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	NTO degradation by direct photolysis: DFT study. Structural Chemistry, 2023, 34, 23-31.	2.0	5
2	SARS-CoV M^{pro} inhibitory activity of aromatic disulfide compounds: QSAR model. Journal of Biomolecular Structure and Dynamics, 2022, 40, 780-786.	3.5	23
3	First-Principles Modeling of Non-covalent Interactions in Molecular Systems and Extended Materials. , 2022, , 71-124.		0
4	Application of Computational Approaches to Analysis of Multistep Chemical Reactions of Energetic Materials: Hydrolysis of Hexahydro-1,3,5-Trinitro-1,3,5-Triazine (RDX) and Octahydro-1,3,5,7-Tetranitro-1,3,5,7-Tetrazocine(HMX). , 2022, , 215-232.		0
5	Metal halide perovskites for photocatalysis applications. Journal of Materials Chemistry A, 2022, 10, 407-429.	10.3	61
6	Enhanced Perovskite Solar Cell Performance via 2-Amino-5-iodobenzoic Acid Passivation. ACS Applied Materials & Interfaces, 2022, 14, 5414-5424.	8.0	17
7	Computational approaches in assessments of mixture toxicity. Current Opinion in Toxicology, 2022, 29, 31-35.	5.0	5
8	Green Chemistry in the Synthesis of Pharmaceuticals. Chemical Reviews, 2022, 122, 3637-3710.	47.7	155
9	In Silico Tools and Software to Predict ADMET of New Drug Candidates. Methods in Molecular Biology, 2022, 2425, 85-115.	0.9	15
10	Identification of potential antivirals against 3CLpro enzyme for the treatment of SARS-CoV-2: A multi-step virtual screening study. SAR and QSAR in Environmental Research, 2022, 33, 357-386.	2.2	9
11	Decomposition of 2,4,6-trinitrotoluene (TNT) and 5-nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (NTO) by Fe13O13 nanoparticle: density functional theory study. Environmental Science and Pollution Research, 2022, 29, 68522-68531.	5.3	2
12	An effect of nitrogen incorporation on the structure and properties of amorphous SiC: First-principles molecular dynamics simulations. Thin Solid Films, 2022, 756, 139349.	1.8	1
13	Repurposing FDA approved drugs as possible anti-SARS-CoV-2 medications using ligand-based computational approaches: sum of ranking difference-based model selection. Structural Chemistry, 2022, 33, 1741-1753.	2.0	9
14	Photophysical Properties of Donorâ€“Acceptorâ^'Ï€ Bridgeâ€“Acceptor Sensitizers with a Naphthobisthiadiazole Auxiliary Acceptor: Toward Longer-Wavelength Access in Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2022, 126, 11875-11888.	3.1	8
15	Protein reliability analysis and virtual screening of natural inhibitors for SARS-CoV-2 main protease (M^{pro}) through docking, molecular mechanic & dynamic, and ADMET profiling. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6810-6827.	3.5	21
16	N-arylnaphthylamines as inhibitors of human immunodeficiency virus integrase - lens epithelium-derived growth factor interactions: theoretical studies. Journal of Biomolecular Structure and Dynamics, 2021, 39, 867-880.	3.5	0
17	Efficient approach for exploring the multiple-channel bimolecular interactions of conformationally flexible reagents. Epoxide ring opening reaction. Structural Chemistry, 2021, 32, 581-589.	2.0	1
18	Evaluating the cytotoxicity of a large pool of metal oxide nanoparticles to Escherichia coli: Mechanistic understanding through InÂVitro and In Silico studies. Chemosphere, 2021, 264, 128428.	8.2	19

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19	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
20	Catalytic role of solvated electron in the spontaneous degradation of insensitive munition compounds: computational chemistry investigation. Structural Chemistry, 2021, 32, 521-527.	2.0	4
21	Drug Databases for Development of Therapeutics Against Coronaviruses. Methods in Pharmacology and Toxicology, 2021, , 761.	0.2	1
22	Application of QSPR Modeling in Designing and Prediction of Power Conversion-Efficient Solar Cell. Challenges and Advances in Computational Chemistry and Physics, 2021, , 167-186.	0.6	0
23	Combining Features of Metal Oxide Nanoparticles. , 2021, , 317-329.		1
24	Computational Screening of Organic Dye-Sensitizers for Dye-Sensitized Solar Cells: DFT/TDDFT Approach. Challenges and Advances in Computational Chemistry and Physics, 2021, , 187-205.	0.6	0
25	Another look at the structure of the (H2O)nâ€¢Ö¾ system: water anion vs. hydrated electron. Structural Chemistry, 2021, 32, 655-665.	2.0	2
26	The kernel-weighted local polynomial regression (KwLPR) approach: an efficient, novel tool for development of QSAR/QSAAR toxicity extrapolation models. Journal of Cheminformatics, 2021, 13, 9.	6.1	9
27	Z,E-Isomerism in a Series of Substituted Iminophosphonates: Quantum Chemical Research. Organics, 2021, 2, 84-97.	1.3	2
28	Zeta potentials (Î¶) of metal oxide nanoparticles: A meta-analysis of experimental data and a predictive neural networks modeling. NanoImpact, 2021, 22, 100317.	4.5	28
29	COMBINED EXPERIMENTAL AND COMPUTATIONAL APPROACH TO THE STRUCTURE OF A NEW NICKEL(II) COMPLEX WITH TRIDENTATE SCHIFF BASE LIGAND. Journal of Structural Chemistry, 2021, 62, 938-946.	1.0	1
30	Preliminary Screening of COVID-19 Infection Employing Machine Learning Techniques From Simple Blood Profile. International Journal of Quantitative Structure-Property Relationships, 2021, 6, 35-47.	0.5	6
31	Interaction of epoxy-based hydrogels and water: A molecular dynamics simulation study. Journal of Molecular Graphics and Modelling, 2021, 106, 107915.	2.4	9
32	Using quasi-SMILES for the predictive modeling of the safety of 574 metal oxide nanoparticles measured in different experimental conditions. Environmental Toxicology and Pharmacology, 2021, 86, 103665.	4.0	19
33	Theoretical DFT Study on the Mechanisms of CO/CO2 Conversion in Chemical Looping Catalyzed by Calcium Ferrite. Journal of Physical Chemistry A, 2021, 125, 8159-8167.	2.5	2
34	Application of quasi-SMILES to the model of gold-nanoparticles uptake in A549Âcells. Computers in Biology and Medicine, 2021, 136, 104720.	7.0	8
35	QSAR and machine learning modeling of toxicity of nanomaterials: a risk assessment approach. , 2021, , 417-441.		2
36	Single site Fe on the (110) surface of Î³-Al₂O₃: insights from a DFT study including the periodic boundary approach. Physical Chemistry Chemical Physics, 2021, 23, 7164-7177.	2.8	9

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37	Jahn-Teller and Pseudo Jahn-Teller Effects: Influences on the Electronic Structures of Small Transition, Main Group and Mixed Metal Clusters. Structural Chemistry, 2020, 31, 7-23.	2.0	2
38	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. Green Chemistry, 2020, 22, 1458-1516.	9.0	86
39	How the CORAL software can be used to select compounds for efficient treatment of neurodegenerative diseases?. Toxicology and Applied Pharmacology, 2020, 408, 115276.	2.8	6
40	From Animal to Human: Interspecies Analysis Provides a Novel Way of Ascertaining and Fighting COVID-19. Innovation(China), 2020, 1, 100021.	9.1	11
41	Effect of Microenvironment on the Geometrical Structure of d(A)₅ d(T)₅ and d(G)₅ d(C)₅ DNA Mini-Helixes and the Dickerson Dodecamer: A Density Functional Theory Study. Journal of Physical Chemistry B, 2020, 124, 9343-9353.	2.6	5
42	Revealing the Photophysical Mechanism of N,Nâ€²-Diphenyl-aniline Based Sensitizers with the Dâ€“Dâ^™Iâ€“A Framework: Theoretical Insights. ACS Sustainable Chemistry and Engineering, 2020, 8, 13328-13341.	6.7	36
43	Advancement of predictive modeling of zeta potentials (Î¶) in metal oxide nanoparticles with correlation intensity index (CII). Journal of Molecular Liquids, 2020, 317, 113929.	4.9	15
44	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
45	Negative thermal quenching of photoluminescence in a copperâ€“organic framework emitter. Chemical Communications, 2020, 56, 12057-12060.	4.1	22
46	Single Fe Site on the Surface of Î³-Al₂O₃: Insights from Density Functional Theory Periodic Boundary Approach. Journal of Physical Chemistry C, 2020, 124, 20931-20941.	3.1	7
47	Evaluating Donor Effects in Isoindigo-Based Small Molecular Fluorophores. Journal of Physical Chemistry A, 2020, 124, 10777-10786.	2.5	9
48	Chemometric Modeling of the Ecotoxicity of Industrial Chemicals to an Avian Species Anas Platyrhynchos. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 1-16.	0.5	3
49	Is intraspecies QSTR model answer to toxicity data gap filling: Ecotoxicity modeling of chemicals to avian species. Science of the Total Environment, 2020, 738, 139858.	8.0	9
50	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
51	A density functional theory study of simplest nanocomposites formed by graphene oxide and polyvinyl alcohol: geometry, interaction energy and vibrational spectrum. Journal of Molecular Modeling, 2020, 26, 183.	1.8	2
52	The index of ideality of correlation: models of the flash points of ternary mixtures. New Journal of Chemistry, 2020, 44, 4858-4868.	2.8	12
53	First-Principles Approach for Assessing Cold Electron Injection Efficiency of Dye-Sensitized Solar Cell: Elucidation of Mechanism of Charge Injection and Recombination. Journal of Physical Chemistry C, 2020, 124, 2817-2836.	3.1	25
54	Cleftâ€Induced Ditopic Binding of Spherical Halides with a Hexaurea Receptor. ChemistrySelect, 2020, 5, 1401-1409.	1.5	4

