Jerzy Leszczynski

List of Publications by Year
in descending order

559 papers	19,147 citations	11651 70 h-index	27406 106 g-index
579 all docs	579 docs citations	579 times ranked	13781 citing authors

#	Article	IF	Citations
1	Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles. Nature Nanotechnology, 2011, 6, 175-178.	31.5	654
2	Electronic properties, hydrogen bonding, stacking, and cation binding of DNA and RNA bases. Biopolymers, 2001, 61, 3-31.	2.4	408
3	Nature of Nucleic Acidâ^'Base Stacking: Nonempirical ab Initio and Empirical Potential Characterization of 10 Stacked Base Dimers. Comparison of Stacked and H-Bonded Base Pairs. The Journal of Physical Chemistry, 1996, 100, 5590-5596.	2.9	404
4	Intramolecular Proton Transfer in Mono- and Dihydrated Tautomers of Guanine:Â An ab Initio Post Hartreeâ^'Fock Study. Journal of the American Chemical Society, 1998, 120, 5024-5032.	13.7	238
5	Quantitative Classification of Covalent and Noncovalent H-Bonds. Journal of Physical Chemistry B, 2006, 110, 6444-6446.	2.6	224
6	Hydrogen Bonding and Stacking of DNA Bases: A Review of Quantum-chemicalab initioStudies. Journal of Biomolecular Structure and Dynamics, 1996, 14, 117-135.	3.5	222
7	Interaction of DNA Base Pairs with Various Metal Cations (Mg2+, Ca2+, Sr2+, Ba2+, Cu+, Ag+, Au+, Zn2+,) Tj ETQq1 1 0.784314 rgBT /O Interaction. Journal of Physical Chemistry B, 1997, 101, 9670-9677.	2.6	222
8	Toward the Development of â€œNanoâ€QSARsâ€• Advances and Challenges. Small, 2009, 5, 2494-2509.	10.0	215
9	Mineralâ€“organic interfacial processes: potential roles in the origins of life. Chemical Society Reviews, 2012, 41, 5502.	38.1	205
10	Double-Proton Transfer in Adenineâ^'Thymine and Guanineâ^'Cytosine Base Pairs. A Post-Hartreeâ^'Fock ab Initio Study. Journal of the American Chemical Society, 2004, 126, 10119-10129.	13.7	201
11	Advancing risk assessment of engineered nanomaterials: Application of computational approaches. Advanced Drug Delivery Reviews, 2012, 64, 1663-1693.	13.7	186
12	Interactions of Electrons with Bare and Hydrated Biomolecules: From Nucleic Acid Bases to DNA Segments. Chemical Reviews, 2012, 112, 5603-5640.	47.7	179
13	Comprehensive Theoretical Study of the Conversion Reactions of Spiropyrans:Â Substituent and Solvent Effects. Journal of Physical Chemistry B, 2004, 108, 16233-16243.	2.6	170
14	Genotoxicity of metal oxide nanomaterials: review of recent data and discussion of possible mechanisms. Nanoscale, 2015, 7, 2154-2198.	5.6	163
15	Green Chemistry in the Synthesis of Pharmaceuticals. Chemical Reviews, 2022, 122, 3637-3710.	47.7	155
16	Zeta Potential for Metal Oxide Nanoparticles: A Predictive Model Developed by a Nano-Quantitative Structureâ€“Property Relationship Approach. Chemistry of Materials, 2015, 27, 2400-2407.	6.7	154
17	Accurate and transferable multitask prediction of chemical properties with an atoms-in-molecules neural network. Science Advances, 2019, 5, eaav6490.	10.3	148
18	Base stacking in cytosine dimer. A comparison of correlatedab initio calculations with three empirical potential models and density functional theory calculations. Journal of Computational Chemistry, 1996, 17, 841-850.	3.3	147

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19	Towards understanding mechanisms governing cytotoxicity of metal oxides nanoparticles: Hints from nano-QSAR studies. Nanotoxicology, 2015, 9, 313-325.	3.0	147
20	Determination of Redox Potentials for the Watsonâ"Crick Base Pairs, DNA Nucleosides, and Relevant Nucleoside Analogues. Journal of Physical Chemistry B, 2007, 111, 5386-5395.	2.6	140
21	Remarkable diversity of carbonâ€"carbon bonds: structures and properties of fullerenes, carbon nanotubes, and graphene. Structural Chemistry, 2010, 21, 1155-1169.	2.0	136
22	QSAR as a random event: Modeling of nanoparticles uptake in PaCa2 cancer cells. Chemosphere, 2013, 92, 31-37.	8.2	133
