

Binh Khanh Mai

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1670773/publications.pdf>

Version: 2024-02-01

46
papers

1,052
citations

361413

20
h-index

454955

30
g-index

57
all docs

57
docs citations

57
times ranked

1088
citing authors

#	ARTICLE	IF	CITATIONS
1	Top Leads for Swine Influenza A/H1N1 Virus Revealed by Steered Molecular Dynamics Approach. Journal of Chemical Information and Modeling, 2010, 50, 2236-2247.	5.4	84
2	Steered Molecular Dynamics-A Promising Tool for Drug Design. Current Bioinformatics, 2012, 7, 342-351.	1.5	73
3	Neuraminidase inhibitor R-125489 "A promising drug for treating influenza virus: Steered molecular dynamics approach. Biochemical and Biophysical Research Communications, 2011, 410, 688-691.	2.1	66
4	Determination of Spin Inversion Probability, H-Tunneling Correction, and Regioselectivity in the Two-State Reactivity of Nonheme Iron(IV)-Oxo Complexes. Journal of Physical Chemistry Letters, 2015, 6, 1472-1476.	4.6	64
5	Efficient Formation of 2,3-Dihydrofurans via Iron-Catalyzed Cycloisomerization of $\hat{\pm}$ -Allenols. ACS Catalysis, 2018, 8, 12-16.	11.2	42
6	Generation of Axially Chiral Fluoroallenes through a Copper-Catalyzed Enantioselective $\hat{2}$ -Fluoride Elimination. Journal of the American Chemical Society, 2021, 143, 13759-13768.	13.7	40
7	Inversion of Enantioselectivity in Allene Gas versus Allyl Acetate Reductive Aldehyde Allylation Guided by Metal-Centered Stereogenicity: An Experimental and Computational Study. ACS Catalysis, 2019, 9, 9158-9163.	11.2	39
8	Highly Selective Palladium-Catalyzed Hydroborylative Carbocyclization of Bisallenes to Seven-Membered Rings. Journal of the American Chemical Society, 2018, 140, 14324-14333.	13.7	38
9	Study of Tamiflu Sensitivity to Variants of A/H5N1 Virus Using Different Force Fields. Journal of Chemical Information and Modeling, 2011, 51, 2266-2276.	5.4	36
10	Mechanisms of Rh-Catalyzed Oxyfluorination and Oxytrifluoromethylation of Diazocarbonyl Compounds with Hypervalent Fluoroiodine. ACS Catalysis, 2018, 8, 4483-4492.	11.2	35
11	Is It Fe(III)-Oxyl Radical That Abstracts Hydrogen in the C-H Activation of TauD? A Theoretical Study Based on the DFT Potential Energy Surfaces. Inorganic Chemistry, 2016, 55, 3844-3852.	4.0	33
12	Confronting the Challenging Asymmetric Carbonyl 1,2-Addition Using Vinyl Heteroarene Pronucleophiles: Ligand-Controlled Regiodivergent Processes through a Dearomatized Allyl-Cu Species. Journal of the American Chemical Society, 2022, 144, 5985-5995.	13.7	32
13	Tropylium-Promoted Hydroboration Reactions: Mechanistic Insights <i>via</i> Experimental and Computational Studies. Journal of Organic Chemistry, 2021, 86, 9117-9133.	3.2	31
14	Mechanical Unfolding of Acylphosphatase Studied by Single-Molecule Force Spectroscopy and MD Simulations. Biophysical Journal, 2010, 99, 238-247.	0.5	26
15	Diastereoselective Synthesis of <i>N</i> -Protected 2,3-Dihydropyrroles via Iron-Catalyzed Cycloisomerization of $\hat{\pm}$ -Allenic Sulfonamides. ACS Catalysis, 2019, 9, 1733-1737.	11.2	26
16	How Does CO ₂ React with Styrene Oxide in Co-MOF-74 and Mg-MOF-74? Catalytic Mechanisms Proposed by QM/MM Calculations. Journal of Physical Chemistry C, 2018, 122, 503-514.	3.1	25
17	Estimation of the Binding Free Energy of AC1NX476 to \hat{HIV} Protease Wild Type and Mutations Using Free-Energy Perturbation Method. Chemical Biology and Drug Design, 2015, 86, 546-558.	3.2	24
18	Proton Transfer Dependence on Hydrogen-Bonding of Solvent to the Water Wire: A Theoretical Study. Journal of Physical Chemistry B, 2013, 117, 307-315.	2.6	23

