

Kendall Houk

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/6409025/kendall-houk-publications-by-year.pdf>

Version: 2024-04-10

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Allylic C(sp ³)H arylation of olefins via ternary catalysis 2022 , 1, 59-68		3
729	Catalytic properties of 4,5-bridged proline methano- and ethanolones in the Hajos-Parrish intramolecular aldol reaction. <i>Organic Chemistry Frontiers</i> , 2022 , 9, 649-659	5.2	0
728	Electrochemical Fluorination of Vinyl Boronates through Donor-Stabilized Vinyl Carbocation Intermediates.. <i>Angewandte Chemie - International Edition</i> , 2022 ,	16.4	2
727	A Diazo-Hooker Reaction, Inspired by the Biosynthesis of Azamerone.. <i>Organic Letters</i> , 2022 , 24, 490-495	5.2	1
726	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
725	Palladium-catalyzed stereospecific C ₃ coupling toward diverse PN-heterocycles. <i>Chem</i> , 2022 , 8, 569-579	16.2	2
724	Extended β -Strands Contribute to Reversible Amyloid Formation.. <i>ACS Nano</i> , 2022 ,	16.7	2
723	Stereodivergent Attached-Ring Synthesis via Non-Covalent Interactions: A Short Formal Synthesis of Merrilactone A. <i>Angewandte Chemie</i> , 2022 , 134, e202114514	3.6	
722	Epoxidation and Late-Stage C _H Functionalization by P450 Tam1 Are Mediated by Variant Heme-Iron Oxidizing Species. <i>ACS Catalysis</i> , 2022 , 12, 3731-3742	13.1	0
721	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
720	Halogen-bond-assisted radical activation of glycosyl donors enables mild and stereoconvergent 1,2-cis-glycosylation.. <i>Nature Chemistry</i> , 2022 ,	17.6	8
719	Discovery and characterization of a terpene biosynthetic pathway featuring a norbornene-forming Diels-Alderase.. <i>Nature Communications</i> , 2022 , 13, 2568	17.4	1
718	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
717	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
716	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
715	An Enzymatic Platform for Primary Amination of 1-Aryl-2-alkyl Alkynes.. <i>Journal of the American Chemical Society</i> , 2021 ,	16.4	8
714	Active Controlled and Tunable Coacervation Using Side-Chain Functional β -Helical Homopolypeptides. <i>Journal of the American Chemical Society</i> , 2021 , 143, 18196-18203	16.4	4

713	Pd(II)-Catalyzed Synthesis of Benzocyclobutenes by β -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
712	Tunable Amine-Reactive Electrophiles for Selective Profiling of Lysine. <i>Angewandte Chemie - International Edition</i> , 2021 ,	16.4	2
711	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
710	Performance-limiting formation dynamics in mixed-halide perovskites. <i>Science Advances</i> , 2021 , 7, eabj1792	14.3	9
709	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. <i>Angewandte Chemie</i> , 2021 , 133, 24298-24308	3.6	3
708	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 24096-24106	16.4	5
707	An enantioselective ambimodal cross-Diels-Alder reaction and applications in synthesis. <i>Nature Catalysis</i> , 2021 , 4, 892-900	36.5	4
706	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
705	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
704	Metal-Free Directed C-H Borylation of Pyrroles. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 8500-8504	16.4	12
703	Photochemical intermolecular dearomative cycloaddition of bicyclic azaarenes with alkenes. <i>Science</i> , 2021 , 371, 1338-1345	33.3	29
702	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
701	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
700	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
699	Sequential C-F bond functionalizations of trifluoroacetamides and acetates via spin-center shifts. <i>Science</i> , 2021 , 371, 1232-1240	33.3	53
698	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
697	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
696	The Influence of Substitution on Thiol-Induced Oxanorbornadiene Fragmentation. <i>Organic Letters</i> , 2021 , 23, 3751-3754	6.2	1

695	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
694	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
693	Structural diversification of hapalindole and fischerindole natural products via cascade biocatalysis. <i>ACS Catalysis</i> , 2021 , 11, 4670-4681	13.1	1
692	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
691	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
690	Post-Transition State Bifurcation in Iron-Catalyzed Arene Aminations. <i>ACS Catalysis</i> , 2021 , 11, 6816-6824	13.1	5
689	Direct Synthesis of Ketones from Methyl Esters by Nickel-Catalyzed Suzuki-Miyaura Coupling. <i>Angewandte Chemie</i> , 2021 , 133, 13588-13595	3.6	3
688	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
687	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
686	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
685	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
684	Origins of Endo Selectivity in Diels-Alder Reactions of Cyclic Allene Dienophiles. <i>Angewandte Chemie</i> , 2021 , 133, 15116-15124	3.6	1
683	An Asymmetric S ₂ Dynamic Kinetic Resolution. <i>Journal of the American Chemical Society</i> , 2021 , 143, 7509-7520	16.4	10
682	Arene-Perfluoroarene Interactions in Solution. <i>Journal of Organic Chemistry</i> , 2021 , 86, 8425-8436	4.2	4
681	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
680	Engineering P450 TamI 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
679	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
678	Computational Exploration of How Enzyme XimE Converts Natural S-Epoxide to Pyran and R-Epoxide to Furan. <i>ACS Catalysis</i> , 2021 , 11, 7928-7942	13.1	6

677	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. <i>Angewandte Chemie</i> , 2021 , 133, 18349-18356	18.5	1
676	Synthetic strategy toward ineleganolide: A cautionary tale. <i>Tetrahedron</i> , 2021 , 93, 132289-132289	2.4	1
675	Nonenzymatic Stereoselective -Glycosylation of Polypeptides and Proteins. <i>Journal of the American Chemical Society</i> , 2021 , 143, 11919-11926	16.4	10
674	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
673	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
672	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
671	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
670	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
669	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
668	A Polyketide Cyclase That Forms Medium-Ring Lactones. <i>Journal of the American Chemical Society</i> , 2021 , 143, 80-84	16.4	8
667	Library construction of stereochemically diverse isomers of spirooliganin: their total synthesis and antiviral activity. <i>Chemical Science</i> , 2021 , 12, 7003-7011	9.4	4
666	Efficient synthesis of isoindolones by intramolecular cyclisation of pyridinylbenzoic acids. <i>Organic and Biomolecular Chemistry</i> , 2021 , 19, 8025-8029	3.9	0
665	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	
664	Overcoming Kinetic and Thermodynamic Challenges of Classic Cope Rearrangements. <i>Journal of Organic Chemistry</i> , 2021 , 86, 2632-2643	4.2	4
663	Phosphorus(III)-assisted regioselective C-H silylation of heteroarenes. <i>Nature Communications</i> , 2021 , 12, 524	17.4	12
662	Computational Redesign of a PETase for Plastic Biodegradation under Ambient Condition by the GRAPE Strategy. <i>ACS Catalysis</i> , 2021 , 11, 1340-1350	13.1	60
661	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
660	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

659	Chlorinated Spiroconjugated Fused Extended Aromatics for Multifunctional Organic Electronics. <i>Advanced Materials</i> , 2021 , 33, e2006120	24	9
658	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
657	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
656	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
655	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
654	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
653	Cyclization by C(sp ³) π Arylation with a Transient Directing Group for the Diastereoselective Preparation of Indanes. <i>ACS Catalysis</i> , 2021 , 11, 3115-3127	13.1	6
652	Dipolar order in an amphidynamic crystalline metal-organic framework through reorienting linkers. <i>Nature Chemistry</i> , 2021 , 13, 278-283	17.6	6
651	Cleaving arene rings for acyclic alkenylnitrile synthesis. <i>Nature</i> , 2021 , 597, 64-69	50.4	10
650	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 18201-18208	16.4	3
649	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
648	Organocatalytic enantioselective dearomatization of thiophenes by 1,10-conjugate addition of indole imine methides. <i>Nature Communications</i> , 2021 , 12, 4881	17.4	10
647	Conformational dynamics of androgen receptors bound to agonists and antagonists. <i>Scientific Reports</i> , 2021 , 11, 15887	4.9	2
646	Probing Catalyst Speciation in Pd-MPAAM-Catalyzed Enantioselective C(sp ³) π Arylation: Catalyst Improvement via Destabilization of Off-Cycle Species. <i>ACS Catalysis</i> , 2021 , 11, 11040-11048	13.1	2
645	Ambimodal Transition States in Diels-Alder Cycloadditions of Tropolone and Tropolonate with N-Methylmaleimide**. <i>Angewandte Chemie</i> , 2021 , 133, 25195	3.6	0
644	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
643	Ambiphilic Reactivity of Vinyl Pd-Oxyallyl for Expeditionary Construction of Highly Functionalized Cyclooctanoids. <i>Organic Letters</i> , 2021 , 23, 7330-7335	6.2	4
642	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

