*, **1990**, 112, 7508-7514 16.4 97
- 625 Enzymatic catalysis of anti-Baldwin ring closure in polyether biosynthesis. *Nature*, **2012**, 483, 355-8 50.4 96
- 624 Octaphyrin-(1.0.1.0.1.0.1.0). *Angewandte Chemie International Edition in English*, **1995**, 34, 2515-2517 96

623	Origins of stereoselectivities in chiral phosphoric acid catalyzed allylboration and propargylations of aldehydes. <i>Journal of Organic Chemistry</i> , 2013 , 78, 1208-15	4.2	95
622	Regioselectivity and reactivity in the 1,3-dipolar cycloadditions of diazonium betaines (dialkylazanes, azides, and nitrous oxide). <i>Journal of the American Chemical Society</i> , 1972 , 94, 8953-8955	16.4	95
621	Diels-Alder exo selectivity in terminal-substituted dienes and dienophiles: experimental discoveries and computational explanations. <i>Journal of the American Chemical Society</i> , 2009 , 131, 1947-57	16.4	94
620	Origins of stereoselectivity in the trans Diels-Alder paradigm. <i>Journal of the American Chemical Society</i> , 2010 , 132, 9335-40	16.4	93
619	Cooperative and Competitive Substituent Effects on the Cope Rearrangements of Phenyl-Substituted 1,5-Hexadienes Elucidated by Becke3LYP/6-31G* Calculations. <i>Journal of the American Chemical Society</i> , 2000 , 122, 7456-7460	16.4	93
618	Metal-free directed sp-C-H borylation. <i>Nature</i> , 2019 , 575, 336-340	50.4	93
617	Dynamically Complex [6+4] and [4+2] Cycloadditions in the Biosynthesis of Spinosyn A. <i>Journal of the American Chemical Society</i> , 2016 , 138, 3631-4	16.4	92
616	Decomposition pathways of Z-selective ruthenium metathesis catalysts. <i>Journal of the American Chemical Society</i> , 2012 , 134, 7861-6	16.4	90
615	Ionic and Neutral Mechanisms for C-H Bond Silylation of Aromatic Heterocycles Catalyzed by Potassium tert-Butoxide. <i>Journal of the American Chemical Society</i> , 2017 , 139, 6880-6887	16.4	89
614	Theoretical transition structures for radical additions to alkenes. <i>Journal of Organic Chemistry</i> , 1986 , 51, 2874-2879	4.2	88
613	Design of catalysts for site-selective and enantioselective functionalization of non-activated primary C-H bonds. <i>Nature Chemistry</i> , 2018 , 10, 1048-1055	17.6	86
612	The relationship between proximity and reactivity. An ab initio study of the flexibility of the OH...bul. + CH ₄ hydrogen abstraction transition state and a force-field model for the transition states of intramolecular hydrogen abstractions. <i>Journal of Organic Chemistry</i> , 1988 , 53, 1650-1664	4.2	86
611	Direct Dynamics Quasiclassical Trajectory Study of the Stereochemistry of the Vinylcyclopropane-Cyclopentene Rearrangement. <i>Journal of the American Chemical Society</i> , 1999 , 121, 4720-4721	16.4	85
610	Bergangsstrukturen in pericyclischen Reaktionen von Kohlenwasserstoffen. <i>Angewandte Chemie</i> , 1992 , 104, 711-739	3.6	85
609	The existence of secondary orbital interactions. <i>Journal of Computational Chemistry</i> , 2007 , 28, 344-61	3.5	84
608	The origin of the halogen effect on reactivity and reversibility of Diels-Alder cycloadditions involving furan. <i>Angewandte Chemie - International Edition</i> , 2006 , 45, 1442-5	16.4	84
607	Transition structures of ene reactions of ethylene and formaldehyde with propene. <i>Journal of the American Chemical Society</i> , 1987 , 109, 6947-6952	16.4	83
606	Pyridine N-Oxide vs Pyridine Substrates for Rh(III)-Catalyzed Oxidative C-H Bond Functionalization. <i>Journal of the American Chemical Society</i> , 2015 , 137, 9843-54	16.4	82

605	Synthesis and reactivity comparisons of 1-methyl-3-substituted cyclopropene mini-tags for tetrazine bioorthogonal reactions. <i>Chemistry - A European Journal</i> , 2014 , 20, 3365-75	4.8	82
604	An efficient computational model to predict the synthetic utility of heterocyclic arynes. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 2758-62	16.4	82
603	Theoretical study of Pd(0)-catalyzed carbohalogenation of alkenes: mechanism and origins of reactivities and selectivities in alkyl halide reductive elimination from Pd(II) species. <i>Chemical Science</i> , 2012 , 3, 1987	9.4	82
602	Cage-Walking: Vertex Differentiation by Palladium-Catalyzed Isomerization of B(9)-Bromo-meta-Carborane. <i>Journal of the American Chemical Society</i> , 2017 , 139, 7729-7732	16.4	80
601	Distortion-accelerated cycloadditions and strain-release-promoted cycloreversions in the organocatalytic carbonyl-olefin metathesis. <i>Chemical Science</i> , 2014 , 5, 471-475	9.4	80
600	1,3-Dipolar cycloaddition reactivities of perfluorinated aryl azides with enamines and strained dipolarophiles. <i>Journal of the American Chemical Society</i> , 2015 , 137, 2958-66	16.4	80
599	Theoretical Prediction and Experimental Tests of Conformational Switches in Transition States of Diels-Alder and 1,3-Dipolar Cycloadditions to Enol Ethers. <i>Journal of Organic Chemistry</i> , 1998 , 63, 1064-1073	4.2	80
598	Calculations of Isotropic Hyperfine Coupling Constants of Organic Radicals. An Evaluation of Semiempirical, Hartree-Fock, and Density Functional Methods. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 18371-18379		80
597	Origin of Huisgen's factor x: staggering of allylic bonds promotes anomalously rapid exo attack on norbornenes. <i>Journal of the American Chemical Society</i> , 1982 , 104, 4974-4976	16.4	80
596	Novel double [6 + 4] cycloaddition of tropone to dimethylfulvene. <i>Journal of the American Chemical Society</i> , 1970 , 92, 6392-6394	16.4	80
595	Transition states and mechanisms of the hetero-Diels-Alder reactions of hyponitrous acid, nitrosoalkanes, nitrosoarenes, and nitrosocarbonyl compounds. <i>Journal of Organic Chemistry</i> , 2001 , 66, 5192-200	4.2	79
594	Enzymatic hydroxylation of an unactivated methylene C-H bond guided by molecular dynamics simulations. <i>Nature Chemistry</i> , 2015 , 7, 653-60	17.6	78
593	Mechanism and Origins of Ligand-Controlled Stereoselectivity of Ni-Catalyzed Suzuki-Miyaura Coupling with Benzylic Esters: A Computational Study. <i>Journal of the American Chemical Society</i> , 2017 , 139, 12994-13005	16.4	78
592	A Becke3LYP/6-31G* Study of the Cope Rearrangements of Substituted 1,5-Hexadienes Provides Computational Evidence for a Chameleonic Transition State. <i>Journal of the American Chemical Society</i> , 1999 , 121, 10529-10537	16.4	78
591	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. <i>Nature Communications</i> , 2018 , 9, 2487	17.4	77
590	Dual Gold Catalysis: Stepwise Catalyst Transfer via Dinuclear Clusters. <i>Journal of the American Chemical Society</i> , 2015 , 137, 10668-76	16.4	76
589	Origins of stereoselectivity in evolved ketoreductases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, E7065-72	11.5	76
588	The energetic advantage of 5-exo versus 6-endo epoxide openings: a preference overwhelmed by antibody catalysis. <i>Journal of the American Chemical Society</i> , 1993 , 115, 8453-8454	16.4	74

587	Cinchona Urea-Catalyzed Asymmetric Sulfa-Michael Reactions: The Brønsted Acid-Hydrogen Bonding Model. <i>Journal of the American Chemical Society</i> , 2016 , 138, 9041-4	16.4	74
586	The Origins of Dramatic Differences in Five-Membered vs Six-Membered Chelation of Pd(II) on Efficiency of C(sp)-H Bond Activation. <i>Journal of the American Chemical Society</i> , 2017 , 139, 8514-8521	16.4	73
585	Theoretical Studies of the Structure, Aromaticity, and Magnetic Properties of o-Benzyne. <i>Angewandte Chemie International Edition in English</i> , 1997 , 36, 2761-2764		73
584	Ground- and Excited-State Reactions of Norbornene and Isomers: A CASSCF Study and Comparison with Femtosecond Experiments. <i>Journal of the American Chemical Society</i> , 1999 , 121, 5772-5786	16.4	72
583	Rational design, enantioselective synthesis and catalytic applications of axially chiral EBINOLs. <i>Nature Catalysis</i> , 2019 , 2, 504-513	36.5	71
582	Biochemical Characterization of a Eukaryotic Decalin-Forming Diels-Alderase. <i>Journal of the American Chemical Society</i> , 2016 , 138, 15837-15840	16.4	71
581	Kinetics and Thermodynamics of Reversible Thiol Additions to Mono- and Diactivated Michael Acceptors: Implications for the Design of Drugs That Bind Covalently to Cysteines. <i>Journal of Organic Chemistry</i> , 2016 , 81, 11726-11733	4.2	71
580	Diels-Alder Reactivities of Benzene, Pyridine, and Di-, Tri-, and Tetrazines: The Roles of Geometrical Distortions and Orbital Interactions. <i>Journal of the American Chemical Society</i> , 2016 , 138, 1660-7	16.4	71
579	MIDA boronates are hydrolysed fast and slow by two different mechanisms. <i>Nature Chemistry</i> , 2016 , 8, 1067-1075	17.6	70
578	Z-Selective ethenolysis with a ruthenium metathesis catalyst: experiment and theory. <i>Journal of the American Chemical Society</i> , 2013 , 135, 5848-58	16.4	70
577	Origin of Substituent Effects in Edge-to-Face Aryl-Aryl Interactions. <i>Molecular Physics</i> , 2009 , 107, 749-760.		70
576	Discovery of new mutually orthogonal bioorthogonal cycloaddition pairs through computational screening. <i>Chemical Science</i> , 2016 , 7, 1257-1261	9.4	69
575	Teaching an old carbocation new tricks: Intermolecular C-H insertion reactions of vinyl cations. <i>Science</i> , 2018 , 361, 381-387	33.3	69
574	Intramolecular Crossed [2+2] Photocycloaddition through Visible Light-Induced Energy Transfer. <i>Journal of the American Chemical Society</i> , 2017 , 139, 9807-9810	16.4	69
573	Dynamics of 1,3-dipolar cycloaddition reactions of diazonium betaines to acetylene and ethylene: bending vibrations facilitate reaction. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 2746-8	16.4	69
572	Experimental Proof of the Non-Least-Motion Cycloadditions of Dichlorocarbene to Alkenes: Kinetic Isotope Effects and Quantum Mechanical Transition States. <i>Journal of the American Chemical Society</i> , 1999 , 121, 3933-3938	16.4	69
571	Transition structures for intramolecular hydrogen-atom transfers: the energetic advantage of seven-membered over six-membered transition structures. <i>Journal of the American Chemical Society</i> , 1987 , 109, 2195-2197	16.4	69
570	Catalytic iron-carbene intermediate revealed in a cytochrome carbene transferase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 7308-7313	11.5	69

569	Molecular dynamics explorations of active site structure in designed and evolved enzymes. <i>Accounts of Chemical Research</i> , 2015 , 48, 1080-9	24.3	68
568	Origins of initiation rate differences in ruthenium olefin metathesis catalysts containing chelating benzylidenes. <i>Journal of the American Chemical Society</i> , 2015 , 137, 5782-92	16.4	68
567	Cycloadditions of cyclohexynes and cyclopentyne. <i>Journal of the American Chemical Society</i> , 2014 , 136, 14706-9	16.4	68
566	Alkene distortion energies and torsional effects control reactivities, and stereoselectivities of azide cycloadditions to norbornene and substituted norbornenes. <i>Journal of Organic Chemistry</i> , 2013 , 78, 1778-83	16.3	68
565	Carbenoid character in transition structures for reactions of ketenes with alkenes. <i>Journal of the American Chemical Society</i> , 1990 , 112, 1754-1756	16.4	68
564	The origins of noncovalent catalysis of intermolecular Diels-Alder reactions by cyclodextrins, self-assembling capsules, antibodies, and RNAses. <i>Journal of Organic Chemistry</i> , 2002 , 67, 4250-60	4.2	67
563	Hyperconjugative, Secondary Orbital, Electrostatic, and Steric Effects on the Reactivities and Endo and Exo Stereoselectivities of Cyclopropene Diels-Alder Reactions. <i>Journal of the American Chemical Society</i> , 2016 , 138, 16731-16736	16.4	67
562	Nitrone Cycloadditions of 1,2-Cyclohexadiene. <i>Journal of the American Chemical Society</i> , 2016 , 138, 2512-15	16.4	66
561	Improving physical properties via C-H oxidation: chemical and enzymatic approaches. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 12091-6	16.4	66
560	Lewis acid catalysis alters the shapes and products of bis-pericyclic Diels-Alder transition states. <i>Journal of the American Chemical Society</i> , 2007 , 129, 4528-9	16.4	66
559	The dichotomy between cycloaddition transition states calculated by semiempirical and ab initio techniques. <i>Journal of the American Chemical Society</i> , 1977 , 99, 4511-4514	16.4	66
558	Controllable catalytic difluorocarbene transfer enables access to diversified fluoroalkylated arenes. <i>Nature Chemistry</i> , 2019 , 11, 948-956	17.6	66
557	Benchmarking pKa Prediction Methods for Residues in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 951-66	6.4	65
556	Efficient Biosynthesis of Fungal Polyketides Containing the Dioxabicyclo-octane Ring System. <i>Journal of the American Chemical Society</i> , 2015 , 137, 11904-7	16.4	64
555	Chiral phosphoric acid catalyzed highly enantioselective desymmetrization of 2-substituted and 2,2-disubstituted 1,3-diols via oxidative cleavage of benzylidene acetals. <i>Journal of the American Chemical Society</i> , 2014 , 136, 12249-52	16.4	64
554	Involvement of Lipocalin-like CghA in Decalin-Forming Stereoselective Intramolecular [4+2] Cycloaddition. <i>ChemBioChem</i> , 2015 , 16, 2294-8	3.8	64
553	A carbonate-forming Baeyer-Villiger monooxygenase. <i>Nature Chemical Biology</i> , 2014 , 10, 552-4	11.7	63
552	Non-Directed Allylic C-H Acetoxylation in the Presence of Lewis Basic Heterocycles. <i>Chemical Science</i> , 2014 , 5, 2352-2361	9.4	63

