

Yun-Dong Wu

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9325321/publications.pdf>

Version: 2024-02-01

127
papers

5,756
citations

57631

44
h-index

88477

70
g-index

130
all docs

130
docs citations

130
times ranked

5458
citing authors

#	ARTICLE	IF	CITATIONS
1	Palladium-Catalyzed <i>meta</i> -Selective C–H Bond Activation with a Nitrile-Containing Template: Computational Study on Mechanism and Origins of Selectivity. <i>Journal of the American Chemical Society</i> , 2014, 136, 344-355.	6.6	317
2	Computational Organic Chemistry: Bridging Theory and Experiment in Establishing the Mechanisms of Chemical Reactions. <i>Journal of the American Chemical Society</i> , 2015, 137, 1706-1725.	6.6	271
3	Role of <i>N</i> -Acyl Amino Acid Ligands in Pd(II)-Catalyzed Remote C–H Activation of Tethered Arenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 894-897.	6.6	263
4	From Porphyrin Isomers to Octapyrrolic Figure Eight Macrocycles. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 2511-2514.	4.4	168
5	A Theoretical Study on the Mechanism, Regiochemistry, and Stereochemistry of Hydrosilylation Catalyzed by Cationic Ruthenium Complexes. <i>Journal of the American Chemical Society</i> , 2003, 125, 11578-11582.	6.6	156
6	Ligand-Controlled Remarkable Regio- and Stereodivergence in Intermolecular Hydrosilylation of Internal Alkynes: Experimental and Theoretical Studies. <i>Journal of the American Chemical Society</i> , 2013, 135, 13835-13842.	6.6	135
7	A Density Functional Study of Substituent Effects on the O–H and O–CH ₃ Bond Dissociation Energies in Phenol and Anisole. <i>Journal of Organic Chemistry</i> , 1996, 61, 7904-7910.	1.7	132
8	Computational Exploration of Rh ^{III} /Rh ^V and Rh ^{III} /Rh ^I Catalysis in Rhodium(III)-Catalyzed C–H Activation Reactions of <i>N</i> -Phenoxyacetamides with Alkynes. <i>Journal of the American Chemical Society</i> , 2016, 138, 6861-6868.	6.6	116
9	Novel Turns and Helices in Peptides of Chiral \pm -Aminoxy Acids. <i>Journal of the American Chemical Society</i> , 1999, 121, 589-590.	6.6	115
10	Theoretical Analysis of Secondary Structures of β -Peptides. <i>Accounts of Chemical Research</i> , 2008, 41, 1418-1427.	7.6	113
11	An In β ether Chiral Center Modulates the Helicity, Cell Permeability, and Target Binding Affinity of a Peptide. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8013-8017.	7.2	111
12	Octaphyrin-(1.0.1.0.1.0.1.0). <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 2515-2517.	4.4	110
13	New Mechanistic Insights on the Selectivity of Transition-Metal-Catalyzed Organic Reactions: The Role of Computational Chemistry. <i>Accounts of Chemical Research</i> , 2016, 49, 1302-1310.	7.6	100
14	Conformational Features and Anion-Binding Properties of Calix[4]pyrrole: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2001, 66, 3739-3746.	1.7	97
15	A Combined IM β MS/DFT Study on [Pd(MPAA)]-Catalyzed Enantioselective C–H Activation: Relay of Chirality through a Rigid Framework. <i>Chemistry - A European Journal</i> , 2015, 21, 11180-11188.	1.7	94
16	Residue-Specific Force Field Based on the Protein Coil Library. RSFF1: Modification of OPLS-AA/L. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6983-6998.	1.2	93
17	Residue-Specific Force Field Based on Protein Coil Library. RSFF2: Modification of AMBER ff99SB. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1035-1047.	1.2	92
18	PACE Force Field for Protein Simulations. 1. Full Parameterization of Version 1 and Verification. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3373-3389.	2.3	89

