

Raghavan B Sunoj

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

160 papers	5,334 citations	43 h-index	62 g-index
176 ext. papers	5,974 ext. citations	7.1 avg, IF	6.35 L-index

#	Paper	IF	Citations
160	Molecular insights into chirality transfer from double axially chiral phosphoric acid in a synergistic enantioselective intramolecular amination.. <i>Chemical Science</i> , 2022 , 13, 1323-1334	9.4	4
159	Machine learning studies on asymmetric relay Heck reaction-Potential avenues for reaction development.. <i>Journal of Chemical Physics</i> , 2022 , 156, 114303	3.9	2
158	Iridium-Catalyzed Regioselective Borylation through C-H Activation and the Origin of Ligand-Dependent Regioselectivity Switching. <i>Journal of Organic Chemistry</i> , 2021 , 86, 15618-15630	4.2	0
157	Tale of the Breslow intermediate, a central player in N-heterocyclic carbene organocatalysis: then and now. <i>Chemical Science</i> , 2021 , 12, 7973-7992	9.4	21
156	On the question of steric repulsion versus noncovalent attractive interactions in chiral phosphoric acid catalyzed asymmetric reactions. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 18936-18950	3.6	2
155	Pd-Catalyzed π (sp)-H Fluorination of Free Amines. <i>Journal of the American Chemical Society</i> , 2020 , 142, 9966-9974	16.4	35
154	Insights on Absolute and Relative Stereocontrol in Stereodivergent Cooperative Catalysis. <i>Journal of the American Chemical Society</i> , 2020 , 142, 9612-9624	16.4	12
153	Palladium-Catalyzed -C-H Allylation of Arenes: A Unique Combination of a Pyrimidine-Based Template and Hexafluoroisopropanol. <i>Journal of the American Chemical Society</i> , 2020 , 142, 12453-12466	16.4	43
152	Energetics of Dynamic Kinetic Asymmetric Transformation in Suzuki-Miyaura Coupling. <i>ACS Catalysis</i> , 2020 , 10, 4349-4360	13.1	3
151	Is silver a mere terminal oxidant in palladium catalyzed C-H bond activation reactions?. <i>Chemical Science</i> , 2020 , 11, 208-216	9.4	29
150	A unified machine-learning protocol for asymmetric catalysis as a proof of concept demonstration using asymmetric hydrogenation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 1339-1345	11.5	30
149	Unraveling the Importance of Noncovalent Interactions in Asymmetric Hydroformylation Reactions. <i>Journal of the American Chemical Society</i> , 2020 , 142, 17079-17092	16.4	15
148	Mechanistic insights into rhodium-catalyzed enantioselective allylic alkylation for quaternary stereogenic centers. <i>Chemical Science</i> , 2020 , 12, 2527-2539	9.4	2
147	Hypercoordinate iodine for catalytic asymmetric diamination of styrene: insights into the mechanism, role of solvent, and stereoselection. <i>Chemical Science</i> , 2019 , 10, 7082-7090	9.4	8
146	Cooperativity and serial ligand catalysis in an allylic amination reaction by Pd(II)-bis-sulfoxide and Brønsted acids. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 7723-7734	3.9	1
145	Mechanism and Origin of Enantioselectivity in Nickel-Catalyzed Alkyl-Alkyl Suzuki Coupling Reaction. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 6701-6710	2.8	9
144	Computational asymmetric catalysis: On the origin of stereoselectivity in catalytic reactions. <i>Advances in Physical Organic Chemistry</i> , 2019 , 53, 1-27	0.3	1

143	On the activation of hypercoordinate iodine(iii) compounds for reactions of current interest. <i>Dalton Transactions</i> , 2019 , 48, 4086-4093	4.3	8
142	Insights into the role of noncovalent interactions in distal functionalization of the aryl C(sp)-H bond. <i>Chemical Science</i> , 2019 , 10, 3826-3835	9.4	17
