Leif A Eriksson

List of Publications by Year
in descending order

306	8,518	44069	79698
papers	citations	48 h-index	73 g-index

319	319	319	8747
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Endoplasmic reticulum stress signalling â€“ from basic mechanisms to clinical applications. FEBS Journal, 2019, 286, 241-278.	4.7	568
2	Electron affinities and ionization potentials of nucleotide bases. Chemical Physics Letters, 2000, 322, 129-135.	2.6	226
3	The calculation of NMR and ESR spectroscopy parameters using density functional theory. Theoretical and Computational Chemistry, 1995, 2, 273-347.	0.4	139
4	Hydrogen Atom Transfer in Ribonucleotide Reductase (RNR). Journal of Physical Chemistry B, 1998, 102, 10622-10629.	2.6	138
5	Catalytic Mechanism of Galactose Oxidase:Â A Theoretical Study. Journal of the American Chemical Society, 2000, 122, 8031-8036.	13.7	134
6	The hyperfine structures of small radicals from density functional calculations. Journal of Chemical Physics, 1994, 100, 5066-5075.	3.0	126
7	Density functional calculations on model tyrosyl radicals. Biophysical Journal, 1997, 72, 1556-1567.	0.5	123
8	A theoretical study of 5-halouracils: electron affinities, ionization potentials and dissociation of the related anions. Chemical Physics Letters, 2001, 343, 151-158.	2.6	118
9	Structure and Dynamics of Monomerâ"Template Complexation: An Explanation for Molecularly Imprinted Polymer Recognition Site Heterogeneity. Journal of the American Chemical Society, 2009, 131, 13297-13304.	13.7	112
10	Theoretical study of phototoxic reactions of psoralens. Journal of Photochemistry and Photobiology A: Chemistry, 2003, 154, 235-243.	3.9	105
11	Theoretical methods that help understanding the structure and reactivity of gas phase ions. International Journal of Mass Spectrometry, 2005, 240, 37-99.	1.5	104
12	Theoretical Study of Cisplatin Binding to DNA:Â The Importance of Initial Complex Stabilization. Journal of Physical Chemistry B, 2005, 109, 11006-11015.	2.6	104
13	Rational design and validation of a Tip60 histone acetyltransferase inhibitor. Scientific Reports, 2014, 4, 5372.	3.3	103
14	Recent Developments in Configuration Interaction and Density Functional Theory Calculations of Radical Hyperfine Structure.. Advances in Quantum Chemistry, 1996, 27, 297-369.	0.8	83
15	Radiation Products of Thymine, 1-Methylthymine, and Uracil Investigated by Density Functional Theory. Journal of Physical Chemistry B, 1998, 102, 5369-5377.	2.6	83
16	Comparison of Experimental and Calculated Hyperfine Coupling Constants. Which Radicals Are Formed in Irradiated Guanine?. Journal of Physical Chemistry B, 1998, 102, 9332-9343.	2.6	82
17	Reaction mechanism of thymine dimer formation in DNA induced by UV light. Journal of Photochemistry and Photobiology A: Chemistry, 2002, 152, 95-101.	3.9	80
18	First principles electrochemistry: Electrons and protons reacting as independent ions. Journal of Chemical Physics, 2002, 117, 10193-10206.	3.0	79

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19	Density functional calculations of isotropic hyperfine coupling constants of radical cations. Journal of Chemical Physics, 1993, 99, 9756-9763.	3.0	77
20	Theoretical Study of the Antioxidant Properties of Pyridoxine. Journal of Physical Chemistry A, 2006, 110, 13068-13072.	2.5	77
21	Assessment of Procedures for Calculating Radical Hyperfine Structures. Journal of Physical Chemistry A, 1997, 101, 1352-1359.	2.5	75
