

Daniel A Singleton

List of Publications by Year in descending order

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114
papers

7,206
citations

43973

48
h-index

62479

80
g-index

124
all docs

124
docs citations

124
times ranked

4667
citing authors

#	ARTICLE	IF	CITATIONS
1	Energy Read-out as a Probe of Kinetically Hidden Transition States. <i>Organic Letters</i> , 2021, 23, 2174-2177.	2.4	6
2	Isotope Effects and the Mechanism of Photoredox-Promoted [2 + 2] Cycloadditions of Enones. <i>Journal of Organic Chemistry</i> , 2021, 86, 6305-6313.	1.7	8
3	Bond Memory in Dynamically Determined Stereoselectivity. <i>Journal of the American Chemical Society</i> , 2020, 142, 85-88.	6.6	10
4	Vibrationally Hot and Cold Triplets. Sensitizer-Dependent Dynamics and Localized Vibrational Promotion of a Di- π -methane Rearrangement. <i>Journal of the American Chemical Society</i> , 2020, 142, 19885-19888.	6.6	7
5	Solvation Dynamics and the Nature of Reaction Barriers and Ion-Pair Intermediates in Carbocation Reactions. <i>Journal of the American Chemical Society</i> , 2020, 142, 12865-12877.	6.6	34
6	Comment on "Activation of methane to CH ₃ ⁺ : A selective industrial route to methanesulfonic acid". <i>Science</i> , 2019, 364, .	6.0	8
7	Labelling and determination of the energy in reactive intermediates in solution enabled by energy-dependent reaction selectivity. <i>Nature Chemistry</i> , 2018, 10, 237-241.	6.6	25
8	Ir-Catalyzed ortho-Borylation of Phenols Directed by Substrate-Ligand Electrostatic Interactions: A Combined Experimental/in Silico Strategy for Optimizing Weak Interactions. <i>Journal of the American Chemical Society</i> , 2017, 139, 7864-7871.	6.6	131
9	Concert along the Edge: Dynamics and the Nature of the Border between General and Specific Acid-Base Catalysis. <i>Journal of the American Chemical Society</i> , 2017, 139, 5965-5972.	6.6	31
10	Failure and Redemption of Statistical and Nonstatistical Rate Theories in the Hydroboration of Alkenes. <i>Journal of the American Chemical Society</i> , 2017, 139, 15710-15723.	6.6	32
11	Mechanistic Studies of Formal Thioboration Reactions of Alkynes. <i>Journal of Organic Chemistry</i> , 2017, 82, 8165-8178.	1.7	24
12	Controlling Selectivity by Controlling Energy Partitioning in a Thermal Reaction in Solution. <i>Journal of the American Chemical Society</i> , 2016, 138, 14534-14537.	6.6	18
13	Dynamics and the Regiochemistry of Nitration of Toluene. <i>Journal of the American Chemical Society</i> , 2016, 138, 15167-15176.	6.6	65
14	Dynamically Complex [6+4] and [4+2] Cycloadditions in the Biosynthesis of Spinosyn A. <i>Journal of the American Chemical Society</i> , 2016, 138, 3631-3634.	6.6	116
15	A Case Study of the Mechanism of Alcohol-Mediated Morita Baylis-Hillman Reactions. The Importance of Experimental Observations. <i>Journal of the American Chemical Society</i> , 2015, 137, 3811-3826.	6.6	368
16	Controlling Selectivity by Controlling the Path of Trajectories. <i>Journal of the American Chemical Society</i> , 2015, 137, 14244-14247.	6.6	49
17	Isotope Effects, Dynamic Matching, and Solvent Dynamics in a Wittig Reaction. Betaines as Bypassed Intermediates. <i>Journal of the American Chemical Society</i> , 2014, 136, 13122-13125.	6.6	71
18	Dynamics and a Unified Understanding of Competitive [2,3]- and [1,2]-Sigmatropic Rearrangements Based on a Study of Ammonium Ylides. <i>Journal of the American Chemical Society</i> , 2014, 136, 3740-3743.	6.6	56

