Jonathan M Goodman

List of Publications by Citations

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	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
182	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
181	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
180	Polymorph control: past, present and future. *Drug Discovery Today*, **2008**, 13, 198-210	8.8	247
179	Enantio- and diastereoselective aldol reactions of achiral ethyl and methyl ketones with aldehydes: the use of enol diisopinocampheylborinates. *Tetrahedron*, **1990**, 46, 4663-4684	2.4	231
178	An unbounded systematic search of conformational space. *Journal of Computational Chemistry*, **1991**, 12, 1110-1117	3.5	221
177	Assigning the stereochemistry of pairs of diastereoisomers using GIAO NMR shift calculation. *Journal of Organic Chemistry*, **2009**, 74, 4597-607	4.2	191
176	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
175	The mechanism of TBD-catalyzed ring-opening polymerization of cyclic esters. *Journal of Organic Chemistry*, **2007**, 72, 9656-62	4.2	154
174	Aldol reactions in polypropionate synthesis: High □face selectivity of enol borinates from □chiral methyl and ethyl ketones under substrate control. *Tetrahedron Letters*, **1989**, 30, 7121-7124	2	148
173	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
172	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
171	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
170	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
169	Defining molecular initiating events in the adverse outcome pathway framework for risk assessment. *Chemical Research in Toxicology*, **2014**, 27, 2100-12	4	109
168	10-Helical conformations in oxetane □amino acid hexamers. *Tetrahedron Letters*, **2001**, 42, 4251-4255	2	106
167	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

166	Diclofenac solubility: independent determination of the intrinsic solubility of three crystal forms. *Journal of Medicinal Chemistry*, **2007**, 50, 979-83	8.3	96
165	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
164	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
163	Mechanism of BINOL--phosphoric acid-catalyzed strecker reaction of benzyl imines. *Journal of the American Chemical Society*, **2009**, 131, 4070-7	16.4	94
162	Findings of the challenge to predict aqueous solubility. *Journal of Chemical Information and Modeling*, **2009**, 49, 1-5	6.1	91
161	Predicting intrinsic aqueous solubility by a thermodynamic cycle. *Molecular Pharmaceutics*, **2008**, 5, 266-79	5.6	91
160	Aldol reactions of methylketones using chiral boron reagents: A reversal in aldehyde enantioface selectivity. *Tetrahedron Letters*, **1989**, 30, 997-1000	2	91
159	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
158	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
157	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
156	Design, synthesis, and evaluation of inhibitors of trypanosomal and leishmanial dihydrofolate reductase. *Journal of Medicinal Chemistry*, **1999**, 42, 4300-12	8.3	75
155	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
154	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
153	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
152	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
151	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
150	Transition-state modeling of the aldol reaction of boron enolates: a force field approach. *Journal of Organic Chemistry*, **1990**, 55, 3576-3581	4.2	59
149	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

148	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
147	Goldilocks Catalysts: Computational Insights into the Role of the 3,3'-Substituents on the Selectivity of BINOL-Derived Phosphoric Acid Catalysts. *Journal of the American Chemical Society*, **2016**, 138, 7910-7	16.4	54
146	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
145	DP4-AI automated NMR data analysis: straight from spectrometer to structure. *Chemical Science*, **2020**, 11, 4351-4359	9.4	51
144	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
143	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
142	A highly enantioselective one-pot sulfur ylide epoxidation reaction. *Tetrahedron Letters*, **2002**, 43, 5427-5430	2	49
141	Theoretical study of the asymmetric conjugate alkenylation of enones catalyzed by binaphthols. *Journal of Organic Chemistry*, **2008**, 73, 5078-89	4.2	48
140	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
139	Mechanistic insights into a BINOL-derived phosphoric acid-catalyzed asymmetric Pictet-Spengler reaction. *Journal of Organic Chemistry*, **2015**, 80, 2634-40	4.2	47
138	Computer Software Review: Reaxys. *Journal of Chemical Information and Modeling*, **2009**, 49, 2897-2898	6.1	47
137	Genetic Algorithms in Conformational Analysis. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 317-320		47
136	ROBIA: a reaction prediction program. *Organic Letters*, **2005**, 7, 3541-4	6.2	46
135	Self-assembly of trehalose molecules on a lysozyme surface: the broken glass hypothesis. *Physical Chemistry Chemical Physics*, **2011**, 13, 2294-9	3.6	45
134	Doubling the power of DP4 for computational structure elucidation. *Organic and Biomolecular Chemistry*, **2017**, 15, 8998-9007	3.9	44
133	What Is the Longest Unbranched Alkane with a Linear Global Minimum Conformation?. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 876-878		44
132	Sulfide–BF3·OEt2 mediated Baylis–Hillman reactions. *Tetrahedron Letters*, **2002**, 43, 8219-8222	2	44
131	Diastereofacial selectivity in the aldol reactions of chiral α-methyl aldehydes: a computer modelling approach.. *Tetrahedron*, **1992**, 48, 4439-4458	2.4	44

