Qiantao Wang

List of Publications by Year
in descending order

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		331670	395702
45	1,221	21	33
papers	citations	h-index	g-index

46	46	46	1487
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis of indoles and quinazolines via additive-controlled selective Câ€“H activation/annulation of N-arylamidines and sulfoxonium ylides. Chemical Communications, 2019, 55, 4039-4042.	4.1	97
2	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. Journal of Chemical Theory and Computation, 2015, 11, 2609-2618.	5.3	93
3	Modeling Organochlorine Compounds and the Ïƒ-Hole Effect Using a Polarizable Multipole Force Field. Journal of Physical Chemistry B, 2014, 118, 6456-6465.	2.6	69
4	An optimized charge penetration model for use with the AMOEBA force field. Physical Chemistry Chemical Physics, 2017, 19, 276-291.	2.8	65
5	Synthesis and biological evaluation of pyrido[2,3-d]pyrimidine-2,4-dione derivatives as eEF-2K inhibitors. Bioorganic and Medicinal Chemistry, 2014, 22, 4910-4916.	3.0	55
6	Iridium-Catalyzed Bâ€“H Bond Insertion Reactions Using Sulfoxonium Ylides as Carbene Precursors toward Î±-Boryl Carbonyls. Organic Letters, 2019, 21, 9005-9008.	4.6	55
7	A stabilized retro-inverso peptide ligand of transferrin receptor for enhanced liposome-based hepatocellular carcinoma-targeted drug delivery. Acta Biomaterialia, 2019, 83, 379-389.	8.3	52
8	Visible light photoredox catalyzed thiophosphate synthesis using methylene blue as a promoter. Organic Chemistry Frontiers, 2018, 5, 1416-1422.	4.5	42
9	The application of the MM/GBSA method in the binding pose prediction of FGFR inhibitors. Physical Chemistry Chemical Physics, 2020, 22, 9656-9663.	2.8	42
10	United polarizable multipole water model for molecular mechanics simulation. Journal of Chemical Physics, 2015, 143, 014504.	3.0	36
11	Graphene oxide mediated thiolation of indoles in water: a green and sustainable approach to synthesize 3-sulfenylindoles. Organic Chemistry Frontiers, 2019, 6, 116-120.	4.5	36
12	1,2,3-Triazole-assisted Câ€“H amidation by cobalt(<scp>iii</scp>) catalysis. Organic Chemistry Frontiers, 2017, 4, 2184-2190.	4.5	34
13	The Molecular Mechanism of Eukaryotic Elongation Factor 2 Kinase Activation. Journal of Biological Chemistry, 2014, 289, 23901-23916.	3.4	32
14	General van der Waals potential for common organic molecules. Bioorganic and Medicinal Chemistry, 2016, 24, 4911-4919.	3.0	30
15	[Cp*Rh^{III}]/Ionic Liquid as a Highly Efficient and Recyclable Catalytic Medium for Câ^'H Amidation. ChemSusChem, 2018, 11, 3672-3678.	6.8	28
16	Practical Synthesis of Benzimidazo[1,2-a]quinolines via Rh(III)-Catalyzed Câ€“H Activation Cascade Reaction from Imidamides and Anthranils. Organic Letters, 2020, 22, 501-504.	4.6	28
17	Polarizable Multipole-Based Force Field for Dimethyl and Trimethyl Phosphate. Journal of Chemical Theory and Computation, 2015, 11, 5326-5339.	5.3	26
18	Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general shortâ€range penetration correction up to quadrupoles. Journal of Computational Chemistry, 2016, 37, 494-506.	3.3	26

