J Raul Alvarez-Idaboy

List of Publications by Citations

131 papers	4,914 citations	42 h-index	65 g-index
138 ext. papers	5,482 ext. citations	3.8 avg, IF	6.08 L-index

#	Paper	IF	Citations
131	Food Antioxidants: Chemical Insights at the Molecular Level. *Annual Review of Food Science and Technology*, **2016**, 7, 335-52	14.7	222
130	On the importance of prereactive complexes in molecule-radical reactions: hydrogen abstraction from aldehydes by OH. *Journal of the American Chemical Society*, **2001**, 123, 2018-24	16.4	211
129	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
128	A Quantum Chemical and Classical Transition State Theory Explanation of Negative Activation Energies in OH Addition To Substituted Ethenes. *Journal of the American Chemical Society*, **2000**, 122, 3715-3720	16.4	193
127	Antioxidant activity of trans-resveratrol toward hydroxyl and hydroperoxyl radicals: a quantum chemical and computational kinetics study. *Journal of Organic Chemistry*, **2012**, 77, 3868-77	4.2	183
126	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
125	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
124	Glutathione: mechanism and kinetics of its non-enzymatic defense action against free radicals. *RSC Advances*, **2011**, 1, 1763	3.7	108
123	Computational strategies for predicting free radical scavengersRprotection against oxidative stress: Where are we and what might follow?. *International Journal of Quantum Chemistry*, **2019**, 119, e25665	2.1	101
122	Can a Single Water Molecule Really Catalyze the Acetaldehyde + OH Reaction in Tropospheric Conditions?. *Journal of Physical Chemistry Letters*, **2010**, 1, 3112-3115	6.4	98
121	ROS initiated oxidation of dopamine under oxidative stress conditions in aqueous and lipidic environments. *Journal of Physical Chemistry B*, **2011**, 115, 12234-46	3.4	91
120	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
119	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
118	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
117	The mechanism of the Baeyer-Villiger rearrangement: quantum chemistry and TST study supported by experimental kinetic data. *Organic and Biomolecular Chemistry*, **2007**, 5, 3682-9	3.9	87
116	A new approach to counterpoise correction to BSSE. *Journal of Computational Chemistry*, **2006**, 27, 1203-10	3.9	85
115	A new specific mechanism for the acid catalysis of the addition step in the Baeyer-Villiger rearrangement. *Organic Letters*, **2006**, 8, 1763-5	6.2	81

114	Quantum chemistry and TST study of the mechanisms and branching ratios for the reactions of OH with unsaturated aldehydes. *Physical Chemistry Chemical Physics*, **2009**, 11, 7649-58	3.6	78
113	Mechanism and kinetics studies on the antioxidant activity of sinapinic acid. *Physical Chemistry Chemical Physics*, **2011**, 13, 11199-205	3.6	72
112	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
111	The Baeyer-Villiger reaction: solvent effects on reaction mechanisms. *Organic and Biomolecular Chemistry*, **2009**, 7, 3682-90	3.9	66
110	Canolol: a promising chemical agent against oxidative stress. *Journal of Physical Chemistry B*, **2011**, 115, 8590-6	3.4	65
109	Piceatannol, a better peroxyl radical scavenger than resveratrol. *RSC Advances*, **2013**, 3, 20209	3.7	64
108	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
107	Glycolaldehyde + OH gas phase reaction: a quantum chemistry + CVT/SCT approach. *Journal of Physical Chemistry A*, **2005**, 109, 169-80	2.8	62
106	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
105	Theoretical determination of the rate constant for OH hydrogen abstraction from toluene. *Journal of Physical Chemistry A*, **2006**, 110, 10155-62	2.8	60
104	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
103	On the possible catalytic role of a single water molecule in the acetone + OH gas phase reaction: a theoretical pseudo-second-order kinetics study. *Theoretical Chemistry Accounts*, **2011**, 129, 209-217	1.9	56
102	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
101	OH hydrogen abstraction reactions from alanine and glycine: A quantum mechanical approach. *Journal of Computational Chemistry*, **2001**, 22, 1138-1153	3.5	55
100	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
99	Mechanism and kinetics of the water-assisted formic acid + OH reaction under tropospheric conditions. *Journal of Physical Chemistry A*, **2011**, 115, 5138-46	2.8	52
98	Theoretical study of the initial reaction between OH and isoprene in tropospheric conditions. *Physical Chemistry Chemical Physics*, **2003**, 5, 1392-1399	3.6	49
97	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

