Miguel Reina

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Comprehensive Investigation of the Antioxidant and Pro-oxidant Effects of Phenolic Compounds: A Double-Edged Sword in the Context of Oxidative Stress?. Journal of Physical Chemistry B, 2018, 122, 6198-6214.	2.6	71
2	Adsorption of melphalan anticancer drug on C24, B12N12, B12C6N6, B6C12N12 and B6C6N12 nanocages: A comparative DFT study. Journal of Molecular Liquids, 2021, 329, 115528.	4.9	34
3	A new free radical scavenging cascade involving melatonin and three of its metabolites (3OHM, AFMK) Tj ETQq1 1	0.78431	4 rgBT /Ov€
4	A Computer-Assisted Systematic Search for Melatonin Derivatives with High Potential as Antioxidants. Melatonin Research, 2018, 1, 27-58.	1.1	29
5	Silybin and 2,3-Dehydrosilybin Flavonolignans as Free Radical Scavengers. Journal of Physical Chemistry B, 2015, 119, 11597-11606.	2.6	15
6	Is Silybin the Best Free Radical Scavenger Compound in Silymarin?. Journal of Physical Chemistry B, 2016, 120, 4568-4578.	2.6	15
7	Silybin interacting with Cu 4 , Ag 4 and Au 4 clusters: Do these constitute antioxidant materials?. Computational and Theoretical Chemistry, 2017, 1112, 1-9.	2.5	15
8	Second generation of Casiopeinas®: A joint experimental and theoretical study. Inorganica Chimica Acta, 2021, 517, 120201.	2.4	15
9	Copper or free radical scavenger?. Computational and Theoretical Chemistry, 2017, 1104, 1-11.	2.5	14
10	How the presence of metal atoms and clusters can modify the properties of Silybin? A computational prediction. Computational and Theoretical Chemistry, 2017, 1099, 174-184.	2.5	14
11	Free radicals interacting with Cu, Ag and Au clusters. Computational and Theoretical Chemistry, 2017, 1120, 24-33.	2.5	13
12	Computationally designed p-coumaric acid analogs: searching for neuroprotective antioxidants. New Journal of Chemistry, 2021, 45, 14369-14380.	2.8	13
13	Cu, Ag and Au clusters as air pollutants hunters. Computational and Theoretical Chemistry, 2018, 1130, 15-23.	2.5	12
14	Understanding of vibrational and thermal behavior of bio-based doped alginate@nickel cross-linked beads: A combined experimental and theoretical study. Journal of Molecular Structure, 2022, 1249, 131524.	3.6	10
15	Identification of descriptors for structure-activity relationship in ruthenium (II) mixed compounds with antiparasitic activity. European Journal of Medicinal Chemistry, 2020, 189, 112084.	5.5	9
16	Compounds and Molecules: Learning How to Distinguish Them through an Educational Game. Journal of Chemical Education, 2022, 99, 1266-1271.	2.3	9
17	Conversion of Methyl Mercaptan to Hydrocarbons over H-ZSM-5 Zeolite: DFT/BOMD Study. ACS Omega, 2017, 2, 4647-4656.	3.5	8
18	CADMIO: Creating and Curating an Educational YouTube Channel with Chemistry Videos. Journal of Chemical Education, 2021, 98, 3593-3599.	2.3	8

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19	Seguridad en el laboratorio: una aproximaciÃ ³ n práctica. Educacion Quimica, 2021, 32, 45.	0.1	8
20	Improving the Understanding of Chemistry by Using the Right Words: A Clear-Cut Strategy to Avoid Misconceptions When Talking about Elements, Atoms, and Molecules. Journal of Chemical Education, 2022, 99, 2999-3006.	2.3	8
21	MET-Organic: A Multilevel Card Game to Promote the Learning of Organic Chemistry Nomenclature. Journal of Chemical Education, 2022, 99, 1948-1956.	2.3	6
22	C ₃₆ and C ₃₅ E (E=N and B) Fullerenes as Potential Nanovehicles for Neuroprotective Drugs: A Comparative DFT Study. ChemistrySelect, 2021, 6, 4844-4858.	1.5	5
23	Are Small Quasiâ€Fullerenes Capable of Encapsulating Trimetallic Nitrides A _{3â€x} B _x N (A, B =Sc, Y, La, <i>x=</i> 0â€3)? A DFT Study. ChemistrySelect, 2018, 3, 6791-6801.	1.5	4
24	Binding of multiple SO 2 molecules to small gold cluster anions (Au N â^' , Au N OH â^' , N = 1â€8). International Journal of Quantum Chemistry, 2019, 119, e25987.	2.0	4
25	Pyridyl based mono and di-selenoethers: Synthesis, characterization and DFT study. Journal of Molecular Structure, 2020, 1205, 127449.	3.6	4
26	Theoretical study of Au20/WS2 composite material as a potential candidate for the capture of XO (X=C, N, S) gases. Computational Condensed Matter, 2021, 28, e00580.	2.1	4
27	C _n and C _{nâ€1} B Fullerenes as Potential Nanovehicles for Piribedil Neuroprotective Drug (n=20, 36 and 60). ChemistrySelect, 2019, 4, 13916-13925.	1.5	3
28	Heteroleptic Nill complexes: Synthesis, structural characterization, computational studies and amoebicidal activity evaluation. Journal of Inorganic Biochemistry, 2020, 206, 111043.	3.5	3
29	The influence of the carbohydrate anomeric linkage on the free radical scavenging activity of enzymatically-synthesized phenolic glycosides. RSC Advances, 2016, 6, 45452-45461.	3.6	2
30	Mixed Rull complexes containing diselenoâ€ligand and α,βâ€diketones donors with anticancer activity. Synthesis, characterization, electrochemical and DFT studies. European Journal of Inorganic Chemistry, 2021, 2021, 4856.	2.0	1