

Per-Ola Norrby

List of Publications by Year in descending order

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211
papers

10,061
citations

27035

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54771

88
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245
all docs

245
docs citations

245
times ranked

8800
citing authors

#	ARTICLE	IF	CITATIONS
1	Automated fitting of transition state force fields for biomolecular simulations. PLoS ONE, 2022, 17, e0264960.	1.1	5
2	Machine learning meets mechanistic modelling for accurate prediction of experimental activation energies. Chemical Science, 2021, 12, 1163-1175.	3.7	102
3	Enantioselective Synthesis of Atropisomeric Biaryls using Biaryl 2,5-Diphenylphospholanes as Ligands for Palladium-Catalysed Suzuki-Miyaura Reactions. Advanced Synthesis and Catalysis, 2021, 363, 259-267.	2.1	15
4	Microsecond timescale MD simulations at the transition state of <i>Pm</i> HMGR predict remote allosteric residues. Chemical Science, 2021, 12, 6413-6418.	3.7	7
5	Stereoselectivity Predictions for the Pd-Catalyzed 1,4-Conjugate Addition Using Quantum-Guided Molecular Mechanics. Journal of Organic Chemistry, 2021, 86, 5660-5667.	1.7	6
6	Organic reactivity from mechanism to machine learning. Nature Reviews Chemistry, 2021, 5, 240-255.	13.8	88
7	Experimental and Computational Models for Side Chain Discrimination in Peptide-Protein Interactions. Chemistry - A European Journal, 2021, 27, 10883-10897.	1.7	6
8	Proofreading experimentally assigned stereochemistry through Q2MM predictions in Pd-catalyzed allylic aminations. Nature Communications, 2021, 12, 6719.	5.8	5
9	Synthetic and mechanistic studies in enantioselective allylic substitutions catalysed by palladium complexes of a modular class of axially chiral quinazoline-containing ligands. Tetrahedron, 2020, 76, 130780.	1.0	8
10	From desktop to benchtop with automated computational workflows for computer-aided design in asymmetric catalysis. Nature Catalysis, 2020, 3, 574-584.	16.1	31
11	Applications of Quantum Chemistry in Pharmaceutical Process Development: Current State and Opportunities. Organic Process Research and Development, 2020, 24, 1496-1507.	1.3	25
12	Palladium Catalyzed Stereoselective Arylation of Biocatalytically Derived Cyclic 1,3-Dienes: Chirality Transfer via a Heck-Type Mechanism. Organic Letters, 2020, 22, 2464-2469.	2.4	4
13	Transition State Force Field for the Asymmetric Redox-Relay Heck Reaction. Journal of the American Chemical Society, 2020, 142, 9700-9707.	6.6	15
14	Degradation of Pharmaceuticals through Sequential Photon Absorption and Photoionization in Amiloride Derivatives. Cell Reports Physical Science, 2020, 1, 100274.	2.8	5
15	Holistic models of reaction selectivity. Nature, 2019, 571, 332-333.	13.7	3
16	Relative Strength of Common Directing Groups in Palladium-Catalyzed Aromatic C-H Activation. Science, 2019, 20, 373-391.	1.9	34
17	An Improved Class of Phosphite-Oxazoline Ligands for Pd-Catalyzed Allylic Substitution Reactions. ACS Catalysis, 2019, 9, 6033-6048.	5.5	18
18	Is Excited-State Aromaticity a Driving Force for Planarization of Dibenzannelated 8-Electron Heterocycles?. ChemPlusChem, 2019, 84, 712-721.	1.3	38

