Jonathan M Goodman

List of Publications by Year in Descending Order

183 papers	7,682 citations	47 h-index	81 g-index
227 ext. papers	8,555 ext. citations	5.6 avg, IF	6.4 L-index

#	Paper	IF	Citations
183	The DP5 probability, quantification and visualisation of structural uncertainty in single molecules.. *Chemical Science*, **2022**, 13, 3507-3518	9.4	2
182	Towards Quantifying the Uncertainty in In Silico Predictions using Bayesian Learning. *Computational Toxicology*, **2022**, 100228	3.1	
181	-Triflylphosphoramides: highly acidic catalysts for asymmetric transformations. *Organic and Biomolecular Chemistry*, **2021**, 19, 9565-9618	3.9	1
180	CATMoS: Collaborative Acute Toxicity Modeling Suite. *Environmental Health Perspectives*, **2021**, 129, 47013	8.4	14
179	InChI version 1.06: now more than 99.99% reliable. *Journal of Cheminformatics*, **2021**, 13, 40	8.6	4
178	Machine Learning in Predictive Toxicology: Recent Applications and Future Directions for Classification Models. *Chemical Research in Toxicology*, **2021**, 34, 217-239	4	14
177	VRAI-selectivity: calculation of selectivity beyond transition state theory. *Organic and Biomolecular Chemistry*, **2021**, 19, 3940-3947	3.9	2
176	Mechanistically driven identification of novel structural alerts for mitochondrial toxicity. *Computational Toxicology*, **2021**, 20, 100183	3.1	
175	Confidence in Inactive and Active Predictions from Structural Alerts. *Chemical Research in Toxicology*, **2020**, 33, 3010-3022	4	3
174	Synergism of anisotropic and computational NMR methods reveals the likely configuration of phormidolide A. *Chemical Communications*, **2020**, 56, 7565-7568	5.8	13
173	In Silico Guidance for In Vitro Androgen and Glucocorticoid Receptor ToxCast Assays. *Environmental Science & Technology*, **2020**, 54, 7461-7470	10.3	2
172	DP4-AI automated NMR data analysis: straight from spectrometer to structure. *Chemical Science*, **2020**, 11, 4351-4359	9.4	51
171	Charge-assisted phosph(v)azane anion receptors. *Dalton Transactions*, **2020**, 49, 3403-3407	4.3	2
170	Neural network activation similarity: a new measure to assist decision making in chemical toxicology. *Chemical Science*, **2020**, 11, 7335-7348	9.4	10
169	Rapid Route-Finding for Bifurcating Organic Reactions. *Journal of the American Chemical Society*, **2020**, 142, 9210-9219	16.4	16
168	Structural Alerts and Random Forest Models in a Consensus Approach for Receptor Binding Molecular Initiating Events. *Chemical Research in Toxicology*, **2020**, 33, 388-401	4	10
167	A Computational and Experimental Investigation of the Origin of Selectivity in the Chiral Phosphoric Acid Catalyzed Enantioselective Minisci Reaction. *Journal of the American Chemical Society*, **2020**, 142, 21091-21101	16.4	17

166	Quantitative Predictions for Molecular Initiating Events Using Three-Dimensional Quantitative Structure-Activity Relationships. *Chemical Research in Toxicology*, **2020**, 33, 324-332	4	9
165	BINOPtimal: a web tool for optimal chiral phosphoric acid catalyst selection. *Chemical Communications*, **2019**, 55, 1778-1781	5.8	4
164	The optimal DFT approach in DP4 NMR structure analysis - pushing the limits of relative configuration elucidation. *Organic and Biomolecular Chemistry*, **2019**, 17, 5886-5890	3.9	27
163	Guest Binding via N-H???Bonding and Kinetic Entrapment by an Inorganic Macrocycle. *Angewandte Chemie - International Edition*, **2019**, 58, 10655-10659	16.4	8
162	Guest Binding via NH???Bonding and Kinetic Entrapment by an Inorganic Macrocycle. *Angewandte Chemie*, **2019**, 131, 10765-10769	3.6	5
161	Reaction Prediction and Synthesis Design **2018**, 86-105		2
160	A synthesis-enabled relative stereochemical assignment of the C1-C28 region of hemicalide. *Chemical Communications*, **2018**, 54, 3247-3250	5.8	17
