Annia Galano

List of Publications by Year
in descending order

205 papers	12,844 citations	20759 60 h-index	27345 106 g-index
208 all docs	208 docs citations	208 times ranked	11621 citing authors

#	Article	IF	Citations
1	Melatonin as a natural ally against oxidative stress: a physicochemical examination. Journal of Pineal Research, 2011, 51, 1-16.	3.4	963
2	Melatonin: an ancient molecule that makes oxygen metabolically tolerable. Journal of Pineal Research, 2015, 59, 403-419.	3.4	751
3	On the free radical scavenging activities of melatonin's metabolites, <scp>AFMK</scp> and <scp>AMK</scp>. Journal of Pineal Research, 2013, 54, 245-257.	3.4	679
4	Melatonin: Exceeding Expectations. Physiology, 2014, 29, 325-333.	1.6	401
5	Melatonin as a mitochondria-targeted antioxidant: one of evolutionâ€™s best ideas. Cellular and Molecular Life Sciences, 2017, 74, 3863-3881.	2.4	369
6	Phytomelatonin: Assisting Plants to Survive and Thrive. Molecules, 2015, 20, 7396-7437.	1.7	294
7	Food Antioxidants: Chemical Insights at the Molecular Level. Annual Review of Food Science and Technology, 2016, 7, 335-352.	5.1	294
8	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, 2430-2445.	1.5	289
9	Mitochondria: Central Organelles for Melatoninâ€²s Antioxidant and Anti-Aging Actions. Molecules, 2018, 23, 509.	1.7	263
10	Melatonin and its metabolites vs oxidative stress: From individual actions to collective protection. Journal of Pineal Research, 2018, 65, e12514.	3.4	225
11	Kinetics of radicalâ€molecule reactions in aqueous solution: A benchmark study of the performance of density functional methods. Journal of Computational Chemistry, 2014, 35, 2019-2026.	1.5	211
12	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.	1.3	210
13	Melatonin: A Versatile Protector against Oxidative DNA Damage. Molecules, 2018, 23, 530.	1.7	192
14	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.	1.0	178
15	Is Caffeine a Good Scavenger of Oxygenated Free Radicals?. Journal of Physical Chemistry B, 2011, 115, 4538-4546.	1.2	177
16	On the direct scavenging activity of melatonin towards hydroxyl and a series of peroxyl radicals. Physical Chemistry Chemical Physics, 2011, 13, 7178.	1.3	160
17	Carbon Nanotubes as Free-Radical Scavengers. Journal of Physical Chemistry C, 2008, 112, 8922-8927.	1.5	150
18	Melatonin and its metabolites as copper chelating agents and their role in inhibiting oxidative stress: a physicochemical analysis. Journal of Pineal Research, 2015, 58, 107-116.	3.4	142

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19	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, 10380-10389.	1.2	139
20	Glutathione: mechanism and kinetics of its non-enzymatic defense action against free radicals. RSC Advances, 2011, 1, 1763.	1.7	136
21	Carbon nanotubes: promising agents against free radicals. Nanoscale, 2010, 2, 373.	2.8	133
22	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.	0.5	130
23	Non-isothermal pyrolysis of pectin: A thermochemical and kinetic approach. Journal of Analytical and Applied Pyrolysis, 2015, 112, 94-104.	2.6	123
24	<i>Eyringpy</i>: A program for computing rate constants in the gas phase and in solution. International Journal of Quantum Chemistry, 2019, 119, e25686.	1.0	122
25	Melatonin reduces lipid peroxidation and membrane viscosity. Frontiers in Physiology, 2014, 5, 377.	1.3	114
26	OH Radical Scavenging Activity of Edaravone: Mechanism and Kinetics. Journal of Physical Chemistry B, 2011, 115, 1306-1314.	1.2	111
27	Ellagic Acid: An Unusually Versatile Protector against Oxidative Stress. Chemical Research in Toxicology, 2014, 27, 904-918.	1.7	110
28	Gas phase reactions of C1â€"C4alcohols with the OH radical: A quantum mechanical approach. Physical Chemistry Chemical Physics, 2002, 4, 4648-4662.	1.3	108
29	A new approach to counterpoise correction to BSSE. Journal of Computational Chemistry, 2006, 27, 1203-1210.	1.5	105
30	Carotenoids can act as antioxidants by oxidizing the superoxideradical anion. Physical Chemistry Chemical Physics, 2010, 12, 193-200.	1.3	105
31	Role of the reacting free radicals on the antioxidant mechanism of curcumin. Chemical Physics, 2009, 363, 13-23.	0.9	104
32	OH Radical Gas Phase Reactions with Aliphatic Ethers: A Variational Transition State Theory Study. Journal of Physical Chemistry A, 2009, 113, 13913-13920.	1.1	103
33	Guanosine + OH Radical Reaction in Aqueous Solution: A Reinterpretation of the UVâˆ'vis Data Based on Thermodynamic and Kinetic Calculations. Organic Letters, 2009, 11, 5114-5117.	2.4	100
34	Deprotonation Mechanism and Acidity Constants in Aqueous Solution of Flavonols: a Combined Experimental and Theoretical Study. Journal of Physical Chemistry B, 2013, 117, 12347-12359.	1.2	99
35	Empirically Fitted Parameters for Calculating p<i>K</i>_a Values with Small Deviations from Experiments Using a Simple Computational Strategy. Journal of Chemical Information and Modeling, 2016, 56, 1714-1724.	2.5	97
36	Oxidative desulfurization (ODS) of organosulfur compounds catalyzed by peroxo-metallate complexes of WOxâ€"ZrO2: Thermochemical, structural, and reactivity indexes analyses. Journal of Catalysis, 2011, 282, 201-208.	3.1	93