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19	A Predictive Tool for Electrophilic Aromatic Substitutions Using Machine Learning. <i>Journal of Organic Chemistry</i> , 2019, 84, 4695-4703.	1.7	70
20	Rapid virtual screening of enantioselective catalysts using CatVS. <i>Nature Catalysis</i> , 2019, 2, 41-45.	16.1	81
21	Nonclassical Mechanism in the Cyclodehydration of Diols Catalyzed by a Bifunctional Iridium Complex. <i>Chemistry - A European Journal</i> , 2019, 25, 2631-2636.	1.7	6
22	Computational prediction of chemical reactions: current status and outlook. <i>Drug Discovery Today</i> , 2018, 23, 1203-1218.	3.2	126
23	Revisiting the Stereodetermining Step in Enantioselective Iridium-Catalyzed Imine Hydrogenation. <i>ACS Catalysis</i> , 2018, 8, 615-623.	5.5	38
24	Designing flexible low-viscous sieving media for capillary electrophoresis analysis of ribonucleic acids. <i>Journal of Chromatography A</i> , 2018, 1562, 108-114.	1.8	17
25	Degradation caused by incompatibility between sodium stearyl fumarate (PRUV) and AZD7986 in the drug product. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2018, 158, 82-87.	1.4	5
26	Enantioselective Synthesis of Sterically Hindered Tertiary α -Aryl Oxindoles via Palladium-Catalyzed Decarboxylative Protonation. An Experimental and Theoretical Mechanistic Investigation. <i>Advanced Synthesis and Catalysis</i> , 2018, 360, 3124-3137.	2.1	11
27	Application of Q2MM to predictions in stereoselective synthesis. <i>Chemical Communications</i> , 2018, 54, 8294-8311.	2.2	37
28	Manganese-Catalyzed Cross-Coupling of Aryl Halides and Grignard Reagents by a Radical Mechanism. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 4758-4764.	1.2	14
29	Competing Pathways in O -Arylations with Diaryliodonium Salts: Mechanistic Insights. <i>Chemistry - A European Journal</i> , 2017, 23, 13249-13258.	1.7	56
30	The Manganese-Catalyzed Cross-Coupling Reaction and the Influence of Trace Metals. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 5269-5274.	1.2	13
31	Kinetic and Theoretical Investigation of Iron(III)-Catalyzed Silane Chlorination. <i>ChemCatChem</i> , 2016, 8, 584-592.	1.8	3
32	Prediction of Stereochemistry using Q2MM. <i>Accounts of Chemical Research</i> , 2016, 49, 996-1005.	7.6	76
33	Anomeric Effects in Sulfamides. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3677-3682.	1.1	9
34	Asymmetric Catalyzed Allylic Substitution Using a Pd/Pa-S Catalyst Library with Exceptional High Substrate and Nucleophile Versatility: DFT and Pd- η -allyl Key Intermediates Studies. <i>Organometallics</i> , 2016, 35, 3323-3335.	1.1	21
35	Mechanistic Insights into the Iridium-Catalyzed Hydrogenations of α,β -Unsaturated Ketones. <i>ChemCatChem</i> , 2016, 8, 3099-3106.	1.8	14
36	Glycerol Upgrading via Hydrogen Borrowing: Direct Ruthenium-Catalyzed Amination of the Glycerol Derivative Solketal. <i>ACS Sustainable Chemistry and Engineering</i> , 2016, 4, 5730-5736.	3.2	18