23	A DFT Study of the Water-Assisted Intramolecular Proton Transfer in the Tautomers of Adenine. Journal of Physical Chemistry A, 1999, 103, 2744-2750.	2.5	130
24	Reactivities of Sites on (5,5) Single-Walled Carbon Nanotubes with and without a Stone-Wales Defect. Journal of Chemical Theory and Computation, 2010, 6, 1351-1357.	5.3	126
25	Molecular Structure and Vibrational IR Spectra of Cytosine and Its Thio and Seleno Analogues by Density Functional Theory and Conventional ab Initio Calculations. The Journal of Physical Chemistry, 1996, 100, 941-953.	2.9	124
26	Prediction of rate constants for radical degradation of aromatic pollutants in water matrix: A QSAR study. Chemosphere, 2009, 75, 1128-1134.	8.2	122
27	Ab Initio Ionization Energy Thresholds of DNA and RNA Bases in Gas Phase and in Aqueous Solution. Journal of Physical Chemistry A, 2004, 108, 6373-6377.	2.5	119
28	Near-UV Resonant Two-Photon Ionization Spectroscopy of Gas Phase Guanine:Â Evidence for the Observation of Three Rare Tautomers. Journal of Physical Chemistry A, 2006, 110, 10921-10924.	2.5	119
29	DNA strand breaks induced by near-zero-electronvolt electron attachment to pyrimidine nucleotides. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 5658-5663.	7.1	116
30	Amino groups in nucleic acid bases, aniline, aminopyridines, and aminotriazine are nonplanar: Results of correlatedabinitioquantum chemical calculations and anharmonic analysis of the aniline inversion motion. Journal of Chemical Physics, 1996, 105, 11042-11050.	3.0	115
31	Base Stacking and Hydrogen Bonding in Protonated Cytosine Dimer: The Role of Molecular ion-dipole and Induction Interactions. Journal of Biomolecular Structure and Dynamics, 1996, 13, 695-706.	3.5	114
32	Thioguanine and Thiouracil:Â Hydrogen-Bonding and Stacking Properties. Journal of Physical Chemistry A, 1997, 101, 9489-9495.	2.5	113
33	Tautomerism N(9)H .dblharw. N(7)H of Purine, Adenine, and 2-Chloroadenine: Combined Experimental IR Matrix Isolation and Ab Initio Quantum Mechanical Studies. The Journal of Physical Chemistry, 1994, 98, 2813-2816.	2.9	112
34	The Potential Energy Surface of Guanine Is Not Flat:Â Anab InitioStudy with Large Basis Sets and Higher Order Electron Correlation Contributions. Journal of Physical Chemistry A, 1998, 102, 2357-2362.	2.5	110
35	Are the amino groups in the nucleic acid bases coplanar with the molecular rings? Ab initioHF/6-31G* andMP2/6-31G* studies. International Journal of Quantum Chemistry, 1992, 44, 43-55.	2.0	104
36	A Remarkable Alteration in the Bonding Pattern:Â An HF and DFT Study of the Interactions between the Metal Cations and the Hoogsteen Hydrogen-Bonded G-Tetrad. Journal of Physical Chemistry A, 2000, 104, 6308-6313.	2.5	104

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37	Periodic table-based descriptors to encode cytotoxicity profile of metal oxide nanoparticles: A mechanistic QSTR approach. Ecotoxicology and Environmental Safety, 2014, 107, 162-169.	6.0	103
38	Interaction of the Adenineâ^'Thymine Watsonâ^'Crick and Adenineâ^'Adenine Reverse-Hoogsteen DNA Base Pairs with Hydrated Group IIa (Mg2+, Ca2+, Sr2+, Ba2+) and IIb (Zn2+, Cd2+, Hg2+) Metal Cations:Â Absence of the Base Pair Stabilization by Metal-Induced Polarization Effects. Journal of Physical Chemistry B, 1999, 103, 2528-2534.	2.6	102
39	Nonplanar DNA Base Pairs. Journal of Biomolecular Structure and Dynamics, 1996, 13, 827-833.	3.5	101
40	TDDFT investigation on nucleic acid bases: Comparison with experiments and standard approach. Journal of Computational Chemistry, 2004, 25, 768-778.	3.3	99
41	Electron Attachment-Induced DNA Single Strand Breaks:Â C3â€˜â^'O3â€˜Ïƒ-Bond Breaking of Pyrimidine Nucleotides Predominates. Journal of the American Chemical Society, 2006, 128, 9322-9323.	13.7	99
42	Open access in silico tools to predict the ADMET profiling of drug candidates. Expert Opinion on Drug Discovery, 2020, 15, 1473-1487.	5.0	99