141	Harnessing Noncovalent Interactions in Dual-Catalytic Enantioselective Heck-Matsuda Arylation. <i>Journal of the American Chemical Society</i> , 2019 , 141, 998-1009	16.4	46
140	Rhodium Catalyzed Asymmetric Hydroamination of Internal Alkynes with Indoline: Mechanism, Origin of Enantioselectivity, and Role of Additives. <i>Journal of Organic Chemistry</i> , 2018 , 83, 2627-2639	4.2	11
139	Insights on the Origin of Regiodivergence in the Parallel Kinetic Resolution of rac-Aziridines Using a Chiral Lanthanum/Strontium Bimetallic Catalyst. <i>ACS Catalysis</i> , 2018 , 8, 7633-7644	13.1	7
138	A quantification scheme for non-covalent interactions in the enantio-controlling transition states in asymmetric catalysis. <i>Organic and Biomolecular Chemistry</i> , 2018 , 16, 5643-5652	3.9	7
137	Two chiral catalysts in action: insights into cooperativity and stereoselectivity in proline and cinchona-thiourea dual organocatalysis. <i>Chemical Science</i> , 2018 , 9, 8738-8747	9.4	19
136	Mechanistic Insights on Orthogonal Selectivity in Heterocycle Synthesis. <i>ACS Catalysis</i> , 2018 , 8, 10111-10118	13.1	16
135	Machine learning for predicting product distributions in catalytic regioselective reactions. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 18311-18318	3.6	22
134	Origin of stereoselectivity in the amination of alcohols using cooperative asymmetric dual catalysis involving chiral counter-ions. <i>Chemical Science</i> , 2018 , 9, 6126-6133	9.4	22
133	Hypercoordinate iodine(III) promoted reactions and catalysis: an update on current mechanistic understanding. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017 , 7, e1299	7.9	27
132	Enantioselective Heck-Matsuda Arylations through Chiral Anion Phase-Transfer of Aryl Diazonium Salts. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 5806-5811	16.4	45
131	Reversing Enantioselectivity Using Noncovalent Interactions in Asymmetric Dearomatization of 1-Naphthols: The Power of 3,3'-Substituents in Chiral Phosphoric Acid Catalysts. <i>Organic Letters</i> , 2017 , 19, 2354-2357	6.2	25
130	Hypercoordinate Iodine Catalysts in Enantioselective Transformation: The Role of Catalyst Folding in Stereoselectivity. <i>ACS Catalysis</i> , 2017 , 7, 4189-4196	13.1	35
129	Enantioselective Heck-Matsuda Arylations through Chiral Anion Phase-Transfer of Aryl Diazonium Salts. <i>Angewandte Chemie</i> , 2017 , 129, 5900-5905	3.6	10
128	Catalytic Arene meta-C-H Functionalization Exploiting a Quinoline-Based Template. <i>ACS Catalysis</i> , 2017 , 7, 3162-3168	13.1	63
127	Origin of Stereoselectivity in Cooperative Asymmetric Catalysis Involving N-Heterocyclic Carbenes and Lewis Acids toward the Synthesis of Spirooxindole Lactone. <i>ACS Catalysis</i> , 2017 , 7, 530-537	13.1	63
126	Transposed Paterni-Büchi Reaction. <i>Journal of the American Chemical Society</i> , 2017 , 139, 655-662	16.4	31

125	Experimental and Computational Studies on Remote $\text{C}(\text{sp}^3)\text{H}$ Silylation and Germanylation of Aliphatic Carboxamides. <i>ACS Catalysis</i> , 2017 , 7, 8171-8175	13.1	76
124	Mechanism and reactivity in the Morita-Baylis-Hillman reaction: the challenge of accurate computations. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 30647-30657	3.6	51
123	Asymmetric Dual Chiral Catalysis using Iridium Phosphoramidites and Diarylprolinol Silyl Ethers: Insights into Stereodivergence. <i>ACS Catalysis</i> , 2017 , 7, 6675-6685	13.1	13
122	Aliphatic $\text{C}(\text{sp})\text{-H}$ Bond Activation Using Nickel Catalysis: Mechanistic Insights on Regioselective Arylation. <i>Journal of Organic Chemistry</i> , 2017 , 82, 9619-9626	4.2	24