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37	Stereoselectivity in (Acyloxy)borane-Catalyzed Mukaiyama Aldol Reactions. <i>Journal of Organic Chemistry</i> , 2016, 81, 5314-5321.	1.7	11
38	Conformational Preferences of a Tropos Biphenyl Phosphinooxazolineâ€“a Ligand with Wide Substrate Scope. <i>ACS Catalysis</i> , 2016, 6, 1701-1712.	5.5	30
39	Theoretical and Experimental Optimization of a New Amino Phosphite Ligand Library for Asymmetric Palladiumâ€“Catalyzed Allylic Substitution. <i>ChemCatChem</i> , 2015, 7, 4091-4107.	1.8	21
40	Singleâ€“Flask Multicomponent Palladiumâ€“Catalyzed β , γ -Coupling of Ketone Enolates: Facile Preparation of Complex Carbon Scaffolds. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11822-11825.	7.2	20
41	Mechanistic Studies on the Alkylation of Amines with Alcohols Catalyzed by a Bifunctional Iridium Complex. <i>ACS Catalysis</i> , 2015, 5, 3704-3716.	5.5	72
42	Ni-Catalyzed Alkenylation of Ketone Enolates under Mild Conditions: Catalyst Identification and Optimization. <i>Journal of the American Chemical Society</i> , 2015, 137, 7019-7022.	6.6	53
43	New insights into the mechanism of iron-catalyzed cross-coupling reactions. <i>Dalton Transactions</i> , 2015, 44, 3959-3962.	1.6	30
44	On the Radical Nature of Ironâ€“Catalyzed Crossâ€“Coupling Reactions. <i>Chemistry - A European Journal</i> , 2015, 21, 5946-5953.	1.7	63
45	Pd- η^3 -C ₆ H ₉ complexes of the Trost modular ligand: high nuclearity columnar aggregation controlled by concentration, solvent and counterion. <i>Chemical Science</i> , 2015, 6, 5793-5801.	3.7	12
46	Improving the Q2MM method for transition state force field modeling. <i>Journal of Computational Chemistry</i> , 2015, 36, 244-250.	1.5	9
47	Epoxyalcohols: Bioactivation and Conjugation Required for Skin Sensitization. <i>Chemical Research in Toxicology</i> , 2014, 27, 1860-1870.	1.7	10
48	Mechanistic Aspects of Submillimolar Copperâ€“Catalyzed C ₁ N Crossâ€“Coupling. <i>ChemCatChem</i> , 2014, 6, 1277-1282.	1.8	16
49	Breaking conjugation: unusual regioselectivity with 2-substituted allylic substrates in the Tsujiâ€“Trost reaction. <i>Chemical Science</i> , 2014, 5, 1241-1250.	3.7	9
50	Mechanistic Investigations of Palladium-Catalyzed Allylic Fluorination. <i>Organometallics</i> , 2014, 33, 2121-2133.	1.1	63
51	Role of the Base in Buchwaldâ€“Hartwig Amination. <i>Journal of Organic Chemistry</i> , 2014, 79, 11961-11969.	1.7	74
52	Investigating the Nature of Palladium Chain-Walking in the Enantioselective Redox-Relay Heck Reaction of Alkenyl Alcohols. <i>Journal of Organic Chemistry</i> , 2014, 79, 11841-11850.	1.7	95
53	Fast and reversible insertion of carbon dioxide into zirconoceneâ€“alkoxide bonds. A mechanistic study. <i>Dalton Transactions</i> , 2014, 43, 8894-8898.	1.6	4
54	Stereoselectivity in Asymmetric Catalysis: The Case of Ruthenium-Catalyzed Ketone Hydrogenation. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2427-2435.	2.3	27

