Dean J Tantillo

List of Publications by Year
in descending order

347 papers	11,970 citations	31902 53 h-index	46693 89 g-index
403 all docs	403 docs citations	403 times ranked	9961 citing authors

#	Article	IF	Citations
1	Computational Prediction of¹H and¹³C Chemical Shifts: A Useful Tool for Natural Product, Mechanistic, and Synthetic Organic Chemistry. Chemical Reviews, 2012, 112, 1839-1862.	23.0	1,027
2	Redox chemistry and chemical biology of H2S, hydropersulfides, and derived species: Implications of their possible biological activity and utility. Free Radical Biology and Medicine, 2014, 77, 82-94.	1.3	340
3	Small Molecule Signaling Agents: The Integrated Chemistry and Biochemistry of Nitrogen Oxides, Oxides of Carbon, Dioxygen, Hydrogen Sulfide, and Their Derived Species. Chemical Research in Toxicology, 2012, 25, 769-793.	1.7	330
4	Biosynthesis via carbocations: Theoretical studies on terpene formation. Natural Product Reports, 2011, 28, 1035.	5.2	312
5	Theozymes and compuzymes: theoretical models for biological catalysis. Current Opinion in Chemical Biology, 1998, 2, 743-750.	2.8	223
6	Total Synthesis of Oxidized Welwitindolinones and (âˆ’)-<i>N</i>-Methylwelwitindolinone C Isonitrile. Journal of the American Chemical Society, 2012, 134, 1396-1399.	6.6	161
7	The Correct Structure of Aquatolideâ€”Experimental Validation of a Theoretically-Predicted Structural Revision. Journal of the American Chemical Society, 2012, 134, 18550-18553.	6.6	148
8	The carbocation continuum in terpene biosynthesisâ€”where are the secondary cations?. Chemical Society Reviews, 2010, 39, 2847.	18.7	147
9	Total synthesis and isolation of citrinalin and cyclopiamine congeners. Nature, 2014, 509, 318-324.	13.7	140
10	Recent excursions to the borderlands between the realms of concerted and stepwise: carbocation cascades in natural products biosynthesis. Journal of Physical Organic Chemistry, 2008, 21, 561-570.	0.9	129
11	Biosynthetic consequences of multiple sequential post-transition-state bifurcations. Nature Chemistry, 2014, 6, 104-111.	6.6	128
12	Post-transition state bifurcations gain momentum â€“ current state of the field. Pure and Applied Chemistry, 2017, 89, 679-698.	0.9	127
13	A gold-catalysed enantioselective Cope rearrangement of achiral 1,5-dienes. Nature Chemistry, 2012, 4, 405-409.	6.6	126
14	Importance of Inherent Substrate Reactivity in Enzymeâ€Promoted Carbocation Cyclization/Rearrangements. Angewandte Chemie - International Edition, 2017, 56, 10040-10045.	7.2	124
15	Formation of the Unusual Semivolatile Diterpene Rhizathalene by the <i>Arabidopsis</i> Class I Terpene Synthase TPS08 in the Root Stele Is Involved in Defense against Belowground Herbivory. Plant Cell, 2013, 25, 1108-1125.	3.1	123
16	Acylammonium Salts as Dienophiles in Dielsâ€“Alder/Lactonization Organocascades. Journal of the American Chemical Society, 2014, 136, 4492-4495.	6.6	120
17	Theoretical Studies on Farnesyl Cation Cyclization:Â Pathways to Pentalenene. Journal of the American Chemical Society, 2006, 128, 6172-6179.	6.6	119
18	Walking in the woods with quantum chemistry â€“ applications of quantum chemical calculations in natural products research. Natural Product Reports, 2013, 30, 1079.	5.2	116

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19	Consequences of Conformational Preorganization in Sesquiterpene Biosynthesis: Theoretical Studies on the Formation of the Bisabolene, Curcumene, Acoradiene, Zizaene, Cedrene, Duprezianene, and Sesquithuriferol Sesquiterpenes. Journal of the American Chemical Society, 2009, 131, 7999-8015.	6.6	113
