

Dean J Tantillo

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335
papers

9,480
citations

48
h-index

80
g-index

403
ext. papers

10,773
ext. citations

8.1
avg, IF

6.94
L-index

#	Paper	IF	Citations
335	Computational prediction of ¹ H and ¹³ C chemical shifts: a useful tool for natural product, mechanistic, and synthetic organic chemistry. <i>Chemical Reviews</i> , 2012 , 112, 1839-62	68.1	809
334	Small molecule signaling agents: the integrated chemistry and biochemistry of nitrogen oxides, oxides of carbon, dioxygen, hydrogen sulfide, and their derived species. <i>Chemical Research in Toxicology</i> , 2012 , 25, 769-93	4	279
333	Redox chemistry and chemical biology of H ₂ S, hydropersulfides, and derived species: implications of their possible biological activity and utility. <i>Free Radical Biology and Medicine</i> , 2014 , 77, 82-94	7.8	271
332	Biosynthesis via carbocations: theoretical studies on terpene formation. <i>Natural Product Reports</i> , 2011 , 28, 1035-53	15.1	253
331	Theozymes and compozymes: theoretical models for biological catalysis. <i>Current Opinion in Chemical Biology</i> , 1998 , 2, 743-50	9.7	196
330	Total synthesis of oxidized welwitindolinones and (-)-N-methylwelwitindolinone C isonitrile. <i>Journal of the American Chemical Society</i> , 2012 , 134, 1396-9	16.4	136
329	The correct structure of aquatolide-experimental validation of a theoretically-predicted structural revision. <i>Journal of the American Chemical Society</i> , 2012 , 134, 18550-3	16.4	127
328	The carbocation continuum in terpene biosynthesis--where are the secondary cations?. <i>Chemical Society Reviews</i> , 2010 , 39, 2847-54	58.5	121
327	Recent excursions to the borderlands between the realms of concerted and stepwise: carbocation cascades in natural products biosynthesis. <i>Journal of Physical Organic Chemistry</i> , 2008 , 21, 561-570	2.1	118
326	Total synthesis and isolation of citrinalin and cyclopiamine congeners. <i>Nature</i> , 2014 , 509, 318-324	50.4	112
325	A gold-catalysed enantioselective Cope rearrangement of achiral 1,5-dienes. <i>Nature Chemistry</i> , 2012 , 4, 405-9	17.6	111
324	Theoretical studies on farnesyl cation cyclization: pathways to pentalenene. <i>Journal of the American Chemical Society</i> , 2006 , 128, 6172-9	16.4	105
323	Biosynthetic consequences of multiple sequential post-transition-state bifurcations. <i>Nature Chemistry</i> , 2014 , 6, 104-11	17.6	103
322	Consequences of conformational preorganization in sesquiterpene biosynthesis: theoretical studies on the formation of the bisabolene, curcumene, acoradiene, zizaene, cedrene, duprezianene, and sesquithuriferol sesquiterpenes. <i>Journal of the American Chemical Society</i> , 2009 , 131, 7999-8015	16.4	100
321	Acylammonium salts as dienophiles in Diels-Alder/lactonization organocascades. <i>Journal of the American Chemical Society</i> , 2014 , 136, 4492-5	16.4	97
320	Formation of the unusual semivolatile diterpene rhizathalene by the Arabidopsis class I terpene synthase TPS08 in the root stele is involved in defense against belowground herbivory. <i>Plant Cell</i> , 2013 , 25, 1108-25	11.6	95
319	Importance of Inherent Substrate Reactivity in Enzyme-Promoted Carbocation Cyclization/Rearrangements. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 10040-10045	16.4	93

