Dejan A MilenkoviÄ

List of Publications by Year
in descending order

59 papers	1,482 citations	257450 24 h-index	330143 37 g-index
59 all docs	59 docs citations	59 times ranked	1423 citing authors

#	Article	IF	Citations
1	Revisiting the solvation enthalpies and free energies of the proton and electron in various solvents. Computational and Theoretical Chemistry, 2016, 1077, 11-17.	2.5	148
2	PM6 and DFT study of free radical scavenging activity of morin. Food Chemistry, 2012, 134, 1754-1760.	8.2	97
3	Antioxidative mechanisms in chlorogenic acid. Food Chemistry, 2017, 237, 390-398.	8.2	93
4	Advanced oxidation process of coumarins by hydroxyl radical: Towards the new mechanism leading to less toxic products. Chemical Engineering Journal, 2020, 395, 124971.	12.7	61
5	Examination of the chemical behavior of the quercetin radical cation towards some bases. Physical Chemistry Chemical Physics, 2013, 15, 7370.	2.8	56
6	Theoretical study of the thermodynamics of the mechanisms underlying antiradical activity of cinnamic acid derivatives. Food Chemistry, 2018, 246, 481-489.	8.2	54
7	Antiradical activity of delphinidin, pelargonidin and malvin towards hydroxyl and nitric oxide radicals: The energy requirements calculations as a prediction of the possible antiradical mechanisms. Food Chemistry, 2017, 218, 440-446.	8.2	52
8	Vibrational and Hirshfeld surface analyses, quantum chemical calculations, and molecular docking studies of coumarin derivative 3-(1-m-toluidinoethylidene)-chromane-2,4-dione and its corresponding palladium(II) complex. Journal of Molecular Structure, 2020, 1209, 127935.	3.6	49
9	Free radical scavenging activity of morin 2â€²-Oâ˜ phenoxide anion. Food Chemistry, 2012, 135, 2070-2077.	8.2	45
10	Antiradical activity of catecholamines and metabolites of dopamine: theoretical and experimental study. Physical Chemistry Chemical Physics, 2017, 19, 12970-12980.	2.8	45
11	Inhibitory activity of quercetin, its metabolite, and standard antiviral drugs towards enzymes essential for SARS-CoV-2: the role of acidâ€“base equilibria. RSC Advances, 2021, 11, 2838-2847.	3.6	41
12	Mechanistic study of the structureâ€“activity relationship for the free radical scavenging activity of baicalein. Journal of Molecular Modeling, 2011, 17, 2575-2584.	1.8	40
13	Antioxidative potential of ferulic acid phenoxyl radical. Phytochemistry, 2020, 170, 112218.	2.9	40
14	Several coumarin derivatives and their Pd(<scp>ii</scp>) complexes as potential inhibitors of the main protease of SARS-CoV-2, anin silicoapproach. RSC Advances, 2020, 10, 35099-35108.	3.6	37
15	Synthesis, spectroscopic characterization (FT-IR, FT-Raman, and NMR), quantum chemical studies and molecular docking of 3-(1-(phenylamino)ethylidene)-chroman-2,4-dione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 195, 31-40.	3.9	36
16	Interpretation of the IR and Raman spectra of morin by density functional theory and comparative analysis. Vibrational Spectroscopy, 2013, 64, 1-9.	2.2	32
17	Synthesis and comprehensive spectroscopic (X-ray, NMR, FTIR, UVâ€“Vis),Âquantum chemical and molecular docking investigation of 3-acetyl-4â€²hydroxyâ€²2-oxo-2H-chromen-7-yl acetate. Journal of Molecular Structure, 2021, 1225, 129256.	3.6	31
18	Synthesis, Crystallographic, Quantum Chemical, Antitumor, and Molecular Docking/Dynamic Studies of 4-Hydroxycoumarin-Neurotransmitter Derivatives. International Journal of Molecular Sciences, 2022, 23, 1001.	4.1	31