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55	Palladium-Catalyzed Alkenylation of Ketone Enolates under Mild Conditions. <i>Organic Letters</i> , 2014, 16, 3970-3973.	2.4	36
56	Mechanism, Reactivity, and Selectivity in Palladium-Catalyzed Redox-Relay Heck Arylations of Alkenyl Alcohols. <i>Journal of the American Chemical Society</i> , 2014, 136, 1960-1967.	6.6	187
57	On the oxidation state of iron in iron-mediated C-C couplings. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 51-55.	0.8	50
58	Chelation-Controlled Addition of Organozincs to α -Chloro Aldimines. <i>Journal of the American Chemical Society</i> , 2012, 134, 17599-17604.	6.6	30
59	Mechanistic Studies of the CuH-Catalyzed Synthesis of α -Hydroxyallenes. <i>Organometallics</i> , 2012, 31, 8024-8030.	1.1	11
60	A computational study of the enantioselective addition of n-BuLi to benzaldehyde in the presence of a chiral lithium N,P amide. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 2807.	1.5	12
61	Mild and Efficient Nickel-Catalyzed Heck Reactions with Electron-Rich Olefins. <i>Journal of the American Chemical Society</i> , 2012, 134, 443-452.	6.6	138
62	New efficient ligand for sub-mol % copper-catalyzed C-N cross-coupling reactions running under air. <i>Beilstein Journal of Organic Chemistry</i> , 2012, 8, 1909-1915.	1.3	9
63	Transmetalation Versus α -Hydride Elimination: The Role of 1,4-Benzoquinone in Chelation-Controlled Arylation Reactions with Arylboronic Acids. <i>Chemistry - A European Journal</i> , 2012, 18, 4714-4722.	1.7	39
64	Aggregation and Solvation of Chiral N,P-Amide Ligands in Coordinating Solvents: A Computational and NMR Spectroscopic Study. <i>ChemPlusChem</i> , 2012, 77, 799-806.	1.3	11
65	<i>t</i> -Bu or not <i>t</i> -Bu?. <i>Chemistry - A European Journal</i> , 2012, 18, 1640-1649.	1.7	35
66	Low Temperature Studies of Iron-Catalyzed Cross-Coupling of Alkyl Grignard Reagents with Aryl Electrophiles. <i>Advanced Synthesis and Catalysis</i> , 2012, 354, 448-456.	2.1	43
67	A highly selective agonist for the metabotropic glutamate receptor mGluR2. <i>MedChemComm</i> , 2011, 2, 1120.	3.5	9
68	Experimental and Theoretical Investigations of the Autoxidation of Geranial: A Dioxolane Hydroperoxide Identified as a Skin Sensitizer. <i>Chemical Research in Toxicology</i> , 2011, 24, 1507-1515.	1.7	19
69	Computational Insights into Palladium-Mediated Allylic Substitution Reactions. <i>Topics in Organometallic Chemistry</i> , 2011, , 65-93.	0.7	24
70	A DFT comparison of the neutral and cationic Heck pathways. <i>Dalton Transactions</i> , 2011, 40, 11308.	1.6	36
71	Sterically Governed Selectivity in Palladium-Assisted Allylic Alkylation. <i>Organometallics</i> , 2011, 30, 230-238.	1.1	15
72	Pyranoside Phosphite-Oxazoline Ligands for the Highly Versatile and Enantioselective Ir-Catalyzed Hydrogenation of Minimally Functionalized Olefins. A Combined Theoretical and Experimental Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 13634-13645.	6.6	163