641	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
640	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
639	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
638	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
637	Origin of Increased Reactivity in Rhenium-Mediated Cycloadditions of Tetrazines. <i>Journal of Organic Chemistry</i> , 2021 , 86, 13129-13133	4.2	5
636	Constructing Saturated Guanidinium Heterocycles by Cycloaddition of α -Amidinyliminium Ions with Indoles. <i>Organic Letters</i> , 2021 , 23, 7618-7623	6.2	2
635	[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
634	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
633	Electric field-catalyzed single-molecule Diels-Alder reaction dynamics. <i>Science Advances</i> , 2021 , 7,	14.3	20
632	Wide-Gap Perovskite via Synergetic Surface Passivation and Its Application toward Efficient Stacked Tandem Photovoltaics. <i>Small</i> , 2021 , e2103887	11	1
631	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
630	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
629	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
628	Catalytic enantioselective synthesis of chiral tetraarylmethanes. <i>Nature Catalysis</i> , 2020 , 3, 1010-1019	36.5	25
627	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
626	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
625	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
624	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

623	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
622	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
621	Stereoselective [4+2]-Cycloaddition with Chiral Alkenylboranes. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 11432-11439	16.4	10
620	Stereoselective [4+2]-Cycloaddition with Chiral Alkenylboranes. <i>Angewandte Chemie</i> , 2020 , 132, 11529-11536	16.36	2
619	Understand the Specific Regio- and Enantioselectivity of Fluostatin Conjugation in the Post-Biosynthesis. <i>Biomolecules</i> , 2020 , 10,	5.9	5
618	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
617	Ligand-Controlled Regiodivergent Palladium-Catalyzed Hydrogermylation of Ynamides. <i>Journal of the American Chemical Society</i> , 2020 , 142, 11153-11164	16.4	25
616	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
615	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
614	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
613	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
612	Selective Enzymatic Oxidation of Silanes to Silanols. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 15507-15511	16.4	23
611	Electrophilic Azides for Materials Synthesis and Chemical Biology. <i>Accounts of Chemical Research</i> , 2020 , 53, 937-948	24.3	24
610	Molecular Spur Gears with Triptycene Rotators and a Norbornane-Based Stator. <i>Organic Letters</i> , 2020 , 22, 4049-4052	6.2	5
609	Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with η -Vinyl Allylboron Reagents. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 10540-10548	16.4	27
608	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
607	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
606	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

605	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
604	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
603	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
602	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
601	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
600	Differentiation and functionalization of remote C-H bonds in adjacent positions. <i>Nature Chemistry</i> , 2020 , 12, 399-404	17.6	42
599	Isoquinoline thiosemicarbazone displays potent anticancer activity with efficacy against aggressive leukemias. <i>RSC Medicinal Chemistry</i> , 2020 , 11, 392-410	3.5	4
598	Aminoperoxide adducts expand the catalytic repertoire of flavin monooxygenases. <i>Nature Chemical Biology</i> , 2020 , 16, 556-563	11.7	26
597	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
596	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
595	Rational Development of Remote C-H Functionalization of Biphenyl: Experimental and Computational Studies. <i>Angewandte Chemie</i> , 2020 , 132, 4800-4807	3.6	2
594	Enantioselective C-H functionalization of bicyclo[1.1.1]pentanes. <i>Nature Catalysis</i> , 2020 , 3, 351-357	36.5	28
593	Selective Enzymatic Oxidation of Silanes to Silanols. <i>Angewandte Chemie</i> , 2020 , 132, 15637-15641	3.6	6
592	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
591	Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with β -Vinyl Allylboron Reagents. <i>Angewandte Chemie</i> , 2020 , 132, 10627-10635	3.6	9
590	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
589	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
588	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	

587	Expanded Helicenes as Synthons for Chiral Macrocyclic Nanocarbons. <i>Journal of the American Chemical Society</i> , 2020 , 142, 11084-11091	16.4	17
586	FAD-dependent enzyme-catalysed intermolecular [4+2] cycloaddition in natural product biosynthesis. <i>Nature Chemistry</i> , 2020 , 12, 620-628	17.6	47
585	Intercepting fleeting cyclic allenes with asymmetric nickel catalysis. <i>Nature</i> , 2020 , 586, 242-247	50.4	17
584	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
583	Bioinspired Synthesis of (±)-PF-1018. <i>Angewandte Chemie</i> , 2020 , 132, 5301-5305	3.6	1
582	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
581	Molecular Basis for Spirocycle Formation in the Paraherquamide Biosynthetic Pathway. <i>Journal of the American Chemical Society</i> , 2020 , 142, 2244-2252	16.4	20
580	Isonitrile-responsive and bioorthogonally removable tetrazine protecting groups. <i>Chemical Science</i> , 2020 , 11, 169-179	9.4	23
579	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
578	Sungeidines from a Non-canonical Ene-alkyne Biosynthetic Pathway. <i>Journal of the American Chemical Society</i> , 2020 , 142, 1673-1679	16.4	10
577	Bioinspired Synthesis of (-)-PF-1018. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 5263-5267	16.4	6
576	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
575	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
574	An enzymatic Alder-ene reaction. <i>Nature</i> , 2020 , 586, 64-69	50.4	14
573	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
572	Enzyme-free synthesis of natural phospholipids in water. <i>Nature Chemistry</i> , 2020 , 12, 1029-1034	17.6	22
571	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
570	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

569	Atroposelective Synthesis of Axially Chiral N-Arylpyrroles by Chiral-at-Rhodium Catalysis. <i>Angewandte Chemie</i> , 2020 , 132, 13654-13658	3.6	9
568	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
567	Photorearrangement of [8]-2,6-Pyridinophane -Oxide. <i>Journal of the American Chemical Society</i> , 2020 , 142, 20717-20724	16.4	3
566	Computational Investigation of the Mechanism of Diels-Alderase Pyl14. <i>Journal of the American Chemical Society</i> , 2020 , 142, 20232-20239	16.4	6
565	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
564	Intramolecular C(sp ³)-H Bond Oxygenation by Transition-Metal Acylnitrenoids. <i>Angewandte Chemie</i> , 2020 , 132, 21890-21894	3.6	2
563	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
562	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
561	Intramolecular C(sp ³)-H Bond Oxygenation by Transition-Metal Acylnitrenoids. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 21706-21710	16.4	12
560	Boron tribromide as a reagent for anti-Markovnikov addition of HBr to cyclopropanes. <i>Chemical Science</i> , 2020 , 11, 9426-9433	9.4	5
559	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
558	Computational Exploration of a Redox-Neutral Organocatalytic Mitsunobu Reaction. <i>Journal of the American Chemical Society</i> , 2020 , 142, 16403-16408	16.4	7
557	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
556	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
555	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
554	Fjord-Edge Graphene Nanoribbons with Site-Specific Nitrogen Substitution. <i>Journal of the American Chemical Society</i> , 2020 , 142, 18093-18102	16.4	11
553	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
552	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

551	Diels-Alder reactivities of cycloalkenediones with tetrazine. <i>Journal of Molecular Modeling</i> , 2019 , 25, 33	2	5
550	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
549	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
548	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
547	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
546	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
545	Sterically Unprotected Nucleophilic Boron Cluster Reagents. <i>CheM</i> , 2019 , 5, 2461-2469	16.2	15
544	Hyperconjugative Antiaromaticity Activates 4-Pyrazoles as Inverse-Electron-Demand Diels-Alder Dienes. <i>Organic Letters</i> , 2019 , 21, 8492-8495	6.2	13
543	Fungal indole alkaloid biogenesis through evolution of a bifunctional reductase/Diels-Alderase. <i>Nature Chemistry</i> , 2019 , 11, 972-980	17.6	34
542	The expanding world of biosynthetic pericyclases: cooperation of experiment and theory for discovery. <i>Natural Product Reports</i> , 2019 , 36, 698-713	15.1	52
541	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
540	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
539	A Biocatalytic Platform for Synthesis of Chiral Trifluoromethylated Organoborons. <i>ACS Central Science</i> , 2019 , 5, 270-276	16.8	51
538	Mechanism and Regioselectivity of an Unsymmetrical Hexadehydro-Diels-Alder (HDDA) Reaction. <i>Journal of Organic Chemistry</i> , 2019 , 84, 1959-1963	4.2	11
537	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
536	Enabling microbial syringol conversion through structure-guided protein engineering. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 13970-13976	11.5	22
535	Synthesis and Target Identification of a Novel Electrophilic Warhead, 2-Chloromethylquinoline. <i>Biochemistry</i> , 2019 , 58, 2715-2719	3.2	3
534	Rational design, enantioselective synthesis and catalytic applications of axially chiral EBINOLs. <i>Nature Catalysis</i> , 2019 , 2, 504-513	36.5	71