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19	Energy requirements of the reactions of kaempferol and selected radical species in different media: towards the prediction of the possible radical scavenging mechanisms. Structural Chemistry, 2014, 25, 1795-1804.	2.0	29
20	Experimental and theoretical elucidation of structural and antioxidant properties of vanillylmandelic acid and its carboxylate anion. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 198, 61-70.	3.9	28
21	Free Radical Scavenging Potency of Dihydroxybenzoic Acids. Journal of Chemistry, 2017, 2017, 1-9.	1.9	27
22	Hydrogen atom transfer versus proton coupled electron transfer mechanism of gallic acid with different peroxy radicals. Reaction Kinetics, Mechanisms and Catalysis, 2018, 123, 215-230.	1.7	27
23	Advanced oxidation processes of coumarins by hydroperoxyl radical: An experimental and theoretical study, and ecotoxicology assessment. Chemical Engineering Journal, 2021, 424, 130331.	12.7	27
24	A DFT and PM6 study of free radical scavenging activity of ellagic acid. Monatshefte FÃ¼r Chemie, 2013, 144, 803-812.	1.8	25
25	The preferred radical scavenging mechanisms of fisetin and baicalein towards oxygen-centred radicals in polar protic and polar aprotic solvents. RSC Advances, 2014, 4, 32228-32236.	3.6	24
26	Comparative antiradical activity and molecular Docking/Dynamics analysis of octopamine and norepinephrine: the role of OH groups. Computational Biology and Chemistry, 2020, 84, 107170.	2.3	24
27	Preparation and antimicrobial activity of a new palladium(II) complexes with a coumarin-derived ligands. Crystal structures of the 3-(1-(o-toluidino)ethylidene)-chroman-2,4-dione and 3-(1-(m-toluidino) ethylidene)-chroman-2,4-dione. Inorganica Chimica Acta, 2019, 484, 52-59.	2.4	22
28	Application of comparative vibrational spectroscopic and mechanistic studies in analysis of fisetin structure. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 83, 120-129.	3.9	21
29	Structural and spectral analysis of 3-metoxytyramine, an important metabolite of dopamine. Journal of Molecular Structure, 2017, 1134, 226-236.	3.6	21
30	Structural, spectral and NBO analysis of 3-(1-(3-hydroxypropylamino)ethylidene)chroman-2,4-dione. Journal of Molecular Structure, 2017, 1147, 69-75.	3.6	18
31	Solvation enthalpies and Gibbs energies of the proton and electron: Influence of solvation models. Journal of the Serbian Society for Computational Mechanics, 2016, 10, 66-76.	0.4	17
32	Structural and electronic features of baicalein and its radicals. Monatshefte FÃ¼r Chemie, 2011, 142, 145-152.	1.8	15
33	Theoretical Study of Radical Inactivation, LOX Inhibition, and Iron Chelation: The Role of Ferulic Acid in Skin Protection against UVA Induced Oxidative Stress. Antioxidants, 2021, 10, 1303.	5.1	15
34	Structural characterization of kaempferol: a spectroscopic and computational study. Macedonian Journal of Chemistry and Chemical Engineering, 2019, 38, 49.	0.6	14
35	Potent 1,2,4â€Triazoleâ€3â€thione Radical Scavengers Derived from Phenolic Acids: Synthesis, Electrochemistry, and Theoretical Study. ChemistrySelect, 2016, 1, 3870-3878.	1.5	13
36	Thermodynamic and kinetic analysis of the reaction between biological catecholamines and chlorinated methylperoxy radicals. Molecular Physics, 2018, 116, 1166-1178.	1.7	13

