Annia Galano

List of Publications by Citations

203 papers	10,085 citations	55 h-index	94 g-index
208 ext. papers	11,394 ext. citations	3.9 avg, IF	6.98 L-index

#	Paper	IF	Citations
203	Melatonin as a natural ally against oxidative stress: a physicochemical examination. *Journal of Pineal Research*, **2011**, 51, 1-16	10.4	816
202	Melatonin: an ancient molecule that makes oxygen metabolically tolerable. *Journal of Pineal Research*, **2015**, 59, 403-19	10.4	595
201	On the free radical scavenging activities of melatonin's metabolites, AFMK and AMK. *Journal of Pineal Research*, **2013**, 54, 245-57	10.4	569
200	Melatonin: exceeding expectations. *Physiology*, **2014**, 29, 325-33	9.8	269
199	Melatonin as a mitochondria-targeted antioxidant: one of evolution's best ideas. *Cellular and Molecular Life Sciences*, **2017**, 74, 3863-3881	10.3	255
198	Phytomelatonin: assisting plants to survive and thrive. *Molecules*, **2015**, 20, 7396-437	4.8	225
197	Food Antioxidants: Chemical Insights at the Molecular Level. *Annual Review of Food Science and Technology*, **2016**, 7, 335-52	14.7	222
196	A computational methodology for accurate predictions of rate constants in solution: application to the assessment of primary antioxidant activity. *Journal of Computational Chemistry*, **2013**, 34, 2430-45	3.5	203
195	Mitochondria: Central Organelles for Melatonin's Antioxidant and Anti-Aging Actions. *Molecules*, **2018**, 23,	4.8	159
194	A physicochemical examination of the free radical scavenging activity of Trolox: mechanism, kinetics and influence of the environment. *Physical Chemistry Chemical Physics*, **2013**, 15, 4642-50	3.6	154
193	Kinetics of radical-molecule reactions in aqueous solution: a benchmark study of the performance of density functional methods. *Journal of Computational Chemistry*, **2014**, 35, 2019-26	3.5	151
192	Is caffeine a good scavenger of oxygenated free radicals?. *Journal of Physical Chemistry B*, **2011**, 115, 4538-46	3.4	150
191	Melatonin and its metabolites vs oxidative stress: From individual actions to collective protection. *Journal of Pineal Research*, **2018**, 65, e12514	10.4	146
190	Carbon Nanotubes as Free-Radical Scavengers. *Journal of Physical Chemistry C*, **2008**, 112, 8922-8927	3.8	133
189	On the direct scavenging activity of melatonin towards hydroxyl and a series of peroxyl radicals. *Physical Chemistry Chemical Physics*, **2011**, 13, 7178-88	3.6	132
188	Melatonin: A Versatile Protector against Oxidative DNA Damage. *Molecules*, **2018**, 23,	4.8	126
187	Melatonin and its metabolites as copper chelating agents and their role in inhibiting oxidative stress: a physicochemical analysis. *Journal of Pineal Research*, **2015**, 58, 107-16	10.4	121

186	Counterpoise corrected interaction energies are not systematically better than uncorrected ones: comparison with CCSD(T) CBS extrapolated values. *Theoretical Chemistry Accounts*, **2010**, 126, 75-85	1.9	114
185	Carbon nanotubes: promising agents against free radicals. *Nanoscale*, **2010**, 2, 373-80	7.7	108
184	Glutathione: mechanism and kinetics of its non-enzymatic defense action against free radicals. *RSC Advances*, **2011**, 1, 1763	3.7	108
183	Computational strategies for predicting free radical scavengers' protection against oxidative stress: Where are we and what might follow?. *International Journal of Quantum Chemistry*, **2019**, 119, e25665	2.1	101
182	Radical scavenging ability of gallic acid toward OH and OOH radicals. Reaction mechanism and rate constants from the density functional theory. *Journal of Physical Chemistry B*, **2014**, 118, 10380-9	3.4	101
181	OH radical scavenging activity of Edaravone: mechanism and kinetics. *Journal of Physical Chemistry B*, **2011**, 115, 1306-14	3.4	97
180	OH radical gas phase reactions with aliphatic ethers: a variational transition state theory study. *Journal of Physical Chemistry A*, **2009**, 113, 13913-20	2.8	91
179	Carotenoids can act as antioxidants by oxidizing the superoxide radical anion. *Physical Chemistry Chemical Physics*, **2010**, 12, 193-200	3.6	89
178	Gas phase reactions of C1□4 alcohols with the OH radical: A quantum mechanical approach. *Physical Chemistry Chemical Physics*, **2002**, 4, 4648-4662	3.6	89
177	Role of the reacting free radicals on the antioxidant mechanism of curcumin. *Chemical Physics*, **2009** , 363, 13-23	2.3	88