22	On the accuracy of gradient corrected density functional methods for transition metal complexes. Journal of Chemical Physics, 1995, 102, 872-878.	3.0	74
23	Evidence of High â€¢OH Radical Quenching Efficiency by Vitamin B₆. Journal of Physical Chemistry B, 2009, 113, 9629-9632.	2.6	73
24	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	3.1	72
25	Theoretical Investigation of Adenine Radicals Generated in Irradiated DNA Components. Journal of Physical Chemistry B, 1998, 102, 10602-10614.	2.6	69
26	Catalytic Mechanism of Pyruvate Formate-Lyase (PFL). A Theoretical Study. Journal of the American Chemical Society, 1998, 120, 11449-11455.	13.7	69
27	Hydroxyl Radical Reactions with Phenol as a Model for Generation of Biologically Reactive Tyrosyl Radicals. Journal of Physical Chemistry B, 2000, 104, 848-855.	2.6	69
28	Mechanism of Photoinduced Decomposition of Ketoprofen. Journal of Medicinal Chemistry, 2007, 50, 1735-1743.	6.4	69
29	Effects of Ionizing Radiation on Crystalline Cytosine Monohydrate. Journal of Physical Chemistry B, 1998, 102, 7484-7491.	2.6	68
30	Substituent effects on OH bond strength and hyperfine properties of phenol, as model for modified tyrosyl radicals in proteins. International Journal of Quantum Chemistry, 2000, 76, 714-723.	2.0	68
31	A Triplet Mechanism for the Formation of Cyclobutane Pyrimidine Dimers in UV-Irradiated DNA. Journal of Physical Chemistry B, 2006, 110, 7556-7562.	2.6	68
32	Resonance Structures of the Amide Bond: The Advantages of Planarity. Chemistry - A European Journal, 2006, 12, 7215-7224.	3.3	68
33	Theoretical study of hypericin. Journal of Photochemistry and Photobiology A: Chemistry, 2005, 172, 293-299.	3.9	66
34	Hydrolysis Process of the Second Generation Platinum-Based Anticancer Drug cis-Amminedichlorocyclohexylamineplatinum(II). Journal of Physical Chemistry B, 2005, 109, 12195-12205.	2.6	63
35	Identification of the Brominated Flame Retardant 1,2-Dibromo-4-(1,2-dibromoethyl)cyclohexane as an Androgen Agonist. Journal of Medicinal Chemistry, 2006, 49, 7366-7372.	6.4	63
36	Linear-muffin-tin-orbital method for helical polymers: A detailed study oftrans-polyacetylene. Physical Review B, 1991, 44, 12713-12736.	3.2	62

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37	Assessment of Basis Set and Functional Dependencies in Density Functional Theory:Â Studies of Atomization and Reaction Energies. Journal of Physical Chemistry A, 1997, 101, 1927-1934.	2.5	61
38	Secretion of protein disulphide isomerase AGR2 confers tumorigenic properties. ELife, 2016, 5, .	6.0	60
39	Pharmacological Targeting of IRE1 in Cancer. Trends in Cancer, 2020, 6, 1018-1030.	7.4	59
40	Electronic Structure of a Transient Histidine Radical in Liquid Aqueous Solution:Â EPR Continuous-Flow Studies and Density Functional Calculations. Journal of Physical Chemistry A, 1999, 103, 1283-1290.	2.5	56
41	Sphingolipids contribute to acetic acid resistance in Zygosaccharomyces bailii. Biotechnology and Bioengineering, 2016, 113, 744-753.	3.3	54
42	Comparative study of DFT methods applied to small titanium/oxygen compounds. International Journal of Quantum Chemistry, 1996, 59, 427-443.	2.0	53
43	Targeting cancer using KAT inhibitors to mimic lethal knockouts. Biochemical Society Transactions, 2016, 44, 979-986.	3.4	52