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19	Racing Carbon Atoms. Atomic Motion Reaction Coordinates and Structural Effects on Newtonian Kinetic Isotope Effects. <i>Organic Letters</i> , 2012, 14, 5238-5241.	2.4	16
20	Isotope Effects and Heavy-Atom Tunneling in the Roush Allylboration of Aldehydes. <i>Organic Letters</i> , 2012, 14, 2370-2373.	2.4	33
21	Outer-Sphere Direction in Iridium C-H Borylation. <i>Journal of the American Chemical Society</i> , 2012, 134, 11350-11353.	6.6	167
22	Entropic Intermediates and Hidden Rate-Limiting Steps in Seemingly Concerted Cycloadditions. Observation, Prediction, and Origin of an Isotope Effect on Recrossing. <i>Journal of the American Chemical Society</i> , 2012, 134, 1914-1917.	6.6	79
23	Dynamic Origin of the Stereoselectivity of a Nucleophilic Substitution Reaction. <i>Organic Letters</i> , 2012, 14, 2528-2531.	2.4	58
24	Isotope-Induced Desymmetrization Can Mimic Isotopic Perturbation of Equilibria. On the Symmetry of Bromonium Ions and Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 2011, 133, 17172-17175.	6.6	38
25	Competition between Reaction and Intramolecular Energy Redistribution in Solution: Observation and Nature of Nonstatistical Dynamics in the Ozonolysis of Vinyl Ethers. <i>Journal of the American Chemical Society</i> , 2011, 133, 13824-13827.	6.6	49
26	Isotope Effect, Mechanism, and Origin of Catalysis in the Decarboxylation of Mandelylthiamin. <i>Journal of the American Chemical Society</i> , 2010, 132, 6896-6897.	6.6	31
27	Experimental Evidence for Heavy-Atom Tunneling in the Ring-Opening of Cyclopropylcarbinyl Radical from Intramolecular ¹² C/ ¹³ C Kinetic Isotope Effects. <i>Journal of the American Chemical Society</i> , 2010, 132, 12548-12549.	6.6	84
28	Electronic effects in iridium C-H borylations: insights from unencumbered substrates and variation of boryl ligand substituents. <i>Chemical Communications</i> , 2010, 46, 7724.	2.2	104
29	Transition-State Geometry Measurements from ¹³ C Isotope Effects. The Experimental Transition State for the Epoxidation of Alkenes with Oxaziridines. <i>Journal of the American Chemical Society</i> , 2009, 131, 2397-2403.	6.6	49
30	Recrossing and Dynamic Matching Effects on Selectivity in a Diels-Alder Reaction. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 9156-9159.	7.2	101
31	Newtonian Kinetic Isotope Effects. Observation, Prediction, and Origin of Heavy-Atom Dynamic Isotope Effects. <i>Journal of the American Chemical Society</i> , 2009, 131, 8382-8383.	6.6	55
32	Dynamics and the Failure of Transition State Theory in Alkene Hydroboration. <i>Journal of the American Chemical Society</i> , 2009, 131, 3130-3131.	6.6	137
33	Control Elements in Dynamically Determined Selectivity on a Bifurcating Surface. <i>Journal of the American Chemical Society</i> , 2008, 130, 14544-14555.	6.6	142
34	Phenomenon of Optical Self-Purification of Chiral Non-Racemic Compounds. <i>Journal of the American Chemical Society</i> , 2007, 129, 12112-12113.	6.6	174
35	Insights into the Mechanism of Flavoprotein-Catalyzed Amine Oxidation from Nitrogen Isotope Effects on the Reaction of N-Methyltryptophan Oxidase. <i>Biochemistry</i> , 2007, 46, 7655-7664.	1.2	69
36	Isotope Effects and the Mechanism of Epoxidation of Cyclohexenone with tert-Butyl Hydroperoxide. <i>Journal of Organic Chemistry</i> , 2007, 72, 6183-6189.	1.7	24