121	Exploring the Mechanism and Stereoselectivity in Chiral Cinchona-Catalyzed Heterodimerization of Ketenes. <i>Journal of Organic Chemistry</i> , 2017 , 82, 13449-13458	4.2	6
120	Mechanistic Insights and the Origin of Regioselective Borylation in an Iridium-Catalyzed Alkyl $\text{C}(\text{sp}^3)\text{H}$ Bond Functionalization. <i>Organometallics</i> , 2017 , 36, 151-158	3.8	13
119	Asymmetric Cooperative Catalysis in a Three-Component Reaction: Mechanism and Origin of Enantio- and Diastereoselectivities. <i>Organic Letters</i> , 2016 , 18, 3746-9	6.2	8
118	Mechanism and Stereoselectivity in an Asymmetric N-Heterocyclic Carbene-Catalyzed Carbon-Carbon Bond Activation Reaction. <i>Organic Letters</i> , 2016 , 18, 5932-5935	6.2	24
117	Directing group assisted α -hydroxylation by C-H activation. <i>Chemical Science</i> , 2016 , 7, 3147-3153	9.4	107
116	Keto-Enol Thermodynamics of Breslow Intermediates. <i>Journal of the American Chemical Society</i> , 2016 , 138, 5044-51	16.4	33
115	Palladium/Silver Cooperativity in an Aryl Amination Reaction through CH Functionalization. <i>ACS Catalysis</i> , 2016 , 6, 696-708	13.1	61
114	Role of Lewis acid additives in a palladium catalyzed directed C-H functionalization reaction of benzohydroxamic acid to isoxazolone. <i>Organic and Biomolecular Chemistry</i> , 2016 , 15, 246-255	3.9	8
113	Cooperative Asymmetric Catalysis by N-Heterocyclic Carbenes and Brønsted Acid in β -Lactam Formation: Insights into Mechanism and Stereoselectivity. <i>ACS Catalysis</i> , 2016 , 6, 3118-3126	13.1	48
112	Transition State Models for Understanding the Origin of Chiral Induction in Asymmetric Catalysis. <i>Accounts of Chemical Research</i> , 2016 , 49, 1019-28	24.3	92
111	Origin of Kinetic Resolution of Hydroxy Esters through Catalytic Enantioselective Lactonization by Chiral Phosphoric Acids. <i>Organic Letters</i> , 2016 , 18, 3730-3	6.2	11
110	Photoreactions with a Twist: Atropisomerism-Driven Divergent Reactivity of Enones with UV and Visible Light. <i>Chemistry - A European Journal</i> , 2016 , 22, 11339-48	4.8	5
109	A phosphonide based PNP ligand, 2,6-{Ph ₂ PC(O)} ₂ (C ₅ H ₃ N), showing PP, PNP and PNO coordination modes. <i>Dalton Transactions</i> , 2015 , 44, 4167-79	4.3	13
108	Synthesis, characterization and DFT studies of 1, 1'-Bis(diphenylphosphino)ferrocene substituted diiron complexes: Bioinspired [FeFe] hydrogenase model complexes. <i>Journal of Chemical Sciences</i> , 2015 , 127, 557-563	1.8	12

107	Mechanistic Studies on Stereoselective Organocatalytic Direct C-H Activation in an Aliphatic Chain by Chiral N-Heterocyclic Carbenes. <i>ACS Catalysis</i> , 2015 , 5, 5794-5802	13.1	33
106	Origin of Stereodivergence in Cooperative Asymmetric Catalysis with Simultaneous Involvement of Two Chiral Catalysts. <i>Journal of the American Chemical Society</i> , 2015 , 137, 15712-22	16.4	66
105	Mechanistic Insights on Cooperative Catalysis through Computational Quantum Chemical Methods. <i>ACS Catalysis</i> , 2015 , 5, 480-503	13.1	78
104	Deciphering the Origin of Stereoinduction in Cooperative Asymmetric Catalysis Involving Pd(II) and a Chiral Brønsted Acid. <i>Organic Letters</i> , 2015 , 17, 2874-7	6.2	11
103	Asymmetric Dual-Catalytic Cascade by Chiral N-Heterocyclic Carbene and Quinuclidine: Mechanism and Origin of Enantioselectivity in Benzofuranone Formation. <i>ACS Catalysis</i> , 2015 , 5, 1596-1603	13.1	42
102	Axial coordination dichotomy in dirhodium carbenoid catalysis: a curious case of cooperative asymmetric dual-catalytic approach toward amino esters. <i>Journal of Organic Chemistry</i> , 2015 , 80, 2192-7	4.2	23