44	The effects of nonlocal gradient corrections in density functional calculations of hydrocarbon radical hyperfine structures. International Journal of Quantum Chemistry, 1994, 52, 879-901.	2.0	51
45	Electronic and Magnetic Properties of Neutral and Charged Quinone and Plastoquinone Radicals. Journal of Physical Chemistry A, 1997, 101, 9496-9504.	2.5	51
46	Activation of anti-cancer drug cisplatin â€" is the activated complex fully aquated?. Molecular Physics, 2004, 102, 2537-2544.	1.7	51
47	Oxidation pathways of adenine and guanine in aqueous solution from first principles electrochemistry. Physical Chemistry Chemical Physics, 2004, 6, 4707.	2.8	51
48	The unfolded protein response modulators GSK2606414 and KIRA6 are potent KIT inhibitors. Cell Death and Disease, 2019, 10, 300.	6.3	51
49	Thermodynamics of the Photoenzymic Repair Mechanism Studied by Density Functional Theory. Journal of the American Chemical Society, 2000, 122, 10126-10132.	13.7	49
50	A Comprehensive Study of Sugar Radicals in Irradiated DNA. Journal of Physical Chemistry B, 1998, 102, 7674-7686.	2.6	48
51	Dehydration of Ribonucleotides Catalyzed by Ribonucleotide Reductase: The Role of the Enzyme. Biophysical Journal, 2006, 90, 2109-2119.	0.5	48
52	Control of anterior <scp>GR</scp> adient 2 (<scp>AGR</scp> 2) dimerization links endoplasmic reticulum proteostasis to inflammation. EMBO Molecular Medicine, 2019, 11, .	6.9	48
53	On the Formation of Cyclobutane Pyrimidine Dimers in UV-irradiated DNA: Why are Thymines More Reactive?Â¶. Photochemistry and Photobiology, 2003, 78, 159.	2.5	47
54	Hydrogen peroxide contributes to the ultravioletâ€B (280â€“315 nm) induced oxidative stress of plant leaves through multiple pathways. FEBS Letters, 2014, 588, 2255-2261.	2.8	47

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55	Theoretical Study of Model Tryptophan Radicals and Radical Cations:Â Comparison with Experimental Data of DNA Photolyase, CytochromecPeroxidase, and Ribonucleotide Reductase. Journal of Physical Chemistry B, 1997, 101, 9811-9819.	2.6	46
56	Theoretical Modeling of Hydroxyl-Radical-Induced Lipid Peroxidation Reactions. Journal of Physical Chemistry B, 2007, 111, 5684-5693.	2.6	46
57	Electronic structure calculations of hydrocarbon radical cations: a density functional study. Journal of the American Chemical Society, 1993, 115, 6896-6900.	13.7	45
58	Photodegradation mechanism of the common non-steroid anti-inflammatory drug diclofenac and its carbazole photoproduct. Physical Chemistry Chemical Physics, 2009, 11, 4601.	2.8	45
59	Hydrolytic Deamination of 5-Methylcytosine in Protic Mediumâ€"A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 2524-2533.	2.5	45
60	The Influence of Cholesterol on the Properties and Permeability of Hypericin Derivatives in Lipid Membranes. Journal of Chemical Theory and Computation, 2011, 7, 560-574.	5.3	45
61	Predictive power of long-range corrected functionals on the spectroscopic properties of tetrapyrrole derivatives for photodynamic therapy. Physical Chemistry Chemical Physics, 2011, 13, 7207.	2.8	44
62	Molecular Dynamics Studies of Liposomes as Carriers for Photosensitizing Drugs: Development, Validation, and Simulations with a Coarse-Grained Model. Journal of Chemical Theory and Computation, 2014, 10, 5-13.	5.3	44
63	A comparative study of the hyperfine structures of neutral nitrogen oxides: DFT vs CISD results. The Journal of Physical Chemistry, 1994, 98, 792-799.	2.9	42