#	ARTICLE	IF	CITATIONS
19	Nickel-catalyzed asymmetric hydrogenation of \hat{I}^2 -acylamino nitroolefins: an efficient approach to chiral amines. <i>Chemical Science</i> , 2017, 8, 6419-6422.	3.7	82
20	Synthesis and Characterization of Chiral N^{α} O Turns Induced by \hat{I}^{\pm} -Aminoxy Acids. <i>Journal of Organic Chemistry</i> , 2001, 66, 7303-7312.	1.7	78
21	Theoretical Studies on Alkene Addition to Molybdenum Alkylidenes. <i>Journal of the American Chemical Society</i> , 1997, 119, 8043-8049.	6.6	77
22	Highly Regio- and Stereoselective Hydrosilylation of Internal Thioalkynes under Mild Conditions. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 5632-5635.	7.2	77
23	Mechanism of Ni-NHC Catalyzed Hydrogenolysis of Aryl Ethers: Roles of the Excess Base. <i>ACS Catalysis</i> , 2016, 6, 483-493.	5.5	76
24	A diversity-oriented synthesis of bioactive benzanilides via a regioselective $C(sp^2) \hat{C}^H$ hydroxylation strategy. <i>Chemical Science</i> , 2016, 7, 2229-2238.	3.7	74
25	Assembling a Hybrid Pd Catalyst from a Chiral Anionic Co^{III} Complex and Ligand for Asymmetric $C(sp^3) \hat{C}^H$ Functionalization. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1803-1807.	7.2	73
26	Enantioselective Addition of Cyclic Ketones to Unactivated Alkenes Enabled by Amine/Pd(II) Cooperative Catalysis. <i>ACS Catalysis</i> , 2019, 9, 791-797.	5.5	72
27	Von Porphyrin-Isomeren zu octapyrrolischen Makrocyclen mit 8α -Konformation. <i>Angewandte Chemie</i> , 1995, 107, 2705-2709.	1.6	71
28	WDSPdb: a database for WD40-repeat proteins. <i>Nucleic Acids Research</i> , 2015, 43, D339-D344.	6.5	68
29	Palladium-catalyzed benzo[d]isoxazole synthesis by $C \hat{C}^H$ activation/[4 + 1] annulation. <i>Chemical Science</i> , 2014, 5, 1574-1578.	3.7	67
30	Folding of Fourteen Small Proteins with a Residue-Specific Force Field and Replica-Exchange Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2014, 136, 9536-9539.	6.6	66
31	Crosslinked Aspartic Acids as Helix-Nucleating Templates. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 12088-12093.	7.2	62
32	A Theoretical Study on the Mechanism and Diastereoselectivity of the Kulinkovich Hydroxycyclopropanation Reaction. <i>Journal of the American Chemical Society</i> , 2001, 123, 5777-5786.	6.6	61
33	Parameterization of PACE Force Field for Membrane Environment and Simulation of Helical Peptides and Helix-Helix Association. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 300-313.	2.3	61
34	A Combined DFT/IM-MS Study on the Reaction Mechanism of Cationic Ru(II)-Catalyzed Hydroboration of Alkynes. <i>ACS Catalysis</i> , 2017, 7, 1361-1368.	5.5	56
35	The intrinsic conformational features of amino acids from a protein coil library and their applications in force field development. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3413.	1.3	55
36	Catalytic Asymmetric Homologation of Ketones with \hat{I}^{\pm} -Alkyl \hat{I}^{\pm} -Diazo Esters. <i>Journal of the American Chemical Society</i> , 2021, 143, 2394-2402.	6.6	53

