Dejan A Milenkovic

List of Publications by Year in Descending Order

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	Synthesis, Crystallographic, Quantum Chemical, Antitumor, and Molecular Docking/Dynamic Studies of 4-Hydroxycoumarin-Neurotransmitter Derivatives.. *International Journal of Molecular Sciences*, **2022**, 23,	6.3	10
50	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**, 115201	5	1
49	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. *Journal of Molecular Structure*, **2021**, 1225, 129256	3.4	15
48	Impact of the phenolic O□H vs. C-ring C□H bond cleavage on the antioxidant potency of dihydrokaempferol. *New Journal of Chemistry*, **2021**, 45, 7977-7986	3.6	7
47	Advanced oxidation processes of coumarins by hydroperoxyl radical: An experimental and theoretical study, and ecotoxicology assessment. *Chemical Engineering Journal*, **2021**, 424, 130331	14.7	4
46	Inhibitory activity of quercetin, its metabolite, and standard antiviral drugs towards enzymes essential for SARS-CoV-2: the role of acid-base equilibria.. *RSC Advances*, **2021**, 11, 2838-2847	3.7	19
45	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	3.4	24
44	Advanced oxidation process of coumarins by hydroxyl radical: Towards the new mechanism leading to less toxic products. *Chemical Engineering Journal*, **2020**, 395, 124971	14.7	28
43	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	0.3	
42	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	3.4	3
41	Antioxidative potential of ferulic acid phenoxyl radical. *Phytochemistry*, **2020**, 170, 112218	4	16
40	Comparative antiradical activity and molecular Docking/Dynamics analysis of octopamine and norepinephrine: the role of OH groups. *Computational Biology and Chemistry*, **2020**, 84, 107170	3.6	17
39	Several coumarin derivatives and their Pd(ii) complexes as potential inhibitors of the main protease of SARS-CoV-2, an approach.. *RSC Advances*, **2020**, 10, 35099-35108	3.7	20
38	Different theoretical approaches in the study of antioxidative mechanisms **2020**, 211-256		
37	Experimental and theoretical investigations of an organic nonlinear optical material p-toluidinium picrate □A comparative study. *Journal of Molecular Structure*, **2019**, 1195, 73-84	3.4	2
36	The role of guaiacyl moiety in free radical scavenging by 3,5-dihydroxy-4-methoxybenzyl alcohol: thermodynamics of 3H+/3e□mechanisms. *Molecular Physics*, **2019**, 117, 207-217	1.7	7
35	Study of Influence of Free Radical Species on Antioxidant Activity of Selected 1,2,4-Triazole-3-thiones. *ChemistrySelect*, **2019**, 4, 7476-7485	1.8	4

34	Structural characterization of kaempferol: a spectroscopic and computational study. *Macedonian Journal of Chemistry and Chemical Engineering*, **2019**, 38, 49	1.1	8
33	The reactivity of dopamine precursors and metabolites towards ABTS□ An experimental and theoretical study. *Journal of the Serbian Chemical Society*, **2019**, 84, 877-889	0.9	6
32	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	2.7	15
31	Effects of conjugation metabolism on radical scavenging and transport properties of quercetin - In silico study. *Journal of Molecular Graphics and Modelling*, **2019**, 86, 278-285	2.8	5
30	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	4.4	21
29	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	4.4	29
28	Thermodynamic and kinetic analysis of the reaction between biological catecholamines and chlorinated methylperoxy radicals. *Molecular Physics*, **2018**, 116, 1166-1178	1.7	11
27	QSAR of the free radical scavenging potency of selected hydroxyanthraquinones. *Chemical Papers*, **2018**, 72, 2785-2793	1.9	2
26	Reactivity of the coumarine derivative towards cartilage proteins: combined NBO, QTAIM, and molecular docking study. *Monatshefte F□ Chemie*, **2018**, 149, 159-166	1.4	7
25	Theoretical study of the thermodynamics of the mechanisms underlying antiradical activity of cinnamic acid derivatives. *Food Chemistry*, **2018**, 246, 481-489	8.5	35
24	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	1.6	18
23	Antiradical activity of catecholamines and metabolites of dopamine: theoretical and experimental study. *Physical Chemistry Chemical Physics*, **2017**, 19, 12970-12980	3.6	21
22	Antioxidative mechanisms in chlorogenic acid. *Food Chemistry*, **2017**, 237, 390-398	8.5	60
21	Structural, spectral and NBO analysis of 3-(1-(3-hydroxypropylamino)ethylidene)chroman-2,4-dione. *Journal of Molecular Structure*, **2017**, 1147, 69-75	3.4	14
20	Synthesis and theoretical investigation of some new 4-substituted flavylium salts. *Food Chemistry*, **2017**, 229, 688-694	8.5	7
19	Structural and spectral analysis of 3-metoxytyramine, an important metabolite of dopamine. *Journal of Molecular Structure*, **2017**, 1134, 226-236	3.4	15
18	Free Radical Scavenging Potency of Dihydroxybenzoic Acids. *Journal of Chemistry*, **2017**, 2017, 1-9	2.3	20
17	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	8.5	37

16	Potent 1,2,4-Triazole-3-thione Radical Scavengers Derived from Phenolic Acids: Synthesis, Electrochemistry, and Theoretical Study. *ChemistrySelect*, **2016**, 1, 3870-3878	1.8	8
15	Revisiting the solvation enthalpies and free energies of the proton and electron in various solvents. *Computational and Theoretical Chemistry*, **2016**, 1077, 11-17	2	94
14	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	3	10
13	Mechanism, kinetics and selectivity of selenocyclization of 5-alkenylhydantoins: an experimental and computational study. *Beilstein Journal of Organic Chemistry*, **2015**, 11, 1865-75	2.5	2
12	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	3.7	20
11	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	1.8	22
10	Interpretation of the IR and Raman spectra of morin by density functional theory and comparative analysis. *Vibrational Spectroscopy*, **2013**, 64, 1-9	2.1	22
9	Examination of the chemical behavior of the quercetin radical cation towards some bases. *Physical Chemistry Chemical Physics*, **2013**, 15, 7370-8	3.6	48
8	A DFT and PM6 study of free radical scavenging activity of ellagic acid. *Monatshefte F Chemie*, **2013**, 144, 803-812	1.4	22
7	Free radical scavenging activity of morin 2 O(-) phenoxide anion. *Food Chemistry*, **2012**, 135, 2070-7	8.5	40
6	A joint application of vibrational spectroscopic and quantum mechanical methods in quantitative analysis of baicalein structure. *Monatshefte F Chemie*, **2012**, 143, 1369-1378	1.4	
5	Structure and reactivity of baicalein radical cation. *International Journal of Quantum Chemistry*, **2012**, 112, 2009-2017	2.1	7
4	PM6 and DFT study of free radical scavenging activity of morin. *Food Chemistry*, **2012**, 134, 1754-60	8.5	86
3	Application of comparative vibrational spectroscopic and mechanistic studies in analysis of fisetin structure. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 83, 120-9	4.4	16
2	Mechanistic study of the structure-activity relationship for the free radical scavenging activity of baicalein. *Journal of Molecular Modeling*, **2011**, 17, 2575-84	2	28
1	Structural and electronic features of baicalein and its radicals. *Monatshefte F Chemie*, **2011**, 142, 145-152	1.4	11