96	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
95	Antioxidant activity of propyl gallate in aqueous and lipid media: a theoretical study. *Physical Chemistry Chemical Physics*, **2013**, 15, 13137-46	3.6	45
94	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
93	Computational and experimental study of the interactions between ionic liquids and volatile organic compounds. *Physical Chemistry Chemical Physics*, **2010**, 12, 9830-8	3.6	44
92	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
91	Mechanism of the OH–propene–O2 reaction: An ab initio study. *International Journal of Chemical Kinetics*, **1999**, 31, 29-36	1.4	44
90	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
89	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
88	Free-radical scavenging by tryptophan and its metabolites through electron transfer based processes. *Journal of Molecular Modeling*, **2015**, 21, 213	2	38
87	Single water-molecule catalysis in the glyoxal+OH reaction under tropospheric conditions: Fact or fiction? A quantum chemistry and pseudo-second order computational kinetic study. *Chemical Physics Letters*, **2010**, 501, 11-15	2.5	38
86	A Quantum Chemical and TST Study of the OH Hydrogen-Abstraction Reaction from Substituted Aldehydes: FCHO and ClCHO. *Journal of Physical Chemistry A*, **2001**, 105, 9034-9039	2.8	38
85	Quantum Chemical and Conventional Transition-State Theory Calculations of Rate Constants for the NO3 + Alkane Reaction. *Journal of Physical Chemistry A*, **2002**, 106, 4645-4650	2.8	37
84	Dihydroxybenzoic acids as free radical scavengers: mechanisms, kinetics, and trends in activity. *New Journal of Chemistry*, **2014**, 38, 2639	3.6	34
83	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
82	A quantum chemical study on the free radical scavenging activity of tyrosol and hydroxytyrosol. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	34
81	Coumarin-Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. *Journal of Chemical Information and Modeling*, **2016**, 56, 662-70	6.1	32
80	Lipoic acid and dihydrolipoic acid. A comprehensive theoretical study of their antioxidant activity supported by available experimental kinetic data. *Journal of Chemical Information and Modeling*, **2014**, 54, 1642-52	6.1	31
79	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

78	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
77	Quantum chemical and conventional TST calculations of rate constants for the OH+alkane reaction. *Chemical Physics*, **2005**, 310, 213-223	2.3	29
76	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
75	Melatonin and its metabolites as chemical agents capable of directly repairing oxidized DNA. *Journal of Pineal Research*, **2019**, 66, e12539	10.4	26
74	Antioxidant activity of fraxetin and its regeneration in aqueous media. A density functional theory study. *RSC Advances*, **2014**, 4, 52920-52932	3.7	25
73	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
72	Thiophenols, Promising Scavengers of Peroxyl Radicals: Mechanisms and kinetics. *Journal of Computational Chemistry*, **2019**, 40, 2103-2110	3.5	24
71	Antioxidant activity of selected natural polyphenolic compounds from soybean via peroxyl radical scavenging. *RSC Advances*, **2014**, 4, 38918-38930	3.7	23
70	Substituent effects in the Baeyer-Villiger reaction of acetophenones: a theoretical study. *Journal of Physical Organic Chemistry*, **2009**, 22, 643-649	2.1	23
69	Reinvestigating the role of multiple hydrogen transfers in Baeyer-Villiger reactions. *Journal of Organic Chemistry*, **2007**, 72, 6580-3	4.2	23
68	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
67	A proton-electron sequential transfer mechanism: theoretical evidence about its biological relevance. *Physical Chemistry Chemical Physics*, **2015**, 17, 28525-8	3.6	21
66	The Baeyer-Villiger reaction of 23-oxosapogenins. *Arkivoc*, **2005**, 2005, 109-126	0.9	21
65	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
64	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
63	Theoretical Model of Furan and 2-Furancarboxaldehyde. The Molecular Structure and Vibrational Spectra, Including Isotopic Effects. *The Journal of Physical Chemistry*, **1994**, 98, 5607-5613		19
62	Non-alkane behavior of cyclopropane and its derivatives: characterization of unconventional hydrogen bond interactions. *Theoretical Chemistry Accounts*, **2007**, 118, 597-606	1.9	18
61	A possible mechanism for furan formation in the tropospheric oxidation of dienes. *Environmental Science & Technology*, **2005**, 39, 8797-802	10.3	18