318	Walking in the woods with quantum chemistry--applications of quantum chemical calculations in natural products research. <i>Natural Product Reports</i> , 2013 , 30, 1079-86	15.1	93
317	Post-transition state bifurcations gain momentum [Current state of the field. <i>Pure and Applied Chemistry</i> , 2017 , 89, 679-698	2.1	91
316	A potential energy surface bifurcation in terpene biosynthesis. <i>Nature Chemistry</i> , 2009 , 1, 384-9	17.6	91
315	Prediction of the structure of nobilisitine a using computed NMR chemical shifts. <i>Journal of Natural Products</i> , 2011 , 74, 1339-43	4.9	85
314	Unearthing a sesterterpene biosynthetic repertoire in the Brassicaceae through genome mining reveals convergent evolution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, E6005-E6014	11.5	81
313	Effect of isotopically sensitive branching on product distribution for pentalenene synthase: support for a mechanism predicted by quantum chemistry. <i>Journal of the American Chemical Society</i> , 2012 , 134, 11369-71	16.4	75
312	Differentiating mechanistic possibilities for the thermal, intramolecular [2 + 2] cycloaddition of allene-ynes. <i>Journal of the American Chemical Society</i> , 2010 , 132, 11952-66	16.4	73
311	Chemical Hermaphroditism: The Potential of the Cr(CO) ₃ Moiety To Stabilize Transition States and Intermediates with Anionic, Cationic, or Radical Character at the Benzylic Position. <i>Journal of the American Chemical Society</i> , 1999 , 121, 3596-3606	16.4	72
310	Formation of beyerene, kaurene, trachylobane, and atiserene diterpenes by rearrangements that avoid secondary carbocations. <i>Journal of the American Chemical Society</i> , 2010 , 132, 5375-86	16.4	67
309	Quantum chemical dissection of the classic terpinyl/pinyl/bornyl/camphyl cation conundrum-the role of pyrophosphate in manipulating pathways to monoterpenes. <i>Organic and Biomolecular Chemistry</i> , 2010 , 8, 4589-600	3.9	65
308	Dyotropic rearrangements of fused tricyclic lactones: application to the synthesis of (-)-curcumanolide A and (-)-curcumalactone. <i>Journal of the American Chemical Society</i> , 2012 , 134, 13348-56	16.4	64
307	The need for enzymatic steering in abietic acid biosynthesis: gas-phase chemical dynamics simulations of carbocation rearrangements on a bifurcating potential energy surface. <i>Journal of the American Chemical Society</i> , 2011 , 133, 8335-43	16.4	64
306	Which is more likely in trichodiene biosynthesis: hydride or proton transfer?. <i>Organic Letters</i> , 2006 , 8, 4601-4	6.2	64
305	The chemical biology of the persulfide (RSSH)/perthiyl (RSS [•]) redox couple and possible role in biological redox signaling. <i>Free Radical Biology and Medicine</i> , 2016 , 101, 20-31	7.8	64
304	The value of universally available raw NMR data for transparency, reproducibility, and integrity in natural product research. <i>Natural Product Reports</i> , 2019 , 36, 35-107	15.1	63
303	Pronounced steric effects of substituents in the nazarov cyclization of aryl dienyl ketones. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 6379-83	16.4	61
302	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
301	Brønsted acid catalyzed enantioselective indole aza-Claisen rearrangement mediated by an arene CH-O interaction. <i>Journal of the American Chemical Society</i> , 2013 , 135, 16380-3	16.4	60