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19	Capturing Many-Body Interactions with Classical Dipole Induction Models. Journal of Chemical Theory and Computation, 2017, 13, 2751-2761.	5.3	26
20	3-Silaazetidine: An Unexplored yet Versatile Organosilane Species for Ring Expansion toward Silaazacycles. Journal of the American Chemical Society, 2021, 143, 11141-11151.	13.7	26
21	GLUT₁â€mediated venlafaxineâ€thiamine disulfide systemâ€glucose conjugates with â€œlockâ€inâ€• function for central nervous system delivery. Chemical Biology and Drug Design, 2018, 91, 707-716.	3.2	25
22	Alpha-asarone improves cognitive function of aged rats by alleviating neuronal excitotoxicity via GABAA receptors. Neuropharmacology, 2020, 162, 107843.	4.1	23
23	Improved Hydrogen Bonding at the NDDO-Type Semiempirical Quantum Mechanical/Molecular Mechanical Interface. Journal of Chemical Theory and Computation, 2009, 5, 2206-2211.	5.3	21
24	Estimating and modeling charge transfer from the SAPT induction energy. Journal of Computational Chemistry, 2017, 38, 2222-2231.	3.3	21
25	Palladium-catalyzed direct Câ€“H ethoxycarbonylation of 2-aryl-1,2,3-triazoles and efficient synthesis of suvorexant. Organic Chemistry Frontiers, 2018, 5, 648-652.	4.5	20
26	A novel immunoliposome mediated by CD123 antibody targeting to acute myeloid leukemia cells. International Journal of Pharmaceutics, 2017, 529, 531-542.	5.2	19
27	Anti-CD123 antibody-modified niosomes for targeted delivery of daunorubicin against acute myeloid leukemia. Drug Delivery, 2017, 24, 882-890.	5.7	19
28	Importance of Three-Body Problems and Proteinâ€“Protein Interactions in Proteolysis-Targeting Chimera Modeling: Insights from Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2022, 62, 523-532.	5.4	19
29	Rhodiumâ€Catalyzed orthoâ€Cyanation of 2â€Arylâ€1,2,3â€triazole: An Alternative Approach to Suvorexant. European Journal of Organic Chemistry, 2018, 2018, 723-729.	2.4	18
30	Using docking and alchemical free energy approach to determine the binding mechanism of eEF2K inhibitors and prioritizing the compound synthesis. Frontiers in Molecular Biosciences, 2015, 2, 9.	3.5	15
31	Total synthesis of the isoquinoline alkaloid decumbenine BviaRu(<scp>iii</scp>)-catalyzed Câ€“H activation. Organic Chemistry Frontiers, 2018, 5, 1604-1607.	4.5	14
32	Alpha-asarone Improves Cognitive Function of APP/PS1 Mice and Reducing Aî²42, P-tau and Neuroinflammation, and Promoting Neuron Survival in the Hippocampus. Neuroscience, 2021, 458, 141-152.	2.3	14
33	Hydration Free Energy from Orthogonal Space Random Walk and Polarizable Force Field. Journal of Chemical Theory and Computation, 2014, 10, 2792-2801.	5.3	13
34	Identification and Validation of Novel PERK Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 1467-1475.	5.4	12
35	The development of an Amber-compatible organosilane force field for drug-like small molecules. Physical Chemistry Chemical Physics, 2021, 23, 12582-12591.	2.8	10
36	Synthesis of isatins by the palladium-catalyzed intramolecular acylation of unactivated aryl C(sp2)â€“H bonds. RSC Advances, 2015, 5, 103280-103283.	3.6	9

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37	Group 9 [Cp*MIII] complex-catalyzed Câ€“H olefination of arenes in water at room temperature: a study on the catalytic activity. Organic Chemistry Frontiers, 2019, 6, 967-971.	4.5	8
38	Novel cyclodextrinâ€modified hâ€BN@Pd(II) nanomaterial: An efficient and recoverable catalyst for ligandâ€free Câ€C crossâ€coupling reactions in water. Applied Organometallic Chemistry, 2017, 31, e3854.	3.5	7
39	Reactions of Disulfides with Silyl Phosphites to Generate Thiophosphates Under Neat Conditions. ChemSusChem, 2018, 11, 1426-1431.	6.8	7
40	An Efficient Method for Sulfonylation of Amines, Alcohols and Phenols with N-Fluorobenzenesulfonimide Under Mild Conditions. Chemical Research in Chinese Universities, 2018, 34, 191-196.	2.6	7
41	Synthesis, antiepileptic effects, and structure-activity relationships of Î±-asarone derivatives: In vitro and in vivo neuroprotective effect of selected derivatives. Bioorganic Chemistry, 2021, 115, 105179.	4.1	7
42	Accounting for non-optimal interactions in molecular recognition: a study of ionâ€“Ï€ complexes using a QM/MM model with a dipole-polarisable MM region. Physical Chemistry Chemical Physics, 2011, 13, 19401.	2.8	5
43	Filling the Gap in Understanding the Mechanism of GABA_AR and Propofol Using Computational Approaches. Journal of Chemical Information and Modeling, 2021, 61, 1889-1901.	5.4	3
44	Reliable Prediction of the Proteinâ€“Ligand Binding Affinity Using a Charge Penetration Corrected AMOEBA Force Field: A Case Study of Drug Resistance Mutations in Abl Kinase. Journal of Chemical Theory and Computation, 2022, , .	5.3	3
45	Calculation of Transport Parameters Using ab initio and AMOEBA Polarizable Force Field Methods. Journal of Physical Chemistry A, 2021, 125, 4918-4927.	2.5	2