176	Guanosine + OH radical reaction in aqueous solution: a reinterpretation of the UV-vis data based on thermodynamic and kinetic calculations. *Organic Letters*, **2009**, 11, 5114-7	6.2	88
175	Melatonin reduces lipid peroxidation and membrane viscosity. *Frontiers in Physiology*, **2014**, 5, 377	4.6	85
174	A new approach to counterpoise correction to BSSE. *Journal of Computational Chemistry*, **2006**, 27, 1203-10	3.9	85
173	Oxidative desulfurization (ODS) of organosulfur compounds catalyzed by peroxo-metallate complexes of WOx□rO2: Thermochemical, structural, and reactivity indexes analyses. *Journal of Catalysis*, **2011**, 282, 201-208	7.3	84
172	Non-isothermal pyrolysis of pectin: A thermochemical and kinetic approach. *Journal of Analytical and Applied Pyrolysis*, **2015**, 112, 94-104	6	82
171	Relative antioxidant efficiency of a large series of carotenoids in terms of one electron transfer reactions. *Journal of Physical Chemistry B*, **2007**, 111, 12898-908	3.4	82
170	Deprotonation mechanism and acidity constants in aqueous solution of flavonols: a combined experimental and theoretical study. *Journal of Physical Chemistry B*, **2013**, 117, 12347-59	3.4	79
169	Capsaicin, a tasty free radical scavenger: mechanism of action and kinetics. *Journal of Physical Chemistry B*, **2012**, 116, 1200-8	3.4	75

168	Free radical scavenger properties of -mangostin: thermodynamics and kinetics of HAT and RAF mechanisms. *Journal of Physical Chemistry B*, **2011**, 115, 12591-8	3.4	73
167	Ellagic acid: an unusually versatile protector against oxidative stress. *Chemical Research in Toxicology*, **2014**, 27, 904-18	4	72
166	Mechanism and kinetics studies on the antioxidant activity of sinapinic acid. *Physical Chemistry Chemical Physics*, **2011**, 13, 11199-205	3.6	72
165	What is important to prevent oxidative stress? A theoretical study on electron-transfer reactions between carotenoids and free radicals. *Journal of Physical Chemistry B*, **2009**, 113, 12113-20	3.4	71
164	Mechanism of the OH radical scavenging activity of nordihydroguaiaretic acid: a combined theoretical and experimental study. *Journal of Physical Chemistry B*, **2010**, 114, 6625-35	3.4	71
163	Rate constant dependence on the size of aldehydes in the NO(3) + aldehydes reaction. An explanation via quantum chemical calculations and CTST. *Journal of the American Chemical Society*, **2001**, 123, 8387-95	16.4	70
162	Reactions of OOH radical with beta-carotene, lycopene, and torulene: hydrogen atom transfer and adduct formation mechanisms. *Journal of Physical Chemistry B*, **2009**, 113, 11338-45	3.4	68
161	Canolol: a promising chemical agent against oxidative stress. *Journal of Physical Chemistry B*, **2011**, 115, 8590-6	3.4	65
160	Piceatannol, a better peroxyl radical scavenger than resveratrol. *RSC Advances*, **2013**, 3, 20209	3.7	64
159	On the chemical repair of DNA radicals by glutathione: hydrogen vs electron transfer. *Journal of Physical Chemistry B*, **2012**, 116, 9316-25	3.4	62
158	Glycolaldehyde + OH gas phase reaction: a quantum chemistry + CVT/SCT approach. *Journal of Physical Chemistry A*, **2005**, 109, 169-80	2.8	62
157	Cyclic-3-hydroxymelatonin (C3HOM), a potent antioxidant, scavenges free radicals and suppresses oxidative reactions. *Current Medicinal Chemistry*, **2014**, 21, 1557-65	4.3	62
156	Antioxidant properties of several coumarin-chalcone hybrids from theoretical insights. *RSC Advances*, **2015**, 5, 565-575	3.7	61
155	Rate Coefficient and Mechanism of the Gas Phase OH Hydrogen Abstraction Reaction from Formic Acid:´ A Quantum Mechanical Approach. *Journal of Physical Chemistry A*, **2002**, 106, 9520-9528	2.8	61
154	Theoretical determination of the rate constant for OH hydrogen abstraction from toluene. *Journal of Physical Chemistry A*, **2006**, 110, 10155-62	2.8	60
153	Empirically Fitted Parameters for Calculating pKa Values with Small Deviations from Experiments Using a Simple Computational Strategy. *Journal of Chemical Information and Modeling*, **2016**, 56, 1714-24	6.1	59
152	Free Radical Scavenging Activity of Ultrashort Single-Walled Carbon Nanotubes with Different Structures through Electron Transfer Reactions. *Journal of Physical Chemistry C*, **2010**, 114, 8184-8191	3.8	57
