

Annia Galano

List of Publications by Year in Descending Order

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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.

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	Potentiating the Benefits of Melatonin through Chemical Functionalization: Possible Impact on Multifactorial Neurodegenerative Disorders. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	1
202	Free radical scavenging activity of newly designed sesamol derivatives. <i>New Journal of Chemistry</i> , 2021 , 45, 11960-11967	3.6	2
201	Computationally designed p-coumaric acid analogs: searching for neuroprotective antioxidants. <i>New Journal of Chemistry</i> , 2021 , 45, 14369-14380	3.6	5
200	Capsaicin, a Powerful OH-Inactivating Ligand. <i>Antioxidants</i> , 2020 , 9,	7.1	5
199	Chalcogen effects on the primary antioxidant activity of chrysin and quercetin. <i>New Journal of Chemistry</i> , 2020 , 44, 9073-9082	3.6	11
198	Chemical repair mechanisms of damaged tyrosyl and tryptophanyl residues in proteins by the superoxide radical anion. <i>New Journal of Chemistry</i> , 2020 , 44, 2505-2513	3.6	
197	The Antioxidant Capability of Higenamine: Insights from Theory. <i>Antioxidants</i> , 2020 , 9,	7.1	11
196	Computer-designed melatonin derivatives: potent peroxy radical scavengers with no pro-oxidant behavior. <i>Theoretical Chemistry Accounts</i> , 2020 , 139, 1	1.9	3
195	Computationally Designed Sesamol Derivatives Proposed as Potent Antioxidants. <i>ACS Omega</i> , 2020 , 5, 9566-9575	3.9	6
194	Computational strategies for predicting free radical scavengers' protection against oxidative stress: Where are we and what might follow?. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25665	2.1	101
193	Synthesis of Dimeric Steroid Trioxabispacetals Scaffolds by Gold(I)-Catalyzed Hydroalkoxylation/Hydration of Diynediols. <i>European Journal of Organic Chemistry</i> , 2019 , 2019, 4916-4927 ²	3.2	5
192	Detailed Investigation of the Outstanding Peroxyl Radical Scavenging Activity of Two Novel Amino-Pyridinol-Based Compounds. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 3494-3505	6.1	2
191	Competitive Gas Phase Reactions for the Production of Isomers COH. Spectroscopic Constants of Methyl Formate. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 9658-9668	2.8	6
190	Melatonin and its metabolites as chemical agents capable of directly repairing oxidized DNA. <i>Journal of Pineal Research</i> , 2019 , 66, e12539	10.4	26
189	Synthesis, Characterization, and Solid State Dynamic Studies of a Hydrogen Bond-Hindered Steroidal Molecular Rotor with a Flexible Axis. <i>Journal of Organic Chemistry</i> , 2018 , 83, 3768-3779	4.2	13
188	Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. <i>Chemistry - A European Journal</i> , 2018 , 24, 8686-8691	4.8	9
187	Citric acid: A promising copper scavenger. <i>Computational and Theoretical Chemistry</i> , 2018 , 1133, 47-50	2	18

