

Daniel BÃ-m

List of Publications by Year in descending order

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Version: 2024-02-01

24
papers

494
citations

687363

13
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677142

22
g-index

27
all docs

27
docs citations

27
times ranked

618
citing authors

#	ARTICLE	IF	CITATIONS
1	Beyond the classical thermodynamic contributions to hydrogen atom abstraction reactivity. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E10287-E10294.	7.1	74
2	Toward Accurate Conformational Energies of Smaller Peptides and Medium-Sized Macrocycles: MPCONF196 Benchmark Energy Data Set. Journal of Chemical Theory and Computation, 2018, 14, 1254-1266.	5.3	69
3	Elucidating the Mechanism of Excited-State Bond Homolysis in Nickel-Bipyridine Photoredox Catalysts. Journal of the American Chemical Society, 2022, 144, 6516-6531.	13.7	47
4	Local Electric Fields As a Natural Switch of Heme-Iron Protein Reactivity. ACS Catalysis, 2021, 11, 6534-6546.	11.2	40
5	Cytosine Radical Cations: A Gas-Phase Study Combining IRMPD Spectroscopy, LVPD Spectroscopy, Ion-Molecule Reactions, and Theoretical Calculations. ChemPhysChem, 2017, 18, 1293-1301.	2.1	29
6	Accurate Prediction of One-Electron Reduction Potentials in Aqueous Solution by Variable-Temperature H-Atom Addition/Abstraction Methodology. Journal of Physical Chemistry Letters, 2016, 7, 7-13.	4.6	24
7	Proton-Electron Transfer to the Active Site Is Essential for the Reaction Mechanism of Soluble β -Desaturase. Journal of the American Chemical Society, 2020, 142, 10412-10423.	13.7	24
8	Structural and computational basis for potent inhibition of glutamate carboxypeptidase II by carbamate-based inhibitors. Bioorganic and Medicinal Chemistry, 2019, 27, 255-264.	3.0	21
9	Copper(II) and Zinc(II) Complexes of Conformationally Constrained Polyazamacrocycles as Efficient Catalysts for RNA Model Substrate Cleavage in Aqueous Solution at Physiological pH. Chemistry - A European Journal, 2016, 22, 10426-10437.	3.3	20
10	Mono- and binuclear non-heme iron chemistry from a theoretical perspective. Journal of Biological Inorganic Chemistry, 2016, 21, 619-644.	2.6	20
11	Macrocycle Conformational Sampling by DFT-D3/COSMO-RS Methodology. Journal of Chemical Information and Modeling, 2018, 58, 48-60.	5.4	19
12	Preparation of (Pentafluorosulfanyl)benzenes by Direct Fluorination of Diaryldisulfides: Synthetic Approach and Mechanistic Aspects. Chemistry - A European Journal, 2019, 25, 11375-11382.	3.3	18
13	Electrostatic regulation of blue copper sites. Chemical Science, 2021, 12, 11406-11413.	7.4	15
14	Increase in Solubility of Poorly-Ionizable Pharmaceuticals by Salt Formation: A Case of Agomelatine Sulfonates. Crystal Growth and Design, 2017, 17, 5283-5294.	3.0	13
15	Computational Electrochemistry as a Reliable Probe of Experimentally Elusive Mononuclear Nonheme Iron Species. Journal of Physical Chemistry C, 2018, 122, 10773-10782.	3.1	12
16	Reactive mode composition factor analysis of transition states: the case of coupled electron-proton transfers. Physical Chemistry Chemical Physics, 2019, 21, 24912-24918.	2.8	12
17	Radical Reactions Affecting Polar Groups in Threonine Peptide Ions. Journal of Physical Chemistry B, 2017, 121, 6557-6569.	2.6	9
18	Predicting Effects of Site-Directed Mutagenesis on Enzyme Kinetics by QM/MM and QM Calculations: A Case of Glutamate Carboxypeptidase II. Journal of Physical Chemistry B, 2022, 126, 132-143.	2.6	9

#	ARTICLE	IF	CITATIONS
19	Dissecting the Temperature Dependence of Electron-Proton Transfer Reactivity. <i>Journal of Physical Chemistry C</i> , 2019, 123, 21422-21428.	3.1	6
20	Preparation and redox properties of fluorinated 1,3-diphenylisobenzofurans. <i>Electrochimica Acta</i> , 2019, 321, 134659.	5.2	4
21	Near-UV Water Splitting by Cu, Ni, and Co Complexes in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2069-2078.	2.5	3
22	From Synthetic to Biological Fe ₄ S ₄ Complexes: Redox Properties Correlated to Function of Radical S-Adenosylmethionine Enzymes. <i>ChemPlusChem</i> , 2020, 85, 2534-2541.	2.8	3
23	Understanding desaturation/hydroxylation activity of castor stearyl Δ^9 -Desaturase through rational mutagenesis. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 1378-1388.	4.1	3
24	Frontispiece: Copper(II) and Zinc(II) Complexes of Conformationally Constrained Polyazamacrocycles as Efficient Catalysts for RNA Model Substrate Cleavage in Aqueous Solution at Physiological pH. <i>Chemistry - A European Journal</i> , 2016, 22, .	3.3	0