- 551 A torquoselective 6 π electrocycloization approach to reserpine alkaloids. *Organic Letters*, **2012**, 14, 5388-91.2 63
- 550 Mechanism and origins of ligand-controlled selectivities in [Ni(NHC)]-catalyzed intramolecular (5 + 2) cycloadditions and homo-ene reactions: a theoretical study. *Journal of the American Chemical Society*, **2013**, 135, 1456-62 16.4 63
- 549 Nitroxyl disulfides, novel intermediates in transnitrosation reactions. *Journal of the American Chemical Society*, **2003**, 125, 6972-6 16.4 63
- 548 Transannular [6 + 4] and Ambimodal Cycloaddition in the Biosynthesis of Heronamide A. *Journal of the American Chemical Society*, **2015**, 137, 13518-23 16.4 62
- 547 Origins of stereoselectivity in intramolecular aldol reactions catalyzed by cinchona amines. *Journal of the American Chemical Society*, **2015**, 137, 2116-27 16.4 62
- 546 Experimental and Computational Development of a Conformationally Flexible Template for the meta-C-H Functionalization of Benzoic Acids. *Journal of the American Chemical Society*, **2017**, 139, 10702-10714 16.4 61
- 545 Origins of stereoselectivity in intramolecular Diels-Alder cycloadditions of dienes and dienophiles linked by ester and amide tethers. *Journal of Organic Chemistry*, **2001**, 66, 1938-40 4.2 61
- 544 Establishing the (3 + 2) Mechanism for the Permanganate Oxidation of Alkenes by Theory and Kinetic Isotope Effects. *Journal of Organic Chemistry*, **1999**, 64, 800-802 4.2 61
- 543 Mechanism and Origins of Chemo- and Stereoselectivities of Aryl Iodide-Catalyzed Asymmetric Difluorinations of β -Substituted Styrenes. *Journal of the American Chemical Society*, **2018**, 140, 15206-15218 16.4 61
- 542 Chronology of CH \cdots O Hydrogen Bonding from Molecular Dynamics Studies of the Phosphoric Acid-Catalyzed Allylboration of Benzaldehyde. *Journal of the American Chemical Society*, **2017**, 139, 7717-7720 16.4 60
- 541 Enhanced reactivity in dioxirane C-H oxidations via strain release: a computational and experimental study. *Journal of Organic Chemistry*, **2013**, 78, 4037-48 4.2 60
- 540 Computational Redesign of a PETase for Plastic Biodegradation under Ambient Condition by the GRAPE Strategy. *ACS Catalysis*, **2021**, 11, 1340-1350 13.1 60
- 539 Ultrafast rotation in an amphidynamic crystalline metal organic framework. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 13613-13618 11.5 59
- 538 Extended Hartree-Fock (EHF) theory of chemical reactions VI: hybrid DFT and post-Hartree-Fock approaches for concerted and non-concerted transition structures of the Diels-Alder reaction. *Molecular Physics*, **2002**, 100, 717-727 1.7 59
- 537 Stereospecificity of 1,3-dipolar cycloadditions of p-nitrobenzonitrile oxide to cis- and trans-dideuterioethylene. *Journal of the American Chemical Society*, **1985**, 107, 7227-7228 16.4 59
- 536 Diels-Alder reactions of allene with benzene and butadiene: concerted, stepwise, and ambimodal transition states. *Journal of Organic Chemistry*, **2014**, 79, 8968-76 4.2 58
- 535 Mechanism of Permanganate Oxidation of Alkanes: 'Hydrogen Abstraction and Oxygen Rebound' *Journal of the American Chemical Society*, **2000**, 122, 7821-7822 16.4 58
- 534 A Theoretical Investigation of Phosphoramidates and Sulfonamides as Protease Transition State Isosteres. *Journal of Organic Chemistry*, **1998**, 63, 1419-1428 4.2 58

533	Molecular Mechanics and Statistical Thermodynamics Studies of Complexes of a Flexible Hemiacetone with Neutral Guests. <i>Journal of the American Chemical Society</i> , 1996 , 118, 8056-8070	16.4	58
532	Cycloaddition reactions of cycloheptatriene and 2,5-dimethyl-3,4-diphenylcyclopentadienone. <i>Journal of the American Chemical Society</i> , 1970 , 92, 4143-4145	16.4	58
531	Mechanisms and Origins of Periselectivity of the Ambimodal [6 + 4] Cycloadditions of Tropone to Dimethylfulvene. <i>Journal of the American Chemical Society</i> , 2017 , 139, 8251-8258	16.4	57
530	Synthesis of N = 8 Armchair Graphene Nanoribbons from Four Distinct Polydiacetylenes. <i>Journal of the American Chemical Society</i> , 2017 , 139, 15878-15890	16.4	57
529	Substrate control in stereoselective lanthionine biosynthesis. <i>Nature Chemistry</i> , 2015 , 7, 57-64	17.6	57
528	Cinchona Alkaloid-Catalyzed Asymmetric Conjugate Additions: The Bifunctional Brønsted Acid-Hydrogen Bonding Model. <i>Journal of the American Chemical Society</i> , 2016 , 138, 1170-3	16.4	57
527	Theoretical analysis of reactivity patterns in Diels-Alder reactions of cyclopentadiene, cyclohexadiene, and cycloheptadiene with symmetrical and unsymmetrical dienophiles. <i>Journal of Organic Chemistry</i> , 2015 , 80, 3530-7	4.2	56
526	Computational assessment of 1,3-dipolar cycloadditions to graphene. <i>Journal of Materials Chemistry</i> , 2011 , 21, 1503-1508		56
525	Dynamics of carbene cycloadditions. <i>Journal of the American Chemical Society</i> , 2011 , 133, 17848-54	16.4	56
524	Carboxylate-assisted C(sp ³)-H activation in olefin metathesis-relevant ruthenium complexes. <i>Journal of the American Chemical Society</i> , 2014 , 136, 6733-43	16.4	55
523	Extraordinary Difference in Reactivity of Ozone (OOO) and Sulfur Dioxide (OSO): A Theoretical Study. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2104-11	6.4	55
522	Structural basis for antibody catalysis of a disfavored ring closure reaction. <i>Biochemistry</i> , 1999 , 38, 7062-7064	3.4	55
521	Von Porphyrin-Isomeren zu octapyrrolischen Makrocyclen mit 8er-Konformation. <i>Angewandte Chemie</i> , 1995 , 107, 2705-2709	3.6	55
520	Transition states of electrophilic radical additions to alkenes. <i>Journal of the American Chemical Society</i> , 1991 , 113, 4324-4325	16.4	55
519	Direct single-molecule dynamic detection of chemical reactions. <i>Science Advances</i> , 2018 , 4, eaar2177	14.3	54
518	How cinchona alkaloid-derived primary amines control asymmetric electrophilic fluorination of cyclic ketones. <i>Journal of the American Chemical Society</i> , 2014 , 136, 9556-9	16.4	54
517	Ketone-Catalyzed Decomposition of Peroxynitrite via Dioxirane Intermediates. <i>Journal of the American Chemical Society</i> , 1999 , 121, 11976-11983	16.4	54
516	Enzyme-catalysed [6+4] cycloadditions in the biosynthesis of natural products. <i>Nature</i> , 2019 , 568, 122-126	16.4	53

- 515 Generation and regioselective trapping of a 3,4-piperidine for the synthesis of functionalized heterocycles. *Journal of the American Chemical Society*, **2015**, 137, 4082-5 16.4 53
- 514 On the Mechanism of Ligand-Assisted, Copper-Catalyzed Benzylic Amination by Chloramine-T. *Organometallics*, **2010**, 29, 3404-3412 3.8 53
- 513 Cycloadditions of dienes to fulvenes. *Journal of Organic Chemistry*, **1973**, 38, 3836-3843 4.2 53
- 512 Sequential C-F bond functionalizations of trifluoroacetamides and acetates via spin-center shifts. *Science*, **2021**, 371, 1232-1240 33.3 53
- 511 Non-Symmetric Chiral-at-Ruthenium Catalyst for Highly Efficient Enantioselective Intramolecular C(sp)-H Amidation. *Journal of the American Chemical Society*, **2019**, 141, 19048-19057 16.4 53
- 510 The expanding world of biosynthetic pericyclases: cooperation of experiment and theory for discovery. *Natural Product Reports*, **2019**, 36, 698-713 15.1 52
- 509 A Biocatalytic Platform for Synthesis of Chiral Trifluoromethylated Organoborons. *ACS Central Science*, **2019**, 5, 270-276 16.8 51
- 508 Ruthenium-Catalyzed Asymmetric Hydrohydroxyalkylation of Butadiene: The Role of the Formyl Hydrogen Bond in Stereochemical Control. *Journal of the American Chemical Society*, **2015**, 137, 8838-50 16.4 51
- 507 Distortion-Controlled Reactivity and Molecular Dynamics of Dehydro-Diels-Alder Reactions. *Journal of the American Chemical Society*, **2016**, 138, 8247-52 16.4 51
- 506 Computational predictions of substituted benzyne and indolyne regioselectivities. *Tetrahedron Letters*, **2015**, 56, 3511-3514 2 51
- 505 Palladium Complexes of the New Porphyrin Isomers (Z)- and (E)-IsoporphycenePdII-Induced Cyclization of Tetrapyrrolealdehydes. *Angewandte Chemie International Edition in English*, **1997**, 36, 353-357 51
- 504 The mechanism and regioselectivity of the ene reactions of nitroso compounds: a theoretical study of reactivity, regioselectivity, and kinetic isotope effects establishes a stepwise path involving polarized diradical intermediates. *Organic and Biomolecular Chemistry*, **2003**, 1, 1389-403 3.9 51
- 503 Theoretical Study of the Concerted and Stepwise Mechanisms of Triazolinedione Diels-Alder Reactions. *Journal of the American Chemical Society*, **1998**, 120, 12303-12309 16.4 51
- 502 Why do some Fischer indolizations fail?. *Journal of the American Chemical Society*, **2011**, 133, 5752-5 16.4 50
- 501 Stereoselectivities and regioselectivities of (4 + 3) cycloadditions between allenamide-derived chiral oxazolidinone-stabilized oxyallyls and furans: experiment and theory. *Journal of the American Chemical Society*, **2011**, 133, 14443-51 16.4 50
- 500 Origins of Stereoselective Carbene 1,2-Shifts and Cycloadditions of 1,2-Dichloroethylidene: A Theoretical Model Based on CBS-Q and B3LYP Calculations. *Journal of the American Chemical Society*, **1997**, 119, 10805-10809 16.4 50
- 499 Rearrangement of Iridabenzvalenes to Iridabenzenes and/or β -Cyclopentadienyliridium(I) Complexes: Experimental and Computational Analysis of the Influence of Silyl Ring Substituents and Phosphine Ligands. *Organometallics*, **2007**, 26, 3957-3968 3.8 50
- 498 Alkynes, Allenes, and Alkenes in [3,3]-Sigmatropy: Functional Diversity and Kinetic Monotony. A Theoretical Analysis. *Journal of the American Chemical Society*, **1998**, 120, 5622-5627 16.4 50

497	Transition State of the Base-Promoted Ring-Opening of Isoxazoles. Theoretical Prediction of Catalytic Functionalities and Design of Haptens for Antibody Production. <i>Journal of the American Chemical Society</i> , 1996 , 118, 6462-6471	16.4	50
496	Mechanism of the P450-Catalyzed Oxidative Cyclization in the Biosynthesis of Griseofulvin. <i>ACS Catalysis</i> , 2016 , 6, 4506-4511	13.1	49
495	Selective gold(I)-catalyzed formation of tetracyclic indolines: a single transition structure and bifurcations lead to multiple products. <i>Journal of Organic Chemistry</i> , 2011 , 76, 3477-83	4.2	49
494	Experimental determination of the absolute enantioselectivity of an antibody-catalyzed Diels-Alder reaction and theoretical explorations of the origins of stereoselectivity. <i>Journal of the American Chemical Society</i> , 2003 , 125, 2489-506	16.4	49
493	Catalytic Enantioselective Intramolecular C(sp ³)-H Amination of 2-Azidoacetamides. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 1088-1093	16.4	49
492	Reversible photochemically gated transformation of a hemicarcerand to a carcerand. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 655-9	16.4	48
491	Role of Orbital Interactions and Activation Strain (Distortion Energies) on Reactivities in the Normal and Inverse Electron-Demand Cycloadditions of Strained and Unstrained Cycloalkenes. <i>Journal of Organic Chemistry</i> , 2017 , 82, 8668-8675	4.2	48
490	Intramolecular cycloadditions of cyclobutadiene with dienes: experimental and computational studies of the competing (2 + 2) and (4 + 2) modes of reaction. <i>Journal of the American Chemical Society</i> , 2003 , 125, 16310-21	16.4	47
489	"Even" regioselectivity in [6 + 4] cycloadditions of unsymmetrical tropones with dienes. <i>Journal of the American Chemical Society</i> , 1984 , 106, 3882-3884	16.4	47
488	Cycloaddition reactions of tropone and 2,5-dimethyl-3,4-diphenylcyclopentadienone. <i>Journal of the American Chemical Society</i> , 1970 , 92, 4145-4147	16.4	47
487	FAD-dependent enzyme-catalysed intermolecular [4+2] cycloaddition in natural product biosynthesis. <i>Nature Chemistry</i> , 2020 , 12, 620-628	17.6	47
486	Enzyme-Catalyzed Inverse-Electron Demand Diels-Alder Reaction in the Biosynthesis of Antifungal Illicicolin H. <i>Journal of the American Chemical Society</i> , 2019 , 141, 5659-5663	16.4	46
485	Altering the allowed/forbidden gap in cyclobutene electrocyclic reactions: experimental and theoretical evaluations of the effect of planarity constraints. <i>Journal of the American Chemical Society</i> , 2003 , 125, 5839-48	16.4	46
484	Theoretical Predictions of Substituent Effects on the Thermal Electrocyclic Ring Openings of Cyclobutenones. <i>Journal of Organic Chemistry</i> , 1996 , 61, 2517-2522	4.2	46
483	On the potential energy surface for ring inversion in cyclohexene and related molecules. <i>Journal of the American Chemical Society</i> , 1992 , 114, 10969-10971	16.4	46
482	Effect of Torsional Strain and Electrostatic Interactions on the Stereochemistry of Nucleophilic Additions to Cyclohexanone and Related Systems. <i>Angewandte Chemie International Edition in English</i> , 1992 , 31, 1019-1021		46
481	Enzymatic Intermolecular Hetero-Diels-Alder Reaction in the Biosynthesis of Tropolonic Sesquiterpenes. <i>Journal of the American Chemical Society</i> , 2019 , 141, 14052-14056	16.4	45
480	Computational Exploration of Mechanism and Selectivities of (NHC)Nickel(II)hydride-Catalyzed Hydroalkenylations of Styrene with β -Olefins. <i>ACS Catalysis</i> , 2015 , 5, 5545-5555	13.1	45

479	Influence of water and enzyme SpnF on the dynamics and energetics of the ambimodal [6+4]/[4+2] cycloaddition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E848-E855	11.5	45
478	Crystal Fluidity Reflected by Fast Rotational Motion at the Core, Branches, and Peripheral Aromatic Groups of a Dendrimeric Molecular Rotor. <i>Journal of the American Chemical Society</i> , 2016 , 138, 4650-6	16.4	45
477	Halo substituent effects on intramolecular cycloadditions involving furanyl amides. <i>Journal of Organic Chemistry</i> , 2006 , 71, 5432-9	4.2	45
476	A cornucopia of cycloadducts: theoretical predictions of the mechanisms and products of the reactions of cyclopentadiene with cycloheptatriene. <i>Journal of the American Chemical Society</i> , 2003 , 125, 8330-9	16.4	45
475	Influence of steric interactions on endo stereoselectivity. <i>Journal of the American Chemical Society</i> , 1971 , 93, 4606-4607	16.4	45
474	Computational evaluation of enantioselective Diels-Alder reactions mediated by Corey's cationic oxazaborolidine catalysts. <i>Journal of Organic Chemistry</i> , 2009 , 74, 861-8	4.2	44
473	Molecular dynamics of the Diels-Alder reactions of tetrazines with alkenes and N ₂ extrusions from adducts. <i>Journal of the American Chemical Society</i> , 2015 , 137, 4749-58	16.4	43
472	Why alkynyl substituents dramatically accelerate hexadehydro-Diels-Alder (HDDA) reactions: stepwise mechanisms of HDDA cycloadditions. <i>Organic Letters</i> , 2014 , 16, 5702-5	6.2	43
471	Catalytic Asymmetric Intermolecular Stetter Reactions of Enolizable Aldehydes with Nitrostyrenes: Computational Study Provides Insight into the Success of the Catalyst. <i>Angewandte Chemie</i> , 2012 , 124, 2441-2444	3.6	43
470	The Dimerization of Cyclobutadiene. An ab Initio CASSCF Theoretical Study. <i>Journal of the American Chemical Society</i> , 1996 , 118, 880-885	16.4	43
469	Octaphyrin-(1.0.1.0.1.0.1.0). <i>Angewandte Chemie</i> , 1995 , 107, 2709-2711	3.6	43
468	Modeling of steric control of facial stereoselectivity. Diels-Alder cycloadditions of unsymmetrically substituted cyclopentadienes. <i>Journal of Organic Chemistry</i> , 1987 , 52, 3050-3059	4.2	43
467	Differentiation and functionalization of remote C-H bonds in adjacent positions. <i>Nature Chemistry</i> , 2020 , 12, 399-404	17.6	42
466	P450-Mediated Coupling of Indole Fragments To Forge Communesin and Unnatural Isomers. <i>Journal of the American Chemical Society</i> , 2016 , 138, 4002-5	16.4	42
465	Does nature click? Theoretical prediction of an enzyme-catalyzed transannular 1,3-dipolar cycloaddition in the biosynthesis of lycojaponicumins A and B. <i>Journal of the American Chemical Society</i> , 2013 , 135, 17638-42	16.4	42
464	Function and Structure of MalA/MalA', Iterative Halogenases for Late-Stage C-H Functionalization of Indole Alkaloids. <i>Journal of the American Chemical Society</i> , 2017 , 139, 12060-12068	16.4	42
463	Origins of Enantioselectivity in Asymmetric Radical Additions to Octahedral Chiral-at-Rhodium Enolates: A Computational Study. <i>Journal of the American Chemical Society</i> , 2017 , 139, 17902-17907	16.4	42
462	Highly selective Diels-Alder reactions of directly connected enyne dienophiles. <i>Journal of the American Chemical Society</i> , 2007 , 129, 645-57	16.4	42