60	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
59	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
58	An experimental and theoretical study of the kinetics and mechanism of hydroxyl radical reaction with 2-aminopyrimidine. *RSC Advances*, **2014**, 4, 14157	3.7	16
57	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
56	Isopropylcyclopropane + OH gas phase reaction: a quantum chemistry + CVT/SCT approach. *Journal of Physical Chemistry A*, **2006**, 110, 1917-24	2.8	16
55	Theoretical investigation of the ethene-ethene radical cation addition reaction. *The Journal of Physical Chemistry*, **1993**, 97, 12737-12741		16
54	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
53	Mechanisms and rate constants in the atmospheric oxidation of saturated esters by hydroxyl radicals: A theoretical study. *International Journal of Quantum Chemistry*, **2012**, 112, 3508-3515	2.1	15
52	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
51	Deprotonation routes of anthocyanidins in aqueous solution, pKa values, and speciation under physiological conditions. *RSC Advances*, **2016**, 6, 53421-53429	3.7	15
50	Primary antioxidant and metal-binding effects of tiopronin: A theoretical investigation of its action mechanism. *Computational and Theoretical Chemistry*, **2016**, 1077, 48-57	2	15
49	Tryptophan: antioxidant or target of oxidative stress? A quantum chemistry elucidation. *RSC Advances*, **2014**, 4, 56128-56131	3.7	14
48	Acid-catalyzed nucleophilic additions to carbonyl groups: is the accepted mechanism the rule or an exception?. *Journal of Organic Chemistry*, **2013**, 78, 2327-35	4.2	14
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46	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
45	Quantum mechanical approach to isoleucine+OH gas phase reaction. Mechanism and kinetics. *Computational and Theoretical Chemistry*, **2004**, 676, 97-103		13
44	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
43	Modelling the chemical repair of protein carbon-centered radicals formed via oxidative damage with dihydrolipoic acid. *RSC Advances*, **2015**, 5, 96714-96719	3.7	12

42	Hydrolysis of a chlorambucil analogue. A DFT study. *Journal of Physical Chemistry A*, **2011**, 115, 2359-66	2.8	12
41	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
40	Chalcogen effects on the primary antioxidant activity of chrysin and quercetin. *New Journal of Chemistry*, **2020**, 44, 9073-9082	3.6	11
39	The Antioxidant Capability of Higenamine: Insights from Theory. *Antioxidants*, **2020**, 9,	7.1	11
38	Tropospheric degradation of ethylene glycol monovinyl and divinyl ethers: A mechanistic and kinetic study. *International Journal of Quantum Chemistry*, **2012**, 112, 3525-3534	2.1	10
37	Molecular description of indigo oxidation mechanisms initiated by OH and OOH radicals. *Journal of Physical Chemistry A*, **2012**, 116, 3643-51	2.8	10
36	A theoretical investigation of the mechanism of the NO3 addition to alkenes. *Computational and Theoretical Chemistry*, **2004**, 684, 51-59		10
35	Reaction mechanism of the acyl-enzyme formation in β-lactam hydrolysis by means of quantum chemical modeling. *Computational and Theoretical Chemistry*, **2000**, 504, 13-28		10
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33	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
32	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
31	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
30	Evidence of A Possible Cycloaddition Channel in the Ethene + NO3 Reaction. *Journal of Physical Chemistry A*, **2001**, 105, 9222-9230	2.8	9
29	Radical scavenging activity of ascorbic acid analogs: kinetics and mechanisms. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	8
28	Influence of the methylation degree on the rate constants of the ·OH addition to alkenes and its temperature dependence. *International Journal of Quantum Chemistry*, **2012**, 112, 3479-3483	2.1	8
27	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
26	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
25	Formation mechanism of glyoxal-DNA adduct, a DNA cross-link precursor. *International Journal of Biological Macromolecules*, **2017**, 98, 664-675	7.9	6