43	Immunotoxicity of nanoparticles: a computational study suggests that CNTs and C₆₀ fullerenes might be recognized as pathogens by Toll-like receptors. Nanoscale, 2014, 6, 3488-3495.	5.6	97
44	Novel application of the CORAL software to model cytotoxicity of metal oxide nanoparticles to bacteria Escherichia coli. Chemosphere, 2012, 89, 1098-1102.	8.2	96
45	Tautomerism of uracil: the final chapter? Fourth-order electron correlation contributions to the relative energies of tautomers. The Journal of Physical Chemistry, 1992, 96, 1649-1653.	2.9	94
46	Hydration of cis- and trans-platin: A pseudopotential treatment in the frame of a G3-type theory for platinum complexes. Journal of Chemical Physics, 2000, 113, 2224-2232.	3.0	94
47	Vibrational Raman and Raman Optical Activity Spectra ofd-Lactic Acid,d-Lactate, andd-Glyceraldehyde:Â Ab Initio Calculations. Journal of Physical Chemistry A, 2002, 106, 11008-11016.	2.5	94
48	Adsorption of 1,3,5-Trinitrobenzene on the Siloxane Sites of Clay Minerals:Â Ab Initio Calculations of Molecular Models. Journal of Physical Chemistry B, 1999, 103, 6886-6890.	2.6	93
49	To stack or not to stack: Performance of a new density functional for the uracil and thymine dimers. Chemical Physics Letters, 2008, 459, 164-166.	2.6	93
50	From basic physics to mechanisms of toxicity: the â€œliquid dropâ€•approach applied to develop predictive classification models for toxicity of metal oxide nanoparticles. Nanoscale, 2014, 6, 13986-13993.	5.6	92
51	A direct-dynamics study of proton transfer through water bridges in guanine and 7-azaindole. Journal of Chemical Physics, 2000, 112, 566-573.	3.0	88
52	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. Green Chemistry, 2020, 22, 1458-1516.	9.0	86
53	Electron density distribution in stacked benzene dimers: A new approach towards the estimation of stacking interaction energies. Journal of Chemical Physics, 2005, 122, 144104.	3.0	85
54	Exploration of Computational Approaches to Predict the Toxicity of Chemical Mixtures. Toxics, 2019, 7, 15.	3.7	84

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55	Intramolecular proton transfer in monohydrated tautomers of cytosine: An ab initio post-Hartree-Fock study. International Journal of Quantum Chemistry, 1998, 70, 855-862.	2.0	83
56	Electronic Spectra, Excited State Structures and Interactions of Nucleic Acid Bases and Base Assemblies: A Review. Journal of Biomolecular Structure and Dynamics, 2007, 25, 93-118.	3.5	83
57	Optimal descriptor as a translator of eclectic data into prediction of cytotoxicity for metal oxide nanoparticles under different conditions. Ecotoxicology and Environmental Safety, 2015, 112, 39-45.	6.0	83
58	Mechanism of Dissolution of Neutral Silica Surfaces:Â Including Effect of Self-Healing. Journal of Physical Chemistry A, 2001, 105, 9528-9532.	2.5	81
59	Stoneâ€“Wales defects with two different orientations in (5, 5) single-walled carbon nanotubes: A theoretical study. Chemical Physics Letters, 2007, 434, 86-91.	2.6	80
60	Structure-toxicity relationships of nitroaromatic compounds. Molecular Diversity, 2006, 10, 233-245.	3.9	79
61	Chemisorption of Hydrogen Atoms on the Sidewalls of Armchair Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 7376-7383.	3.1	79
62	Endocrine-disrupting activity of per- and polyfluoroalkyl substances: Exploring combined approaches of ligand and structure based modeling. Chemosphere, 2017, 184, 514-523.	8.2	79
63	Interaction of Water Molecules with Cytosine Tautomers:Â An Excited-State Quantum Chemical Investigation. Journal of Physical Chemistry A, 2002, 106, 11338-11346.	2.5	78
64	Does the Hydrated Cytosine Molecule Retain the Canonical Structure? A DFT Study. Journal of Physical Chemistry B, 2000, 104, 5357-5361.	2.6	77
65	A new theoretical insight into the nature of intermolecular interactions in the molecular crystal of urea. Journal of Chemical Physics, 2002, 117, 1031-1039.	3.0	75