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55	Chemometric modeling of power conversion efficiency of organic dyes in dye sensitized solar cells for the future renewable energy. Nano Energy, 2020, 70, 104537.	16.0	35
56	Ecotoxicity Databases for QSAR Modeling. Methods in Pharmacology and Toxicology, 2020, , 709-758.	0.2	6
57	First-principles investigations of the pressure-induced phase transformations and properties of crystalline and amorphous AlN. Physical Review Materials, 2020, 4, .	2.4	7
58	Semi-correlations combined with the index of ideality of correlation: a tool to build up model of mutagenic potential. Molecular and Cellular Biochemistry, 2019, 452, 133-140.	3.1	13
59	Accurate and transferable multitask prediction of chemical properties with an atoms-in-molecules neural network. Science Advances, 2019, 5, eaav6490.	10.3	148
60	Role of Singlet Oxygen in the Degradation of Selected Insensitive Munitions Compounds: A Comprehensive, Quantum Chemical Investigation. Journal of Physical Chemistry A, 2019, 123, 7597-7608.	2.5	5
61	Computational and experimental approach to understanding the structural interplay of self-assembled end-terminated alkanethiolates on gold surfaces. Physical Chemistry Chemical Physics, 2019, 21, 23320-23328.	2.8	6
62	Optoelectronic Properties of C60 and C70 Fullerene Derivatives: Designing and Evaluating Novel Candidates for Efficient P3HT Polymer Solar Cells. Materials, 2019, 12, 2282.	2.9	15
63	Characterization and Simulation of Natural Pyrite Surfaces: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 26397-26405.	3.1	13
64	Evaluating genotoxicity of metal oxide nanoparticles: Application of advanced supervised and unsupervised machine learning techniques. Ecotoxicology and Environmental Safety, 2019, 185, 109733.	6.0	34
65	A first-principles study of the stability and mechanical properties of ternary transition metal carbide alloys. Journal of Applied Physics, 2019, 125, .	2.5	16
66	Combining Features of Metal Oxide Nanoparticles. International Journal of Quantitative Structure-Property Relationships, 2019, 4, 28-40.	0.5	5
67	InÂvitro and in silico modeling of perfluoroalkyl substances mixture toxicity in an amphibian fibroblast cell line. Chemosphere, 2019, 233, 25-33.	8.2	44
68	Exploration of Computational Approaches to Predict the Toxicity of Chemical Mixtures. Toxics, 2019, 7, 15.	3.7	84
69	â€œIdeal correlationsâ€•for biological activity of peptides. BioSystems, 2019, 181, 51-57.	2.0	11
70	Predicting Thermal Conductivity Enhancement of Al2O3/Water and CuO/Water Nanofluids Using Quantitative Structure-Property Relationship Approach. International Journal of Quantitative Structure-Property Relationships, 2019, 4, 18-27.	0.5	4
71	Modeling of Glass Transition Temperatures for Polymeric Coating Materials: Application of QSPR Mixtureâ€based Approach. Molecular Informatics, 2019, 38, e1800150.	2.5	3
72	Stability of SiC and SiN interfaces in titanium carbide and nitride based heterostructures. Journal of Applied Physics, 2019, 125, 075303.	2.5	3

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73	Theoretical study of formate, tartrate, tartronate, and glycolate production from 6-carbon trioxylate intermediate in the citric acid cycle. Journal of Molecular Modeling, 2019, 25, 347.	1.8	0
74	How water affects mercuryâ€“halogen interaction in the atmosphere. Journal of Molecular Modeling, 2019, 25, 357.	1.8	1
75	A density functional theory investigation of degradation of Nitroguanidine in the photoactivated triplet state. Journal of Molecular Modeling, 2019, 25, 372.	1.8	0
76	Adsorption of nitrogen-containing compounds on hydroxylated Î±-quartz surfaces. RSC Advances, 2019, 9, 36066-36074.	3.6	0
77	Ecotoxicological Modeling, Ranking and Prioritization of Pharmaceuticals Using QSTR and iâ€QSTTR Approaches: Application of 2D and Fragment Based Descriptors. Molecular Informatics, 2019, 38, e1800078.	2.5	24
78	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
79	Is clay-polycation adsorbent future of the greener society? In silico modeling approach with comprehensive virtual screening. Chemosphere, 2019, 220, 1108-1117.	8.2	6
80	Toward comprehension of multiple human cells uptake of engineered nano metal oxides: quantitative inter cell line uptake specificity (QICLUS) modeling. Nanotoxicology, 2019, 13, 14-34.	3.0	23
81	Multiple e-Pharmacophore modeling to identify a single molecule that could target both streptomycin and paromomycin binding sites for 30S ribosomal subunit inhibition. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1582-1596.	3.5	13
82	Diffusion of energetic compounds through biological membrane: Application of classical MD and COSMOmic approximations. Journal of Biomolecular Structure and Dynamics, 2019, 37, 247-255.	3.5	6
83	Recent Advances of In-Silico Modeling of Potent Antagonists for the Adenosine Receptors. Current Pharmaceutical Design, 2019, 25, 750-773.	1.9	14
84	Virtual Screening of Anti-Cancer Compounds: Application of Monte Carlo Technique. Anti-Cancer Agents in Medicinal Chemistry, 2019, 19, 148-153.	1.7	4
85	Interactions of Substituted Nitroaromatics with Model Graphene Systems: Applicability of Hammett Substituent Constants To Predict Binding Energies. ACS Omega, 2018, 3, 2773-2785.	3.5	3
86	Structure and Energetics of (111) Surface of Î³-Al₂O₃: Insights from DFT Including Periodic Boundary Approach. ACS Omega, 2018, 3, 1881-1888.	3.5	34
87	Fullerene quinazolinone conjugates targeting Mycobacterium tuberculosis: a combined molecular docking, QSAR, and ONIOM approach. Structural Chemistry, 2018, 29, 765-775.	2.0	6
88	QSPR modeling of optical rotation of amino acids using specific quantum chemical descriptors. Journal of Molecular Modeling, 2018, 24, 59.	1.8	8
89	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
90	Second generation periodic table-based descriptors to encode toxicity of metal oxide nanoparticles to multiple species: QSTR modeling for exploration of toxicity mechanisms. Environmental Science: Nano, 2018, 5, 2742-2760.	4.3	26

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91	Reply to the comment on â€œCausation or only correlation? Application of causal inference graphs for evaluating causality in nano-QSAR modelsâ€•by D. A. Tasi, J. Csontos, B. Nagy, Z. KÃ³nya and G. Tasi, Nanoscale, 2018, 10, C8NR02377H. Nanoscale, 2018, 10, 20867-20868.	5.6	2
92	Light-dependent isomeric effects of polycyclic aromatic hydrocarbons on the predication of DNA cleavage factor efficiency. Structural Chemistry, 2018, 29, 1697-1707.	2.0	1
93	The index of ideality of correlation: hierarchy of Monte Carlo models for glass transition temperatures of polymers. Journal of Polymer Research, 2018, 25, 1.	2.4	12
94	QSAR modeling of adipose/blood partition coefficients of Alcohols, PCBs, PBDEs, PCDDs and PAHs: A data gap filling approach. Environment International, 2018, 121, 1193-1203.	10.0	17
95	Prediction of antimicrobial activity of large pool of peptides using quasi-SMILES. BioSystems, 2018, 169-170, 5-12.	2.0	13
96	Impact of Pharmaceuticals on the Environment: Risk Assessment Using QSAR Modeling Approach. Methods in Molecular Biology, 2018, 1800, 395-443.	0.9	32
97	Applicability Domain: A Step Toward Confident Predictions and Decidability for QSAR Modeling. Methods in Molecular Biology, 2018, 1800, 141-169.	0.9	61
98	Insight into mechanism of iron-oxides reduction in atmospheres of CH4 and CO. Chemical Physics Letters, 2018, 706, 708-714.	2.6	8
99	Single or mixture halogenated chemicals? Risk assessment and developmental toxicity prediction on zebrafish embryos based on weighted descriptors approach. Chemosphere, 2018, 210, 588-596.	8.2	23
100	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
101	High-temperature thermoelectric transport behavior of the Al/Î³-Al‹sub›2‹/sub›O‹sub›3‹/sub›interface: impact of electron and phonon scattering at nanoscale metalâ€“ceramic contacts. Physical Chemistry Chemical Physics, 2018, 20, 14513-14524.	2.8	4
102	Catalytic abiotic synthesis of uracil from cysteine and urea: Theoretical studies. Chemical Physics Letters, 2018, 710, 16-25.	2.6	0
103	Towards the Development of Global Nano-Quantitative Structureâ€“Property Relationship Models: Zeta Potentials of Metal Oxide Nanoparticles. Nanomaterials, 2018, 8, 243.	4.1	31
104	Recent Advances of Computational Modeling for Predicting Drug Metabolism: A Perspective. Current Drug Metabolism, 2018, 18, 1106-1122.	1.2	19
105	Novel Imprinted Polymer for the Preconcentration of Cadmium with Determination by Inductively Coupled Plasma Mass Spectrometry. Analytical Letters, 2017, 50, 482-499.	1.8	14
106	Geometry optimization of steroid sulfatase inhibitors - the influence on the free binding energy with STS. Structural Chemistry, 2017, 28, 1017-1032.	2.0	10
107	Computational Modeling of DNA and RNA Fragments. , 2017, , 1803-1826.		1
108	Application of Quantum Mechanics and Molecular Mechanics in Chemoinformatics. , 2017, , 2041-2063.		0

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109	Chlorophenol sorption on multi-walled carbon nanotubes: DFT modeling and structureâ€“property relationship analysis. Journal of Molecular Modeling, 2017, 23, 39.	1.8	4
110	CORAL and Nano-QFAR: Quantitative feature â€“ Activity relationships (QFAR) for bioavailability of nanoparticles (ZnO, CuO, Co 3 O 4 , and TiO 2). Ecotoxicology and Environmental Safety, 2017, 139, 404-407.	6.0	29
111	A quantum chemical based toxicity study of estimated reduction potential and hydrophobicity in series of nitroaromatic compounds. SAR and QSAR in Environmental Research, 2017, 28, 133-150.	2.2	12
112	In silico modeling of functionalized graphene oxide-metal cluster conjugates as Raman probe: Raman activity of pyridine. Structural Chemistry, 2017, 28, 379-389.	2.0	2
113	In vivo toxicity of nitroaromatics: A comprehensive quantitative structureâ€“activity relationship study. Environmental Toxicology and Chemistry, 2017, 36, 2227-2233.	4.3	26
114	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
115	Predicting Physical Properties of Nanofluids by Computational Modeling. Journal of Physical Chemistry C, 2017, 121, 1910-1917.	3.1	23
116	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
117	4d and 5d bimetal doped tubular silicon clusters Si₁₂M₂ with M = Nb, Ta, Mo and W: a bimetallic configuration model. Physical Chemistry Chemical Physics, 2017, 19, 3115-3124.	2.8	36
118	In silico kinetics of alkaline hydrolysis of 1,3,5-trinitro-1,3,5-triazinane (RDX): M06-2X investigation. Environmental Sciences: Processes and Impacts, 2017, 19, 388-394.	3.5	18
119	Binding of Alkali Metal Ions with 1,3,5-Tri(phenyl)benzene and 1,3,5-Tri(naphthyl)benzene: The Effect of Phenyl and Naphthyl Ring Substitution on Cationâ^'Î€ Interactions Revealed by DFT Study. Journal of Physical Chemistry A, 2017, 121, 8927-8938.	2.5	5
120	d(A)3d(T)3 and d(G)3d(C)3 B-DNA mini-helixes: the DFT/M06-2x and DFT/B97-D3 comparison of geometrical and energetic characteristics. Journal of Molecular Modeling, 2017, 23, 289.	1.8	8
121	Exploiting a single intramolecular conformational switching Ni-TPP molecule to probe charge transfer dynamics at the nanoscale on bare Si(100)-2 Ã— 1. Physical Chemistry Chemical Physics, 2017, 19, 28982-28992.	2.8	2
122	An Ideal C₃-Symmetric Sulfate Complex: Molecular Recognition of Oxoanions by m-Nitrophenyl- and Pentafluorophenyl-Functionalized Hexaurea Receptors. ACS Omega, 2017, 2, 5840-5849.	3.5	14
123	Remarkable hexafunctional anion receptor with operational urea-based inner cleft and thiourea-based outer cleft: Novel design with high-efficiency for sulfate binding. Scientific Reports, 2017, 7, 6032.	3.3	18
124	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
125	Inhibitors or toxins? Large library target-specific screening of fullerene-based nanoparticles for drug design purpose. Nanoscale, 2017, 9, 10263-10276.	5.6	29
126	Understanding the influence of low-frequency vibrations on the hydrogen bonds of acetic acid and acetamide dimers. Physical Chemistry Chemical Physics, 2017, 19, 24866-24878.	2.8	10