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37	Capsaicin, a Tasty Free Radical Scavenger: Mechanism of Action and Kinetics. Journal of Physical Chemistry B, 2012, 116, 1200-1208.	1.2	91
38	Free Radical Scavenger Properties of Î±-Mangostin: Thermodynamics and Kinetics of HAT and RAF Mechanisms. Journal of Physical Chemistry B, 2011, 115, 12591-12598.	1.2	88
39	Relative Antioxidant Efficiency of a Large Series of Carotenoids in Terms of One Electron Transfer Reactions. Journal of Physical Chemistry B, 2007, 111, 12898-12908.	1.2	85
40	On the Chemical Repair of DNA Radicals by Glutathione: Hydrogen vs Electron Transfer. Journal of Physical Chemistry B, 2012, 116, 9316-9325.	1.2	85
41	Piceatannol, a better peroxyl radical scavenger than resveratrol. RSC Advances, 2013, 3, 20209.	1.7	85
42	Mechanism of the OH Radical Scavenging Activity of Nordihydroguaiaretic Acid: A Combined Theoretical and Experimental Study. Journal of Physical Chemistry B, 2010, 114, 6625-6635.	1.2	82
43	Mechanism and kinetics studies on the antioxidant activity of sinapinic acid. Physical Chemistry Chemical Physics, 2011, 13, 11199.	1.3	80
44	Melatonin Mitigates Mitochondrial Meltdown: Interactions with SIRT3. International Journal of Molecular Sciences, 2018, 19, 2439.	1.8	80
45	Antioxidant properties of several coumarinâ€"chalcone hybrids from theoretical insights. RSC Advances, 2015, 5, 565-575.	1.7	79
46	Reactions of OOH Radical with Î²-Carotene, Lycopene, and Torulene: Hydrogen Atom Transfer and Adduct Formation Mechanisms. Journal of Physical Chemistry B, 2009, 113, 11338-11345.	1.2	77
47	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, 12113-12120.	1.2	77
48	Canolol: A Promising Chemical Agent against Oxidative Stress. Journal of Physical Chemistry B, 2011, 115, 8590-8596.	1.2	77
49	Rate Constant Dependence on the Size of Aldehydes in the NO3+ Aldehydes Reaction. An Explanation via Quantum Chemical Calculations and CTST. Journal of the American Chemical Society, 2001, 123, 8387-8395.	6.6	71
50	Rate Coefficient and Mechanism of the Gas Phase OH Hydrogen Abstraction Reaction from Formic Acid:Â A Quantum Mechanical Approach. Journal of Physical Chemistry A, 2002, 106, 9520-9528.	1.1	71
51	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.	1.2	71
52	Adrenaline and Noradrenaline: Protectors against Oxidative Stress or Molecular Targets?. Journal of Physical Chemistry B, 2015, 119, 3479-3491.	1.2	70
53	Theoretical Determination of the Rate Constant for OH Hydrogen Abstraction from Toluene. Journal of Physical Chemistry A, 2006, 110, 10155-10162.	1.1	69
54	Cyclic-3-hydroxymelatonin (C3HOM), A Potent Antioxidant, Scavenges Free Radicals and Suppresses Oxidative Reactions. Current Medicinal Chemistry, 2014, 21, 1557-1565.	1.2	69