66	NanoSolveIT Project: Driving nanoinformatics research to develop innovative and integrated tools for in silico nanosafety assessment. Computational and Structural Biotechnology Journal, 2020, 18, 583-602.	4.1	74
67	Metal ions in non-complementary DNA base pairs: an ab initio study of Cu(I), Ag(I), and Au(I) complexes with the cytosine-adenine base pair. Journal of Biological Inorganic Chemistry, 1999, 4, 537-545.	2.6	73
68	Molecular Structure and Hydrogen Bonding in Polyhydrated Complexes of Adenine:Â A DFT Study. Journal of Physical Chemistry B, 2003, 107, 2846-2852.	2.6	73
69	A theoretical investigation of tautomeric equilibria and proton transfer in isolated and monohydrated cytosine and isocytosine molecules. Computational and Theoretical Chemistry, 1999, 487, 47-55.	1.5	72
70	An analysis of stable forms of CL-20: A DFT study of conformational transitions, infrared and Raman spectra. Journal of Molecular Structure, 2007, 843, 14-25.	3.6	72
71	Adsorption of the Phosphate Groups on Silica Hydroxyls:Â An ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 1228-1238.	2.5	70
72	Nano meets bio at the interface. Nature Nanotechnology, 2010, 5, 633-634.	31.5	70

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73	Comprehension of drug toxicity: Software and databases. Computers in Biology and Medicine, 2014, 45, 20-25.	7.0	69
74	Infrared spectra of tautomers and rotamers of 9-methylguanine. An experimental and theoretical study. Canadian Journal of Chemistry, 1991, 69, 1705-1720.	1.1	65
75	Structural nonrigidity of nucleic acid bases. Post-Hartree-Fock ab initio study. International Journal of Quantum Chemistry, 2000, 80, 1116-1124.	2.0	62
76	Surface Reactivity for Chlorination on Chlorinated (5,5) Armchair SWCNT: A Computational Approach. Journal of Physical Chemistry C, 2012, 116, 22399-22410.	3.1	62
77	A Theoretical Study of Excited State Properties of Adenineâ˜'Thymine and Guanineâ˜'Cytosine Base Pairs. Journal of Physical Chemistry A, 2002, 106, 4709-4717.	2.5	61
78	Novel approach for efficient predictions properties of large pool of nanomaterials based on limited set of species: nano-read-across. Nanotechnology, 2015, 26, 015701.	2.6	61
79	Applicability Domain: A Step Toward Confident Predictions and Decidability for QSAR Modeling. Methods in Molecular Biology, 2018, 1800, 141-169.	0.9	61
80	Metal halide perovskites for photocatalysis applications. Journal of Materials Chemistry A, 2022, 10, 407-429.	10.3	61
81	Comprehensive theoretical study towards the accurate proton affinity values of naturally occurring amino acids. International Journal of Quantum Chemistry, 2006, 106, 2920-2933.	2.0	60
82	Receptor- and ligand-based study of fullerene analogues: comprehensive computational approach including quantum-chemical, QSAR and molecular docking simulations. Organic and Biomolecular Chemistry, 2013, 11, 5798.	2.8	60
83	The Shielding Constants and Scalar Couplings in Nâ˜'HÂ·Â·Â·OC and Nâ˜'HÂ·Â·Â·NC Hydrogen Bonded Systems:Â An ab Initio MO Study. Journal of Physical Chemistry A, 2000, 104, 8105-8113.	2.5	59
84	Nature of binding in the alkalineâ€“earth clusters: Be3, Mg3, and Ca3. Journal of Chemical Physics, 2000, 113, 6245-6252.	3.0	59
85	Modeling of the Hydration Shell of Uracil and Thymine. International Journal of Molecular Sciences, 2000, 1, 17-27.	4.1	58
86	Predicting water solubility and octanol water partition coefficient for carbon nanotubes based on the chiral vector. Computational Biology and Chemistry, 2007, 31, 127-128.	2.3	58
87	CORAL: QSAR modeling of toxicity of organic chemicals towards Daphnia magna. Chemometrics and Intelligent Laboratory Systems, 2012, 110, 177-181.	3.5	57
88	Interaction of nucleic acid bases with single-walled carbon nanotube. Chemical Physics Letters, 2009, 480, 269-272.	2.6	55
89	Ab Initio Kinetic Simulation of Gas-Phase Experiments: Tautomerization of Cytosine and Guanine. Journal of Physical Chemistry B, 2009, 113, 6140-6150.	2.6	55