101	Non-innocent additives in a palladium(II)-catalyzed C-H bond activation reaction: insights into multimetallic active catalysts. <i>Journal of the American Chemical Society</i> , 2014 , 136, 5535-8	16.4	99
100	Importance of ligand exchanges in Pd(II)-Brønsted acid cooperative catalytic approach to spirocyclic rings. <i>Journal of the American Chemical Society</i> , 2014 , 136, 15998-6008	16.4	50
99	The mechanism of catalytic methylation of 2-phenylpyridine using di-tert-butyl peroxide. <i>Dalton Transactions</i> , 2014 , 43, 10183-201	4.3	12
98	Mechanistic insights on cooperative asymmetric multicatalysis using chiral counterions. <i>Journal of Organic Chemistry</i> , 2014 , 79, 7600-6	4.2	36
97	The mechanism of the NHC catalyzed aza-Morita-Baylis-Hillman reaction: insights into a new substrate-catalyzed bimolecular pathway. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 2176-9	3.9	24
96	Axially chiral imidodiphosphoric Acid catalyst for asymmetric sulfoxidation reaction: insights on asymmetric induction. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 4432-6	16.4	65
95	Rational design of catalysts for asymmetric diamination reaction using transition state modeling. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 2745-53	3.9	24
94	Deciphering the origin of cooperative catalysis by dirhodium acetate and chiral spiro phosphoric acid in an asymmetric amination reaction. <i>Chemical Communications</i> , 2014 , 50, 14639-42	5.8	23
93	Mechanistic insights on iodine(III) promoted metal-free dual C-H activation involved in the formation of a spirocyclic bis-oxindole. <i>Organic Letters</i> , 2014 , 16, 6224-7	6.2	34
92	Axially Chiral Imidodiphosphoric Acid Catalyst for Asymmetric Sulfoxidation Reaction: Insights on Asymmetric Induction. <i>Angewandte Chemie</i> , 2014 , 126, 4521-4525	3.6	15
91	Mechanism and stereoselectivity of biologically important oxygenation reactions of the 7-dehydrocholesterol radical. <i>Journal of Organic Chemistry</i> , 2013 , 78, 7023-9	4.2	7
90	Mechanism of catalytic functionalization of primary C-H bonds using a silylation strategy. <i>Organic Letters</i> , 2013 , 15, 4066-9	6.2	26

89	Synthesis of 3,3-Disubstituted Oxindoles by Palladium-Catalyzed Asymmetric Intramolecular γ -Arylation of Amides: Reaction Development and Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2013 , 19, 11916-27	4.8	74
88	Rationalizing Reactivity and Selectivity in Aminocatalytic Reactions 2013 , 463-494		
87	N-heterocyclic carbene catalyzed asymmetric intermolecular Stetter reaction: origin of enantioselectivity and role of counterions. <i>Organic Letters</i> , 2013 , 15, 5040-3	6.2	45
86	Cyclopalladation of dimesityl selenide: synthesis, reactivity, structural characterization, isolation of an intermediate complex with C-H \cdots Pd intra-molecular interaction and computational studies. <i>Dalton Transactions</i> , 2013 , 42, 10828-37	4.3	11
85	On the mechanism of the dehydroaromatization of hexane to benzene by an iridium pincer catalyst. <i>Chemistry - A European Journal</i> , 2013 , 19, 4069-77	4.8	18
84	New bisphosphonate ligands, 1,3-phenylenebis((diphenylphosphino)methanone) and (2-bromo-1,3-phenylene)bis((diphenylphosphino)methanone): synthesis, coordination behavior, DFT calculations and catalytic studies. <i>Dalton Transactions</i> , 2013 , 42, 11385-99	4.3	19
83	Mechanistic insights on organocatalytic enantioselective decarboxylative protonation by epicinchona-thiourea hybrid derivatives. <i>Journal of Organic Chemistry</i> , 2012 , 77, 10525-36	4.2	29
82	Refined transition-state models for proline-catalyzed asymmetric Michael reactions under basic and base-free conditions. <i>Journal of Organic Chemistry</i> , 2012 , 77, 10516-24	4.2	20
