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List of Publications by Year
in descending order

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81 papers	1,910 citations	236612 25 h-index	288905 40 g-index
92 all docs	92 docs citations	92 times ranked	2073 citing authors

#	Article	IF	Citations
1	Autodock Vina Adopts More Accurate Binding Poses but Autodock4 Forms Better Binding Affinity. Journal of Chemical Information and Modeling, 2020, 60, 204-211.	2.5	233
2	Fe2O3 nanoporous network fabricated from Fe3O4/reduced graphene oxide for high-performance ethanol gas sensor. Sensors and Actuators B: Chemical, 2018, 255, 3275-3283.	4.0	120
3	The Sâˆ'H Bond Dissociation Enthalpies and Acidities of Para and Meta Substituted Thiophenols:Â A Quantum Chemical Study. Journal of Physical Chemistry A, 2003, 107, 9182-9188.	1.1	74
4	Theoretical and Experimental Studies of the Antioxidant and Antinitrosant Activity of Syringic Acid. Journal of Organic Chemistry, 2020, 85, 15514-15520.	1.7	74
5	A highly sensitive fluorescent chemosensor for simultaneous determination of Ag(I), Hg(II), and Cu(II) ions: Design, synthesis, characterization and application. Dyes and Pigments, 2015, 116, 89-96.	2.0	63
6	Density functional theory study of the role of benzylic hydrogen atoms in the antioxidant properties of lignans. Scientific Reports, 2018, 8, 12361.	1.6	63
7	Antioxidant Motifs in Flavonoids: Oâ€"H versus Câ€"H Bond Dissociation. ACS Omega, 2019, 4, 8935-8942.	1.6	53
8	Singletâˆ'Triplet Energy Gaps of Gas-Phase RNA and DNA Bases. A Quantum Chemical Study. Journal of Physical Chemistry A, 2004, 108, 6554-6561.	1.1	52
9	Is Vitamin A an Antioxidant or a Pro-oxidant?. Journal of Physical Chemistry B, 2017, 121, 9348-9357.	1.2	52
10	Antioxidant properties of xanthones extracted from the pericarp of Garcinia mangostana (Mangosteen): A theoretical study. Chemical Physics Letters, 2015, 625, 30-35.	1.2	51
11	The triplet state of cytosine and its derivatives: Electron impact and quantum chemical study. Journal of Chemical Physics, 2004, 121, 11668-11674.	1.2	47
12	Coumarin-Based Dual Chemosensor for Colorimetric and Fluorescent Detection of Cu²⁺ in Water Media. ACS Omega, 2020, 5, 21241-21249.	1.6	47
13	Effect of the Structure and Temperature on Corrosion Inhibition of Thiourea Derivatives in 1.0 M HCl Solution. ACS Omega, 2019, 4, 14478-14489.	1.6	46
14	The Câˆ'H and Î±(Câˆ'X) Bond Dissociation Enthalpies of Toluene, C6H5-CH2X (X = F, Cl), and Their Substituted Derivatives:â€‰ A DFT Study. Journal of Physical Chemistry A, 2005, 109, 10342-10347.	1.1	45
15	A theoretical study of the radical scavenging activity of natural stilbenes. RSC Advances, 2019, 9, 42020-42028.	1.7	41
16	Facile post-synthesis and gas sensing properties of highly porous NiO microspheres. Sensors and Actuators A: Physical, 2019, 296, 110-120.	2.0	40
17	Is Indolinonic Hydroxylamine a Promising Artificial Antioxidant?. Journal of Physical Chemistry B, 2019, 123, 7777-7784.	1.2	40
18	Insight into the antioxidant properties of non-phenolic terpenoids contained in essential oils extracted from the buds of Cleistocalyx operculatus: a DFT study. RSC Advances, 2016, 6, 30824-30834.	1.7	37

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19	Ring Versus Nitrogen Protonation of Anilines. Letters in Organic Chemistry, 2004, 1, 23-30.	0.2	32
20	Oversampling Free Energy Perturbation Simulation in Determination of the Ligandâ€Binding Free Energy. Journal of Computational Chemistry, 2020, 41, 611-618.	1.5	30