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127	Drug-Nanoparticle Composites. Journal of Nanotoxicology and Nanomedicine, 2017, 2, 1-10.	0.7	4
128	Modeling of Interactions between the Zebrafish Hatching Enzyme ZHE1 and A Series of Metal Oxide Nanoparticles: Nano-QSAR and Causal Analysis of Inactivation Mechanisms. Nanomaterials, 2017, 7, 330.	4.1	17
129	Power Conversion Efficiency of Arylamine Organic Dyes for Dye-Sensitized Solar Cells (DSSCs) Explicit to Cobalt Electrolyte: Understanding the Structural Attributes Using a Direct QSPR Approach. Computation, 2017, 5, 2.	2.0	17
130	Evaluating the toxicity of TiO2-based nanoparticles to Chinese hamster ovary cells and Escherichia coli: a complementary experimental and computational approach. Beilstein Journal of Nanotechnology, 2017, 8, 2171-2180.	2.8	29
131	Review of Current and Emerging Approaches for Quantitative Nanostructure-Activity Relationship Modeling. , 2017, , 1704-1721.		1
132	Exploring Simple, Interpretable, and Predictive QSPR Model of Fullerene C60 Solubility in Organic Solvents. Journal of Nanotoxicology and Nanomedicine, 2017, 2, 28-43.	0.7	6
133	QSPR/QSAR Analyses by Means of the CORAL Software. , 2017, , 929-955.		0
134	Theoretical Studies on Hydrogen Bonds in Anions Encapsulated by an Azamacrocyclic Receptor. Crystals, 2016, 6, 31.	2.2	2
135	Review of Current and Emerging Approaches for Quantitative Nanostructure-Activity Relationship Modeling. Journal of Nanotoxicology and Nanomedicine, 2016, 1, 1-16.	0.7	20
136	Can Toxicity for Different Species be Correlated?. International Journal of Quantitative Structure-Property Relationships, 2016, 1, 23-51.	0.5	20
137	pHâ€controlled reaction divergence of decarboxylation versus fragmentation in reactions of dihydroxyfumarate with glyoxylate and formaldehyde: parallels to biological pathways. Journal of Physical Organic Chemistry, 2016, 29, 352-360.	1.9	5
138	Efficacy of topological informational potentials for analysis of nonequivalent atoms in molecular graphs: the case of chiral fullerenes. Journal of Mathematical Chemistry, 2016, 54, 1986-1996.	1.5	1
139	Novel enhanced applications of QSPR models: Temperature dependence of aqueous solubility. Journal of Computational Chemistry, 2016, 37, 2045-2051.	3.3	15
140	Structure and electrochemical properties for complexes of nitrocompounds with inorganic ions: A theoretical approach. Journal of Computational Chemistry, 2016, 37, 1206-1213.	3.3	2
141	International conference on â€œModeling Interaction in Biomolecules VIIâ€• held in Prague, 14â€“18 September 2015. Journal of Molecular Modeling, 2016, 22, 1.	1.8	0
142	Application of ligand- and receptor-based approaches for prediction of the HIV-RT inhibitory activity of fullerene derivatives. Journal of Nanoparticle Research, 2016, 18, 1.	1.9	12
143	Advantages and limitations of classic and 3D QSAR approaches in nano-QSAR studies based on biological activity of fullerene derivatives. Journal of Nanoparticle Research, 2016, 18, 256.	1.9	37
144	In Silico Alkaline Hydrolysis of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine: Density Functional Theory Investigation. Environmental Science & Technology, 2016, 50, 10039-10046.	10.0	14

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145	A DFT-based QSAR study on inhibition of human dihydrofolate reductase. Journal of Molecular Graphics and Modelling, 2016, 70, 23-29.	2.4	19
146	Quantitative structure-property relationship model leading to virtual screening of fullerene derivatives: Exploring structural attributes critical for photoconversion efficiency of polymer solar cell acceptors. Nano Energy, 2016, 26, 677-691.	16.0	25
147	A comprehensive computational analysis of cathinone and its metabolites using quantum mechanical approaches and docking studies. Structural Chemistry, 2016, 27, 1291-1302.	2.0	5
148	Monte Carloâ€“based quantitative structureâ€“activity relationship models for toxicity of organic chemicals to Daphnia magna. Environmental Toxicology and Chemistry, 2016, 35, 2691-2697.	4.3	24
149	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
150	Computational assessment of environmental hazards of nitroaromatic compounds: influence of the type and position of aromatic ring substituents on toxicity. Structural Chemistry, 2016, 27, 191-198.	2.0	11
151	Introduction of simplex-informational descriptors for QSPR analysis of fullerene derivatives. Journal of Mathematical Chemistry, 2016, 54, 698-706.	1.5	10
152	Experimental and Theoretical Aspects of Anion Complexes with a Thiophene-Based Cryptand. Comments on Inorganic Chemistry, 2016, 36, 305-326.	5.2	6
153	Estimation of melting points of large set of persistent organic pollutants utilizing QSPR approach. Journal of Molecular Modeling, 2016, 22, 55.	1.8	14
154	Adsorption of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) on a soil organic matter. A DFT M05 computational study. Chemosphere, 2016, 148, 294-299.	8.2	6
155	Experimental and computational study of membrane affinity for selected energetic compounds. Chemosphere, 2016, 148, 322-327.	8.2	10
156	Causation or only correlation? Application of causal inference graphs for evaluating causality in nano-QSAR models. Nanoscale, 2016, 8, 7203-7208.	5.6	23
157	Conformations, vibrational spectra and force field of 1-methyl-2-(2â€²-pyridyl)benzimidazole: experimental data and density functional theory investigation in comparison with 2-(2â€²-pyridyl)benzimidazole. Structural Chemistry, 2016, 27, 209-219.	2.0	5
158	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
159	Application of Quantum Mechanics and Molecular Mechanics in Chemoinformatics. , 2016, , 1-23.		4
160	Computational Modeling of DNA and RNA Fragments. , 2016, , 1-24.		0
161	Modeling the Dispersibility of Single Walled Carbon Nanotubes in Organic Solvents by Quantitative Structure-Activity Relationship Approach. Nanomaterials, 2015, 5, 778-791.	4.1	16
162	Computational study of NTO (5-nitro-2,4-dihydro-3H-1,2,4-triazol-3-one) tautomeric properties in aqueous solution. Structural Chemistry, 2015, 26, 1281-1286.	2.0	11

#	Article	IF	Citations
163	QSAR model as a random event: A case of rat toxicity. Bioorganic and Medicinal Chemistry, 2015, 23, 1223-1230.	3.0	36
164	Alkaline hydrolysis of hexahydro-1,3,5-trinitro-1,3,5-triazine: M06-2X investigation. Chemosphere, 2015, 134, 31-38.	8.2	11
165	Toward Selection of Efficient Density Functionals for van der Waals Molecular Complexes: Comparative Study of Câ€“HÂ·Â·Â·Ï€ and Nâ€“HÂ·Â·Â·Ï€ Interactions. Journal of Physical Chemistry A, 2015, 119, 1190-1200.	2.5	22
166	Photoinduced Electron Detachment and Proton Transfer: The Proposal for Alternative Path of Formation of Triplet States of Guanine (G) and Cytosine (C) Pair. Journal of Physical Chemistry B, 2015, 119, 2454-2458.	2.6	6
167	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
168	Synthesis and anion binding studies of tris(3-aminopropyl)amine-based tripodal urea and thiourea receptors: proton transfer-induced selectivity for hydrogen sulfate over sulfate. RSC Advances, 2015, 5, 17606-17614.	3.6	27
169	Structure and Redox Properties of 5-Amino-3-nitro-1H-1,2,4-triazole (ANTA) Adsorbed on a Silica Surface: A DFT M05 Computational Study. Journal of Physical Chemistry A, 2015, 119, 8139-8145.	2.5	14
170	Amino substituted nitrogen heterocycle ureas as kinase insert domain containing receptor (KDR) inhibitors: Performance of structureâ€“activity relationship approaches. Journal of Food and Drug Analysis, 2015, 23, 168-175.	1.9	7
171	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
172	Are the reduction and oxidation properties of nitrocompounds dissolved in water different from those produced when adsorbed on a silica surface? A DFT M05-2X computational study. Journal of Computational Chemistry, 2015, 36, 1029-1035.	3.3	12
173	Causal inference methods to assist in mechanistic interpretation of classification nano-SAR models. RSC Advances, 2015, 5, 77739-77745.	3.6	16
174	Computational study of nitroguanidine (NQ) tautomeric properties in aqueous solution. Structural Chemistry, 2015, 26, 1273-1280.	2.0	5
175	How the â€œLiquid Dropâ€•Approach Could Be Efficiently Applied for Quantitative Structureâ€“Property Relationship Modeling of Nanofluids. Journal of Physical Chemistry C, 2015, 119, 25542-25547.	3.1	18
176	Structure and Binding Energy of Double-Stranded A-DNA Mini-helices: Quantum-Chemical Study. Journal of Physical Chemistry B, 2015, 119, 12741-12749.	2.6	10
177	Synthesis and anion binding properties of a urea-based molecular cleft. Tetrahedron Letters, 2015, 56, 657-661.	1.4	17
178	Genotoxicity of metal oxide nanomaterials: review of recent data and discussion of possible mechanisms. Nanoscale, 2015, 7, 2154-2198.	5.6	163
179	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
180	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

