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	Structure-Based Drug Discovery of IRE1 Modulators. Methods in Molecular Biology, 2022, 2378, 293-315.	0.9	0
2	Dynamics of 5R-Tg Base Flipping in DNA Duplexes Based on Simulationsâ”€Agreement with Experiments and Beyond. Journal of Chemical Information and Modeling, 2022, 62, 386-398.	5.4	3
3	Sensor dimer disruption as a new mode of action to block the IRE1-mediated unfolded protein response. Computational and Structural Biotechnology Journal, 2022, 20, 1584-1592.	4.1	6
4	Stress-induced tyrosine phosphorylation of RtcB modulates IRE1 activity and signaling outputs. Life Science Alliance, 2022, 5, e202201379.	2.8	8
5	A novel DPH5-related diphthamide-deficiency syndrome causing embryonic lethality or profound neurodevelopmental disorder. Genetics in Medicine, 2022, 24, 1567-1582.	2.4	5
6	Virtual Screening Expands the Non-Natural Amino Acid Palette for Peptide Optimization. Journal of Chemical Information and Modeling, 2022, 62, 2999-3007.	5.4	9
7	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
8	Reconstruction of the Fas-Based Death-Inducing Signaling Complex (DISC) Using a Proteinâ€“Protein Docking Meta-Approach. Journal of Chemical Information and Modeling, 2021, 61, 3543-3558.	5.4	8
9	Molecular-dynamics-simulation-guided membrane engineering allows the increase of membrane fatty acid chain length in Saccharomyces cerevisiae. Scientific Reports, 2021, 11, 17333.	3.3	3
10	Apoptosome Formation through Disruption of the K192-D616 Salt Bridge in the Apaf-1 Closed Form. ACS Omega, 2021, 6, 22551-22558.	3.5	12
11	The stressosome, a caspaseâ€8â€activating signalling complex assembled in response to cell stress in an ATG5â€mediated manner. Journal of Cellular and Molecular Medicine, 2021, 25, 8809-8820.	3.6	9
12	Structural and molecular bases to IRE1 activity modulation. Biochemical Journal, 2021, 478, 2953-2975.	3.7	7
13	SARS-CoV-2 integral membrane proteins shape the serological responses of patients with COVID-19. IScience, 2021, 24, 103185.	4.1	13
14	Peptidomimeticâ€based identification of FDAâ€approved compounds inhibiting IRE1 activity. FEBS Journal, 2021, 288, 945-960.	4.7	18
15	Molecular modeling provides a structural basis for PERK inhibitor selectivity towards RIPK1. RSC Advances, 2020, 10, 367-375.	3.6	17
16	Pharmacological Targeting of IRE1 in Cancer. Trends in Cancer, 2020, 6, 1018-1030.	7.4	59
17	Protein kinase A controls yeast growth in visible light. BMC Biology, 2020, 18, 168.	3.8	17
18	New insights on human IRE1 tetramer structures based on molecular modeling. Scientific Reports, 2020, 10, 17490.	3.3	5

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19	Deciphering the selectivity of inhibitor MKC9989 towards residue K907 in IRE1Î±; a multiscalein silicoapproach. RSC Advances, 2020, 10, 19720-19729.	3.6	5
20	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
21	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
22	Interaction of cobalt and iron hydroperoxo bleomycin with deoxyribonucleic acid (DNA): Dynamic vs. electronic structure considerations. Inorganica Chimica Acta, 2020, 509, 119682.	2.4	4
23	Molecular dynamics study of the recognition of ATP by nucleic acid aptamers. Nucleic Acids Research, 2020, 48, 6471-6480.	14.5	32
24	Endoplasmic reticulum stress signalling â€“ from basic mechanisms to clinical applications. FEBS Journal, 2019, 286, 241-278.	4.7	568
25	Effect of Kinase Inhibiting RNase Attenuator (KIRA) Compounds on the Formation of Face-to-Face Dimers of Inositol-Requiring Enzyme 1: Insights from Computational Modeling. International Journal of Molecular Sciences, 2019, 20, 5538.	4.1	6
26	Proline 411 biases the conformation of the intrinsically disordered plant UVR8 photoreceptor C27 domain altering the functional properties of the peptide. Scientific Reports, 2019, 9, 818.	3.3	5
27	A new splitâ€luciferase complementation assay identifies pentachlorophenol as an inhibitor of apoptosome formation. FEBS Open Bio, 2019, 9, 1194-1203.	2.3	11
28	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
29	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
30	Selective Inhibition of IRE1 Signalling mediated by MKC9989: New Insights from Molecular Docking and Molecular Dynamics Simulations. ChemistrySelect, 2019, 4, 3199-3203.	1.5	4
