

Dejan A Milenkovic

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

51 papers	948 citations	19 h-index	29 g-index
59 ext. papers	1,197 ext. citations	3.8 avg, IF	4.64 L-index

#	Paper	IF	Citations
51	Revisiting the solvation enthalpies and free energies of the proton and electron in various solvents. <i>Computational and Theoretical Chemistry</i> , 2016 , 1077, 11-17	2	94
50	PM6 and DFT study of free radical scavenging activity of morin. <i>Food Chemistry</i> , 2012 , 134, 1754-60	8.5	86
49	Antioxidative mechanisms in chlorogenic acid. <i>Food Chemistry</i> , 2017 , 237, 390-398	8.5	60
48	Examination of the chemical behavior of the quercetin radical cation towards some bases. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 7370-8	3.6	48
47	Free radical scavenging activity of morin 2HO(-) phenoxide anion. <i>Food Chemistry</i> , 2012 , 135, 2070-7	8.5	40
46	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. <i>Food Chemistry</i> , 2017 , 218, 440-446	8.5	37
45	Theoretical study of the thermodynamics of the mechanisms underlying antiradical activity of cinnamic acid derivatives. <i>Food Chemistry</i> , 2018 , 246, 481-489	8.5	35
44	Synthesis, spectroscopic characterization (FT-IR, FT-Raman, and NMR), quantum chemical studies and molecular docking of 3-(1-(phenylamino)ethylidene)-chroman-2,4-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018 , 195, 31-40	4.4	29
43	Advanced oxidation process of coumarins by hydroxyl radical: Towards the new mechanism leading to less toxic products. <i>Chemical Engineering Journal</i> , 2020 , 395, 124971	14.7	28
42	Mechanistic study of the structure-activity relationship for the free radical scavenging activity of baicalein. <i>Journal of Molecular Modeling</i> , 2011 , 17, 2575-84	2	28
41	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. <i>Journal of Molecular Structure</i> , 2020 , 1209, 127935	3.4	24
40	Energy requirements of the reactions of kaempferol and selected radical species in different media: towards the prediction of the possible radical scavenging mechanisms. <i>Structural Chemistry</i> , 2014 , 25, 1795-1804	1.8	22
39	Interpretation of the IR and Raman spectra of morin by density functional theory and comparative analysis. <i>Vibrational Spectroscopy</i> , 2013 , 64, 1-9	2.1	22
38	A DFT and PM6 study of free radical scavenging activity of ellagic acid. <i>Monatshefte für Chemie</i> , 2013 , 144, 803-812	1.4	22
37	Antiradical activity of catecholamines and metabolites of dopamine: theoretical and experimental study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 12970-12980	3.6	21
36	Experimental and theoretical elucidation of structural and antioxidant properties of vanillylmandelic acid and its carboxylate anion. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018 , 198, 61-70	4.4	21
35	Free Radical Scavenging Potency of Dihydroxybenzoic Acids. <i>Journal of Chemistry</i> , 2017 , 2017, 1-9	2.3	20

34	The preferred radical scavenging mechanisms of fisetin and baicalein towards oxygen-centred radicals in polar protic and polar aprotic solvents. <i>RSC Advances</i> , 2014 , 4, 32228-32236	3.7	20
33	Several coumarin derivatives and their Pd(II) complexes as potential inhibitors of the main protease of SARS-CoV-2, an approach.. <i>RSC Advances</i> , 2020 , 10, 35099-35108	3.7	20
32	Inhibitory activity of quercetin, its metabolite, and standard antiviral drugs towards enzymes essential for SARS-CoV-2: the role of acid-base equilibria.. <i>RSC Advances</i> , 2021 , 11, 2838-2847	3.7	19
31	Hydrogen atom transfer versus proton coupled electron transfer mechanism of gallic acid with different peroxy radicals. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2018 , 123, 215-230	1.6	18
30	Comparative antiradical activity and molecular Docking/Dynamics analysis of octopamine and norepinephrine: the role of OH groups. <i>Computational Biology and Chemistry</i> , 2020 , 84, 107170	3.6	17
29	Application of comparative vibrational spectroscopic and mechanistic studies in analysis of fisetin structure. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 83, 120-9	4.4	16
28	Antioxidative potential of ferulic acid phenoxyl radical. <i>Phytochemistry</i> , 2020 , 170, 112218	4	16
27	Structural and spectral analysis of 3-methoxytyramine, an important metabolite of dopamine. <i>Journal of Molecular Structure</i> , 2017 , 1134, 226-236	3.4	15
26	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. <i>Inorganica Chimica Acta</i> , 2019 , 484, 52-59	2.7	15
25	Synthesis and comprehensive spectroscopic (X-ray, NMR, FTIR, UV-Vis), quantum chemical and molecular docking investigation of 3-acetyl-4-hydroxy-2-oxo-2H-chromen-7-yl acetate. <i>Journal of Molecular Structure</i> , 2021 , 1225, 129256	3.4	15
24	Structural, spectral and NBO analysis of 3-(1-(3-hydroxypropylamino)ethylidene)chroman-2,4-dione. <i>Journal of Molecular Structure</i> , 2017 , 1147, 69-75	3.4	14
23	Thermodynamic and kinetic analysis of the reaction between biological catecholamines and chlorinated methylperoxy radicals. <i>Molecular Physics</i> , 2018 , 116, 1166-1178	1.7	11
22	Structural and electronic features of baicalein and its radicals. <i>Monatshefte Für Chemie</i> , 2011 , 142, 145-152.	2.4	11
21	Synthesis, Crystallographic, Quantum Chemical, Antitumor, and Molecular Docking/Dynamic Studies of 4-Hydroxycoumarin-Neurotransmitter Derivatives.. <i>International Journal of Molecular Sciences</i> , 2022 , 23,	6.3	10
20	Solvation enthalpies and Gibbs energies of the proton and electron: Influence of solvation models. <i>Journal of the Serbian Society for Computational Mechanics</i> , 2016 , 10, 66-76	3	10
19	Potent 1,2,4-Triazole-3-thione Radical Scavengers Derived from Phenolic Acids: Synthesis, Electrochemistry, and Theoretical Study. <i>ChemistrySelect</i> , 2016 , 1, 3870-3878	1.8	8
18	Structural characterization of kaempferol: a spectroscopic and computational study. <i>Macedonian Journal of Chemistry and Chemical Engineering</i> , 2019 , 38, 49	1.1	8
17	Synthesis and theoretical investigation of some new 4-substituted flavylum salts. <i>Food Chemistry</i> , 2017 , 229, 688-694	8.5	7