#	Article	IF	Citations
181	Towards understanding mechanisms governing cytotoxicity of metal oxides nanoparticles: Hints from nano-QSAR studies. Nanotoxicology, 2015, 9, 313-325.	3.0	147
182	<i>Ab Initio</i> Studies of Anatase TiO₂ (101) Surface-supported Au₈ Clusters. Current Topics in Medicinal Chemistry, 2015, 15, 1859-1867.	2.1	16
183	QSPR/QSAR Analyses by Means of the CORAL Software. Advances in Chemical and Materials Engineering Book Series, 2015, , 560-585.	0.3	10
184	Reliable but Timesaving: In Search of an Efficient Quantum-chemical Method for the Description of Functional Fullerenes. Current Topics in Medicinal Chemistry, 2015, 15, 1845-1858.	2.1	0
185	Nucleic Acids: Ground-State and Excited-State Properties, Structures, and Interactions and Environmental Aspects as Revealed by Computational Studies. , 2014, , .		1
186	Fundamental Properties of Graphene. World Scientific Series on Carbon Nanoscience, 2014, , 1-37.	0.1	4
187	Intermediate carbene formation in the reaction of thioamides with phosphorus (III) derivatives: Quantum chemical investigation. International Journal of Quantum Chemistry, 2014, 114, 241-248.	2.0	3
188	Accurate calculations of dynamic first hyperpolarizability: Construction of physically justified slaterâ€type basis sets. International Journal of Quantum Chemistry, 2014, 114, 689-695.	2.0	2
189	Homodimers of Cytosine and 1-MethylCytosine. A DFT study of geometry, relative stability and H-NMR shifts in gas-phase and selected solvents. Journal of Molecular Modeling, 2014, 20, 2115.	1.8	6
190	Optimal descriptors as a tool to predict the thermal decomposition of polymers. Journal of Mathematical Chemistry, 2014, 52, 1171-1181.	1.5	15
191	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
192	Toward Accurate and Efficient Predictions of Entropy and Gibbs Free Energy of Adsorption of High Nitrogen Compounds on Carbonaceous Materials. Journal of Physical Chemistry C, 2014, 118, 4774-4783.	3.1	17
193	Comprehension of drug toxicity: Software and databases. Computers in Biology and Medicine, 2014, 45, 20-25.	7.0	69
194	Adsorption of Nitrogen-Containing Compounds on the (100) Î±-Quartz Surface: Ab Initio Cluster Approach. Journal of Physical Chemistry C, 2014, 118, 3023-3034.	3.1	17
195	AconitumandDelphiniumDiterpenoid Alkaloids of Local Anesthetic Activity: Comparative QSAR Analysis Based on GA-MLRA/PLS and Optimal Descriptors Approach. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2014, 32, 213-238.	2.9	13
196	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
197	Optimal descriptor as a translator of eclectic information into the prediction of membrane damage: The case of a group of ZnO and TiO2 nanoparticles. Ecotoxicology and Environmental Safety, 2014, 108, 203-209.	6.0	27
198	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

#	Article	IF	Citations
199	A Theoretical Investigation of the Relative Stability of Isomeric Dihydropyridines. Chemistry of Heterocyclic Compounds, 2014, 50, 327-335.	1.2	1
200	Theoretical Study of One-Electron Reduction And Oxidation Potentials of N-Heterocyclic Compounds. Chemistry of Heterocyclic Compounds, 2014, 50, 311-318.	1.2	13
201	Thermal racemization of spiropyrans: implication of substituent and solvent effects revealed by computational study. Structural Chemistry, 2014, 25, 667-677.	2.0	10
202	Direct QSPR: the most efficient way of predicting organic carbon/water partition coefficient (log K) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	2.0	21
203	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
204	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
205	Hints from Computational Chemistry: Mechanisms of Transformations of Simple Species into Purine and Adenine by Feasible Abiotic Processes. , 2014, , 393-427.		4
206	Ð†ÐŹÐµÐ½Ñ‚Ð¸Ñ„Ð¸Ñ†Ð¸Ñ€Ð¾Ð²Ð°Ð½Ð¾-4-Ñ‚Ñ€Ð¸Ñ„Ñ‚Ð¾Ñ€Ð¼ÐµÑ‚Ð¸Ð»-1-(4-Ð±Ñ€Ð¾Ð¼Ð¾Ð½Ð°Ñ„Ñ‚Ð¸Ð»)Ð°Ð¼Ð¸Ð½Ð¾Ð½Ð¸Ñ‚Ñ Ñ‚Ð° N-Ñ„Ðµ		
207	Optimal descriptor as a translator of eclectic information into the prediction of thermal conductivity of micro-electro-mechanical systems. Journal of Mathematical Chemistry, 2013, 51, 2230-2237.	1.5	12
208	Role of the Multipolar Electrostatic Interaction Energy Components in Strong and Weak Cationâ^Ï€ Interactions. Journal of Physical Chemistry A, 2013, 117, 7989-8000.	2.5	12
209	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
210	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
211	Computational study on Câ^'Hâ€¦Ï€ interactions of acetylene with benzene, 1,3,5-trifluorobenzene and coronene. Journal of Molecular Modeling, 2013, 19, 2855-2864.	1.8	30
212	Structural, energetic, spectroscopic and QTAIM analyses of cationâ€“Ï€ interactions involving mono- and bi-cyclic ring fused benzene systems. Physical Chemistry Chemical Physics, 2013, 15, 20839.	2.8	21
213	Comparative Theoretical Study on the Positional Preference for Functionalization of Two OH and SH Groups with (5,5) Armchair SWCNT. Journal of Physical Chemistry C, 2013, 117, 14441-14450.	3.1	10
214	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
215	B-DNA characteristics are preserved in double stranded d(A)3Â·d(T)3 and d(G)3Â·d(C)3 mini-helixes: conclusions from DFT/M06-2X study. Physical Chemistry Chemical Physics, 2013, 15, 18155.	2.8	36
216	From Formamide to Purine: An Energetically Viable Mechanistic Reaction Pathway. Journal of Physical Chemistry B, 2013, 117, 2314-2320.	2.6	37

#	Article	IF	Citations
217	Theoretical study of ionization and oneâ€electron oxidation potentials of Nâ€heterocyclic compounds. Journal of Computational Chemistry, 2013, 34, 1094-1100.	3.3	17
218	Tautomerism in nucleic acid bases and base pairs: a brief overview. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 637-649.	14.6	45
219	QSAR as a random event: Modeling of nanoparticles uptake in PaCa2 cancer cells. Chemosphere, 2013, 92, 31-37.	8.2	133
220	DFT-based reactivity study of (5,5) armchair boron nitride nanotube (BNNT). Chemical Physics Letters, 2013, 565, 69-73.	2.6	39
221	Exploring Relative Thermodynamic Stabilities of Formic Acid and Formamide Dimers â€“ Role of Low-Frequency Hydrogen-Bond Vibrations. Journal of Chemical Theory and Computation, 2013, 9, 1016-1026.	5.3	17
222	CORAL: QSPRs of enthalpies of formation of organometallic compounds. Journal of Mathematical Chemistry, 2013, 51, 1684-1693.	1.5	7
223	From Formamide to Adenine: A Self-Catalytic Mechanism for an Abiotic Approach. Journal of Physical Chemistry B, 2013, 117, 14039-14045.	2.6	33
224	CORAL: Monte Carlo Method as a Tool for the Prediction of the Bioconcentration Factor of Industrial Pollutants. Molecular Informatics, 2013, 32, 145-154.	2.5	21
225	Chapter 10. Nano-QSAR: Advances and Challenges. RSC Nanoscience and Nanotechnology, 2012, , 220-256.	0.2	11
226	In search of active RGD peptides: Theoretical study of hydrogen bonding in five-member ring cyclic-RGD isomers. Computational and Theoretical Chemistry, 2012, 998, 141-147.	2.5	6
227	Comprehensive Study on the Dissociative Chemisorption of NH₃ on the Sidewalls of Stoneâ€“Wales Defective Armchair (5,5) Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 6012-6021.	3.1	31
228	CORAL: Models of toxicity of binary mixtures. Chemometrics and Intelligent Laboratory Systems, 2012, 119, 39-43.	3.5	23
229	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
230	Could hydrolysis of arsenic substituted DNA be prevented? Protection arises from stacking interactions. Chemical Communications, 2012, 48, 3626.	4.1	8
231	Electron Attachment to the Cytosine-Centered DNA Single Strands: Does Base Stacking Matter?. Journal of Physical Chemistry B, 2012, 116, 1458-1466.	2.6	11
232	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
233	QSAR models for ACE-inhibitor activity of tri-peptides based on representation of the molecular structure by graph of atomic orbitals and SMILES. Structural Chemistry, 2012, 23, 1873-1878.	2.0	27
234	Adsorption of Formamide on Kaolinite Surfaces: A Combined Infrared Experimental and Theoretical Study. Journal of Physical Chemistry C, 2012, 116, 23981-23991.	3.1	36

#	Article	IF	Citations
235	Advancing risk assessment of engineered nanomaterials: Application of computational approaches. Advanced Drug Delivery Reviews, 2012, 64, 1663-1693.	13.7	186
236	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
237	Predictions of Gibbs Free Energies for the Adsorption of Polyaromatic and Nitroaromatic Environmental Contaminants on Carbonaceous Materials: Efficient Computational Approach. Langmuir, 2012, 28, 13307-13317.	3.5	20
238	Relativistic study of tautomerism and core electron binding energies of thio- and selenocytosine. Structural Chemistry, 2012, 23, 1293-1299.	2.0	5
239	Metal Oxide Nanoparticles: Size-Dependence of Quantum-Mechanical Properties. Nanoscience and Nanotechnology - Asia, 2012, 1, 53-58.	0.7	12
240	Mechanical properties of silicon nanowires. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 817-828.	14.6	12
241	Room temperature synthesis of PbSe quantum dots in aqueous solution: stabilization by interactions with ligands. Nanoscale, 2012, 4, 1312.	5.6	39
242	The electronic spectra and the Hâ€bonding pattern of the sulfur and selenium substituted guanines. Journal of Computational Chemistry, 2012, 33, 1587-1593.	3.3	19
243	Coral: QSPR modeling of rate constants of reactions between organic aromatic pollutants and hydroxyl radical. Journal of Computational Chemistry, 2012, 33, 1902-1906.	3.3	30
244	QSPR Prediction of Lipophilicity for Organic Compounds Using Random Forest Technique on the Basis of Simplex Representation of Molecular Structure. Molecular Informatics, 2012, 31, 273-280.	2.5	8
245	A theoretical study of cation-Ï€ interactions: Li+, Na+, K+, Be2+, Mg2+ and Ca2+ complexation with mono- and bicyclic ring-fused benzene derivatives. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	30
246	Theoretical studies on the structure and electronic properties of cubic gold nanoclusters. Canadian Journal of Chemical Engineering, 2012, 90, 852-859.	1.7	4
247	Interactions of Electrons with Bare and Hydrated Biomolecules: From Nucleic Acid Bases to DNA Segments. Chemical Reviews, 2012, 112, 5603-5640.	47.7	179
248	Fundamental Structural, Electronic, and Chemical Properties of Carbon Nanostructures: Graphene, Fullerenes, Carbon Nanotubes, and Their Derivatives. , 2012, , 793-867.		17
249	Mineralâ€“organic interfacial processes: potential roles in the origins of life. Chemical Society Reviews, 2012, 41, 5502.	38.1	205
250	Density functional theory study of interactions of cyclotrimethylene trinitramine (RDX) and triacetone triperoxide (TATP) with metalâ€“organic framework (IRMOF-1(Be)). Structural Chemistry, 2012, 23, 1143-1154.	2.0	5
251	Molecular simulations of adsorption of RDX and TATP on IRMOF-1(Be). Journal of Molecular Modeling, 2012, 18, 3363-3378.	1.8	11
252	CORAL: QSAR modeling of toxicity of organic chemicals towards Daphnia magna. Chemometrics and Intelligent Laboratory Systems, 2012, 110, 177-181.	3.5	57