533	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
532	Bacterial Tetrabromopyrrole Debrominase Shares a Reductive Dehalogenation Strategy with Human Thyroid Deiodinase. <i>Biochemistry</i> , 2019 , 58, 5329-5338	3.2	8
531	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
530	Stable, Reactive, and Orthogonal Tetrazines: Dispersion Forces Promote the Cycloaddition with Isonitriles. <i>Angewandte Chemie</i> , 2019 , 131, 9141-9146	3.6	6
529	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
528	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
527	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
526	Evaluation of DFT Methods and Implicit Solvation Models for Anion-Binding Host-Guest Systems. <i>Helvetica Chimica Acta</i> , 2019 , 102, e1900032	2	7
525	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
524	Enzyme-catalysed [6+4] cycloadditions in the biosynthesis of natural products. <i>Nature</i> , 2019 , 568, 122-126	16.4	53
523	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
522	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
521	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
520	Generation of Dithianyl and Dioxolanyl Radicals Using Photoredox Catalysis: Application in the Total Synthesis of the Danshenspiroketallactones via Radical Relay Chemistry. <i>Organic Letters</i> , 2019 , 21, 1708-1712	6.2	24
519	Cycloadditions of Oxacyclic Allenes and a Catalytic Asymmetric Entryway to Enantioenriched Cyclic Allenes. <i>Angewandte Chemie</i> , 2019 , 131, 5709-5713	3.6	2
518	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
517	Isomeric triazines exhibit unique profiles of bioorthogonal reactivity. <i>Chemical Science</i> , 2019 , 10, 9109-9114	16.4	16
516	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

515	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
514	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
513	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
512	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
511	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	
510	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
509	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
508	Asymmetric Desymmetrization of Oxetanes for the Synthesis of Chiral Tetrahydrothiophenes and Tetrahydroselenophenes. <i>Angewandte Chemie</i> , 2019 , 131, 18223-18228	3.6	9
507	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
506	Constructive molecular configurations for surface-defect passivation of perovskite photovoltaics. <i>Science</i> , 2019 , 366, 1509-1513	33.3	434
505	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
504	Non--Symmetric Chiral-at-Ruthenium Catalyst for Highly Efficient Enantioselective Intramolecular C(sp)-H Amidation. <i>Journal of the American Chemical Society</i> , 2019 , 141, 19048-19057	16.4	53
503	Expanding the Frontiers of Higher-Order Cycloadditions. <i>Accounts of Chemical Research</i> , 2019 , 52, 3488-3501	14.9	39
502	Controllable catalytic difluorocarbene transfer enables access to diversified fluoroalkylated arenes. <i>Nature Chemistry</i> , 2019 , 11, 948-956	17.6	66
501	Metal-free directed sp-C-H borylation. <i>Nature</i> , 2019 , 575, 336-340	50.4	93
500	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
499	��facial Selectivities in Hydride Reductions of Hindered Endocyclic Iminium Ions. <i>Journal of Organic Chemistry</i> , 2019 , 84, 273-281	4.2	2
498	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

497	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
496	Catalytic Enantioselective Intramolecular C(sp ³)-H Amination of 2-Azidoacetamides. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 1088-1093	16.4	49
495	Sydnone-Based Approach to Heterohelices through 1,3-Dipolar-Cycloadditions. <i>Journal of the American Chemical Society</i> , 2019 , 141, 1435-1440	16.4	32
494	Ambimodal Trisperiocyclic Transition State and Dynamic Control of Periselectivity. <i>Journal of the American Chemical Society</i> , 2019 , 141, 1217-1221	16.4	28
493	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
492	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
491	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
490	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
489	Nucleophilic ¹⁸ F-Fluorination of Anilines via N-Arylsydnone Intermediates. <i>Synlett</i> , 2018 , 29, 1131-1135	2.2	9
488	Origins of halogen effects in bioorthogonal sydnone cycloadditions. <i>Chemical Communications</i> , 2018 , 54, 5082-5085	5.8	22
487	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
486	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
485	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
484	Formation of Aminocyclopentadienes from Silyldihydropyridines: Ring Contractions Driven by Anion Stabilization. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 6605-6609	16.4	1
483	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	
482	Origins of Stereoselectivity in Mannich Reactions Catalyzed by Chiral Vicinal Diamines. <i>Journal of Organic Chemistry</i> , 2018 , 83, 3171-3176	4.2	6
481	Bridged [2.2.1] bicyclic phosphine oxide facilitates catalytic π -umpolung addition-Wittig olefination. <i>Chemical Science</i> , 2018 , 9, 1867-1872	9.4	32
480	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

479	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
478	Direct single-molecule dynamic detection of chemical reactions. <i>Science Advances</i> , 2018 , 4, eaar2177	14.3	54
477	Origin of π -Facial Stereoselectivity in Thiophene 1-Oxide Cycloadditions. <i>Journal of Organic Chemistry</i> , 2018 , 83, 2611-2616	4.2	11
476	Oxidation of rubrene, and implications for device stability. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 3757-3761	7.3	11
475	The Distortion/Interaction Model for Analysis of Activation Energies of Organic Reactions 2018 , 371-402		2
474	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
473	Formation of Aminocyclopentadienes from Silyldihydropyridines: Ring Contractions Driven by Anion Stabilization. <i>Angewandte Chemie</i> , 2018 , 130, 6715-6719	3.6	
472	Readily Accessible Ambiphilic Cyclopentadienes for Bioorthogonal Labeling. <i>Journal of the American Chemical Society</i> , 2018 , 140, 6426-6431	16.4	14
471	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
470	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
469	Arylketone π -Conjugation Controls Enantioselectivity in Asymmetric Alkynylations Catalyzed by Centrochiral Ruthenium Complexes. <i>Journal of the American Chemical Society</i> , 2018 , 140, 5146-5152	16.4	22
468	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
467	Structural basis of the Cope rearrangement and cyclization in hapalindole biogenesis. <i>Nature Chemical Biology</i> , 2018 , 14, 345-351	11.7	26
466	Diels-Alder cycloadditions of strained azacyclic allenes. <i>Nature Chemistry</i> , 2018 , 10, 953-960	17.6	40
465	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
464	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
463	Teaching an old carbocation new tricks: Intermolecular C-H insertion reactions of vinyl cations. <i>Science</i> , 2018 , 361, 381-387	33.3	69
462	Metathesis and Decomposition of Fischer Carbenes of Cyclometalated Z-Selective Ruthenium Metathesis Catalysts. <i>Organometallics</i> , 2018 , 37, 2212-2216	3.8	11

461	Enzymatic one-step ring contraction for quinolone biosynthesis. <i>Nature Communications</i> , 2018 , 9, 2826	17.4	11
460	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
459	The mechanism of the triple aryne-tetrazine reaction cascade: theory and experiment. <i>Chemical Science</i> , 2018 , 9, 7688-7693	9.4	18
458	Biosynthesis of thiocarboxylic acid-containing natural products. <i>Nature Communications</i> , 2018 , 9, 2362	17.4	16
457	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	
456	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. <i>Frontiers in Chemistry</i> , 2018 , 6, 663	5	8
455	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
454	Bioorthogonal release of sulfonamides and mutually orthogonal liberation of two drugs. <i>Chemical Communications</i> , 2018 , 54, 14089-14092	5.8	32
453	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
452	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
451	Hyperconjugative Aromaticity and Antiaromaticity Control the Reactivities and E -Facial Stereoselectivities of 5-Substituted Cyclopentadiene Diels-Alder Cycloadditions. <i>Journal of Organic Chemistry</i> , 2018 , 83, 14658-14666	4.2	31
450	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
449	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
448	Origins of Selectivities in the Stork Diels-Alder Cycloaddition for the Synthesis of (\pm)-4-Methylenegermine. <i>Organic Letters</i> , 2018 , 20, 6108-6111	6.2	3
447	Organocatalytic [6+4] Cycloadditions via Zwitterionic Intermediates: Chemo-, Regio-, and Stereoselectivities. <i>Journal of the American Chemical Society</i> , 2018 , 140, 13726-13735	16.4	23
446	Mechanism and Origins of Chemo- and Stereoselectivities of Aryl Iodide-Catalyzed Asymmetric Difluorinations of E -Substituted Styrenes. <i>Journal of the American Chemical Society</i> , 2018 , 140, 15206-15218	16.4	61
445	Mild Ring-Opening 1,3-Hydroborations of Non-Activated Cyclopropanes. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 16861-16865	16.4	34
444	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