31	The unfolded protein response modulators GSK2606414 and KIRA6 are potent KIT inhibitors. Cell Death and Disease, 2019, 10, 300.	6.3	51
32	Theoretical Insights on the Inefficiency of RNA Oxidative Damage under Aerobic Conditions. Journal of Physical Chemistry A, 2018, 122, 431-438.	2.5	3
33	Binding Analysis of the Inositol-Requiring Enzyme 1 Kinase Domain. ACS Omega, 2018, 3, 13313-13322.	3.5	9
34	QM/MM Studies of Dph5 â€“ A Promiscuous Methyltransferase in the Eukaryotic Biosynthetic Pathway of Diphthamide. Journal of Chemical Information and Modeling, 2018, 58, 1406-1414.	5.4	8
35	Exploring Polypharmacology in Drug Design. Methods in Molecular Biology, 2018, 1824, 229-243.	0.9	7
36	In silico and in vitro studies of the reduction of unsaturated Î±,Î² bonds of trans-2-hexenedioic acid and 6-amino-trans-2-hexenoic acid â€“ Important steps towards biobased production of adipic acid. PLoS ONE, 2018, 13, e0193503.	2.5	12

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37	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
38	On the formation of a side product with hexahydroaporphine-like structure in the Grewe cyclization of dextromethorphan. Research on Chemical Intermediates, 2017, 43, 1689-1708.	2.7	1
39	Analysis of Biphenyl-Type Inhibitors Targeting the Eg5 Î±4/Î±6 Allosteric Pocket. ACS Omega, 2017, 2, 1836-1849.	3.5	2
40	Ligand Selectivity between the ADP-Ribosylating Toxins: An Inverse-Docking Study for Multitarget Drug Discovery. ACS Omega, 2017, 2, 1710-1719.	3.5	7
41	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. Scientific Reports, 2017, 7, 8885.	3.3	19
42	Homology model of the human tRNA splicing ligase RtcB. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1983-1993.	2.6	24
43	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
44	Improved Homology Model of the Human all-trans Retinoic Acid Metabolizing Enzyme CYP26A1. Molecules, 2016, 21, 351.	3.8	5
45	Exploration of multiple Sortase A protein conformations in virtual screening. Scientific Reports, 2016, 6, 20413.	3.3	14
46	Sphingolipids contribute to acetic acid resistance in Zygosaccharomyces bailii. Biotechnology and Bioengineering, 2016, 113, 744-753.	3.3	54
47	Targeting cancer using KAT inhibitors to mimic lethal knockouts. Biochemical Society Transactions, 2016, 44, 979-986.	3.4	52
48	Estimation of Liposome Penetration Barriers of Drug Molecules with All-Atom and Coarse-Grained Models. Journal of Chemical Theory and Computation, 2016, 12, 4651-4661.	5.3	11
49	Structures, Properties, and Dynamics of Intermediates in eEF2-Diphthamide Biosynthesis. Journal of Chemical Information and Modeling, 2016, 56, 1776-1786.	5.4	3
50	Permeability of 5-aminolevulinic acid oxime derivatives in lipid membranes. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	0
51	Defects in the calcium-binding region drastically affect the cadherin-like domains of RET tyrosine kinase. Physical Chemistry Chemical Physics, 2016, 18, 8673-8681.	2.8	2
52	DNA Distortion Caused by Uracil-Containing Intrastrand Cross-Links. Journal of Physical Chemistry B, 2016, 120, 1195-1204.	2.6	10
53	Secretion of protein disulphide isomerase AGR2 confers tumorigenic properties. ELife, 2016, 5, .	6.0	60
54	Characterization of interactions and pharmacophore development for DFG-out inhibitors to RET tyrosine kinase. Journal of Molecular Modeling, 2015, 21, 167.	1.8	11

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55	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
56	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
57	De novo tertiary structure prediction using RNA123â€"benchmarking and application to Macugen. Journal of Molecular Modeling, 2014, 20, 2389.	1.8	7
58	Deamination features of 5-hydroxymethylcytosine, a radical and enzymatic DNA oxidation product. Journal of Molecular Modeling, 2014, 20, 2290.	1.8	3
59	Improved homology model of cyclohexanone monooxygenase from Acinetobacter calcoaceticus based on multiple templates. Computational Biology and Chemistry, 2014, 49, 14-22.	2.3	7
60	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
61	Rational design and validation of a Tip60 histone acetyltransferase inhibitor. Scientific Reports, 2014, 4, 5372.	3.3	103