64	On the bathochromic shift of the absorption by astaxanthin in crustacyanin: a quantum chemical study. Chemical Physics Letters, 2003, 375, 30-38.	2.6	42
65	Theoretical Study of the Reaction of Vitamin B6 with1O2. Chemistry - A European Journal, 2007, 13, 4636-4642.	3.3	41
66	Density functional theory investigation of hyperfine coupling constants in peroxyl radicals. Journal of Chemical Physics, 1997, 106, 7738-7748.	3.0	40
67	Sandwich Complexes Based on the â€œAll-Metalâ€•Al42â^' Aromatic Ring. Chemistry - A European Journal, 2006, 12, 4495-4502.	3.3	40
68	Electron-Transfer Induced Repair of 6-4 Photoproducts in DNA:â€‰ A Computational Study. Journal of Physical Chemistry A, 2007, 111, 2351-2361.	2.5	39
69	Theoretical Study of Ibuprofen Phototoxicity. Journal of Physical Chemistry B, 2007, 111, 13345-13352.	2.6	38
70	Diazasilene (SiNN): a comparative study of electron density distributions derived from Hartree-Fock, second-order Moller-Plesset perturbation theory, and density functional methods. The Journal of Physical Chemistry, 1994, 98, 1844-1850.	2.9	37
71	Calculation of the hyperfine constants of phosphorus-containing radicals. Molecular Physics, 1997, 91, 537-550.	1.7	37
72	Theoretical Study of the Insertion Reactions of Aluminum with H2O, NH3, HCl, and Cl2. Journal of Physical Chemistry A, 1998, 102, 1005-1017.	2.5	37

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73	pH-Dependent Electronic and Spectroscopic Properties of Pyridoxine (Vitamin B6). Journal of Physical Chemistry B, 2006, 110, 16774-16780.	2.6	37
74	Protein-bound chromophores astaxanthin and phytochromobilin: excited state quantum chemical studies. Physical Chemistry Chemical Physics, 2006, 8, 4053.	2.8	37
75	The role of the pyridoxine (vitamin B6) biosynthesis enzyme PDX1 in ultraviolet-B radiation responses in plants. Plant Physiology and Biochemistry, 2011, 49, 284-292.	5.8	36
76	Mechanistic Insight into Self-Propagation of Organo-Mediated Beckmann Rearrangement: A Combined Experimental and Computational Study. Journal of Organic Chemistry, 2013, 78, 4297-4302.	3.2	36
77	A density functional theory study of the hyperfine structures of the atoms B to O and the species NH2 and NH+3. Chemical Physics Letters, 1994, 217, 24-30.	2.6	35
78	Electron Densities of Several Small Molecules As Calculated from Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 6317-6324.	2.9	35
79	Theoretical Studies of the Cross-Linking Mechanisms between Cytosine and Tyrosine. Journal of the American Chemical Society, 2002, 124, 2753-2761.	13.7	35
80	Computational Evidence for the Role of Arabidopsis thaliana UVR8 as UVâ€“B Photoreceptor and Identification of Its Chromophore Amino Acids. Journal of Chemical Information and Modeling, 2011, 51, 1287-1295.	5.4	34
81	Accurate density functional theory study of cationic magnesium clusters and Mg+â€“rare gas interactions. Journal of Chemical Physics, 1995, 103, 1050-1056.	3.0	33
82	Mechanism of Hydroxyl Radical Addition to Imidazole and Subsequent Water Elimination. Journal of Physical Chemistry B, 1999, 103, 5598-5607.	2.6	33
83	Can Range-Separated and Hybrid DFT Functionals Predict Low-Lying Excitations? A Tookad Case Study. Journal of Chemical Theory and Computation, 2010, 6, 2086-2094.	5.3	33
84	A density functional theory study of the free radicals NH2, NF2, NCl2, PH2, PF2, and PCl2. Canadian Journal of Chemistry, 1994, 72, 695-704.	1.1	32