443	Asymmetric phosphoric acid-catalyzed four-component Ugi reaction. <i>Science</i> , 2018 , 361,	33.3	100
442	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
441	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. <i>Nature Communications</i> , 2018 , 9, 2487	17.4	77
440	Enzyme-catalyzed cationic epoxide rearrangements in quinolone alkaloid biosynthesis. <i>Nature Chemical Biology</i> , 2017 , 13, 325-332	11.7	28
439	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
438	A potassium tert-butoxide and hydrosilane system for ultra-deep desulfurization of fuels. <i>Nature Energy</i> , 2017 , 2,	62.3	39
437	Enzyme-Catalyzed Intramolecular Enantioselective Hydroalkoxylation. <i>Journal of the American Chemical Society</i> , 2017 , 139, 3639-3642	16.4	14
436	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
435	Potassium tert-Butoxide-Catalyzed Dehydrogenative C-H Silylation of Heteroaromatics: A Combined Experimental and Computational Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2017 , 139, 6867-6879	16.4	122
434	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
433	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
432	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
431	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
430	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
429	Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 10070-10086	16.4	649
428	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
427	Das Distortion/Interaction-Activation-Strain-Modell zur Analyse von Reaktionsgeschwindigkeiten. <i>Angewandte Chemie</i> , 2017 , 129, 10204-10221	3.6	136
426	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

425	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
424	Chronology of CH ₃ OH Hydrogen Bonding from Molecular Dynamics Studies of the Phosphoric Acid-Catalyzed Allylboration of Benzaldehyde. <i>Journal of the American Chemical Society</i> , 2017 , 139, 7717-7720	16.4	60
423	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
422	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
421	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
420	(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
419	Design and Applications of N-tert-Butyl Sulfinyl Squaramide Catalysts. <i>Organic Letters</i> , 2017 , 19, 1926-1929	16.4	12
418	Holy Grails for Computational Organic Chemistry and Biochemistry. <i>Accounts of Chemical Research</i> , 2017 , 50, 539-543	24.3	100
417	Palladium-Catalyzed Suzuki-Miyaura Coupling of Aryl Esters. <i>Journal of the American Chemical Society</i> , 2017 , 139, 1311-1318	16.4	165
416	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
415	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
414	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
413	Origins of Stereoselectivity in Chiral Aminoalcohol Catalysis of Oxyallyl Cation-Indole Reactions. <i>Organic Letters</i> , 2017 , 19, 5685-5688	6.2	5
412	Synthesis and Evaluation of Sterically Demanding Ruthenium Dithiolate Catalysts for Stereoretentive Olefin Metathesis. <i>Organometallics</i> , 2017 , 36, 3940-3953	3.8	9
411	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
410	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
409	Understanding and Interrupting the Fischer Azaindolization Reaction. <i>Journal of the American Chemical Society</i> , 2017 , 139, 14833-14836	16.4	15
408	Synthesis of [18F]Fluoroarenes by Nucleophilic Radiofluorination of N-Arylsydnone. <i>Angewandte Chemie</i> , 2017 , 129, 13186-13190	3.6	9

407	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
406	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
405	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
404	Synthesis of [F]Fluoroarenes by Nucleophilic Radiofluorination of N-Arylsydnone. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 13006-13010	16.4	32
403	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
402	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
401	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	
400	SAM-dependent enzyme-catalysed pericyclic reactions in natural product biosynthesis. <i>Nature</i> , 2017 , 549, 502-506	50.4	108
399	Bioorthogonal Cycloadditions: Computational Analysis with the Distortion/Interaction Model and Predictions of Reactivities. <i>Accounts of Chemical Research</i> , 2017 , 50, 2297-2308	24.3	101
398	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	4.2	19
397	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
396	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
395	Model for the Enantioselectivity of Asymmetric Intramolecular Alkylations by Bis-Quaternized Cinchona Alkaloid-Derived Catalysts. <i>Journal of Organic Chemistry</i> , 2017 , 82, 8645-8650	4.2	22
394	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
393	Experimental and Computational Development of a Conformationally Flexible Template for the meta-C-H Functionalization of Benzoic Acids. <i>Journal of the American Chemical Society</i> , 2017 , 139, 10702-10714	16.4	61
392	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
391	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
390	Chirality Sensing of β -Hydroxyphosphonates by N-tert-Butyl Sulfinyl Squaramide. <i>Organic Letters</i> , 2017 , 19, 4191-4194	6.2	9

389	Ultrafast rotation in an amphidynamic crystalline metal organic framework. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 13613-13618	11.5	59
388	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
387	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
386	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
385	Computational Exploration of Concerted and Zwitterionic Mechanisms of Diels-Alder Reactions between 1,2,3-Triazines and Enamines and Acceleration by Hydrogen-Bonding Solvents. <i>Journal of the American Chemical Society</i> , 2017 , 139, 18213-18221	16.4	22
384	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
383	Experimental-Computational Synergy for Selective Pd(II)-Catalyzed C-H Activation of Aryl and Alkyl Groups. <i>Accounts of Chemical Research</i> , 2017 , 50, 2853-2860	24.3	150
382	Effect of trehalose polymer regioisomers on protein stabilization. <i>Polymer Chemistry</i> , 2017 , 8, 4781-4788	4.9	23
381	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
380	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
379	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
378	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
377	A resorcinarene for inhibition of A β Fibrillation. <i>Chemical Science</i> , 2017 , 8, 2003-2009	9.4	37
376	Tautomerization and Dimerization of 6,13-Disubstituted Derivatives of Pentacene. <i>Chemistry - A European Journal</i> , 2017 , 23, 6111-6117	4.8	6
375	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
374	Ligand-accelerated enantioselective methylene C(sp ³)-H bond activation. <i>Science</i> , 2016 , 353, 1023-1027	33.3	248
373	On the prevalence of bridged macrocyclic pyrroloindolines formed in regiodivergent alkylations of tryptophan. <i>Chemical Science</i> , 2016 , 7, 4158-4166	9.4	10
372	Biochemical Characterization of a Eukaryotic Decalin-Forming Diels-Alderase. <i>Journal of the American Chemical Society</i> , 2016 , 138, 15837-15840	16.4	71

371	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
370	MIDA boronates are hydrolysed fast and slow by two different mechanisms. <i>Nature Chemistry</i> , 2016 , 8, 1067-1075	17.6	70
369	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
368	Origins of Stereoselectivity of Chiral Vicinal Diamine-Catalyzed Aldol Reactions. <i>Journal of Organic Chemistry</i> , 2016 , 81, 12408-12415	4.2	10
367	Biocatalytic trifluoromethylation of unprotected phenols. <i>Nature Communications</i> , 2016 , 7, 13323	17.4	21
366	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
365	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
364	Nickel-Catalyzed Activation of Acyl C=O Bonds of Methyl Esters. <i>Angewandte Chemie</i> , 2016 , 128, 2860-2864	15.4	33
363	Mechanism of the P450-Catalyzed Oxidative Cyclization in the Biosynthesis of Griseofulvin. <i>ACS Catalysis</i> , 2016 , 6, 4506-4511	13.1	49
362	Distortion-Controlled Reactivity and Molecular Dynamics of Dehydro-Diels-Alder Reactions. <i>Journal of the American Chemical Society</i> , 2016 , 138, 8247-52	16.4	51
361	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
360	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
359	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
358	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
357	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
356	Schleyer hyperconjugative aromaticity and Diels-Alder reactivity of 5-substituted cyclopentadienes. <i>Journal of Computational Chemistry</i> , 2016 , 37, 117-23	3.5	33
355	Nitrone Cycloadditions of 1,2-Cyclohexadiene. <i>Journal of the American Chemical Society</i> , 2016 , 138, 2512-15	15.4	66
354	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

