Binh Khanh Mai

List of Publications by Year
in descending order

46	1,052	361296 20	454834 30
papers	citations	h-index	g-index

57	57	57	1088
all docs	docs citations	times ranked	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.	2.5	84
2	Steered Molecular Dynamics-A Promising Tool for Drug Design. Current Bioinformatics, 2012, 7, 342-351.	0.7	73
3	Neuraminidase inhibitor R-125489 â€“ A promising drug for treating influenza virus: Steered molecular dynamics approach. Biochemical and Biophysical Research Communications, 2011, 410, 688-691.	1.0	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.	2.1	64
5	Efficient Formation of 2,3-Dihydrofurans via Iron-Catalyzed Cycloisomerization of Î±-Allenols. ACS Catalysis, 2018, 8, 12-16.	5.5	42
6	Generation of Axially Chiral Fluoroallenes through a Copper-Catalyzed Enantioselective Î²-Fluoride Elimination. Journal of the American Chemical Society, 2021, 143, 13759-13768.	6.6	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.	5.5	39
8	Highly Selective Palladium-Catalyzed Hydroborylative Carbocyclization of Bisallenes to Seven-Membered Rings. Journal of the American Chemical Society, 2018, 140, 14324-14333.	6.6	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.	2.5	36
10	Mechanisms of Rh-Catalyzed Oxyfluorination and Oxytrifluoromethylation of Diazocarbonyl Compounds with Hypervalent Fluoroiodine. ACS Catalysis, 2018, 8, 4483-4492.	5.5	35
11	Is It Fe(III)-Oxyl Radical That Abstracts Hydrogen in the Câ€“H Activation of TauD? A Theoretical Study Based on the DFT Potential Energy Surfaces. Inorganic Chemistry, 2016, 55, 3844-3852.	1.9	33
12	Confronting the Challenging Asymmetric Carbonyl 1,2-Addition Using Vinyl Heteroarene Pronucleophiles: Ligand-Controlled Regiodivergent Processes through a Dearomatized Allylâ€“Cu Species. Journal of the American Chemical Society, 2022, 144, 5985-5995.	6.6	32
13	Tropylium-Promoted Hydroboration Reactions: Mechanistic Insights Via Experimental and Computational Studies. Journal of Organic Chemistry, 2021, 86, 9117-9133.	1.7	31
14	Mechanical Unfolding of Acylphosphatase Studied by Single-Molecule Force Spectroscopy and MD Simulations. Biophysical Journal, 2010, 99, 238-247.	0.2	26
15	Diastereoselective Synthesis of N-Protected 2,3-Dihydropyrroles via Iron-Catalyzed Cycloisomerization of Î±-Allenic Sulfonamides. ACS Catalysis, 2019, 9, 1733-1737.	5.5	26
16	How Does CO₂ 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.	1.5	25
17	Estimation of the Binding Free Energy of AC1NX476 toÂHIVâ€1 Protease Wild Type and Mutations Using FreeÂEnergy Perturbation Method. Chemical Biology and Drug Design, 2015, 86, 546-558.	1.5	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.	1.2	23