#	Article	IF	Citations
253	CORAL: Predictions of rate constants of hydroxyl radical reaction using representation of the molecular structure obtained by combination of SMILES and Graph approaches. Chemometrics and Intelligent Laboratory Systems, 2012, 112, 65-70.	3.5	23
254	DFT M06-2X investigation of alkaline hydrolysis of nitroaromatic compounds. Chemosphere, 2012, 88, 635-643.	8.2	49
255	Use of quantitative structureâ€“enantioselective retention relationship for the liquid chromatography chiral separation prediction of the series of pyrrolidinâ€2â€one compounds. Chirality, 2012, 24, 72-77.	2.6	14
256	Structural and electronic property responses to the arsenic/phosphorus exchange in GCâ€related DNA of the Bâ€form. Journal of Computational Chemistry, 2012, 33, 817-821.	3.3	4
257	Theoretical study of the surface properties of poly(dimethylsiloxane) and poly(tetrafluoroethylene). Journal of Molecular Modeling, 2012, 18, 239-250.	1.8	3
258	Metal Oxide Nanoparticles: Size-Dependence of Quantum-Mechanical Properties. Nanoscience and Nanotechnology - Asia, 2012, 1, 53-58.	0.7	15
259	Application of Quantum-Chemical Techniques to Model Environmental Mercury Depletion Reactions. , 2012, , 435-470.		0
260	Potential Path of DNA Damage: Electron Attachmentâ€“Induced DNA Single-Strand Breaks. , 2012, , 511-536.		0
261	Theoretical studies on interactions between low energy electrons and proteinâ€“DNA fragments: valence anions of AT-amino acids side chain complexes. Physical Chemistry Chemical Physics, 2011, 13, 19499.	2.8	5
262	Carâ€“Parrinello Molecular Dynamics Simulations of Tensile Tests on SiâŸ001âŸ© Nanowires. Journal of Physical Chemistry C, 2011, 115, 12283-12292.	3.1	5
263	Dynamical Nonplanarity of Benzene. Evidences from the Carâ€“Parrinello Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2011, 2, 2881-2884.	4.6	12
264	Low Energy Electron Attachment to the Adenosine Site of DNA. Journal of Physical Chemistry B, 2011, 115, 14831-14837.	2.6	18
265	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
266	Do Stoneâ€“Wales Defects Alter the Magnetic and Transport Properties of Single-Walled Carbon Nanotubes?. Journal of Physical Chemistry C, 2011, 115, 22232-22241.	3.1	28
267	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
268	Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles. Nature Nanotechnology, 2011, 6, 175-178.	31.5	654
269	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
270	Evaluation of the dependence of aqueous solubility of nitro compounds on temperature and salinity: A COSMO-RS simulation. Chemosphere, 2011, 83, 287-294.	8.2	19

#	Article	IF	Citations
271	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
272	Calibration and applications of the Î”MP2 method for calculating core electron binding energies. Physical Chemistry Chemical Physics, 2011, 13, 5703.	2.8	27
273	QSAR modeling of anxiolytic activity taking into account the presence of keto- and enol-tautomers by balance of correlations with ideal slopes. Open Chemistry, 2011, 9, 846-854.	1.9	5
274	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
275	Toward robust computational electrochemical predicting the environmental fate of organic pollutants. Journal of Computational Chemistry, 2011, 32, 2195-2203.	3.3	40
276	Probing the structures and thermodynamic characteristics of the environment polluting mercuric halides, cyanides and thiocyanates. Chemical Physics Letters, 2011, 501, 308-314.	2.6	4
277	Interaction of nucleic acid bases and Watsonâ€“Crick base pairs with fullerene: Computational study. Chemical Physics Letters, 2010, 493, 130-134.	2.6	17
278	Choosing safe dispersing media for C60 fullerenes by using cytotoxicity tests on the bacterium Escherichia coli. Journal of Hazardous Materials, 2010, 176, 367-373.	12.4	19
279	The effect of ring annelation to benzene on cation-Ï€ interactions: DFT study. Journal of Molecular Structure, 2010, 976, 320-323.	3.6	16
280	Use of the international chemical identifier for constructing QSPR-model of normal boiling points of acyclic carbonyl substances. Journal of Mathematical Chemistry, 2010, 47, 355-369.	1.5	6
281	QSAR analysis of 1,4-dihydro-4-oxo-1-(2-thiazolyl)-1,8-naphthyridines exhibiting anticancer activity by optimal SMILES-based descriptors. Journal of Mathematical Chemistry, 2010, 47, 647-666.	1.5	10
282	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
283	Adsorption of RDX and TATP on IRMOF-1: an ab initio study. Structural Chemistry, 2010, 21, 391-404.	2.0	13
284	Remarkable diversity of carbonâ€“carbon bonds: structures and properties of fullerenes, carbon nanotubes, and graphene. Structural Chemistry, 2010, 21, 1155-1169.	2.0	136
285	One-electron standard reduction potentials of nitroaromatic and cyclic nitramine explosives. Environmental Pollution, 2010, 158, 3048-3053.	7.5	42
286	Comprehensive Analysis of DNA Strand Breaks at the Guanosine Site Induced by Lowâ€Energy Electron Attachment. ChemPhysChem, 2010, 11, 175-181.	2.1	22
287	Lowâ€Energyâ€Barrier Proton Transfer Induced by Electron Attachment to the Guanineâ‹…â‹…â‹…Cytosine Base Pair. ChemPhysChem, 2010, 11, 880-888.	2.1	31
288	Exploration of density functional methods for oneâ€electron reduction potential of nitrobenzenes. Journal of Computational Chemistry, 2010, 31, 144-150.	3.3	25

#	Article	IF	Citations
289	DFT Study on Tautomerism of Dihydroâ€2Hâ€1,5â€benzodiazepinâ€2â€ones and Dihydroâ€2Hâ€1,5â€benzodiazepineâ€2â€thiones. European Journal of Organic Chemistry, 2010, 2010, 280-291.	2.4	19
290	Application of Random Forest and Multiple Linear Regression Techniques to QSPR Prediction of an Aqueous Solubility for Military Compounds. Molecular Informatics, 2010, 29, 394-406.	2.5	37
291	Evaluation of functionalized isoreticular metal organic frameworks (IRMOFs) as smart nanoporous preconcentrators of RDX. Sensors and Actuators B: Chemical, 2010, 148, 459-468.	7.8	38
292	Density functional theory investigation of interaction of zigzag (7,0) single-walled carbon nanotube with Watsonâ€“Crick DNA base pairs. Chemical Physics Letters, 2010, 496, 128-132.	2.6	31
293	Aconitum and Delphinium alkaloids of curare-like activity. QSAR analysis and molecular docking of alkaloids into AChBP. European Journal of Medicinal Chemistry, 2010, 45, 3885-3894.	5.5	29
294	Guanine in water solution: Comprehensive study of hydration cage versus continuum solvation model. International Journal of Quantum Chemistry, 2010, 110, 3027-3039.	2.0	13
295	Nano meets bio at the interface. Nature Nanotechnology, 2010, 5, 633-634.	31.5	70
296	Electron attachment-induced DNA single-strand breaks at the pyrimidine sites. Nucleic Acids Research, 2010, 38, 5280-5290.	14.5	50
297	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
298	Local and Global Electronic Effects in Single and Double Boron-Doped Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 1528-1533.	3.1	26
299	Effect of Charge Distribution on RDX Adsorption in IRMOF-10. Langmuir, 2010, 26, 5942-5950.	3.5	27
300	Density Functional Theory Based Studies on the Nature of Raman and Resonance Raman Scattering of Nerve Agent Bound to Gold and Oxide-Supported Gold Clusters: A Plausible Way of Detection. Journal of Physical Chemistry A, 2010, 114, 4340-4353.	2.5	10
301	Comprehensive evaluation of medium and long range correlated density functionals in TD-DFT investigation of DNA bases and base pairs: gas phase and water solution study. Molecular Physics, 2010, 108, 3131-3146.	1.7	19
302	New QSPR equations for prediction of aqueous solubility for military compounds. Chemosphere, 2010, 79, 887-890.	8.2	17
303	Nanomaterials â€“ the Next Great Challenge for Qsar Modelers. Challenges and Advances in Computational Chemistry and Physics, 2010, , 383-409.	0.6	34
304	QSAR modeling of acute toxicity on mammals caused by aromatic compounds: the case study using oral LD50 for rats. Journal of Environmental Monitoring, 2010, 12, 1037.	2.1	28
305	In the pursuit of small â€œred shiftâ€•of Câ€“H stretching vibrational frequency of Câ€“Hâ‹¯Ï€ interactions for benzene dimer: How to amend MP2 calculations to reproduce the experimental results. Journal of Chemical Physics, 2009, 130, 081101.	3.0	26
306	Toward Understanding of Hydrogen Storage in Single-Walled Carbon Nanotubes by Investigations of Chemisorption Mechanism. , 2009, , 297-313.		7

#	Article	IF	Citations
307	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
308	Conformational flexibility of pyrimidine rings of nucleic acid bases in polar environment: PCM study. Structural Chemistry, 2009, 20, 743-749.	2.0	23
309	Additive InChI-based optimal descriptors: QSPR modeling of fullerene C 60 solubility in organic solvents. Journal of Mathematical Chemistry, 2009, 46, 1232-1251.	1.5	36
310	Toward the Development of â€œNanoâ€QSARsâ€• Advances and Challenges. Small, 2009, 5, 2494-2509.	10.0	215
311	Consensus QSAR Modeling of Phosphorâ€Containing Chiral AChE Inhibitors. QSAR and Combinatorial Science, 2009, 28, 664-677.	1.4	40
312	Structureâ€hepatoprotective activity relationship study of sesquiterpene lactones: A QSAR analysis. International Journal of Quantum Chemistry, 2009, 109, 17-27.	2.0	13
313	MaSK: A visualization tool for teaching and research in computational chemistry. International Journal of Quantum Chemistry, 2009, 109, 8-16.	2.0	38
314	Theoretical investigations of the structure and bonding of several transition metal complexes to probe their carbon monoxide releasing properties. International Journal of Quantum Chemistry, 2009, 109, 2263-2272.	2.0	8
315	Predicting water solubility of congeners: Chloronaphthalenesâ€”A case study. Journal of Hazardous Materials, 2009, 170, 1014-1022.	12.4	37
316	Fullerene (C60) forms stable complex with nucleic acid base guanine. Chemical Physics Letters, 2009, 469, 207-209.	2.6	17
317	Reply to â€˜Comment on â€˜To stack or not to stack: Performance of a new density functional for the uracil and thymine dimersâ€™ [Chem. Phys. Lett. 459 (2008) 164]â€™. Chemical Physics Letters, 2009, 473, 209-210.	2.6	10
318	Hydration of guanine: Electronic singlet excited states for complexes with 19 and 27 water molecules. Chemical Physics Letters, 2009, 478, 254-259.	2.6	15
319	Interaction of nucleic acid bases with single-walled carbon nanotube. Chemical Physics Letters, 2009, 480, 269-272.	2.6	55
320	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
321	Application of Quantum Chemical Approximations to Environmental Problems: Prediction of Water Solubility for Nitro Compounds. Environmental Science & Technology, 2009, 43, 9208-9215.	10.0	30
322	An Analysis of Substituent Effects in Ethane Derivatives: The Quantum Theory of Atoms in Molecules Approach. Journal of Physical Chemistry A, 2009, 113, 1105-1110.	2.5	19
323	Valence Anions of 9-Methylguanineâ€”1-Methylcytosine Complexes. Computational and Photoelectron Spectroscopy Studies. Journal of the American Chemical Society, 2009, 131, 2663-2669.	13.7	33
324	Prediction of rate constants for radical degradation of aromatic pollutants in water matrix: A QSAR study. Chemosphere, 2009, 75, 1128-1134.	8.2	122