#	ARTICLE	IF	CITATIONS
19	Efficient Stereoselective Carbocyclization to <i>cis</i> -1,4-Disubstituted Heterocycles Enabled by Dual Pd/Electron Transfer Mediator (ETM) Catalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 5751-5759.	13.7	21
20	Mechanisms of Rh-Catalyzed Oxyaminofluorination and Oxyaminotrifluoromethylthiolation of Diazocarbonyl Compounds with Electrophilic Reagents. <i>Organic Letters</i> , 2018, 20, 6646-6649.	4.6	20
21	Unusual Alternating Crystallization-Induced Emission Enhancement Behavior in Nonconjugated β -Phenylalkyl Tropylium Salts. <i>Journal of the American Chemical Society</i> , 2021, 143, 20384-20394.	13.7	20
22	The Kinetic Isotope Effect as a Probe of Spin Crossover in the C \equiv H Activation of Methane by the Fe ⁺ Cation. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 3946-3951.	13.8	19
23	Controlling cyclization pathways in palladium(ⁱⁱ)-catalyzed intramolecular alkene hydro-functionalization <i>via</i> substrate directivity. <i>Chemical Science</i> , 2020, 11, 11307-11314.	7.4	19
24	Improving \langle ligand ranking \rangle of \langle AutoDock \rangle Vina by changing the empirical parameters. <i>Journal of Computational Chemistry</i> , 2022, 43, 160-169.	3.3	19
25	Insights into the binding and covalent inhibition mechanism of PF-07321332 to SARS-CoV-2 M ^{pro} . <i>RSC Advances</i> , 2022, 12, 3729-3737.	3.6	19
26	Enantioselective Iridium-Catalyzed Allylation of Nitroalkanes: Entry to \hat{I}^2 -Stereogenic $\hat{I}\pm$ -Quaternary Primary Amines. <i>Journal of the American Chemical Society</i> , 2021, 143, 9343-9349.	13.7	18
27	Adequate prediction for inhibitor affinity of Al^{2+} protofibril using the linear interaction energy method. <i>RSC Advances</i> , 2019, 9, 12455-12461.	3.6	16
28	C \equiv N Bond Forming Radical Rebound Is the Enantioselectivity-Determining Step in P411-Catalyzed Enantioselective C(sp ³) -- H Amination: A Combined Computational and Experimental Investigation. <i>Journal of the American Chemical Society</i> , 2022, 144, 11215-11225.	13.7	15
29	Development and Characterization of Monomeric N-End Rule Inhibitors through <i>In Vitro</i> Model Substrates. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 2540-2546.	6.4	13
30	Tropolonate Salts as Acyl-Transfer Catalysts under Thermal and Photochemical Conditions: Reaction Scope and Mechanistic Insights. <i>ACS Catalysis</i> , 2020, 10, 12596-12606.	11.2	13
31	Theoretical Studies for Large Tunneling and the Hydrogen-Transfer Mechanism in the C \equiv H Activation of CH ₃ CN by a Di($\frac{1}{4}$ -oxo)diiron(IV) Complex: A Model for Intermediate Q in Soluble Methane Monooxygenase. <i>Chemistry - A European Journal</i> , 2013, 19, 3568-3572.	3.3	12
32	Lithium Cuprate Coupling Reactions: Evaluation of Computational Methods for Determination of the Reaction Mechanisms. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5005-5015.	2.5	11
33	Characterization of mammalian N-degrons and development of heterovalent inhibitors of the N-end rule pathway. <i>Chemical Science</i> , 2013, 4, 3339.	7.4	10
34	Substrate-Dependent H/D Kinetic Isotope Effects and the Role of the Di($\frac{1}{4}$ -oxo)diiron(IV) Core in Soluble Methane Monooxygenase: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2014, 20, 6532-6541.	3.3	9
35	Kinetic Isotope Effects as a Probe for the Protonolysis Mechanism of Alkylmetal Complexes: VTST/MT Calculations Based on DFT Potential Energy Surfaces. <i>Inorganic Chemistry</i> , 2016, 55, 9822-9829.	4.0	9
36	Carbenoid Alkene Insertion Reactions of Oxiranyllithiums. <i>Journal of Organic Chemistry</i> , 2012, 77, 8605-8614.	3.2	7

#	ARTICLE	IF	CITATIONS
37	VTST/MT studies of the catalytic mechanism of C-H activation by transition metal complexes with [Cu ₂ (μ -O ₂)], [Fe ₂ (μ -O ₂)] and Fe(IV)=O cores based on DFT potential energy surfaces. <i>Journal of Biological Inorganic Chemistry</i> , 2017, 22, 321-338.	2.6	7
38	Excited-State Multiple Proton Transfer Depending on the Acidity and Basicity of Mediating Alcohols in 7-Azaindole (ROH) ₂ (R=H, CH_3) Complexes: A Theoretical Study. <i>Photochemistry and Photobiology</i> , 2015, 91, 306-314.	2.5	6
39	Esterification of Tertiary Amides: Remarkable Additive Effects of Potassium Alkoxides for Generating Hetero Manganese-Potassium Dinuclear Active Species. <i>Chemistry - A European Journal</i> , 2020, 26, 10735-10742.	3.3	6
40	Kinetic, ESI-MS, and Computational Studies of η^5 -Allyliridium-C ₆ O ₂ -Benzoate-Catalyzed Allylic Amination: Understanding the Effect of Cesium Ion. <i>ACS Catalysis</i> , 2022, 12, 3660-3668.	11.2	6
41	The Antipsychotic Drug Clozapine Suppresses the RGS4 Polyubiquitylation and Proteasomal Degradation Mediated by the Arg/N-Degron Pathway. <i>Neurotherapeutics</i> , 2021, 18, 1768-1782.	4.4	5
42	Unraveling the Mechanism of the Ir ^{III} -Catalyzed Regiospecific Synthesis of α -Chlorocarbonyl Compounds from Allylic Alcohols. <i>Chemistry - A European Journal</i> , 2020, 26, 14978-14986.	3.3	4
43	Ring Contraction of Tropylium Ions into Benzenoid Derivatives. <i>Organic Letters</i> , 2022, 24, 2520-2525.	4.6	3
44	Long-range proton relay shows an inverse linear free energy relationship depending on the pK _a of the hydrogen-bonded wire. <i>RSC Advances</i> , 2015, 5, 2669-2676.	3.6	2
45	Mechanisms of Metal-Catalyzed Electrophilic F/CF ₃ /SCF ₃ Transfer Reactions from Quantum Chemical Calculations. <i>Topics in Organometallic Chemistry</i> , 2020, , 39-56.	0.7	2
46	Esterification of Tertiary Amides: Remarkable Additive Effects of Potassium Alkoxides for Generating Hetero Manganese-Potassium Dinuclear Active Species. <i>Chemistry - A European Journal</i> , 2020, 26, 10647-10647.	3.3	0