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73	Dispersion and Back-Donation Gives Tetracoordinate [Pd(PPh ₃) ₄]. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11794-11797.	7.2	77
74	β- and γ-Lactams through Palladium-Catalyzed Intramolecular Allylic Alkylation: Enantioselective Synthesis, NMR Investigation, and DFT Rationalization. <i>Chemistry - A European Journal</i> , 2011, 17, 2885-2896.	1.7	36
75	Iron-Catalyzed Coupling of Aryl Grignard Reagents with Alkyl Halides: A Competitive Hammett Study. <i>Chemistry - A European Journal</i> , 2011, 17, 11991-11993.	1.7	48
76	Palladium-Catalyzed Allylic Sulfinylation and the Mislow-Braverman-Evans Rearrangement. <i>Chemistry - A European Journal</i> , 2011, 17, 13963-13965.	1.7	5
77	Application of Q2MM to Stereoselective Reactions. <i>Current Organic Chemistry</i> , 2010, 14, 1629-1645.	0.9	19
78	γ-Arylation by Rearrangement: On the Reaction of Enolates with Diaryliodonium Salts. <i>Chemistry - A European Journal</i> , 2010, 16, 8251-8254.	1.7	122
79	DFT Investigation of the Palladium-Catalyzed Ene-Yne Coupling. <i>Chemistry - A European Journal</i> , 2010, 16, 9494-9501.	1.7	15
80	Kinetic Investigation of a Ligand-Accelerated Substituted Copper-Catalyzed C ₁₂ N Cross-Coupling Reaction. <i>Chemistry - A European Journal</i> , 2010, 16, 13613-13616.	1.7	40
81	On the mechanism of the rhodium catalyzed acrylamide hydrogenation. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 9-14.	4.8	11
82	Trans effects in the Heck reaction: A model study. <i>Journal of Molecular Catalysis A</i> , 2010, 328, 108-113.	4.8	18
83	Memory and dynamics in Pd-catalyzed allylic alkylation with P,N-ligands. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 1585-1592.	1.8	26
84	Copper-Catalyzed Cross-Couplings with Part-per-Million Catalyst Loadings. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 5691-5693.	7.2	238
85	Mechanistic Investigation of Iron-Catalyzed Coupling Reactions. <i>ChemCatChem</i> , 2009, 1, 152-161.	1.8	119
86	DFT-Based Explanation of the Effect of Simple Anionic Ligands on the Regioselectivity of the Heck Arylation of Acrolein Acetals. <i>Organometallics</i> , 2009, 28, 6201-6205.	1.1	23
87	Structure-Based Rationale for Selectivity in the Asymmetric Allylic Alkylation of Cycloalkenyl Esters Employing the Trost <i>Standard Ligand</i> TM (TSL): Isolation, Analysis and Alkylation of the Monomeric form of the Cationic <i>η</i> ³ -Cyclohexenyl Complex [(<i>η</i> ³ -C ₆ H ₉)Pd(TSL)] ⁺ . <i>Journal of the American Chemical Society</i> , 2009, 131, 9945-9957.	6.6	166
88	Prediction of Enantioselectivity in Rhodium Catalyzed Hydrogenations. <i>Journal of the American Chemical Society</i> , 2009, 131, 410-411.	6.6	110
89	Acid-Catalyzed Nucleophilic Aromatic Substitution: Experimental and Theoretical Exploration of a Multistep Mechanism. <i>Chemistry - A European Journal</i> , 2008, 14, 3954-3960.	1.7	23
90	Mechanisms of Air Oxidation of Ethoxylated Surfactants: Computational Estimations of Energies and Reaction Behaviors. <i>Chemistry - A European Journal</i> , 2008, 14, 9549-9554.	1.7	8

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91	Asymmetric Synthesis of Iridoid Derivatives Using Resolved 2-Phenylindoline as a Chiral Auxiliary. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 5915-5921.	1.2	9
92	Mechanism of Air Oxidation of the Fragrance Terpene Geraniol. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 101-106.	2.3	34
93	Unusual Selectivity-Determining Factors in the Phosphine-Free Heck Arylation of Allyl Ethers. <i>Organometallics</i> , 2008, 27, 3187-3195.	1.1	28
94	Steric Influence on the Excited-State Lifetimes of Ruthenium Complexes with Bipyridyl-Alkylene-Pyridyl Ligands. <i>Inorganic Chemistry</i> , 2008, 47, 3540-3548.	1.9	127
95	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 673-681.	2.3	26
96	Combined Experimental and Theoretical Study of the Mechanism and Enantioselectivity of Palladium-Catalyzed Intermolecular Heck Coupling. <i>Journal of the American Chemical Society</i> , 2008, 130, 10414-10421.	6.6	97
97	Development of a Q2MM Force Field for the Asymmetric Rhodium Catalyzed Hydrogenation of Enamides. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1313-1323.	2.3	63
98	On the Nature of the Intermediates and the Role of Chloride Ions in Pd-Catalyzed Allylic Alkylations: Added Insight from Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12862-12867.	1.1	46
99	The Mechanism for the Rhodium-Catalyzed Decarbonylation of Aldehydes: A Combined Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 5206-5215.	6.6	180
100	General Transition-State Force Field for Cytochrome P450 Hydroxylation. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1765-1773.	2.3	54
101	Oxidative Addition of Aryl Chlorides to Monoligated Palladium(0): A DFT-SCRF Study. <i>Organometallics</i> , 2007, 26, 550-553.	1.1	190
102	Memory Effects in Palladium-Catalyzed Allylic Alkylations of Cyclohexenyl Acetate. <i>Advanced Synthesis and Catalysis</i> , 2007, 349, 2631-2640.	2.1	27
103	The Mechanism of the Phosphine-Free Palladium-Catalyzed Hydroarylation of Alkynes. <i>Journal of the American Chemical Society</i> , 2006, 128, 12785-12793.	6.6	61
104	Regioselectivity in lithiation of 1-methylpyrazole: experimental, density functional theory and multinuclear NMR study. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 1261.	1.5	13
105	Modulation of the reactivity, stability and substrate- and enantioselectivity of an epoxidation catalyst by noncovalent dynamic attachment of a receptor functionality aspects on the mechanism of the Jacobsen-Katsuki epoxidation applied to a supramolecular system. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 1927-1948.	1.5	45
106	Divergence en Route to Nonclassical Annonaceous Acetogenins. Synthesis of Pyranicin and Pyragonicin. <i>Journal of Organic Chemistry</i> , 2006, 71, 1879-1891.	1.7	37
107	Direct Determination of Absolute Configuration of Methyl-Substituted Phenylloxiranes: Combined Experimental and Theoretical Approach. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9123-9129.	1.1	9
108	On the Performance of Continuum Solvation Models for the Solvation Energy of Small Anions. <i>Organometallics</i> , 2006, 25, 45-47.	1.1	23