- 300 Branching out from the bisabolyl cation. Unifying mechanistic pathways to barbatene, bazzanene, chamigrene, chamipinene, cumacrene, cuprenene, dunniene, isobazzanene, iso- β -bisabolene, isochamigrene, laurene, microbiotene, sesquithujene, sesquisabinene, thujopsene, trichodiene, and widdradiene sesquiterpenes. *Journal of the American Chemical Society*, **2014**, 136, 2450-63 16.4 58
- 299 Stereocontrol in a combined allylic azide rearrangement and intramolecular Schmidt reaction. *Journal of the American Chemical Society*, **2012**, 134, 6528-31 16.4 58
- 298 Metal promoted vinylcyclopropane-cyclopentene rearrangements: Reactions ripe for mechanism-based catalyst design. *Journal of Organometallic Chemistry*, **2006**, 691, 4386-4392 2.3 58
- 297 Mechanistic studies on the stereoselective formation of beta-mannosides from mannosyl iodides using alpha-deuterium kinetic isotope effects. *Journal of Organic Chemistry*, **2007**, 72, 4663-72 4.2 56
- 296 Computational studies on biosynthetic carbocation rearrangements leading to sativene, cyclosativene, alpha-ylangene, and beta-ylangene. *Journal of Organic Chemistry*, **2008**, 73, 6570-9 4.2 55
- 295 Multicomponent assembly of highly substituted indoles by dual palladium-catalyzed coupling reactions. *Angewandte Chemie - International Edition*, **2012**, 51, 10588-91 16.4 52
- 294 How cyclobutanes are assembled in nature--insights from quantum chemistry. *Chemical Society Reviews*, **2014**, 43, 5042-50 58.5 51
- 293 A cytochrome P450 serves as an unexpected terpene cyclase during fungal meroterpenoid biosynthesis. *Journal of the American Chemical Society*, **2013**, 135, 16805-8 16.4 51
- 292 Cryptic post-transition state bifurcations that reduce the efficiency of lactone-forming Rh-carbenoid C-H insertions. *Chemical Science*, **2017**, 8, 1442-1449 9.4 51
- 291 Heterocycle-heterocycle strategies: (2-nitrophenyl)isoxazole precursors to 4-aminoquinolines, 1H-indoles, and quinolin-4(1H)-ones. *Organic Letters*, **2013**, 15, 2062-5 6.2 50
- 290 They Came From the Deep: Syntheses, Applications, and Biology of Ladderanes. *Current Organic Chemistry*, **2006**, 10, 2055-2074 1.7 50
- 289 Perturbing the structure of the 2-norbornyl cation through C-H...N and C-H... π interactions. *Journal of Organic Chemistry*, **2007**, 72, 8877-81 4.2 49
- 288 Mechanism of the Ni(0)-catalyzed vinylcyclopropane-cyclopentene rearrangement. *Journal of Organic Chemistry*, **2009**, 74, 7822-33 4.2 48
- 287 Dynamic behavior of rearranging carbocations - implications for terpene biosynthesis. *Beilstein Journal of Organic Chemistry*, **2016**, 12, 377-90 2.5 48
- 286 Traversing Biosynthetic Carbocation Landscapes in the Total Synthesis of Andrastin and Terretonin Meroterpenes. *Angewandte Chemie - International Edition*, **2017**, 56, 12498-12502 16.4 47
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- 284 Mechanistic studies of copper(I)-catalyzed 1,3-halogen migration. *Journal of the American Chemical Society*, **2015**, 137, 5346-54 16.4 46
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281	A divergent approach to the synthesis of the yohimbinoid alkaloids venenatine and alstovenine. <i>Nature Chemistry</i> , 2013 , 5, 126-31	17.6	46
280	Transition-state complexation in palladium-promoted [3,3] sigmatropic shifts. <i>Journal of the American Chemical Society</i> , 2007 , 129, 8686-7	16.4	46
279	Applied Computational Chemistry for the Blind and Visually Impaired. <i>Journal of Chemical Education</i> , 2012 , 89, 1400-1404	2.4	45
278	Potent s-cis-locked bithiazole correctors of DeltaF508 cystic fibrosis transmembrane conductance regulator cellular processing for cystic fibrosis therapy. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 6044-54	8.3	45
277	Theoretical Studies on Pentadienyl Cation Electrocyclizations. <i>Current Organic Chemistry</i> , 2010 , 14, 1561-1577	15.77	44
276	Prediction of a new pathway to presilphiperfolanol. <i>Organic Letters</i> , 2008 , 10, 4827-30	6.2	44
275	Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1212-22	6.4	43
274	The taxadiene-forming carbocation cascade. <i>Journal of the American Chemical Society</i> , 2011 , 133, 18249-56	56.4	43
273	Theoretical studies on synthetic and biosynthetic oxidopyrylium-alkene cycloadditions: pericyclic pathways to intricarene. <i>Journal of Organic Chemistry</i> , 2008 , 73, 1516-23	4.2	43
272	Analogies between synthetic and biosynthetic reactions in which [1,2]-alkyl shifts are combined with other events: dyotropic, Schmidt, and carbocation rearrangements. <i>Journal of Organic Chemistry</i> , 2012 , 77, 8845-50	4.2	42
271	Hisotropic rearrangements: hybrids of electrocyclic and sigmatropic reactions. <i>Journal of Organic Chemistry</i> , 2006 , 71, 3686-95	4.2	42
270	Diverged Plant Terpene Synthases Reroute the Carbocation Cyclization Path towards the Formation of Unprecedented 6/11/5 and 6/6/7/5 Sesterterpene Scaffolds. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 1291-1295	16.4	42
269	Biological production of 2-butanone in Escherichia coli. <i>ChemSusChem</i> , 2014 , 7, 92-5	8.3	41
268	Mechanistic Insight into the Dehydro-Diels-Alder Reaction of Styrene-Ynes. <i>Journal of Organic Chemistry</i> , 2015 , 80, 11686-98	4.2	41
267	Fidelity in Hapten Design: How Analogous Are Phosphonate Haptens to the Transition States for Alkaline Hydrolyses of Aryl Esters?. <i>Journal of Organic Chemistry</i> , 1999 , 64, 3066-3076	4.2	41
266	Synthesis and Utility of Dihydropyridine Boronic Esters. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 2205-9	16.4	41
265	Switching between concerted and stepwise mechanisms for dyotropic rearrangements of lactones leading to spirocyclic, bridged butyrolactones. <i>Journal of Organic Chemistry</i> , 2011 , 76, 7167-74	4.2	40

