# 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 | 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 |
| 2 | 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 |
| 3 | Synthesis and comprehensive spectroscopic (X-ray, NMR, FTIR, UVâ€“Vis),Âquantum chemical and molecular docking investigation of 3-acetyl-4â€hydroxyâ€2-oxo-2H-chromen-7-yl acetate. Journal of Molecular Structure, 2021, 1225, 129256. | 3.6 | 31 |
| 4 | 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 |
| 5 | 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 |
| 6 | 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 |
| 7 | 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 |
| 8 | MOLECULAR DOCKING AND MOLECULAR DYNAMICS STUDIES OF THE INTERACTION BETWEEN COUMARIN-NEUROTRANSMITTER DERIVATIVES AND CARBONIC ANHYDRASE IX. , 2021, , . | | 0 |
| 9 | 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 |
| 10 | Different theoretical approaches in the study of antioxidative mechanisms. , 2020, , 211-256. | | 0 |
| 11 | 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 |
| 12 | Antioxidative potential of ferulic acid phenoxyl radical. Phytochemistry, 2020, 170, 112218. | 2.9 | 40 |
| 13 | 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 |
| 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 | 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | Antioxidative Capacity of Evernic Acid and Its Interactions with TDP1. , 2019, , . | | 0 |
| 23 | 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 |
| 24 | 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 |
| 25 | Structural characterization of kaempferol: a spectroscopic and computational study. Macedonian Journal of Chemistry and Chemical Engineering, 2019, 38, 49. | 0.6 | 14 |
| 26 | 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 |
| 27 | 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 |
| 28 | 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 |
| 29 | Thermodynamic and kinetic analysis of the reaction between biological catecholamines and chlorinated methylperoxy radicals. Molecular Physics, 2018, 116, 1166-1178. | 1.7 | 13 |
| 30 | 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 |
| 31 | Theoretical study of the thermodynamics of the mechanisms underlying antiradical activity of cinnamic acid derivatives. Food Chemistry, 2018, 246, 481-489. | 8.2 | 54 |
| 32 | 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 |
| 33 | QSAR of the free radical scavenging potency of selected hydroxyanthraquinones. Chemical Papers, 2018, 72, 2785-2793. | 2.2 | 10 |
| 34 | Antiradical activity of catecholamines and metabolites of dopamine: theoretical and experimental study. Physical Chemistry Chemical Physics, 2017, 19, 12970-12980. | 2.8 | 45 |
| 35 | Antioxidative mechanisms in chlorogenic acid. Food Chemistry, 2017, 237, 390-398. | 8.2 | 93 |
| 36 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Synthesis and theoretical investigation of some new 4-substituted flavylium salts. Food Chemistry, 2017, 229, 688-694. | 8.2 | 7 |
| 38 | Structural and spectral analysis of 3-metoxytyramine, an important metabolite of dopamine. Journal of Molecular Structure, 2017, 1134, 226-236. | 3.6 | 21 |
| 39 | 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 |
| 40 | Free Radical Scavenging Potency of Dihydroxybenzoic Acids. Journal of Chemistry, 2017, 2017, 1-9. | 1.9 | 27 |
| 41 | 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 |
| 42 | 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 |
| 43 | 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 |
| 44 | Study of electron transfer mechanism of gallic acid. , 2015, , . | | 0 |
| 45 | DFT investigation of the reaction of cyanidin with hydroxyl radical. , 2015, , . | | 2 |
| 46 | 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 |
| 47 | 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 |
| 48 | 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 |
| 49 | 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 |
| 50 | Examination of the chemical behavior of the quercetin radical cation towards some bases. Physical Chemistry Chemical Physics, 2013, 15, 7370. | 2.8 | 56 |
| 51 | A DFT and PM6 study of free radical scavenging activity of ellagic acid. Monatshefte FÃ¼r Chemie, 2013, 144, 803-812. | 1.8 | 25 |
| 52 | Free radical scavenging activity of morin 2â€²-Oâ˜ phenoxide anion. Food Chemistry, 2012, 135, 2070-2077. | 8.2 | 45 |
| 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 | Structure and reactivity of baicalein radical cation. International Journal of Quantum Chemistry, 2012, 112, 2009-2017. | 2.0 | 7 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | PM6 and DFT study of free radical scavenging activity of morin. Food Chemistry, 2012, 134, 1754-1760. | 8.2 | 97 |
| 56 | 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 |
| 57 | 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 |
| 58 | Structural and electronic features of baicalein and its radicals. Monatshefte FÃ¼r Chemie, 2011, 142, 145-152. | 1.8 | 15 |
| 59 | Synthesis and theoretical investigation of some new 4-substituted flavylium salts. , 0, , . | | 0 |