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55	On the peroxyl scavenging activity of hydroxycinnamic acid derivatives: mechanisms, kinetics, and importance of the acidâ€“base equilibrium. Physical Chemistry Chemical Physics, 2012, 14, 12534.	1.3	68
56	Glycolaldehyde + OH Gas Phase Reaction:â€‰ A Quantum Chemistry + CVT/SCT Approach. Journal of Physical Chemistry A, 2005, 109, 169-180.	1.1	65
57	Physicochemical Insights on the Free Radical Scavenging Activity of Sesamol: Importance of the Acid/Base Equilibrium. Journal of Physical Chemistry B, 2011, 115, 13101-13109.	1.2	64
58	Surface acidâ€“basic properties of WOxâ€“ZrO2 and catalytic efficiency in oxidative desulfurization. Applied Catalysis B: Environmental, 2009, 92, 1-8.	10.8	63
59	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.	1.5	63
60	Searching for Computational Strategies to Accurately Predict p<i>K</i>_as of Large Phenolic Derivatives. Journal of Chemical Theory and Computation, 2011, 7, 2528-2538.	2.3	62
61	Peroxyl-Radical-Scavenging Activity of Garlic: 2-Propenesulfenic Acid versus Allicin. Journal of Physical Chemistry B, 2009, 113, 16077-16081.	1.2	59
62	OH hydrogen abstraction reactions from alanine and glycine: A quantum mechanical approach. Journal of Computational Chemistry, 2001, 22, 1138-1153.	1.5	57
63	Theoretical Explanation of Nonexponential OH Decay in Reactions with Benzene and Toluene under Pseudo-First-Order Conditions. Journal of Physical Chemistry A, 2008, 112, 7608-7615.	1.1	57
64	Hydrogen Abstraction Reactions from Phenolic Compounds by Peroxyl Radicals: Multireference Character and Density Functional Theory Rate Constants. Journal of Physical Chemistry A, 2016, 120, 4634-4642.	1.1	55
65	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, 8813-8821.	1.1	53
66	Structureâ^'Reactivity Relationship in Ketones + OH Reactions:Â A Quantum Mechanical and TST Approach. Journal of Physical Chemistry A, 2004, 108, 2740-2749.	1.1	52
67	Theoretical study of the initial reaction between OH and isoprene in tropospheric conditions. Physical Chemistry Chemical Physics, 2003, 5, 1392-1399.	1.3	51
68	<i>N</i>-Acetylserotonin and 6-Hydroxymelatonin against Oxidative Stress: Implications for the Overall Protection Exerted by Melatonin. Journal of Physical Chemistry B, 2015, 119, 8535-8543.	1.2	50
69	Mechanism and Kinetics of the Reaction of OH Radicals with Glyoxal and Methylglyoxal: A Quantum Chemistry+CVT/SCT Approach. ChemPhysChem, 2004, 5, 1379-1388.	1.0	49
70	OH radical reactions with phenylalanine in free and peptide forms. Organic and Biomolecular Chemistry, 2008, 6, 732.	1.5	49
71	Cyclic 3-hydroxymelatonin, a key metabolite enhancing the peroxyl radical scavenging activity of melatonin. RSC Advances, 2014, 4, 5220.	1.7	49
72	Influence of Silicon Defects on the Adsorption of Thiophene-like Compounds on Polycyclic Aromatic Hydrocarbons:Â A Theoretical Study Using Thiophene + Coronene as the Simplest Model. Journal of Physical Chemistry A, 2007, 111, 1677-1682.	1.1	47