130	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
129	Novel inhibitors of Leishmanial dihydrofolate reductase. *Bioorganic and Medicinal Chemistry Letters*, **2001**, 11, 977-80	2.9	41
128	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
127	Theoretical study on the selectivity of asymmetric sulfur ylide epoxidation reaction. *Organic Letters* , **2004**, 6, 2559-62	6.2	38
126	Origins of stereoselectivity in chiral boron enolate aldol reactions: A computational study using transition state modellings. *Tetrahedron*, **1991**, 47, 3471-3484	2.4	38
125	Mechanistic insights into the catalytic asymmetric allylboration of ketones: Brønsted or Lewis acid activation?. *Organic Letters*, **2009**, 11, 37-40	6.2	37
124	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
123	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
122	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
121	Synthesis and post-assembly modification of some functionalised, neutral □-associated [2]catenanes. *New Journal of Chemistry*, **1999**, 23, 897-903	3.6	35
120	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
119	A History of the Molecular Initiating Event. *Chemical Research in Toxicology*, **2016**, 29, 2060-2070	4	34
118	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
117	Interactive analysis of selectivity in kinetic resolutions. *Tetrahedron Letters*, **1999**, 40, 8715-8718	2	33
116	Theoretical studies of aldol stereoselectivity: the development of a force field model for enol borinates and the investigation of chiral enolate .pi.-face selectivity. *Journal of Organic Chemistry*, **1990**, 55, 3295-3303	4.2	33
115	Expanding DP4: application to drug compounds and automation. *Organic and Biomolecular Chemistry*, **2016**, 14, 3943-9	3.9	30
114	Hydrogen-bond stabilization in oxyanion holes: grand jeté to three dimensions. *Organic and Biomolecular Chemistry*, **2012**, 10, 1905-13	3.9	29
113	Organocatalytic domino reaction of cyanosulfones: access to complex cyclohexane systems with quaternary carbon centers. *Organic Letters*, **2013**, 15, 1386-9	6.2	28

112	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
111	Enantioselectivity in the boron aldol reactions of methyl ketones. *Chemical Communications*, **2007**, 2124-6	5.8	28
110	The ROBIA program for predicting organic reactivity. *Journal of Chemical Information and Modeling*, **2006**, 46, 606-14	6.1	28
109	A configurational model for siphonariid polypropionates derived from structural and biosynthetic considerations. *Tetrahedron Letters*, **1994**, 35, 6929-6932	2	28
108	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
107	Mechanism of amination of Eketo 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
106	What is the smallest saturated acyclic alkane that cannot be made?. *Journal of Chemical Information and Modeling*, **2005**, 45, 81-7	6.1	27
105	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
104	Some calculations for organic chemists: boiling point variation, Boltzmann factors and the Eyring equation. *Tetrahedron Letters*, **2000**, 41, 9879-9882	2	27
103	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
102	A DFT study on the regioselectivity of the reaction of dichloropropynylborane with isoprene. *Journal of Organic Chemistry*, **2003**, 68, 4059-66	4.2	26
101	Enolisation of ketones by dialkylboron chlorides and trifiates: A model for the effect of reagent leaving group substrate structure and amine base.. *Tetrahedron Letters*, **1992**, 33, 7223-7226	2	26
100	The effect of sodium chloride on poly-l-glutamate conformation. *Chemical Communications*, **2009**, 896-8	5.8	25
99	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
98	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
97	Nitrone cyclisations: the development of a semi-quantitative model from ab initio calculations. *Tetrahedron*, **2002**, 58, 3667-3671	2.4	24
96	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
95	Concomitant Hydrate Polymorphism in the Precipitation of Sparfloxacin from Aqueous Solution. *Crystal Growth and Design*, **2008**, 8, 114-118	3.5	23