#	Article	IF	Citations
325	Comprehensive Investigation of the Energetics of Pyrimidine Nucleoside Formation in a Model Prebiotic Reaction. Journal of the American Chemical Society, 2009, 131, 16088-16095.	13.7	32
326	Effect of a pH Change on the Conformational Stability of the Modified Nucleotide Queuosine Monophosphate. Journal of Physical Chemistry A, 2009, 113, 9386-9395.	2.5	12
327	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
328	Structure and hydrogen bonding in polyhydrated complexes of guanine. Structural Chemistry, 2008, 19, 171-180.	2.0	30
329	Adsorption of dimethyl methylphosphonate and trimethyl phosphate on calcium oxide: an abÂinitio study. Structural Chemistry, 2008, 19, 307-320.	2.0	33
330	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
331	Multiple Linear Regression Analysis and Optimal Descriptors: Predicting the Cholesteryl Ester Transfer Protein Inhibition Activity. QSAR and Combinatorial Science, 2008, 27, 595-606.	1.4	14
332	Aconitum and Delphinium sp. alkaloids as antagonist modulators of voltage-gated Na+ channels. Computational Biology and Chemistry, 2008, 32, 88-101.	2.3	29
333	Multiplicative SMILES-based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. Chemical Physics Letters, 2008, 457, 332-336.	2.6	43
334	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
335	QSAR modeling of acute toxicity by balance of correlations. Bioorganic and Medicinal Chemistry, 2008, 16, 5999-6008.	3.0	53
336	Structures and Energetics of the Cationâ^Ï€ Interactions of Li⁺, Na⁺, and K⁺ with Cup-Shaped Molecules: Effect of Ring Addition to Benzene and Cavity Selectivity. Journal of Physical Chemistry A, 2008, 112, 7916-7924.	2.5	32
337	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
338	Electronic structure, absorption spectra, and hyperpolarisabilities of some novel pushâ€“pull zinc porphyrins. A DFT/TDDFT study. Molecular Physics, 2008, 106, 147-160.	1.7	14
339	Hydration-Dependent Structural Deformation of Guanine in the Electronic Singlet Excited State. Journal of Physical Chemistry B, 2008, 112, 5139-5152.	2.6	42
340	Thio- versus oxo-derivatives of DNA bases: theoretical study on possible mutagenic effect of sulfur atom. Journal of Sulfur Chemistry, 2008, 29, 401-413.	2.0	1
341	Chapter 7 Toward nanomaterials: Structural, energetic and reactivity aspects of single-walled carbon nanotubes. Theoretical and Computational Chemistry, 2007, 18, 167-199.	0.4	13
342	Relativistic two-component infinite order method for atomic core ionization potentials. Journal of Chemical Physics, 2007, 126, 154106.	3.0	8

#	Article	IF	Citations
343	Application of quantum-chemical approximations to environmental problems: Prediction of physical and chemical properties of TNT and related species. Chemosphere, 2007, 69, 1144-1150.	8.2	21
344	Molecular modelling and QSAR analysis of the estrogenic activity of terpenoids isolated fromFerulaplants. SAR and QSAR in Environmental Research, 2007, 18, 663-673.	2.2	31
345	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
346	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
347	Do the low-energy conformers of nerve agents (NAs) really have cholinesterase inhibition properties? Investigations of the low-energy conformers of acetylcholine and the two NAs sarin and soman. Molecular Physics, 2007, 105, 2551-2564.	1.7	9
348	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
349	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
350	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
351	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
352	Effect of ring annelation on Li+â€“benzene interaction: A computational study. Chemical Physics Letters, 2007, 443, 205-210.	2.6	26
353	Additive SMILES based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. Chemical Physics Letters, 2007, 444, 209-214.	2.6	37
354	Evidence of structural non-planarity in excited state: New findings provided by vibrational analysis of the guanineâ€“cytosine base pair. Chemical Physics Letters, 2007, 447, 330-334.	2.6	6
355	Probing the role of PO stretching mode enhancement in nerve-agent sensors: Simulation of the adsorption of diisopropylfluorophosphate on the model MgO and CaO surfaces. Chemical Physics Letters, 2007, 450, 138-143.	2.6	15
356	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
357	QSAR Modeling of Acute Toxicity for Nitrobenzene Derivatives Towards Rats: Comparative Analysis by MLRA and Optimal Descriptors. QSAR and Combinatorial Science, 2007, 26, 686-693.	1.4	30
358	Effect of tube length on the chemisorptions of one and two hydrogen atoms on the sidewalls of (3,3) and (4,4) single-walled carbon nanotubes: A theoretical study. International Journal of Quantum Chemistry, 2007, 107, 2211-2219.	2.0	32
359	Predicting thermal conductivity of nanomaterials by correlation weighting technological attributes codes. Materials Letters, 2007, 61, 4777-4780.	2.6	24
360	Photochemical syn-anti Isomerization Reactions in N2-Hydroxyisocytosines-An Experimental Matrix Isolation and Theoretical StudyÂ¶. Photochemistry and Photobiology, 2007, 77, 243-252.	2.5	0

#	Article	IF	Citations
361	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
362	Quantitative Classification of Covalent and Noncovalent H-Bonds. Journal of Physical Chemistry B, 2006, 110, 6444-6446.	2.6	224
363	Theoretical Study of Adsorption of Sarin and Soman on Tetrahedral Edge Clay Mineral Fragments. Journal of Physical Chemistry B, 2006, 110, 21175-21183.	2.6	37
364	Towards the Elucidation of the Activation of Cisplatin in Anticancer Treatment. Computational Chemistry - Reviews of Current Trends, 2006, , 265-321.	0.4	2
365	First-order interaction energies and the basis set truncation effects. Molecular Physics, 2006, 104, 395-407.	1.7	5
366	Aromaticity-induced changes in electronic properties of size-expanded DNA bases: Case of xC. International Journal of Quantum Chemistry, 2006, 106, 2339-2346.	2.0	17
367	Ab initio insight on the interaction of ascorbate with Li+, Na+, K+, Be2+, Mg2+, and Ca2+ metal cations. International Journal of Quantum Chemistry, 2006, 106, 2366-2372.	2.0	12
368	Conformational studies on parathion. International Journal of Quantum Chemistry, 2006, 106, 2356-2365.	2.0	3
369	Structure and hydrolysis of the heavy alkaline earth cations: Relativistic studies. International Journal of Quantum Chemistry, 2006, 106, 2422-2427.	2.0	3
370	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
371	Ab initio study of the structural properties of ascorbic acid (vitamin C). International Journal of Quantum Chemistry, 2006, 106, 2934-2943.	2.0	28
372	Local minima conformations of the Sc3N @C80 endohedral complex: Ab initio quantum chemical study and suggestions for experimental verification. International Journal of Quantum Chemistry, 2006, 106, 2975-2980.	2.0	16
373	Spectral origins and ionization potentials of guanine tautomers: Theoretical elucidation of experimental findings. Chemical Physics Letters, 2006, 429, 261-265.	2.6	53
374	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
375	The origin of the interaction of 1,3,5-trinitrobenzene with siloxane surface of clay minerals. Computational and Theoretical Chemistry, 2006, 766, 151-157.	1.5	28
376	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
377	Structure-toxicity relationships of nitroaromatic compounds. Molecular Diversity, 2006, 10, 233-245.	3.9	79
378	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

#	Article	IF	Citations
379	Is a Dihydrogen Bond a Unique Phenomenon?. Computational Chemistry - Reviews of Current Trends, 2005, , 195-235.	0.4	1
380	Probing ab initio MP2 approach towards the prediction of vibrational infrared spectra of DNA base pairs. Journal of Molecular Structure, 2005, 744-747, 19-34.	3.6	10
381	Remarkable effect of base pairing on the geometry of guanine under electronic excitation: A theoretical investigation. Chemical Physics Letters, 2005, 414, 92-97.	2.6	13
382	Adsorption of 2,4-Dinitrotoluene on Dickite: The Role of H-Bonding. Structural Chemistry, 2005, 16, 325-337.	2.0	27
383	Theoretical study of adsorption of methyltert-butyl ether on broken clay minerals surfaces. International Journal of Quantum Chemistry, 2005, 105, 325-340.	2.0	9
384	Time-dependent density functional theory (TD-DFT) study of the excited state proton transfer in hypoxanthine. International Journal of Quantum Chemistry, 2005, 105, 387-395.	2.0	22
385	Ab initio quantum chemical studies of fullerene molecules with substitutes C59X [Xï£¾Si, Ge, Sn], C59Xâ¯ [Xï£¾B, Al, Ga, In], and C59X [Xï£¾N, P, As, Sb]. International Journal of Quantum Chemistry, 2005, 105, 429-436.	2.0	37
386	Environmentally Induced H-Bond Transformation as a Source of Anilâ€“Type Molecule Specific Solvatochromy. Molecular Crystals and Liquid Crystals, 2005, 427, 245/[557]-258/[570].	0.9	2
387	The chemistry of lithium-modified carbonium cations. Molecular Physics, 2005, 103, 2215-2222.	1.7	0
388	Effect of Hydration on the Lowest Singlet Ï€Ï€* Excited-State Geometry of Guanine:Â A Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 17333-17339.	2.6	37
389	The Nature of Interactions in the Ionic Crystal of 3-Pentenenitrile, 2-Nitro-5-oxo, Ion(â¯1), Sodium. Journal of Physical Chemistry B, 2005, 109, 2027-2033.	2.6	38
390	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
391	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
392	Modelling of the Stabilization of the Complex of a Single Walled (5,5) Carbon Nanotube C60H20 with Cumulenic or Acetylenic Chain. AIP Conference Proceedings, 2005, , .	0.4	6
393	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
394	Charges of Phosphate Groups. A Role in Stabilization of 2â€²-deoxyribonucleotides. A DFT Investigation. Journal of Biomolecular Structure and Dynamics, 2005, 22, 441-454.	3.5	25
395	Clusters, the intermediate state of matter. Theoretical and Computational Chemistry, 2004, 15, 67-84.	0.4	3
396	The Influence of Intermolecular Interactions on Second-Order Susceptibilities of Molecular Crystals: Application to the m-Nitroaniline Crystal. Structural Chemistry, 2004, 15, 363-368.	2.0	11