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73	Water Complexes of Important Air Pollutants: Geometries, Complexation Energies, Concentrations, Infrared Spectra, and Intrinsic Reactivity. Journal of Physical Chemistry A, 2010, 114, 5796-5809.	1.1	47
74	Free-radical scavenging by tryptophan and its metabolites through electron transfer based processes. Journal of Molecular Modeling, 2015, 21, 213.	0.8	47
75	Branching Ratios of Aliphatic Amines + OH Gas-Phase Reactions:â€‰ A Variational Transition-State Theory Study. Journal of Chemical Theory and Computation, 2008, 4, 322-327.	2.3	43
76	Phenolic Melatonin-Related Compounds: Their Role as Chemical Protectors against Oxidative Stress. Molecules, 2016, 21, 1442.	1.7	43
77	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.	0.9	42
78	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.	2.6	42
79	Influence of Point Defects on the Free-Radical Scavenging Capability of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 8302-8308.	1.5	41
80	Coumarinâ€"Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. Journal of Chemical Information and Modeling, 2016, 56, 662-670.	2.5	41
81	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.	1.3	39
82	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.	1.5	38
83	On the free radical scavenging mechanism of protocatechuic acid, regeneration of the catechol group in aqueous solution. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	38
84	A quantum chemical study on the free radical scavenging activity of tyrosol and hydroxytyrosol. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	38
85	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.	5.2	38
86	Theoretical Study on the Reaction of Tropospheric Interest:â€‰ Hydroxyacetone + OH. Mechanism and Kinetics. Journal of Physical Chemistry A, 2006, 110, 9153-9160.	1.1	37
87	Reactivity of silicon and germanium doped CNTs toward aromatic sulfur compounds: A theoretical approach. Chemical Physics, 2008, 345, 87-94.	0.9	37
88	Xanthones as antioxidants: A theoretical study on the thermodynamics and kinetics of the single electron transfer mechanism. Food and Function, 2012, 3, 442.	2.1	37
89	Dihydroxybenzoic acids as free radical scavengers: mechanisms, kinetics, and trends in activity. New Journal of Chemistry, 2014, 38, 2639.	1.4	37
90	Melatonin and its metabolites as chemical agents capable of directly repairing oxidized DNA. Journal of Pineal Research, 2019, 66, e12539.	3.4	37

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91	First principles calculations of p<i>K</i>_a values of amines in aqueous solution: Application to neurotransmitters. International Journal of Quantum Chemistry, 2012, 112, 3449-3460.	1.0	36
92	Theoretical study on the chemical fate of adducts formed through free radical addition reactions to carotenoids. Theoretical Chemistry Accounts, 2010, 127, 595-603.	0.5	33
93	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, 7129-7137.	1.2	33
94	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.	1.4	33
95	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.	1.5	32
96	On the Free Radical Scavenging Capability of Carboxylated Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 6363-6370.	1.5	32
97	Role of Allyl Group in the Hydroxyl and Peroxyl Radical Scavenging Activity of<i>S</i>-Allylcysteine. Journal of Physical Chemistry B, 2011, 115, 13408-13417.	1.2	32
98	On the Outstanding Antioxidant Capacity of Edaravone Derivatives through Single Electron Transfer Reactions. Journal of Physical Chemistry B, 2012, 116, 1180-1188.	1.2	32
99	Free Radicals Induced Oxidative Stress at a Molecular Level: The Current Status, Challenges and Perspectives of Computational Chemistry Based Protocols. Journal of the Mexican Chemical Society, 2017, 59, .	0.2	32
100	Theoretical study on the peroxyl radicals scavenging activity of esculetin and its regeneration in aqueous solution. Physical Chemistry Chemical Physics, 2014, 16, 1197-1207.	1.3	31
101	NEW INSIGTHS ON THE KINETICS AND MECHANISM OF THE ELECTROCHEMICAL OXIDATION OF DICLOFENAC IN NEUTRAL AQUEOUS MEDIUM. Electrochimica Acta, 2016, 199, 92-98.	2.6	31
102	Citric acid: A promising copper scavenger. Computational and Theoretical Chemistry, 2018, 1133, 47-50.	1.1	29
103	A Computer-Assisted Systematic Search for Melatonin Derivatives with High Potential as Antioxidants. Melatonin Research, 2018, 1, 27-58.	0.7	29
104	Mechanism of OH Radical Reactions with HCN and CH3CN:â€‰ OH Regeneration in the Presence of O2. Journal of Physical Chemistry A, 2007, 111, 5086-5091.	1.1	28
105	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.	1.5	28
106	Mechanism and kinetics of the hydroxyl and hydroperoxyl radical scavenging activity of N-acetylcysteine amide. Theoretical Chemistry Accounts, 2011, 130, 51-60.	0.5	28
107	Radical grafting of carbon surfaces with alkylic groups by mediated oxidation of carboxylates. Journal of Electroanalytical Chemistry, 2007, 610, 137-146.	1.9	27
108	<i>Cis</i> Carotenoids: Colorful Molecules and Free Radical Quenchers. Journal of Physical Chemistry B, 2013, 117, 4050-4061.	1.2	27