353	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
352	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
351	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
350	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
349	Theory and Modeling of Asymmetric Catalytic Reactions. <i>Accounts of Chemical Research</i> , 2016 , 49, 750-624.3	11.1	
348	Discovery of new mutually orthogonal bioorthogonal cycloaddition pairs through computational screening. <i>Chemical Science</i> , 2016 , 7, 1257-1261	9.4	69
347	Molecular Dynamics of Dimethyldioxirane C-H Oxidation. <i>Journal of the American Chemical Society</i> , 2016 , 138, 4237-42	16.4	37
346	Transition States of Vicinal Diamine-Catalyzed Aldol Reactions. <i>Journal of the American Chemical Society</i> , 2016 , 138, 503-6	16.4	20
345	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
344	Organocatalysis: Fundamentals and Comparisons to Metal and Enzyme Catalysis. <i>Catalysts</i> , 2016 , 6, 128 4	19	
343	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
342	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
341	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
340	Nickel-Catalyzed Activation of Acyl C-O Bonds of Methyl Esters. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 2810-4	16.4	115
339	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
338	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
337	In Situ Catalyst Modification in Atom Transfer Radical Reactions with Ruthenium Benzylidene Complexes. <i>Journal of the American Chemical Society</i> , 2016 , 138, 7171-7	16.4	13
336	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

335	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
334	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. <i>Journal of the American Chemical Society</i> , 2016 , 138, 6861-8	16.4	101
333	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
332	Unexpected, Latent Radical Reaction of Methane Propagated by Trifluoromethyl Radicals. <i>Journal of Organic Chemistry</i> , 2016 , 81, 9820-9825	4.2	4
331	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
330	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
329	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
328	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
327	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
326	Ruthenium-Catalyzed Asymmetric Hydrohydroxyalkylation of Butadiene: The Role of the Formyl Hydrogen Bond in Stereochemical Control. <i>Journal of the American Chemical Society</i> , 2015 , 137, 8838-50	16.4	51
325	1,2,4-Triazines Are Versatile Bioorthogonal Reagents. <i>Journal of the American Chemical Society</i> , 2015 , 137, 8388-91	16.4	101
324	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
323	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
322	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
321	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
320	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
319	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, 5596-601	16.4	23
318	Concerted Ring Opening and Cycloaddition of Chiral Epoxy Enolsilanes with Dienes. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 7422-5	16.4	16

3 ¹⁷	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
3 ¹⁶	(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
3 ¹⁵	Generation and regioselective trapping of a 3,4-piperidine for the synthesis of functionalized heterocycles. <i>Journal of the American Chemical Society</i> , 2015 , 137, 4082-5	16.4	53
3 ¹⁴	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
3 ¹³	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
3 ¹²	Computational Studies of Ruthenium-Catalyzed Olefin Metathesis 2015 , 199-252		8
3 ¹¹	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
3 ¹⁰	Transannular [6 + 4] and Ambimodal Cycloaddition in the Biosynthesis of Heronamide A. <i>Journal of the American Chemical Society</i> , 2015 , 137, 13518-23	16.4	62
3 ⁰⁹	Mechanistic Insights into Two-Phase Radical C-H Arylations. <i>ACS Central Science</i> , 2015 , 1, 456-462	16.8	22
3 ⁰⁸	Dual Gold Catalysis: Stepwise Catalyst Transfer via Dinuclear Clusters. <i>Journal of the American Chemical Society</i> , 2015 , 137, 10668-76	16.4	76
3 ⁰⁷	Computational Exploration of Mechanism and Selectivities of (NHC)Nickel(II)hydride-Catalyzed Hydroalkenylations of Styrene with π -Olefins. <i>ACS Catalysis</i> , 2015 , 5, 5545-5555	13.1	45
3 ⁰⁶	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
3 ⁰⁵	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
3 ⁰⁴	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
3 ⁰³	Ligand-Controlled Diastereoselective 1,3-Dipolar Cycloadditions of Azomethine Ylides with Methacrylonitrile. <i>Organic Letters</i> , 2015 , 17, 6166-9	6.2	14
3 ⁰²	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
3 ⁰¹	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
3 ⁰⁰	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

299	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
298	Substrate control in stereoselective lanthionine biosynthesis. <i>Nature Chemistry</i> , 2015 , 7, 57-64	17.6	57
297	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
296	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
295	Involvement of Lipocalin-like CghA in Decalin-Forming Stereoselective Intramolecular [4+2] Cycloaddition. <i>ChemBioChem</i> , 2015 , 16, 2294-8	3.8	64
294	Evolution of a Unified Strategy for Complex Sesterterpenoids: Progress toward Astellatol and the Total Synthesis of (-)-Nitidasin. <i>Chemistry - A European Journal</i> , 2015 , 21, 13646-65	4.8	23
293	Iodoarene-Catalyzed Stereospecific Intramolecular sp(3) C-H Amination: Reaction Development and Mechanistic Insights. <i>Journal of the American Chemical Society</i> , 2015 , 137, 7564-7	16.4	111
292	Mechanistic analysis of an asymmetric palladium-catalyzed conjugate addition of arylboronic acids to α -substituted cyclic enones. <i>Chemical Science</i> , 2015 , 6, 1917-1922	9.4	23
291	Cyclometalated Z-Selective Ruthenium Metathesis Catalysts with Modified N-Chelating Groups. <i>Organometallics</i> , 2015 , 34, 2858-2869	3.8	37
290	Can acyclic conformational control be achieved a sulfur-fluorine effect?. <i>Chemical Science</i> , 2015 , 6, 3565-3571	3.7	23
289	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
288	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
287	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
286	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
285	Origins of stereoselectivity in intramolecular aldol reactions catalyzed by cinchona amines. <i>Journal of the American Chemical Society</i> , 2015 , 137, 2116-27	16.4	62
284	Theoretical study of the molecular ordering, paracrystallinity, and charge mobilities of oligomers in different crystalline phases. <i>Journal of the American Chemical Society</i> , 2015 , 137, 2856-66	16.4	136
283	Computational predictions of substituted benzyne and indolyne regioselectivities. <i>Tetrahedron Letters</i> , 2015 , 56, 3511-3514	2	51
282	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

281	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
280	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
279	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
278	The role of distant mutations and allosteric regulation on LovD active site dynamics. <i>Nature Chemical Biology</i> , 2014 , 10, 431-6	11.7	132
277	A carbonate-forming Baeyer-Villiger monooxygenase. <i>Nature Chemical Biology</i> , 2014 , 10, 552-4	11.7	63
276	Non-Directed Allylic C-H Acetoxylation in the Presence of Lewis Basic Heterocycles. <i>Chemical Science</i> , 2014 , 5, 2352-2361	9.4	63
275	Torquoselective ring opening of fused cyclobutenamides: evidence for a cis,trans-cyclooctadienone intermediate. <i>Journal of the American Chemical Society</i> , 2014 , 136, 9802-5	16.4	22
274	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
273	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
272	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
271	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
270	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
269	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
268	Diels-Alder reactions of allene with benzene and butadiene: concerted, stepwise, and ambimodal transition states. <i>Journal of Organic Chemistry</i> , 2014 , 79, 8968-76	4.2	58
267	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
266	Theoretical elucidation of the origins of substituent and strain effects on the rates of Diels-Alder reactions of 1,2,4,5-tetrazines. <i>Journal of the American Chemical Society</i> , 2014 , 136, 11483-93	16.4	113
265	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
264	Cycloadditions of cyclohexynes and cyclopentyne. <i>Journal of the American Chemical Society</i> , 2014 , 136, 14706-9	16.4	68

