Qiantao Wang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5054460/publications.pdf

Version: 2024-02-01

		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	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
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	Alpha-asarone improves cognitive function of aged rats by alleviating neuronal excitotoxicity via GABAA receptors. Neuropharmacology, 2020, 162, 107843.	4.1	23
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	Reactions of Disulfides with Silyl Phosphites to Generate Thiophosphates Under Neat Conditions. ChemSusChem, 2018, 11, 1426-1431.	6.8	7
18	Visible light photoredox catalyzed thiophosphate synthesis using methylene blue as a promoter. Organic Chemistry Frontiers, 2018, 5, 1416-1422.	4.5	42

#	Article	IF	Citations
19	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
20	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
21	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
22	GLUT₁â€mediated venlafaxineâ€thiamine disulfide systemâ€glucose conjugates with â€œlockâ€•function for central nervous system delivery. Chemical Biology and Drug Design, 2018, 91, 707-716.	3.2	25
23	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
24	[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
25	Capturing Many-Body Interactions with Classical Dipole Induction Models. Journal of Chemical Theory and Computation, 2017, 13, 2751-2761.	5.3	26
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	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
28	Anti-CD123 antibody-modified niosomes for targeted delivery of daunorubicin against acute myeloid leukemia. Drug Delivery, 2017, 24, 882-890.	5.7	19
29	Estimating and modeling charge transfer from the SAPT induction energy. Journal of Computational Chemistry, 2017, 38, 2222-2231.	3.3	21
30	1,2,3-Triazole-assisted Câ€“H amidation by cobalt(<scp>iii</scp>) catalysis. Organic Chemistry Frontiers, 2017, 4, 2184-2190.	4.5	34
31	An optimized charge penetration model for use with the AMOEBA force field. Physical Chemistry Chemical Physics, 2017, 19, 276-291.	2.8	65
32	General van der Waals potential for common organic molecules. Bioorganic and Medicinal Chemistry, 2016, 24, 4911-4919.	3.0	30
33	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
34	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
35	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
36	United polarizable multipole water model for molecular mechanics simulation. Journal of Chemical Physics, 2015, 143, 014504.	3.0	36

#	Article	IF	Citations
37	Polarizable Multipole-Based Force Field for Dimethyl and Trimethyl Phosphate. Journal of Chemical Theory and Computation, 2015, 11, 5326-5339.	5.3	26
38	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
39	The Molecular Mechanism of Eukaryotic Elongation Factor 2 Kinase Activation. Journal of Biological Chemistry, 2014, 289, 23901-23916.	3.4	32
40	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
41	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
42	Identification and Validation of Novel PERK Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 1467-1475.	5.4	12
43	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
44	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
45	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