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109	Non-alkane behavior of cyclopropane and its derivatives: characterization of unconventional hydrogen bond interactions. Theoretical Chemistry Accounts, 2007, 118, 597-606.	0.5	25
110	On the ^{â€¢}OH and ^{â€¢}OOH scavenging activity of 3â€methylâ€1â€pyridinâ€2â€ylâ€5â€pyrazolone: Comparisons with its parent compound, edaravone. International Journal of Quantum Chemistry, 2012, 112, 3441-3448.	1.0	25
111	The role of acidâ€“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.	1.3	24
112	Chalcogen effects on the primary antioxidant activity of chrysin and quercetin. New Journal of Chemistry, 2020, 44, 9073-9082.	1.4	24
113	The Baeyer-Villiger reaction of 23-oxosapogenins. Arkivoc, 2005, 2005, 109-126.	0.3	24
114	Uric and 1-Methyluric Acids: Metabolic Wastes or Antiradical Protectors?. Journal of Physical Chemistry B, 2011, 115, 15430-15438.	1.2	23
115	Assessing the Protective Activity of a Recently Discovered Phenolic Compound against Oxidative Stress Using Computational Chemistry. Journal of Chemical Information and Modeling, 2015, 55, 2552-2561.	2.5	23
116	A Possible Mechanism for Furan Formation in the Tropospheric Oxidation of Dienes. Environmental Science & Technology, 2005, 39, 8797-8802.	4.6	22
117	Deprotonation routes of anthocyanidins in aqueous solution, pK_avalues, and speciation under physiological conditions. RSC Advances, 2016, 6, 53421-53429.	1.7	22
118	Capsaicin, a Powerful â€¢OH-Inactivating Ligand. Antioxidants, 2020, 9, 1247.	2.2	22
119	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.	1.0	21
120	On the role of s-cis conformers in the reaction of dienes with OH radicals. Physical Chemistry Chemical Physics, 2004, 6, 2237-2244.	1.3	21
121	A combined theoreticalâ€“experimental study on the acidity of WOx-ZrO2 systems. Physical Chemistry Chemical Physics, 2008, 10, 4181.	1.3	21
122	On the chemical behavior of C60 hosting H2O and other isoelectronic neutral molecules. Journal of Molecular Modeling, 2014, 20, 2412.	0.8	21
123	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.	1.1	21
124	Computationally Designed Sesamol Derivatives Proposed as Potent Antioxidants. ACS Omega, 2020, 5, 9566-9575.	1.6	21
125	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.	1.5	20
126	Ionization Energies, Proton Affinities, and p<i>K</i>_aValues of a Large Series of Edaravone Derivatives: Implication for Their Free Radical Scavenging Activity. Journal of Physical Chemistry B, 2011, 115, 10375-10384.	1.2	20