151	Melatonin Mitigates Mitochondrial Meltdown: Interactions with SIRT3. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	55

150	Physicochemical insights on the free radical scavenging activity of sesamol: importance of the acid/base equilibrium. *Journal of Physical Chemistry B*, **2011**, 115, 13101-9	3.4	55
149	OH hydrogen abstraction reactions from alanine and glycine: A quantum mechanical approach. *Journal of Computational Chemistry*, **2001**, 22, 1138-1153	3.5	55
148	On the peroxyl scavenging activity of hydroxycinnamic acid derivatives: mechanisms, kinetics, and importance of the acid-base equilibrium. *Physical Chemistry Chemical Physics*, **2012**, 14, 12534-43	3.6	54
147	Peroxyl-radical-scavenging activity of garlic: 2-propenesulfenic acid versus allicin. *Journal of Physical Chemistry B*, **2009**, 113, 16077-81	3.4	53
146	Searching for Computational Strategies to Accurately Predict pKas of Large Phenolic Derivatives. *Journal of Chemical Theory and Computation*, **2011**, 7, 2528-38	6.4	52
145	Surface acid-basic properties of WOx/ZrO2 and catalytic efficiency in oxidative desulfurization. *Applied Catalysis B: Environmental*, **2009**, 92, 1-8	21.8	52
144	Theoretical study of the initial reaction between OH and isoprene in tropospheric conditions. *Physical Chemistry Chemical Physics*, **2003**, 5, 1392-1399	3.6	49
143	Hydrogen Abstraction Reactions from Phenolic Compounds by Peroxyl Radicals: Multireference Character and Density Functional Theory Rate Constants. *Journal of Physical Chemistry A*, **2016**, 120, 4634-42	2.8	47
142	Adrenaline and noradrenaline: protectors against oxidative stress or molecular targets?. *Journal of Physical Chemistry B*, **2015**, 119, 3479-91	3.4	46
141	OH radical reactions with phenylalanine in free and peptide forms. *Organic and Biomolecular Chemistry*, **2008**, 6, 732-8	3.9	46
140	Theoretical explanation of nonexponential OH decay in reactions with benzene and toluene under pseudo-first-order conditions. *Journal of Physical Chemistry A*, **2008**, 112, 7608-15	2.8	46
139	Structure-Reactivity Relationship in Ketones + OH Reactions: A Quantum Mechanical and TST Approach. *Journal of Physical Chemistry A*, **2004**, 108, 2740-2749	2.8	45
138	Influence of silicon defects on the adsorption of thiophene-like compounds on polycyclic aromatic hydrocarbons: a theoretical study using thiophene + coronene as the simplest model. *Journal of Physical Chemistry A*, **2007**, 111, 1677-82	2.8	44
137	Mechanism and kinetics of the reaction of OH radicals with glyoxal and methylglyoxal: a quantum chemistry + CVT/SCT approach. *ChemPhysChem*, **2004**, 5, 1379-88	3.2	44
136	N-Acetylserotonin and 6-Hydroxymelatonin against Oxidative Stress: Implications for the Overall Protection Exerted by Melatonin. *Journal of Physical Chemistry B*, **2015**, 119, 8535-43	3.4	42
135	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	3.4	42
134	Water complexes of important air pollutants: geometries, complexation energies, concentrations, infrared spectra, and intrinsic reactivity. *Journal of Physical Chemistry A*, **2010**, 114, 5796-809	2.8	41
133	Cyclic 3-hydroxymelatonin, a key metabolite enhancing the peroxyl radical scavenging activity of melatonin. *RSC Advances*, **2014**, 4, 5220	3.7	40

132	Branching Ratios of Aliphatic Amines + OH Gas-Phase Reactions: A Variational Transition-State Theory Study. *Journal of Chemical Theory and Computation*, **2008**, 4, 322-7	6.4	39
131	Free-radical scavenging by tryptophan and its metabolites through electron transfer based processes. *Journal of Molecular Modeling*, **2015**, 21, 213	2	38
130	On the influence of diameter and length on the properties of armchair single-walled carbon nanotubes: A theoretical chemistry approach. *Chemical Physics*, **2006**, 327, 159-170	2.3	37
129	NR2 and P3+: Accurate, Efficient Electron-Propagator Methods for Calculating Valence, Vertical Ionization Energies of Closed-Shell Molecules. *Journal of Physical Chemistry A*, **2015**, 119, 8813-21	2.8	36
128	Theoretical and experimental studies of highly active graphene nanosheets to determine catalytic nitrogen sites responsible for the oxygen reduction reaction in alkaline media. *Journal of Materials Chemistry A*, **2016**, 4, 976-990	13	36
127	Influence of Point Defects on the Free-Radical Scavenging Capability of Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2010**, 114, 8302-8308	3.8	36