20	A potential energy surface bifurcation in terpene biosynthesis. Nature Chemistry, 2009, 1, 384-389.	6.6	109
21	Unearthing a sesterterpene biosynthetic repertoire in the Brassicaceae through genome mining reveals convergent evolution. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6005-E6014.	3.3	102
22	Branching Out from the Bisabolyl Cation. Unifying Mechanistic Pathways to Barbatene, Bazzanene, Chamigrene, Chamipinene, Cumacrene, Cuprenene, Dunniene, Isobazzanene, Iso-Î³-bisabolene, Isochamigrene, Laurene, Microbiotene, Sesquithujene, Sesquisabinene, Thujopsene, Trichodiene, and Widdradiene Sesquiterpenes. Journal of the American Chemical Society, 2014, 136, 2450-2463.	6.6	95
23	Differentiating Mechanistic Possibilities for the Thermal, Intramolecular [2 + 2] Cycloaddition of Alleneâˆ'Ynes. Journal of the American Chemical Society, 2010, 132, 11952-11966.	6.6	94
24	Prediction of the Structure of Nobilisitine A Using Computed NMR Chemical Shifts. Journal of Natural Products, 2011, 74, 1339-1343.	1.5	93
25	The value of universally available raw NMR data for transparency, reproducibility, and integrity in natural product research. Natural Product Reports, 2019, 36, 35-107.	5.2	92
26	The chemical biology of the persulfide (RSSH)/perthiyl (RSSÂ·) redox couple and possible role in biological redox signaling. Free Radical Biology and Medicine, 2016, 101, 20-31.	1.3	89
27	Effect of Isotopically Sensitive Branching on Product Distribution for Pentalenene Synthase: Support for a Mechanism Predicted by Quantum Chemistry. Journal of the American Chemical Society, 2012, 134, 11369-11371.	6.6	82
28	Chemical Hermaphroditism:Â The Potential of the Cr(CO)3Moiety To Stabilize Transition States and Intermediates with Anionic, Cationic, or Radical Character at the Benzylic Position. Journal of the American Chemical Society, 1999, 121, 3596-3606.	6.6	80
29	BrÃ¸nsted Acid Catalyzed Enantioselective Indole Aza-Claisen Rearrangement Mediated by an Arene CHâ€"O Interaction. Journal of the American Chemical Society, 2013, 135, 16380-16383.	6.6	80
30	Dynamic behavior of rearranging carbocations â€" implications for terpene biosynthesis. Beilstein Journal of Organic Chemistry, 2016, 12, 377-390.	1.3	79
31	Formation of Beyerene, Kaurene, Trachylobane, and Atiserene Diterpenes by Rearrangements That Avoid Secondary Carbocations. Journal of the American Chemical Society, 2010, 132, 5375-5386.	6.6	77
32	Dyotropic Rearrangements of Fused Tricyclic Î²-Lactones: Application to the Synthesis of (âˆ')-Curcumanolide A and (âˆ')-Curcumalactone. Journal of the American Chemical Society, 2012, 134, 13348-13356.	6.6	74
33	Quantum chemical dissection of the classic terpinyl/pinyl/bornyl/camphyl cation conundrumâ€"the role of pyrophosphate in manipulating pathways to monoterpenes. Organic and Biomolecular Chemistry, 2010, 8, 4589.	1.5	73
34	Which Is More Likely in Trichodiene Biosynthesis:â€‰ Hydride or Proton Transfer?. Organic Letters, 2006, 8, 4601-4604.	2.4	69
35	The Need for Enzymatic Steering in Abietic Acid Biosynthesis: Gas-Phase Chemical Dynamics Simulations of Carbocation Rearrangements on a Bifurcating Potential Energy Surface. Journal of the American Chemical Society, 2011, 133, 8335-8343.	6.6	69
36	Traversing Biosynthetic Carbocation Landscapes in the Total Synthesis of Andrastin and Terretonin Meroterpenes. Angewandte Chemie - International Edition, 2017, 56, 12498-12502.	7.2	69

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37	Cryptic post-transition state bifurcations that reduce the efficiency of lactone-forming Rh-carbenoid Câ€“H insertions. Chemical Science, 2017, 8, 1442-1449.	3.7	69