186	Role of purines on the copper-catalyzed oxidative damage in biological systems: Protection versus promotion. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25527	2.1	7
185	Mitochondria: Central Organelles for Melatonin's Antioxidant and Anti-Aging Actions. <i>Molecules</i> , 2018 , 23,	4.8	159
184	Melatonin: A Versatile Protector against Oxidative DNA Damage. <i>Molecules</i> , 2018 , 23,	4.8	126
183	Scavenging Ability of Homogentisic Acid and Ergosterol toward Free Radicals Derived from Ethanol Consumption. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 7514-7521	3.4	8
182	Melatonin Mitigates Mitochondrial Meltdown: Interactions with SIRT3. <i>International Journal of Molecular Sciences</i> , 2018 , 19,	6.3	55
181	Melatonin and its metabolites vs oxidative stress: From individual actions to collective protection. <i>Journal of Pineal Research</i> , 2018 , 65, e12514	10.4	146
180	A Computer-Assisted Systematic Search for Melatonin Derivatives with High Potential as Antioxidants. <i>Melatonin Research</i> , 2018 , 1, 27-58	5.1	17
179	Estimation of empirically fitted parameters for calculating pK a values of thiols in a fast and reliable way. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	10
178	How to identify promising metal scavengers? d-penicillamine with copper as a study case. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25457	2.1	10
177	The other side of the superoxide radical anion: its ability to chemically repair DNA oxidized sites. <i>Chemical Communications</i> , 2018 , 54, 13710-13713	5.8	7
176	Chemical Protectors against the Toxic Effects of Paracetamol (Acetaminophen) and Its Meta Analogue: Preventing Protein Arylation. <i>ACS Omega</i> , 2018 , 3, 18582-18591	3.9	3
175	The reactions of plant hormones with reactive oxygen species: chemical insights at a molecular level. <i>Journal of Molecular Modeling</i> , 2018 , 24, 255	2	4
174	Comprehensive Investigation of the Antioxidant and Pro-oxidant Effects of Phenolic Compounds: A Double-Edged Sword in the Context of Oxidative Stress?. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 6198-6214 ⁴²	3.4	4
173	Non-covalent π -stacking interactions turn off non-adiabatic effects in proton-coupled electron transfer reactions. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 6969-6972	3.6	15
172	Dual antioxidant/pro-oxidant behavior of the tryptophan metabolite 3-hydroxyanthranilic acid: a theoretical investigation of reaction mechanisms and kinetics. <i>New Journal of Chemistry</i> , 2017 , 41, 3829-3845	3.6	21
171	Exploring Chemical Routes Relevant to the Toxicity of Paracetamol and Its meta-Analogue at a Molecular Level. <i>Chemical Research in Toxicology</i> , 2017 , 30, 1286-1301	4	13
170	Direct and cluster-assisted dehydrogenation of methane by Nb and Ta: a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 16178-16188	3.6	5
169	The spontaneous decarboxylation of strong carboxylic acid π -carboxylate mixtures and the use of carbon surfaces to trap the released free radicals. <i>Electrochimica Acta</i> , 2017 , 245, 472-481	6.7	6

168	The role of acid-base equilibria in formal hydrogen transfer reactions: tryptophan radical repair by uric acid as a paradigmatic case. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 15296-15309	3.6	17
167	A combined theoretical-experimental investigation on the mechanism of lignin pyrolysis: Role of heating rates and residence times. <i>Journal of Analytical and Applied Pyrolysis</i> , 2017 , 128, 208-216	6	28
166	Melatonin and Related Compounds: Chemical Insights into their Protective Effects Against Oxidative Stress. <i>Current Organic Chemistry</i> , 2017 , 21,	1.7	10
165	Systematic Search for Chemical Reactions in Gas Phase Contributing to Methanol Formation in Interstellar Space. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 7393-7400	2.8	2
164	Melatonin as a mitochondria-targeted antioxidant: one of evolution's best ideas. <i>Cellular and Molecular Life Sciences</i> , 2017 , 74, 3863-3881	10.3	255
163	Combined experimental-theoretical investigation on the interactions of Diuron with a urea-formaldehyde matrix: implications for its use as an intelligent pesticide. <i>Chemical Papers</i> , 2017 , 71, 2495-2503	1.9	3
162	Elucidation of the complex deprotonation routes of Changrolin, the antihypertensives LQM-303 and LQM-303b, and their derivatives. <i>Computational and Theoretical Chemistry</i> , 2017 , 1115, 229-238	2	2
161	Radical-trapping and preventive antioxidant effects of 2-hydroxymelatonin and 4-hydroxymelatonin: Contributions to the melatonin protection against oxidative stress. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017 , 1861, 2206-2217	4	13
160	Reactivity Indexes and O-H Bond Dissociation Energies of a Large Series of Polyphenols: Implications for their Free Radical Scavenging Activity 2017 , 56,		4
159	Free Radicals Induced Oxidative Stress at a Molecular Level: The Current Status, Challenges and Perspectives of Computational Chemistry Based Protocols 2017 , 59,		15
158	Empirically Fitted Parameters for Calculating pKa Values with Small Deviations from Experiments Using a Simple Computational Strategy. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 1714-24	6.1	59
157	Silicon-Doped Carbon Nanotubes: Promising CO ₂ /N ₂ Selective Agents for Sequestering Carbon Dioxide. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 24476-24481	3.8	8
156	A combined experimental-theoretical study of the acid-base behavior of mangiferin: implications for its antioxidant activity. <i>RSC Advances</i> , 2016 , 6, 51171-51182	3.7	7
155	A first principles investigation on the electron donor ability of synthetic melatonin derivatives: implications for their antioxidant activity. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	4
154	Food Antioxidants: Chemical Insights at the Molecular Level. <i>Annual Review of Food Science and Technology</i> , 2016 , 7, 335-52	14.7	222
153	NEW INSIGHTS ON THE KINETICS AND MECHANISM OF THE ELECTROCHEMICAL OXIDATION OF DICLOFENAC IN NEUTRAL AQUEOUS MEDIUM. <i>Electrochimica Acta</i> , 2016 , 199, 92-98	6.7	22
152	Coumarin-Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 662-70	6.1	32
151	The key role of the sequential proton loss electron transfer mechanism on the free radical scavenging activity of some melatonin-related compounds. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	16