461	Gating and Entropy in Guest Exchange by Rebek's Sportsballs. Theoretical Studies of One-Door, Side-Door, and Back-Door Gating. <i>Organic Letters</i> , 1999 , 1, 591-594	6.2	42
460	Polyether Catalysis of Ester Aminolysis: A Computational and Experimental Study. <i>Liebigs Annalen</i> , 1996 , 1996, 1511-1522		42
459	Origin of Stereoselectivities in Asymmetric Alkoxyseleenylation. <i>Journal of the American Chemical Society</i> , 1999 , 121, 8567-8576	16.4	41
458	Strained Allenes as Dienophiles in the Diels-Alder Reaction: An Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 1999 , 64, 976-983	4.2	41
457	Genome-Mined Diels-Alderase Catalyzes Formation of the cis-Octahydrodecalins of Varicidin A and B. <i>Journal of the American Chemical Society</i> , 2019 , 141, 769-773	16.4	41
456	Relationships between Product Ratios in Ambimodal Pericyclic Reactions and Bond Lengths in Transition Structures. <i>Journal of the American Chemical Society</i> , 2018 , 140, 3061-3067	16.4	40
455	Origins of Selectivity and General Model for Chiral Phosphoric Acid-Catalyzed Oxetane Desymmetrizations. <i>Journal of the American Chemical Society</i> , 2016 , 138, 12356-9	16.4	40
454	Diels-Alder cycloadditions of strained azacyclic allenes. <i>Nature Chemistry</i> , 2018 , 10, 953-960	17.6	40
453	Intramolecular Diels-Alder reactions of cycloalkenones: stereoselectivity, Lewis acid acceleration, and halogen substituent effects. <i>Journal of the American Chemical Society</i> , 2014 , 136, 2397-403	16.4	40
452	Solid-State Order and Charge Mobility in [5]- to [12]Cycloparaphenylenes. <i>Journal of the American Chemical Society</i> , 2019 , 141, 952-960	16.4	40
451	A potassium tert-butoxide and hydrosilane system for ultra-deep desulfurization of fuels. <i>Nature Energy</i> , 2017 , 2,	62.3	39
450	Chiral Brønsted Acid-Catalyzed Asymmetric Allyl(propargyl)boration Reaction of ortho-Alkynyl Benzaldehydes: Synthetic Applications and Factors Governing the Enantioselectivity. <i>ACS Catalysis</i> , 2016 , 6, 2506-2514	13.1	39
449	Expanding the Frontiers of Higher-Order Cycloadditions. <i>Accounts of Chemical Research</i> , 2019 , 52, 3488-3501	14.9	39
448	Origins of the Stereoselectivity in a Thiourea-Primary Amine-Catalyzed Nazarov Cyclization. <i>Journal of the American Chemical Society</i> , 2015 , 137, 13191-9	16.4	38
447	QM/MM Protocol for Direct Molecular Dynamics of Chemical Reactions in Solution: The Water-Accelerated Diels-Alder Reaction. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5606-12	6.4	38
446	Thermodynamic control of the electrocyclic ring opening of cyclobutenes: C=X substituents at C-3 mask the kinetic torquoselectivity. <i>Journal of the American Chemical Society</i> , 2009 , 131, 6664-5	16.4	38
445	Stable, Reactive, and Orthogonal Tetrazines: Dispersion Forces Promote the Cycloaddition with Isonitriles. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 9043-9048	16.4	37
444	Molecular Dynamics of Dimethyldioxirane C-H Oxidation. <i>Journal of the American Chemical Society</i> , 2016 , 138, 4237-42	16.4	37

443	Mechanisms and transition states of 1,3-dipolar cycloadditions of phenyl azide with enamines: a computational analysis. <i>Journal of Organic Chemistry</i> , 2013 , 78, 1576-82	4.2	37
442	Conjugated Trimeric Scaffolds Accessible from Indolyne Cyclotrimerizations: Synthesis, Structures, and Electronic Properties. <i>Journal of the American Chemical Society</i> , 2017 , 139, 10447-10455	16.4	37
441	A resorcinarene for inhibition of A β fibrillation. <i>Chemical Science</i> , 2017 , 8, 2003-2009	9.4	37
440	Cyclometalated Z-Selective Ruthenium Metathesis Catalysts with Modified N-Chelating Groups. <i>Organometallics</i> , 2015 , 34, 2858-2869	3.8	37
439	Origins of boat or chair preferences in the Ireland-Claisen rearrangements of cyclohexenyl esters: a theoretical study. <i>Journal of Organic Chemistry</i> , 2003 , 68, 572-7	4.2	37
438	Construction of linear-fused tricyclopentanoids by intramolecular [6 + 2] cycloadditions of fulvenes with enamines. <i>Journal of the American Chemical Society</i> , 1985 , 107, 5308-5309	16.4	37
437	Diazo Esters as Dienophiles in Intramolecular (4 + 2) Cycloadditions: Computational Explorations of Mechanism. <i>Journal of the American Chemical Society</i> , 2017 , 139, 2766-2770	16.4	36
436	Torsional Control of Stereoselectivities in Electrophilic Additions and Cycloadditions to Alkenes. <i>Chemical Science</i> , 2014 , 5,	9.4	36
435	Intramolecular oxyallyl-carbonyl (3 + 2) cycloadditions. <i>Journal of the American Chemical Society</i> , 2013 , 135, 5242-5	16.4	36
434	Conformational Transmission of Chirality: The Origin of 1,4-Asymmetric Induction in Michael Reactions of Chiral Imines. <i>Journal of the American Chemical Society</i> , 1997 , 119, 826-827	16.4	36
433	Activation Mode and Origin of Selectivity in Chiral Phosphoric Acid-Catalyzed Oxacycle Formation by Intramolecular Oxetane Desymmetrizations. <i>ACS Catalysis</i> , 2017 , 7, 7332-7339	13.1	34
432	Fungal indole alkaloid biogenesis through evolution of a bifunctional reductase/Diels-Alderase. <i>Nature Chemistry</i> , 2019 , 11, 972-980	17.6	34
431	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. <i>Chemistry - A European Journal</i> , 2019 , 25, 6342-6348	4.8	34
430	Periselectivity in the [4 + 2] and [6 + 4] cycloadditions of diphenylnitrilimine to tropone. <i>Journal of Organic Chemistry</i> , 1978 , 43, 817-821	4.2	34
429	Mild Ring-Opening 1,3-Hydroborations of Non-Activated Cyclopropanes. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 16861-16865	16.4	34
428	(2 + 2) Cycloaddition of Benzyne to Endohedral Metallofullerenes M ₃ N@C ₈₀ (M = Sc, Y): A Rotating-Intermediate Mechanism. <i>Journal of the American Chemical Society</i> , 2015 , 137, 6820-8	16.4	33
427	Nickel-Catalyzed Activation of Acyl C=O Bonds of Methyl Esters. <i>Angewandte Chemie</i> , 2016 , 128, 2860-2864	9.4	33
426	Schleyer hyperconjugative aromaticity and Diels-Alder reactivity of 5-substituted cyclopentadienes. <i>Journal of Computational Chemistry</i> , 2016 , 37, 117-23	3.5	33

425	Overriding Traditional Electronic Effects in Biocatalytic Baeyer-Villiger Reactions by Directed Evolution. <i>Journal of the American Chemical Society</i> , 2018 , 140, 10464-10472	16.4	33
424	Regioselectivities of (4 + 3) cycloadditions between furans and oxazolidinone-substituted oxyallyls. <i>Organic Letters</i> , 2010 , 12, 5506-9	6.2	33
423	Computation of Accurate Activation Barriers for Methyl-Transfer Reactions of Sulfonium and Ammonium Salts in Aqueous Solution. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1028-35	6.4	33
422	Studies of Diastereoselectivity in Conjugate Addition of Organoaluminum Reagents to (R)-[(p-Tolylsulfinyl)methyl]quinols and Derivatives. <i>Journal of Organic Chemistry</i> , 1998 , 63, 3687-3693	4.2	33
421	Catalytic Enantioselective Hetero-[6+4] and -[6+2] Cycloadditions for the Construction of Condensed Polycyclic Pyrroles, Imidazoles, and Pyrazoles. <i>Journal of the American Chemical Society</i> , 2019 , 141, 3288-3297	16.4	32
420	Highly Diastereoselective Functionalization of Piperidines by Photoredox-Catalyzed β -Amino C-H Arylation and Epimerization. <i>Journal of the American Chemical Society</i> , 2020 , 142, 8194-8202	16.4	32
419	Enzymatic control of dioxygen binding and functionalization of the flavin cofactor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 4909-4914	11.5	32
418	Bridged [2.2.1] bicyclic phosphine oxide facilitates catalytic β -umpolung addition-Wittig olefination. <i>Chemical Science</i> , 2018 , 9, 1867-1872	9.4	32
417	Synthesis of [F]Fluoroarenes by Nucleophilic Radiofluorination of N-Arylsydnone. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 13006-13010	16.4	32
416	"H/Vinyl" and "Alkyl/Vinyl" conical intersections leading to carbene formation from the excited states of cyclohexene and norbornene. <i>Journal of the American Chemical Society</i> , 2002 , 124, 11182-90	16.4	32
415	Mechanism and Thermodynamics of Guest Escape from a Carcerand. <i>Journal of the American Chemical Society</i> , 1995 , 117, 1853-1854	16.4	32
414	Z-Selective Cross-Metathesis and Homodimerization of 3E-1,3-Dienes: Reaction Optimization, Computational Analysis, and Synthetic Applications. <i>Journal of the American Chemical Society</i> , 2016 , 138, 14039-14046	16.4	32
413	Open-Shell Fluorination of Alkyl Bromides: Unexpected Selectivity in a Silyl Radical-Mediated Chain Process. <i>Journal of the American Chemical Society</i> , 2019 , 141, 20031-20036	16.4	32
412	Sydnone-Based Approach to Heterohelicones through 1,3-Dipolar-Cycloadditions. <i>Journal of the American Chemical Society</i> , 2019 , 141, 1435-1440	16.4	32
411	Bioorthogonal release of sulfonamides and mutually orthogonal liberation of two drugs. <i>Chemical Communications</i> , 2018 , 54, 14089-14092	5.8	32
410	Mechanism and Origins of Enantioselectivities in Spirobiindane-Based Hypervalent Iodine(III)-Induced Asymmetric Dearomatizing Spirolactonizations. <i>Journal of the American Chemical Society</i> , 2019 , 141, 16046-16056	16.4	31
409	Enantioselective Diarylcarbene Insertion into Si-H Bonds Induced by Electronic Properties of the Carbenes. <i>Journal of the American Chemical Society</i> , 2020 , 142, 12394-12399	16.4	31
408	Unprecedented Dearomatized Spirocyclopropane in a Sequential Rhodium(III)-Catalyzed C-H Activation and Rearrangement Reaction. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 5520-5524	16.4	31

407	The Dynamics of Chemical Reactions: Atomistic Visualizations of Organic Reactions, and Homage to van 't Hoff. <i>Chemistry - A European Journal</i> , 2018 , 24, 3916-3924	4.8	31
406	Origins of the Endo and Exo Selectivities in Cyclopropenone, Iminocyclopropene, and Triafulvene Diels-Alder Cycloadditions. <i>Journal of Organic Chemistry</i> , 2018 , 83, 3164-3170	4.2	31
405	Probing Stereoselectivity in Ring-Opening Metathesis Polymerization Mediated by Cyclometalated Ruthenium-Based Catalysts: A Combined Experimental and Computational Study. <i>Journal of the American Chemical Society</i> , 2016 , 138, 1394-405	16.4	31
404	The [6 + 4] cycloadditions of diethylaminobutadiene to fulvenes. A new synthesis of azulenes. <i>Journal of the American Chemical Society</i> , 1976 , 98, 7095-7096	16.4	31
403	Hyperconjugative Aromaticity and Antiaromaticity Control the Reactivities and π -Facial Stereoselectivities of 5-Substituted Cyclopentadiene Diels-Alder Cycloadditions. <i>Journal of Organic Chemistry</i> , 2018 , 83, 14658-14666	4.2	31
402	Arynes and Cyclic Alkynes as Synthetic Building Blocks for Stereodefined Quaternary Centers. <i>Journal of the American Chemical Society</i> , 2018 , 140, 7605-7610	16.4	30
401	Molecular Dynamics Analysis of Binding of Kinase Inhibitors to WT EGFR and the T790M Mutant. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2066-78	6.4	30
400	Building on Cram's legacy: stimulated gating in hemicarcerands. <i>Accounts of Chemical Research</i> , 2014 , 47, 2168-76	24.3	30
399	A Single Active Site Mutation in the Pikromycin Thioesterase Generates a More Effective Macrocyclization Catalyst. <i>Journal of the American Chemical Society</i> , 2017 , 139, 13456-13465	16.4	30
398	On the mechanism of peripentacene formation from pentacene: computational studies of a prototype for graphene formation from smaller acenes. <i>Journal of the American Chemical Society</i> , 2007 , 129, 6536-46	16.4	30
397	New Paradigm for Anionic Heteroatom Cope Rearrangements. <i>Journal of the American Chemical Society</i> , 1998 , 120, 205-206	16.4	30
396	Asymmetric Desymmetrization of Oxetanes for the Synthesis of Chiral Tetrahydrothiophenes and Tetrahydroselenophenes. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 18055-18060	16.4	29
395	Self-Assembling Ternary Complex Stabilities and Template Ratios in Carceplex Formation. <i>Journal of the American Chemical Society</i> , 1997 , 119, 4321-4322	16.4	29
394	Experimental Determination of the Activation Parameters and Stereoselectivities of the Intramolecular Diels-Alder Reactions of 1,3,8-Nonatriene, 1,3,9-Decatriene, and 1,3,10-Undecatriene and Transition State Modeling with the Monte Carlo-Jumping Between Wells/Molecular Dynamics Method. <i>Journal of the American Chemical Society</i> , 1997 , 119, 10255-10259	16.4	29
393	Photoelectron and ultraviolet spectra of small-ring fused aromatic molecules as probes of aromatic ring distortions. <i>Journal of the American Chemical Society</i> , 1978 , 100, 3730-3737	16.4	29
392	Photochemical intermolecular dearomative cycloaddition of bicyclic azaarenes with alkenes. <i>Science</i> , 2021 , 371, 1338-1345	33.3	29
391	Enzyme-catalyzed cationic epoxide rearrangements in quinolone alkaloid biosynthesis. <i>Nature Chemical Biology</i> , 2017 , 13, 325-332	11.7	28
390	Enantioselective C-H functionalization of bicyclo[1.1.1]pentanes. <i>Nature Catalysis</i> , 2020 , 3, 351-357	36.5	28