159	Using 2D Structural Alerts to Define Chemical Categories for Molecular Initiating Events. *Toxicological Sciences*, **2018**, 165, 213-223	4.4	20
158	International chemical identifier for reactions (RInChI). *Journal of Cheminformatics*, **2018**, 10, 22	8.6	19
157	Using Transition State Modeling To Predict Mutagenicity for Michael Acceptors. *Journal of Chemical Information and Modeling*, **2018**, 58, 1266-1271	6.1	12
156	A possible extension to the RInChI as a means of providing machine readable process data. *Journal of Cheminformatics*, **2017**, 9, 23	8.6	5
155	Doubling the power of DP4 for computational structure elucidation. *Organic and Biomolecular Chemistry*, **2017**, 15, 8998-9007	3.9	44
154	Transfer hydrogenation of ortho-hydroxybenzophenone ketimines catalysed by BINOL-derived phosphoric acid occurs by a 14-membered bifunctional transition structure. *Organic and Biomolecular Chemistry*, **2017**, 15, 6943-6947	3.9	12
153	Selecting Chiral BINOL-Derived Phosphoric Acid Catalysts: General Model To Identify Steric Features Essential for Enantioselectivity. *Chemistry - A European Journal*, **2017**, 23, 14248-14260	4.8	47
152	()-Selective Takai olefination of salicylaldehydes. *Beilstein Journal of Organic Chemistry*, **2017**, 13, 323-328	2.5	3
151	A History of the Molecular Initiating Event. *Chemical Research in Toxicology*, **2016**, 29, 2060-2070	4	34
150	Goldilocks Catalysts: Computational Insights into the Role of the 3,3Substituents on the Selectivity of BINOL-Derived Phosphoric Acid Catalysts. *Journal of the American Chemical Society*, **2016**, 138, 7910-7	16.4	54
149	Toward the stereochemical assignment and synthesis of hemicalide: DP4f GIAO-NMR analysis and synthesis of a reassigned C16-C28 subunit. *Chemical Communications*, **2016**, 52, 4632-5	5.8	24

148	Expanding DP4: application to drug compounds and automation. *Organic and Biomolecular Chemistry*, **2016**, 14, 3943-9	3.9	30
147	A Practical Guide for Predicting the Stereochemistry of Bifunctional Phosphoric Acid Catalyzed Reactions of Imines. *Accounts of Chemical Research*, **2016**, 49, 1029-41	24.3	102
146	Using Molecular Initiating Events To Generate 2D Structure-Activity Relationships for Toxicity Screening. *Chemical Research in Toxicology*, **2016**, 29, 1611-1627	4	12
145	The most reactive amide as a transition-state mimic for cis-trans interconversion. *Journal of the American Chemical Society*, **2015**, 137, 926-30	16.4	56
144	Dial-a-molecule workshop: computational prediction of reaction outcomes and optimum synthetic routes. *Chemistry Central Journal*, **2015**, 9,		3
143	Mechanistic insights into a BINOL-derived phosphoric acid-catalyzed asymmetric Pictet-Spengler reaction. *Journal of Organic Chemistry*, **2015**, 80, 2634-40	4.2	47
142	Asymmetric boronate addition to o-quinone methides: ligand exchange, solvent effects, and Lewis acid catalysis. *Journal of Organic Chemistry*, **2015**, 80, 2056-61	4.2	28
141	Base-mediated cascade rearrangements of aryl-substituted diallyl ethers. *Journal of Organic Chemistry*, **2015**, 80, 1472-98	4.2	16
140	Synthesis of 2,3-O-benzyl-ribose and xylose and their equilibration. *Tetrahedron: Asymmetry*, **2014**, 25, 1424-1429		2
139	Defining molecular initiating events in the adverse outcome pathway framework for risk assessment. *Chemical Research in Toxicology*, **2014**, 27, 2100-12	4	109
138	Lewis acid catalysis and ligand exchange in the asymmetric binaphthol-catalyzed propargylation of ketones. *Journal of Organic Chemistry*, **2013**, 78, 8796-801	4.2	22
137	Reversal of facial selectivity in a thia-Claisen rearrangement by incorporation of a vinylic bromine substituent. *Organic and Biomolecular Chemistry*, **2013**, 11, 7530-9	3.9	4
136	The formation of high-purity isocyanurate through proazaphosphatrane-catalysed isocyanate cyclo-trimerisation: computational insights. *Organic and Biomolecular Chemistry*, **2013**, 11, 90-7	3.9	20