126	Reactivity of silicon and germanium doped CNTs toward aromatic sulfur compounds: A theoretical approach. *Chemical Physics*, **2008**, 345, 87-94	2.3	36
125	Dihydroxybenzoic acids as free radical scavengers: mechanisms, kinetics, and trends in activity. *New Journal of Chemistry*, **2014**, 38, 2639	3.6	34
124	On the evolution of one-electron-oxidized deoxyguanosine in damaged DNA under physiological conditions: a DFT and ONIOM study on proton transfer and equilibrium. *Physical Chemistry Chemical Physics*, **2012**, 14, 12476-84	3.6	34
123	A quantum chemical study on the free radical scavenging activity of tyrosol and hydroxytyrosol. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	34
122	Theoretical study on the reaction of tropospheric interest: hydroxyacetone + OH. Mechanism and kinetics. *Journal of Physical Chemistry A*, **2006**, 110, 9153-60	2.8	34
121	Xanthones as antioxidants: a theoretical study on the thermodynamics and kinetics of the single electron transfer mechanism. *Food and Function*, **2012**, 3, 442-50	6.1	33
120	Phenolic Melatonin-Related Compounds: Their Role as Chemical Protectors against Oxidative Stress. *Molecules*, **2016**, 21,	4.8	33
119	Coumarin-Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. *Journal of Chemical Information and Modeling*, **2016**, 56, 662-70	6.1	32
118	On the free radical scavenging mechanism of protocatechuic acid, regeneration of the catechol group in aqueous solution. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	32
117	Theoretical study on the chemical fate of adducts formed through free radical addition reactions to carotenoids. *Theoretical Chemistry Accounts*, **2010**, 127, 595-603	1.9	32
116	Influence of Diameter, Length, and Chirality of Single-Walled Carbon Nanotubes on Their Free Radical Scavenging Capability. *Journal of Physical Chemistry C*, **2009**, 113, 18487-18491	3.8	31
115	First principles calculations of pKa values of amines in aqueous solution: Application to neurotransmitters. *International Journal of Quantum Chemistry*, **2012**, 112, 3449-3460	2.1	30

114	Influence of the environment on the protective effects of guaiacol derivatives against oxidative stress: mechanisms, kinetics, and relative antioxidant activity. *Journal of Physical Chemistry B*, **2012**, 116, 7129-37	3.4	30
113	Mechanism and rate coefficients of the gas phase OH hydrogen abstraction reaction from asparagine: a quantum mechanical approach. *Computational and Theoretical Chemistry*, **2002**, 617, 77-86		30
112	A combined theoretical-experimental investigation on the mechanism of lignin pyrolysis: Role of heating rates and residence times. *Journal of Analytical and Applied Pyrolysis*, **2017**, 128, 208-216	6	28
111	On the outstanding antioxidant capacity of edaravone derivatives through single electron transfer reactions. *Journal of Physical Chemistry B*, **2012**, 116, 1180-8	3.4	28
110	Theoretical study on the peroxyl radicals scavenging activity of esculetin and its regeneration in aqueous solution. *Physical Chemistry Chemical Physics*, **2014**, 16, 1197-207	3.6	27
109	On the Free Radical Scavenging Capability of Carboxylated Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2010**, 114, 6363-6370	3.8	27
108	Melatonin and its metabolites as chemical agents capable of directly repairing oxidized DNA. *Journal of Pineal Research*, **2019**, 66, e12539	10.4	26
107	Effect of Different Functional Groups on the Free Radical Scavenging Capability of Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2010**, 114, 14734-14739	3.8	25
106	Role of allyl group in the hydroxyl and peroxyl radical scavenging activity of S-allylcysteine. *Journal of Physical Chemistry B*, **2011**, 115, 13408-17	3.4	25
105	Mechanism of OH radical reactions with HCN and CH3CN: OH regeneration in the presence of O2. *Journal of Physical Chemistry A*, **2007**, 111, 5086-91	2.8	24
104	Radical grafting of carbon surfaces with alkylic groups by mediated oxidation of carboxylates. *Journal of Electroanalytical Chemistry*, **2007**, 610, 137-146	4.1	23
103	NEW INSIGTHS ON THE KINETICS AND MECHANISM OF THE ELECTROCHEMICAL OXIDATION OF DICLOFENAC IN NEUTRAL AQUEOUS MEDIUM. *Electrochimica Acta*, **2016**, 199, 92-98	6.7	22
