

Martha C Daza

List of Publications by Year in descending order

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23
papers

511
citations

759233

12
h-index

642732

23
g-index

23
all docs

23
docs citations

23
times ranked

829
citing authors

#	ARTICLE	IF	CITATIONS
1	Ion mobility spectrometry experiments should be carried out at high temperatures to reduce uncertainties in the measurement of reduced mobilities. <i>Analytical Methods</i> , 2021, 13, 2878-2887.	2.7	4
2	Effect of the acyl-group length on the chemoselectivity of the lipase-catalyzed acylation of propranolol—a computational study. <i>Journal of Molecular Modeling</i> , 2021, 27, 198.	1.8	1
3	Hydrogen Bonds and $n \rightarrow \pi^*$ Interactions in the Acetylation of Propranolol Catalyzed by <i>Candida antarctica</i> Lipase B: A QTAIM Study. <i>ACS Omega</i> , 2021, 6, 20992-21004.	3.5	2
4	Finite-temperature effect in the O-acylation of (R,S)-propranolol catalyzed by <i>Candida antarctica</i> lipase B. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 107, 107951.	2.4	1
5	The Dimer-of-Trimers Assembly Prevents Catalysis at the Transferase Site of Prokaryotic FAD Synthase. <i>Biophysical Journal</i> , 2018, 115, 988-995.	0.5	11
6	Concerted double proton-transfer electron-transfer between catechol and superoxide radical anion. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26179-26190.	2.8	30
7	Protonation-State-Driven Photophysics in Phenothiazinium Dyes: Intersystem Crossing and Singlet-Oxygen Production. <i>ChemPhotoChem</i> , 2017, 1, 459-469.	3.0	5
8	Quantum Mechanics/Molecular Mechanics Insights into the Enantioselectivity of the O-Acetylation of (R,S)-Propranolol Catalyzed by <i>Candida antarctica</i> Lipase B. <i>ACS Catalysis</i> , 2017, 7, 115-127.	11.2	23
9	Internal heavy atom effects in phenothiazinium dyes: enhancement of intersystem crossing via vibronic spin-orbit coupling. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11350-11358.	2.8	55
10	Computational study of the enantioselectivity of the O-acetylation of (R,S)-propranolol catalyzed by <i>Candida antarctica</i> lipase B. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2014, 108, 21-31.	1.8	12
11	Acetylation of (R,S)-propranolol catalyzed by <i>Candida antarctica</i> lipase B: An experimental and computational study. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2013, 98, 21-29.	1.8	20
12	Visible light singlet oxygen production with tetra(4-carboxyphenyl)porphyrin/SiO ₂ . <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 259, 47-52.	3.9	22
13	A theoretical study of thionine: spin-orbit coupling and intersystem crossing. <i>Photochemical and Photobiological Sciences</i> , 2012, 11, 1860-1867.	2.9	24
14	A quantum chemical investigation of the electronic structure of thionine. <i>Photochemical and Photobiological Sciences</i> , 2012, 11, 397-408.	2.9	32
15	CoH _n (n=1-3): Classical and non-classical cobalt polyhydride. <i>Chemical Physics Letters</i> , 2010, 490, 143-147.	2.6	5
16	Visible light superoxide radical anion generation by tetra(4-carboxyphenyl)porphyrin/TiO ₂ : EPR characterization. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2010, 215, 172-178.	3.9	97
17	On the nature of copper-hydrogen bonding: AIM and NBO analysis of CuH _n (1) Tj ETQq1 1 0,784314 rgBT /Ove	2.0	4
18	Hydrogen bonds C-H...O in superoxide radical 1,4-Pentadiene complexes. <i>Computational and Theoretical Chemistry</i> , 2009, 893, 77-83.	1.5	5

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19	Photophysics of phenalenone: quantum-mechanical investigation of singlet \leftrightarrow triplet intersystem crossing. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1688.	2.8	31
20	Quantum chemical and chemotopological study of fourth row monohydrides. <i>Chemical Physics Letters</i> , 2006, 428, 55-61.	2.6	10
21	Structure and bonding of weak hydrogen peroxide complexes. <i>Computational and Theoretical Chemistry</i> , 2002, 580, 117-126.	1.5	25
22	Structure and bonding of H ₂ O ₂ $\cdot\cdot$ X complexes with (X = NO ⁺ , CN ⁻ , HCN, HNC, CO). <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4089-4094.	2.8	21
23	Basis set superposition error-counterpoise corrected potential energy surfaces. Application to hydrogen peroxide $\cdot\cdot$ X (X=F \cdot , \cdot Cl \cdot , Br \cdot , \cdot Li ⁺ , \cdot Na ⁺) complexes. <i>Journal of Chemical Physics</i> , 1999, 110, 11806-11813.	3.0	71