135	Understanding the mechanism of the asymmetric propargylation of aldehydes promoted by 1,1′-bi-2-naphthol-derived catalysts. *Journal of the American Chemical Society*, **2013**, 135, 6142-8	16.4	81
134	Organocatalytic domino reaction of cyanosulfones: access to complex cyclohexane systems with quaternary carbon centers. *Organic Letters*, **2013**, 15, 1386-9	6.2	28
133	International chemical identifier for reactions (RInChI). *Journal of Cheminformatics*, **2013**, 5, 45	8.6	17
132	1,3-Dipolar cycloaddition of nitrones with phenylvinyl sulfone. An experimental and theoretical study. *Tetrahedron: Asymmetry*, **2012**, 23, 76-85		12
131	Mechanism of amination of α-keto esters by azadicarboxylates catalyzed by an axially chiral guanidine: acyclic keto esters react through an E enolate. *Journal of the American Chemical Society*, **2012**, 134, 16869-76	16.4	27

130	Hydrogen-bond stabilization in oxyanion holes: grand jet to three dimensions. *Organic and Biomolecular Chemistry*, **2012**, 10, 1905-13	3.9	29
129	Mechanistic insights into the BINOL-derived phosphoric acid-catalyzed asymmetric allylboration of aldehydes. *Journal of the American Chemical Society*, **2012**, 134, 2716-22	16.4	139
128	In Silico Inspired Total Synthesis of (-)-Dolabriferol. *Angewandte Chemie*, **2012**, 124, 4773-4775	3.6	2
127	In silico inspired total synthesis of (-)-dolabriferol. *Angewandte Chemie - International Edition*, **2012**, 51, 4695-7	16.4	15
126	The molecular basis for selective inhibition of unconventional mRNA splicing by an IRE1-binding small molecule. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, E869-78	11.5	360
125	A model for the enantioselectivity of imine reactions catalyzed by BINOL-phosphoric acid catalysts. *Journal of Organic Chemistry*, **2011**, 76, 1775-88	4.2	133
124	How reliable are DFT transition structures? Comparison of GGA, hybrid-meta-GGA and meta-GGA functionals. *Organic and Biomolecular Chemistry*, **2011**, 9, 689-700	3.9	186
123	Structure-activity studies of the pelorusides: new congeners and semi-synthetic analogues. *Organic and Biomolecular Chemistry*, **2011**, 9, 4456-66	3.9	19
122	Self-assembly of trehalose molecules on a lysozyme surface: the broken glass hypothesis. *Physical Chemistry Chemical Physics*, **2011**, 13, 2294-9	3.6	45
121	Synthetic and computational studies on the tricarboxylate core of 6,7-dideoxysqualestatin H5 involving a carbonyl ylide cycloaddition-rearrangement. *Organic and Biomolecular Chemistry*, **2010**, 8, 3975-84	3.9	15
120	Enzyme catalysis by hydrogen bonds: the balance between transition state binding and substrate binding in oxyanion holes. *Journal of Organic Chemistry*, **2010**, 75, 1831-40	4.2	86
119	DFT study on the factors determining the enantioselectivity of Friedel-Crafts reactions of indole with N-acyl and N-tosylimines catalyzed by BINOL-phosphoric acid derivatives. *Journal of Organic Chemistry*, **2010**, 75, 589-97	4.2	95
118	Assigning stereochemistry to single diastereoisomers by GIAO NMR calculation: the DP4 probability. *Journal of the American Chemical Society*, **2010**, 132, 12946-59	16.4	524
117	The stereochemical assignment of acyclic polyols: a computational study of the NMR data of a library of stereopentad sequences from polyketide natural products. *Tetrahedron*, **2010**, 66, 6437-6444	2.4	20
116	Proline-catalyzed aldol reactions of cyclic diketones: fluorine modifies pathways as well as transition states. *Tetrahedron*, **2010**, 66, 8021-8028	2.4	10
115	The regioselective photochemical rearrangement of alpha-[PN(t)Bu](4). *Chemical Communications*, **2009**, 6637-9	5.8	9
114	A route to enantiomerically pure 5-(2?-hydroxyethyl)cyclopent-2-en-1-ol and its absolute configuration by Mosher esters. *Tetrahedron: Asymmetry*, **2009**, 20, 449-456		6