102	Mechanism and kinetics of the hydroxyl and hydroperoxyl radical scavenging activity of N-acetylcysteine amide. *Theoretical Chemistry Accounts*, **2011**, 130, 51-60	1.9	22
101	Dual antioxidant/pro-oxidant behavior of the tryptophan metabolite 3-hydroxyanthranilic acid: a theoretical investigation of reaction mechanisms and kinetics. *New Journal of Chemistry*, **2017**, 41, 3829-3845	3.6	21
100	The Baeyer-Villiger reaction of 23-oxosapogenins. *Arkivoc*, **2005**, 2005, 109-126	0.9	21
99	Cis carotenoids: colorful molecules and free radical quenchers. *Journal of Physical Chemistry B*, **2013**, 117, 4050-61	3.4	20
98	Uric and 1-methyluric acids: metabolic wastes or antiradical protectors?. *Journal of Physical Chemistry B*, **2011**, 115, 15430-8	3.4	20
97	On the role of s-cis conformers in the reaction of dienes with OH radicals. *Physical Chemistry Chemical Physics*, **2004**, 6, 2237-2244	3.6	20

96	On the •OH and •OOH scavenging activity of 3-methyl-1-pyridin-2-yl-5-pyrazolone: Comparisons with its parent compound, edaravone. *International Journal of Quantum Chemistry*, **2012**, 112, 3441-3448	2.1	19
95	Kinetics and mechanism of the gas-phase OH hydrogen abstraction reaction from methionine: A quantum mechanical approach. *International Journal of Chemical Kinetics*, **2003**, 35, 212-221	1.4	19
94	Citric acid: A promising copper scavenger. *Computational and Theoretical Chemistry*, **2018**, 1133, 47-50	2	18
93	On the chemical behavior of C60 hosting H2O and other isoelectronic neutral molecules. *Journal of Molecular Modeling*, **2014**, 20, 2412	2	18
92	Ionization energies, proton affinities, and pKa values of a large series of edaravone derivatives: implication for their free radical scavenging activity. *Journal of Physical Chemistry B*, **2011**, 115, 10375-84	3.4	18
91	Non-alkane behavior of cyclopropane and its derivatives: characterization of unconventional hydrogen bond interactions. *Theoretical Chemistry Accounts*, **2007**, 118, 597-606	1.9	18
90	A possible mechanism for furan formation in the tropospheric oxidation of dienes. *Environmental Science & Technology*, **2005**, 39, 8797-802	10.3	18
89	Rate coefficients and mechanism of the gas phase OH hydrogen abstraction reaction from serine: a quantum mechanical approach. *Computational and Theoretical Chemistry*, **2003**, 629, 165-174		18
88	The role of acid-base equilibria in formal hydrogen transfer reactions: tryptophan radical repair by uric acid as a paradigmatic case. *Physical Chemistry Chemical Physics*, **2017**, 19, 15296-15309	3.6	17
87	Theoretical investigation of the OH*-initiated oxidation of benzaldehyde in the troposphere. *ChemPhysChem*, **2008**, 9, 1453-9	3.2	17
86	A Computer-Assisted Systematic Search for Melatonin Derivatives with High Potential as Antioxidants. *Melatonin Research*, **2018**, 1, 27-58	5.1	17
85	The key role of the sequential proton loss electron transfer mechanism on the free radical scavenging activity of some melatonin-related compounds. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	16
84	Assessing the Protective Activity of a Recently Discovered Phenolic Compound against Oxidative Stress Using Computational Chemistry. *Journal of Chemical Information and Modeling*, **2015**, 55, 2552-61	6.1	16
83	Isopropylcyclopropane + OH gas phase reaction: a quantum chemistry + CVT/SCT approach. *Journal of Physical Chemistry A*, **2006**, 110, 1917-24	2.8	16
82	Quantum mechanical based approaches for predicting pKa values of carboxylic acids: evaluating the performance of different strategies. *RSC Advances*, **2016**, 6, 112057-112064	3.7	16
81	Non-covalent π-stacking interactions turn off non-adiabatic effects in proton-coupled electron transfer reactions. *Physical Chemistry Chemical Physics*, **2017**, 19, 6969-6972	3.6	15
80	Vertical ionization energies of free radicals and electron detachment energies of their anions: a comparison of direct and indirect methods versus experiment. *Journal of Physical Chemistry A*, **2014**, 118, 6125-31	2.8	15
79	Mechanism and branching ratios of hydroxy ethers + (*)OH gas phase reactions: relevance of h bond interactions. *Journal of Physical Chemistry A*, **2010**, 114, 7525-36	2.8	15

78	A combined theoretical-experimental study on the acidity of WO(x)-ZrO(2) systems. *Physical Chemistry Chemical Physics*, **2008**, 10, 4181-8	3.6	15