150	Anthranilic acid as a secondary antioxidant: Implications to the inhibition of OH production and the associated oxidative stress. <i>Computational and Theoretical Chemistry</i> , 2016 , 1077, 18-24	2	12
149	A deeper insight on the radical scavenger activity of two simple coumarins toward OOH radical. <i>Computational and Theoretical Chemistry</i> , 2016 , 1077, 133-138	2	8
148	Theoretical and experimental studies of highly active graphene nanosheets to determine catalytic nitrogen sites responsible for the oxygen reduction reaction in alkaline media. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 976-990	13	36
147	Hydrogen Abstraction Reactions from Phenolic Compounds by Peroxyl Radicals: Multireference Character and Density Functional Theory Rate Constants. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 4634-42	2.8	47
146	Phenolic Melatonin-Related Compounds: Their Role as Chemical Protectors against Oxidative Stress. <i>Molecules</i> , 2016 , 21,	4.8	33
145	Quantum mechanical based approaches for predicting pKa values of carboxylic acids: evaluating the performance of different strategies. <i>RSC Advances</i> , 2016 , 6, 112057-112064	3.7	16
144	Deprotonation routes of anthocyanidins in aqueous solution, pKa values, and speciation under physiological conditions. <i>RSC Advances</i> , 2016 , 6, 53421-53429	3.7	15
143	Computational-aided design of melatonin analogues with outstanding multifunctional antioxidant capacity. <i>RSC Advances</i> , 2016 , 6, 22951-22963	3.7	14
142	Numerical test of SAC-CI methods for calculating vertical ionization energies. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	4
141	Site reactivity in the free radicals induced damage to leucine residues: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 4970-6	3.6	12
140	Free-radical scavenging by tryptophan and its metabolites through electron transfer based processes. <i>Journal of Molecular Modeling</i> , 2015 , 21, 213	2	38
139	N-Acetylserotonin and 6-Hydroxymelatonin against Oxidative Stress: Implications for the Overall Protection Exerted by Melatonin. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 8535-43	3.4	42
138	NR2 and P3+: Accurate, Efficient Electron-Propagator Methods for Calculating Valence, Vertical Ionization Energies of Closed-Shell Molecules. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 8813-21	2.8	36
137	Antioxidant properties of several coumarin-chalcone hybrids from theoretical insights. <i>RSC Advances</i> , 2015 , 5, 565-575	3.7	61
136	Melatonin: an ancient molecule that makes oxygen metabolically tolerable. <i>Journal of Pineal Research</i> , 2015 , 59, 403-19	10.4	595
135	Theoretical study on the oxidative damage to cholesterol induced by peroxyl radicals. <i>Journal of Physical Organic Chemistry</i> , 2015 , 28, 504-508	2.1	8
134	Phytomelatonin: assisting plants to survive and thrive. <i>Molecules</i> , 2015 , 20, 7396-437	4.8	225
133	Assessing the Protective Activity of a Recently Discovered Phenolic Compound against Oxidative Stress Using Computational Chemistry. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2552-61	6.1	16