85	Ribonucleotide activation by enzyme ribonucleotide reductase: Understanding the role of the enzyme. Journal of Computational Chemistry, 2004, 25, 2031-2037.	3.3	32
86	Properties and Permeability of Hypericin and Brominated Hypericin in Lipid Membranes. Journal of Chemical Theory and Computation, 2009, 5, 3139-3149.	5.3	32
87	Catalysts or Initiators? Beckmann Rearrangement Revisited. Journal of Organic Chemistry, 2013, 78, 6782-6785.	3.2	32
88	Molecular dynamics study of the recognition of ATP by nucleic acid aptamers. Nucleic Acids Research, 2020, 48, 6471-6480.	14.5	32
89	COMPARE analysis of the toxicity of an iminoquinone derivative of the imidazo[5,4-f]benzimidazoles with NAD(P)H:quinone oxidoreductase 1 (NQO1) activity and computational docking of quinones as NQO1 substrates. Bioorganic and Medicinal Chemistry, 2012, 20, 3223-3232.	3.0	31
90	Antioxidant Properties of Î²-Carotene Isomers and Their Role in Photosystems: Insights from Ab Initio Simulations. Journal of Physical Chemistry A, 2012, 116, 3498-3506.	2.5	30

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91	Structure of a Transient Neutral Histidine Radical in Solution:Â EPR Continuous-Flow Studies in a Ti3+/EDTAâ˜Fenton System and Density Functional Calculations. Journal of Physical Chemistry A, 2000, 104, 9144-9152.	2.5	28
92	Proton catalyzed hydrolytic deamination of cytosine: a computational study. Theoretical Chemistry Accounts, 2008, 120, 429-435.	1.4	28
93	Catalytic Mechanism and Roles of Arg197 and Thr183 in theStaphylococcus aureusSortase A Enzyme. Journal of Physical Chemistry B, 2011, 115, 13003-13011.	2.6	28
94	Some calculated properties of phenylphosphinidene (C6H5P). Chemical Physics Letters, 1996, 254, 307-313.	2.6	27
95	Tyrosyl radical in galactose oxidase not strongly perturbed by cysteine cross-link. Chemical Physics Letters, 1999, 313, 374-378.	2.6	27
96	Conformational Analysis of Quinone Anion Radicals in Photosystem II and Photosynthetic Bacteria. Journal of Physical Chemistry A, 1999, 103, 3745-3749.	2.5	27
97	Oxidative Degradation of Pyruvate Formate-Lyase. Journal of the American Chemical Society, 2000, 122, 2035-2040.	13.7	27
98	Permeability of Psoralen Derivatives in Lipid Membranes. Biophysical Journal, 2006, 91, 2464-2474.	0.5	27
99	Photophysics, photochemistry, and reactivity: Molecular aspects of perylenequinone reactions. Photochemical and Photobiological Sciences, 2007, 6, 1089-1096.	2.9	27
100	Endohedral (X@ZniSi)i=4-160,Â± Nanoclusters, X = Li, Na, K, Cl, Br. Journal of Physical Chemistry C, 2007, 111, 3560-3565.	3.1	27
101	Photochemical Reaction Mechanism of UV-B-Induced Monomerization of UVR8 Dimers as the First Signaling Event in UV-B-Regulated Gene Expression in Plants. Journal of Physical Chemistry B, 2014, 118, 951-965.	2.6	27
102	Analysis of aquaporins from the euryhaline barnacle Balanus improvisus reveals differential expression in response to changes in salinity. PLoS ONE, 2017, 12, e0181192.	2.5	27
103	Electronic and hyperfine structures of hydrocarbon radical cations. Computational and Theoretical Chemistry, 1991, 230, 263-286.	1.5	26
104	Experimental and Theoretical Investigation of the Mechanism of Radiation-Induced Radical Formation in Hydrogen-Bonded Cocrystals of 1-Methylcytosine and 5-Fluorouracil. Journal of Physical Chemistry B, 2000, 104, 9343-9350.	2.6	26
105	Theoretical Studies of Chemical Reactivity of Metabolically Activated Forms of Aromatic Amines toward DNA. Chemical Research in Toxicology, 2012, 25, 2236-2252.	3.3	26