94	Sulfonium ylide epoxidation reactions: methylene transfer. *Chemical Communications*, **2004**, 1076-7	5.8	23
93	Seven-Membered Lactams as Constraints for Amide Self-Recognition. *Journal of the American Chemical Society*, **1995**, 117, 9768-9769	16.4	23
92	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
91	Molecular orbital calculations on R1R2C?O□H2BF complexes: Anomeric stabilisation and conformational preferences.. *Tetrahedron Letters*, **1992**, 33, 7219-7222	2	21
90	Diels-Alder reactions of vinylboranes: A computational study on the boron substituent effects. *Arkivoc*, **2003**, 2003, 556-565	0.9	21
89	Using 2D Structural Alerts to Define Chemical Categories for Molecular Initiating Events. *Toxicological Sciences*, **2018**, 165, 213-223	4.4	20
88	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
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86	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
85	Conformational preferences of R1R2CO□H2BF complexes. *Chemical Communications*, **1997**, 2383-2384	5.8	20
84	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
83	International chemical identifier for reactions (RInChI). *Journal of Cheminformatics*, **2018**, 10, 22	8.6	19
82	Structure-activity studies of the pelorusides: new congeners and semi-synthetic analogues. *Organic and Biomolecular Chemistry*, **2011**, 9, 4456-66	3.9	19
81	Chemical documents: machine understanding and automated information extraction. *Organic and Biomolecular Chemistry*, **2004**, 2, 3294-300	3.9	19
80	A synthesis-enabled relative stereochemical assignment of the C1-C28 region of hemicalide. *Chemical Communications*, **2018**, 54, 3247-3250	5.8	17
79	International chemical identifier for reactions (RInChI). *Journal of Cheminformatics*, **2013**, 5, 45	8.6	17
78	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
77	Rapid Route-Finding for Bifurcating Organic Reactions. *Journal of the American Chemical Society*, **2020**, 142, 9210-9219	16.4	16

76	Base-mediated cascade rearrangements of aryl-substituted diallyl ethers. *Journal of Organic Chemistry*, **2015**, 80, 1472-98	4.2	16
75	Synthetic studies on siphonariid polypropionates: synthesis and isomerization of the caloundrin B trioxaadamantane ring system. *Organic Letters*, **2009**, 11, 1373-6	6.2	16
74	MM2 force field parameters for compounds containing the diazoketone function. *Journal of the Chemical Society Perkin Transactions II*, **1994**, 109		16
73	In silico inspired total synthesis of (-)-dolabriferol. *Angewandte Chemie - International Edition*, **2012**, 51, 4695-7	16.4	15
72	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
71	Computer-assisted design of chiral boron enolates: The role of ate complexes in determining aldol stereoselectivity.. *Tetrahedron*, **1994**, 50, 1227-1242	2.4	15
70	Experimental data checker: better information for organic chemists. *Organic and Biomolecular Chemistry*, **2004**, 2, 3067-70	3.9	14
69	Aziridinium ring opening: a simple ionic reaction pathway with sequential transition states. *Tetrahedron Letters*, **2005**, 46, 2067-2069	2	14
68	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
67	CATMoS: Collaborative Acute Toxicity Modeling Suite. *Environmental Health Perspectives*, **2021**, 129, 47013	8.4	14
66	Machine Learning in Predictive Toxicology: Recent Applications and Future Directions for Classification Models. *Chemical Research in Toxicology*, **2021**, 34, 217-239	4	14
65	Synergism of anisotropic and computational NMR methods reveals the likely configuration of phormidolide A. *Chemical Communications*, **2020**, 56, 7565-7568	5.8	13
64	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
63	Amodiaquinium dichloride dihydrate from laboratory powder diffraction data. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, o4196-o4199		13
62	Controlling neighbouring group participation from thioacetals. *Tetrahedron Letters*, **2003**, 44, 2841-2844	2	13
61	1,3-Dipolar cycloaddition of nitrones with phenylvinyl sulfone. An experimental and theoretical study. *Tetrahedron: Asymmetry*, **2012**, 23, 76-85		12
60	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
59	Studies on the formation of a tricyclic C2-symmetric sulfide. *Tetrahedron Letters*, **2001**, 42, 7091-7093	2	12

