## Misaela Francisco-Marquez

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Detailed Investigation of the Outstanding Peroxyl Radical Scavenging Activity of Two Novel Amino-Pyridinol-Based Compounds. Journal of Chemical Information and Modeling, 2019, 59, 3494-3505.	2.5	8
2	Computational study of substituent effects on the acidity, toxicity and chemical reactivity of bacteriostatic sulfonamides. Journal of Molecular Graphics and Modelling, 2018, 81, 116-124.	1.3	41
3	Polymorphism, Intermolecular Interactions, and Spectroscopic Properties in Crystal Structures of Sulfonamides. Journal of Pharmaceutical Sciences, 2018, 107, 273-285.	1.6	17
4	The reactions of plant hormones with reactive oxygen species: chemical insights at a molecular level. Journal of Molecular Modeling, 2018, 24, 255.	0.8	5
5	Adsorption of Sulfonamides on Phyllosilicate Surfaces by Molecular Modeling Calculations. Journal of Physical Chemistry C, 2017, 121, 2905-2914.	1.5	23
6	Silicon-Doped Carbon Nanotubes: Promising CO2/N2 Selective Agents for Sequestering Carbon Dioxide. Journal of Physical Chemistry C, 2016, 120, 24476-24481.	1.5	10
7	Anthranilic acid as a secondary antioxidant: Implications to the inhibition of OH production and the associated oxidative stress. Computational and Theoretical Chemistry, 2016, 1077, 18-24.	1.1	16
8	On the chemical behavior of C60 hosting H2O and other isoelectronic neutral molecules. Journal of Molecular Modeling, 2014, 20, 2412.	0.8	21
9	Ellagic Acid: An Unusually Versatile Protector against Oxidative Stress. Chemical Research in Toxicology, 2014, 27, 904-918.	1.7	110
10	Crystal structure, stability and spectroscopic properties of methane and CO2 hydrates. Journal of Molecular Graphics and Modelling, 2013, 44, 253-265.	1.3	44
11	A quantum chemical study on the free radical scavenging activity of tyrosol and hydroxytyrosol. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	38
12	Physicochemical Insights on the Free Radical Scavenging Activity of Sesamol: Importance of the Acid/Base Equilibrium. Journal of Physical Chemistry B, 2011, 115, 13101-13109.	1.2	64
13	Mechanism and kinetics studies on the antioxidant activity of sinapinic acid. Physical Chemistry Chemical Physics, 2011, 13, 11199.	1.3	80
14	Canolol: A Promising Chemical Agent against Oxidative Stress. Journal of Physical Chemistry B, 2011, 115, 8590-8596.	1.2	77
15	Adsorption of polyaromatic heterocycles on pyrophyllite surface by means of different theoretical approaches. Environmental Chemistry, 2011, 8, 429.	0.7	18
16	Molecular structure and spectroscopic properties of polyaromatic heterocycles by first principle calculations: spectroscopic shifts with the adsorption of thiophene on phyllosilicate surface. Theoretical Chemistry Accounts, 2010, 125, 83-95.	0.5	42
17	Water Complexes of Important Air Pollutants: Geometries, Complexation Energies, Concentrations, Infrared Spectra, and Intrinsic Reactivity. Journal of Physical Chemistry A, 2010, 114, 5796-5809.	1.1	47
18	Mechanism and Branching Ratios of Hydroxy Ethers + <sup>•</sup> OH Gas phase Reactions: Relevance of H Bond Interactions. Journal of Physical Chemistry A, 2010, 114, 7525-7536.	1.1	17

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19	On the Free Radical Scavenging Capability of Carboxylated Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 6363-6370.	1.5	32
20	Effect of Different Functional Groups on the Free Radical Scavenging Capability of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 14734-14739.	1.5	28
21	Influence of Point Defects on the Free-Radical Scavenging Capability of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 8302-8308.	1.5	41
22	Rate constants of the gasâ€phase reactions of OH radicals with <i>trans</i> â€2â€hexenal, <i>trans</i> â€2â€octenal, and <i>trans</i> â€2â€nonenal. International Journal of Chemical Kinetics, 2009, 41, 483-489.	1.0	15
23	Reactions of OOH Radical with Î <sup>2</sup> -Carotene, Lycopene, and Torulene: Hydrogen Atom Transfer and Adduct Formation Mechanisms. Journal of Physical Chemistry B, 2009, 113, 11338-11345.	1.2	77
24	Role of the Sulfur Atom on the Reactivity of Methionine toward OH Radicals: Comparison with Norleucine. Journal of Physical Chemistry B, 2009, 113, 4947-4952.	1.2	14
25	Peroxyl-Radical-Scavenging Activity of Garlic: 2-Propenesulfenic Acid versus Allicin. Journal of Physical Chemistry B, 2009, 113, 16077-16081.	1.2	59
26	Quantum chemistry and TST study of the mechanism and kinetics of the butadiene and isoprene reactions with mercapto radicals. Chemical Physics, 2008, 344, 273-280.	0.9	12
27	Reactivity of silicon and germanium doped CNTs toward aromatic sulfur compounds: A theoretical approach. Chemical Physics, 2008, 345, 87-94.	0.9	37
28	A Possible Mechanism for Furan Formation in the Tropospheric Oxidation of Dienes. Environmental Science & Technology, 2005, 39, 8797-8802.	4.6	22
29	On the role of s-cis conformers in the reaction of dienes with OH radicals. Physical Chemistry Chemical Physics, 2004, 6, 2237-2244.	1.3	21
30	Theoretical study of the initial reaction between OH and isoprene in tropospheric conditions. Physical Chemistry Chemical Physics, 2003, 5, 1392-1399.	1.3	51