21	Pivotal Role of Heteroatoms in Improving the Corrosion Inhibition Ability of Thiourea Derivatives. ACS Omega, 2020, 5, 27655-27666.	1.6	29
22	Theoretical Study of the Substituent Effects on the Sâ^'H Bond Dissociation Energy and Ionization Energy of 3-Pyridinethiol:Â Prediction of Novel Antioxidant. Journal of Physical Chemistry A, 2006, 110, 10904-10911.	1.1	28
23	Surface enhanced Raman scattering of melamine on silver substrate: An experimental and DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 169, 230-237.	2.0	28
24	A thermodynamic and kinetic study of the antioxidant activity of natural hydroanthraquinones. RSC Advances, 2020, 10, 20089-20097.	1.7	27
25	A DFT analysis on the radical scavenging activity of oxygenated terpenoids present in the extract of the buds of Cleistocalyx operculatus. RSC Advances, 2017, 7, 39686-39698.	1.7	25
26	Theoretical Study for Exploring the Diglycoside Substituent Effect on the Antioxidative Capability of Isorhamnetin Extracted from Anoectochilus roxburghii. ACS Omega, 2019, 4, 14996-15003.	1.6	25
27	Netropsin interactions in the minor groove of d(GGCCAATTGG) studied by a combination of resolution enhancement and ab initio calculations. FEBS Journal, 2005, 272, 3531-3541.	2.2	24
28	Electronic structure of zwitterionic diamino-meta-quinonoid molecules: identity of UV absorption bands. Chemical Physics Letters, 2003, 382, 349-354.	1.2	20
29	Effect of Substituents on the Pâ^'H Bond Dissociation Enthalpies of Phenylphosphines and Proton Affinities of Phenylphosphine Anions:Â A DFT Study. Journal of Physical Chemistry A, 2004, 108, 11362-11368.	1.1	20
30	Binding of inhibitors to the monomeric and dimeric SARS-CoV-2 Mpro. RSC Advances, 2021, 11, 2926-2934.	1.7	19
31	Effects of fluorine-substitution on the molecular properties of dimethyl ethers: A theoretical investigation. Computational and Theoretical Chemistry, 2007, 821, 71-81.	1.5	18
32	Theoretical investigation on the bond dissociation enthalpies of phenolic compounds extracted from Artocarpus altilis using ONIOM(ROB3LYP/6-311++G(2df,2p):PM6) method. Chemical Physics Letters, 2014, 613, 139-145.	1.2	18
33	Theoretical Study on the Antioxidant Activity of Natural Depsidones. ACS Omega, 2020, 5, 7895-7902.	1.6	18
34	Computational estimation of potential inhibitors from known drugs against the main protease of SARS-CoV-2. RSC Advances, 2021, 11, 17478-17486.	1.7	17
35	Antioxidant activity of thiourea derivatives: An experimental and theoretical study. Journal of Molecular Liquids, 2021, 340, 117149.	2.3	17
36	Decarboxylation of metastable methyl benzoate molecular ions. Journal of the American Society for Mass Spectrometry, 2006, 17, 807-814.	1.2	16

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37	Methyl and Phenyl Substitution Effects on the Proton Affinities of Hydrides of First and Second Row Elements and Substituent Effects on the Proton Affinities of Ring Carbons in Benzene:Â A DFT Study. Journal of Physical Chemistry A, 2006, 110, 4509-4515.	1.1	15
38	Exceptional case of Kasha's rule: Emission from higher-lying singlet electron excited states into ground states in coumarin-based biothiol sensing. Dyes and Pigments, 2018, 152, 118-126.	2.0	15
39	In Silico Evaluation of the Radical Scavenging Mechanism of Mactanamide. ACS Omega, 2020, 5, 24106-24110.	1.6	15