77	Free Radicals Induced Oxidative Stress at a Molecular Level: The Current Status, Challenges and Perspectives of Computational Chemistry Based Protocols **2017**, 59,		15
76	Deprotonation routes of anthocyanidins in aqueous solution, pKa values, and speciation under physiological conditions. *RSC Advances*, **2016**, 6, 53421-53429	3.7	15
75	Free radical scavenging activity of caffeine's metabolites. *International Journal of Quantum Chemistry*, **2012**, 112, 3472-3478	2.1	14
74	Computational-aided design of melatonin analogues with outstanding multifunctional antioxidant capacity. *RSC Advances*, **2016**, 6, 22951-22963	3.7	14
73	Exploring Chemical Routes Relevant to the Toxicity of Paracetamol and Its meta-Analogue at a Molecular Level. *Chemical Research in Toxicology*, **2017**, 30, 1286-1301	4	13
72	Synthesis, Characterization, and Solid State Dynamic Studies of a Hydrogen Bond-Hindered Steroidal Molecular Rotor with a Flexible Axis. *Journal of Organic Chemistry*, **2018**, 83, 3768-3779	4.2	13
71	The mechanism of mediated oxidation of carboxylates with ferrocene as redox catalyst in absence of grafting effects. An experimental and theoretical approach. *Electrochimica Acta*, **2014**, 136, 542-549	6.7	13
70	Radical-trapping and preventive antioxidant effects of 2-hydroxymelatonin and 4-hydroxymelatonin: Contributions to the melatonin protection against oxidative stress. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 2206-2217	4	13
69	Atmospheric Reactions of Oxygenated Volatile Organic Compounds+OH Radicals: Role of Hydrogen-Bonded Intermediates and Transition States. *Advances in Quantum Chemistry*, **2008**, 245-274	1.4	13
68	Quantum mechanical approach to isoleucine+OH gas phase reaction. Mechanism and kinetics. *Computational and Theoretical Chemistry*, **2004**, 676, 97-103		13
67	Site reactivity in the free radicals induced damage to leucine residues: a theoretical study. *Physical Chemistry Chemical Physics*, **2015**, 17, 4970-6	3.6	12
66	Anthranilic acid as a secondary antioxidant: Implications to the inhibition of OH production and the associated oxidative stress. *Computational and Theoretical Chemistry*, **2016**, 1077, 18-24	2	12
65	Role of the sulfur atom on the reactivity of methionine toward OH radicals: comparison with norleucine. *Journal of Physical Chemistry B*, **2009**, 113, 4947-52	3.4	12
64	CBS-QB3 + VTST Study of Methyl N-Methylcarbamate + OH Gas-Phase Reaction: Mechanism, Kinetics, and Branching Ratios. *Journal of Chemical Theory and Computation*, **2009**, 5, 1295-303	6.4	12
63	On the mechanism of gas-phase reaction of C1-C3 aliphatic thiols + OH radicals. *Journal of Physical Chemistry A*, **2007**, 111, 1523-9	2.8	12
62	Kinetics and mechanism of the beta-alanine + OH gas phase reaction: a quantum mechanical approach. *Physical Chemistry Chemical Physics*, **2006**, 8, 285-92	3.6	12
61	Chalcogen effects on the primary antioxidant activity of chrysin and quercetin. *New Journal of Chemistry*, **2020**, 44, 9073-9082	3.6	11

60	The Antioxidant Capability of Higenamine: Insights from Theory. *Antioxidants*, **2020**, 9,	7.1	11
59	On the mechanism of the OH initiated oxidation of acetylene in the presence of O2 and NO x. *Theoretical Chemistry Accounts*, **2008**, 121, 219-225	1.9	11
58	Melatonin and Related Compounds: Chemical Insights into their Protective Effects Against Oxidative Stress. *Current Organic Chemistry*, **2017**, 21,	1.7	10
57	Ab initio study of □alanine conformers in gas phase. *Arkivoc*, **2005**, 2005, 7-18	0.9	10
56	Estimation of empirically fitted parameters for calculating pK a values of thiols in a fast and reliable way. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	10
55	How to identify promising metal scavengers? d-penicillamine with copper as a study case. *International Journal of Quantum Chemistry*, **2018**, 118, e25457	2.1	10
54	Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. *Chemistry - A European Journal*, **2018**, 24, 8686-8691	4.8	9
53	Synthesis of new ZnS□bipy based hybrid organic□inorganic materials for photocatalytic reduction of 4-nitrophenol. *New Journal of Chemistry*, **2015**, 39, 2188-2194	3.6	9
52	Stability and electronic structure of Si, Ge, and Ti substituted single walled carbon nanotubes. *Physical Review B*, **2008**, 77,	3.3	9