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37	Dynamic Effects on the Periselectivity, Rate, Isotope Effects, and Mechanism of Cycloadditions of Ketenes with Cyclopentadiene. <i>Journal of the American Chemical Society</i> , 2006, 128, 7594-7607.	6.6	179
38	Isotope effects and the mechanism of fragmentation of epoxy imino-1,3,4-oxadiazolines. <i>Tetrahedron Letters</i> , 2005, 46, 819-822.	0.7	2
39	Isotope effects and the mechanism of palladium-catalyzed allylic alkylation. <i>Tetrahedron Letters</i> , 2005, 46, 1631-1634.	0.7	8
40	Isotope effects and the mechanism of deoxygenation of epoxides with dichlorocarbene. <i>Tetrahedron Letters</i> , 2005, 46, 2033-2036.	0.7	9
41	The Normal Range for Secondary Swain ² Schaad Exponents without Tunneling or Kinetic Complexity. <i>Journal of the American Chemical Society</i> , 2005, 127, 3294-3295.	6.6	35
42	Isotope Effects, Dynamics, and the Mechanism of Solvolysis of Aryldiazonium Cations in Water. <i>Journal of the American Chemical Society</i> , 2005, 127, 2888-2899.	6.6	39
43	Isotope Effects and the Nature of Enantioselectivity in the Shi Epoxidation. The Importance of Asynchronicity. <i>Journal of the American Chemical Society</i> , 2005, 127, 6679-6685.	6.6	71
44	Mechanism and Origin of Enantioselectivity in the Rh ₂ (OAc)(DPTI) ₃ -Catalyzed Cyclopropanation of Alkynes. <i>Journal of the American Chemical Society</i> , 2005, 127, 6190-6191.	6.6	54
45	Concerted Transition State, Stepwise Mechanism. Dynamics Effects in C ₂ -C ₆ Enyne Allene Cyclizations. <i>Journal of the American Chemical Society</i> , 2005, 127, 9216-9223.	6.6	129
46	Isotope Effects and the Nature of Stereo- and Regioselectivity in Hydroaminations of Vinylarenes Catalyzed by Palladium(II) ² Diphosphine Complexes. <i>Organic Letters</i> , 2004, 6, 2469-2472.	2.4	49
47	A Few Molecules Can Control the Enantiomeric Outcome. Evidence Supporting Absolute Asymmetric Synthesis Using the Soai Asymmetric Autocatalysis. <i>Organic Letters</i> , 2003, 5, 4337-4339.	2.4	114
48	A New Form of Kinetic Isotope Effect. Dynamic Effects on Isotopic Selectivity and Regioselectivity. <i>Journal of the American Chemical Society</i> , 2003, 125, 1176-1177.	6.6	100
49	Isotope Effects and the Nature of Selectivity in Rhodium-Catalyzed Cyclopropanations. <i>Journal of the American Chemical Society</i> , 2003, 125, 15902-15911.	6.6	142
50	Mechanism of Ene Reactions of Singlet Oxygen. A Two-Step No-Intermediate Mechanism. <i>Journal of the American Chemical Society</i> , 2003, 125, 1319-1328.	6.6	259
51	Exo-Selective Diels ² Alder Reactions of Vinylazepines. Origin of Divergent Stereoselectivity in Diels ² Alder Reactions of Vinylazepines, Vinylpiperideines, and Vinylcycloalkenes. <i>Journal of Organic Chemistry</i> , 2003, 68, 8991-8995.	1.7	22
52	Isotope Effects and the Mechanism of Atom Transfer Radical Polymerization. <i>Macromolecules</i> , 2003, 36, 8609-8616.	2.2	48
53	Isotope Effects and the Mechanism of an Electron-Transfer-Catalyzed Diels ² Alder Reaction. <i>Journal of the American Chemical Society</i> , 2002, 124, 11552-11559.	6.6	52
54	Mechanism and Origin of Stereoselectivity in Lewis Acid Catalyzed [2+2] Cycloadditions of Ketenes with Aldehydes. <i>Angewandte Chemie</i> , 2002, 114, 1642-1645.	1.6	4