113	Conformational changes of trialanine in sodium halide solutions: An in silico study. *Journal of Molecular Liquids*, **2009**, 147, 117-123	6	11

112	Mechanistic insights into the catalytic asymmetric allylboration of ketones: Brønsted or Lewis acid activation?. *Organic Letters*, **2009**, 11, 37-40	6.2	37
111	Computer Software Review: Reaxys. *Journal of Chemical Information and Modeling*, **2009**, 49, 2897-2898	6.1	47
110	Mechanism of BINOL--phosphoric acid-catalyzed strecker reaction of benzyl imines. *Journal of the American Chemical Society*, **2009**, 131, 4070-7	16.4	94
109	Synthetic studies on siphonariid polypropionates: synthesis and isomerization of the caloundrin B trioxaadamantane ring system. *Organic Letters*, **2009**, 11, 1373-6	6.2	16
108	Findings of the challenge to predict aqueous solubility. *Journal of Chemical Information and Modeling*, **2009**, 49, 1-5	6.1	91
107	The effect of sodium chloride on poly-l-glutamate conformation. *Chemical Communications*, **2009**, 896-8	5.8	25
106	Joining the crown family; the tetrameric, O-bridged macrocycle [{P(micro-N(t)Bu)}2(micro-O)]4. *Dalton Transactions*, **2009**, 1293-6	4.3	25
105	To switch or not to switch: the effects of potassium and sodium ions on alpha-poly-L-glutamate conformations in aqueous solutions. *Journal of the American Chemical Society*, **2009**, 131, 10854-6	16.4	50
104	Assigning the stereochemistry of pairs of diastereoisomers using GIAO NMR shift calculation. *Journal of Organic Chemistry*, **2009**, 74, 4597-607	4.2	191
103	Hydrogen bonding and pi-stacking: how reliable are force fields? A critical evaluation of force field descriptions of nonbonded interactions. *Journal of Chemical Information and Modeling*, **2009**, 49, 944-55	6.1	146
102	What is the mechanism of amine conjugate additions to pyrazole crotonate catalyzed by thiourea catalysts?. *Organic and Biomolecular Chemistry*, **2009**, 7, 483-7	3.9	20
101	Polymorph control: past, present and future. *Drug Discovery Today*, **2008**, 13, 198-210	8.8	247
100	Dynamic combinatorial discovery of a [2]-catenane and its guest-induced conversion into a molecular square host. *Journal of the American Chemical Society*, **2008**, 130, 10834-5	16.4	70
99	Theoretical study of the mechanism of hantzsch ester hydrogenation of imines catalyzed by chiral BINOL-phosphoric acids. *Journal of the American Chemical Society*, **2008**, 130, 8741-7	16.4	257
98	Predicting intrinsic aqueous solubility by a thermodynamic cycle. *Molecular Pharmaceutics*, **2008**, 5, 266-79	5.6	91
97	Solubility challenge: can you predict solubilities of 32 molecules using a database of 100 reliable measurements?. *Journal of Chemical Information and Modeling*, **2008**, 48, 1289-303	6.1	142
96	Stereostructure assignment of flexible five-membered rings by GIAO 13C NMR calculations: prediction of the stereochemistry of elatenyne. *Journal of Organic Chemistry*, **2008**, 73, 4053-62	4.2	75
95	Enantiopure 2-substituted glyceraldehyde derivatives by aza-Claisen rearrangement or C-alkylation of enamines. *Organic Letters*, **2008**, 10, 4537-40	6.2	7

94	Concomitant Hydrate Polymorphism in the Precipitation of Sparfloxacin from Aqueous Solution. *Crystal Growth and Design*, **2008**, 8, 114-118	3.5	23
93	Theoretical study of the asymmetric conjugate alkenylation of enones catalyzed by binaphthols. *Journal of Organic Chemistry*, **2008**, 73, 5078-89	4.2	48
92	1,5-anti stereocontrol in the boron-mediated aldol reactions of beta-alkoxy methyl ketones: the role of the formyl hydrogen bond. *Journal of Organic Chemistry*, **2008**, 73, 1253-63	4.2	60
91	Enantioselectivity in the boron aldol reactions of methyl ketones. *Chemical Communications*, **2007**, 2124-6	3.8	28
90	Diclofenac solubility: independent determination of the intrinsic solubility of three crystal forms. *Journal of Medicinal Chemistry*, **2007**, 50, 979-83	8.3	96