106	Hydrogen Atom Addition to Hydrocarbon Guests in Radiolyzed Zeolites. Journal of Physical Chemistry B, 1999, 103, 9219-9230.	2.6	25
107	Conformational dependence of the electronic absorption by astaxanthin and its implications for the bathochromic shift in crustacyanin. Physical Chemistry Chemical Physics, 2004, 6, 4190.	2.8	25
108	Absorption Spectra of Riboflavinâ€"A Difficult Case for Computational Chemistry. Journal of Physical Chemistry A, 2010, 114, 10234-10242.	2.5	25

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109	Merits and pitfalls of conventional and covalent docking in identifying new hydroxyl aryl aldehyde like compounds as human IRE1 inhibitors. Scientific Reports, 2019, 9, 3407.	3.3	25
110	The reduction of ribonucleotides catalyzed by the enzyme ribonucleotide reductase. Theoretical Chemistry Accounts, 2002, 108, 352-364.	1.4	24
111	Hydrolytic Deamination of 5,6-Dihydrocytosine in a Protic Medium: A Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 1826-1834.	2.5	24
112	Computational studies on Schiff-base formation: Implications for the catalytic mechanism of porphobilinogen synthase. Computational and Theoretical Chemistry, 2011, 963, 479-489.	2.5	24
113	Homology model of the human tRNA splicing ligase RtcB. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1983-1993.	2.6	24
114	On the local structure of the glycyl radical in different enzymes. Journal of the Chemical Society Perkin Transactions II, 1998, , 305-308.	0.9	23
115	Photo-oxidation of lipids by singlet oxygen: a theoretical study. Chemical Physics Letters, 2004, 398, 336-342.	2.6	23
116	Hydrogen abstraction from deoxyribose by a neighbouring uracil-5-yl radical. Physical Chemistry Chemical Physics, 2007, 9, 5975.	2.8	23
117	â€¢H Atom andâ€¢OH Radical Reactions with 5-Methylcytosine. Journal of Physical Chemistry A, 2007, 111, 8968-8972.	2.5	23
118	Photodegradation Mechanism of Nonsteroidal Anti-Inflammatory Drugs Containing Thiophene Moieties: Suprofen and Tiaprofenic Acid. Journal of Physical Chemistry B, 2009, 113, 11306-11313.	2.6	23
119	The effect of a neon matrix on the hyperfine structure of CH+4. A model study. Chemical Physics Letters, 1993, 211, 88-93.	2.6	22
120	Computational evidence in favor of a protonated chromophore in the photoactivation of phytochrome. Chemical Physics Letters, 2005, 416, 83-88.	2.6	22
121	Theoretical Assessment of Norfloxacin Redox and Photochemistry. Journal of Physical Chemistry A, 2009, 113, 10803-10810.	2.5	22
122	Catalytic Roles of Active-Site Residues in 2-Methyl-3-hydroxypyridine-5-carboxylic Acid Oxygenase: An ONIOM/DFT Study. Journal of Physical Chemistry B, 2011, 115, 1918-1926.	2.6	22
123	Catalytic Mechanism and Product Specificity of Oxidosqualene-Lanosterol Cyclase: A QM/MM Study. Journal of Physical Chemistry B, 2012, 116, 13857-13862.	2.6	22
124	Alcohols enhance the rate of acetic acid diffusion in S. cerevisiae: biophysical mechanisms and implications for acetic acid tolerance. Microbial Cell, 2018, 5, 42-55.	3.2	22
125	Influence of C5-methylation of cytosine on the formation of cyclobutane pyrimidine dimers. Chemical Physics Letters, 2005, 401, 99-103.	2.6	21
126	Theoretical Study of the Phototoxicity of Naproxen and the Active Form of Nabumetone. Journal of Physical Chemistry A, 2008, 112, 10921-10930.	2.5	21