16	The role of guaiacyl moiety in free radical scavenging by 3,5-dihydroxy-4-methoxybenzyl alcohol: thermodynamics of 3H+/3e ⁻ mechanisms. <i>Molecular Physics</i> , 2019 , 117, 207-217	1.7	7
15	Structure and reactivity of baicalein radical cation. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 2009-2017	2.1	7
14	Impact of the phenolic O-H vs. C-ring C-H bond cleavage on the antioxidant potency of dihydrokaempferol. <i>New Journal of Chemistry</i> , 2021 , 45, 7977-7986	3.6	7
13	Reactivity of the coumarine derivative towards cartilage proteins: combined NBO, QTAIM, and molecular docking study. <i>Monatshefte Für Chemie</i> , 2018 , 149, 159-166	1.4	7
12	The reactivity of dopamine precursors and metabolites towards ABTS: An experimental and theoretical study. <i>Journal of the Serbian Chemical Society</i> , 2019 , 84, 877-889	0.9	6
11	Effects of conjugation metabolism on radical scavenging and transport properties of quercetin - In silico study. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 86, 278-285	2.8	5
10	Study of Influence of Free Radical Species on Antioxidant Activity of Selected 1,2,4-Triazole-3-thiones. <i>ChemistrySelect</i> , 2019 , 4, 7476-7485	1.8	4
9	Advanced oxidation processes of coumarins by hydroperoxyl radical: An experimental and theoretical study, and ecotoxicology assessment. <i>Chemical Engineering Journal</i> , 2021 , 424, 130331	14.7	4
8	Vibrational spectroscopic studies (FTIR and FT-Raman) and molecular dynamics analysis of industry inspired 3-amino-4-hydroxybenzene sulfonic acid. <i>Journal of Molecular Structure</i> , 2020 , 1205, 127579	3.4	3
7	Experimental and theoretical investigations of an organic nonlinear optical material p-toluidinium picrate: A comparative study. <i>Journal of Molecular Structure</i> , 2019 , 1195, 73-84	3.4	2
6	QSAR of the free radical scavenging potency of selected hydroxyanthraquinones. <i>Chemical Papers</i> , 2018 , 72, 2785-2793	1.9	2
5	Mechanism, kinetics and selectivity of selenocyclization of 5-alkenylhydantoins: an experimental and computational study. <i>Beilstein Journal of Organic Chemistry</i> , 2015 , 11, 1865-75	2.5	2
4	In vitro, in vivo and in silico evaluation of the anti-inflammatory potential of Hyssopus officinalis L. subsp. aristatus (Godr.) Nyman (Lamiaceae).. <i>Journal of Ethnopharmacology</i> , 2022 , 115201	5	1
3	A joint application of vibrational spectroscopic and quantum mechanical methods in quantitative analysis of baicalein structure. <i>Monatshefte Für Chemie</i> , 2012 , 143, 1369-1378	1.4	
2	Investigation of Coumarin Derivative 3-(1-o-toluidinoethylidene)-chromane-2,4-dione: IR Spectroscopic Characterization, NBO, and AIM Analysis and Molecular Docking Studies. <i>Learning and Analytics in Intelligent Systems</i> , 2020 , 127-142	0.3	
1	Different theoretical approaches in the study of antioxidative mechanisms 2020 , 211-256		