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55	Mechanism and Origin of Stereoselectivity in Lewis Acid Catalyzed [2+2] Cycloadditions of Ketenes with Aldehydes. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1572-1575.	7.2	43
56	Enantioselective Synthesis without Discrete Optically Active Additives. <i>Journal of the American Chemical Society</i> , 2002, 124, 10010-10011.	6.6	112
57	Minimum Energy Structure of Hydridotris(pyrazolyl)borato Iridium(V) Tetrahydride Is Not a C _{3v} Capped Octahedron. <i>Journal of the American Chemical Society</i> , 2001, 123, 9822-9829.	6.6	20
58	Isotope effects and the distinction between synchronous, asynchronous, and stepwise Diels-Alder reactions. <i>Tetrahedron</i> , 2001, 57, 5149-5160.	1.0	87
59	¹³ C and ² H Kinetic Isotope Effects and the Mechanism of Lewis Acid-Catalyzed Ene Reactions of Formaldehyde. <i>Journal of Organic Chemistry</i> , 2000, 65, 895-899.	1.7	26
60	Isotope Effects and the Mechanism of Chlorotrimethylsilane-Mediated Addition of Cuprates to Enones. <i>Journal of the American Chemical Society</i> , 2000, 122, 3288-3295.	6.6	73
61	Isotope Effects and the Mechanism of Allylic Hydroxylation of Alkenes with Selenium Dioxide. <i>Journal of Organic Chemistry</i> , 2000, 65, 7554-7560.	1.7	48
62	Resolution of Conflicting Mechanistic Observations in Ester Aminolysis. A Warning on the Qualitative Prediction of Isotope Effects for Reactive Intermediates. <i>Journal of the American Chemical Society</i> , 2000, 122, 11035-11036.	6.6	48
63	¹³ C Kinetic Isotope Effects and the Mechanism of the Uncatalyzed Decarboxylation of Orotic Acid. <i>Journal of the American Chemical Society</i> , 2000, 122, 3296-3300.	6.6	46
64	Separation of the primary and secondary kinetic isotope effects at a reactive center using starting material reactivities. Application to the FeCl ₃ -Catalyzed oxidation of C-H bonds with tert-butyl hydroperoxide. <i>Tetrahedron Letters</i> , 1999, 40, 3847-3850.	0.7	15
65	Isotope effects for Lewis acid catalyzed Diels-Alder reactions. The experimental transition state. <i>Tetrahedron Letters</i> , 1999, 40, 5817-5821.	0.7	36
66	Isotope effects and the experimental transition state for a prototypical thermal ene reaction. <i>Tetrahedron Letters</i> , 1999, 40, 8939-8943.	0.7	16
67	Stereochemical labeling at natural abundance. Stereochemistry, isotope effects, and mechanism of the Diels-Alder reaction of hexachlorocyclopentadiene with ethyl vinyl ether. <i>Tetrahedron Letters</i> , 1999, 40, 639-642.	0.7	9
68	Reinvestigation of the Isotope Effects for the Claisen and Aromatic Claisen Rearrangements: The Nature of the Claisen Transition States. <i>Journal of the American Chemical Society</i> , 1999, 121, 10865-10874.	6.6	126
69	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.	6.6	77
70	Carbometalations of Simple Alkenes with Allyldibromoborane. <i>Organic Letters</i> , 1999, 1, 485-486.	2.4	17
71	Isotope Effects and the Mechanism of Triazolinedione Ene Reactions. Aziridinium Imides Are Innocent Bystanders. <i>Journal of the American Chemical Society</i> , 1999, 121, 11885-11893.	6.6	42
72	¹³ C and ² H Kinetic Isotope Effects and the Mechanism of Bromination of 1-Pentene under Synthetic Conditions. <i>Organic Letters</i> , 1999, 1, 327-330.	2.4	4