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127	Electron Densities of Homonuclear Diatomic Molecules As Calculated from Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 5274-5280.	2.9	20
128	Hydrogen Abstraction by Soybean Lipoxygenase-1. Density Functional Theory Study on Active Site Models in Terms of Gibbs Free Energies. Journal of Physical Chemistry B, 2004, 108, 13831-13838.	2.6	20
129	Phytochromobilin C15-Z,syn? C15-E,anti isomerization: concerted or stepwise?. Physical Chemistry Chemical Physics, 2004, 6, 5066.	2.8	20
130	First principles electrochemical study of redox events in DNA bases and chemical repair in aqueous solution. Physical Chemistry Chemical Physics, 2004, 6, 2426.	2.8	20
131	Effects of OH Radical Addition on Proton Transfer in the Guanineâ^'Cytosine Base Pair. Journal of Physical Chemistry B, 2007, 111, 6571-6576.	2.6	20
132	A triplet mechanism for the formation of thymineâ€“thymine (6-4) dimers in UV-irradiated DNA. Physical Chemistry Chemical Physics, 2011, 13, 8961.	2.8	20
133	Hyperfine Structures of the Series C2HnF5-n, n = 0-5: A Density Functional Theory Study. The Journal of Physical Chemistry, 1995, 99, 623-629.	2.9	19
134	Effects of Steric Congestion on Stilbene Radical Anions and Dianions:Â DFT Calculations in the Interpretation of Stilbene Radical Anion ESR Spectra. Journal of Organic Chemistry, 1996, 61, 6739-6743.	3.2	19
135	Hybrid DFTâ€MD simulations of geometry and hyperfine structure of the CCH radical in argon matrices at low temperatures. Journal of Chemical Physics, 1996, 105, 8195-8203.	3.0	19
136	7-Nitro-4-(phenylthio)benzofurazan is a potent generator of superoxide and hydrogen peroxide. Archives of Toxicology, 2012, 86, 1613-1625.	4.2	19
137	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. Scientific Reports, 2017, 7, 8885.	3.3	19
138	Oxygen Dependent Purine Lesions in Double-Stranded Oligodeoxynucleotides: Kinetic and Computational Studies Highlight the Mechanism for 5â€²,8-Cyclopurine Formation. Journal of the American Chemical Society, 2020, 142, 5825-5833.	13.7	19
139	Structure and dynamics of the silacyclobutane radical cation, studied by ab initio and density functional theory and electron spin resonance spectroscopy. Journal of Chemical Physics, 1997, 107, 297-306.	3.0	18
140	Theoretical study of the tandem cross-linkage lesion in DNA. Chemical Physics Letters, 2006, 417, 303-308.	2.6	18
141	Deamination of the Radical Cation of the Base Moiety of 2â€²â€Deoxycytidine: A Theoretical Study. ChemPhysChem, 2008, 9, 1195-1203.	2.1	18
142	Peptidomimeticâ€based identification of FDAâ€approved compounds inhibiting IRE1 activity. FEBS Journal, 2021, 288, 945-960.	4.7	18
143	Hydroxyl radical â€“ Thymine adduct induced DNA damages. Chemical Physics Letters, 2008, 458, 186-189.	2.6	17
144	Modelling the behavior of 5-aminolevulinic acid and its alkyl esters in a lipid bilayer. Chemical Physics Letters, 2008, 463, 178-182.	2.6	17

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145	Computational Insights into the Mechanism of Porphobilinogen Synthase. Journal of Physical Chemistry B, 2010, 114, 16860-16870.	2.6	17
146	The first branching point in porphyrin biosynthesis: A systematic docking, molecular dynamics and quantum mechanical/molecular mechanical study of substrate binding and mechanism of uroporphyrinogenâ€III decarboxylase. Journal of Computational Chemistry, 2011, 32, 822-834.	3.3	17
