

Martha C Daza

List of Publications by Year in descending order

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23
papers

511
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759233

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642732

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23
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23
times ranked

829
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	Basis set superposition error-counterpoise corrected potential energy surfaces. Application to hydrogen peroxide- X^- ($X = F^-, Cl^-, Br^-, Li^+, Na^+$) complexes. <i>Journal of Chemical Physics</i> , 1999, 110, 11806-11813.	3.0	71
3	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
4	A quantum chemical investigation of the electronic structure of thionine. <i>Photochemical and Photobiological Sciences</i> , 2012, 11, 397-408.	2.9	32
5	Photophysics of phenalenone: quantum-mechanical investigation of singlet-triplet intersystem crossing. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1688.	2.8	31
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	Structure and bonding of weak hydrogen peroxide complexes. <i>Computational and Theoretical Chemistry</i> , 2002, 580, 117-126.	1.5	25
8	A theoretical study of thionine: spin-orbit coupling and intersystem crossing. <i>Photochemical and Photobiological Sciences</i> , 2012, 11, 1860-1867.	2.9	24
9	Quantum Mechanics/Molecular Mechanics Insights into the Enantioselectivity of the <i>O</i> -Acetylation of <i>(R,S)</i> -Propranolol Catalyzed by <i>Candida antarctica</i> Lipase B. <i>ACS Catalysis</i> , 2017, 7, 115-127.	11.2	23
10	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
11	Structure and bonding of H ₂ O ₂ - X complexes with ($X = NO^+, CN^-, HCN, HNC, CO$). <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4089-4094.	2.8	21
12	Acetylation of <i>(R,S)</i> -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
13	Computational study of the enantioselectivity of the <i>O</i> -acetylation of <i>(R,S)</i> -propranolol catalyzed by <i>Candida antarctica</i> lipase B. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2014, 108, 21-31.	1.8	12
14	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
15	Quantum chemical and chemotopological study of fourth row monohydrides. <i>Chemical Physics Letters</i> , 2006, 428, 55-61.	2.6	10
16	Hydrogen bonds $H\cdots O$ in superoxide anion radical $^{\cdot-}O_2$ 1,4-Pentadiene complexes. <i>Computational and Theoretical Chemistry</i> , 2009, 893, 77-83.	1.5	5
17	CoH _n ($n=1-3$): Classical and non-classical cobalt polyhydride. <i>Chemical Physics Letters</i> , 2010, 490, 143-147.	2.6	5
18	Protonation-State-Driven Photophysics in Phenothiazinium Dyes: Intersystem Crossing and Singlet-Oxygen Production. <i>ChemPhotoChem</i> , 2017, 1, 459-469.	3.0	5

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19	On the nature of copperâ€“hydrogen bonding: AIM and NBO analysis of CuH_n(1) Tj ETQq1 1 0,784314 rgBT /Ove	2.0	7
20	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
21	Hydrogen Bonds and n â†“ Î€* 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
22	Effect of the acyl-group length on the chemoselectivity of the lipase-catalyzed acylation of propranololâ€“a computational study. <i>Journal of Molecular Modeling</i> , 2021, 27, 198.	1.8	1
23	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