62	Insight into reaction mechanism and product formation a C8-purine radical in RNA: a theoretical perspective. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	1
63	Interactions and Stabilities of the UV RESISTANCE LOCUS8 (UVR8) Protein Dimer and Its Key Mutants. Journal of Chemical Information and Modeling, 2013, 53, 1736-1746.	5.4	8
64	Predicting Enzymeâ€"Substrate Specificity with QM/MM Methods: A Case Study of the Stereospecificity of <scp>d</scp>-Glucarate Dehydratase. Biochemistry, 2013, 52, 5511-5513.	2.5	6
65	Development of non-standard arginine residue parameters for use with the AMBER force fields. Chemical Physics Letters, 2013, 584, 188-194.	2.6	3
66	UV-induced formation of the thymine-thymine pyrimidine (6-4) pyrimidone photoproduct â€" a DFT study of the oxetane intermediate ring opening. Photochemical and Photobiological Sciences, 2013, 12, 1509-1516.	2.9	13
67	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
68	Theoretical prediction of the proteinâ€"protein interaction between Arabidopsis thaliana COP1 and UVR8. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	8
69	Catalysts or Initiators? Beckmann Rearrangement Revisited. Journal of Organic Chemistry, 2013, 78, 6782-6785.	3.2	32
70	OF MICE AND MEN: DISSECTING THE INTERACTION BETWEEN LISTERIA MONOCYTOGENES INTERNALIN A AND E-CADHERIN. Computational and Structural Biotechnology Journal, 2013, 6, e201303022.	4.1	1
71	Modification of the anticancer drug tamoxifen to avoid CYP2D6 polymorphism. Canadian Journal of Chemistry, 2013, 91, 916-924.	1.1	2
72	Comparison of the mechanism of deamination of 5,6-dihydro-5-methylcytosine with other cytosine derivatives. Highlights in Theoretical Chemistry, 2013, , 307-317.	0.0	0

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73	Identifying the sarco(endo)plasmic reticulum Ca2+ ATPase (SERCA) as a potential target for hypericin â€“ a theoretical study. Physical Chemistry Chemical Physics, 2012, 14, 12637.	2.8	9
74	7-Nitro-4-(phenylthio)benzofurazan is a potent generator of superoxide and hydrogen peroxide. Archives of Toxicology, 2012, 86, 1613-1625.	4.2	19
75	Computational Studies of Drugs in Lipid Membranes and Liposomes. Procedia Engineering, 2012, 44, 1777-1780.	1.2	0
76	Homology Models of Human All-Trans Retinoic Acid Metabolizing Enzymes CYP26B1 and CYP26B1 Spliced Variant. Journal of Chemical Information and Modeling, 2012, 52, 2631-2637.	5.4	8
77	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
78	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
79	Synthesis, kinase activity and molecular modeling of a resorcylic acid lactone incorporating an amide and a trans-enone in the macrocycle. Tetrahedron, 2012, 68, 5533-5540.	1.9	10
80	Stability and iron coordination in DNA adducts of Anthracycline based anti-cancer drugs. Physical Chemistry Chemical Physics, 2012, 14, 12505.	2.8	10
81	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
82	Catalytic Mechanism of Porphobilinogen Synthase: The Chemical Step Revisited by QM/MM Calculations. Journal of Physical Chemistry B, 2012, 116, 12105-12112.	2.6	6
83	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
84	Cloning and Functional Studies of a Splice Variant of CYP26B1 Expressed in Vascular Cells. PLoS ONE, 2012, 7, e36839.	2.5	9
85	Comparison of the mechanism of deamination of 5,6-dihydro-5-methylcytosine with other cytosine derivatives. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
86	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
87	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
88	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
89	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
90	Formation Mechanism and Structure of a Guanineâ€“Uracil DNA Intrastrand Cross-Link. Chemical Research in Toxicology, 2011, 24, 2189-2199.	3.3	15

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91	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
92	A Theoretical Rationale for Why Azetidine Has a Faster Rate of Formation Than Oxetane in TC(6â€“4) Photoproducts. Journal of Physical Chemistry B, 2011, 115, 9681-9686.	2.6	9
93	Conformational Enantiomerization and Estrogen Receptor Î± Binding of Anti-Cancer Drug Tamoxifen and Its Derivatives. Journal of Chemical Information and Modeling, 2011, 51, 306-314.	5.4	8
