

Leonardo Muñoz-Rugeles

List of Publications by Year in descending order

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Version: 2024-02-01

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papers

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1163117

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15
docs citations

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times ranked

322
citing authors

#	ARTICLE	IF	CITATIONS
1	Empirically Fitted Parameters for Calculating pK_a Values with Small Deviations from Experiments Using a Simple Computational Strategy. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1714-1724.	5.4	97
2	Hydrogen Abstraction Reactions from Phenolic Compounds by Peroxyl Radicals: Multireference Character and Density Functional Theory Rate Constants. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4634-4642.	2.5	55
3	A proton-electron sequential transfer mechanism: theoretical evidence about its biological relevance. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28525-28528.	2.8	26
4	The role of acid-base equilibria in formal hydrogen transfer reactions: tryptophan radical repair by uric acid as a paradigmatic case. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15296-15309.	2.8	24
5	Tryptophan: antioxidant or target of oxidative stress? A quantum chemistry elucidation. <i>RSC Advances</i> , 2014, 4, 56128-56131.	3.6	21
6	Non-covalent π - π stacking interactions turn off non-adiabatic effects in proton-coupled electron transfer reactions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6969-6972.	2.8	20
7	Synthesis and Photodynamics of Stilbenyl-Azopyrroles: Two-Photon Controllable Photoswitching Systems. <i>ChemPhotoChem</i> , 2020, 4, 144-154.	3.0	15
8	The other side of the superoxide radical anion: its ability to chemically repair DNA oxidized sites. <i>Chemical Communications</i> , 2018, 54, 13710-13713.	4.1	11
9	Tryptophan versus nitric oxide, nitrogen dioxide and carbonate radicals: differences in reactivity and implications for oxidative damage to proteins. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	7
10	Wettability of graphene oxide functionalized with <i>N</i> -alkylamines: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11412-11419.	2.8	6
11	Two-photon induced isomerization through a cyaninic molecular antenna in azo compounds. <i>Chemical Communications</i> , 2021, 57, 3123-3126.	4.1	5
12	Sensitization of Nd^{3+} Luminescence by Simultaneous Two-Photon Excitation through a Coordinating Polymethinic Antenna. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2498-2510.	2.5	5
13	Chemical repair of damaged leucine and tryptophane by thiophenols at close to diffusion-controlled rates: Mechanisms and kinetics. <i>Journal of Computational Chemistry</i> , 2022, , .	3.3	4
14	Chemical repair mechanisms of damaged tyrosyl and tryptophanyl residues in proteins by the superoxide radical anion. <i>New Journal of Chemistry</i> , 2020, 44, 2505-2513.	2.8	0
15	Molecular Dynamics study of the effect on the interfacial activity of Alkylamine-Modified graphene oxide. <i>Journal of Molecular Liquids</i> , 2022, 362, 119724.	4.9	0