90	Optimal methods for calculation of the amount of intermolecular electron transfer. Journal of Chemical Physics, 2002, 117, 6952-6958.	3.0	53

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91	Spectral origins and ionization potentials of guanine tautomers: Theoretical elucidation of experimental findings. Chemical Physics Letters, 2006, 429, 261-265.	2.6	53
92	QSAR modeling of acute toxicity by balance of correlations. Bioorganic and Medicinal Chemistry, 2008, 16, 5999-6008.	3.0	53
93	Using a holistic approach to assess the impact ofÂengineered nanomaterials inducing toxicity in aquatic systems. Journal of Food and Drug Analysis, 2014, 22, 128-146.	1.9	53
94	Therapeutics for COVID-19: from computation to practicesâ€"where we are, where we are heading to. Molecular Diversity, 2021, 25, 625-659.	3.9	53
95	QSAR analysis of the toxicity of nitroaromatics inTetrahymena pyriformis: structural factors and possible modes of action. SAR and QSAR in Environmental Research, 2011, 22, 575-601.	2.2	52
96	Bonding in hypohalous acids HOX (X=F, Cl, Br, and I) from the topological analysis of the electron localization function. Journal of Chemical Physics, 1999, 111, 2542-2555.	3.0	51
97	Improved model for fullerene C60 solubility in organic solvents based on quantum-chemical and topological descriptors. Journal of Nanoparticle Research, 2011, 13, 3235-3247.	1.9	51
98	Electron attachment-induced DNA single-strand breaks at the pyrimidine sites. Nucleic Acids Research, 2010, 38, 5280-5290.	14.5	50
99	Stacking and H-bonding patterns of dGpdC and dGpdCpdG: Performance of the M05-2X and M06-2X Minnesota density functionals for the single strand DNA. Chemical Physics Letters, 2011, 512, 108-112.	2.6	50
100	Comprehensive ab initio studies of nuclear magnetic resonance shielding and coupling constants in XHâ‹¯O hydrogen-bonded complexes of simple organic molecules. Journal of Chemical Physics, 2000, 112, 7930-7938.	3.0	49
101	New theoretical insight into the thermal cisâ€"trans isomerization of azo compounds: Protonation lowers the activation barrier. Journal of Chemical Physics, 2001, 114, 5504-5508.	3.0	49
102	The effect of nitroaromaticsâ€™ composition on their toxicity in vivo: Novel, efficient non-additive 1D QSAR analysis. Chemosphere, 2008, 72, 1373-1380.	8.2	49
103	DFT M06-2X investigation of alkaline hydrolysis of nitroaromatic compounds. Chemosphere, 2012, 88, 635-643.	8.2	49
104	Evaluation criteria for the quality of published experimental data on nanomaterials and their usefulness for QSAR modelling. SAR and QSAR in Environmental Research, 2013, 24, 995-1008.	2.2	49
105	Stabilization of the Purineâ€¢Purineâ€¢Pyrimidine DNA Base Triplets by Divalent Metal Cations. Journal of Biomolecular Structure and Dynamics, 1998, 16, 139-143.	3.5	48
106	The influence of square planar platinum complexes on DNA base pairing. An ab initio DFT study. Physical Chemistry Chemical Physics, 2001, 3, 4404-4411.	2.8	48
107	Electronic Transitions of Thiouracils in the Gas Phase and in Solutions:Â Time-Dependent Density Functional Theory (TD-DFT) Study. Journal of Physical Chemistry A, 2004, 108, 10367-10375.	2.5	47
108	Adsorption of Sarin and Soman on Dickite:Â An ab Initio ONIOM Study. Journal of Physical Chemistry B, 2004, 108, 1918-1930.	2.6	47

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109	Adsorption of thymine and uracil on 1â€‰:â€‰1 clay mineral surfaces: comprehensive ab initio study on influence of sodium cation and water. Physical Chemistry Chemical Physics, 2011, 13, 7862.	2.8	47
110	Comprehensive Investigations of Kinetics of Alkaline Hydrolysis of TNT (2,4,6-Trinitrotoluene), DNT (2,4-Dinitrotoluene), and DNAN (2,4-Dinitroanisole). Environmental Science & Technology, 2014, 48, 10465-10474.	10.0	47