132	Synthesis of new ZnSBipy based hybrid organic/inorganic materials for photocatalytic reduction of 4-nitrophenol. <i>New Journal of Chemistry</i> , 2015 , 39, 2188-2194	3.6	9
131	Non-isothermal pyrolysis of pectin: A thermochemical and kinetic approach. <i>Journal of Analytical and Applied Pyrolysis</i> , 2015 , 112, 94-104	6	82
130	Melatonin and its metabolites as copper chelating agents and their role in inhibiting oxidative stress: a physicochemical analysis. <i>Journal of Pineal Research</i> , 2015 , 58, 107-16	10.4	121
129	Adrenaline and noradrenaline: protectors against oxidative stress or molecular targets?. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 3479-91	3.4	46
128	Theoretical study on the peroxy radicals scavenging activity of esculetin and its regeneration in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 1197-207	3.6	27
127	Dihydroxybenzoic acids as free radical scavengers: mechanisms, kinetics, and trends in activity. <i>New Journal of Chemistry</i> , 2014 , 38, 2639	3.6	34
126	Melatonin: exceeding expectations. <i>Physiology</i> , 2014 , 29, 325-33	9.8	269
125	New free radicals to measure antiradical capacity: a theoretical study. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 10092-100	3.4	2
124	Cyclic 3-hydroxymelatonin, a key metabolite enhancing the peroxy radical scavenging activity of melatonin. <i>RSC Advances</i> , 2014 , 4, 5220	3.7	40
123	Radical scavenging ability of gallic acid toward OH and OOH radicals. Reaction mechanism and rate constants from the density functional theory. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 10380-9	3.4	101
122	Vertical ionization energies of free radicals and electron detachment energies of their anions: a comparison of direct and indirect methods versus experiment. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 6125-31	2.8	15
121	On the chemical behavior of C60 hosting H2O and other isoelectronic neutral molecules. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2412	2	18
120	Computational study on the kinetics and mechanism of the carbaryl + OH reaction. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 7776-81	2.8	3
119	Ellagic acid: an unusually versatile protector against oxidative stress. <i>Chemical Research in Toxicology</i> , 2014 , 27, 904-18	4	72
118	The mechanism of mediated oxidation of carboxylates with ferrocene as redox catalyst in absence of grafting effects. An experimental and theoretical approach. <i>Electrochimica Acta</i> , 2014 , 136, 542-549	6.7	13
117	Melatonin reduces lipid peroxidation and membrane viscosity. <i>Frontiers in Physiology</i> , 2014 , 5, 377	4.6	85
116	Kinetics of radical-molecule reactions in aqueous solution: a benchmark study of the performance of density functional methods. <i>Journal of Computational Chemistry</i> , 2014 , 35, 2019-26	3.5	151
115	Cyclic-3-hydroxymelatonin (C3HOM), a potent antioxidant, scavenges free radicals and suppresses oxidative reactions. <i>Current Medicinal Chemistry</i> , 2014 , 21, 1557-65	4.3	62

114	A computational methodology for accurate predictions of rate constants in solution: application to the assessment of primary antioxidant activity. <i>Journal of Computational Chemistry</i> , 2013 , 34, 2430-45	3.5	203
113	Piceatannol, a better peroxy radical scavenger than resveratrol. <i>RSC Advances</i> , 2013 , 3, 20209	3.7	64
112	Deprotonation mechanism and acidity constants in aqueous solution of flavonols: a combined experimental and theoretical study. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 12347-59	3.4	79
111	Self-decarboxylation of trichloroacetic acid redox catalyzed by trichloroacetate ions in acetonitrile solutions. <i>Organic and Biomolecular Chemistry</i> , 2013 , 11, 318-25	3.9	7
110	On the free radical scavenging activities of melatonin's metabolites, AFMK and AMK. <i>Journal of Pineal Research</i> , 2013 , 54, 245-57	10.4	569
109	Spectro-electrochemical and DFT study of tenoxicam metabolites formed by electrochemical oxidation. <i>Electrochimica Acta</i> , 2013 , 111, 314-323	6.7	6
108	Cis carotenoids: colorful molecules and free radical quenchers. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 4050-61	3.4	20
107	A physicochemical examination of the free radical scavenging activity of Trolox: mechanism, kinetics and influence of the environment. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 4642-50	3.6	154
106	On the hydroperoxyl radical scavenging activity of two Edaravone derivatives: mechanism and kinetics. <i>Journal of Physical Organic Chemistry</i> , 2013 , 26, 261-268	2.1	4
105	Unambiguous assignment of ¹³ C 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. <i>Arkivoc</i> , 2013 , 2013, 107-125	0.9	7
104	Electrochemical characterization of tenoxicam using a bare carbon paste electrode under stagnant and forced convection conditions. <i>Electrochimica Acta</i> , 2012 , 59, 150-155	6.7	8
103	On the chemical repair of DNA radicals by glutathione: hydrogen vs electron transfer. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 9316-25	3.4	62
102	On the outstanding antioxidant capacity of edaravone derivatives through single electron transfer reactions. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 1180-8	3.4	28
101	On the evolution of one-electron-oxidized deoxyguanosine in damaged DNA under physiological conditions: a DFT and ONIOM study on proton transfer and equilibrium. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 12476-84	3.6	34
100	Correlation between hydrogen bonding association constants in solution with quantum chemistry indexes: the case of successive association between reduced species of quinones and methanol. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 10638-45	2.8	5
99	On the free radical scavenging mechanism of protocatechuic acid, regeneration of the catechol group in aqueous solution. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	32
98	Capsaicin, a tasty free radical scavenger: mechanism of action and kinetics. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 1200-8	3.4	75
97	On the DH and DOH scavenging activity of 3-methyl-1-pyridin-2-yl-5-pyrazolone: Comparisons with its parent compound, edaravone. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 3441-3448 ^{2.1}	2.1	19