#	Article	IF	Citations
397	Sarin and Soman: Structure and Properties. Structural Chemistry, 2004, 15, 517-525.	2.0	36
398	A Nonempirical Quantum-Chemical Study and Natural Bond Orbital Analysis of C6H5XCY3Species (X =) Tj ETQq0 0 0 rgBT /Overlock 10	2.0	10
399	Ab initio study of dissolution reactions of five-membered aluminosilicate framework rings. International Journal of Quantum Chemistry, 2004, 96, 365-373.	2.0	8
400	C1?C2 bond cleavage in vinylidenecyclopropanes: Theoretical density functional theory study. International Journal of Quantum Chemistry, 2004, 96, 343-348.	2.0	9
401	Electron transport throughout the DNA base pair. International Journal of Quantum Chemistry, 2004, 96, 436-442.	2.0	6
402	Theoretical study of the ground-state gas-phase unimolecular decomposition channels of propynoic acid. International Journal of Quantum Chemistry, 2004, 100, 779-787.	2.0	4
403	A theoretical study of the structure and properties of uric acid: A potent antioxidant. International Journal of Quantum Chemistry, 2004, 100, 801-809.	2.0	15
404	Modeling of the molecular structure and catalytic activity of the new fullerene-based catalyst (?2-c60)pd(PPh3)2: An application in the reaction of selective hydrogenation of acetylenic alcohols. International Journal of Quantum Chemistry, 2004, 100, 810-817.	2.0	13
405	Theoretical study of adsorption of methyltert-butyl ether on the substituted tetrahedral surface of dickite. International Journal of Quantum Chemistry, 2004, 100, 818-831.	2.0	3
406	TDDFT investigation on nucleic acid bases: Comparison with experiments and standard approach. Journal of Computational Chemistry, 2004, 25, 768-778.	3.3	99
407	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
408	Hydrolysis of the heavy metal cations: Relativistic effects. Physical Chemistry Chemical Physics, 2004, 6, 4553-4557.	2.8	14
409	Cooperative Effects:Â Stabilization of the Isoguanine Trimer. Journal of Physical Chemistry B, 2004, 108, 8017-8022.	2.6	15
410	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
411	Sn2BrxI4-x(g) and Sn2BryI3-y+(x= 0â^'4,y= 0â^'3) Species:Â Mass Spectrometric Evidence and Quantum-Chemical Studies. Journal of Physical Chemistry A, 2004, 108, 2418-2425.	2.5	8
412	Multiconfigurational Self-Consistent Field Study of the Excited State Properties of 4-Thiouracil in the Gas Phase. Journal of Physical Chemistry A, 2004, 108, 7241-7246.	2.5	11
413	Modeling the Gas-Phase Reduction of Nitrobenzene to Nitrosobenzene by Iron Monoxide:Â A Density Functional Theory Study. Journal of Physical Chemistry A, 2004, 108, 4878-4886.	2.5	11
414	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

#	Article	IF	Citations
415	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
416	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
417	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
418	Theoretical Study of the Substituent and Solvent Effects on the Molecular Structures, Absorption and Emission Spectra of Open-Form Spiropyrans. Collection of Czechoslovak Chemical Communications, 2004, 69, 47-62.	1.0	4
419	Model Calculations of Radiation-Induced Damage in Thymine Derivatives. Structural Chemistry, 2003, 14, 451-454.	2.0	8
420	A DFT and MP2 Study on the Molecular Structure and Vibrational Spectra of Halogenosubstituted Phosphoryl and Thiophosphoryl Compounds. Structural Chemistry, 2003, 14, 511-525.	2.0	4
421	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
422	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
423	Reply to Comment on â€œRationalizing the Strength of Hydrogen-Bonded Complexes. Ab Initio HF and DFT Studiesâ€• Journal of Physical Chemistry A, 2003, 107, 9251-9252.	2.5	5
424	Ab Initio Studies of the Microsolvation of Ions. Journal of Physical Chemistry A, 2003, 107, 949-955.	2.5	26
425	Isoguanine:Â From Base Pair to Tetrad. Journal of Physical Chemistry A, 2003, 107, 9447-9455.	2.5	10
426	Molecular properties of protonated homogeneous and mixed carbon oxide and carbon dioxide clusters. Journal of Chemical Physics, 2003, 119, 6560-6570.	3.0	8
427	Interactions of model organic species and explosives with clay minerals. Theoretical and Computational Chemistry, 2003, 12, 341-388.	0.4	1
428	Excited States of Nucleic Acid Bases. Computational Chemistry - Reviews of Current Trends, 2003, , 249-344.	0.4	13
429	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
430	A theoretical study of protonated argon clusters: ArnH+â€,(n=1â€“7). Journal of Chemical Physics, 2002, 117, 4803-4809.	3.0	28
431	Acetone n-radical cation conformational preference and torsional barrier. Journal of Chemical Physics, 2002, 116, 7049-7056.	3.0	10
432	Interactions of Water with Mono- and Diamino Derivatives ofN,Nâ€˜-Dimethyluracil. Journal of Physical Chemistry A, 2002, 106, 7828-7833.	2.5	9

#	Article	IF	Citations
433	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
434	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
435	Optimal methods for calculation of the amount of intermolecular electron transfer. Journal of Chemical Physics, 2002, 117, 6952-6958.	3.0	53
436	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
437	A Theoretical Investigation of Excited-State Properties of the Adenineâ^'Uracil Base Pair. Journal of Physical Chemistry A, 2002, 106, 1011-1018.	2.5	30
438	cis-Diamminedichloropalladium and its interaction with guanine and guanine-cytosine base pair. International Journal of Quantum Chemistry, 2002, 90, 1121-1128.	2.0	6
439	Ab initio study of electronic spectra of merocyanine 540 and its photoproducts. International Journal of Quantum Chemistry, 2002, 87, 265-269.	2.0	7
440	cis-Diamminodichloronickel and Its Interaction with Guanine and Guanineâ€“Cytosine Base Pair. Structural Chemistry, 2002, 13, 133-140.	2.0	14
441	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
442	Quantum Chemical Calculations of the First- and Second-Order Hyperpolarizabilities of Molecules in Solutions. Journal of Physical Chemistry A, 2001, 105, 10702-10710.	2.5	38
443	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
444	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
445	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
446	Ab initio calculations of the NMR spectra of [1.1.1]propellane and bicyclo[1.1.1]pentane. Physical Chemistry Chemical Physics, 2001, 3, 1986-1991.	2.8	36
447	Iâ^'H2O and its neutral precursors: Similarities and differences. Journal of Chemical Physics, 2001, 115, 9260-9265.	3.0	18
448	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
449	An ab initio post-Hartree-Fock study of vibrational infrared spectra of 5-azacytosine and cytosine. International Journal of Quantum Chemistry, 2001, 83, 203-212.	2.0	6
450	The structures and properties ofcis- andtrans-MeCl2(NH3)2, Me=Pd and Pt complexes, in ground and excited states. International Journal of Quantum Chemistry, 2001, 83, 213-219.	2.0	8

#	Article	IF	Citations
451	Electronic properties, hydrogen bonding, stacking, and cation binding of DNA and RNA bases. Biopolymers, 2001, 61, 3-31.	2.4	408
452	Title is missing!. Structural Chemistry, 2001, 12, 121-126.	2.0	12
453	An ab initio theoretical study of the stereoisomers of tetrahydrocannabinols. , 2001, 15, 323-333.		3
454	The influence of the molecular charge on potential energy curves for the proton transfer in electronic ground and excited states. Journal of Chemical Physics, 2001, 114, 8251-8256.	3.0	16
455	The influence of the detachment of electrons on the properties and the nature of interactions in Xâ^'H2Oâ€‰(X=Cl,â€ŠBr) complexes. Journal of Chemical Physics, 2001, 115, 3469-3473.	3.0	12
456	The molecular structures and nature of interactions in CH3+Arn(n=1â€“8) complexes. Journal of Chemical Physics, 2001, 115, 771-777.	3.0	17
457	Ionic Clusters with Weakly Interacting Components-Magic Numbers Rationalized by the Shell Structure. Computational Chemistry - Reviews of Current Trends, 2001, , 179-196.	0.4	2
458	Investigations of the excited-state properties of isocytosine: An ab initio approach. International Journal of Quantum Chemistry, 2000, 77, 240-254.	2.0	22
459	Structural nonrigidity of nucleic acid bases. Post-Hartree-Fock ab initio study. International Journal of Quantum Chemistry, 2000, 80, 1116-1124.	2.0	62
460	A DFT investigation on effects of hydration on the tautomeric equilibria of hypoxanthine. Computational and Theoretical Chemistry, 2000, 529, 99-112.	1.5	28
461	Molecular structure and IR spectra of bromomethanes by DFT and post-Hartree-Fock MP2 and CCSD(T) calculations. Molecular Physics, 2000, 98, 371-386.	1.7	22
462	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
463	Modeling of the Hydration Shell of Uracil and Thymine. International Journal of Molecular Sciences, 2000, 1, 17-27.	4.1	58
464	Transition from Regular to Stochastic Vibrational Motion in H+ 3 Molecule: An ab initio Classical Trajectory Study. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2000, 55, 478-480.	1.5	1
465	Aromatic DNA Base Stacking and H-Bonding. Computational Chemistry - Reviews of Current Trends, 2000, , 171-210.	0.4	7
466	Molecular Structure and Vibrational IR Spectra of Fluoro, Chloro and Bromosubstituted Methanes, Silanes and Germanes: An Ab Initio Approach. Computational Chemistry - Reviews of Current Trends, 2000, , 243-306.	0.4	1
467	The structure and properties of H3+Arnâ€Š(n=1â€“9) cations. Journal of Chemical Physics, 2000, 113, 3615-3620.	3.0	17
468	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

#	Article	IF	Citations
469	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
470	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
471	Cationâ€"Ï€ and Amino-Acceptor Interactions Between Hydrated Metal Cations and DNA Bases. A Quantum-Chemical View. Journal of Biomolecular Structure and Dynamics, 2000, 17, 1087-1096.	3.5	32
472	Does the Hydrated Cytosine Molecule Retain the Canonical Structure? A DFT Study. Journal of Physical Chemistry B, 2000, 104, 5357-5361.	2.6	77
473	Theoretical Study of Proton Transfer in Hypoxanthine Tautomers:â€‰ Effects of Hydration. Journal of Physical Chemistry A, 2000, 104, 3021-3027.	2.5	44
474	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
475	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
476	Nature of binding in the alkalineâ€"earth clusters: Be3, Mg3, and Ca3. Journal of Chemical Physics, 2000, 113, 6245-6252.	3.0	59
477	Aromatic Base Stacking in DNA: Fromab initioCalculations to Molecular Dynamics Simulations. Journal of Biomolecular Structure and Dynamics, 2000, 17, 1-24.	3.5	14
478	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
479	EXPLOSIVE ADVANCES IN COMPUTATIONAL CHEMISTRY â€" APPLICATIONS OF PARALLEL COMPUTING IN BIOMEDICAL AND MATERIAL SCIENCE RESEARCH. , 2000, , .		0
480	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
481	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
482	The contribution of ring conformational flexibility to the relative stability of isomeric cyclohexadienes. Chemical Physics Letters, 1999, 302, 262-266.	2.6	6
483	Stability of Allylbenzene Conformers Revised: A Quantum-Chemical Study. Structural Chemistry, 1999, 10, 79-83.	2.0	1
484	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
485	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
486	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