- 264 Cation-Controlled Enantioselective and Diastereoselective Synthesis of Indolines: An Autoinductive Phase-Transfer Initiated 5-endo-trig Process. *Journal of the American Chemical Society*, **2015**, 137, 13414-24^{16.4} 39
- 263 A promiscuous proton in taxadiene biosynthesis?. *Organic Letters*, **2007**, 9, 1069-71 6.2 39
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- 261 Proton sandwiches: nonclassical carbocations with tetracoordinate protons. *Angewandte Chemie - International Edition*, **2005**, 44, 2719-2723 16.4 38
- 260 Blocking Deprotonation with Retention of Aromaticity in a Plant ent-Copalyl Diphosphate Synthase Leads to Product Rearrangement. *Angewandte Chemie - International Edition*, **2016**, 55, 634-8 16.4 38
- 259 C-H \cdots N Interactions as modulators of carbocation structure – Implications for terpene biosynthesis. *Chemical Science*, **2013**, 4, 2512 9.4 37
- 258 Mechanism of the acid-promoted intramolecular schmidt reaction: theoretical assessment of the importance of lone pair-cation, cation- π and steric effects in controlling regioselectivity. *Journal of Organic Chemistry*, **2012**, 77, 640-7 4.2 37
- 257 Multicenter bonding in organic chemistry. Geometry-sensitive 3c-2e bonding in (C...H...C) fragments of organic cations. *Journal of Organic Chemistry*, **2004**, 69, 2992-6 4.2 37
- 256 Navigating Past a Fork in the Road: Carbocation- π Interactions Can Manipulate Dynamic Behavior of Reactions Facing Post-Transition-State Bifurcations. *Journal of the American Chemical Society*, **2017**, 139, 7485-7493 16.4 36
- 255 The energetic viability of an unexpected skeletal rearrangement in cyclooctatin biosynthesis. *Organic and Biomolecular Chemistry*, **2015**, 13, 10273-8 3.9 34
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- 253 Trapping and Electron Paramagnetic Resonance Characterization of the 5'dAdo Radical in a Radical -Adenosyl Methionine Enzyme Reaction with a Non-Native Substrate. *ACS Central Science*, **2019**, 5, 1777-1785^{16.8} 33
- 252 The many roles of quantum chemical predictions in synthetic organic chemistry. *Chemistry - an Asian Journal*, **2014**, 9, 674-80 4.5 33
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- 250 Biosynthesis of lycosantalonal, a cis-prenyl derived diterpenoid. *Journal of the American Chemical Society*, **2014**, 136, 16951-3 16.4 32
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- 248 Toward Structural Correctness: Aquatolide and the Importance of 1D Proton NMR FID Archiving. *Journal of Organic Chemistry*, **2016**, 81, 878-89 4.2 31
- 247 Stereodivergent, Diels-Alder-initiated organocascades employing π -unsaturated acylammonium salts: scope, mechanism, and application. *Chemical Science*, **2017**, 8, 1511-1524 9.4 31