389	Phenalenone Polyketide Cyclization Catalyzed by Fungal Polyketide Synthase and Flavin-Dependent Monooxygenase. <i>Journal of the American Chemical Society</i> , 2016 , 138, 4249-59	16.4	28
388	Computational study of factors controlling the boat and chair transition states of Ireland-Claisen rearrangements. <i>Journal of Organic Chemistry</i> , 2010 , 75, 2115-8	4.2	28
387	CH.O Hydrogen Bonding Influences pi-Facial Stereoselective Epoxidations We are grateful to the National Institute of General Medical Sciences, National Institutes of Health (GM-36700) for financial support of this research and the National Computational Science Alliance (Illinois) for computer time and support. <i>Angewandte Chemie - International Edition</i> , 2001 , 40, 4485-4488	16.4	28
386	[5,5] Sigmatropic Rearrangement. DFT Prediction of a Diradical Mechanism for a Woodward-Hoffmann Allowed Thermal Pericyclic Reaction. <i>Journal of the American Chemical Society</i> , 1998 , 120, 10490-10493	16.4	28
385	A Convergent Strategy for the Asymmetric Synthesis of Enantiomerically Pure Bicyclic Compounds by Using a Silicon-Directed Cycloaddition Reaction: The Synthesis of Enantiomerically Pure Bicyclo. <i>Angewandte Chemie - International Edition</i> , 1999 , 38, 2728-2730	16.4	28
384	Ambimodal Trispericyclic Transition State and Dynamic Control of Periselectivity. <i>Journal of the American Chemical Society</i> , 2019 , 141, 1217-1221	16.4	28
383	Catalytic Asymmetric Staudinger-aza-Wittig Reaction for the Synthesis of Heterocyclic Amines. <i>Journal of the American Chemical Society</i> , 2019 , 141, 9537-9542	16.4	27
382	Development of Chiral Bis-hydrazone Ligands for the Enantioselective Cross-Coupling Reactions of Aryldimethylsilanolates. <i>Journal of Organic Chemistry</i> , 2015 , 80, 313-66	4.2	27
381	Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with β -Vinyl Allylboron Reagents. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 10540-10548	16.4	27
380	Design, Synthesis, and Validation of an Effective, Reusable Silicon-Based Transfer Agent for Room-Temperature Pd-Catalyzed Cross-Coupling Reactions of Aryl and Heteroaryl Chlorides with Readily Available Aryl Lithium Reagents. <i>Journal of the American Chemical Society</i> , 2016 , 138, 1836-9	16.4	27
379	Origin of Regiochemical Control in Rh(III)/Rh(V)-Catalyzed Reactions of Unsaturated Oximes and Alkenes to Form Pyridines. <i>ACS Catalysis</i> , 2019 , 9, 7154-7165	13.1	27
378	N-Type Conjugated Polymer-Enabled Selective Dispersion of Semiconducting Carbon Nanotubes for Flexible CMOS-Like Circuits. <i>Advanced Functional Materials</i> , 2015 , 25, 1837-1844	15.6	27
377	Mechanism of S(H)2 reactions of disulfides: frontside vs backside, stepwise vs concerted. <i>Journal of Organic Chemistry</i> , 2009 , 74, 5356-60	4.2	27
376	Evolution of the Diels-Alder Reaction Mechanism since the 1930s: Woodward, Houk with Woodward, and the Influence of Computational Chemistry on Understanding Cycloadditions. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 12660-12681	16.4	27
375	Atroposelective Synthesis of Axially Chiral N-Arylpyrroles by Chiral-at-Rhodium Catalysis. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 13552-13556	16.4	26
374	Aminoperoxide adducts expand the catalytic repertoire of flavin monooxygenases. <i>Nature Chemical Biology</i> , 2020 , 16, 556-563	11.7	26
373	Structural basis of the Cope rearrangement and cyclization in hapalindole biogenesis. <i>Nature Chemical Biology</i> , 2018 , 14, 345-351	11.7	26
372	Molecular Dynamics Simulations of Selective Metabolite Transport across the Propanediol Bacterial Microcompartment Shell. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 8149-8154	3.4	26

371	Catalytic enantioselective synthesis of chiral tetraarylmethanes. <i>Nature Catalysis</i> , 2020 , 3, 1010-1019	36.5	25
370	Ligand-Controlled Regiodivergent Palladium-Catalyzed Hydrogermylation of Ynamides. <i>Journal of the American Chemical Society</i> , 2020 , 142, 11153-11164	16.4	25
369	Synthesis of ent-ketorfanol via a C-H alkenylation/torquoselective 6 π electrocyclization cascade. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 12044-8	16.4	25
368	Experimental Diels-Alder Reactivities of Cycloalkenones and Cyclic Dienes Explained through Transition-State Distortion Energies. <i>Angewandte Chemie</i> , 2011 , 123, 10550-10552	3.6	25
367	Origins of the regioselectivities in the Diels-Alder reactions of vinylindenes with 1,4-quinone monoketal and acrolein dienophiles. <i>Journal of Organic Chemistry</i> , 2009 , 74, 6770-6	4.2	25
366	Transition states for the dimerization of 1,3-cyclohexadiene: a DFT, CASPT2, and CBS-QB3 quantum mechanical investigation. <i>Journal of Organic Chemistry</i> , 2008 , 73, 7586-92	4.2	25
365	Mechanism of the Vinylcyclobutane Rearrangement of Scepterin to Ageliferin and Nagelamide E. <i>Angewandte Chemie</i> , 2006 , 118, 4232-4236	3.6	25
364	Development of β,β -Disubstituted Crotylboronate Reagents and Stereoselective Crotylation via Brønsted or Lewis Acid Catalysis. <i>Journal of the American Chemical Society</i> , 2020 , 142, 18355-18368	16.4	25
363	Origins of the Unfavorable Activation and Reaction Energies of 1-Azadiene Heterocycles Compared to 2-Azadiene Heterocycles in Diels-Alder Reactions. <i>Journal of Organic Chemistry</i> , 2017 , 82, 1912-1919	4.2	24
362	Generation of Dithianyl and Dioxolanyl Radicals Using Photoredox Catalysis: Application in the Total Synthesis of the Danshenspiroketalactones via Radical Relay Chemistry. <i>Organic Letters</i> , 2019 , 21, 1708-1712	6.2	24
361	Cycloadditions of Oxacyclic Allenes and a Catalytic Asymmetric Entryway to Enantioenriched Cyclic Allenes. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 5653-5657	16.4	24
360	Electrophilic Azides for Materials Synthesis and Chemical Biology. <i>Accounts of Chemical Research</i> , 2020 , 53, 937-948	24.3	24
359	Rational Development of Remote C-H Functionalization of Biphenyl: Experimental and Computational Studies. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 4770-4777	16.4	24
358	Biosynthesis of Heptacyclic Duclauxins Requires Extensive Redox Modifications of the Phenalenone Aromatic Polyketide. <i>Journal of the American Chemical Society</i> , 2018 , 140, 6991-6997	16.4	24
357	Structural basis for stereoselective dehydration and hydrogen-bonding catalysis by the SAM-dependent pericyclase LepI. <i>Nature Chemistry</i> , 2019 , 11, 812-820	17.6	24
356	Inverted Binding of Non-natural Substrates in Strictosidine Synthase Leads to a Switch of Stereochemical Outcome in Enzyme-Catalyzed Pictet-Spengler Reactions. <i>Journal of the American Chemical Society</i> , 2020 , 142, 792-800	16.4	24
355	AlCl ₃ -Catalyzed Ring Expansion Cascades of Bicyclic Cyclobutenamides Involving Highly Strained Cis,Trans-Cycloheptadienone Intermediates. <i>Journal of the American Chemical Society</i> , 2015 , 137, 5596-6011	16.4	23
354	Selective Enzymatic Oxidation of Silanes to Silanols. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 15507-15511	16.4	23

- 353 Competition between concerted and stepwise dynamics in the triplet di- π -methane rearrangement. *Angewandte Chemie - International Edition*, **2014**, 53, 8664-7 16.4 23
- 352 Effect of trehalose polymer regioisomers on protein stabilization. *Polymer Chemistry*, **2017**, 8, 4781-4788 4.9 23
- 351 Evolution of a Unified Strategy for Complex Sesterterpenoids: Progress toward Astellatol and the Total Synthesis of (-)-Nitidasin. *Chemistry - A European Journal*, **2015**, 21, 13646-65 4.8 23
- 350 Mechanistic analysis of an asymmetric palladium-catalyzed conjugate addition of arylboronic acids to β -substituted cyclic enones. *Chemical Science*, **2015**, 6, 1917-1922 9.4 23
- 349 Can acyclic conformational control be achieved a sulfur-fluorine effect?. *Chemical Science*, **2015**, 6, 3565-3571 9.4 23
- 348 π -Facial Diastereoselection in Diels-Alder Reactions of (R)-4-[(p-Tolylsulfinyl)methyl]quinols. *Journal of Organic Chemistry*, **1997**, 62, 9128-9137 4.2 23
- 347 Aromaticity and Antiaromaticity in Small Ring Transition States, Assessed by NICS Values and Energetics. *Journal of Molecular Modeling*, **2000**, 6, 158-165 2 23
- 346 Isonitrile-responsive and bioorthogonally removable tetrazine protecting groups. *Chemical Science*, **2020**, 11, 169-179 9.4 23
- 345 Organocatalytic [6+4] Cycloadditions via Zwitterionic Intermediates: Chemo-, Regio-, and Stereoselectivities. *Journal of the American Chemical Society*, **2018**, 140, 13726-13735 16.4 23
- 344 Enabling microbial syringol conversion through structure-guided protein engineering. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 13970-13976 11.5 22
- 343 Mechanistic Insights into Two-Phase Radical C-H Arylations. *ACS Central Science*, **2015**, 1, 456-462 16.8 22
- 342 Origins of halogen effects in bioorthogonal sydnone cycloadditions. *Chemical Communications*, **2018**, 54, 5082-5085 5.8 22
- 341 Arylketone π -Conjugation Controls Enantioselectivity in Asymmetric Alkynylations Catalyzed by Centrochiral Ruthenium Complexes. *Journal of the American Chemical Society*, **2018**, 140, 5146-5152 16.4 22
- 340 Torquoselective ring opening of fused cyclobutenamides: evidence for a cis,trans-cyclooctadienone intermediate. *Journal of the American Chemical Society*, **2014**, 136, 9802-5 16.4 22
- 339 Model for the Enantioselectivity of Asymmetric Intramolecular Alkylations by Bis-Quaternized Cinchona Alkaloid-Derived Catalysts. *Journal of Organic Chemistry*, **2017**, 82, 8645-8650 4.2 22
- 338 Computational Exploration of Concerted and Zwitterionic Mechanisms of Diels-Alder Reactions between 1,2,3-Triazines and Enamines and Acceleration by Hydrogen-Bonding Solvents. *Journal of the American Chemical Society*, **2017**, 139, 18213-18221 16.4 22
- 337 Stereoselective Diels-Alder Reactions of Hexachlorocyclopentadiene with Chiral Alkenes: New Insights Into the Inside-Alkoxy Model of Stereoselectivity. *Journal of Organic Chemistry*, **1997**, 62, 5728-5731 4.3 22
- 336 Theoretical investigation of the stereoselective stepwise cope rearrangement of a 3-vinylmethylenecyclobutane. *Journal of the American Chemical Society*, **2006**, 128, 11106-13 16.4 22

335	Concerted rearrangement versus heterolytic cleavage in anionic [2,3]- and [3,3]-sigmatropic shifts. A DFT study of relationships among anion stabilities, mechanisms, and rates. <i>Journal of Organic Chemistry</i> , 2003 , 68, 2310-6	4.2	22
334	Mechanistic Variations and Rate Effects of Alkoxy and Thioalkoxy Substituents on Anionic Oxy-Cope Rearrangements. <i>Journal of the American Chemical Society</i> , 1999 , 121, 11880-11884	16.4	22
333	Experimental and theoretical studies of substituent effects on an orbital-symmetry-forbidden electrocyclization. <i>Journal of the American Chemical Society</i> , 1989 , 111, 5356-5367	16.4	22
332	Enzyme-free synthesis of natural phospholipids in water. <i>Nature Chemistry</i> , 2020 , 12, 1029-1034	17.6	22
331	Reactivity Profiles of Diazo Amides, Esters, and Ketones in Transition-Metal-Free C-H Insertion Reactions. <i>Journal of the American Chemical Society</i> , 2019 , 141, 3558-3565	16.4	22
330	Vinyl Carbocations Generated under Basic Conditions and Their Intramolecular C-H Insertion Reactions. <i>Journal of the American Chemical Society</i> , 2019 , 141, 9140-9144	16.4	21
329	Mechanism and Dynamics of Intramolecular C-H Insertion Reactions of 1-Aza-2-azoniaallene Salts. <i>Journal of the American Chemical Society</i> , 2015 , 137, 9100-7	16.4	21
328	Computational analysis of the stereochemical outcome in the imidazolidinone-catalyzed enantioselective (4 + 3)-cycloaddition reaction. <i>Journal of Organic Chemistry</i> , 2015 , 80, 744-50	4.2	21
327	Biocatalytic trifluoromethylation of unprotected phenols. <i>Nature Communications</i> , 2016 , 7, 13323	17.4	21
326	How tethers control the chemo- and regioselectivities of intramolecular cycloadditions between aryl-1-aza-2-azoniaallenes and alkenes. <i>Organic Letters</i> , 2014 , 16, 4260-3	6.2	21
325	Intramolecular hetero-Diels-Alder reactions of imine and iminium dienophiles: quantum mechanical exploration of mechanisms and stereoselectivities. <i>Journal of Organic Chemistry</i> , 2008 , 73, 2679-86	4.2	21
324	Importance of Intermolecular Hydrogen Bonding for the Stereochemical Control of Allene-Enone (3+2) Annulations Catalyzed by a Bifunctional, Amino Acid Derived Phosphine Catalyst. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 2022-7	16.4	21
323	QM/QM' Direct Molecular Dynamics of Water-Accelerated Diels-Alder Reaction. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 6250-4	3.4	21
322	Anthracene-Triphenylamine-Based Platinum(II) Metallacages as Synthetic Light-Harvesting Assembly. <i>Journal of the American Chemical Society</i> , 2021 , 143, 2908-2919	16.4	21
321	Type II Anion Relay Chemistry: Conformational Constraints To Achieve Effective [1,5]-Vinyl Brook Rearrangements. <i>Journal of the American Chemical Society</i> , 2017 , 139, 8710-8717	16.4	20
320	Torsional Barriers to Rotation and Planarization in Heterocyclic Oligomers of Value in Organic Electronics. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5624-5638	6.4	20
319	Demystifying the asymmetry-amplifying, autocatalytic behaviour of the Soai reaction through structural, mechanistic and computational studies. <i>Nature Chemistry</i> , 2020 , 12, 412-423	17.6	20
318	An Initiation Kinetics Prediction Model Enables Rational Design of Ruthenium Olefin Metathesis Catalysts Bearing Modified Chelating Benzylidenes. <i>ACS Catalysis</i> , 2018 , 8, 4600-4611	13.1	20