24	Theoretical study of copper complexes with lipoic and dihydrolipoic acids. *RSC Advances*, **2016**, 6, 107924-107932	3.7	6
23	Computational Quantum Chemistry: A Reliable Tool in the Understanding of Gas-Phase Reactions. *Journal of Chemical Education*, **2006**, 83, 481	2.4	6
22	On the correlation between ionization potentials and bond angles in heterocyclic compounds. *Journal of Molecular Structure*, **1991**, 249, 305-312	3.4	6
21	Theoretical model of the electrophilic substitution in pentagonal unsaturated heterocycles. *Computational and Theoretical Chemistry*, **1990**, 209, 361-372		6
20	Chemical repair of protein carbon-centred radicals: long-distance dynamic factors. *Canadian Journal of Chemistry*, **2016**, 94, 1119-1126	0.9	6
19	Computationally Designed Sesamol Derivatives Proposed as Potent Antioxidants. *ACS Omega*, **2020**, 5, 9566-9575	3.9	6
18	A theoretical and experimental evaluation of imidazolium-based ionic liquids for atmospheric mercury capture. *Journal of Molecular Modeling*, **2014**, 20, 2186	2	5
17	A study of the nucleophilic attack of the beta-lactamic bond of antibiotics in water solution. *Computational and Theoretical Chemistry*, **2001**, 539, 233-243		5
16	Theoretical modelling of the electrophilic substitution mechanism in furan. *Computational and Theoretical Chemistry*, **1992**, 253, 243-259		5
15	Contrasting reactions of hydrated electron and formate radical with 2-thio analogues of cytosine and uracil. *Physical Chemistry Chemical Physics*, **2016**, 18, 28781-28790	3.6	5
14	Modelling the repair of carbon-centred protein radicals by the antioxidants glutathione and Trolox. *New Journal of Chemistry*, **2019**, 43, 2085-2097	3.6	4
13	Formation of 2-hexene by cationic dimerization of propene: an ab initio and density functional theory study. *Theoretical Chemistry Accounts*, **1997**, 97, 277-282	1.9	4
12	Theoretical study of reactions of the 1-butene radical cation in frozen halocarbon matrixes. *The Journal of Physical Chemistry*, **1993**, 97, 12742-12744		4
11	Tryptophan versus nitric oxide, nitrogen dioxide and carbonate radicals: differences in reactivity and implications for oxidative damage to proteins. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
10	Theoretical Study of the Reactivity and Selectivity of Various Free Radicals with Cysteine Residues. *ACS Omega*, **2018**, 3, 16519-16528	3.9	4
9	Insights into the Mechanism of Hydroxyl Radical Mediated Oxidations of 2-Aminopurine: A Computational and Sonochemical Product Analysis Study. *Journal of Physical Chemistry B*, **2020**, 124, 6245-6256	3.4	3
8	Theoretical study of the complex reaction of O(3P) with trans-2-butene. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	3
7	Theoretical and experimental study demonstrates kinetic control in chalcone-flavanone transformation of naphthalene derivatives. *Journal of Molecular Structure*, **2018**, 1157, 631-637	3.4	2

6	Model Calculations of Base-Catalysed 1,3-Proton Transfer Reactions in Indene-like Systems.. *Acta Chemica Scandinavica*, **1994**, 48, 423-427		2
5	Free radical scavenging activity of newly designed sesamol derivatives. *New Journal of Chemistry*, **2021**, 45, 11960-11967	3.6	2
4	Mechanism of the OHβpropeneD2 reaction: An ab initio study **1999**, 31, 29		1
3	Reinvestigation of Acetophenones Oxidation by Performic Acid in Formic Acid. *Journal of Physical Chemistry A*, **2019**, 123, 1968-1972	2.8	0
2	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	
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	