#	ARTICLE	IF	CITATIONS
37	Octaphyrin(1.0.1.0.1.0.1.0). <i>Angewandte Chemie</i> , 1995, 107, 2709-2711.	1.6	52
38	Mechanistic Study on Cu(II)-Catalyzed Oxidative Cross-Coupling Reaction between Arenes and Boronic Acids under Aerobic Conditions. <i>Journal of the American Chemical Society</i> , 2018, 140, 5579-5587.	6.6	52
39	A Combined Computational and Experimental Study of Rh-Catalyzed C-H Silylation with Silacyclobutanes: Insights Leading to a More Efficient Catalyst System. <i>Journal of the American Chemical Society</i> , 2021, 143, 3571-3582.	6.6	52
40	PACE Force Field for Protein Simulations. 2. Folding Simulations of Peptides. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3390-3402.	2.3	51
41	Accurate Structure Prediction and Conformational Analysis of Cyclic Peptides with Residue-Specific Force Fields. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1805-1810.	2.1	50
42	Why does Togni's reagent I exist in the high-energy hypervalent iodine form? Re-evaluation of benziodoxole based hypervalent iodine reagents. <i>Chemical Communications</i> , 2016, 52, 5371-5374.	2.2	50
43	Iron-Catalyzed Enantioselective Radical Carboazidation and Diazidation of α,β -Unsaturated Carbonyl Compounds. <i>Journal of the American Chemical Society</i> , 2021, 143, 11856-11863.	6.6	50
44	Ru-Catalyzed Geminal Hydroboration of Silyl Alkynes via a New <i>gem</i> -Addition Mechanism. <i>Journal of the American Chemical Society</i> , 2020, 142, 13867-13877.	6.6	46
45	Thermal Activation of Methane and Ethene by Bare MO ₂ (M=Ge, Sn, and Pb): A Combined Theoretical/Experimental Study. <i>Chemistry - A European Journal</i> , 2011, 17, 9619-9625.	1.7	45
46	Influence of Side Chain Conformations on Local Conformational Features of Amino Acids and Implication for Force Field Development. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5840-5850.	1.2	44
47	Theoretical Study of α -Peptide Models: Intrinsic Preferences of Helical Structures. <i>Helvetica Chimica Acta</i> , 2002, 85, 3144-3160.	1.0	43
48	Genome-wide Analysis of WD40 Protein Family in Human. <i>Scientific Reports</i> , 2016, 6, 39262.	1.6	43
49	Coarse-Grained Protein Model Coupled with a Coarse-Grained Water Model: A Molecular Dynamics Study of Polyalanine-Based Peptides. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2146-2161.	2.3	42
50	Computational Studies on the Mechanism of the Copper-Catalyzed $\text{sp}^3\text{-C}\ddot{\text{C}}\text{H}$ Cross-Dehydrogenative Coupling Reaction. <i>ChemPlusChem</i> , 2013, 78, 943-951.	1.3	42
51	Enantioselective Formal Vinylogous N-H Insertion of Secondary Aliphatic Amines Catalyzed by a High-Spin Cobalt(II) Complex. <i>Journal of the American Chemical Society</i> , 2021, 143, 9648-9656.	6.6	41
52	Ir-Catalyzed Regio- and Stereoselective Hydrosilylation of Internal Thioalkynes: A Combined Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2016, 81, 6157-6164.	1.7	40
53	Toward a Coarse-Grained Protein Model Coupled with a Coarse-Grained Solvent Model: Solvation Free Energies of Amino Acid Side Chains. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1891-1901.	2.3	39
54	Hybrid Palladium Catalyst Assembled from Chiral Phosphoric Acid and Thioamide for Enantioselective $\alpha\text{-C}(\text{sp}^3)\text{-H}$ Arylation. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12774-12778.	7.2	39

#	ARTICLE	IF	CITATIONS
55	Isoporphycene: The Fourth Constitutional Isomer of Porphyrin with an N4 Core—Occurrence of E/Z Isomerism. <i>Angewandte Chemie - International Edition</i> , 1999, 38, 2919-2923.	7.2	38
56	Ru-Catalyzed Migratory Geminal Semihydrogenation of Internal Alkynes to Terminal Olefins. <i>Journal of the American Chemical Society</i> , 2019, 141, 17441-17451.	6.6	38
57	Contracted Porphyrins: Octaethylisocorrole. <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 2612-2615.	4.4	36
58	Prokaryotic and Highly-Repetitive WD40 Proteins: A Systematic Study. <i>Scientific Reports</i> , 2017, 7, 10585.	1.6	36
59	Enantioselective Intermolecular Heck and Reductive Heck Reactions of Aryl Triflates, Mesylates, and Tosylates Catalyzed by Nickel. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 2828-2832.	7.2	36
60	Metal-Free Synthesis of 3-Arylquinolin-2-ones from Acrylic Amides via a Highly Regioselective 1,2-Aryl Migration: An Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2016, 81, 4058-4065.	1.7	35
61	A Twist of the Twist Mechanism, 2-Iodoxybenzoic Acid (IBX)-Mediated Oxidation of Alcohol Revisited: Theory and Experiment. <i>Organic Letters</i> , 2017, 19, 6502-6505.	2.4	35
62	Self-Assembling Nanotubes Consisting of Rigid Cyclic Peptides. <i>Advanced Functional Materials</i> , 2012, 22, 3051-3056.	7.8	33
63	Significantly Improved Protein Folding Thermodynamics Using a Dispersion-Corrected Water Model and a New Residue-Specific Force Field. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3199-3205.	2.1	33
64	Non-manifesting AHI1 truncations indicate localized loss-of-function tolerance in a severe Mendelian disease gene. <i>Human Molecular Genetics</i> , 2015, 24, 2594-2603.	1.4	32
65	Universal Implementation of a Residue-Specific Force Field Based on CMAP Potentials and Free Energy Decomposition. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4474-4486.	2.3	30
66	Folding Thermodynamics and Mechanism of Five Trp-Cage Variants from Replica-Exchange MD Simulations with RSFF2 Force Field. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5473-5480.	2.3	27
67	Directing Effects on the Copper-Catalyzed Site-Selective Arylation of Indoles. <i>Organic Letters</i> , 2018, 20, 6502-6505.	2.4	26
68	Mechanistic understanding of catalysis by combining mass spectrometry and computation. <i>Chemical Communications</i> , 2019, 55, 12749-12764.	2.2	25
69	Radical Reactivity, Catalysis, and Reaction Mechanism of Arylcopper(II) Compounds: The Missing Link in Organocopper Chemistry. <i>Journal of the American Chemical Society</i> , 2019, 141, 18341-18348.	6.6	24
70	Rh-Catalyzed [4 + 2] Annulation with a Removable Monodentate Structure toward Iminopyranes and Pyranones by C-H Annulation. <i>Organic Letters</i> , 2022, 24, 3003-3008.	2.4	24
71	Significant Refinement of Protein Structure Models Using a Residue-Specific Force Field. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1949-1956.	2.3	23
72	Asymmetric Reductive and Alkynylative Heck Bicyclization of Enynes to Access Conformationally Restricted Aza[3.1.0]bicycles. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 10814-10818.	7.2	23