58	Using Molecular Initiating Events To Generate 2D Structure-Activity Relationships for Toxicity Screening. *Chemical Research in Toxicology*, **2016**, 29, 1611-1627	4	12
57	Using Transition State Modeling To Predict Mutagenicity for Michael Acceptors. *Journal of Chemical Information and Modeling*, **2018**, 58, 1266-1271	6.1	12
56	Conformational changes of trialanine in sodium halide solutions: An in silico study. *Journal of Molecular Liquids*, **2009**, 147, 117-123	6	11
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53	Developing a force field for the transition state of the aldol reaction of enolborinates: Evaluation of the use of fixed point charges.. *Tetrahedron*, **1992**, 48, 4183-4192	2.4	11
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51	Proline-catalyzed aldol reactions of cyclic diketones: fluorine modifies pathways as well as transition states. *Tetrahedron*, **2010**, 66, 8021-8028	2.4	10
50	Stereochemical elucidation of the 1,4 polyketide amphidinoketide I. *Chemical Communications*, **2003**, 2616-7	5.8	10
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48	A force field model for boron enolates. *Tetrahedron Letters*, **1987**, 28, 5209-5212	2	10
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43	Ligand atom partial charges assignment for complementary electrostatic potentials. *Journal of Computer-Aided Molecular Design*, **1992**, 6, 461-74	4.2	9
42	Quantitative Predictions for Molecular Initiating Events Using Three-Dimensional Quantitative Structure-Activity Relationships. *Chemical Research in Toxicology*, **2020**, 33, 324-332	4	9
41	Guest Binding via N-H???Bonding and Kinetic Entrapment by an Inorganic Macrocycle. *Angewandte Chemie - International Edition*, **2019**, 58, 10655-10659	16.4	8

40	Enantiopure 2-substituted glyceraldehyde derivatives by aza-Claisen rearrangement or C-alkylation of enamines. *Organic Letters*, **2008**, 10, 4537-40	6.2	7
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38	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
37	Computer-assisted design of asymmetric 1,3-dipolar cycloadditions between dimethylvinylborane and chiral nitrones. *Tetrahedron*, **2005**, 61, 10886-10893	2.4	6
36	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
35	A possible extension to the RInChI as a means of providing machine readable process data. *Journal of Cheminformatics*, **2017**, 9, 23	8.6	5
34	Guest Binding via NH???Bonding and Kinetic Entrapment by an Inorganic Macrocycle. *Angewandte Chemie*, **2019**, 131, 10765-10769	3.6	5
33	Computational assessment of synthetic procedures. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 351-7	4.2	5
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30	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
29	InChI version 1.06: now more than 99.99% reliable. *Journal of Cheminformatics*, **2021**, 13, 40	8.6	4
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27	()-Selective Takai olefination of salicylaldehydes. *Beilstein Journal of Organic Chemistry*, **2017**, 13, 323-328	2.5	3
26	Dial-a-molecule workshop: computational prediction of reaction outcomes and optimum synthetic routes. *Chemistry Central Journal*, **2015**, 9,		3
25	A tricycloheptane product in cationic rearrangements. *Organic and Biomolecular Chemistry*, **2003**, 1, 3570-1	3.9	3
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19	Reaction Prediction and Synthesis Design **2018**, 86-105		2
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