317	Quantitative prediction of morphology and electron transport in crystal and disordered organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 11238-11243	7.1	20
316	Transition States of Vicinal Diamine-Catalyzed Aldol Reactions. <i>Journal of the American Chemical Society</i> , 2016 , 138, 503-6	16.4	20
315	Computational investigation of the competition between the concerted Diels-Alder reaction and formation of diradicals in reactions of acrylonitrile with nonpolar dienes. <i>Journal of Organic Chemistry</i> , 2013 , 78, 6582-92	4.2	20
314	Photoelectron spectra of 3-substituted cyclopentenes. Correlations between ionization potentials and cycloaddition regioselectivity. <i>Journal of the American Chemical Society</i> , 1978 , 100, 105-110	16.4	20
313	Molecular Basis for Spirocyclic Formation in the Paraherquamide Biosynthetic Pathway. <i>Journal of the American Chemical Society</i> , 2020 , 142, 2244-2252	16.4	20
312	Synthetic, Mechanistic, and Biological Interrogation of Chemical Space En Route to (-)-Bilobalide. <i>Journal of the American Chemical Society</i> , 2020 , 142, 18599-18618	16.4	20
311	Reactivity of Single-Walled Carbon Nanotubes in the Diels-Alder Cycloaddition Reaction: Distortion-Interaction Analysis along the Reaction Pathway. <i>Chemistry - A European Journal</i> , 2016 , 22, 12819-24	4.8	20
310	Electric field-catalyzed single-molecule Diels-Alder reaction dynamics. <i>Science Advances</i> , 2021 , 7,	14.3	20
309	Asymmetric Photocatalysis by Intramolecular Hydrogen-Atom Transfer in Photoexcited Catalyst-Substrate Complex. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 14462-14466	16.4	19
308	Pd-Catalyzed Decarboxylative Olefination: Stereoselective Synthesis of Polysubstituted Butadienes and Macrocyclic P-glycoprotein Inhibitors. <i>Journal of the American Chemical Society</i> , 2020 , 142, 9982-9992	16.4	19
307	Influence of Endo- and Exocyclic Heteroatoms on Stabilities and 1,3-Dipolar Cycloaddition Reactivities of Mesoionic Azomethine Ylides and Imines. <i>Journal of Organic Chemistry</i> , 2017 , 82, 10980-10988	16.3	19
306	An Efficient Computational Model to Predict the Synthetic Utility of Heterocyclic Arynes. <i>Angewandte Chemie</i> , 2012 , 124, 2812-2816	3.6	19
305	H/vinyl conical intersections of hexatrienes related to the hula-twist photoisomerization. <i>Molecular Physics</i> , 2006 , 104, 993-1008	1.7	19
304	Photolysis of heptanal. <i>Journal of Organic Chemistry</i> , 2006 , 71, 6403-8	4.2	19
303	Thermodynamic and Quantum Chemical Study of the Conversion of Chorismate to (Pyruvate + 4-Hydroxybenzoate). <i>Journal of Physical Chemistry B</i> , 1998 , 102, 8634-8639	3.4	19
302	Schizophrenic substituents: the origin of anomalous substituent effects on cycloaddition regioselectivity. <i>Journal of the American Chemical Society</i> , 1978 , 100, 6531-6533	16.4	19
301	Organocatalysis: Fundamentals and Comparisons to Metal and Enzyme Catalysis. <i>Catalysts</i> , 2016 , 6, 1284	4	19
300	Ambimodal Dipolar/Diels-Alder Cycloaddition Transition States Involving Proton Transfers. <i>Journal of the American Chemical Society</i> , 2018 , 140, 18124-18131	16.4	19

299	Using Ring Strain to Control 4E-Electrocyclization Reactions: Torquoselectivity in Ring Closing of Medium-Ring Dienes and Ring Opening of Bicyclic Cyclobutenes. <i>Journal of Organic Chemistry</i> , 2017 , 82, 4613-4624	4.2	18
298	Bimodal Evans-Polanyi Relationships in Dioxirane Oxidations of sp C-H: Non-perfect Synchronization in Generation of Delocalized Radical Intermediates. <i>Journal of the American Chemical Society</i> , 2017 , 139, 16650-16656	16.4	18
297	Mono-, Di-, and Trifluoroalkyl Substituent Effects on the Torquoselectivities of Cyclobutene and Oxetene Electrocyclic Ring Openings. <i>Journal of Organic Chemistry</i> , 2015 , 80, 11768-72	4.2	18
296	The mechanism of the triple aryne-tetrazine reaction cascade: theory and experiment. <i>Chemical Science</i> , 2018 , 9, 7688-7693	9.4	18
295	Investigation of Trimethyllysine Binding by the HP1 Chromodomain via Unnatural Amino Acid Mutagenesis. <i>Journal of the American Chemical Society</i> , 2017 , 139, 17253-17256	16.4	18
294	H/Allyl and Alkyl/Allyl Conical Intersections: Ubiquitous Control Elements in Photochemical Sigmatropic Shifts. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2651-2652	16.4	18
293	Why are isoxazoles unreactive in Diels-Alder reactions? An ab initio computational study. <i>Journal of Organic Chemistry</i> , 1992 , 57, 3753-3755	4.2	18
292	Efficient -Selective Olefin-Acrylamide Cross-Metathesis Enabled by Sterically Demanding Cyclometalated Ruthenium Catalysts. <i>Journal of the American Chemical Society</i> , 2020 , 142, 20987-20993	16.4	18
291	Iterative Catalysis in the Biosynthesis of Mitochondrial Complex II Inhibitors Harzianopyridone and Atpenin B. <i>Journal of the American Chemical Society</i> , 2020 , 142, 8550-8554	16.4	17
290	Origins of the Stereoretentive Mechanism of Olefin Metathesis with Ru-Dithiolate Catalysts. <i>Journal of Organic Chemistry</i> , 2017 , 82, 10595-10600	4.2	17
289	New Class of Anion-Accelerated Amino-Cope Rearrangements as Gateway to Diverse Chiral Structures. <i>Journal of the American Chemical Society</i> , 2017 , 139, 13141-13146	16.4	17
288	Synthesis of Diverse 11- and 12-Membered Macrolactones from a Common Linear Substrate Using a Single Biocatalyst. <i>ACS Central Science</i> , 2017 , 3, 1304-1310	16.8	17
287	A theoretical study of cyclohexyne addition to carbonyl-C \equiv bonds: allowed and forbidden electrocyclic and nonpericyclic ring-openings of strained cyclobutenes. <i>Journal of Organic Chemistry</i> , 2012 , 77, 4939-48	4.2	17
286	Origins of regioselectivity of Diels-Alder reactions for the synthesis of bisanthraquinone antibiotic BE-43472B. <i>Journal of Organic Chemistry</i> , 2010 , 75, 922-8	4.2	17
285	Combining Quantum Mechanical Reaction Pathways with Force Field Lattice Interactions To Model a Solid-State Phototransformation. <i>Journal of the American Chemical Society</i> , 1997 , 119, 1474-1475	16.4	17
284	The three corrugated surfaces of 1,4-divinyldimethyltetramethylene diradical intermediates and their connections to 1,2-divinylcyclobutane, 4-vinylcyclohexene, 1,5-cyclooctadiene, and two butadienes. <i>Journal of Organic Chemistry</i> , 2005 , 70, 2994-3008	4.2	17
283	Why 6-methylpentacene deconjugates but avoids the thermally allowed unimolecular mechanism. <i>Organic Letters</i> , 2006 , 8, 4915-8	6.2	17
282	Catalysis on the coastline: theozyme, molecular dynamics, and free energy perturbation analysis of antibody 21D8 catalysis of the decarboxylation of 5-nitro-3-carboxybenzisoxazole. <i>Journal of Computational Chemistry</i> , 2003 , 24, 98-110	3.5	17

281	Transition structures and exo/endo stereoselectivities of concerted [6 + 4] cycloadditions with density functional theory. <i>Theoretical Chemistry Accounts</i> , 1999 , 103, 81-84	1.9	17
280	"Anomalous" selectivities in electrophilic aromatic substitutions. <i>Journal of the American Chemical Society</i> , 1979 , 101, 1337-1340	16.4	17
279	Elucidation of the structure of the double [6 + 4] adduct of tropone and dimethylfulvene by nuclear magnetic resonance and the nuclear overhauser effect. <i>Challenge</i> , 1971 , 109	0.8	17
278	Expanded Helicenes as Synthons for Chiral Macrocyclic Nanocarbons. <i>Journal of the American Chemical Society</i> , 2020 , 142, 11084-11091	16.4	17
277	Intercepting fleeting cyclic allenes with asymmetric nickel catalysis. <i>Nature</i> , 2020 , 586, 242-247	50.4	17
276	Catalytic mechanism and endo-to-exo selectivity reversion of an octalin-forming natural Diels-Alderase. <i>Nature Catalysis</i> , 2021 , 4, 223-232	36.5	17
275	Efficient Lewis acid catalysis of an abiological reaction in a de novo protein scaffold. <i>Nature Chemistry</i> , 2021 , 13, 231-235	17.6	17
274	Transient [3,3] Cope rearrangement of 3,3-dicyano-1,5-dienes: computational analysis and 2-step synthesis of arylcycloheptanes. <i>Chemical Science</i> , 2018 , 9, 8760-8764	9.4	17
273	Concerted Ring Opening and Cycloaddition of Chiral Epoxy Enolsilanes with Dienes. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 7422-5	16.4	16
272	Electronic complementarity permits hindered butenolide heterodimerization and discovery of novel cGAS/STING pathway antagonists. <i>Nature Chemistry</i> , 2020 , 12, 310-317	17.6	16
271	Biosynthesis of thiocarboxylic acid-containing natural products. <i>Nature Communications</i> , 2018 , 9, 2362	17.4	16
270	Isomeric triazines exhibit unique profiles of bioorthogonal reactivity. <i>Chemical Science</i> , 2019 , 10, 9109-9114	11.4	16
269	Dynamic Ligand Exchange as a Mechanistic Probe in Pd-Catalyzed Enantioselective C-H Functionalization Reactions Using Monoprotected Amino Acid Ligands. <i>Journal of the American Chemical Society</i> , 2017 , 139, 18500-18503	16.4	16
268	Aromatic Claisen Rearrangements of O-prenylated tyrosine and model prenyl aryl ethers: Computational study of the role of water on acceleration of Claisen rearrangements. <i>European Journal of Organic Chemistry</i> , 2013 , 2013, 2823	3.2	16
267	The Origin of the Halogen Effect on Reactivity and Reversibility of Diels-Alder Cycloadditions Involving Furan. <i>Angewandte Chemie</i> , 2006 , 118, 1470-1473	3.6	16
266	Understanding and Interrupting the Fischer Azaindolization Reaction. <i>Journal of the American Chemical Society</i> , 2017 , 139, 14833-14836	16.4	15
265	Sterically Unprotected Nucleophilic Boron Cluster Reagents. <i>Chem</i> , 2019 , 5, 2461-2469	16.2	15
264	Confined organization of fullerene units along high polymer chains. <i>Journal of Materials Chemistry C</i> , 2013 , 1, 5747	7.1	15

263	Enzyme-Catalyzed Intramolecular Enantioselective Hydroalkoxylation. <i>Journal of the American Chemical Society</i> , 2017 , 139, 3639-3642	16.4	14
262	Stereospecific Synthesis of Substituted Aziridines by a Crystal-to-Crystal Photodenitrogenation of (2)-1,2,3-Triazolines. <i>Organic Letters</i> , 2015 , 17, 4568-71	6.2	14
261	Ligand-Controlled Diastereoselective 1,3-Dipolar Cycloadditions of Azomethine Ylides with Methacrylonitrile. <i>Organic Letters</i> , 2015 , 17, 6166-9	6.2	14
260	Readily Accessible Ambiphilic Cyclopentadienes for Bioorthogonal Labeling. <i>Journal of the American Chemical Society</i> , 2018 , 140, 6426-6431	16.4	14
259	Reversible Photochemically Gated Transformation of a Hemicarcerand to a Carcerand. <i>Angewandte Chemie</i> , 2013 , 125, 683-687	3.6	14
258	Pressure-Induced Cycloadditions of Dicyanoacetylene to Strained Arenes: The Formation of Cyclooctatetraene, 9,10-Dihydronaphthalene, and Azulene Derivatives; A Degenerate [1,5] Sigmatropic Shift—Comparison between Theory and Experiment. <i>Chemistry - A European Journal</i> , 2009 , 15, 2118-2132	4.8	14
257	An enzymatic Alder-ene reaction. <i>Nature</i> , 2020 , 586, 64-69	50.4	14
256	Hyperconjugative Antiaromaticity Activates 4-Pyrazoles as Inverse-Electron-Demand Diels-Alder Dienes. <i>Organic Letters</i> , 2019 , 21, 8492-8495	6.2	13
255	Computational and experimental investigations of the formal dyotropic rearrangements of Himbert arene/allene cycloadducts. <i>Journal of the American Chemical Society</i> , 2015 , 137, 6956-64	16.4	13
254	Computational Design of Enhanced Enantioselectivity in Chiral Phosphoric Acid-Catalyzed Oxidative Desymmetrization of 1,3-Diol Acetals. <i>Journal of the American Chemical Society</i> , 2020 , 142, 8506-8513	16.4	13
253	autoDIAS: a python tool for an automated distortion/interaction activation strain analysis. <i>Journal of Computational Chemistry</i> , 2019 , 40, 2509-2515	3.5	13
252	The mechanism and regioselectivities of (NHC)nickel(ii)hydride-catalyzed cycloisomerization of dienes: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2017 , 15, 7131-7139	3.9	13
251	Catalytic Effects of Ammonium and Sulfonium Salts and External Electric Fields on Aza-Diels-Alder Reactions. <i>Journal of Organic Chemistry</i> , 2020 , 85, 2618-2625	4.2	13
250	Structure and Function of NzeB, a Versatile C-C and C-N Bond-Forming Diketopiperazine Dimerase. <i>Journal of the American Chemical Society</i> , 2020 , 142, 17413-17424	16.4	13
249	Organocatalysis Intermediates as Platforms to Study Noncovalent Interactions: Integrating Fluorine Gauche Effects in Iminium Systems to Facilitate Acyclic Conformational Control. <i>Synlett</i> , 2016 , 27, 1051-1055	2.2	13
248	In Situ Catalyst Modification in Atom Transfer Radical Reactions with Ruthenium Benzyldiene Complexes. <i>Journal of the American Chemical Society</i> , 2016 , 138, 7171-7	16.4	13
247	Controlling, Understanding, and Redirecting the Thermal Rearrangement of 3,3-Dicyano-1,5-enynes. <i>Journal of the American Chemical Society</i> , 2018 , 140, 16134-16139	16.4	13
246	Unveiling the full reaction path of the Suzuki-Miyaura cross-coupling in a single-molecule junction. <i>Nature Nanotechnology</i> , 2021 , 16, 1214-1223	28.7	13