#	ARTICLE	IF	CITATIONS
73	A Bulky and Electron-Rich π -N-Heterocyclic Carbene-Palladium Complex (SIPr) ^{Ph} ₂ /Pd(cin)Cl: Highly Efficient and Versatile for the Buchwald-Hartwig Amination of (Hetero)aryl Chlorides with (Hetero)aryl Amines at Room Temperature. ACS Catalysis, 2021, 11, 9252-9261.	5.5	23
74	Chiral Sulfoxide-Induced Single Turn Peptide \pm -Helicity. Scientific Reports, 2016, 6, 38573.	1.6	22
75	Mechanistic Study on Pd/Mono-N-protected Amino Acid Catalyzed Vinyl-Vinyl Coupling Reactions: Reactivity and E/Z Selectivity. Organic Letters, 2016, 18, 5240-5243.	2.4	22
76	Assembling a Hybrid Pd Catalyst from a Chiral Anionic Co(III) Complex and Ligand for Asymmetric C(sp ³) Tj ETQq000 rgBT /Overlock 10	1.6	22
77	Systematic investigation of the aza-Cope reaction for fluorescence imaging of formaldehyde <i>in vitro</i> and <i>in vivo</i> . Chemical Science, 2021, 12, 13857-13869.	3.7	22
78	Ligand-Assisted Palladium(II)/(IV) Oxidation for α -C-H Fluorination. Advanced Synthesis and Catalysis, 2016, 358, 1946-1957.	2.1	20
79	Enantioselective Synthesis of Nitriles Containing a Quaternary Carbon Center by Michael Reactions of Silyl Ketene Imines with 1-Acylpyrazoles. Journal of the American Chemical Society, 2021, 143, 19091-19098.	6.6	20
80	An In π -ether Chiral Center Modulates the Helicity, Cell Permeability, and Target Binding Affinity of a Peptide. Angewandte Chemie, 2016, 128, 8145-8149.	1.6	19
81	Intrinsically disordered regions stabilize the helical form of the C-terminal domain of RfaH: A molecular dynamics study. Bioorganic and Medicinal Chemistry, 2016, 24, 4970-4977.	1.4	19
82	A Missing Piece of the Mechanism in Metal-Catalyzed Hydrogenation: Co(π -I)/Co(0)/Co(+I) Catalytic Cycle for Co(π -I)-Catalyzed Hydrogenation. Organic Letters, 2019, 21, 360-364.	2.4	19
83	WDSPdb: an updated resource for WD40 proteins. Bioinformatics, 2019, 35, 4824-4826.	1.8	18
84	Reactivities of d0 transition metal complexes toward oxygen: Synthetic and mechanistic studies. Science in China Series B: Chemistry, 2009, 52, 1723-1733.	0.8	17
85	Structures and conformations of heteroatom-bridged calixarenes. Journal of Physical Organic Chemistry, 2011, 24, 1157-1165.	0.9	17
86	Protein dynamics and structural waters in bromodomains. PLoS ONE, 2017, 12, e0186570.	1.1	17
87	Mechanism of Phosphorylation-Induced Folding of 4E-BP2 Revealed by Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 320-328.	2.3	16
88	Ruthenium-Catalyzed Geminal Hydroborative Cyclization of Enynes. Angewandte Chemie - International Edition, 2022, 61, .	7.2	16
89	Folding Simulations of an \pm -Helical Hairpin Motif \pm with Residue-Specific Force Fields. Journal of Physical Chemistry B, 2016, 120, 33-41.	1.2	14
90	Asymmetric Catalytic (2+1) Cycloaddition of Thioketones to Synthesize Tetrasubstituted Thiiranes. Angewandte Chemie - International Edition, 2022, 61, .	7.2	14