38	Metal promoted vinylcyclopropaneâ€“cyclopentene rearrangements: Reactions ripe for mechanism-based catalyst design. Journal of Organometallic Chemistry, 2006, 691, 4386-4392.	0.8	68
39	Pronounced Steric Effects of Substituents in the Nazarov Cyclization of Aryl Dienyl Ketones. Angewandte Chemie - International Edition, 2008, 47, 6379-6383.	7.2	67
40	Stereocontrol in a Combined Allylic Azide Rearrangement and Intramolecular Schmidt Reaction. Journal of the American Chemical Society, 2012, 134, 6528-6531.	6.6	67
41	A Cytochrome P450 Serves as an Unexpected Terpene Cyclase during Fungal Meroterpenoid Biosynthesis. Journal of the American Chemical Society, 2013, 135, 16805-16808.	6.6	65
42	The chemical biology of hydropersulfides (RSSH): Chemical stability, reactivity and redox roles. Archives of Biochemistry and Biophysics, 2015, 588, 15-24.	1.4	65
43	Origins of Stereoselectivity in Intramolecular Dielsâˆ’Alder Cycloadditions of Dienes and Dienophiles Linked by Ester and Amide Tethers. Journal of Organic Chemistry, 2001, 66, 1938-1940.	1.7	62
44	How cyclobutanes are assembled in nature â€“ insights from quantum chemistry. Chemical Society Reviews, 2014, 43, 5042.	18.7	62
45	Blocking Deprotonation with Retention of Aromaticity in a Plant <i>ent</i>â€Copalyl Diphosphate Synthase Leads to Product Rearrangement. Angewandte Chemie - International Edition, 2016, 55, 634-638.	7.2	61
46	Mechanism of the Ni(0)-Catalyzed Vinylcyclopropaneâˆ’Cyclopentene Rearrangement. Journal of Organic Chemistry, 2009, 74, 7822-7833.	1.7	59
47	Multicomponent Assembly of Highly Substituted Indoles by Dual Palladiumâ€Catalyzed Coupling Reactions. Angewandte Chemie - International Edition, 2012, 51, 10588-10591.	7.2	59
48	Mechanistic Studies on the Stereoselective Formation of Î²-Mannosides from Mannosyl Iodides Using Î±-Deuterium Kinetic Isotope Effects. Journal of Organic Chemistry, 2007, 72, 4663-4672.	1.7	58
49	Computational Studies on Biosynthetic Carbocation Rearrangements Leading to Sativene, Cyclosativene, Î±-Ylangene, and Î²-Ylangene. Journal of Organic Chemistry, 2008, 73, 6570-6579.	1.7	57
50	Applied Computational Chemistry for the Blind and Visually Impaired. Journal of Chemical Education, 2012, 89, 1400-1404.	1.1	57
51	They Came From the Deep: Syntheses, Applications, and Biology of Ladderanes. Current Organic Chemistry, 2006, 10, 2055-2074.	0.9	56
52	Heterocycleâ€“Heterocycle Strategies: (2-Nitrophenyl)isoxazole Precursors to 4-Aminoquinolines, 1<i>H</i>-Indoles, and Quinolin-4(1<i>H</i>)-ones. Organic Letters, 2013, 15, 2062-2065.	2.4	56
53	Diverged Plant Terpene Synthases Reroute the Carbocation Cyclization Path towards the Formation of Unprecedented 6/11/5 and 6/6/7/5 Sesterterpene Scaffolds. Angewandte Chemie - International Edition, 2018, 57, 1291-1295.	7.2	55
54	Carbocations and the Complex Flavor and Bouquet of Wine: Mechanistic Aspects of Terpene Biosynthesis in Wine Grapes. Molecules, 2015, 20, 10781-10792.	1.7	54

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55	Biomimetic Total Synthesis of Santalinâ€…Y. Angewandte Chemie - International Edition, 2015, 54, 5079-5083.	7.2	54
56	Synthesis and Utility of Dihydropyridine Boronic Esters. Angewandte Chemie - International Edition, 2016, 55, 2205-2209.	7.2	54
57	A divergent approach to the synthesis of the yohimbinoid alkaloids venenatine and alstovenine. Nature Chemistry, 2013, 5, 126-131.	6.6	53
58	Mechanism of Rh₂(II)-Catalyzed Indole Formation: The Catalyst Does Not Control Product Selectivity. Journal of the American Chemical Society, 2016, 138, 487-490.	6.6	53