245	Mechanism, Regio-, and Diastereoselectivity of Rh(III)-Catalyzed Cyclization Reactions of N-Arylnitrones with Alkynes: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 4496-4504	2.8	12
244	Design and Applications of N-tert-Butyl Sulfinyl Squaramide Catalysts. <i>Organic Letters</i> , 2017 , 19, 1926-1929	12	12
243	Mesoscale Ordering and Charge-Transport of Crystalline Spiro-OMeTAD Organic Semiconductors. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 993-999	3.8	12
242	Highly torquoselective electrocyclizations and competing 1,7-hydrogen shifts of 1-azatrienes with silyl substitution at the allylic carbon. <i>Organic Letters</i> , 2015 , 17, 2138-41	6.2	12
241	Isotopically Directed Symmetry Breaking and Enantioenrichment in Attrition-Enhanced Deracemization. <i>Journal of the American Chemical Society</i> , 2020 , 142, 3873-3879	16.4	12
240	Catalase Involved in Oxidative Cyclization of the Tetracyclic Ergoline of Fungal Ergot Alkaloids. <i>Journal of the American Chemical Society</i> , 2019 , 141, 17517-17521	16.4	12
239	Theoretical exploration of the mechanism of riboflavin formation from 6,7-dimethyl-8-ribityllumazine: nucleophilic catalysis, hydride transfer, hydrogen atom transfer, or nucleophilic addition?. <i>Journal of the American Chemical Society</i> , 2013 , 135, 6658-68	16.4	12
238	Terminal substituent effects on the reactivity, thermodynamics, and stereoselectivity of the 8E electrocyclization cascades of 1,3,5,7-tetraenes. <i>Journal of Organic Chemistry</i> , 2014 , 79, 11370-7	4.2	12
237	Unexpected Complexity in the Thermal $[2 + 2 + 2]$ Cycloaddition Reactions of Quadricyclane: Theory and Isotope Effects. <i>Journal of the American Chemical Society</i> , 1999 , 121, 4334-4339	16.4	12
236	Intramolecular C(sp ³)-H Bond Oxygenation by Transition-Metal Acylnitrenoids. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 21706-21710	16.4	12
235	Metal-Free Directed C-H Borylation of Pyrroles. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 8500-8504	16.4	12
234	Phosphorus(III)-assisted regioselective C-H silylation of heteroarenes. <i>Nature Communications</i> , 2021 , 12, 524	17.4	12
233	Mechanism and Regioselectivity of an Unsymmetrical Hexadehydro-Diels-Alder (HDDA) Reaction. <i>Journal of Organic Chemistry</i> , 2019 , 84, 1959-1963	4.2	11
232	An Unexpected Ireland-Claisen Rearrangement Cascade During the Synthesis of the Tricyclic Core of Curcusone C: Mechanistic Elucidation by Trial-and-Error and Automatic Artificial Force-Induced Reaction (AFIR) Computations. <i>Journal of the American Chemical Society</i> , 2019 , 141, 6995-7004	16.4	11
231	Origin of π -Facial Stereoselectivity in Thiophene 1-Oxide Cycloadditions. <i>Journal of Organic Chemistry</i> , 2018 , 83, 2611-2616	4.2	11
230	Oxidation of rubrene, and implications for device stability. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 3757-3761	11	11
229	Quinine-Promoted, Enantioselective Boron-Tethered Diels-Alder Reaction by Anomeric Control of Transition-State Conformation. <i>Journal of Organic Chemistry</i> , 2018 , 83, 5756-5765	4.2	11
228	Metathesis and Decomposition of Fischer Carbenes of Cyclometalated Z-Selective Ruthenium Metathesis Catalysts. <i>Organometallics</i> , 2018 , 37, 2212-2216	3.8	11

227	Enzymatic one-step ring contraction for quinolone biosynthesis. <i>Nature Communications</i> , 2018 , 9, 2826	17.4	11
226	The effect of hexyl side chains on molecular conformations, crystal packing, and charge transport of oligothiophenes. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 582-588	7.1	11
225	Manifestation of Felkin-Anh Control in Enantioselective Acyl Transfer Catalysis: Kinetic Resolution of Carboxylic Acids. <i>Angewandte Chemie</i> , 2012 , 124, 9776-9780	3.6	11
224	Theoretical Study of a Termolecular Mechanism for the Reaction of (Trimethylsilyl)thiazole with Carbonyl Compounds. <i>Journal of Organic Chemistry</i> , 1996 , 61, 1922-1926	4.2	11
223	Transition Structures of the Electrocyclic Reactions of cis,cis,cis-1,3,5-Cyclooctatriene. <i>Israel Journal of Chemistry</i> , 1993 , 33, 287-293	3.4	11
222	Fjord-Edge Graphene Nanoribbons with Site-Specific Nitrogen Substitution. <i>Journal of the American Chemical Society</i> , 2020 , 142, 18093-18102	16.4	11
221	Total Synthesis and Computational Investigations of Sesquiterpene-Tropolones Ameliorate Stereochemical Inconsistencies and Resolve an Ambiguous Biosynthetic Relationship. <i>Journal of the American Chemical Society</i> , 2021 , 143, 6006-6017	16.4	11
220	Rhodium-Catalyzed Intramolecular [5+2] Cycloaddition of Inverted 3-Acyloxy-1,4-enyne and Alkyne: Experimental and Theoretical Studies. <i>Chemistry - A European Journal</i> , 2016 , 22, 7079-83	4.8	11
219	Palladium-Catalyzed Silacyclization of (Hetero)Arenes with a Tetrasilane Reagent through Twofold C-H Activation. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 7066-7071	16.4	11
218	Mechanisms and Origins of Selectivities of the Lewis Acid-Catalyzed Diels-Alder Reactions between Arylallenes and Acrylates. <i>Journal of Organic Chemistry</i> , 2017 , 82, 6398-6402	4.2	10
217	Stereoselective [4+2]-Cycloaddition with Chiral Alkenylboranes. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 11432-11439	16.4	10
216	Intramolecular Diels-Alder Approaches to the Decalin Core of Verongidolide: The Origin of the exo-Selectivity, a DFT Analysis. <i>Journal of Organic Chemistry</i> , 2018 , 83, 5975-5985	4.2	10
215	On the prevalence of bridged macrocyclic pyrroloindolines formed in regiodivergent alkylations of tryptophan. <i>Chemical Science</i> , 2016 , 7, 4158-4166	9.4	10
214	Origins of Stereoselectivity of Chiral Vicinal Diamine-Catalyzed Aldol Reactions. <i>Journal of Organic Chemistry</i> , 2016 , 81, 12408-12415	4.2	10
213	Sungeidines from a Non-canonical Eneidyne Biosynthetic Pathway. <i>Journal of the American Chemical Society</i> , 2020 , 142, 1673-1679	16.4	10
212	Computational-Based Mechanistic Study and Engineering of Cytochrome P450 MycG for Selective Oxidation of 16-Membered Macrolide Antibiotics. <i>Journal of the American Chemical Society</i> , 2020 , 142, 17981-17988	16.4	10
211	An Asymmetric S ₂ Dynamic Kinetic Resolution. <i>Journal of the American Chemical Society</i> , 2021 , 143, 7509-7520	16.4	10
210	Nonenzymatic Stereoselective -Glycosylation of Polypeptides and Proteins. <i>Journal of the American Chemical Society</i> , 2021 , 143, 11919-11926	16.4	10

209	Variations in Rotational Barriers of Allyl and Benzyl Cations, Anions, and Radicals. <i>Journal of Organic Chemistry</i> , 2016 , 81, 9576-9584	4.2	10
208	A Four-Step Synthesis of Substituted 5,11-Dicyano-6,12-diaryltetracenes with Enhanced Stability and High Fluorescence Emission. <i>Chemistry - A European Journal</i> , 2018 , 24, 159-168	4.8	10
207	Mechanism of Permanganate-Promoted Dihydroxylation of Complex Diketopiperazines: Critical Roles of Counter-cation and Ion-Pairing. <i>Journal of the American Chemical Society</i> , 2018 , 140, 13375-13386	16.4	10
206	Cleaving arene rings for acyclic alkenylnitrile synthesis. <i>Nature</i> , 2021 , 597, 64-69	50.4	10
205	Organocatalytic enantioselective dearomatization of thiophenes by 1,10-conjugate addition of indole imine methides. <i>Nature Communications</i> , 2021 , 12, 4881	17.4	10
204	High Site Selectivity in Electrophilic Aromatic Substitutions: Mechanism of C-H Thianthrenation. <i>Journal of the American Chemical Society</i> , 2021 , 143, 16041-16054	16.4	10
203	Origins of Regioselectivity in the Fischer Indole Synthesis of a Selective Androgen Receptor Modulator. <i>Journal of Organic Chemistry</i> , 2017 , 82, 5904-5909	4.2	9
202	Synthesis and Evaluation of Sterically Demanding Ruthenium Dithiolate Catalysts for Stereoretentive Olefin Metathesis. <i>Organometallics</i> , 2017 , 36, 3940-3953	3.8	9
201	Activating Pyrimidines by Pre-distortion for the General Synthesis of 7-Aza-indazoles from 2-Hydrazonylpyrimidines via Intramolecular Diels-Alder Reactions. <i>Journal of the American Chemical Society</i> , 2019 , 141, 15901-15909	16.4	9
200	Secondary Orbital Interactions Enhance the Reactivity of Alkynes in Diels-Alder Cycloadditions. <i>Journal of the American Chemical Society</i> , 2019 , 141, 2224-2227	16.4	9
199	Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with η -Vinyl Allylboron Reagents. <i>Angewandte Chemie</i> , 2020 , 132, 10627-10635	3.6	9
198	Nucleophilic ¹⁸ F-Fluorination of Anilines via N-Arylsydnone Intermediates. <i>Synlett</i> , 2018 , 29, 1131-1135	2.2	9
197	Origins of Selective Formation of 5-Vinyl-2-methylene Furans from Oxyallyl/Diene (3+2) Cycloadditions with Pd(0) Catalysis. <i>Journal of the American Chemical Society</i> , 2019 , 141, 12382-12387	16.4	9
196	Asymmetric Desymmetrization of Oxetanes for the Synthesis of Chiral Tetrahydrothiophenes and Tetrahydroselenophenes. <i>Angewandte Chemie</i> , 2019 , 131, 18223-18228	3.6	9
195	Synthesis of [¹⁸ F]Fluoroarenes by Nucleophilic Radiofluorination of N-Arylsydnone. <i>Angewandte Chemie</i> , 2017 , 129, 13186-13190	3.6	9
194	Chirality Sensing of η -Hydroxyphosphonates by N-tert-Butyl Sulfinyl Squaramide. <i>Organic Letters</i> , 2017 , 19, 4191-4194	6.2	9
193	Elucidation of Strong Cooperative Effects Caused by Dispersion Interactions in a Recognition-Mediated Diels-Alder Reaction. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 5064-5071	6.4	9
192	Performance-limiting formation dynamics in mixed-halide perovskites. <i>Science Advances</i> , 2021 , 7, eabj1792	12.3	9

191	Atroposelective Synthesis of Axially Chiral N-Arylpyrroles by Chiral-at-Rhodium Catalysis. <i>Angewandte Chemie</i> , 2020 , 132, 13654-13658	3.6	9
190	Chlorinated Spiroconjugated Fused Extended Aromatics for Multifunctional Organic Electronics. <i>Advanced Materials</i> , 2021 , 33, e2006120	24	9
189	Theoretical Study of Diastereoselective NHC-Catalyzed Cross-Benzoin Reactions between Furfural and -Boc-Protected β -Amino Aldehydes. <i>Journal of Organic Chemistry</i> , 2019 , 84, 13565-13571	4.2	8
188	Impact of morphology, side-chains, and crystallinity on charge-transport properties of β -extended double helicenes. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 901-914	3.6	8
187	Bacterial Tetrabromopyrrole Debrominase Shares a Reductive Dehalogenation Strategy with Human Thyroid Deiodinase. <i>Biochemistry</i> , 2019 , 58, 5329-5338	3.2	8
186	Computational Studies of Ruthenium-Catalyzed Olefin Metathesis 2015 , 199-252		8
185	Simulations of Molecular Ordering and Charge-Transport of Oligo-Didodecylquaterthiophenes (DDQT). <i>Journal of Physical Chemistry C</i> , 2015 , 119, 158-165	3.8	8
184	Beispielloses dearomatisiertes Spirocyclopropan in einer sequenziellen Rhodium(III)-katalysierten C-H-Aktivierung und Umlagerungsreaktion. <i>Angewandte Chemie</i> , 2018 , 130, 5618-5622	3.6	8
183	Origins of regioselectivity in 1,3-dipolar cycloadditions of nitrile oxides with alkynylboronates. <i>Bioorganic and Medicinal Chemistry</i> , 2016 , 24, 4787-4790	3.4	8
182	Theoretical Analysis of the Retro-Diels-Alder Reactivity of Oxanorbornadiene Thiol and Amine Adducts. <i>Organic Letters</i> , 2017 , 19, 4504-4507	6.2	8
181	Medium-Ring Effects on the Endo/Exo Selectivity of the Organocatalytic Intramolecular Diels-Alder Reaction. <i>Journal of Organic Chemistry</i> , 2015 , 80, 12058-75	4.2	8
180	An Enzymatic Platform for Primary Amination of 1-Aryl-2-alkyl Alkynes.. <i>Journal of the American Chemical Society</i> , 2021 ,	16.4	8
179	More Than π -Stacking: Contribution of Amide- π and CH- π Interactions to Crotonyllysine Binding by the AF9 YEATS Domain. <i>Journal of the American Chemical Society</i> , 2020 , 142, 17048-17056	16.4	8
178	Computational Exploration of the Mechanism of Critical Steps in the Biomimetic Synthesis of Preisolactone A, and Discovery of New Ambimodal (5 + 2)/(4 + 2) Cycloadditions. <i>Journal of the American Chemical Society</i> , 2021 , 143, 6601-6608	16.4	8
177	Origins of Endo Selectivity in Diels-Alder Reactions of Cyclic Allene Dienophiles. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 14989-14997	16.4	8
176	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. <i>Frontiers in Chemistry</i> , 2018 , 6, 663	5	8
175	A Polyketide Cyclase That Forms Medium-Ring Lactones. <i>Journal of the American Chemical Society</i> , 2021 , 143, 80-84	16.4	8
174	Fungal Dioxygenase AsqJ Is Promiscuous and Bimodal: Substrate-Directed Formation of Quinolones versus Quinazolinones. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 8297-8302	16.4	8

173	Halogen-bond-assisted radical activation of glycosyl donors enables mild and stereoconvergent 1,2-cis-glycosylation.. <i>Nature Chemistry</i> , 2022 ,	17.6	8
172	Evaluation of DFT Methods and Implicit Solvation Models for Anion-Binding Host-Guest Systems. <i>Helvetica Chimica Acta</i> , 2019 , 102, e1900032	2	7
171	Concerted [4 + 2] and Stepwise (2 + 2) Cycloadditions of Tetrafluoroethylene with Butadiene: DFT and DLPNO-UCCSD(T) Explorations. <i>Journal of Organic Chemistry</i> , 2020 , 85, 3858-3864	4.2	7
170	Stereospecific Ring Contraction of Bromocycloheptenes through Dyotropic Rearrangements via Nonclassical Carbocation-Anion Pairs. <i>Journal of the American Chemical Society</i> , 2018 , 140, 4986-4990	16.4	7
169	Intramolecular C-H Activation Reactions of Ru(NHC) Complexes Combined with H ₂ Transfer to Alkenes: A Theoretical Elucidation of Mechanisms and Effects of Ligands on Reactivities. <i>Organometallics</i> , 2017 , 36, 3613-3623	3.8	7
168	Thermodynamic and stereochemical aspects of the polymerizability of glycolide and lactide. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	7
167	Perspective on the theoretical interpretation of 1-2 asymmetric induction. The importance of antiperiplanarity. <i>Theoretical Chemistry Accounts</i> , 2000 , 103, 330-331	1.9	7
166	Eine konvergente Strategie zur asymmetrischen Synthese enantiomerenreiner Bicyclen über eine siliciumgesteuerte Cycloaddition: Synthese von enantiomerenreinem Bicyclo[3.2.0]hept-2-en-6-on. <i>Angewandte Chemie</i> , 1999 , 111, 2897-2899	3.6	7
165	Dispersion and Steric Effects on Enantio-/Diastereoselectivities in Synergistic Dual Transition-Metal Catalysis.. <i>Journal of the American Chemical Society</i> , 2022 ,	16.4	7
164	Computational Exploration of a Redox-Neutral Organocatalytic Mitsunobu Reaction. <i>Journal of the American Chemical Society</i> , 2020 , 142, 16403-16408	16.4	7
163	Mechanism of an Organocatalytic Cope Rearrangement Involving Iminium Intermediates: Elucidating the Role of Catalyst Ring Size. <i>Journal of the American Chemical Society</i> , 2020 , 142, 16877-16886	16.4	7
162	Taming Radical Pairs in the Crystalline Solid State: Discovery and Total Synthesis of Psychotriadine. <i>Journal of the American Chemical Society</i> , 2021 , 143, 4043-4054	16.4	7
161	Biosynthesis of Cyclophane-Containing Hirsutellone Family of Fungal Natural Products. <i>Journal of the American Chemical Society</i> , 2021 , 143, 5605-5609	16.4	7
160	Accelerated Development of a Scalable Ring-Closing Metathesis to Manufacture AMG 176 Using a Combined High-Throughput Experimentation and Computational Modeling Approach. <i>Organic Process Research and Development</i> , 2021 , 25, 442-451	3.9	7
159	Cooperative Stapling of Native Peptides at Lysine and Tyrosine or Arginine with Formaldehyde. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 6646-6652	16.4	7
158	Computational Exploration of a Pd(II)-Catalyzed C-H Arylation Where Stereoselectivity Arises from Attractive Aryl-Aryl Interactions. <i>Journal of Organic Chemistry</i> , 2018 , 83, 14786-14790	4.2	7
157	Stable, Reactive, and Orthogonal Tetrazines: Dispersion Forces Promote the Cycloaddition with Isonitriles. <i>Angewandte Chemie</i> , 2019 , 131, 9141-9146	3.6	6
156	Molecular Basis of Iterative C-H Oxidation by TamI, a Multifunctional P450 monooxygenase from the Tirandamycin Biosynthetic Pathway. <i>ACS Catalysis</i> , 2020 , 10, 13445-13454	13.1	6