51	Computational study on the antifreeze glycoproteins as inhibitors of clathrate-hydrate formation. *ChemPhysChem*, **2008**, 9, 1630-5	3.2	9
50	Quantum chemistry and TST study of the mechanism and kinetics of the butadiene and isoprene reactions with mercapto radicals. *Chemical Physics*, **2008**, 344, 273-280	2.3	9
49	Ground-state and some excited states of Li2 by the half-projected Hartree□Fock method. *International Journal of Quantum Chemistry*, **1995**, 54, 305-311	2.1	9
48	Silicon-Doped Carbon Nanotubes: Promising CO2/N2 Selective Agents for Sequestering Carbon Dioxide. *Journal of Physical Chemistry C*, **2016**, 120, 24476-24481	3.8	8
47	A deeper insight on the radical scavenger activity of two simple coumarins toward OOH radical. *Computational and Theoretical Chemistry*, **2016**, 1077, 133-138	2	8
46	Scavenging Ability of Homogentisic Acid and Ergosterol toward Free Radicals Derived from Ethanol Consumption. *Journal of Physical Chemistry B*, **2018**, 122, 7514-7521	3.4	8
45	Electrochemical characterization of tenoxicam using a bare carbon paste electrode under stagnant and forced convection conditions. *Electrochimica Acta*, **2012**, 59, 150-155	6.7	8
44	Theoretical study on the oxidative damage to cholesterol induced by peroxyl radicals. *Journal of Physical Organic Chemistry*, **2015**, 28, 504-508	2.1	8
43	Role of purines on the copper-catalyzed oxidative damage in biological systems: Protection versus promotion. *International Journal of Quantum Chemistry*, **2018**, 118, e25527	2.1	7

42	A combined experimental–theoretical study of the acid–base behavior of mangiferin: implications for its antioxidant activity. *RSC Advances*, **2016**, 6, 51171-51182	3.7	7
41	Self-decarboxylation of trichloroacetic acid redox catalyzed by trichloroacetate ions in acetonitrile solutions. *Organic and Biomolecular Chemistry*, **2013**, 11, 318-25	3.9	7
40	Deprotonation mechanism of new antihypertensive piperidinylmethylphenols: a combined experimental and theoretical study. *Journal of Physical Chemistry B*, **2009**, 113, 11765-74	3.4	7
39	Unambiguous assignment of 13C NMR signals in epimeric 4,5-epoxy-3-oxo-steroids assisted by X-ray diffraction and gauge invariant atomic orbitals calculation of absolute isotropic shieldings. *Arkivoc*, **2013**, 2013, 107-125	0.9	7
38	The other side of the superoxide radical anion: its ability to chemically repair DNA oxidized sites. *Chemical Communications*, **2018**, 54, 13710-13713	5.8	7
37	The spontaneous decarboxylation of strong carboxylic acid–carboxylate mixtures and the use of carbon surfaces to trap the released free radicals. *Electrochimica Acta*, **2017**, 245, 472-481	6.7	6
36	Competitive Gas Phase Reactions for the Production of Isomers COH. Spectroscopic Constants of Methyl Formate. *Journal of Physical Chemistry A*, **2019**, 123, 9658-9668	2.8	6
35	Spectro-electrochemical and DFT study of tenoxicam metabolites formed by electrochemical oxidation. *Electrochimica Acta*, **2013**, 111, 314-323	6.7	6
34	Role of Hydrolysis Degree in the Drug–Matrix Interactions of Nanosized Sol–Gel Titania Reservoirs for Epilepsy Treatment. *Journal of Physical Chemistry C*, **2010**, 114, 20022-20027	3.8	6
33	Drug–Matrix Interactions in Nanostructured Materials Containing Acetyl Salicylic Acid Using an Enteric Polymer As a Coating. *Journal of Physical Chemistry C*, **2008**, 112, 20222-20226	3.8	6
32	Computational Quantum Chemistry: A Reliable Tool in the Understanding of Gas-Phase Reactions. *Journal of Chemical Education*, **2006**, 83, 481	2.4	6
31	Computationally Designed Sesamol Derivatives Proposed as Potent Antioxidants. *ACS Omega*, **2020**, 5, 9566-9575	3.9	6
30	Direct and cluster-assisted dehydrogenation of methane by Nb and Ta: a theoretical investigation. *Physical Chemistry Chemical Physics*, **2017**, 19, 16178-16188	3.6	5
29	Capsaicin, a Powerful OH-Inactivating Ligand. *Antioxidants*, **2020**, 9,	7.1	5
28	Synthesis of Dimeric Steroid Trioxabispiroacetals Scaffolds by Gold(I)-Catalyzed Hydroalkoxylation–Hydration of Diynediols. *European Journal of Organic Chemistry*, **2019**, 2019, 4916-4927	2.2	5
27	Correlation between hydrogen bonding association constants in solution with quantum chemistry indexes: the case of successive association between reduced species of quinones and methanol. *Journal of Physical Chemistry A*, **2012**, 116, 10638-45	2.8	5