81	Mechanism of cooperative catalysis in a Lewis acid promoted nickel-catalyzed dual C-H activation reaction. <i>Organic Letters</i> , 2012 , 14, 4584-7	6.2	26
80	Noninnocent role of N-methyl pyrrolidinone in thiazolidinethione-promoted asymmetric aldol reactions. <i>Organic Letters</i> , 2012 , 14, 5752-5	6.2	15
79	Revisiting sesquiterpene biosynthetic pathways leading to santalene and its analogues: a comprehensive mechanistic study. <i>Organic and Biomolecular Chemistry</i> , 2012 , 10, 7996-8006	3.9	13
78	Conformational mapping and energetics of saccharide-aromatic residue interactions: implications for the discrimination of anomers and epimers and in protein engineering. <i>Organic and Biomolecular Chemistry</i> , 2012 , 10, 4186-200	3.9	11
77	Mechanistic insights on platinum- and palladium-pincer catalyzed coupling and cyclopropanation reactions between olefins. <i>Dalton Transactions</i> , 2012 , 41, 8430-40	4.3	17
76	Microsolvated transition state models for improved insight into chemical properties and reaction mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 12715-36	3.6	71
75	On the origin of regio- and stereoselectivity in singlet oxygen addition to enecarbamates. <i>Journal of Organic Chemistry</i> , 2012 , 77, 2474-85	4.2	12
74	Role of Explicit Solvents in Palladium(II)-Catalyzed Alkoxylation of Arenes: An Interesting Paradigm for Preferred Outer-Sphere Reductive Elimination over Inner-Sphere Pathway. <i>Organometallics</i> , 2012 , 31, 6466-6481	3.8	38
73	Exploration of CH \cdots O mediated stacking interactions in saccharide: aromatic residue complexes through conformational sampling. <i>Carbohydrate Research</i> , 2012 , 361, 133-40	2.9	16
72	Origin of stereoselectivity in a chiral N-heterocyclic carbene-catalyzed desymmetrization of substituted cyclohexyl 1,3-diketones. <i>Organic Letters</i> , 2012 , 14, 2810-3	6.2	40

71	Mechanistic insights into the role of chiral ligands in asymmetric diamination reactions. <i>Chemistry - A European Journal</i> , 2012 , 18, 7045-9	4.8	20
70	Mechanistic insights on N-heterocyclic carbene-catalyzed annulations: the role of base-assisted proton transfers. <i>Journal of Organic Chemistry</i> , 2011 , 76, 5606-13	4.2	84
69	Quantification of binding affinities of essential sugars with a tryptophan analogue and the ubiquitous role of C-H...interactions. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 6517-30	3.6	24
68	A computational insight into a metal mediated pathway for the ring-opening polymerization (ROP) of lactides by an ionic {(NHC)2Ag}{+}X(-) (X = halide) type N-heterocyclic carbene (NHC) complex. <i>Dalton Transactions</i> , 2011 , 40, 10156-61	4.3	20
67	Stereocontrol in proline-catalyzed asymmetric amination: a comparative assessment of the role of enamine carboxylic acid and enamine carboxylate. <i>Chemical Communications</i> , 2011 , 47, 5759-61	5.8	29
66	Palladium(II)-catalyzed direct alkoxylation of arenes: evidence for solvent-assisted concerted metalation deprotonation. <i>Organic Letters</i> , 2011 , 13, 4802-5	6.2	58
65	Mechanism and electronic effects in nitrogen ylide-promoted asymmetric aziridination reaction. <i>Organic and Biomolecular Chemistry</i> , 2011 , 9, 2123-32	3.9	8
64	Proline-derived organocatalysis and synergism between theory and experiments. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011 , 1, 920-931	7.9	24
63	Chemo-, regio-, and diastereoselectivity preferences in the reaction of a sulfur ylide with a dienal and an enone. <i>Organic and Biomolecular Chemistry</i> , 2011 , 9, 1642-52	3.9	6