59	Navigating Past a Fork in the Road: Carbocationâˆ'Ï€ Interactions Can Manipulate Dynamic Behavior of Reactions Facing Post-Transition-State Bifurcations. Journal of the American Chemical Society, 2017, 139, 7485-7493.	6.6	51
60	Perturbing the Structure of the 2-Norbornyl Cation through Câˆ'HÂ·Â·Â·N and Câˆ'HÂ·Â·Â·Ï€ Interactions. Journal of Organic Chemistry, 2007, 72, 8877-8881.	1.7	50
61	Transition-State Complexation in Palladium-Promoted [3,3] Sigmatropic Shifts. Journal of the American Chemical Society, 2007, 129, 8686-8687.	6.6	50
62	Biological Production of 2â€Butanone in <i>Escherichia coli</i>. ChemSusChem, 2014, 7, 92-95.	3.6	50
63	Potent <i>s-cis</i>-Locked Bithiazole Correctors of Î"F508 Cystic Fibrosis Transmembrane Conductance Regulator Cellular Processing for Cystic Fibrosis Therapy. Journal of Medicinal Chemistry, 2008, 51, 6044-6054.	2.9	49
64	Prediction of a New Pathway to Presilphiperfolanol. Organic Letters, 2008, 10, 4827-4830.	2.4	49
65	Theoretical Studies on Pentadienyl Cation Electrocyclizations. Current Organic Chemistry, 2010, 14, 1561-1577.	0.9	49
66	The Taxadiene-Forming Carbocation Cascade. Journal of the American Chemical Society, 2011, 133, 18249-18256.	6.6	49
67	Analogies between Synthetic and Biosynthetic Reactions in Which [1,2]-Alkyl Shifts Are Combined with Other Events: Dyotropic, Schmidt, and Carbocation Rearrangements. Journal of Organic Chemistry, 2012, 77, 8845-8850.	1.7	49
68	Mechanistic Studies of Copper(I)-Catalyzed 1,3-Halogen Migration. Journal of the American Chemical Society, 2015, 137, 5346-5354.	6.6	49
69	Trapping and Electron Paramagnetic Resonance Characterization of the 5â€²dAdo^{â€¢} Radical in a Radical <i>S</i>-Adenosyl Methionine Enzyme Reaction with a Non-Native Substrate. ACS Central Science, 2019, 5, 1777-1785.	5.3	49
70	Fidelity in Hapten Design:Â How Analogous Are Phosphonate Haptens to the Transition States for Alkaline Hydrolyses of Aryl Esters?. Journal of Organic Chemistry, 1999, 64, 3066-3076.	1.7	47
71	Hiscotropic Rearrangements: Hybrids of Electrocyclic and Sigmatropic Reactions. Journal of Organic Chemistry, 2006, 71, 3686-3695.	1.7	47
72	Theoretical Studies on Synthetic and Biosynthetic Oxidopyryliumâˆ'Alkene Cycloadditions:â€‰ Pericyclic Pathways to Intricarene. Journal of Organic Chemistry, 2008, 73, 1516-1523.	1.7	47

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73	Mechanistic Insight into the Dehydro-Dielsâ€“Alder Reaction of Styreneâ€“Ynes. Journal of Organic Chemistry, 2015, 80, 11686-11698.	1.7	47
74	Quantum Chemistry Calculations for Metabolomics. Chemical Reviews, 2021, 121, 5633-5670.	23.0	47
75	Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. Journal of Chemical Theory and Computation, 2012, 8, 1212-1222.	2.3	46
76	Cyclols Revisited: Facile Synthesis of Mediumâ€Sized Cyclic Peptides. Chemistry - A European Journal, 2017, 23, 13319-13322.	1.7	46
77	Proton Sandwiches: Nonclassical Carbocations with Tetracoordinate Protons. Angewandte Chemie - International Edition, 2005, 44, 2719-2723.	7.2	45
78	Câ€“Hâ‹¯Ï€ interactions as modulators of carbocation structure â€“ implications for terpene biosynthesis. Chemical Science, 2013, 4, 2512.	3.7	45
79	Post-transition state bifurcations induce dynamical detours in Pummerer-like reactions. Chemical Science, 2018, 9, 8937-8945.	3.7	45
80	Switching between Concerted and Stepwise Mechanisms for Dyotropic Rearrangements of Î²-Lactones Leading to Spirocyclic, Bridged Î³-Butyrolactones. Journal of Organic Chemistry, 2011, 76, 7167-7174.	1.7	44