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73	Nonlinear Effects in Kinetic Resolutions. <i>Journal of the American Chemical Society</i> , 1999, 121, 9307-9312.	6.6	57
74	Simultaneous Determination of Intermolecular and Intramolecular ¹³ C and ² H Kinetic Isotope Effects at Natural Abundance. <i>Journal of the American Chemical Society</i> , 1999, 121, 9455-9456.	6.6	76
75	Evidence for a Concerted Mechanism in a Palladium Trimethylenemethane Cycloaddition. <i>Journal of the American Chemical Society</i> , 1999, 121, 9313-9317.	6.6	39
76	Deuterium Kinetic Isotope Effects and the Mechanism of the Bacterial Luciferase Reaction. <i>Biochemistry</i> , 1998, 37, 2596-2606.	1.2	38
77	¹³ C Kinetic Isotope Effects for the Addition of Lithium Dibutylcuprate to Cyclohexenone. Reductive Elimination Is Rate-Determining. <i>Journal of the American Chemical Society</i> , 1997, 119, 3383-3384.	6.6	105
78	Cycloalkenylboranes as Highly Reactive and Selective Diels-Alder Dienophiles. A Simple Synthesis of Bridgehead Bicyclic Alcohols. <i>Journal of Organic Chemistry</i> , 1997, 62, 2255-2258.	1.7	30
79	Experimental Geometry of the Epoxidation Transition State. <i>Journal of the American Chemical Society</i> , 1997, 119, 3385-3386.	6.6	158
80	Reactions of Alkynyl dihaloboranes with 1,3-Dienes. 1,4-Alkynylborations and Stepwise Diels-Alder Reactions. <i>Journal of Organic Chemistry</i> , 1997, 62, 1955-1960.	1.7	36
81	Experimental and Theoretical Kinetic Isotope Effects for Asymmetric Dihydroxylation. Evidence Supporting a Rate-Limiting [3+2] Cycloaddition. <i>Journal of the American Chemical Society</i> , 1997, 119, 9907-9908.	6.6	238
82	In situ formation of alkenyl- and alkynylboranes for Diels-Alder reactions by boron-silicon exchange with alkenyl- and alkynylsilanes. <i>Journal of Organometallic Chemistry</i> , 1997, 544, 157-161.	0.8	27
83	Catalysis by temporary covalent activation. A novel catalysis of unactivated Diels-Alder reactions. <i>Tetrahedron Letters</i> , 1997, 38, 3163-3166.	0.7	15
84	Vinylboranes as diels-Alder Dienophiles. <i>Advances in Cycloaddition</i> , 1997, , 121-148.	0.5	8
85	Allylboration of Alkenes with Allyl dihaloboranes. <i>Journal of the American Chemical Society</i> , 1996, 118, 9986-9987.	6.6	37
86	Synchronous or Asynchronous? An Experimental Transition State from a Direct Comparison of Experimental and Theoretical Kinetic Isotope Effects for a Diels-Alder Reaction. <i>Journal of the American Chemical Society</i> , 1996, 118, 9984-9985.	6.6	147
87	Intramolecular Diels-Alder reactions of vinylboranes. A highly stereoselective two-step decalin synthesis. <i>Tetrahedron Letters</i> , 1995, 36, 3473-3476.	0.7	27
88	High-Precision Simultaneous Determination of Multiple Small Kinetic Isotope Effects at Natural Abundance. <i>Journal of the American Chemical Society</i> , 1995, 117, 9357-9358.	6.6	358
89	A conjunctive diquinane synthesis using a free-radical catalyzed intramolecular [3 + 2] methylenecyclopentane annulation. <i>Tetrahedron Letters</i> , 1994, 35, 689-690.	0.7	16
90	Vinylboranes as trans-dihydroxyethylene equivalents for diels-alder reactions. <i>Tetrahedron Letters</i> , 1994, 35, 509-512.	0.7	45