111	The influence of a sugar-phosphate backbone on the cisplatin-bridged BpB? models of DNA purine bases. Quantum chemical calculations of Pt(ii) bonding characteristics. Physical Chemistry Chemical Physics, 2004, 6, 3585.	2.8	46
112	QSPR study on solubility of fullerene C60 in organic solvents using optimal descriptors calculated with SMILES. Chemical Physics Letters, 2007, 441, 119-122.	2.6	46
113	QSAR modeling of measured binding affinity for fullerene-based HIV-1 PR inhibitors by CORAL. Journal of Mathematical Chemistry, 2010, 48, 959-987.	1.5	46
114	Open and capped (5,5) armchair SWCNTs: A comparative study of DFT-based reactivity descriptors. Chemical Physics Letters, 2012, 541, 85-91.	2.6	46
115	Electronic Structure and Optical Properties of Designed Photo-Efficient Indoline-Based Dye-Sensitizers with Dâ€“Aâ€“Ï€â€“A Framework. Journal of Physical Chemistry C, 2019, 123, 3309-3320.	3.1	46
116	Tautomers of 6-thioguanine: structures and properties. The Journal of Physical Chemistry, 1993, 97, 3520-3524.	2.9	45
117	A new approach to the characterization of nanomaterials: Predicting Youngâ€™s modulus by correlation weighting of nanomaterials codes. Chemical Physics Letters, 2006, 433, 125-129.	2.6	45
118	Tautomerism in nucleic acid bases and base pairs: a brief overview. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 637-649.	14.6	45
119	Addressing a bottle neck for regulation of nanomaterials: quantitative read-across (Nano-QRA) algorithm for cases when only limited data is available. Environmental Science: Nano, 2017, 4, 346-358.	4.3	45
120	How the toxicity of nanomaterials towards different species could be simultaneously evaluated: a novel multi-nano-read-across approach. Nanoscale, 2018, 10, 582-591.	5.6	45
121	Interactions of Hydrated IIa and IIb Group Metal Cations with Thioguanine-Cytosine DNA Base Pair: Ab initio and Density Functional Theory Investigation of Polarization Effects, Differences Among Cations, and Flexibility of the Cation Hydration Shell. Journal of Biomolecular Structure and Dynamics, 1999, 17, 61-77.	3.5	44
122	From the nonplanarity of the amino group to the structural nonrigidity of the molecule: A post-Hartree-Fock ab initio study of 2-aminoimidazole. International Journal of Quantum Chemistry, 1999, 75, 245-253.	2.0	44
123	Theoretical Study of Proton Transfer in Hypoxanthine Tautomers:â€‰ Effects of Hydration. Journal of Physical Chemistry A, 2000, 104, 3021-3027.	2.5	44
124	The interaction of the most stable guanine tautomers with water. The structure and properties of monohydratesElectronic supplementary information (ESI) available: Geometries of a guanine moiety in isolated molecules and monohydrates of the Gua9, Gua7 and Gua9* tautomers (Tables S1, S2 and S3). See http://www.rsc.org/suppdata/cp/b2/b205351a/. Physical Chemistry Chemical Physics, 2002, 4, 5359-5364.	2.8	44
125	Thermodynamics and Kinetics of Intramolecular Proton Transfer in Guanine. Post Hartreeâ€“Fock Study. Journal of Physical Chemistry B, 2005, 109, 13770-13776.	2.6	44
126	Extrapolating between toxicity endpoints of metal oxide nanoparticles: Predicting toxicity to Escherichia coli and human keratinocyte cell line (HaCaT) with Nano-QTTR. Ecotoxicology and Environmental Safety, 2016, 126, 238-244.	6.0	44

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127	Insight into the optoelectronic properties of designed solar cells efficient tetrahydroquinoline dye-sensitizers on TiO2(101) surface: first principles approach. Scientific Reports, 2018, 8, 10997.	3.3	44
128	InÂvitro and in silico modeling of perfluoroalkyl substances mixture toxicity in an amphibian fibroblast cell line. Chemosphere, 2019, 233, 25-33.	8.2	44
129	Prototropic Equilibria in 4-Thiouracil:Â A Combined Spectroscopic and ab Initio SCF-MO Investigation. Journal of Physical Chemistry A, 1998, 102, 2194-2200.	2.5	43
130	Phototautomeric Reaction, Tautomerism, and Infrared Spectra of 6-Thiopurine. Experimental Matrix Isolation and Quantum-Mechanical (Conventional ab Initio and Density-Functional Theory) Studies. Journal of Physical Chemistry A, 1999, 103, 280-288.	2.5	43