#	ARTICLE	IF	CITATIONS
91	Theoretical Study of a Termolecular Mechanism for the Reaction of (Trimethylsilyl)thiazole with Carbonyl Compounds. <i>Journal of Organic Chemistry</i> , 1996, 61, 1922-1926.	1.7	13
92	Theoretical Study Of $\beta^{2,3}$ -Peptide Models. <i>Journal of the Chinese Chemical Society</i> , 2000, 47, 129-134.	0.8	13
93	Mechanism and Selectivity in the Pd-Catalyzed Difunctionalization of Isoprene. <i>Journal of Organic Chemistry</i> , 2016, 81, 7604-7611.	1.7	13
94	Hybrid Palladium Catalyst Assembled from Chiral Phosphoric Acid and Thioamide for Enantioselective β^2 -H Arylation. <i>Angewandte Chemie</i> , 2020, 132, 12874-12878.	1.6	13
95	Synthesis of Benzofurans and Benzoxazoles through a [3,3]-Sigmatropic Rearrangement: OAc as a Multitasking Functional Group. <i>Organic Process Research and Development</i> , 2019, 23, 1646-1653.	1.3	12
96	Developments and Applications of Coil-Library-Based Residue-Specific Force Fields for Molecular Dynamics Simulations of Peptides and Proteins. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2761-2773.	2.3	11
97	Precise Introduction of the β^{CH} -X (X = F, Cl, Br, I) Moiety to Target Molecules by a Radical Strategy: A Theoretical and Experimental Study. <i>Journal of the American Chemical Society</i> , 2021, 143, 13195-13204.	6.6	11
98	Whole-body PET tracking of a d-dodecapeptide and its radiotheranostic potential for PD-L1 overexpressing tumors. <i>Acta Pharmaceutica Sinica B</i> , 2022, 12, 1363-1376.	5.7	11
99	Reactions of d ⁰ alkylidene and amide complexes with silanes. <i>Pure and Applied Chemistry</i> , 2001, 73, 331-335.	0.9	10
100	PPI network analyses of human WD40 protein family systematically reveal their tendency to assemble complexes and facilitate the complex predictions. <i>BMC Systems Biology</i> , 2018, 12, 41.	3.0	9
101	Effects of Aromatic Substitutions on the Photoreactions in Mg ⁺ (C ₆ H _n F ₂ X _{4-n}) (X = F, CH ₃) Complexes: π Formation and Decomposition of Benzynes Radical Cations. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3356-3366.	1.1	8
102	Density Functional Theory Study of the Reaction between d ⁰ Tungsten Alkylidyne Complexes and H ₂ O: Addition versus Hydrolysis. <i>Inorganic Chemistry</i> , 2017, 56, 7111-7119.	1.9	8
103	Computational Study on the Fate of Oxidative Directing Groups in Ru(II), Rh(III), and Pd(II) Catalyzed C-H Functionalization. <i>Journal of Organic Chemistry</i> , 2020, 85, 12594-12602.	1.7	8
104	Asymmetric Reductive and Alkynylative Heck Bicyclization of Enynes to Access Conformationally Restricted Aza[3.1.0]bicycles. <i>Angewandte Chemie</i> , 2020, 132, 10906-10910.	1.6	8
105	Enantioselective Intermolecular Heck and Reductive Heck Reactions of Aryl Triflates, Mesylates, and Tosylates Catalyzed by Nickel. <i>Angewandte Chemie</i> , 2021, 133, 2864-2868.	1.6	7
106	Accurate Structure Prediction for Protein Loops Based on Molecular Dynamics Simulations with RSFF2C. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4614-4628.	2.3	7
107	Asymmetric Domino Heck Arylation and Alkylation of Nonconjugated Dienes: Double π - π -Sodium Attractive Noncovalent Interaction. <i>Organic Letters</i> , 2021, 23, 7064-7068.	2.4	7
108	A THEORETICAL COMPARISON OF CONFORMATIONAL FEATURES OF CALIX[4]AROMATICS. <i>Journal of Theoretical and Computational Chemistry</i> , 2004, 03, 51-68.	1.8	6