263	Building on Cram's legacy: stimulated gating in hemicarcerands. <i>Accounts of Chemical Research</i> , 2014 , 47, 2168-76	24.3	30
262	Improving physical properties via C-H oxidation: chemical and enzymatic approaches. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 12091-6	16.4	66
261	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
260	Competition between concerted and stepwise dynamics in the triplet di- π -methane rearrangement. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 8664-7	16.4	23
259	Chromium Tricarbonyl-Coordinated Carbocations 2014 , 279-289		
258	Terminal substituent effects on the reactivity, thermodynamics, and stereoselectivity of the 8 π electrocyclization cascades of 1,3,5,7-tetraenes. <i>Journal of Organic Chemistry</i> , 2014 , 79, 11370-7	4.2	12
257	Competition Between Concerted and Stepwise Dynamics in the Triplet Di- π -Methane Rearrangement. <i>Angewandte Chemie</i> , 2014 , 126, 8808-8811	3.6	1
256	Torsional Control of Stereoselectivities in Electrophilic Additions and Cycloadditions to Alkenes. <i>Chemical Science</i> , 2014 , 5,	9.4	36
255	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	4.3	68
254	Aromatic interactions as control elements in stereoselective organic reactions. <i>Accounts of Chemical Research</i> , 2013 , 46, 979-89	24.3	183
253	Analysis of supramolecular complex energetics in artificial replicators. <i>Chemical Science</i> , 2013 , 4, 3591	9.4	6
252	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
251	Isomeric cyclopropenes exhibit unique bioorthogonal reactivities. <i>Journal of the American Chemical Society</i> , 2013 , 135, 13680-3	16.4	125
250	Dynamics in Carbene Reactions 2013 , 131-165		1
249	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
248	Confined organization of fullerene units along high polymer chains. <i>Journal of Materials Chemistry C</i> , 2013 , 1, 5747	7.1	15
247	Reversible Photochemically Gated Transformation of a Hemicarcerand to a Carcerand. <i>Angewandte Chemie</i> , 2013 , 125, 683-687	3.6	14
246	Reversible photochemically gated transformation of a hemicarcerand to a carcerand. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 655-9	16.4	48

245	Enhanced reactivity in dioxirane C-H oxidations via strain release: a computational and experimental study. <i>Journal of Organic Chemistry</i> , 2013 , 78, 4037-48	4.2	60
244	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
243	Computational enzyme design. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 5700-25	16.4	351
242	Intramolecular oxyallyl-carbonyl (3 + 2) cycloadditions. <i>Journal of the American Chemical Society</i> , 2013 , 135, 5242-5	16.4	36
241	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
240	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
239	Mechanism and origins of ligand-controlled selectivities in [Ni(NHC)]-catalyzed intramolecular (5 + 2) cycloadditions and homo-ene reactions: a theoretical study. <i>Journal of the American Chemical Society</i> , 2013 , 135, 1456-62	16.4	63
238	Covalently patterned graphene surfaces by a force-accelerated Diels-Alder reaction. <i>Journal of the American Chemical Society</i> , 2013 , 135, 9240-3	16.4	106
237	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
236	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
235	Diels-Alder reactivities of strained and unstrained cycloalkenes with normal and inverse-electron-demand dienes: activation barriers and distortion/interaction analysis. <i>Journal of the American Chemical Society</i> , 2013 , 135, 15642-9	16.4	146
234	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
233	Brønsted acid catalyzed asymmetric propargylation of aldehydes. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 1391-4	16.4	108
232	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, 5064-71	6.4	9
231	Enzymatic catalysis of anti-Baldwin ring closure in polyether biosynthesis. <i>Nature</i> , 2012 , 483, 355-8	50.4	96
230	Steric effects compete with aryne distortion to control regioselectivities of nucleophilic additions to 3-silylarynes. <i>Journal of the American Chemical Society</i> , 2012 , 134, 13966-9	16.4	117
229	A torquoselective 6 π electrocycization approach to reserpine alkaloids. <i>Organic Letters</i> , 2012 , 14, 5388-91	16.2	63
228	Z-Selectivity in olefin metathesis with chelated Ru catalysts: computational studies of mechanism and selectivity. <i>Journal of the American Chemical Society</i> , 2012 , 134, 1464-7	16.4	157

227	Dynamics, transition states, and timing of bond formation in Diels-Alder reactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 12860-5	11.5	144
226	Control and design of mutual orthogonality in bioorthogonal cycloadditions. <i>Journal of the American Chemical Society</i> , 2012 , 134, 17904-7	16.4	125
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	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
223	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		
222	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
221	Decomposition pathways of Z-selective ruthenium metathesis catalysts. <i>Journal of the American Chemical Society</i> , 2012 , 134, 7861-6	16.4	90
220	Reactivity of biarylazacyclooctynones in copper-free click chemistry. <i>Journal of the American Chemical Society</i> , 2012 , 134, 9199-208	16.4	200
219	Understanding reactivity and stereoselectivity in palladium-catalyzed diastereoselective sp ³ C-H bond activation: intermediate characterization and computational studies. <i>Journal of the American Chemical Society</i> , 2012 , 134, 14118-26	16.4	106
218	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
217	An Efficient Computational Model to Predict the Synthetic Utility of Heterocyclic Arynes. <i>Angewandte Chemie</i> , 2012 , 124, 2812-2816	3.6	19
216	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
215	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
214	Thermodynamic and stereochemical aspects of the polymerizability of glycolide and lactide. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	7
213	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. <i>Journal of the American Chemical Society</i> , 2011 , 133, 6956-9	16.4	97
212	Computational assessment of 1,3-dipolar cycloadditions to graphene. <i>Journal of Materials Chemistry</i> , 2011 , 21, 1503-1508		56
211	Dynamics of carbene cycloadditions. <i>Journal of the American Chemical Society</i> , 2011 , 133, 17848-54	16.4	56
210	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

209	Why do some Fischer indolizations fail?. <i>Journal of the American Chemical Society</i> , 2011 , 133, 5752-5	16.4	50
208	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
207	Computational methods to calculate accurate activation and reaction energies of 1,3-dipolar cycloadditions of 24 1,3-dipoles. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 13906-20	2.8	104
206	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
205	Experimental Diels-Alder reactivities of cycloalkenones and cyclic dienes explained through transition-state distortion energies. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 10366-8	16.4	110
204	Selective gold(II)-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
203	Stereoselectivities and regioselectivities of (4 + 3) cycloadditions between allenamide-derived chiral oxazolidinone-stabilized oxyallyls and furans: experiment and theory. <i>Journal of the American Chemical Society</i> , 2011 , 133, 14443-51	16.4	50
202	Probing substituent effects in aryl-aryl interactions using stereoselective Diels-Alder cycloadditions. <i>Journal of the American Chemical Society</i> , 2010 , 132, 3304-11	16.4	159
201	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
200	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
199	Computational design of an enzyme catalyst for a stereoselective bimolecular Diels-Alder reaction. <i>Science</i> , 2010 , 329, 309-13	33.3	652
198	Ligand-controlled regioselectivity in palladium-catalyzed cross coupling reactions. <i>Journal of the American Chemical Society</i> , 2010 , 132, 2496-7	16.4	201
197	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
196	Dynamics of 1,3-dipolar cycloadditions: energy partitioning of reactants and quantitation of synchronicity. <i>Journal of the American Chemical Society</i> , 2010 , 132, 3029-37	16.4	115
195	On the Mechanism of Ligand-Assisted, Copper-Catalyzed Benzylic Amination by Chloramine-T. <i>Organometallics</i> , 2010 , 29, 3404-3412	3.8	53
194	Origins of stereoselectivity in the trans Diels-Alder paradigm. <i>Journal of the American Chemical Society</i> , 2010 , 132, 9335-40	16.4	93
193	Regioselectivities of (4 + 3) cycloadditions between furans and oxazolidinone-substituted oxyallyls. <i>Organic Letters</i> , 2010 , 12, 5506-9	6.2	33
192	Indolyne and aryne distortions and nucleophilic regioselectivities. <i>Journal of the American Chemical Society</i> , 2010 , 132, 1267-9	16.4	204

191	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
190	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
189	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
188	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
187	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
186	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
185	Origin of Substituent Effects in Edge-to-Face Aryl-Aryl Interactions. <i>Molecular Physics</i> , 2009 , 107, 749-760	10.7	70
184	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
183	Transition state distortion energies correlate with activation energies of 1,4-dihydrogenations and Diels-Alder cycloadditions of aromatic molecules. <i>Journal of the American Chemical Society</i> , 2009 , 131, 4084-9	16.4	128
182	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
181	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
180	A hierarchy of homodesmotic reactions for thermochemistry. <i>Journal of the American Chemical Society</i> , 2009 , 131, 2547-60	16.4	418
179	Computational prediction of small-molecule catalysts. <i>Nature</i> , 2008 , 455, 309-13	50.4	244
178	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
177	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
176	Why delta-valerolactone polymerizes and gamma-butyrolactone does not. <i>Journal of Organic Chemistry</i> , 2008 , 73, 2674-8	4.2	130
175	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
174	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