155	Huisgen's 1,3-Dipolar Cycloadditions to Fulvenes Proceed via Ambimodal [6+4]/[4+2] Transition States. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 12412-12416	16.4	6
154	Enhanced Rotation by Ground State Destabilization in Amphidynamic Crystals of a Dipolar 2,3-Difluorophenylene Rotator as Established by Solid State 2H NMR and Dielectric Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 15391-15398	3.8	6
153	Selective Enzymatic Oxidation of Silanes to Silanols. <i>Angewandte Chemie</i> , 2020 , 132, 15637-15641	3.6	6
152	Origins of Stereoselectivity in Mannich Reactions Catalyzed by Chiral Vicinal Diamines. <i>Journal of Organic Chemistry</i> , 2018 , 83, 3171-3176	4.2	6
151	Thermodynamic Control of Isomerizations of Bicyclic Radicals: Interplay of Ring Strain and Radical Stabilization. <i>Organic Letters</i> , 2016 , 18, 32-5	6.2	6
150	Analysis of supramolecular complex energetics in artificial replicators. <i>Chemical Science</i> , 2013 , 4, 3591	9.4	6
149	Origins of Stereoselectivity of Enamine-Iminium-Activated Nazarov Cyclizations by Vicinal Diamines. <i>Journal of Organic Chemistry</i> , 2017 , 82, 8186-8190	4.2	6
148	Tautomerization and Dimerization of 6,13-Disubstituted Derivatives of Pentacene. <i>Chemistry - A European Journal</i> , 2017 , 23, 6111-6117	4.8	6
147	Distortion, Tether, and Entropy Effects on Transannular Diels-Alder Cycloaddition Reactions of 10-18-Membered Rings. <i>Journal of Organic Chemistry</i> , 2015 , 80, 11039-47	4.2	6
146	Pd(II)-Catalyzed Synthesis of Benzocyclobutenes by η^6 Methylene-Selective C(sp)-H Arylation with a Transient Directing Group. <i>Journal of the American Chemical Society</i> , 2021 , 143, 20035-20041	16.4	6
145	Bioinspired Synthesis of (-)-PF-1018. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 5263-5267	16.4	6
144	Structural Contributions to Autocatalysis and Asymmetric Amplification in the Soai Reaction. <i>Journal of the American Chemical Society</i> , 2020 , 142, 18387-18406	16.4	6
143	Computational Investigation of the Mechanism of Diels-Alderase PyrI4. <i>Journal of the American Chemical Society</i> , 2020 , 142, 20232-20239	16.4	6
142	Direct Synthesis of Ketones from Methyl Esters by Nickel-Catalyzed Suzuki-Miyaura Coupling. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 13476-13483	16.4	6
141	Computational Exploration of How Enzyme XimE Converts Natural S-Epoxy to Pyran and R-Epoxy to Furan. <i>ACS Catalysis</i> , 2021 , 11, 7928-7942	13.1	6
140	Cyclization by C(sp ³) η^6 Arylation with a Transient Directing Group for the Diastereoselective Preparation of Indanes. <i>ACS Catalysis</i> , 2021 , 11, 3115-3127	13.1	6
139	Dipolar order in an amphidynamic crystalline metal-organic framework through reorienting linkers. <i>Nature Chemistry</i> , 2021 , 13, 278-283	17.6	6
138	[8+2] vs [4+2] Cycloadditions of Cyclohexadienamines to Tropone and Heptafulvenes-Mechanisms and Selectivities. <i>Journal of the American Chemical Society</i> , 2021 , 143, 934-944	16.4	6

137	1,3-Dipolar Cycloaddition Reactions of Low-Valent Rhodium and Iridium Complexes with Arylnitrile N-Oxides. <i>Journal of Organic Chemistry</i> , 2017 , 82, 5096-5101	4.2	5
136	Origins of Stereoselectivity in Chiral Aminoalcohol Catalysis of Oxyallyl Cation-Indole Reactions. <i>Organic Letters</i> , 2017 , 19, 5685-5688	6.2	5
135	Diels-Alder reactivities of cycloalkenediones with tetrazine. <i>Journal of Molecular Modeling</i> , 2019 , 25, 33	2	5
134	Hyperconjugative $\sigma \rightarrow \pi^*$ Interactions Stabilize the Enol Form of Perfluorinated Cyclic Keto-Enol Systems. <i>Journal of Organic Chemistry</i> , 2019 , 84, 6432-6436	4.2	5
133	Global Diastereoconvergence in the Ireland-Claisen Rearrangement of Isomeric Enolates: Synthesis of Tetrasubstituted β -Amino Acids. <i>Journal of the American Chemical Society</i> , 2020 , 142, 21938-21947	16.4	5
132	Understand the Specific Regio- and Enantioselectivity of Fluostatin Conjugation in the Post-Biosynthesis. <i>Biomolecules</i> , 2020 , 10,	5.9	5
131	Molecular Spur Gears with Triptycene Rotators and a Norbornane-Based Stator. <i>Organic Letters</i> , 2020 , 22, 4049-4052	6.2	5
130	Interception of the Bycroft-Gowland Intermediate in the Enzymatic Macrocyclization of Thiopeptides. <i>Journal of the American Chemical Society</i> , 2020 , 142, 13170-13179	16.4	5
129	Amentotaxins C-V, Structurally Diverse Diterpenoids from the Leaves and Twigs of the Vulnerable Conifer and Their Cytotoxic Effects. <i>Journal of Natural Products</i> , 2020 , 83, 2129-2144	4.9	5
128	Factors Controlling Reactivity in the Hydrogen Atom Transfer and Radical Addition Steps of a Radical Relay Cascade. <i>Organic Letters</i> , 2019 , 21, 5894-5897	6.2	5
127	Pyridine-Based Cavitands for Acid and Carboxylate Recognition. <i>Molecular Crystals and Liquid Crystals</i> , 2006 , 456, 175-192	0.5	5
126	Theozymes and Catalyst Design 2005 , 79-88		5
125	Bis-periazulene: a simple Kekulébiradical with a triplet ground state. <i>Theoretical Chemistry Accounts</i> , 1999 , 102, 397-400	1.9	5
124	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 24096-24106	16.4	5
123	General Light-Mediated, Highly Diastereoselective Piperidine Epimerization: From Most Accessible to Most Stable Stereoisomer. <i>Journal of the American Chemical Society</i> , 2021 , 143, 126-131	16.4	5
122	Boron tribromide as a reagent for anti-Markovnikov addition of HBr to cyclopropanes. <i>Chemical Science</i> , 2020 , 11, 9426-9433	9.4	5
121	Cycloadditions of Cyclopentadiene and Cycloheptatriene with Tropones: All -[6+4] Cycloadditions Are Ambimodal. <i>Journal of the American Chemical Society</i> , 2021 , 143, 3918-3926	16.4	5
120	Post-Transition State Bifurcation in Iron-Catalyzed Arene Aminations. <i>ACS Catalysis</i> , 2021 , 11, 6816-6824	13.1	5

119	Total Synthesis of (-)-Strictosidine and Interception of Aryne Natural Product Derivatives "Strictosidyne" and "Strictosamidyne". <i>Journal of the American Chemical Society</i> , 2021 , 143, 7471-7479	16.4	5
118	How the Lewis Base F Catalyzes the 1,3-Dipolar Cycloaddition between Carbon Dioxide and Nitrilimines. <i>Journal of Organic Chemistry</i> , 2021 , 86, 4320-4325	4.2	5
117	Origin of Increased Reactivity in Rhenium-Mediated Cycloadditions of Tetrazines. <i>Journal of Organic Chemistry</i> , 2021 , 86, 13129-13133	4.2	5
116	Lattice strain suppresses point defect formation in halide perovskites. <i>Nano Research</i> , 2021 , 14, 101-110	10	5
115	Violations. How Nature Circumvents the Woodward-Hoffmann Rules and Promotes the Forbidden Conrotatory 4 + 2 Electron Electrocyclization of Prinzbach's Vinylogous Sesquifulvalene.. <i>Journal of the American Chemical Society</i> , 2021 , 143, 21694-21704	16.4	5
114	Exploring the molecular basis for substrate specificity in homologous macrolide biosynthetic cytochromes P450. <i>Journal of Biological Chemistry</i> , 2019 , 294, 15947-15961	5.4	4
113	Isoquinoline thiosemicarbazone displays potent anticancer activity with efficacy against aggressive leukemias. <i>RSC Medicinal Chemistry</i> , 2020 , 11, 392-410	3.5	4
112	Active Controlled and Tunable Coacervation Using Side-Chain Functional π -Helical Homopolypeptides. <i>Journal of the American Chemical Society</i> , 2021 , 143, 18196-18203	16.4	4
111	An enantioselective ambimodal cross-Diels-Alder reaction and applications in synthesis. <i>Nature Catalysis</i> , 2021 , 4, 892-900	36.5	4
110	Noncovalent π -stacked robust topological organic framework. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 20397-20403	11.5	4
109	Computational Exploration of Ambiphilic Reactivity of Azides and Sustmann's Paradigmatic Parabola. <i>Journal of Organic Chemistry</i> , 2021 , 86, 5792-5804	4.2	4
108	Energy of Concert and Origins of Regioselectivity for 1,3-Dipolar Cycloadditions of Diazomethane. <i>Journal of Organic Chemistry</i> , 2021 , 86, 6840-6846	4.2	4
107	Origin and Control of Chemoselectivity in Cytochrome Catalyzed Carbene Transfer into Si-H and N-H bonds. <i>Journal of the American Chemical Society</i> , 2021 , 143, 7114-7123	16.4	4
106	Arene-Perfluoroarene Interactions in Solution. <i>Journal of Organic Chemistry</i> , 2021 , 86, 8425-8436	4.2	4
105	Engineering P450 Tam1 as an Iterative Biocatalyst for Selective Late-Stage C-H Functionalization and Epoxidation of Tirandamycin Antibiotics.. <i>ACS Catalysis</i> , 2021 , 11, 8304-8316	13.1	4
104	Study of Ground State Interactions of Enantiopure Chiral Quaternary Ammonium Salts and Amides, Nitroalkanes, Nitroalkenes, Esters, Heterocycles, Ketones and Fluoroamides. <i>Chemistry - A European Journal</i> , 2021 , 27, 11352-11366	4.8	4
103	Mechanisms and Dynamics of Synthetic and Biosynthetic Formation of Delitschiapyrones: Solvent Control of Ambimodal Periselectivity. <i>Journal of the American Chemical Society</i> , 2021 , 143, 11734-11740	16.4	4
102	Unexpected, Latent Radical Reaction of Methane Propagated by Trifluoromethyl Radicals. <i>Journal of Organic Chemistry</i> , 2016 , 81, 9820-9825	4.2	4

101	Die Evolution des Diels-Alder-Reaktionsmechanismus seit den 1930er Jahren: Woodward, Houk zusammen mit Woodward und der Einfluss der Computerchemie auf das Verständnis von Cycloadditionen. <i>Angewandte Chemie</i> , 2021 , 133, 12768-12790	3.6	4
100	Library construction of stereochemically diverse isomers of spiroooliganin: their total synthesis and antiviral activity. <i>Chemical Science</i> , 2021 , 12, 7003-7011	9.4	4
99	Overcoming Kinetic and Thermodynamic Challenges of Classic Cope Rearrangements. <i>Journal of Organic Chemistry</i> , 2021 , 86, 2632-2643	4.2	4
98	Mechanism and Origins of Stereoselectivity of the Aldol-Tishchenko Reaction of Sulfinimines. <i>Journal of Organic Chemistry</i> , 2021 , 86, 4296-4303	4.2	4
97	Ambiphilic Reactivity of Vinyl Pd-Oxyallyl for Expeditious Construction of Highly Functionalized Cyclooctanoids. <i>Organic Letters</i> , 2021 , 23, 7330-7335	6.2	4
96	Isolation and X-ray Crystal Structure of an Electrogenated TEMPO-N Charge-Transfer Complex. <i>Organic Letters</i> , 2021 , 23, 454-458	6.2	4
95	Organocatalytic Discrimination of Non-Directing Aryl and Heteroaryl Groups: Enantioselective Synthesis of Bioactive Indole-Containing Triarylmethanes. <i>Chemical Science</i> ,	9.4	4
94	(2+1)-Cycloaddition Reactions Give Further Evidence of the Nitrenium-like Character of 1-Aza-2-azoniaallene Salts. <i>Journal of Organic Chemistry</i> , 2017 , 82, 4001-4005	4.2	3
93	Acyclic Stereocontrol in the Additions of Nucleophilic Alkenes to β -Chiral N-Sulfonyl Imines. <i>Chemistry - A European Journal</i> , 2019 , 25, 12214-12220	4.8	3
92	Synthesis and Target Identification of a Novel Electrophilic Warhead, 2-Chloromethylquinoline. <i>Biochemistry</i> , 2019 , 58, 2715-2719	3.2	3
91	Computational Investigation into Ligand Effects on Correlated Geared Dynamics in Dirhodium Supramolecular Gears-Insights Beyond the NMR Experimental Window. <i>Journal of Organic Chemistry</i> , 2020 , 85, 8695-8701	4.2	3
90	An Experimental Stereoselective Photochemical [1s,3s]-Sigmatropic Silyl Shift and the Existence of Silyl/Allyl Conical Intersections. <i>Journal of the American Chemical Society</i> , 2020 , 142, 6030-6035	16.4	3
89	Influence of Terminal Carboxyl Groups on the Structure and Reactivity of Functionalized m-Carboranethiolate Self-Assembled Monolayers. <i>Chemistry of Materials</i> , 2020 , 32, 6800-6809	9.6	3
88	Mechanism of the Manolikakes Enamide-Based Domino Reaction for the Stereospecific Construction of Tetrahydropyrans. <i>Journal of Organic Chemistry</i> , 2020 , 85, 3806-3811	4.2	3
87	H ₂ Vinyl Conical Intersections for Dienes: A Mechanism for the Photochemical Hula Twist¶. <i>Photochemistry and Photobiology</i> , 2007 , 76, 616-621	3.6	3
86	Allylic C(sp ³)H arylation of olefins via ternary catalysis 2022 , 1, 59-68		3
85	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. <i>Angewandte Chemie - International Edition</i> , 2021 ,	16.4	3
84	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. <i>Angewandte Chemie</i> , 2021 , 133, 24298-24308	3.6	3