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245	Theoretical Studies on NG-Hydroxy-L-arginine and Derived Radicals: Implications for the Mechanism of Nitric Oxide Synthase. <i>Journal of the American Chemical Society</i> , 2000 , 122, 536-537	16.4	31
244	Cyclols Revisited: Facile Synthesis of Medium-Sized Cyclic Peptides. <i>Chemistry - A European Journal</i> , 2017 , 23, 13319-13322	4.8	30
243	Post-transition state bifurcations induce dynamical detours in Pummerer-like reactions. <i>Chemical Science</i> , 2018 , 9, 8937-8945	9.4	29
242	Theoretical and experimental analysis of the reaction mechanism of MrTPS2, a triquinane-forming sesquiterpene synthase from chamomile. <i>Chemistry - A European Journal</i> , 2013 , 19, 13590-600	4.8	28
241	Using theory and experiment to discover catalysts for electrocyclizations. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 31-2	16.4	28
240	A highly selective rearrangement of a housane-derived cation radical: an electrochemically mediated transformation. <i>Journal of Organic Chemistry</i> , 2007 , 72, 4351-7	4.2	28
239	Bedeutung der inhärenten Substratreaktivität bei enzymvermittelten Cyclisierungen/Umlagerungen von Carbokationen. <i>Angewandte Chemie</i> , 2017 , 129, 10172-10178	3.6	27
238	A Fluorescent Adenosine Analogue as a Substrate for an A-to-I RNA Editing Enzyme. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 8713-6	16.4	27
237	Modulation of inherent dynamical tendencies of the bisabolyl cation preorganization in -isozizaene synthase. <i>Chemical Science</i> , 2015 , 6, 2347-2353	9.4	27
236	Feasibility of intramolecular proton transfers in terpene biosynthesis--guiding principles. <i>Journal of the American Chemical Society</i> , 2015 , 137, 4134-40	16.4	26
235	Synthesis and Structure Revision of Dichrocephones A and B. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 2419-2422	16.4	26
234	The viability of nitron-alkene (3 + 2) cycloadditions in alkaloid biosynthesis. <i>Journal of Organic Chemistry</i> , 2014 , 79, 432-5	4.2	26
233	Inherent dynamical preferences in carbocation rearrangements leading to terpene natural products. <i>Pure and Applied Chemistry</i> , 2013 , 85, 1949-1957	2.1	26
232	Matching active site and substrate structures for an RNA editing reaction. <i>Journal of the American Chemical Society</i> , 2009 , 131, 11882-91	16.4	26
231	Lifetimes of carbocations encountered along reaction coordinates for terpene formation. <i>Chemical Science</i> , 2014 , 5, 3301	9.4	25
230	Prospecting for a 5-center 4-electron (C - - H - - C - - H - - C)+ bonding array. <i>Journal of the American Chemical Society</i> , 2003 , 125, 4042-3	16.4	25
229	Speeding Up Sigmatropic Shifts-To Halve or to Hold. <i>Accounts of Chemical Research</i> , 2016 , 49, 741-9	24.3	25

228	Product Rearrangement from Altering a Single Residue in the Rice syn-Copalyl Diphosphate Synthase. <i>Organic Letters</i> , 2016 , 18, 1060-3	6.2	24
227	Intramolecular Chirality Transfer [2 + 2] Cycloadditions of Allenolates and Alkenes. <i>Organic Letters</i> , 2017 , 19, 3703-3706	6.2	24
226	Modes of inactivation of trichodiene synthase by a cyclopropane-containing farnesyl diphosphate analog. <i>Organic and Biomolecular Chemistry</i> , 2009 , 7, 4101-9	3.9	24
225	Origins of diastereoselectivity in Lewis acid promoted ketene-alkene [2 + 2] cycloadditions. <i>Organic Letters</i> , 2014 , 16, 5168-71	6.2	23
224	Complicated goings-on in the metal-manipulated ring-opening of cyclobutene. <i>Journal of the American Chemical Society</i> , 2001 , 123, 9855-9	16.4	23
223	A detailed analysis of the mechanism of a carbocationic triple shift rearrangement. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 9771-9	3.6	22
222	Pentalene formation mechanisms redux. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 887-94	3.9	22
221	Predicting pathways for terpene formation from first principles ¶ routes to known and new sesquiterpenes. <i>Chemical Science</i> , 2014 , 5, 1555	9.4	22
220	Structure-activity relationships of cyanoquinolines with corrector-potentiator activity in β 508 cystic fibrosis transmembrane conductance regulator protein. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 1242-51	8.3	22
219	Caryolene-forming carbocation rearrangements. <i>Beilstein Journal of Organic Chemistry</i> , 2013 , 9, 323-31	2.5	22
218	Sigmatropic shiftamers: fluxionality in broken ladderane polymers. <i>Angewandte Chemie - International Edition</i> , 2002 , 41, 1033-6	16.4	22
217	Extended barbaralanes: sigmatropic shiftamers or sigma-polyacenes?. <i>Journal of the American Chemical Society</i> , 2004 , 126, 4256-63	16.4	22
216	Predicting Productive Binding Modes for Substrates and Carbocation Intermediates in Terpene Synthases-Bornyl Diphosphate Synthase as a Representative Case. <i>ACS Catalysis</i> , 2018 , 8, 3322-3330	13.1	21
215	Nobody Can See Atoms: Science Camps Highlighting Approaches for Making Chemistry Accessible to Blind and Visually Impaired Students. <i>Journal of Chemical Education</i> , 2014 , 91, 188-194	2.4	21
214	Identification and optimization of short helical peptides with novel reactive functionality as catalysts for acyl transfer by reactive tagging. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 1488-94	3.9	21
213	Carbocations and the Complex Flavor and Bouquet of Wine: Mechanistic Aspects of Terpene Biosynthesis in Wine Grapes. <i>Molecules</i> , 2015 , 20, 10781-92	4.8	21
212	Tetracoordinate carbon as a nucleophile? Interconversion of carbenium ions with carbonium ions possessing nearly square-pyramidal pentacoordinate carbons. <i>Journal of Organic Chemistry</i> , 2006 , 71, 645-54	4.2	21
211	Total Synthesis of the Galbulimima Alkaloids Himandravine and GB17 Using Biomimetic Diels-Alder Reactions of Double Diene Precursors. <i>Journal of the American Chemical Society</i> , 2015 , 137, 11197-204	16.4	20