173	Benchmarking pKa Prediction Methods for Residues in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 951-66	6.4	65
172	Bifurcations on potential energy surfaces of organic reactions. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 7592-601	16.4	262
171	Sources of error in DFT computations of C-C bond formation thermochemistries: pi->sigma transformations and error cancellation by DFT methods. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 7746-9	16.4	148
170	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
169	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
168	Rearrangement of Iridabenzvalenes to Iridabenzenes and/or B-Cyclopentadienyliridium(I) Complexes: Experimental and Computational Analysis of the Influence of Silyl Ring Substituents and Phosphine Ligands. <i>Organometallics</i> , 2007 , 26, 3957-3968	3.8	50
167	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
166	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
165	The existence of secondary orbital interactions. <i>Journal of Computational Chemistry</i> , 2007 , 28, 344-61	3.5	84
164	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
163	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
162	H/Vinyl Conical Intersections for Dienes: A Mechanism for the Photochemical Hula Twist. <i>Photochemistry and Photobiology</i> , 2007 , 76, 616-621	3.6	3
161	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
160	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
159	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
158	Mechanism of the Vinylcyclobutane Rearrangement of Scepterin to Ageliferin and Nagelamide E. <i>Angewandte Chemie</i> , 2006 , 118, 4232-4236	3.6	25
157	H/vinyl conical intersections of hexatrienes related to the hula-twist photoisomerization. <i>Molecular Physics</i> , 2006 , 104, 993-1008	1.7	19
156	Pyridine-Based Cavitands for Acid and Carboxylate Recognition. <i>Molecular Crystals and Liquid Crystals</i> , 2006 , 456, 175-192	0.5	5

155	Halo substituent effects on intramolecular cycloadditions involving furanyl amides. <i>Journal of Organic Chemistry</i> , 2006 , 71, 5432-9	4.2	45
154	Dynamics of the degenerate rearrangement of bicyclo[3.1.0]hex-2-ene. <i>Journal of the American Chemical Society</i> , 2006 , 128, 90-4	16.4	104
153	Theoretical investigation of the stereoselective stepwise cope rearrangement of a 3-vinylmethylenecyclobutane. <i>Journal of the American Chemical Society</i> , 2006 , 128, 11106-13	16.4	22
152	Why 6-methylpentacene deconjugates but avoids the thermally allowed unimolecular mechanism. <i>Organic Letters</i> , 2006 , 8, 4915-8	6.2	17
151	Photolysis of heptanal. <i>Journal of Organic Chemistry</i> , 2006 , 71, 6403-8	4.2	19
150	Theoretical studies of stereoselectivities of intramolecular aldol cyclizations catalyzed by amino acids. <i>Journal of the American Chemical Society</i> , 2005 , 127, 11294-302	16.4	106
149	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
148	Theozymes and Catalyst Design 2005 , 79-88		5
147	The three corrugated surfaces of 1,4-divinyltetramethylene 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
146	Theoretical Studies of Antibody Catalysis 2005 , 72-117		1
145	Computational predictions of stereochemistry in asymmetric thiazolium- and triazolium-catalyzed benzoin condensations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004 , 101, 5770-5	11.5	109
144	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
143	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
142	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
141	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
140	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
139	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
138	Nitroxyl disulfides, novel intermediates in transnitrosation reactions. <i>Journal of the American Chemical Society</i> , 2003 , 125, 6972-6	16.4	63

137	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
136	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
135	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
134	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
133	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
132	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. <i>Organic and Biomolecular Chemistry</i> , 2003 , 1, 1389-403	3.9	51
131	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
130	Diels-Alder and ene reactions of singlet oxygen, nitroso compounds and triazolinediones: transition states and mechanisms from contemporary theory. <i>Chemical Communications</i> , 2002 , 1243-55	5.8	129
129	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
128	"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
127	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. <i>Molecular Physics</i> , 2002 , 100, 717-727	1.7	59
126	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	16.4	28
125	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
124	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
123	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	4.2	275
122	Origins of stereoselectivity in intramolecular Diels-Alder cycloadditions of dienes and dienophiles linked by ester and amide tethers. <i>Journal of Organic Chemistry</i> , 2001 , 66, 1938-40	4.2	61
121	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
120	Perspective on theoretical interpretation of 1-2 asymmetric induction. The importance of antiperiplanarity. <i>Theoretical Chemistry Accounts</i> , 2000 , 103, 330-331	1.9	7

119	Aromaticity and Antiaromaticity in Small Ring Transition States, Assessed by NICS Values and Energetics. <i>Journal of Molecular Modeling</i> , 2000 , 6, 158-165	2	23
118	Mechanism of Permanganate Oxidation of Alkanes: Hydrogen Abstraction and Oxygen Rebound. <i>Journal of the American Chemical Society</i> , 2000 , 122, 7821-7822	16.4	58
117	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
116	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
115	Perspective on the theoretical interpretation of the asymmetric induction. The importance of antiperiplanarity. <i>Journal of the American Chemical Society</i> , 2000 , 122, 330-331		0
114	Establishing the (3 + 2) Mechanism for the Permanganate Oxidation of Alkenes by Theory and Kinetic Isotope Effects. <i>Journal of Organic Chemistry</i> , 1999 , 64, 800-802	4.2	61
113	Transition State Modeling of Asymmetric Epoxidation Catalysts. <i>ACS Symposium Series</i> , 1999 , 33-48	0.4	0
112	Bis-periazulene: a simple Kekulé biradical with a triplet ground state. <i>Theoretical Chemistry Accounts</i> , 1999 , 102, 397-400	1.9	5
111	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
110	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
109	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> , 1999 , 5, 2119-2132	4.8	14
108	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[3.2.0]hept-2-en-6-on. <i>Angewandte Chemie - International Edition</i> , 1999 , 38, 2728-2730	16.4	28
107	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
106	Structural basis for antibody catalysis of a disfavored ring closure reaction. <i>Biochemistry</i> , 1999 , 38, 7062-7064	3.4	55
105	Evolution of shape complementarity and catalytic efficiency from a primordial antibody template. <i>Science</i> , 1999 , 286, 2345-8	33.3	106
104	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
103	Ketone-Catalyzed Decomposition of Peroxynitrite via Dioxirane Intermediates. <i>Journal of the American Chemical Society</i> , 1999 , 121, 11976-11983	16.4	54
102	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

101	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
100	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
99	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
98	Origin of Stereoselectivities in Asymmetric Alkoxyseleenylation. <i>Journal of the American Chemical Society</i> , 1999 , 121, 8567-8576	16.4	41
97	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
96	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
95	Theozymes and compuzymes: theoretical models for biological catalysis. <i>Current Opinion in Chemical Biology</i> , 1998 , 2, 743-50	9.7	196
94	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
93	[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
92	The Mechanism of the Slippage Approach to Rotaxanes. Origin of the All-or-Nothing Substituent Effect. <i>Journal of the American Chemical Society</i> , 1998 , 120, 9318-9322	16.4	128
91	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
90	New Paradigm for Anionic Heteroatom Cope Rearrangements. <i>Journal of the American Chemical Society</i> , 1998 , 120, 205-206	16.4	30
89	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
88	Alkynes, Allenes, and Alkenes in [3,3]-Sigmatropy: Functional Diversity and Kinetic Monotony. A Theoretical Analysis. <i>Journal of the American Chemical Society</i> , 1998 , 120, 5622-5627	16.4	50
87	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. <i>Journal of Organic Chemistry</i> , 1998 , 63, 4611-4619	4.2	127
86	A Theoretical Investigation of Phosphoramidates and Sulfonamides as Protease Transition State Isosteres. <i>Journal of Organic Chemistry</i> , 1998 , 63, 1419-1428	4.2	58
85	An antibody exo Diels-Alderase inhibitor complex at 1.95 angstrom resolution. <i>Science</i> , 1998 , 279, 1934-1939	39.3	127
84	Theoretical Study of the Concerted and Stepwise Mechanisms of Triazolinedione Diels-Alder Reactions. <i>Journal of the American Chemical Society</i> , 1998 , 120, 12303-12309	16.4	51