147	Molecular modeling provides a structural basis for PERK inhibitor selectivity towards RIPK1. RSC Advances, 2020, 10, 367-375.	3.6	17
148	Protein kinase A controls yeast growth in visible light. BMC Biology, 2020, 18, 168.	3.8	17
149	Theoretical investigation of the ethene-ethene radical cation addition reaction. The Journal of Physical Chemistry, 1993, 97, 12737-12741.	2.9	16
150	The interactions between alkali metals and C2H2. Density functional theory as an analytic tool. Chemical Physics Letters, 1995, 235, 422-429.	2.6	16
151	A combined quantum mechanics and molecular dynamics study of small Jahnâ€“Teller distorted hydrocarbons: Another difficult test for density-functional theory. Journal of Chemical Physics, 1999, 110, 12059-12069.	3.0	16
152	Molecular dynamics simulations of plastoquinone in solution. Molecular Physics, 2001, 99, 247-253.	1.7	16
153	Pyruvate Formate Lyase:Â A New Perspective. Journal of Physical Chemistry B, 2003, 107, 5751-5757.	2.6	16
154	New insights into a critical biological control step of the mechanism of Ribonucleotide reductase. Computational and Theoretical Chemistry, 2004, 709, 53-65.	1.5	16
155	Electronic excitation energies of ZniSinanoparticles. Nanotechnology, 2006, 17, 4100-4105.	2.6	16
156	Homology Models and Molecular Modeling of Human Retinoic Acid Metabolizing Enzymes Cytochrome P450 26A1 (CYP26A1) and P450 26B1 (CYP26B1). Journal of Chemical Theory and Computation, 2008, 4, 1021-1027.	5.3	16
157	Characterization of Agonist Binding to His524 in the Estrogen Receptor Î± Ligand Binding Domain. Journal of Physical Chemistry B, 2012, 116, 4823-4830.	2.6	16
158	Footprints of natural selection at the mannose-6-phosphate isomerase locus in barnacles. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5376-5385.	7.1	16
159	Loss of WD2 subdomain of Apaf-1 forms an apoptosome structure which blocks activation of caspase-3 and caspase-9. Biochimie, 2021, 180, 23-29.	2.6	16
160	Investigation of Mï¿½ssbauer parameters for a set of iodine compounds using gradient-corrected density functional theory. International Journal of Quantum Chemistry, 1997, 63, 575-583.	2.0	15
161	Molecular dynamics simulations of ubiquinone; a survey over torsional potentials and hydrogen bonds. Molecular Physics, 2001, 99, 1795-1804.	1.7	15
162	B3LYP studies of the formation of neutral tyrosyl radical Yz? and regeneration of neutral tyrosine Yz in PSII. International Journal of Quantum Chemistry, 2001, 83, 220-229.	2.0	15

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163	Theoretical study on conformational preferences of ribose in 2-thiouridineâ€"the role of the 2â€²OH group. Physical Chemistry Chemical Physics, 2010, 12, 3690.	2.8	15
164	Formation Mechanism and Structure of a Guanineâ€“Uracil DNA Intrastrand Cross-Link. Chemical Research in Toxicology, 2011, 24, 2189-2199.	3.3	15
165	The Role of Nucleobase Carboradical and Carbanion on DNA Lesions:Â A Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 23583-23589.	2.6	14
166	Photochemical and photophysical properties, and photodegradation mechanism, of the non-steroid anti-inflammatory drug Flurbiprofen. Journal of Photochemistry and Photobiology A: Chemistry, 2009, 202, 48-56.	3.9	14
167	Exploration of multiple Sortase A protein conformations in virtual screening. Scientific Reports, 2016, 6, 20413.	3.3	14
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