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127	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, 6125-6131.	1.1	20
128	Non-covalent Ï€â€“Ï€ stacking interactions turn off non-adiabatic effects in proton-coupled electron transfer reactions. Physical Chemistry Chemical Physics, 2017, 19, 6969-6972.	1.3	20
129	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.	1.7	20
130	Theoretical Investigation of the OH[.]â€Initiated Oxidation of Benzaldehyde in the Troposphere. ChemPhysChem, 2008, 9, 1453-1459.	1.0	19
131	Quantum mechanical based approaches for predicting pK_a values of carboxylic acids: evaluating the performance of different strategies. RSC Advances, 2016, 6, 112057-112064.	1.7	19
132	On the Mechanism of Gas-Phase Reaction of C1âˆ'C3 Aliphatic Thiols + OH Radicals. Journal of Physical Chemistry A, 2007, 111, 1523-1529.	1.1	18
133	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.	2.6	18
134	Site reactivity in the free radicals induced damage to leucine residues: a theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 4970-4976.	1.3	18
135	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.	0.5	18
136	Isopropylcyclopropane + OH Gas Phase Reaction:â€‰ A Quantum Chemistry + CVT/SCT Approach. Journal of Physical Chemistry A, 2006, 110, 1917-1924.	1.1	17
137	Mechanism and Branching Ratios of Hydroxy Ethers + ^{â€¢}OH Gas phase Reactions: Relevance of H Bond Interactions. Journal of Physical Chemistry A, 2010, 114, 7525-7536.	1.1	17
138	Free radical scavenging activity of caffeine's metabolites. International Journal of Quantum Chemistry, 2012, 112, 3472-3478.	1.0	17
139	Atmospheric Reactions of Oxygenated Volatile Organic Compounds+OH Radicals: Role of Hydrogen-Bonded Intermediates and Transition States. Advances in Quantum Chemistry, 2008, , 245-274.	0.4	16
140	Computational-aided design of melatonin analogues with outstanding multifunctional antioxidant capacity. RSC Advances, 2016, 6, 22951-22963.	1.7	16
141	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.	1.1	16
142	Estimation of empirically fitted parameters for calculating pK a values of thiols in a fast and reliable way. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	16
143	The Antioxidant Capability of Higenamine: Insights from Theory. Antioxidants, 2020, 9, 358.	2.2	16
144	Kinetics and mechanism of the Î²-alanine + OH gas phase reaction: A quantum mechanical approach. Physical Chemistry Chemical Physics, 2006, 8, 285-292.	1.3	15

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145	Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. Chemistry - A European Journal, 2018, 24, 8686-8691.	1.7	15
146	Role of the Sulfur Atom on the Reactivity of Methionine toward OH Radicals: Comparison with Norleucine. Journal of Physical Chemistry B, 2009, 113, 4947-4952.	1.2	14
147	Theoretical study on the oxidative damage to cholesterol induced by peroxyl radicals. Journal of Physical Organic Chemistry, 2015, 28, 504-508.	0.9	14
148	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.	1.7	14
149	Quantum mechanical approach to isoleucine+OH gas phase reaction. Mechanism and kinetics. Computational and Theoretical Chemistry, 2004, 676, 97-103.	1.5	13
150	Synthesis of Dimeric Steroid Trioxabispiroacetals Scaffolds by Gold(I)â€Catalyzed Hydroalkoxylationâ€"Hydration of Diynediols. European Journal of Organic Chemistry, 2019, 2019, 4916-4927.	1.2	13
151	Computationally designed p-coumaric acid analogs: searching for neuroprotective antioxidants. New Journal of Chemistry, 2021, 45, 14369-14380.	1.4	13
152	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.	0.9	12
153	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, 1295-1303.	2.3	12
154	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.	0.5	11
155	Determination of pKa Values of Diclofenac and Ibuprofen in Aqueous Solutions by Capillary Zone Electrophoresis. ECS Transactions, 2010, 29, 443-448.	0.3	11
156	Synthesis of new ZnSâ€"Bipy based hybrid organicâ€"inorganic materials for photocatalytic reduction of 4-nitrophenol. New Journal of Chemistry, 2015, 39, 2188-2194.	1.4	11
157	A combined experimentalâ€"theoretical study of the acidâ€"base behavior of mangiferin: implications for its antioxidant activity. RSC Advances, 2016, 6, 51171-51182.	1.7	11
158	Melatonin and Related Compounds: Chemical Insights into their Protective Effects Against Oxidative Stress. Current Organic Chemistry, 2017, 21, .	0.9	11
159	Role of purines on the copperâ€catalyzed oxidative damage in biological systems: Protection versus promotion. International Journal of Quantum Chemistry, 2018, 118, e25527.	1.0	11
160	The other side of the superoxide radical anion: its ability to chemically repair DNA oxidized sites. Chemical Communications, 2018, 54, 13710-13713.	2.2	11
161	Ab initio study of ÃŸ-alanine conformers in gas phase. Arkivoc, 2005, 2005, 7-18.	0.3	11
162	Computational Study on the Antifreeze Glycoproteins as Inhibitors of Clathrateâ€Hydrate Formation. ChemPhysChem, 2008, 9, 1630-1635.	1.0	10

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