62	[5+3] Cycloaddition of 3-Oxidopyrylium: A Novel Route to Functionalized Cyclooctanoids from Furans. <i>Synthesis</i> , 2010 , 2010, 320-328	2.9	6
61	Transition state models for probing stereoiduction in Evans chiral auxiliary-based asymmetric aldol reactions. <i>Journal of the American Chemical Society</i> , 2010 , 132, 12319-30	16.4	48
60	Organoselenium chemistry: role of intramolecular interactions. <i>Chemical Reviews</i> , 2010 , 110, 4357-416	68.1	377
59	The pivotal role of chelation as a stereochemical control element in non-Evans anti aldol product formation. <i>Organic Letters</i> , 2010 , 12, 2868-71	6.2	20
58	TiCl4-promoted Baylis-Hillman reaction: mechanistic rationale toward product distribution and stereoselectivity. <i>Journal of Organic Chemistry</i> , 2010 , 75, 359-67	4.2	21
57	Ni-, Pd-, or Pt-catalyzed ethylene dimerization: a mechanistic description of the catalytic cycle and the active species. <i>Organic and Biomolecular Chemistry</i> , 2010 , 8, 1040-51	3.9	19
56	Importance of the nature of β -substituents in pyrrolidine organocatalysts in asymmetric Michael additions. <i>Journal of Organic Chemistry</i> , 2010 , 75, 7310-21	4.2	30
55	Enamine versus oxazolidinone: what controls stereoselectivity in proline-catalyzed asymmetric aldol reactions?. <i>Angewandte Chemie - International Edition</i> , 2010 , 49, 6373-7	16.4	91
54	Design of Catalysts for Asymmetric Organic Reactions Through Density Functional Calculations. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010 , 107-136	0.7	2

53	On the origin of reversible hydrogen activation by phosphine-boranes. <i>Chemistry - A European Journal</i> , 2009 , 15, 12846-55	4.8	39
52	On the relative preference of enamine/iminium pathways in an organocatalytic Michael addition reaction. <i>Chemistry - an Asian Journal</i> , 2009 , 4, 714-24	4.5	24
51	Mechanistic insights and the role of cocatalysts in Aza-Morita-Baylis-hillman and Morita-Baylis-Hillman reactions. <i>Journal of Organic Chemistry</i> , 2009 , 74, 6936-43	4.2	62
50	Conformational and isomeric preferences of six-membered inorganic heterocycles [EtNP(E)(OR)] ₃ (E = Lone Pair, O, S, or Se): a synthetic, spectroscopic, structural, and computational study. <i>Inorganic Chemistry</i> , 2009 , 48, 2048-59	5.1	9
49	Synthesis of azoaromatic dyes via redox driven C-N bond fusion. <i>Organic Letters</i> , 2009 , 11, 3218-21	6.2	21
48	On the origins of kinetic resolution of cyclohexane-1,2-diols through stereoselective acylation by chiral tetrapeptides. <i>Organic Letters</i> , 2009 , 11, 3242-5	6.2	39
47	Na(I)/Cu(I-II) heterometallic cages interconnected by unusual linear 2-coordinate OCN-Cu(I)-NCO links: synthesis, structural, magnetostructural correlation and computational studies. <i>Dalton Transactions</i> , 2009 , 9510-9	4.3	20
46	Unraveling high precision stereocontrol in a triple cascade organocatalytic reaction. <i>Organic and Biomolecular Chemistry</i> , 2008 , 6, 3921-9	3.9	42
45	Enantio- and diastereoselectivities in chiral sulfur ylide promoted asymmetric aziridination reactions. <i>Journal of Organic Chemistry</i> , 2008 , 73, 8163-74	4.2	40
44	Face-selective Diels-Alder reactions between unsymmetrical cyclohexadienes and symmetric trans-dienophile: an experimental and computational investigation. <i>Journal of Organic Chemistry</i> , 2008 , 73, 435-44	4.2	10
43	Probing intramolecular interactions in arylselenides using a property descriptor based approach. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 8797-803	2.8	9
42	Mixed-valent metals bridged by a radical ligand: fact or fiction based on structure-oxidation state correlations. <i>Journal of the American Chemical Society</i> , 2008 , 130, 3532-42	16.4	97