83	Stereoselective DielsAlder Reactions of Hexachlorocyclopentadiene with Chiral Alkenes: New Insights Into the Inside-Alkoxy Model of Stereoselectivity. <i>Journal of Organic Chemistry</i> , 1997 , 62, 5728-5731	4.2	22
82	Origins of Stereoselective Carbene 1,2-Shifts and Cycloadditions of 1,2-Dichloroethylidene: A Theoretical Model Based on CBS-Q and B3LYP Calculations. <i>Journal of the American Chemical Society</i> , 1997 , 119, 10805-10809	16.4	50
81	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
80	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
79	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
78	Facial Diastereoselection in DielsAlder Reactions of (R)-4-[(p-Tolylsulfinyl)methyl]quinols. <i>Journal of Organic Chemistry</i> , 1997 , 62, 9128-9137	4.2	23
77	Transition States of Epoxidations: Diradical Character, Spiro Geometries, Transition State Flexibility, and the Origins of Stereoselectivity. <i>Journal of the American Chemical Society</i> , 1997 , 119, 10147-10152	16.4	164
76	Experimental and Theoretical Kinetic Isotope Effects for Asymmetric Dihydroxylation. Evidence Supporting a Rate-Limiting (B + 2) Cycloaddition. <i>Journal of the American Chemical Society</i> , 1997 , 119, 9907-9908	16.4	204
75	Experimental Determination of the Activation Parameters and Stereoselectivities of the Intramolecular DielsAlder 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
74	Palladium Complexes of the New Porphyrin Isomers (Z)- and (E)-IsoporphyceneBdII-Induced Cyclization of Tetrapyrrolealdehydes. <i>Angewandte Chemie International Edition in English</i> , 1997 , 36, 353-357		51
73	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
72	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
71	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
70	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
69	Molecular Mechanics and Statistical Thermodynamics Studies of Complexes of a Flexible Hemiacerand with Neutral Guests. <i>Journal of the American Chemical Society</i> , 1996 , 118, 8056-8070	16.4	58
68	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
67	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
66	Synchronous or Asynchronous? An Experimental Transition State from a Direct Comparison of Experimental and Theoretical Kinetic Isotope Effects for a DielsAlder Reaction. <i>Journal of the American Chemical Society</i> , 1996 , 118, 9984-9985	16.4	128

65	Gating as a control element in constrictive binding and guest release by hemicarcerands. <i>Science</i> , 1996 , 273, 627-9	33.3	97
64	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
63	Polyether Catalysis of Ester Aminolysis I A Computational and Experimental Study. <i>Liebigs Annalen</i> , 1996 , 1996, 1511-1522		42
62	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
61	Pericyclic Reaction Transition States: Passions and Punctilios, 1935-1995. <i>Accounts of Chemical Research</i> , 1995 , 28, 81-90	24.3	558
60	Mechanism and Thermodynamics of Guest Escape from a Carcerand. <i>Journal of the American Chemical Society</i> , 1995 , 117, 1853-1854	16.4	32
59	Von Porphyrin-Isomeren zu octapyrrolischen Makrocyclen mit 8er-Konformation. <i>Angewandte Chemie</i> , 1995 , 107, 2705-2709	3.6	55
58	Octaphyrin-(1.0.1.0.1.0.1.0). <i>Angewandte Chemie</i> , 1995 , 107, 2709-2711	3.6	43
57	From Porphyrin Isomers to Octapyrrolic Figure Eight-Macrocycles. <i>Angewandte Chemie International Edition in English</i> , 1995 , 34, 2511-2514		143
56	Octaphyrin-(1.0.1.0.1.0.1.0). <i>Angewandte Chemie International Edition in English</i> , 1995 , 34, 2515-2517		96
55	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
54	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
53	Hetero-Diels-Alder reaction transition structures: reactivity, stereoselectivity, catalysis, solvent effects, and the exo-lone-pair effect. <i>Journal of Organic Chemistry</i> , 1993 , 58, 3330-3343	4.2	163
52	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
51	Torquoselectivity in the electrocyclic conversion of benzocyclobutenes to o-xylenes. <i>Journal of the American Chemical Society</i> , 1992 , 114, 1157-1165	16.4	121
50	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
49	Theoretical secondary kinetic isotope effects and the interpretation of transition state geometries. 1. The Cope rearrangement. <i>Journal of the American Chemical Society</i> , 1992 , 114, 8565-8572	16.4	98
48	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

47	exo-Lone-pair effect on hetero-Diels-Alder cycloaddition stereochemistry. <i>Journal of the American Chemical Society</i> , 1992 , 114, 1499-1500	16.4	98
46	Transition Structures of Hydrocarbon Pericyclic Reactions. <i>Angewandte Chemie International Edition in English</i> , 1992 , 31, 682-708		512
45	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
44	Bergangsstrukturen in pericyclischen Reaktionen von Kohlenwasserstoffen. <i>Angewandte Chemie</i> , 1992 , 104, 711-739	3.6	85
43	Transition states of electrophilic radical additions to alkenes. <i>Journal of the American Chemical Society</i> , 1991 , 113, 4324-4325	16.4	55
42	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
41	Transition structures for hydrogen atom transfers to oxygen. Comparisons of intermolecular and intramolecular processes, and open- and closed-shell systems. <i>Journal of the American Chemical Society</i> , 1990 , 112, 7508-7514	16.4	97
40	Experimental and theoretical studies of substituent effects on an orbital-symmetry-forbidden electrocycization. <i>Journal of the American Chemical Society</i> , 1989 , 111, 5356-5367	16.4	22
39	Extended Hartree-Fock (EHF) theory of chemical reactions. <i>Theoretica Chimica Acta</i> , 1988 , 73, 337-364		185
38	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
37	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
36	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
35	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
34	Theoretical transition structures for radical additions to alkenes. <i>Journal of Organic Chemistry</i> , 1986 , 51, 2874-2879	4.2	88
33	Evidence for the concerted mechanism of the Diels-Alder reaction of butadiene with ethylene. <i>Journal of the American Chemical Society</i> , 1986 , 108, 554-6	16.4	122
32	Stereospecificity of 1,3-dipolar cycloadditions of p-nitrobenzonitrile oxide to cis- and trans-dideuterioethylene. <i>Journal of the American Chemical Society</i> , 1985 , 107, 7227-7228	16.4	59
31	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
30	"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

29	Stereoselective substituent effects on conrotatory electrocyclic reactions of cyclobutenes. <i>Journal of the American Chemical Society</i> , 1984 , 106, 7989-7991	16.4	225
28	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
27	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
26	Nonplanar alkenes and carbonyls: a molecular distortion which parallels addition stereoselectivity. <i>Journal of the American Chemical Society</i> , 1981 , 103, 2436-2438	16.4	123
25	"Anomalous" selectivities in electrophilic aromatic substitutions. <i>Journal of the American Chemical Society</i> , 1979 , 101, 1337-1340	16.4	17
24	Influence of molecular distortions upon reactivity and stereochemistry in nucleophilic additions to acetylenes. <i>Journal of the American Chemical Society</i> , 1979 , 101, 1340-1343	16.4	103
23	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
22	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
21	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
20	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
19	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
18	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
17	Frontier molecular orbital theory of cycloaddition reactions. <i>Accounts of Chemical Research</i> , 1975 , 8, 361-369	16.4	619
16	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
15	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
14	Lewis acid catalysis of Diels-Alder reactions. <i>Journal of the American Chemical Society</i> , 1973 , 95, 4094-4096	16.4	224
13	Frontier molecular orbitals of 1,3 dipoles and dipolarophiles. <i>Journal of the American Chemical Society</i> , 1973 , 95, 7287-7301	16.4	507
12	Cycloadditions of dienes to fulvenes. <i>Journal of Organic Chemistry</i> , 1973 , 38, 3836-3843	4.2	53

11	Regioselectivity and reactivity in the 1,3-dipolar cycloadditions of diazonium betaines (diazalkanes, azides, and nitrous oxide). <i>Journal of the American Chemical Society</i> , 1972 , 94, 8953-8955	16.4	95
10	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
9	Influence of steric interactions on endo stereoselectivity. <i>Journal of the American Chemical Society</i> , 1971 , 93, 4606-4607	16.4	45
8	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
7	Novel double [6 + 4] cycloaddition of tropone to dimethylfulvene. <i>Journal of the American Chemical Society</i> , 1970 , 92, 6392-6394	16.4	80
6	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
5	Electrochemical Fluorination of Vinyl Boronates through Donor-Stabilized Vinyl Carbocation Intermediates**. <i>Angewandte Chemie</i> , e202113972	3.6	
4	Computations on Pericyclic Reactions Reveal the Richness of Ambimodal Transition States and Pericyclases. <i>Israel Journal of Chemistry</i> ,	3.4	0
3	Lattice strain suppresses point defect formation in halide perovskites. <i>Nano Research</i> , 1	10	5
2	Organocatalytic Discrimination of Non-Directing Aryl and Heteroaryl Groups: Enantioselective Synthesis of Bioactive Indole-Containing Triarylmethanes. <i>Chemical Science</i> ,	9.4	4
1	Application of the Spin-Center Shift in Organic Synthesis. <i>Jacs Au</i> ,		3