89	Exploration of the accessible chemical space of acyclic alkanes. *Journal of Chemical Information and Modeling*, **2007**, 47, 2124-32	6.1	11
88	Structural, solid-state NMR and theoretical studies of the inverse-coordination of lithium chloride using group 13 phosphide hosts. *Chemistry - A European Journal*, **2007**, 13, 1251-60	4.8	13
87	A new method for the reproducible generation of polymorphs: two forms of sulindac with very different solubilities. *Journal of Applied Crystallography*, **2007**, 40, 379-381	3.8	35
86	Computational assessment of synthetic procedures. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 351-7	4.2	5
85	The effect of haem in red and processed meat on the endogenous formation of N-nitroso compounds in the upper gastrointestinal tract. *Carcinogenesis*, **2007**, 28, 685-90	4.6	66
84	Solvent effects and hydration of a tripeptide in sodium halide aqueous solutions: an in silico study. *Physical Chemistry Chemical Physics*, **2007**, 9, 5423-35	3.6	34
83	The mechanism of TBD-catalyzed ring-opening polymerization of cyclic esters. *Journal of Organic Chemistry*, **2007**, 72, 9656-62	4.2	154
82	Solvent Effects and Conformational Stability of a Tripeptide. *Lecture Notes in Computer Science*, **2006**, 141-149	0.9	1
81	Asymmetric conjugate addition of alkynylboronates to enones: rationale for the intriguing catalysis exerted by binaphthols. *Journal of the American Chemical Society*, **2006**, 128, 3116-7	16.4	53
80	Understanding the origins of remote asymmetric induction in the boron aldol reactions of beta-alkoxy methyl ketones. *Organic Letters*, **2006**, 8, 4299-302	6.2	65
79	The ROBIA program for predicting organic reactivity. *Journal of Chemical Information and Modeling*, **2006**, 46, 606-14	6.1	28
78	Amodiaquinium dichloride dihydrate from laboratory powder diffraction data. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, o4196-o4199		13
77	Selection of the cis and trans phosph(III)azane macrocycles [{P(mu-NtBu)}2(1-Y-2-NH-C6H4)]2(Y=O, S). *Dalton Transactions*, **2005**, 1764-73	4.3	26

76	Intramolecular general acid catalysis of phosphate transfer. nucleophilic attack by oxyanions on the PO3 2- group. *Journal of the American Chemical Society*, **2005**, 127, 7033-40	16.4	41
75	What is the smallest saturated acyclic alkane that cannot be made?. *Journal of Chemical Information and Modeling*, **2005**, 45, 81-7	6.1	27
74	ROBIA: a reaction prediction program. *Organic Letters*, **2005**, 7, 3541-4	6.2	46
73	Aziridinium ring opening: a simple ionic reaction pathway with sequential transition states. *Tetrahedron Letters*, **2005**, 46, 2067-2069	2	14
72	Computational evaluation of asymmetric Diels Alder reactions of vinylboranes with chiral dienes. *Tetrahedron Letters*, **2005**, 46, 2461-2464	2	3
71	Computer-assisted design of asymmetric 1,3-dipolar cycloadditions between dimethylvinylborane and chiral nitrones. *Tetrahedron*, **2005**, 61, 10886-10893	2.4	6
70	Sulfonium ylide epoxidation reactions: methylene transfer. *Chemical Communications*, **2004**, 1076-7	5.8	23
69	A promising enantioselective Diels-Alder dienophile by computer-assisted rational design: 2,5-diphenyl-1-vinyl-borolane. *Journal of Computer-Aided Molecular Design*, **2004**, 18, 209-14	4.2	9
68	Selection of a pentameric host in the host-guest complexes [[[[P(mu-NtBu)]2(mu-NH)]5].I]-[Li(thf)4]+ and [[[P(mu-NtBu)]2(mu-NH)]5].HBr.THF. *Chemistry - A European Journal*, **2004**, 10, 6066-72	4.8	50
67	Chemistry on the world-wide-web: a ten year experiment. *Organic and Biomolecular Chemistry*, **2004**, 2, 3222-5	3.9	2
66	Chemical documents: machine understanding and automated information extraction. *Organic and Biomolecular Chemistry*, **2004**, 2, 3294-300	3.9	19
65	Theoretical study on the selectivity of asymmetric sulfur ylide epoxidation reaction. *Organic Letters*, **2004**, 6, 2559-62	6.2	38