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19	Efficient Stereoselective Carbocyclization to cis-1,4-Disubstituted Heterocycles Enabled by Dual Pd/Electron Transfer Mediator (ETM) Catalysis. Journal of the American Chemical Society, 2020, 142, 5751-5759.	6.6	21
20	Mechanisms of Rh-Catalyzed Oxyaminofluorination and Oxyaminotrifluoromethylthiolation of Diazocarbonyl Compounds with Electrophilic Reagents. Organic Letters, 2018, 20, 6646-6649.	2.4	20
21	Unusual Alternating Crystallization-Induced Emission Enhancement Behavior in Nonconjugated Ï‰-Phenylalkyl Tropylium Salts. Journal of the American Chemical Society, 2021, 143, 20384-20394.	6.6	20
22	The Kinetic Isotope Effect as a Probe of Spin Crossover in the Cï£¿H Activation of Methane by the FeO⁺ Cation. Angewandte Chemie - International Edition, 2015, 54, 3946-3951.	7.2	19
23	Controlling cyclization pathways in palladium(<scp>II</scp>)-catalyzed intramolecular alkene hydro-functionalization via substrate directivity. Chemical Science, 2020, 11, 11307-11314.	3.7	19
24	Improving <scp>ligandâ€ranking</scp> of <scp>AutoDock</scp> Vina by changing the empirical parameters. Journal of Computational Chemistry, 2022, 43, 160-169.	1.5	19
25	Insights into the binding and covalent inhibition mechanism of PF-07321332 to SARS-CoV-2 M^{pro}. RSC Advances, 2022, 12, 3729-3737.	1.7	19
26	Enantioselective Iridium-Catalyzed Allylation of Nitroalkanes: Entry to Î²-Stereogenic Î±-Quaternary Primary Amines. Journal of the American Chemical Society, 2021, 143, 9343-9349.	6.6	18
27	Adequate prediction for inhibitor affinity of AÎ²₄₀ protofibril using the linear interaction energy method. RSC Advances, 2019, 9, 12455-12461.	1.7	16
28	Câ€“N Bond Forming Radical Rebound Is the Enantioselectivity-Determining Step in P411-Catalyzed Enantioselective C(sp³)â€“H Amination: A Combined Computational and Experimental Investigation. Journal of the American Chemical Society, 2022, 144, 11215-11225.	6.6	15
29	Development and Characterization of Monomeric N-End Rule Inhibitors through In Vitro Model Substrates. Journal of Medicinal Chemistry, 2013, 56, 2540-2546.	2.9	13
30	Tropolonate Salts as Acyl-Transfer Catalysts under Thermal and Photochemical Conditions: Reaction Scope and Mechanistic Insights. ACS Catalysis, 2020, 10, 12596-12606.	5.5	13
31	Theoretical Studies for Large Tunneling and the Hydrogenâ€Transfer Mechanism in the Cï£¿H Activation of CH₃CN by a Di(Î¼â€oxo)diiron(IV) Complex: A Model for Intermediate Q in Soluble Methane Monooxygenase. Chemistry - A European Journal, 2013, 19, 3568-3572.	1.7	12
32	Lithium Cuprate Coupling Reactions: Evaluation of Computational Methods for Determination of the Reaction Mechanisms. Journal of Physical Chemistry A, 2010, 114, 5005-5015.	1.1	11
33	Characterization of mammalian N-degrons and development of heterovalent inhibitors of the N-end rule pathway. Chemical Science, 2013, 4, 3339.	3.7	10
34	Substrate-Dependent H/D Kinetic Isotope Effects and the Role of the Di(Î¼-oxo)diiron(IV) Core in Soluble Methane Monooxygenase: A Theoretical Study. Chemistry - A European Journal, 2014, 20, 6532-6541.	1.7	9
35	Kinetic Isotope Effects as a Probe for the Protonolysis Mechanism of Alkylmetal Complexes: VTST/MT Calculations Based on DFT Potential Energy Surfaces. Inorganic Chemistry, 2016, 55, 9822-9829.	1.9	9
36	Carbenoid Alkene Insertion Reactions of Oxiranyllithiums. Journal of Organic Chemistry, 2012, 77, 8605-8614.	1.7	7

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37	VTST/MT studies of the catalytic mechanism of Câ€“H activation by transition metal complexes with [Cu2(Î¼-O2)], [Fe2(Î¼-O2)] and Fe(IV)â€“O cores based on DFT potential energy surfaces. Journal of Biological Inorganic Chemistry, 2017, 22, 321-338.	1.1	7
38	Excitedâ€State Multiple Proton Transfer Depending on the Acidity and Basicity of Mediating Alcohols in 7â€Azaindoleâ€“(<scp>ROH</scp>)₂ (R=H, <scp>CH</scp>₃) Complexes: A Theoretical Study. Photochemistry and Photobiology, 2015, 91, 306-314.	1.3	6
39	Esterification of Tertiary Amides: Remarkable Additive Effects of Potassium Alkoxides for Generating Hetero Manganeseâ€“Potassium Dinuclear Active Species. Chemistry - A European Journal, 2020, 26, 10735-10742.	1.7	6
40	Kinetic, ESIâ€“CIDâ€“MS, and Computational Studies of Ï€-AllyliridiumC,O-Benzoate-Catalyzed Allylic Amination: Understanding the Effect of Cesium Ion. ACS Catalysis, 2022, 12, 3660-3668.	5.5	6
41	The Antipsychotic Drug Clozapine Suppresses the RGS4 Polyubiquitylation and Proteasomal Degradation Mediated by the Arg/N-Degron Pathway. Neurotherapeutics, 2021, 18, 1768-1782.	2.1	5
42	Unraveling the Mechanism of the Ir^{III}â€Catalyzed Regiospecific Synthesis of Î±â€Chlorocarbonyl Compounds from Allylic Alcohols. Chemistry - A European Journal, 2020, 26, 14978-14986.	1.7	4
43	Ring Contraction of Tropylium Ions into Benzenoid Derivatives. Organic Letters, 2022, 24, 2520-2525.	2.4	3
44	Long-range proton relay shows an inverse linear free energy relationship depending on the pKa of the hydrogen-bonded wire. RSC Advances, 2015, 5, 2669-2676.	1.7	2
45	Mechanisms of Metal-Catalyzed Electrophilic F/CF3/SCF3 Transfer Reactions from Quantum Chemical Calculations. Topics in Organometallic Chemistry, 2020, , 39-56.	0.7	2
46	Esterification of Tertiary Amides: Remarkable Additive Effects of Potassium Alkoxides for Generating Hetero Manganeseâ€“Potassium Dinuclear Active Species. Chemistry - A European Journal, 2020, 26, 10647-10647.	1.7	0