96	First principles calculations of pKa values of amines in aqueous solution: Application to neurotransmitters. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 3449-3460	2.1	30
95	Free radical scavenging activity of caffeine's metabolites. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 3472-3478	2.1	14
94	On the peroxy scavenging activity of hydroxycinnamic acid derivatives: mechanisms, kinetics, and importance of the acid-base equilibrium. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 12534-43	3.6	54
93	Xanthenes as antioxidants: a theoretical study on the thermodynamics and kinetics of the single electron transfer mechanism. <i>Food and Function</i> , 2012 , 3, 442-50	6.1	33
92	Influence of the environment on the protective effects of guaiacol derivatives against oxidative stress: mechanisms, kinetics, and relative antioxidant activity. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 7129-37	3.4	30
91	A quantum chemical study on the free radical scavenging activity of tyrosol and hydroxytyrosol. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	34
90	Is caffeine a good scavenger of oxygenated free radicals?. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 4538-46	3.4	150
89	Searching for Computational Strategies to Accurately Predict pKas of Large Phenolic Derivatives. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2528-38	6.4	52
88	Uric and 1-methyluric acids: metabolic wastes or antiradical protectors?. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 15430-8	3.4	20
87	Mechanism and kinetics studies on the antioxidant activity of sinapinic acid. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 11199-205	3.6	72
86	On the direct scavenging activity of melatonin towards hydroxyl and a series of peroxy radicals. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7178-88	3.6	132
85	Canolol: a promising chemical agent against oxidative stress. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 8590-6	3.4	65
84	Ionization energies, proton affinities, and pKa values of a large series of edaravone derivatives: implication for their free radical scavenging activity. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 10375-84	3.4	18
83	Melatonin as a natural ally against oxidative stress: a physicochemical examination. <i>Journal of Pineal Research</i> , 2011 , 51, 1-16	10.4	816
82	Oxidative desulfurization (ODS) of organosulfur compounds catalyzed by peroxy-metalate complexes of W ₂ O ₇ /rO ₂ : Thermochemical, structural, and reactivity indexes analyses. <i>Journal of Catalysis</i> , 2011 , 282, 201-208	7.3	84
81	Mechanism and kinetics of the hydroxyl and hydroperoxyl radical scavenging activity of N-acetylcysteine amide. <i>Theoretical Chemistry Accounts</i> , 2011 , 130, 51-60	1.9	22
80	Glutathione: mechanism and kinetics of its non-enzymatic defense action against free radicals. <i>RSC Advances</i> , 2011 , 1, 1763	3.7	108
79	Role of allyl group in the hydroxyl and peroxy radical scavenging activity of S-allylcysteine. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 13408-17	3.4	25