64	Investigation of conjugate addition/intramolecular nitrone dipolar cycloadditions and their use in the synthesis of dendrobatid alkaloid precursors. *Organic and Biomolecular Chemistry*, **2004**, 2, 1258-65	3.9	27
63	Experimental data checker: better information for organic chemists. *Organic and Biomolecular Chemistry*, **2004**, 2, 3067-70	3.9	14
62	QRC: a rapid method for connecting transition structures to reactants in the computational analysis of organic reactivity. *Tetrahedron Letters*, **2003**, 44, 8233-8236	2	35
61	Controlling neighbouring group participation from thioacetals. *Tetrahedron Letters*, **2003**, 44, 2841-2844	2	13
60	A DFT study on the regioselectivity of the reaction of dichloropropynylborane with isoprene. *Journal of Organic Chemistry*, **2003**, 68, 4059-66	4.2	26
59	How Accurate is the Steady State Approximation?. *Journal of Chemical Education*, **2003**, 80, 839	2.4	1

58	A tricycloheptane product in cationic rearrangements. *Organic and Biomolecular Chemistry*, **2003**, 1, 3570-1	3.9	3
57	Stereochemical elucidation of the 1,4 polyketide amphidinoketide I. *Chemical Communications*, **2003**, 2616-7	5.8	10
56	Rotavap simulation and the estimation of boiling points. *Chemical Communications*, **2003**, 2654-5	5.8	
55	Diels-Alder reactions of vinylboranes: A computational study on the boron substituent effects. *Arkivoc*, **2003**, 2003, 556-565	0.9	21
54	Nitrone cyclisations: the development of a semi-quantitative model from ab initio calculations. *Tetrahedron*, **2002**, 58, 3667-3671	2.4	24
53	A highly enantioselective one-pot sulfur ylide epoxidation reaction. *Tetrahedron Letters*, **2002**, 43, 5427-5430	2	49
52	Sulfide□BF3□OEt2 mediated Baylis□Hillman reactions. *Tetrahedron Letters*, **2002**, 43, 8219-8222	2	44
51	A theoretical study of the reaction of alkynylboranes with butadiene: competition between cycloaddition and alkynylboration. *Journal of Organic Chemistry*, **2002**, 67, 8203-9	4.2	20
50	Gas phase versus solution chemistry: on the reversal of regiochemistry of methylation of sp2- and sp3-nitrogens. *Tetrahedron Letters*, **2001**, 42, 6949-6952	2	14
49	Studies on the formation of a tricyclic C2-symmetric sulfide. *Tetrahedron Letters*, **2001**, 42, 7091-7093	2	12
48	The stereochemistry of glabrescol. *Tetrahedron Letters*, **2001**, 42, 7477-7479	2	11
47	10-Helical conformations in oxetane □amino acid hexamers. *Tetrahedron Letters*, **2001**, 42, 4251-4255	2	106
46	Novel inhibitors of Leishmanial dihydrofolate reductase. *Bioorganic and Medicinal Chemistry Letters*, **2001**, 11, 977-80	2.9	41
45	Site-specific examination of secondary structure and orientation determination in membrane proteins: the peptidic (13)C=(18)O group as a novel infrared probe. *Biopolymers*, **2001**, 59, 396-401	2.2	96
44	Stereocontrol in a one-pot procedure for anionic oxy-Cope rearrangement followed by intramolecular aldol reaction. *Journal of the Chemical Society, Perkin Transactions 1*, **2001**, 1051-1061		6
43	Theoretical evaluation of the origin of the regio- and stereoselectivity in the Diels-Alder reactions of dialkylvinylboranes: studies on the reactions of vinylborane, dimethylvinylborane, and vinyl-9-BBN with trans-piperylene and isoprene. *Journal of the American Chemical Society*, **2001**, 123, 8832-7	16.4	35
42	A double ring closing metathesis reaction in the rapid, enantioselective synthesis of NK-1 receptor antagonists. *Organic Letters*, **2001**, 3, 671-4	6.2	61
41	Site-specific examination of secondary structure and orientation determination in membrane proteins: The peptidic 13C?18O group as a novel infrared probe **2001**, 59, 396		5

40	Some calculations for organic chemists: boiling point variation, Boltzmann factors and the Eyring equation. *Tetrahedron Letters*, **2000**, 41, 9879-9882	2	27