83	Photorearrangement of [8]-2,6-Pyridinophane -Oxide. <i>Journal of the American Chemical Society</i> , 2020 , 142, 20717-20724	16.4	3
82	Dramatic Effect of π -Heteroatom Dienolate Substituents on Counterion Assisted Asymmetric Anionic Amino-Cope Reaction Cascades. <i>Journal of the American Chemical Society</i> , 2021 , 143, 5793-5804	16.4	3
81	Direct Synthesis of Ketones from Methyl Esters by Nickel-Catalyzed Suzuki-Miyaura Coupling. <i>Angewandte Chemie</i> , 2021 , 133, 13588-13595	3.6	3
80	Computations Reveal That Electron-Withdrawing Leaving Groups Facilitate Intramolecular Conjugate Displacement Reactions by Negative Hyperconjugation. <i>Journal of Organic Chemistry</i> , 2016 , 81, 4290-4	4.2	3
79	Understanding the R882H mutation effects of DNA methyltransferase DNMT3A: a combination of molecular dynamics simulations and QM/MM calculations.. <i>RSC Advances</i> , 2019 , 9, 31425-31434	3.7	3
78	Origins of Selectivities in the Stork Diels-Alder Cycloaddition for the Synthesis of (–)-4-Methylenegermine. <i>Organic Letters</i> , 2018 , 20, 6108-6111	6.2	3
77	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 18201-18208	16.4	3
76	Total Syntheses of (+)-Peniciketals A-B and (-)-Diocollettines A Exploiting a Photoisomerization/Cyclization Union Protocol. <i>Journal of Organic Chemistry</i> , 2021 , 86, 13583-13597	4.2	3
75	Enzymatic control of endo- and exo-stereoselective Diels-Alder reactions with broad substrate scope. <i>Nature Catalysis</i> , 2021 , 4, 1059-1069	36.5	3
74	Application of the Spin-Center Shift in Organic Synthesis. <i>Jacs Au</i> ,		3
73	Ab initio molecular metadynamics simulation for S-nitrosylation by nitric oxide: S-nitroxide as the key intermediate. <i>Molecular Simulation</i> , 2017 , 43, 1134-1141	2	2
72	Development of indazole mineralocorticoid receptor antagonists and investigation into their selective late-stage functionalization. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2019 , 29, 1854-1858	2.9	2
71	Cycloadditions of Oxacyclic Allenes and a Catalytic Asymmetric Entryway to Enantioenriched Cyclic Allenes. <i>Angewandte Chemie</i> , 2019 , 131, 5709-5713	3.6	2
70	Rolf Huisgen's Classic Studies of Cyclic Triene Diels-Alder Reactions Elaborated by Modern Computational Analysis. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 12506-12519	16.4	2
69	Stereoselective [4+2]-Cycloaddition with Chiral Alkenylboranes. <i>Angewandte Chemie</i> , 2020 , 132, 11529-11536	16.36	2
68	Thermodynamic consequences of Tyr to Trp mutations in the cation-mediated binding of trimethyllysine by the HP1 chromodomain. <i>Chemical Science</i> , 2020 , 11, 3495-3500	9.4	2
67	Rational Development of Remote C-H Functionalization of Biphenyl: Experimental and Computational Studies. <i>Angewandte Chemie</i> , 2020 , 132, 4800-4807	3.6	2
66	The Distortion/Interaction Model for Analysis of Activation Energies of Organic Reactions 2018 , 371-402		2

65	Electrochemical Fluorination of Vinyl Boronates through Donor-Stabilized Vinyl Carbocation Intermediates.. <i>Angewandte Chemie - International Edition</i> , 2022 ,	16.4	2
64	Palladium-catalyzed stereospecific CB coupling toward diverse PN-heterocycles. <i>Chem</i> , 2022 , 8, 569-579	16.2	2
63	Extended β -Strands Contribute to Reversible Amyloid Formation.. <i>ACS Nano</i> , 2022 ,	16.7	2
62	Tunable Amine-Reactive Electrophiles for Selective Profiling of Lysine. <i>Angewandte Chemie - International Edition</i> , 2021 ,	16.4	2
61	Mechanisms and Conformational Control of (4 + 2) and (2 + 2) Cycloadditions of Dienes to Keteniminium Cations. <i>Journal of Organic Chemistry</i> , 2020 , 85, 2597-2606	4.2	2
60	Computational NMR Spectra of o-Benzyne and Stable Guests and Their Hemicarceplexes. <i>Chemistry - A European Journal</i> , 2020 , 26, 2626-2634	4.8	2
59	Intramolecular C(sp ³)H Bond Oxygenation by Transition-Metal Acylnitrenoids. <i>Angewandte Chemie</i> , 2020 , 132, 21890-21894	3.6	2
58	Diversification of Nucleophile-Intercepted Beckmann Fragmentation Products and Related Density Functional Theory Studies. <i>Journal of Organic Chemistry</i> , 2020 , 85, 11396-11408	4.2	2
57	Biosynthesis of the fungal glyceraldehyde-3-phosphate dehydrogenase inhibitor heptelidic acid and mechanism of self-resistance. <i>Chemical Science</i> , 2020 , 11, 9554-9562	9.4	2
56	Synthesis of 2-Ethenylcyclopropyl Aryl Ketones via Intramolecular S ₂ -like Displacement of an Ester. <i>Organic Letters</i> , 2016 , 18, 5138-5141	6.2	2
55	Facial Selectivities in Hydride Reductions of Hindered Endocyclic Iminium Ions. <i>Journal of Organic Chemistry</i> , 2019 , 84, 273-281	4.2	2
54	Conformational dynamics of androgen receptors bound to agonists and antagonists. <i>Scientific Reports</i> , 2021 , 11, 15887	4.9	2
53	Probing Catalyst Speciation in Pd-MPAAM-Catalyzed Enantioselective C(sp ³)H Arylation: Catalyst Improvement via Destabilization of Off-Cycle Species. <i>ACS Catalysis</i> , 2021 , 11, 11040-11048	13.1	2
52	Constructing Saturated Guanidinium Heterocycles by Cycloaddition of -Amidinylium Ions with Indoles. <i>Organic Letters</i> , 2021 , 23, 7618-7623	6.2	2
51	Facile access to fused 2D/3D rings via intermolecular cascade dearomative [2 + 2] cycloaddition/rearrangement reactions of quinolines with alkenes. <i>Nature Catalysis</i> , 2022 , 5, 405-413	36.5	2
50	Aromatic Ring Substituted Aaptamine Analogues as Potential Cytotoxic Agents against Extranodal Natural Killer/T-Cell Lymphoma. <i>Journal of Natural Products</i> , 2020 , 83, 3758-3763	4.9	1
49	Rolf Huisgen's Classic Studies of Cyclic Triene Diels-Alder Reactions Elaborated by Modern Computational Analysis. <i>Angewandte Chemie</i> , 2020 , 132, 12606-12619	3.6	1
48	Formation of Aminocyclopentadienes from Silyldihydropyridines: Ring Contractions Driven by Anion Stabilization. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 6605-6609	16.4	1

47	Dynamics in Carbene Reactions 2013 , 131-165		1
46	Multiple Mechanisms for the Thermal Decomposition of Metallaisoxazolin-5-ones from Computational Investigations. <i>Journal of Organic Chemistry</i> , 2017 , 82, 8438-8443	4.2	1
45	Competition Between Concerted and Stepwise Dynamics in the Triplet Di- π -Methane Rearrangement. <i>Angewandte Chemie</i> , 2014 , 126, 8808-8811	3.6	1
44	Forming Tertiary Organolithiums and Organocuprates from Nitrile Precursors and their Bimolecular Reactions with Carbon Electrophiles to Form Quaternary Carbon Stereocenters. <i>Angewandte Chemie</i> , 2012 , 124, 9719-9724	3.6	1
43	Control of Hetero-Diels-Alder Stereoselectivity through Solvent Polarity and Brønsted or Lewis Acid Catalysis; Theory and Experiment. <i>Synlett</i> , 2013 , 24, 2446-2450	2.2	1
42	Theoretical Studies of Antibody Catalysis 2005 , 72-117		1
41	A Diazo-Hooker Reaction, Inspired by the Biosynthesis of Azamerone.. <i>Organic Letters</i> , 2022 , 24, 490-495	6.2	1
40	Bioinspired Synthesis of (E)-PF-1018. <i>Angewandte Chemie</i> , 2020 , 132, 5301-5305	3.6	1
39	Huisgen's 1,3-Dipolar Cycloadditions to Fulvenes Proceed via Ambimodal [6+4]/[4+2] Transition States. <i>Angewandte Chemie</i> , 2020 , 132, 12512-12516	3.6	1
38	Computational generation of an annotated gigalibrary of synthesizable, composite peptidic macrocycles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 24679-24690	11.5	1
37	The Influence of Substitution on Thiol-Induced Oxanorbornadiene Fragmentation. <i>Organic Letters</i> , 2021 , 23, 3751-3754	6.2	1
36	Structural diversification of hapalindole and fischerindole natural products via cascade biocatalysis. <i>ACS Catalysis</i> , 2021 , 11, 4670-4681	13.1	1
35	Enhanced Gearing Fidelity Achieved Through Macrocyclization of a Solvated Molecular Spur Gear. <i>Journal of the American Chemical Society</i> , 2021 , 143, 7740-7747	16.4	1
34	Origins of Endo Selectivity in Diels-Alder Reactions of Cyclic Allene Dienophiles. <i>Angewandte Chemie</i> , 2021 , 133, 15116-15124	3.6	1
33	Deciphering Reactivity and Selectivity Patterns in Aliphatic C-H Bond Oxygenation of Cyclopentane and Cyclohexane Derivatives. <i>Journal of Organic Chemistry</i> , 2021 , 86, 9925-9937	4.2	1
32	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. <i>Angewandte Chemie</i> , 2021 , 133, 18349-18356	13.5	1
31	Synthetic strategy toward ineleganolide: A cautionary tale. <i>Tetrahedron</i> , 2021 , 93, 132289-132289	2.4	1
30	Molecular dynamics of the intramolecular 1, 3-dipolar ene reaction of a nitrile oxide and an alkene: non-statistical behavior of a reaction involving a diradical intermediate** Dedicated to the memory of the great theoretician and friend, Dieter Cremer. View all notes. <i>Molecular Physics</i> , 2019 , 117, 1360-1366	1.7	1

29	The role of CuI in the siloxane-mediated Pd-catalyzed cross-coupling reactions of aryl iodides with aryl lithium reagents. <i>Chinese Chemical Letters</i> , 2021 , 32, 441-444	8.1	1
28	Fungal Dioxygenase AsqJ Is Promiscuous and Bimodal: Substrate-Directed Formation of Quinolones versus Quinazolinones. <i>Angewandte Chemie</i> , 2021 , 133, 8378-8383	3.6	1
27	Stereoselective Installation of Five Contiguous Stereogenic Centers in a Double Aldol-Tishchenko Cascade and Evaluation of the Key Transition State through DFT Calculation. <i>Organic Letters</i> , 2021 , 23, 6372-6376	6.2	1
26	A shared mechanistic pathway for pyridoxal phosphate-dependent arginine oxidases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021 , 118,	11.5	1
25	Wide-Gap Perovskite via Synergetic Surface Passivation and Its Application toward Efficient Stacked Tandem Photovoltaics. <i>Small</i> , 2021 , e2103887	11	1
24	Origin of iodine preferential attack at sulfur in phosphorothioate and subsequent P-O or P-S bond dissociation.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022 , 119, e2119032119	11.5	1
23	Discovery and characterization of a terpene biosynthetic pathway featuring a norbornene-forming Diels-Alderase.. <i>Nature Communications</i> , 2022 , 13, 2568	17.4	1
22	Uncovering the Key Role of Distortion in Bioorthogonal Tetrazine Tools That Defy the Reactivity/Stability Trade-Off.. <i>Journal of the American Chemical Society</i> , 2022 ,	16.4	1
21	Transition State Modeling of Asymmetric Epoxidation Catalysts. <i>ACS Symposium Series</i> , 1999 , 33-48	0.4	0
20	Catalytic properties of 4,5-bridged proline methano- and ethanologues in the HajosParrish intramolecular aldol reaction. <i>Organic Chemistry Frontiers</i> , 2022 , 9, 649-659	5.2	0
19	Facial Stereoselectivity in Acyl Nitroso Cycloadditions to 5,5-Unsymmetrically Substituted Cyclopentadienes: Computational Exploration of Origins of Selectivity and the Role of Substituent Conformations on Selectivity. <i>Journal of Organic Chemistry</i> , 2021 , 86, 17082-17089	4.2	0
18	Perspective on Theoretical interpretation of 1D asymmetric induction. The importance of antiperiplanarity 2000 , 330-331		0
17	Efficient synthesis of isoindolones by intramolecular cyclisation of pyridinylbenzoic acids. <i>Organic and Biomolecular Chemistry</i> , 2021 , 19, 8025-8029	3.9	0
16	Ambimodal Transition States in DielsAlder Cycloadditions of Tropolone and Tropolonate with N-Methylmaleimide**. <i>Angewandte Chemie</i> , 2021 , 133, 25195	3.6	0
15	Ambimodal Transition States in Diels-Alder Cycloadditions of Tropolone and Tropolonate with N-Methylmaleimide*. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 24991-24996	16.4	0
14	Facile generation of bridged medium-sized polycyclic systems by rhodium-catalysed intramolecular (3+2) dipolar cycloadditions. <i>Nature Communications</i> , 2021 , 12, 5239	17.4	0
13	Computations on Pericyclic Reactions Reveal the Richness of Ambimodal Transition States and Pericyclases. <i>Israel Journal of Chemistry</i> ,	3.4	0
12	Epoxidation and Late-Stage C-H Functionalization by P450 TamI Are Mediated by Variant Heme-Iron Oxidizing Species. <i>ACS Catalysis</i> , 2022 , 12, 3731-3742	13.1	0

11	John D. Roberts, his beginnings at UCLA, his transformation of physical organic chemistry, and his impact on science. <i>Journal of Physical Organic Chemistry</i> , 2018 , 31, e3810	2.1
10	Formation of Aminocyclopentadienes from Silyldihydropyridines: Ring Contractions Driven by Anion Stabilization. <i>Angewandte Chemie</i> , 2018 , 130, 6715-6719	3.6
9	R&Ktitelbild: Stable, Reactive, and Orthogonal Tetrazines: Dispersion Forces Promote the Cycloaddition with Isonitriles (Angew. Chem. 27/2019). <i>Angewandte Chemie</i> , 2019 , 131, 9390-9390	3.6
8	Chromium Tricarbonyl-Coordinated Carbocations 2014 , 279-289	
7	Innentitelbild: Das Distortion/Interaction-Activation-Strain-Modell zur Analyse von Reaktionsgeschwindigkeiten (Angew. Chem. 34/2017). <i>Angewandte Chemie</i> , 2017 , 129, 10134-10134	3.6
6	Chem Is Try Computationally and Experimentally: How Will Computational Organic Chemistry Impact Organic Theories, Mechanisms, and Synthesis in the Twenty-First Century? 2012 , 561-601	
5	Electrochemical Fluorination of Vinyl Boronates through Donor-Stabilized Vinyl Carbocation Intermediates**. <i>Angewandte Chemie</i> , e202113972	3.6
4	Stereodivergent Attached-Ring Synthesis via Non-Covalent Interactions: A Short Formal Synthesis of Merrilactone A. <i>Angewandte Chemie</i> , 2022 , 134, e202114514	3.6
3	Comparative Analysis of Bacterial Cytochromes P450 Involved in the Biosynthesis of 16- Membered Ring Macrolide Antibiotics. <i>FASEB Journal</i> , 2018 , 32, 529.4	0.9
2	François N. Diederich: Pioneer of carbon allotropes and molecular recognition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 32827-32829	11.5
1	Computational determination of the mechanism of the Pd-catalyzed formation of isatoic anhydrides from -haloanilines, CO, and CO. <i>Dalton Transactions</i> , 2021 , 50, 14453-14461	4.3