78	Physicochemical insights on the free radical scavenging activity of sesamol: importance of the acid/base equilibrium. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 13101-9	3.4	55
77	OH radical scavenging activity of Edaravone: mechanism and kinetics. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 1306-14	3.4	97
76	Free radical scavenger properties of Mangostin: thermodynamics and kinetics of HAT and RAF mechanisms. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 12591-8	3.4	73
75	Water complexes of important air pollutants: geometries, complexation energies, concentrations, infrared spectra, and intrinsic reactivity. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 5796-809	2.8	41
74	Mechanism and branching ratios of hydroxy ethers + (*OH) gas phase reactions: relevance of H-bond interactions. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 7525-36	2.8	15
73	Free Radical Scavenging Activity of Ultrashort Single-Walled Carbon Nanotubes with Different Structures through Electron Transfer Reactions. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 8184-8191	3.8	57
72	Role of Hydrolysis Degree in the Drug-Matrix Interactions of Nanosized Sol-Gel Titania Reservoirs for Epilepsy Treatment. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 20022-20027	3.8	6
71	On the Free Radical Scavenging Capability of Carboxylated Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 6363-6370	3.8	27
70	Effect of Different Functional Groups on the Free Radical Scavenging Capability of Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 14734-14739	3.8	25
69	Carbon nanotubes: promising agents against free radicals. <i>Nanoscale</i> , 2010 , 2, 373-80	7.7	108
68	Determination of pKa Values of Diclofenac and Ibuprofen in Aqueous Solutions by Capillary Zone Electrophoresis. <i>ECS Transactions</i> , 2010 , 29, 443-448	1	3
67	Deprotonation Mechanism and logP Values of New Antihypertensive Thiomorpholinylmethylphenols: A Combined Experimental and Theoretical Study. <i>Journal of Chemical & Engineering Data</i> , 2010 , 55, 4323-4331	2.8	
66	Carotenoids can act as antioxidants by oxidizing the superoxide radical anion. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 193-200	3.6	89
65	Influence of Point Defects on the Free-Radical Scavenging Capability of Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 8302-8308	3.8	36
64	La ecuación de Charlot, la gráfica de Flood y la gráfica de Gordus 2010 , 21, 306-313		4
63	Mechanism of the OH radical scavenging activity of nordihydroguaiaretic acid: a combined theoretical and experimental study. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 6625-35	3.4	71
62	Counterpoise corrected interaction energies are not systematically better than uncorrected ones: comparison with CCSD(T) CBS extrapolated values. <i>Theoretical Chemistry Accounts</i> , 2010 , 126, 75-85	1.9	114
61	Theoretical study on the chemical fate of adducts formed through free radical addition reactions to carotenoids. <i>Theoretical Chemistry Accounts</i> , 2010 , 127, 595-603	1.9	32

60	Electrochemical Characterization of Quercetin in Aqueous Solution. <i>ECS Transactions</i> , 2009 , 20, 115-122	1	4
59	Role of the reacting free radicals on the antioxidant mechanism of curcumin. <i>Chemical Physics</i> , 2009 , 363, 13-23	2.3	88
58	Surface acid/basic properties of WO _x /ZrO ₂ and catalytic efficiency in oxidative desulfurization. <i>Applied Catalysis B: Environmental</i> , 2009 , 92, 1-8	21.8	52
57	Influence of Diameter, Length, and Chirality of Single-Walled Carbon Nanotubes on Their Free Radical Scavenging Capability. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 18487-18491	3.8	31
56	Reactions of OOH radical with beta-carotene, lycopene, and torulene: hydrogen atom transfer and adduct formation mechanisms. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 11338-45	3.4	68
55	Deprotonation mechanism of new antihypertensive piperidinylmethylphenols: a combined experimental and theoretical study. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 11765-74	3.4	7
54	Guanosine + OH radical reaction in aqueous solution: a reinterpretation of the UV-vis data based on thermodynamic and kinetic calculations. <i>Organic Letters</i> , 2009 , 11, 5114-7	6.2	88
53	Role of the sulfur atom on the reactivity of methionine toward OH radicals: comparison with norleucine. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 4947-52	3.4	12
52	What is important to prevent oxidative stress? A theoretical study on electron-transfer reactions between carotenoids and free radicals. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 12113-20	3.4	71
51	OH radical gas phase reactions with aliphatic ethers: a variational transition state theory study. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 13913-20	2.8	91
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