26	Computationally designed p-coumaric acid analogs: searching for neuroprotective antioxidants. *New Journal of Chemistry*, **2021**, 45, 14369-14380	3.6	5
25	A first principles investigation on the electron donor ability of synthetic melatonin derivatives: implications for their antioxidant activity. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4

24	On the hydroperoxyl radical scavenging activity of two Edaravone derivatives: mechanism and kinetics. *Journal of Physical Organic Chemistry*, **2013**, 26, 261-268	2.1	4
23	Electrochemical Characterization of Quercetin in Aqueous Solution. *ECS Transactions*, **2009**, 20, 115-122	1	4
22	La ecuaci□n de Charlot, la gr□fica de Flood y la gr□fica de Gordus **2010**, 21, 306-313		4
21	Reactivity Indexes and O-H Bond Dissociation Energies of a Large Series of Polyphenols: Implications for their Free Radical Scavenging Activity **2017**, 56,		4
20	Numerical test of SAC-CI methods for calculating vertical ionization energies. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
19	The reactions of plant hormones with reactive oxygen species: chemical insights at a molecular level. *Journal of Molecular Modeling*, **2018**, 24, 255	2	4
18	Computational study on the kinetics and mechanism of the carbaryl + OH reaction. *Journal of Physical Chemistry A*, **2014**, 118, 7776-81	2.8	3
17	Combined experimental□theoretical investigation on the interactions of Diuron with a urea□formaldehyde matrix: implications for its use as an □ntelligent pesticide□ *Chemical Papers*, **2017**, 71, 2495-2503	1.9	3
16	Determination of pKa Values of Diclofenac and Ibuprofen in Aqueous Solutions by Capillary Zone Electrophoresis. *ECS Transactions*, **2010**, 29, 443-448	1	3
15	Computer-designed melatonin derivatives: potent peroxyl radical scavengers with no pro-oxidant behavior. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	3
14	Chemical Protectors against the Toxic Effects of Paracetamol (Acetaminophen) and Its Meta Analogue: Preventing Protein Arylation. *ACS Omega*, **2018**, 3, 18582-18591	3.9	3
13	Detailed Investigation of the Outstanding Peroxyl Radical Scavenging Activity of Two Novel Amino-Pyridinol-Based Compounds. *Journal of Chemical Information and Modeling*, **2019**, 59, 3494-3505	6.1	2
12	New free radicals to measure antiradical capacity: a theoretical study. *Journal of Physical Chemistry B*, **2014**, 118, 10092-100	3.4	2
11	Systematic Search for Chemical Reactions in Gas Phase Contributing to Methanol Formation in Interstellar Space. *Journal of Physical Chemistry A*, **2017**, 121, 7393-7400	2.8	2
10	Elucidation of the complex deprotonation routes of Changrolin, the antihypertensives LQM-303 and LQM-303b, and their derivatives. *Computational and Theoretical Chemistry*, **2017**, 1115, 229-238	2	2
9	Electrochemical Determination of the Antioxidant Capacity of Organic Compounds. *ECS Transactions*, **2008**, 15, 471-478	1	2
8	Free radical scavenging activity of newly designed sesamol derivatives. *New Journal of Chemistry*, **2021**, 45, 11960-11967	3.6	2
7	Rate coefficient and mechanism of the gas phase OPSCN-□PNCS isomerization: a density functional theory study. *Computational and Theoretical Chemistry*, **2004**, 676, 127-132		1

6	The FC(O)OF torsional potential: thermochemistry and kinetics. *Journal of Molecular Structure*, **2005**, 737, 83-89	3.4	1
5	A spectroscopic study of ground state of lithium hydride with the HPHF model. *Computational and Theoretical Chemistry*, **1993**, 287, 107-110		1
4	Potentiating the Benefits of Melatonin through Chemical Functionalization: Possible Impact on Multifactorial Neurodegenerative Disorders. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
3	Chemical repair mechanisms of damaged tyrosyl and tryptophanyl residues in proteins by the superoxide radical anion. *New Journal of Chemistry*, **2020**, 44, 2505-2513	3.6	
2	Deprotonation Mechanism and logPValues of New Antihypertensive Thiomorpholinylmethylphenols: A Combined Experimental and Theoretical Study *Journal of Chemical & Engineering Data*, **2010**, 55, 4323-4331	2.8	
1	Theoretical approach to cationic polymerization of alkenylfurans. II. Ab initio and semiempirical study of relevant steps in the reaction mechanism. *Journal of Polymer Science Part A*, **1992**, 30, 2497-2502	2.5	