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109	Combining Q2MM modeling and kinetic studies for refinement of the osmium-catalyzed asymmetric dihydroxylation (AD) mnemonic. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 2182-2198.	0.8	33
110	Theoretical Evidence for Low-Ligated Palladium(0): η^6 [Pd η^6 L] as the Active Species in Oxidative Addition Reactions. <i>Organometallics</i> , 2006, 25, 2066-2073.	1.1	174
111	Steric Effects in Release of Amides from Linkers in Solid-Phase Synthesis. Molecular Mechanics Modeling of Key Step in Peptide and Combinatorial Chemistry. <i>International Journal of Peptide Research and Therapeutics</i> , 2006, 12, 335-339.	0.9	3
112	An Experimental and Theoretical Study of the Mechanism of Stannylcupration of $\hat{1}\pm, \hat{1}2$ -Acetylenic Ketones and Esters. <i>Chemistry - A European Journal</i> , 2006, 12, 2866-2873.	1.7	12
113	Deconvoluting the Memory Effect in Pd-Catalyzed Allylic Alkylation: Effect of Leaving Group and Added Chloride. <i>Chemistry - A European Journal</i> , 2006, 12, 5352-5360.	1.7	61
114	Heck Coupling with Nonactivated Alkenyl Tosylates and Phosphates: Examples of Effective 1,2-Migrations of the Alkenyl Palladium(II) Intermediates. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 3349-3353.	7.2	196
115	An Intramolecular Heck Reaction that Prefers a 5-endo- to a 6-exo-trig Cyclization Pathway. <i>Synlett</i> , 2006, 2006, 3140-3144.	1.0	5
116	A Dynamic Supramolecular System Exhibiting Substrate Selectivity in the Catalytic Epoxidation of Olefins.. <i>ChemInform</i> , 2005, 36, no.	0.1	0
117	Surprisingly Mild $\hat{a}\epsilon\epsilon$ Enolate-Counterion-Free $\hat{a}\epsilon$ Pd(0)-Catalyzed Intramolecular Allylic Alkylations.. <i>ChemInform</i> , 2005, 36, no.	0.1	0
118	ZnMe ₂ -Mediated Addition of Acetylenes to Aldehydes and Ketones.. <i>ChemInform</i> , 2005, 36, no.	0.1	0
119	Design and Synthesis of a New Type of Ferrocene-Based Planar Chiral DMAP Analogues. A New Catalyst System for Asymmetric Nucleophilic Catalysis $\hat{a}\epsilon$. <i>Journal of Organic Chemistry</i> , 2005, 70, 8332-8337.	1.7	81
120	New Insights into the Stereoselectivity of the Aryl Zinc Addition to Aldehydes. <i>Journal of the American Chemical Society</i> , 2005, 127, 1548-1552.	6.6	79
121	A dynamic supramolecular system exhibiting substrate selectivity in the catalytic epoxidation of olefins. <i>Chemical Communications</i> , 2005, , 549-551.	2.2	39
122	Surprisingly Mild $\hat{a}\epsilon\epsilon$ Enolate-Counterion-Free $\hat{a}\epsilon$ Pd(0)-Catalyzed Intramolecular Allylic Alkylations. <i>Organic Letters</i> , 2005, 7, 995-998.	2.4	48
123	Palladium(0) alkyne complexes as active species: a DFT investigation. <i>Chemical Communications</i> , 2005, , 4196.	2.2	24
124	A New Strategy for the Improvement of Photophysical Properties in Ruthenium(II) Polypyridyl Complexes. Synthesis and Photophysical and Electrochemical Characterization of Six Mononuclear Ruthenium(II) Bisterpyridine-Type Complexes. <i>Inorganic Chemistry</i> , 2005, 44, 3215-3225.	1.9	97
125	Me ₂ Zn-Mediated Addition of Acetylenes to Aldehydes and Ketones. <i>Journal of Organic Chemistry</i> , 2005, 70, 5733-5736.	1.7	54
126	Nonradical Zinc $\hat{a}\epsilon$ Barbier Reaction for Diastereoselective Synthesis of Vicinal Amino Alcohols. <i>Journal of the American Chemical Society</i> , 2005, 127, 15756-15761.	6.6	67