40	Molecular and electronic structure of zwitterionic diamino-meta-quinonoid molecules. Molecular Physics, 2003, 101, 2347-2355.	0.8	14
41	Hydroxyl Radical Scavenging of Indole-3-Carbinol: A Mechanistic and Kinetic Study. ACS Omega, 2019, 4, 19375-19381.	1.6	14
42	Gas phase nitrosation of substituted benzenes. International Journal of Mass Spectrometry, 2004, 232, 31-40.	0.7	13
43	Synthesis of aromatic and indole alpha-glucosinolates. Carbohydrate Research, 2018, 455, 45-53.	1.1	13
44	Protonation and methylation of thiophenol, thioanisole and their halogenated derivatives: mass spectrometric and computational study. International Journal of Mass Spectrometry, 2003, 228, 151-165.	0.7	12
45	Insights into the mechanisms and kinetics of the hydroperoxyl radical scavenging activity of Artepillin C. New Journal of Chemistry, 2021, 45, 7774-7780.	1.4	12
46	Is natural fraxin an overlooked radical scavenger?. RSC Advances, 2021, 11, 14269-14275.	1.7	12
47	Radical Scavenging Activity of Natural Anthraquinones: a Theoretical Insight. ACS Omega, 2021, 6, 13391-13397.	1.6	11
48	A Specific Gas-Phase Substitution Reaction between Enol Radical Cations and t-Butyl Nitrite. European Journal of Mass Spectrometry, 2004, 10, 889-898.	0.5	10
49	Experimental and theoretical study of corrosion inhibition performance of N-phenylthiourea for mild steel in hydrochloric acid and sodium chloride solution. Journal of Molecular Modeling, 2019, 25, 204.	0.8	10
50	Performance of an integrated approach for prediction of bond dissociation enthalpies of phenols extracted from ginger and tea. Chemical Physics Letters, 2013, 555, 44-50.	1.2	9
51	Functionalization and antioxidant activity of polyanilineâ€“fullerene hybrid nanomaterials: a theoretical investigation. RSC Advances, 2020, 10, 14595-14605.	1.7	9
52	A Quantum Chemical Study of the Protonation of Phenylphosphine and its Halogenated Derivatives. European Journal of Mass Spectrometry, 2003, 9, 257-266.	0.5	8
53	Unimolecular chemistry of metastable dimethyl isophthalate radical cations. International Journal of Mass Spectrometry, 2008, 275, 110-116.	0.7	8
54	Ab initio chemical kinetics for the HCCO + OH reaction. Chemical Physics Letters, 2014, 592, 175-181.	1.2	8

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55	DFT study of the interactions between thiophene-based corrosion inhibitors and an Fe4 cluster. Journal of Molecular Modeling, 2017, 23, 260.	0.8	8
56	C-Terminal Plays as the Possible Nucleation of the Self-Aggregation of the S-Shape AÎ²_{11â€“42} Tetramer in Solution: Intensive MD Study. ACS Omega, 2019, 4, 11066-11073.	1.6	8
57	A coumarin derivative-Cu²⁺ complex-based fluorescent chemosensor for detection of biothiols. RSC Advances, 2020, 10, 36265-36274.	1.7	8
58	Characterization of a distonic isomer C6H5C+(OH)OCH2 of methyl benzoate radical cation by associative ionâ€“molecule reactions. International Journal of Mass Spectrometry, 2006, 249-250, 484-492.	0.7	7
59	Functionalization of fullerene via the Bingel reaction with Î±-chlorocarbanions: an ONIOM approach. Journal of Molecular Modeling, 2016, 22, 113.	0.8	7
60	Using calculations of the electronically excited states for investigation of fluorescent sensors: A review. Vietnam Journal of Chemistry, 2019, 57, 389-400.	0.7	7
61	Internal energy effects on charge stripping spectra of [C7H8]+ and [C5H6]+ radical cations. Chemical Physics Letters, 2006, 419, 139-143.	1.2	6