81	Cation-Controlled Enantioselective and Diastereoselective Synthesis of Indolines: An Autoinductive Phase-Transfer Initiated 5-<i>endo</i>-<i>trig</i> Process. Journal of the American Chemical Society, 2015, 137, 13414-13424.	6.6	43
82	Synthesis of Benzodihydrofurans by Asymmetric Câˆ’H Insertion Reactions of Donor/Donor Rhodium Carbenes. Chemistry - A European Journal, 2017, 23, 11843-11855.	1.7	43
83	Nonclassical Carbocations as Câˆ’H Hydrogen Bond Donors. Journal of Physical Chemistry A, 2006, 110, 4810-4816.	1.1	41
84	Mechanism of the Acid-Promoted Intramolecular Schmidt Reaction: Theoretical Assessment of the Importance of Lone Pairâ€“Cation, Cationâˆ’Ï€, and Steric Effects in Controlling Regioselectivity. Journal of Organic Chemistry, 2012, 77, 640-647.	1.7	41
85	Biosynthesis of Lycosantalonol, a <i>cis</i>-Prenyl Derived Diterpenoid. Journal of the American Chemical Society, 2014, 136, 16951-16953.	6.6	41
86	Lessons in Strain and Stability: Enantioselective Synthesis of (+)â€[5]â€Ladderanoic Acid. Angewandte Chemie - International Edition, 2020, 59, 436-441.	7.2	41
87	A Promiscuous Proton in Taxadiene Biosynthesis?. Organic Letters, 2007, 9, 1069-1071.	2.4	40
88	The energetic viability of an unexpected skeletal rearrangement in cyclooctatin biosynthesis. Organic and Biomolecular Chemistry, 2015, 13, 10273-10278.	1.5	40
89	Product Rearrangement from Altering a Single Residue in the Rice <i>syn</i>-Copalyl Diphosphate Synthase. Organic Letters, 2016, 18, 1060-1063.	2.4	40
90	The Many Roles of Quantum Chemical Predictions in Synthetic Organic Chemistry. Chemistry - an Asian Journal, 2014, 9, 674-680.	1.7	39

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91	Stereodivergent, Dielsâ€"Alder-initiated organocascades employing Î±,Î²-unsaturated acylammonium salts: scope, mechanism, and application. Chemical Science, 2017, 8, 1511-1524.	3.7	39
92	Multicenter Bonding in Organic Chemistry. Geometry-Sensitive 3c-2e Bonding in (CÂ·Â·Â·HÂ·Â·Â·C) Fragments of Organic Cations. Journal of Organic Chemistry, 2004, 69, 2992-2996.	1.7	38
93	How Many Secondary Carbocations Are Involved in the Biosynthesis of Avermitilol?. Organic Letters, 2011, 13, 1294-1297.	2.4	37
94	Toward Structural Correctness: Aquatolide and the Importance of 1D Proton NMR FID Archiving. Journal of Organic Chemistry, 2016, 81, 878-889.	1.7	36
95	Sigmatropic Shiftamers: Fluxionality in Broken Ladderane Polymers. Angewandte Chemie - International Edition, 2002, 41, 1033-1036.	7.2	35
96	Theoretical Studies on NG-Hydroxy-l-arginine and Derived Radicals:â€‰ Implications for the Mechanism of Nitric Oxide Synthase. Journal of the American Chemical Society, 2000, 122, 536-537.	6.6	34
97	Predicting Productive Binding Modes for Substrates and Carbocation Intermediates in Terpene Synthasesâ€"Bornyl Diphosphate Synthase As a Representative Case. ACS Catalysis, 2018, 8, 3322-3330.	5.5	34
98	Synthesis and Structure Revision of Dichrocephonesâ€…A and B. Angewandte Chemie - International Edition, 2018, 57, 2419-2422.	7.2	34
99	A Highly Selective Rearrangement of a Housane-Derived Cation Radical:â€‰ An Electrochemically Mediated Transformation. Journal of Organic Chemistry, 2007, 72, 4351-4357.	1.7	33
100	Lifetimes of carbocations encountered along reaction coordinates for terpene formation. Chemical Science, 2014, 5, 3301.	3.7	33
101	Speeding Up Sigmatropic Shiftsâ€"To Halve or to Hold. Accounts of Chemical Research, 2016, 49, 741-749.	7.6	33
102	Bedeutung der inhÃrenten SubstratreaktivitÃt bei enzymvermittelten Cyclisierungen/Umlagerungen von Carbokationen. Angewandte Chemie, 2017, 129, 10172-10178.	1.6	33