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91	Versatile [3 + 2] methylenecyclopentane annulations of unactivated and electron-rich olefins with [(trimethylsilyl)methylene]cyclopropanedicarboxylates. <i>Journal of Organic Chemistry</i> , 1994, 59, 2020-2024.	1.7	52
92	Direct free-radical substitutions on allyl and vinyl halides using alkyl halides/hexabutyliditin. <i>Tetrahedron Letters</i> , 1993, 34, 3041-3042.	0.7	46
93	Diels-Alder reactions of 2-Alkenylboranes and cis-1-alkenylboranes. Anomalous selectivity that allows a choice of regiochemistry. <i>Tetrahedron Letters</i> , 1993, 34, 3071-3074.	0.7	29
94	In situ formation of vinylboranes for use in Diels Alder reactions. An easy one-pot Diels-Alder synthesis of cyclohexenols. <i>Journal of Organic Chemistry</i> , 1992, 57, 5768-5771.	1.7	54
95	A [4 + 3] transition state for a [4 + 2] cycloaddition. A new secondary orbital interaction in Diels-Alder reactions. <i>Journal of the American Chemical Society</i> , 1992, 114, 6563-6564.	6.6	61
96	Silyl group-transfer-mediated serial Michael additions. <i>Journal of Organic Chemistry</i> , 1992, 57, 1733-1740.	1.7	43
97	An unprecedented electronic preference for the "meta" product in Diels-Alder reactions of ethynyldialkylboranes. [(Trimethylsilyl)ethynyl]-9-BBN as a reactive and versatile dienophile. <i>Journal of Organic Chemistry</i> , 1992, 57, 4796-4797.	1.7	52
98	Tuning of Vinylborane Dienophilicity. Optimization of Reactivity, Regioselectivity, endo-Stereoselectivity, and Reagent Stability. <i>Tetrahedron</i> , 1992, 48, 5831-5838.	1.0	49
99	Vinylboranes are omniphilic dienophiles. Some unusual and useful properties of vinylboranes in diels-alder reactions. <i>Tetrahedron Letters</i> , 1992, 33, 1017-1020.	0.7	37
100	The unsymmetrical 1,1,3,3-tetramethylallyl cation. <i>Journal of the American Chemical Society</i> , 1991, 113, 6271-6272.	6.6	8
101	2-Trimethylsilylvinylboranes: highly reactive and selective diels-alder equivalents of 2-trimethylsilylvinyl alcohol and acetylene. <i>Tetrahedron Letters</i> , 1991, 32, 7365-7368.	0.7	46
102	Methylenecyclopropanedicarboxylates and -dicarboxylates, efficient reagents for the [3 + 2] methylenecyclopentane annulation of unactivated and electron-rich alkenes. <i>Tetrahedron Letters</i> , 1991, 32, 5765-5768.	0.7	37
103	Catalytic stereocontrol of a radical cyclization. <i>Tetrahedron Letters</i> , 1990, 31, 5551-5554.	0.7	42
104	High reactivity, regioselectivity, and endo-stereoselectivity of vinyl boranes in Diels-Alder reactions. <i>Journal of the American Chemical Society</i> , 1990, 112, 7423-7424.	6.6	75
105	[3 + 2] Methylenecyclopentane annulations of unactivated and electron-rich olefins with 2-(phenylsulfonyl)-1-methylenecyclopropanes. <i>Journal of Organic Chemistry</i> , 1990, 55, 4780-4782.	1.7	59
106	Acrolein acetals as allyl cation precursors in the ionic Diels-Alder reaction. <i>Journal of the American Chemical Society</i> , 1987, 109, 2182-2184.	6.6	86
107	Propargyl cations " powerful ambient temperature dienophiles in the diels-lder reaction. <i>Tetrahedron Letters</i> , 1987, 28, 5969-5972.	0.7	14
108	Control of regiospecificity in ionic Diels-Alder reactions. The use of allylic alcohols and allylic ethers as precursors of dienophilic allyl cations. <i>Journal of Organic Chemistry</i> , 1986, 51, 3075-3076.	1.7	37

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109	Chemical reaction of polychlorinated biphenyls on soils with poly(ethylene glycol)/KOH. Chemosphere, 1985, 14, 173-181.	4.2	22
110	Reaction removal of polychlorinated biphenyls from transformer oil: treatment of contaminated oil with poly(ethylene glycol)/potassium hydroxide. Environmental Science & Technology, 1985, 19, 740-746.	4.6	38
111	N-alkyl-4-(N,N-dialkylamino)pyridinium salts: thermally stable phase transfer catalysts for nucleophilic aromatic displacement. Tetrahedron Letters, 1984, 25, 3383-3386.	0.7	38
112	Acid-catalyzed intramolecular "Diels-Alder" reactions. The cycloaddition of allyl cations to 1,3-dienes. Journal of the American Chemical Society, 1984, 106, 6085-6086.	6.6	64
113	Distinction between aminium cation radical and protic acid catalyzed Diels-Alder reactions. Journal of the American Chemical Society, 1984, 106, 7993-7994.	6.6	97
114	Destruction/removal of polychlorinated biphenyls from non-polar media. Reaction of PCB with poly(ethylene glycol)/KOH. Chemosphere, 1983, 12, 183-196.	4.2	33