131	The 19Fâ€“1H coupling constants transmitted through covalent, hydrogen bond, and van der Waals interactions. Journal of Chemical Physics, 2001, 115, 5498-5506.	3.0	43
132	Multiplicative SMILES-based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. Chemical Physics Letters, 2008, 457, 332-336.	2.6	43
133	In silico designing of power conversion efficient organic lead dyes for solar cells using todays innovative approaches to assure renewable energy for future. Npj Computational Materials, 2017, 3, .	8.7	43
134	A density functional theory study of vibrational coupling between ribose and base rings of nucleic acids with ribosyl guanosine as a model system. Journal of Chemical Physics, 2000, 113, 5986-5990.	3.0	42
135	Structure and conformational flexibility of uracil: A comprehensive study of performance of the MP2, B3LYP and SCC-DFTB methods. Computational and Theoretical Chemistry, 2003, 625, 295-303.	1.5	42
136	Hydration-Dependent Structural Deformation of Guanine in the Electronic Singlet Excited State. Journal of Physical Chemistry B, 2008, 112, 5139-5152.	2.6	42
137	Geometries and stabilities of various configurations of benzene dimer: details of novel V-shaped structure revealed. Structural Chemistry, 2009, 20, 11-20.	2.0	42
138	Recovering four-component solutions by the inverse transformation of the infinite-order two-component wave functions. Journal of Chemical Physics, 2009, 130, 164114.	3.0	42
139	One-electron standard reduction potentials of nitroaromatic and cyclic nitramine explosives. Environmental Pollution, 2010, 158, 3048-3053.	7.5	42
140	From Formamide to Purine: A Self-Catalyzed Reaction Pathway Provides a Feasible Mechanism for the Entire Process. Journal of Physical Chemistry B, 2013, 117, 9333-9342.	2.6	42
141	Ab initio prediction of the geometry and IR frequencies of the mono- and dihydrated complexes of the oxo-amino-tautomers of guanine. International Journal of Quantum Chemistry, 1997, 65, 759-765.	2.0	41
142	The effects of characteristics of substituents on toxicity of the nitroaromatics: HiT QSAR study. Journal of Computer-Aided Molecular Design, 2008, 22, 747-759.	2.9	41
143	Optimal nano-descriptors as translators of eclectic data into prediction of the cell membrane damage by means of nano metal-oxides. Environmental Science and Pollution Research, 2015, 22, 745-757.	5.3	41
144	Excited State Proton Transfer in Guanine in the Gas Phase and in Water Solution:Â A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 7775-7780.	2.5	40

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145	Consensus QSAR Modeling of Phosphorâ€Containing Chiral AChE Inhibitors. QSAR and Combinatorial Science, 2009, 28, 664-677.	1.4	40
146	Can the Gibbs Free Energy of Adsorption Be Predicted Efficiently and Accurately: An M05-2X DFT Study. Journal of Physical Chemistry A, 2011, 115, 2423-2430.	2.5	40
147	Toward robust computational electrochemical predicting the environmental fate of organic pollutants. Journal of Computational Chemistry, 2011, 32, 2195-2203.	3.3	40
148	Nano-QSAR: Model of mutagenicity of fullerene as a mathematical function of different conditions. Ecotoxicology and Environmental Safety, 2016, 124, 32-36.	6.0	40
149	The interaction of nitrobenzene with the hydrate basal surface of montmorillonite: an ab initio study. Physical Chemistry Chemical Physics, 2000, 2, 5007-5012.	2.8	39
150	Room temperature synthesis of PbSe quantum dots in aqueous solution: stabilization by interactions with ligands. Nanoscale, 2012, 4, 1312.	5.6	39
151	DFT-based reactivity study of (5,5) armchair boron nitride nanotube (BNNT). Chemical Physics Letters, 2013, 565, 69-73.	2.6	39
152	Tautomeric equilibria in 8-oxopurines: implications for mutagenicity. , 1998, 12, 373-373.		38
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