94	Properties and behaviour of tetracyclic allopsoralen derivatives inside a DPPC lipid bilayer model. Physical Chemistry Chemical Physics, 2011, 13, 10174.	2.8	5
95	Computational design of chlorin based photosensitizers with enhanced absorption properties. Physical Chemistry Chemical Physics, 2011, 13, 11590.	2.8	10
96	Theoretical Study of Pyridoxine (Vitamin B6) Photolysis. Journal of Physical Chemistry A, 2011, 115, 13556-13563.	2.5	12
97	A Mechanistic Hypothesis for the Cytochrome P450-Catalyzed Cisâ€“Trans Isomerization of 4-Hydroxytamoxifen: An Unusual Redox Reaction. Journal of Chemical Information and Modeling, 2011, 51, 2293-2301.	5.4	9
98	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
99	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
100	1,2â€Bis(methylsulfonyl)â€1â€(2â€chloroethyl)â€2â€[1â€(4â€nitrophenyl)ethoxy]carbonyl]hydrazine (KS119): a Cytotoxic Prodrug with Two Stable Conformations Differing in Biological and Physical Properties. Chemical Biology and Drug Design, 2011, 78, 513-526.	3.2	10
101	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
102	Structural changes of Listeria monocytogenes sortase A: A key to understanding the catalytic mechanism. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1564-1572.	2.6	9
103	New nonsteroidal antiâ€inflammatory molecules with reduced photodegradation side effects and enhanced COXâ€2 selectivity. International Journal of Quantum Chemistry, 2011, 111, 1184-1195.	2.0	6
104	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
105	Towards echinomycin mimetics by grafting quinoxaline residues on glycophane scaffolds. Bioorganic and Medicinal Chemistry, 2011, 19, 826-835.	3.0	11
106	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
107	The Pea SAD Short-Chain Dehydrogenase/Reductase: Quinone Reduction, Tissue Distribution, and Heterologous Expression Â Â. Plant Physiology, 2011, 155, 1839-1850.	4.8	8
108	Hydroxylation and Ringâ€Opening Mechanism of an Unusual Flavoprotein Monooxygenase, 2â€Methylâ€3â€hydroxypyridineâ€5â€carboxylic Acid Oxygenase: A Theoretical Study. Chemistry - A European Journal, 2010, 16, 2557-2566.	3.3	10

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109	DFT study of five naphthalimide derivatives: Structures and redox properties. Computational and Theoretical Chemistry, 2010, 941, 133-137.	1.5	3
110	Absorption Spectra of Riboflavinâ€"A Difficult Case for Computational Chemistry. Journal of Physical Chemistry A, 2010, 114, 10234-10242.	2.5	25
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	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
113	The Fate of H Atom Adducts to 3â€²-Uridine Monophosphate. Journal of Physical Chemistry B, 2010, 114, 9617-9621.	2.6	4
114	Computational Insights into the Mechanism of Porphobilinogen Synthase. Journal of Physical Chemistry B, 2010, 114, 16860-16870.	2.6	17
115	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
116	Distinct Hydroxyâ€Radicalâ€Induced Damage of 3â€²â€Uridine Monophosphate in RNA: A Theoretical Study. Chemistry - A European Journal, 2009, 15, 2394-2402.	3.3	8
117	Theoretical study of the structure of neutral, radical and anionic monoperoxo carbonic acid. Computational and Theoretical Chemistry, 2009, 913, 131-138.	1.5	5
118	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
119	Interaction and photobinding between 8-methoxypsoralen and thymine. Chemical Physics Letters, 2009, 471, 128-132.	2.6	7
120	Hydrogen Abstraction from Deoxyribose by a Neighboring 3â€²-Uracil Peroxyl Radical. Journal of Physical Chemistry B, 2009, 113, 6574-6578.	2.6	7
121	Theoretical Assessment of Norfloxacin Redox and Photochemistry. Journal of Physical Chemistry A, 2009, 113, 10803-10810.	2.5	22
122	Properties and Permeability of Hypericin and Brominated Hypericin in Lipid Membranes. Journal of Chemical Theory and Computation, 2009, 5, 3139-3149.	5.3	32
123	Evidence of High â€¢OH Radical Quenching Efficiency by Vitamin B₆. Journal of Physical Chemistry B, 2009, 113, 9629-9632.	2.6	73
124	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
125	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
126	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