103	Using Theory and Experiment to Discover Catalysts for Electrocyclizations. Angewandte Chemie - International Edition, 2009, 48, 31-32.	7.2	32
104	A tangled webâ€"interconnecting pathways to amorphadiene and the amorphene sesquiterpenes. Chemical Science, 2010, 1, 609.	3.7	32
105	Modulation of inherent dynamical tendencies of the bisabolyl cation via preorganization in epi-isozizaene synthase. Chemical Science, 2015, 6, 2347-2353.	3.7	32
106	Crystal Structures of Orotidine Monophosphate Decarboxylase: Does the Structure Reveal the Mechanism of Nature's Most Proficient Enzyme?. ChemBioChem, 2001, 2, 113-118.	1.3	31
107	Feasibility of Intramolecular Proton Transfers in Terpene Biosynthesis â€" Guiding Principles. Journal of the American Chemical Society, 2015, 137, 4134-4140.	6.6	31
108	Intramolecular Chirality Transfer [2 + 2] Cycloadditions of Allenoates and Alkenes. Organic Letters, 2017, 19, 3703-3706.	2.4	31

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109	Prediction of ¹⁹F NMR Chemical Shifts for Fluorinated Aromatic Compounds. Journal of Organic Chemistry, 2018, 83, 3220-3225.	1.7	31
110	Enantioselective synthesis of isochromans and tetrahydroisoquinolines by Câ€“H insertion of donor/donor carbenes. Chemical Science, 2020, 11, 494-498.	3.7	31
111	Theoretical and Experimental Analysis of the Reaction Mechanism of MrTPS2, a Triquinaneâ€Forming Sesquiterpene Synthase from Chamomile. Chemistry - A European Journal, 2013, 19, 13590-13600.	1.7	30
112	A Fluorescent Adenosine Analogue as a Substrate for an Aâ€toâ€I RNA Editing Enzyme. Angewandte Chemie - International Edition, 2015, 54, 8713-8716.	7.2	30
113	Using ¹H and ¹³C NMR chemical shifts to determine cyclic peptide conformations: a combined molecular dynamics and quantum mechanics approach. Physical Chemistry Chemical Physics, 2018, 20, 14003-14012.	1.3	30
114	Metal Bound or Free Ylides as Reaction Intermediates in Metal-Catalyzed [2,3]-Sigmatropic Rearrangements? It Depends. ACS Catalysis, 2021, 11, 829-839.	5.5	30
115	Nobody Can See Atoms: Science Camps Highlighting Approaches for Making Chemistry Accessible to Blind and Visually Impaired Students. Journal of Chemical Education, 2014, 91, 188-194.	1.1	29
116	Faster, Catalyst! React! React! Exploiting Computational Chemistry for Catalyst Development and Design. Accounts of Chemical Research, 2016, 49, 1079-1079.	7.6	29
117	Trapping a cross-linked lysineâ€“tryptophan radical in the catalytic cycle of the radical SAM enzyme SuiB. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	29
118	Inherent dynamical preferences in carbocation rearrangements leading to terpene natural products. Pure and Applied Chemistry, 2013, 85, 1949-1957.	0.9	28
119	The Viability of Nitroneâ€“Alkene (3 + 2) Cycloadditions in Alkaloid Biosynthesis. Journal of Organic Chemistry, 2014, 79, 432-435.	1.7	28
120	Origins of Diastereoselectivity in Lewis Acid Promoted Keteneâ€“Alkene [2 + 2] Cycloadditions. Organic Letters, 2014, 16, 5168-5171.	2.4	28
121	Nâ€“N Bond Formation between Primary Amines and Nitrosos: Direct Synthesis of 2-Substituted Indazolones with Mechanistic Insights. Organic Letters, 2018, 20, 4736-4739.	2.4	28
122	Questions in natural products synthesis research that can (and cannot) be answered using computational chemistry. Chemical Society Reviews, 2018, 47, 7845-7850.	18.7	28
123	Designing Reactions with Post-Transition-State Bifurcations: Asynchronous Nitrene Insertions into Câ€“C Ïƒ Bonds. CheM, 2019, 5, 227-236.	5.8	28