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127	Probing Competitive Enantioselective Approach Vectors Operating in the Jacobsen-Katsuki Epoxidation: A Kinetic Study of Methyl-Substituted Styrenes. <i>Journal of the American Chemical Society</i> , 2005, 127, 13672-13679.	6.6	41
128	Chiral Diamine-Silver(I)-Alkene Complexes: A Quantum Chemical and NMR Study. <i>Organometallics</i> , 2005, 24, 3737-3745.	1.1	10
129	Structure Investigation of TiIV-BODOLates Involved in the Catalytic Asymmetric Reduction of Ketones Using Catecholborane. <i>Chemistry - A European Journal</i> , 2004, 10, 182-189.	1.7	11
130	Reactivity and Regioselectivity in the Heck Reaction: Hammett Study of 4-Substituted Styrenes. <i>Organometallics</i> , 2004, 23, 6160-6165.	1.1	87
131	Transition states from empirical force fields. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 1-7.	0.5	71
132	An Unprecedented [2+3] Cycloadditive Dimerization of a Transient Thiocarbonyl S-Ylide. <i>European Journal of Organic Chemistry</i> , 2003, 2003, 813-815.	1.2	15
133	Diastereoselective Addition of $\hat{\pm}$ -Metalated Sulfoxides to Imines Revisited: Mechanism, Computational Studies, and the Effect of External Chiral Ligands.. <i>ChemInform</i> , 2003, 34, no.	0.1	0
134	Updating the asymmetric osmium-catalyzed dihydroxylation (AD) mnemonic: Q2MM modeling and new kinetic measurements. <i>Chirality</i> , 2003, 15, 360-368.	1.3	44
135	Phenyl versus Ethyl Transfer in the Addition of Organozinc Reagents to Aldehydes: A Theoretical Study. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 3002-3005.	7.2	62
136	A DFT exploration of the enantioselective rearrangement of cyclohexene oxide to cyclohexenol. <i>Tetrahedron</i> , 2003, 59, 9695-9700.	1.0	8
137	Modeling the Stereoselectivity of the \hat{I}^2 -Amino Alcohol-Promoted Addition of Dialkylzinc to Aldehydes. <i>Journal of the American Chemical Society</i> , 2003, 125, 5130-5138.	6.6	65
138	Rationalizing Ring-Size Selectivity in Intramolecular Pd-Catalyzed Allylations of Resonance-Stabilized Carbanions. <i>Organometallics</i> , 2003, 22, 1849-1855.	1.1	21
139	A DFT Study of R ^X Bond Dissociation Enthalpies of Relevance to the Initiation Process of Atom Transfer Radical Polymerization. <i>Macromolecules</i> , 2003, 36, 8551-8559.	2.2	161
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