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127	Hydrolytic Deamination of 5-Methylcytosine in Protic Mediumâ€"A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 2524-2533.	2.5	45
128	Mechanism of nitric oxide induced deamination of cytosine. Physical Chemistry Chemical Physics, 2009, 11, 2379.	2.8	10
129	Computational study of khellin excited states and photobinding to DNA. Photochemical and Photobiological Sciences, 2009, 8, 1179-1186.	2.9	3
130	Proton catalyzed hydrolytic deamination of cytosine: a computational study. Theoretical Chemistry Accounts, 2008, 120, 429-435.	1.4	28
131	Redox and debromination reactions of brominated hypericin. International Journal of Quantum Chemistry, 2008, 108, 1921-1929.	2.0	4
132	Theoretical Studies of Damage to 3â€²â€Uridine Monophosphate Induced by Electron Attachment. Chemistry - A European Journal, 2008, 14, 2850-2856.	3.3	13
133	Deamination of the Radical Cation of the Base Moiety of 2â€²â€Deoxycytidine: A Theoretical Study. ChemPhysChem, 2008, 9, 1195-1203.	2.1	18
134	Hydroxyl radical â€" Thymine adduct induced DNA damages. Chemical Physics Letters, 2008, 458, 186-189.	2.6	17
135	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
136	Multivariate characterisation and quantitative structureâ€"property relationship modelling of nitroaromatic compounds. Analytica Chimica Acta, 2008, 621, 155-162.	5.4	6
137	Theoretical Study of 5-Aminolevulinic Acid Tautomerization:â€‰ A Novel Self-Catalyzed Mechanism. Journal of Physical Chemistry A, 2008, 112, 4367-4374.	2.5	2
138	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
139	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
140	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	3.1	72
141	Hydrogen abstraction from deoxyribose by a neighbouring uracil-5-yl radical. Physical Chemistry Chemical Physics, 2007, 9, 5975.	2.8	23
142	Photophysics, photochemistry, and reactivity: Molecular aspects of perylenequinone reactions. Photochemical and Photobiological Sciences, 2007, 6, 1089-1096.	2.9	27
143	â€¢H Atom andâ€¢OH Radical Reactions with 5-Methylcytosine. Journal of Physical Chemistry A, 2007, 111, 8968-8972.	2.5	23
144	Radical-Induced Damage in 3â€˜dTMP Insights into a Mechanism for DNA Strand Cleavage. Journal of Chemical Theory and Computation, 2007, 3, 803-810.	5.3	10

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145	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
146	Mechanism of Photoinduced Decomposition of Ketoprofen. Journal of Medicinal Chemistry, 2007, 50, 1735-1743.	6.4	69
147	Theoretical Study of Ibuprofen Phototoxicity. Journal of Physical Chemistry B, 2007, 111, 13345-13352.	2.6	38
148	Theoretical Modeling of Hydroxyl-Radical-Induced Lipid Peroxidation Reactions. Journal of Physical Chemistry B, 2007, 111, 5684-5693.	2.6	46
149	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
150	Theoretical Assessment of Naphazoline Redoxchemistry and Photochemistry. Journal of Physical Chemistry B, 2007, 111, 3977-3981.	2.6	2
151	Metal Ion Dependent Adhesion Sites in Integrins:â€‰ A Combined DFT and QMC Study on Mn2+. Journal of Physical Chemistry B, 2007, 111, 9099-9103.	2.6	1
152	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
153	Theoretical Study of Sequence Selectivity and Preferred Binding Mode of Psoralen with DNA. Research Letters in Physical Chemistry, 2007, 2007, 1-5.	0.3	3
154	Theoretical Study of the Reaction of Vitamin B6 with1O2. Chemistry - A European Journal, 2007, 13, 4636-4642.	3.3	41
155	Theoretical study of 5-aminolevulinic acid (5ALA) and some pharmaceutically important derivatives. Chemical Physics Letters, 2007, 434, 101-106.	2.6	4
156	Theoretical prediction of binding modes and hot sequences for allopsoralenâ€“DNA interaction. Chemical Physics Letters, 2007, 450, 127-131.	2.6	3
157	Second International Theoretical Biophysics Symposium, Ã–rebro University, Sweden, June 28â€“July 1, 2005. International Journal of Quantum Chemistry, 2007, 107, 259-260.	2.0	0
158	Solvating, manipulating, damaging, and repairing DNA in a computer. International Journal of Quantum Chemistry, 2007, 107, 279-291.	2.0	3
159	On the Formation of Cyclobutane Pyrimidine Dimers in UV-irradiated DNA: Why are Thymines More Reactive?Â¶. Photochemistry and Photobiology, 2007, 78, 159-167.	2.5	5
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