41	The role of noninnocent solvent molecules in organocatalyzed asymmetric Michael addition reactions. <i>Chemistry - A European Journal</i> , 2008 , 14, 10472-85	4.8	49
40	Water catalysis in the Morita-Baylis-Hillman reaction: a mechanistic perspective. <i>Chemistry - A European Journal</i> , 2008 , 14, 10530-4	4.8	60
39	Density functional theory investigations on sulfur ylide promoted cyclopropanation reactions: insights on mechanism and diastereoselection issues. <i>Journal of Organic Chemistry</i> , 2007 , 72, 331-41	4.2	33
38	Insights on co-catalyst-promoted enamine formation between dimethylamine and propanal through ab initio and density functional theory study. <i>Journal of Organic Chemistry</i> , 2007 , 72, 8202-15	4.2	67
37	Computational investigations on the general reaction profile and diastereoselectivity in sulfur ylide promoted aziridination. <i>Chemistry - A European Journal</i> , 2007 , 13, 4805-15	4.8	34
36	Valence-State Distribution in the Ruthenium o-Quinonoid Systems [Ru(trpy)(Cl)(L1)] ⁺ and [Ru(trpy)(Cl)(L2)] ⁺ (L1 = o-Iminobenzoquinone, L2 = o-Diiminobenzoquinone; trpy = 2,2':6',2''-Terpyridine). <i>European Journal of Inorganic Chemistry</i> , 2007 , 2007, 314-323	2.3	34

35	Intramolecular nonbonding interactions in organoseleniums: Quantification using a computational thermochemical approach. <i>Computational and Theoretical Chemistry</i> , 2007 , 809, 145-152		5
34	Multiple one-electron oxidation and reduction of trinuclear bis(2,4-pentanedionato)ruthenium complexes with substituted diquinoxalino[2,3-a:2',3'-c]phenazine ligands. <i>Polyhedron</i> , 2007 , 26, 3409-3418	2.7	20
33	Bicyclic proline analogues as organocatalysts for stereoselective aldol reactions: an in silico DFT study. <i>Organic and Biomolecular Chemistry</i> , 2007 , 5, 1287-94	3.9	64
32	Ab initio and density functional theory evidence on the rate-limiting step in the Morita-Baylis-Hillman reaction. <i>Organic Letters</i> , 2007 , 9, 4873-6	6.2	71
31	A Cationic (N-Heterocyclic carbene)silver Complex as Catalyst for Bulk Ring-Opening Polymerization of L-Lactides. <i>European Journal of Inorganic Chemistry</i> , 2006 , 2006, 2975-2984	2.3	84
30	An Experimental and Density Functional Theory Approach Towards the Establishment of Preferential Metal- or Ligand-Based Electron-Transfer Processes in Large Quinonoid-Bridged Diruthenium Complexes $[(\text{aap})_2\text{Ru}]_2(\text{EBL}_2)]^n+$ (aap = 2-Arylazopyridine). <i>European Journal of Inorganic Chemistry</i> , 2006 , 2006, 1136-1144	2.3	31
29	Retro Diels-Alder reaction under mild conditions: experimental and theoretical studies. <i>Organic and Biomolecular Chemistry</i> , 2006 , 4, 1854-6	3.9	21
28	Density functional theory and atoms-in-molecule study on the role of two-electron stabilizing interactions in retro Diels-Alder reaction of cycloadducts derived from substituted cyclopentadiene and p-benzoquinone. <i>Organic and Biomolecular Chemistry</i> , 2006 , 4, 3923-30	3.9	9
27	Anomalous excited-state dynamics of lucifer yellow CH in solvents of high polarity: evidence for an intramolecular proton transfer. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 5585-91	2.8	23
26	Quantification of intramolecular nonbonding interactions in organochalcogens. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 5942-7	2.8	44
25	Experimental and theoretical studies of a silver complex of O-functionalized N-heterocyclic carbene. <i>Journal of Organometallic Chemistry</i> , 2006 , 691, 3797-3805	2.3	38
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