39	Solutions for chemistry: synthesis of experiment and calculation. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2000**, 358, 387-398	3	1
38	On the Need for Multiple Lists of Chemical Information. *Molecules*, **2000**, 5, 33-36	4.8	
37	Interactive analysis of selectivity in kinetic resolutions. *Tetrahedron Letters*, **1999**, 40, 8715-8718	2	33
36	Synthesis and post-assembly modification of some functionalised, neutral □-associated [2]catenanes. *New Journal of Chemistry*, **1999**, 23, 897-903	3.6	35
35	How Do Approximations Affect the Solutions to Kinetic Equations?. *Journal of Chemical Education*, **1999**, 76, 275	2.4	2
34	Design, synthesis, and evaluation of inhibitors of trypanosomal and leishmanial dihydrofolate reductase. *Journal of Medicinal Chemistry*, **1999**, 42, 4300-12	8.3	75
33	An Experimental and Theoretical Study of a Bicyclic Acetal Equilibrium. *Organic Letters*, **1999**, 1, 473-476	6.2	7
32	Genetic Algorithms in Conformational Analysis. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 317-320		47
31	Stereoselective Synthesis of 1-Hydroxymethyl-4-phenylsulfonylbutadienes. *Synlett*, **1998**, 1998, 1361-1363	2.2	3
30	What Is the Longest Unbranched Alkane with a Linear Global Minimum Conformation?. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 876-878		44
29	Conformational preferences of R1R2CO□H2BF complexes. *Chemical Communications*, **1997**, 2383-2384	5.8	20
28	Medium ring lactams in molecular recognition. *Materials Science and Engineering C*, **1996**, 4, 59-62	8.3	3
27	Eadfrith: a molecular rendering program for Silicon Graphics workstations. *Journal of Molecular Graphics*, **1996**, 14, 59-61, 91		
26	The rational design and systematic analysis of asymmetric aldol reactions using enol borinates: Applications of transition state computer modelling. *Tetrahedron: Asymmetry*, **1995**, 6, 2613-2636		57
25	Mechanistic insights from ab initio calculations on a nitrogen analogue of the boron-mediated aldol reaction. *Tetrahedron*, **1995**, 51, 4853-4866	2.4	10
24	On the configuration and conformation of oxyallyls in medium and large rings. *Tetrahedron Letters*, **1995**, 36, 7757-7760	2	9
23	The case for content integrity in electronic chemistry journals: The CLIC project. *New Review of Information Networking*, **1995**, 1, 61-69	0.5	1

22	Seven-Membered Lactams as Constraints for Amide Self-Recognition. *Journal of the American Chemical Society*, **1995**, 117, 9768-9769	16.4	23
21	Computer-assisted design of chiral boron enolates: The role of ate complexes in determining aldol stereoselectivity.. *Tetrahedron*, **1994**, 50, 1227-1242	2.4	15
20	A configurational model for siphonariid polypropionates derived from structural and biosynthetic considerations. *Tetrahedron Letters*, **1994**, 35, 6929-6932	2	28
19	MM2 force field parameters for compounds containing the diazoketone function. *Journal of the Chemical Society Perkin Transactions II*, **1994**, 109		16
18	Electrostatic Complementarity in Protein-Substrate Interactions and Ligand Design. *NATO ASI Series Series B: Physics*, **1994**, 373-380		
17	Molecular Mechanics: Problems and Potential **1994**, 53-88		
16	Origins of stereoselectivity in the addition of chiral allyl- and crotylboranes to aldehydes: the development and application of a force field model of the transition state. *Journal of Organic Chemistry*, **1993**, 58, 1711-1718	4.2	24
15	Origins of □face selectivity in the aldol reactions of chiral E-enol borinates: a computational study using transition state modelling.. *Tetrahedron*, **1993**, 49, 685-696	2.4	35
14	The rational design of highly stereoselective boron enolates using transition-state computer modeling: a novel, asymmetric anti aldol reaction for ketones. *Journal of Organic Chemistry*, **1992**, 57, 5173-5177	4.2	41
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