210	Changes in charge distribution, molecular volume, accessible surface area and electronic structure along the reaction coordinate for a carbocationic triple shift rearrangement of relevance to diterpene biosynthesis. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 8902-9	2.8	20
209	Gold(I)-catalyzed formation of bicyclo[4.2.0]oct-1-enes. <i>Journal of Organic Chemistry</i> , 2013 , 78, 5685-90	4.2	20
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206	Fickle hexadienes. Manipulating the relative energies of chairlike and boatlike transition structures for the cope rearrangement. <i>Journal of Organic Chemistry</i> , 2002 , 67, 1419-26	4.2	20
205	Tension between Internal and External Modes of Stabilization in Carbocations Relevant to Terpene Biosynthesis: Modulating Minima Depth via C-H···π Interactions. <i>Organic Letters</i> , 2015 , 17, 5388-91	6.2	19
204	Enzyme inhibition by hydroamination: design and mechanism of a hybrid carmaphycin-syringolin enone proteasome inhibitor. <i>Chemistry and Biology</i> , 2014 , 21, 782-91		19
203	Short interfering RNA guide strand modifiers from computational screening. <i>Journal of the American Chemical Society</i> , 2013 , 135, 17069-77	16.4	19
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201	How an enzyme might accelerate an intramolecular Diels-Alder reaction: theozymes for the formation of salvileucalin B. <i>Organic Letters</i> , 2010 , 12, 1164-7	6.2	19
200	Selective stabilization of transition state structures for cope rearrangements of semibullvalene and barbaralane through interactions with halogens. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 7149-53	2.8	19
199	Breaking down barriers: the liaison between sigmatropic shifts, electrocyclic reactions, and three-center cations. <i>Angewandte Chemie - International Edition</i> , 2003 , 42, 5877-82	16.4	19
198	Enantioselective synthesis of isochromans and tetrahydroisoquinolines by C-H insertion of donor/donor carbenes. <i>Chemical Science</i> , 2020 , 11, 494-498	9.4	19
197	Accessing Multiple Classes of 2-H-Indazoles: Mechanistic Implications for the Cadogan and Davis-Beirut Reactions. <i>Journal of the American Chemical Society</i> , 2019 , 141, 6247-6253	16.4	18
196	Using H and C NMR chemical shifts to determine cyclic peptide conformations: a combined molecular dynamics and quantum mechanics approach. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 14003-14012	3.6	18
195	Questions in natural products synthesis research that can (and cannot) be answered using computational chemistry. <i>Chemical Society Reviews</i> , 2018 , 47, 7845-7850	58.5	18
194	Inhibition of myeloperoxidase: evaluation of 2H-indazoles and 1H-indazolones. <i>Bioorganic and Medicinal Chemistry</i> , 2014 , 22, 6422-9	3.4	18
193	Constrained bithiazoles: small molecule correctors of defective B508-CFTR protein trafficking. <i>Journal of Medicinal Chemistry</i> , 2014 , 57, 6729-38	8.3	18

192	Synthesis of substituted chromanones: an organocatalytic aldol/oxa-Michael reaction. <i>Organic Letters</i> , 2010 , 12, 3410-3	6.2	18
191	Cycloaddition/Ring opening reaction sequences of N-alkenyl aziridines: influence of the aziridine nitrogen on stereoselectivity. <i>Organic Letters</i> , 2008 , 10, 57-60	6.2	18
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