#	ARTICLE	IF	CITATIONS
109	Biophysical and structural characterization of the thermostable WD40 domain of a prokaryotic protein, <i>Thermomonospora curvata</i> PkwA. <i>Scientific Reports</i> , 2018, 8, 12965.	1.6	5
110	IDRMutPred: predicting disease-associated germline nonsynonymous single nucleotide variants (nsSNVs) in intrinsically disordered regions. <i>Bioinformatics</i> , 2020, 36, 4977-4983.	1.8	5
111	Cobalt-Catalyzed 2-(1-Methylhydrazinyl)pyridine-Assisted C-H Alkylation/Annulation: Mechanistic Insights and Rapid Access to Cyclopenta[<i>c</i>]isoquinolinone Derivatives. <i>Journal of Organic Chemistry</i> , 2021, 86, 14915-14927.	1.7	4
112	How to strike a conformational balance in protein force fields for molecular dynamics simulations?. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, e1578.	6.2	4
113	Theoretical Study of the Mechanism and Stereochemistry of Molybdenum Alkylidene Catalyzed Ring-Opening Metathesis Polymerization. <i>ACS Symposium Series</i> , 1999, , 187-197.	0.5	3
114	A novel self-promoted Morita-Baylis-Hillman-like dimerization. <i>Science Bulletin</i> , 2010, 55, 2794-2798.	1.7	3
115	Multifunnel Energy Landscapes for Phosphorylated Translation Repressor 4E-BP2 and Its Mutants. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 800-810.	2.3	3
116	CRISP: accurate structure prediction of disulfide-rich peptides with cystine-specific sequence alignment and machine learning. <i>Bioinformatics</i> , 2020, 36, 3385-3392.	1.8	3
117	Significantly different contact patterns between A ¹²⁴⁰ and A ¹²⁴² monomers involving the N-terminal region. <i>Chemical Biology and Drug Design</i> , 2019, 94, 1615-1625.	1.5	2
118	Critical Computational Evidence Regarding the Long-Standing Controversy over the Main Electrophilic Species in Hypochlorous Acid Solution. <i>Molecules</i> , 2022, 27, 1843.	1.7	2
119	Asymmetric Catalytic (2+1) Cycloaddition of Thioketones to Synthesize Tetrasubstituted Thiiranes. <i>Angewandte Chemie</i> , 0, , .	1.6	2
120	Frontispiece: Asymmetric Catalytic (2+1) Cycloaddition of Thioketones to Synthesize Tetrasubstituted Thiiranes. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	2
121	Ruthenium-Catalyzed Geminal Hydroborative Cyclization of Enynes. <i>Angewandte Chemie</i> , 0, , .	1.6	2
122	Theoretical study of the secondary structures of unionized Poly(¹³ C-D-glutamic acid). <i>Molecular Physics</i> , 2004, 102, 2491-2498.	0.8	1
123	Front Cover Picture: Ligand-Assisted Palladium(II)/(IV) Oxidation for sp ³ C-H Fluorination (<i>Adv. Synth. J.</i> 2021, 10, 2111-2112)	0.1	0
124	Innenr ³ 4cktitelbild: Assembling a Hybrid Pd Catalyst from a Chiral Anionic Co ^{III} Complex and Ligand for Asymmetric C(sp ³) ³ -H Functionalization (<i>Angew. Chem.</i> 6/2019). <i>Angewandte Chemie</i> , 2019, 131, 1863-1863.	1.6	0
125	Phosphate binding sites prediction in phosphorylation-dependent protein-protein interactions. <i>Bioinformatics</i> , 2021, 37, 4712-4718.	1.8	0
126	Total synthesis of monoterpene indole alkaloid (â€)-arbophyllidine. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	0

#	ARTICLE	IF	CITATIONS
127	Frontispiz: Asymmetric Catalytic (2+1) Cycloaddition of Thioketones to Synthesize Tetrasubstituted Thiiranes. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	0