124	Exploiting the Potential of Meroterpenoid Cyclases to Expand the Chemical Space of Fungal Meroterpenoids. Angewandte Chemie - International Edition, 2020, 59, 23772-23781.	7.2	28
125	Prospecting for a 5-Center 4-Electron (C-Â-Â-H-Â-Â-C-Â-Â-H-Â-Â-C)+Bonding Array. Journal of the American Chemical Society, 2003, 125, 4042-4043.	6.6	27
126	Matching Active Site and Substrate Structures for an RNA Editing Reaction. Journal of the American Chemical Society, 2009, 131, 11882-11891.	6.6	27

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127	Enzyme Inhibition by Hydroamination: Design and Mechanism of a Hybrid Carmaphycin-Syringolin Enone Proteasome Inhibitor. Chemistry and Biology, 2014, 21, 782-791.	6.2	27
128	Catalyst-Controlled Regiodivergence in Rearrangements of Indole-Based Onium Ylides. Journal of the American Chemical Society, 2021, 143, 9016-9025.	6.6	27
129	Extended Barbaralanes:Â Sigmatropic Shiftamers or Ïƒ-Polyacenes?. Journal of the American Chemical Society, 2004, 126, 4256-4263.	6.6	26
130	Modes of inactivation of trichodiene synthase by a cyclopropane-containing farnesyldiphosphate analog. Organic and Biomolecular Chemistry, 2009, 7, 4101.	1.5	26
131	Structureâ€“Activity Relationships of Cyanoquinolines with Correctorâ€“Potentiator Activity in Î”F508 Cystic Fibrosis Transmembrane Conductance Regulator Protein. Journal of Medicinal Chemistry, 2012, 55, 1242-1251.	2.9	26
132	Predicting pathways for terpene formation from first principles â€“ routes to known and new sesquiterpenes. Chemical Science, 2014, 5, 1555.	3.7	26
133	Complicated Goings-On in the Metal-Manipulated Ring-Opening of Cyclobutene. Journal of the American Chemical Society, 2001, 123, 9855-9859.	6.6	25
134	Pentalenene formation mechanisms redux. Organic and Biomolecular Chemistry, 2014, 12, 887-894.	1.5	24
135	A detailed analysis of the mechanism of a carbocationic triple shift rearrangement. Physical Chemistry Chemical Physics, 2015, 17, 9771-9779.	1.3	24
136	Total Synthesis of the <i>Galbulimima</i> Alkaloids Himandravine and GB17 Using Biomimetic Dielsâ€“Alder Reactions of Double Diene Precursors. Journal of the American Chemical Society, 2015, 137, 11197-11204.	6.6	24
137	Dissecting a Dyotropic Rearrangement. Journal of Organic Chemistry, 2010, 75, 1693-1700.	1.7	23
138	Caryolene-forming carbocation rearrangements. Beilstein Journal of Organic Chemistry, 2013, 9, 323-331.	1.3	23
139	Accessing Multiple Classes of 2<i>H</i>-Indazoles: Mechanistic Implications for the Cadogan and Davisâ€“Beirut Reactions. Journal of the American Chemical Society, 2019, 141, 6247-6253.	6.6	23
140	Catalysis of decarboxylation by a preorganized heterogeneous microenvironment: crystal structures of abzyme 21D8 1 1Edited by D. Rees. Journal of Molecular Biology, 2000, 302, 1213-1225.	2.0	22
141	Catalysis on the coastline: Theozyme, molecular dynamics, and free energy perturbation analysis of antibody 21D8 catalysis of the decarboxylation of 5-nitro-3-carboxybenzisoxazole. Journal of Computational Chemistry, 2003, 24, 98-110.	1.5	22
142	Tetracoordinate Carbon as a Nucleophile? Interconversion of Carbenium Ions with Carbonium Ions Possessing Nearly Square-Pyramidal Pentacoordinate Carbons. Journal of Organic Chemistry, 2006, 71, 645-654.	1.7	22
143	Short Interfering RNA Guide Strand Modifiers from Computational Screening. Journal of the American Chemical Society, 2013, 135, 17069-17077.	6.6	22
144	Gold(I)-Catalyzed Formation of Bicyclo[4.2.0]oct-1-enes. Journal of Organic Chemistry, 2013, 78, 5685-5690.	1.7	22

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