62	On the loss of a methyl radical from metastable dimethyl terephthalate molecular ions. International Journal of Mass Spectrometry, 2007, 261, 134-139.	0.7	6
63	Antioxidant activities of [60]fullerene derivatives from chalcone, flavone and flavanone: A ONIOM approach via H-atom and electron transfer mechanism. Chemical Physics Letters, 2016, 652, 56-61.	1.2	6
64	The cyclohexadienylidenemethanone radical cation is a more stable distonic isomer of ionized benzaldehyde. Chemical Physics Letters, 2008, 456, 141-145.	1.2	5
65	Ion/molecule reactions involving ionized toluene or ionized methyl benzoate and neutral methyl isocyanide. International Journal of Mass Spectrometry, 2008, 270, 101-110.	0.7	5
66	The Seâ€“H bond of benzeneselenols (ArSe-H): Relationship between bond dissociation enthalpy and spin density of radicals. Chemical Physics, 2013, 415, 18-25.	0.9	4
67	Hg2+-Promoted Spirolactam Hydrolysis Reaction: A Design Strategy for the Highly Selective Sensing of Hg2+ over other Metal Ions in Aqueous Media. Sensors, 2019, 19, 128.	2.1	4
68	Ab Initio Chemical Kinetics for the HCCO + H Reaction. Combustion Science and Technology, 2016, 188, 1095-1114.	1.2	3
69	An experimental and computational study of antioxidant activity of N-phenylthiourea and N-phenylselenourea analogues. Vietnam Journal of Chemistry, 2019, 57, 469-479.	0.7	3
70	Substituent Effects on the Nâ€“H Bond Dissociation Enthalpies, Ionization Energies, Acidities, and Radical Scavenging Behavior of 3,7-Disubstituted Phenoxazines and 3,7-Disubstituted Phenothiazines. ACS Omega, 2020, 5, 27572-27581.	1.6	3
71	Thermodynamics and kinetics in antibody resistance of the 501Y.V2 SARS-CoV-2 variant. RSC Advances, 2021, 11, 33438-33446.	1.7	3
72	Gas-Phase Nitrosation of Ethylene and Related Events in the C₂H₄NO⁺ Landscape. Journal of Physical Chemistry A, 2008, 112, 5418-5428.	1.1	2

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73	Theoretical Investigation on Antioxidant Activity of Phenolic Compounds Extracted from Artocarpus Altilis. IFMBE Proceedings, 2015, , 464-469.	0.2	2
74	A Study of 1-Benzyl-3-phenyl-2-thiourea as an Effective Steel Corrosion Inhibitor in 1.0â€‰M HCl Solution. Journal of Chemistry, 2021, 2021, 1-14.	0.9	2
75	Mechanistic and kinetic studies of the radical scavenging activity of natural abietanes: A theoretical insight. Chemical Physics Letters, 2021, 777, 138737.	1.2	2
76	Insight into Anticorrosion Mechanism of Ampicillin on Mild Steel in Acidic Environment: A Combined Experimental and Theoretical Approach. Journal of Chemistry, 2021, 2021, 1-12.	0.9	2
77	Antibacterial activities of the extracts of Mimosa pudica L. an in-vitro study. International Journal on Advanced Science, Engineering and Information Technology, 2015, 5, 358.	0.2	2
78	Isolation, Quantification and Antioxidant Activity of Extracts and Compounds from the Aerial Parts of Archidendron bauchei (Jack) I. Niels. Letters in Organic Chemistry, 2018, 15, 972-980.	0.2	2
79	Oxoberberine: a promising natural antioxidant in physiological environments. RSC Advances, 2022, 12, 9738-9743.	1.7	2
80	Substituent effects on antioxidant activity of monosubstituted indole-3-carbinols: A DFT study. Vietnam Journal of Chemistry, 2019, 57, 728-734.	0.7	1
81	Prediction of stability constants of Cu2+ complexes with organic fluorescent ligands using thermodynamic cycle in combination with DFT theory and SMD solvent model. Hue University Journal of Science: Natural Science, 2020, 129, 15-23.	0.4	1