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37	Vibrational spectroscopic studies (FTIR and FT-Raman) and molecular dynamics analysis of industry inspired 3-amino-4-hydroxybenzene sulfonic acid. Journal of Molecular Structure, 2020, 1205, 127579.	3.6	13
38	Impact of the phenolic Oâ€“H vs. C-ring Câ€“H bond cleavage on the antioxidant potency of dihydrokaempferol. New Journal of Chemistry, 2021, 45, 7977-7986.	2.8	12
39	QSAR of the free radical scavenging potency of selected hydroxyanthraquinones. Chemical Papers, 2018, 72, 2785-2793.	2.2	10
40	In vitro, in vivo and in silico evaluation of the anti-inflammatory potential of Hyssopus officinalis L. subsp. aristatus (Godr.) Nyman (Lamiaceae). Journal of Ethnopharmacology, 2022, 293, 115201.	4.1	10
41	Reactivity of the coumarine derivative towards cartilage proteins: combined NBO, QTAIM, and molecular docking study. Monatshefte FÃ¼r Chemie, 2018, 149, 159-166.	1.8	8
42	The reactivity of dopamine precursors and metabolites towards ABTSâ€¢-: An experimental and theoretical study. Journal of the Serbian Chemical Society, 2019, 84, 877-889.	0.8	8
43	Mechanism of Antiradical Activity of Newly Synthesized 4,7-Dihydroxycoumarin Derivatives-Experimental and Kinetic DFT Study. International Journal of Molecular Sciences, 2021, 22, 13273.	4.1	8
44	Structure and reactivity of baicalein radical cation. International Journal of Quantum Chemistry, 2012, 112, 2009-2017.	2.0	7
45	Synthesis and theoretical investigation of some new 4-substituted flavylium salts. Food Chemistry, 2017, 229, 688-694.	8.2	7
46	The role of guaiacyl moiety in free radical scavenging by 3,5-dihydroxy-4-methoxybenzyl alcohol: thermodynamics of 3H+/3eâ^' mechanisms. Molecular Physics, 2019, 117, 207-217.	1.7	7
47	Mechanism, kinetics and selectivity of selenocyclization of 5-alkenylhydantoins: an experimental and computational study. Beilstein Journal of Organic Chemistry, 2015, 11, 1865-1875.	2.2	5
48	Study of Influence of Free Radical Species on Antioxidant Activity of Selected 1,2,4â€Triazoleâ€3â€thiones. ChemistrySelect, 2019, 4, 7476-7485.	1.5	5
49	Effects of conjugation metabolism on radical scavenging and transport properties of quercetin â€“ In silico study. Journal of Molecular Graphics and Modelling, 2019, 86, 278-285.	2.4	5
50	Experimental and theoretical investigations of an organic nonlinear optical material p-toluidinium picrate â€“ A comparative study. Journal of Molecular Structure, 2019, 1195, 73-84.	3.6	4
51	DFT investigation of the reaction of cyanidin with hydroxyl radical. , 2015, , .		2
52	DO EQUOLâ€™S C-RING HYDROGENS CONTRIBUTE TO FREE RADICAL SCAVENGING?. Journal of the Serbian Society for Computational Mechanics, 2020, , 45-58.	0.4	2
53	A joint application of vibrational spectroscopic and quantum mechanical methods in quantitative analysis of baicalein structure. Monatshefte FÃ¼r Chemie, 2012, 143, 1369-1378.	1.8	1
54	Study of electron transfer mechanism of gallic acid. , 2015, , .		0

#	Article	IF	Citations
55	Antioxidative Capacity of Evernic Acid and Its Interactions with TDP1. , 2019, , .		0
56	Different theoretical approaches in the study of antioxidative mechanisms. , 2020, , 211-256.		0
57	Synthesis and theoretical investigation of some new 4-substituted flavylium salts. , 0, , .		0
58	Investigation of Coumarin Derivative 3-(1-o-toluidinoethylidene)-chromane-2,4-dione: IR Spectroscopic Characterization, NBO, and AIM Analysis and Molecular Docking Studies. Learning and Analytics in Intelligent Systems, 2020, , 127-142.	0.6	0
59	MOLECULAR DOCKING AND MOLECULAR DYNAMICS STUDIES OF THE INTERACTION BETWEEN COUMARIN-NEUROTRANSMITTER DERIVATIVES AND CARBONIC ANHYDRASE IX. , 2021, , .		0