#	Article	IF	Citations
487	An ab initio study of the structures and properties of the XH42+ and XH62+ (X=C, Si, Ge) dications. International Journal of Quantum Chemistry, 1999, 72, 319-324.	2.0	6
488	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
489	Quantum chemical study of ground-state merocyanine 540 model compounds. International Journal of Quantum Chemistry, 1999, 75, 741-750.	2.0	4
490	Possibility of the Existence of Non-Carbon Fullerenes:â€‰ Ab Initio HF and DFT/B3LYP Studies of the IV Main Group Fullerene-Like Species. Journal of Physical Chemistry A, 1999, 103, 396-401.	2.5	38
491	An Active Site Model and the Catalytic Activity Mechanism of the new Fullerene-Based Catalyst - (Î·²-C₆₀)Pd(PPh₃)₂. Fullerenes, Nanotubes, and Carbon Nanostructures, 1999, 7, 467-484.	0.6	9
492	Atomization Energies, Formation Enthalpies, Bond Dissociation Energies, and Adiabatic Electron Affinities of the PFn/PFn-Series,n= 1â^'6. Journal of Physical Chemistry A, 1999, 103, 7856-7860.	2.5	6
493	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
494	Structure and Nature of the Interaction of the CH3N2+Ion Shellvated by H2Molecules:Â CH3N2+(H2)n=1-9. Journal of Physical Chemistry A, 1999, 103, 9138-9143.	2.5	8
495	Specific Solvation Effects on the Structures and Properties of Neutral and One-Electron Oxidized Formamidineâ^'Formamide Complexes. A Theoretical ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 8317-8327.	2.5	20
496	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
497	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
498	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
499	Tautomeric equilibria in 8-oxopurines: implications for mutagenicity. , 1998, 12, 373-373.		38
500	A DFT Study of the Models of the Bronsted Acid Sites of Zeolite Catalysts. Structural Chemistry, 1998, 9, 319-326.	2.0	0
501	Theoretical Study of Rotational Isomerism in Ethyl Pseudohalides. Structural Chemistry, 1998, 9, 161-167.	2.0	4
502	Ab initio study of the structure of isocytosine-cytosine standard Watson-Crick base pairs in the gas phase and in water. International Journal of Quantum Chemistry, 1998, 69, 37-47.	2.0	27
503	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
504	Searches on the potential energy hypersurfaces of GeCH2, GeSiH2, and Ge2H2. International Journal of Quantum Chemistry, 1998, 70, 925-932.	2.0	31

#	Article	IF	Citations
505	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
506	Tautomerism and Proton Transfer in 6-Selenoguanine:Â A Post Hartreeâ˜'Fock Level ab Initio SCF-MO Investigation. Journal of Physical Chemistry A, 1998, 102, 6161-6166.	2.5	22
507	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
508	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
509	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
510	Ab InitioHF and Density Functional Theory Studies of C₆₀@Si₆₀. Fullerenes, Nanotubes, and Carbon Nanostructures, 1998, 6, 271-281.	0.6	17
511	Searches on the potential energy hypersurfaces of GeCH2, GeSiH2, and Ge2H2. International Journal of Quantum Chemistry, 1998, 70, 925-932.	2.0	1
512	Molecular Structure and Infrared Spectra of the DNA Bases and Their Derivatives: Theory and Experiment. Computational Chemistry - Reviews of Current Trends, 1997, , 140-216.	0.4	30
513	Comment on â€œElectron-Correlated Calculations of Electric Properties of Nucleic Acid Basesâ€• Journal of Physical Chemistry B, 1997, 101, 8038-8039.	2.6	24
514	Tautomerism of Thioguanine:Â From Gas Phase to DNA. Journal of Physical Chemistry A, 1997, 101, 4753-4760.	2.5	37
515	Thioguanine and Thiouracil:Â Hydrogen-Bonding and Stacking Properties. Journal of Physical Chemistry A, 1997, 101, 9489-9495.	2.5	113
516	Molecular Structure of the GeH2Â·Â·Â·OH2 Complex. Journal of Physical Chemistry A, 1997, 101, 3784-3788.	2.5	12
517	Theoretical ab Initio Study of CN2O3Structures:Â Prediction of New High-Energy Molecules. Journal of Physical Chemistry A, 1997, 101, 2709-2714.	2.5	13
518	Interaction of DNA Base Pairs with Various Metal Cations (Mg2+, Ca2+, Sr2+, Ba2+, Cu+, Ag+, Au+, Zn2+,) Tj ETQq0 0 0 rgBT /Overlock Interaction. Journal of Physical Chemistry B, 1997, 101, 9670-9677.	2.6	222
519	Ionic to covalent bonding: a density functional theory study of linear and bent X2Y3 monomers (X = B,) Tj ETQq1 1 0.784314 rgBT /O		12
520	Structures and energies of seleno derivatives of biuret.Ab Initio comparative studies of diselenobiuret, selenobiuret, and selenothiobiuret. Structural Chemistry, 1997, 8, 245-256.	2.0	0
521	Density functional theory and post-Hartree-Fock studies on molecular structure and harmonic vibrational spectrum of formaldehyde. Theoretical Chemistry Accounts, 1997, 97, 195-202.	1.4	8
522	Density functional theory study on molecular structure and vibrational IR spectra of isocytosine. International Journal of Quantum Chemistry, 1997, 61, 453-465.	2.0	37

#	Article	IF	Citations
523	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
524	Nonplanar DNA Base Pairs. Journal of Biomolecular Structure and Dynamics, 1996, 13, 827-833.	3.5	101
525	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
526	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
527	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
528	Existence of Two Distinct Isomeric Forms of Me(OH)SiCH2. A Theoretical Confirmation. The Journal of Physical Chemistry, 1996, 100, 11616-11619.	2.9	4
529	Ab initio study on the stability and properties of XYCOâ‹…â€‰â‹…â€‰â‹…HZ complexes. III. A comparative study of basis set and electron correlation effects for H2COâ‹…â€‰â‹…â€‰â‹…HCl. Journal of Chemical Physics, 1996, 104, 1441-1451.	3.0	17
530	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
531	An ab initio study on HXC(double bond)O ? HY molecular complexes (X, Y = F, Cl). International Journal of Quantum Chemistry, 1996, 57, 757-766.	2.0	5
532	Post-Hartree-Fock and DFT level studies on the Cl2CO ? Cl2 complex: Accurate molecular parameters, harmonic vibrational frequencies, and interaction energies. International Journal of Quantum Chemistry, 1996, 60, 1007-1013.	2.0	1
533	Theoreticalab InitioStudy of CN2O2Structures:Â Prediction of Nitryl Cyanide as a High-Energy Molecule. The Journal of Physical Chemistry, 1996, 100, 19840-19846.	2.9	23
534	Postâ€Hartreeâ€"Fock study on Arâ€"HCO+ and Heâ€"HCO+ complexes: A critical examination of experimental data. Journal of Chemical Physics, 1996, 105, 6388-6394.	3.0	23
535	Interactions of DNA Bases and the Structure of DNA: A Nonempirical Ab Initio Study with Inclusion of Electron Correlation. Computational Chemistry - Reviews of Current Trends, 1996, , 185-218.	0.4	17
536	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
537	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
538	Molecular Structures of 10-Valence Electron Species. 4. Potential Energy Surfaces and Properties of HSiX+(X = O, S, Se). The Journal of Physical Chemistry, 1996, 100, 7361-7366.	2.9	7
539	What changes occur in vibrational spectra of guanine and cytosine when they form the Watson-Crick base pair? A quantum chemicalSCRFHF/6-31G* study. International Journal of Quantum Chemistry, 1995, 56, 207-225.	2.0	23
540	Ab initiostudy of the structure of guanine-cytosine base pair conformers in gas phase and polar solvents. Molecular Physics, 1995, 84, 469-480.	1.7	33

#	Article	IF	Citations
541	Ab initio prediction of the structure, harmonic vibrational frequencies, and dissociation energy of the H2â€“GeH+3â€“H2 cluster ion. Journal of Chemical Physics, 1995, 102, 3667-3673.	3.0	11
542	Partitioned energetics for propene internal rotation. Journal of Chemical Physics, 1995, 103, 1523-1529.	3.0	11
543	Theoretical Investigation of the Molecular Structure of the Ï€Î° DNA Base Pair. Journal of Biomolecular Structure and Dynamics, 1995, 12, 1055-1062.	3.5	34
544	Electronic structure of X2 Y3 molecules (X = B, Al, Ga; Y = O,S): A theoretical study. Journal of Chemical Sciences, 1995, 107, 423-429.	1.5	0
545	Diborane, Dialane, and Digallane: Accurate geometries and vibrational frequencies. International Journal of Quantum Chemistry, 1994, 52, 579-594.	2.0	7
546	Guanine, 6-thioguanine and 6-selenoguanine: ab initio HF/DZP and MP2/DZP comparative studies. Computational and Theoretical Chemistry, 1994, 311, 37-44.	1.5	35
547	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
548	Molecular structure and vibrational infrared spectra of formaldehyde, selenoformaldehyde and their dihalogenoderivatives byab initiopost-Hartree-Fock calculation. Molecular Physics, 1994, 81, 119-131.	1.7	26
549	Tautomers of 6-thioguanine: structures and properties. The Journal of Physical Chemistry, 1993, 97, 3520-3524.	2.9	45
550	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
551	Ab initiopost-Hartree-Fock study on tautomeric stabilities of phosphine oxide, phosphinous acid and their thio analogues. Molecular Physics, 1992, 76, 475-483.	1.7	15
552	Biuret and its sulfur analogs: Structures and energies. International Journal of Quantum Chemistry, 1992, 44, 301-313.	2.0	10
553	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
554	Ab initio post-Hartree-Fock studies on molecular structure and vibrational IR spectrum of formaldehyde. International Journal of Quantum Chemistry, 1992, 44, 421-426.	2.0	7
555	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
556	Structure and properties of uracil and its sulfur analogs: A systematic study of basis set effects inAb InitioSCF calculations. International Journal of Quantum Chemistry, 1991, 40, 9-21.	2.0	24
557	Theoretical and experimental study on small molecular ions. I.Ab Initio calculations on CSe, CSe+, and HCSe+ species. International Journal of Quantum Chemistry, 1991, 40, 451-459.	2.0	4
558	Nanoparticles. , 0, , 92-110.		1

#	Article	IF	Citations
559	A density functional theory study of the simplest adsorption forms of perfluorooctanoic and perfluorooctanesulphonic acids by graphene oxide and fluorinated graphene oxide*. Molecular Physics, 0, , .	1.7	0