Mariusz Makowski

List of Publications by Year
in descending order

104	1,772	279487 23	344852 36
papers	citations	h-index	g-index

105	105	105	1579
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Physics-based protein-structure prediction using a hierarchical protocol based on the UNRES force field: Assessment in two blind tests. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 7547-7552.	3.3	140
2	A unified coarse-grained model of biological macromolecules based on mean-field multipoleâ€“multipole interactions. Journal of Molecular Modeling, 2014, 20, 2306.	0.8	123
3	Potential of Mean Force of Association of Large Hydrophobic Particles: Toward the Nanoscale Limit. Journal of Physical Chemistry B, 2010, 114, 993-1003.	1.2	79
4	Potential of Mean Force of Hydrophobic Association:â€‰ Dependence on Solute Size. Journal of Physical Chemistry B, 2007, 111, 10765-10774.	1.2	63
5	Further Evidence for the Absence of Polyproline II Stretch in the XAO Peptide. Biophysical Journal, 2007, 92, 2904-2917.	0.2	51
6	A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. I. Backbone potentials of coarse-grained polypeptide chains. Journal of Chemical Physics, 2017, 146, 124106.	1.2	48
7	Quantum-Chemical Studies on the Favored and Rare Tautomers of Neutral and Redox Adenine. Journal of Physical Chemistry A, 2013, 117, 1548-1559.	1.1	47
8	Geometric and energetic consequences of prototropy for adenine and its structural models â€“ a review. RSC Advances, 2015, 5, 36587-36604.	1.7	44
9	Ab Initio Studies on the Preferred Site of Protonation in Cytisine in the Gas Phase and Water. International Journal of Molecular Sciences, 2005, 6, 143-156.	1.8	43
10	Influence of Ionic Strength on Hydrophobic Interactions in Water: Dependence on Solute Size and Shape. Journal of Physical Chemistry B, 2020, 124, 10326-10336.	1.2	39
11	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force for the Interaction of Amino Acid Side Chains in Water. IV. Pairs of Different Hydrophobic Side Chains. Journal of Physical Chemistry B, 2008, 112, 11385-11395.	1.2	36
12	Acidâ€“base equilibria in systems involving substituted pyridines in polar aprotic protophobic media and in the amphiprotic methanol. Analytica Chimica Acta, 2000, 418, 233-240.	2.6	35
13	Acidâ€“base and hydrogen-bonding equilibria in aliphatic amine and carboxylic acid systems in non-aqueous solutions. Analytica Chimica Acta, 1999, 401, 317-321.	2.6	33
14	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force for the Interaction of Amino Acid Side Chains in Water. 3. Calculation and Parameterization of the Potentials of Mean Force of Pairs of Identical Hydrophobic Side Chains. Journal of Physical Chemistry B, 2007, 111, 2925-2931.	1.2	33
15	Ab initiostudy of tautomerism and of basicity center preference in histamine, from gas phase to solution-comparison with experimental data (gas phase, solution, solid state). Journal of Physical Organic Chemistry, 2003, 16, 783-796.	0.9	30
16	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 1. Tests of the Approach Using Simple Lattice Protein Models. Journal of Physical Chemistry B, 2004, 108, 16918-16933.	1.2	30
17	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino-Acid Side Chains in Water. VI. Oppositely Charged Side Chains. Journal of Physical Chemistry B, 2011, 115, 6130-6137.	1.2	30
18	Ab Initio Study of Possible and Preferred Basic Site(s) in Polyfunctional N,N1-Dimethyl-N-cyanoformamidine. Journal of Physical Chemistry A, 2001, 105, 869-874.	1.1	29

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19	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino-Acid Side Chains in Water. V. Like-Charged Side Chains. Journal of Physical Chemistry B, 2011, 115, 6119-6129.	1.2	28
20	A comprehensive approach to the analysis of antibiotic-metal complexes. TrAC - Trends in Analytical Chemistry, 2020, 123, 115771.	5.8	28
21	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force for the Interaction of Amino Acid Side Chains in Water. 2. Tests with Simple Spherical Systems. Journal of Physical Chemistry B, 2007, 111, 2917-2924.	1.2	27
22	Ab Initio Study of Energetics of Protonation and Hydrogen Bonding of PyridineN-Oxide and Its Derivatives. Journal of Physical Chemistry A, 1999, 103, 11104-11108.	1.1	26
23	Ab Initio Study of the Energetics of Protonation and Homocomplexed Cation Formation in Systems with Pyridine and Its Derivatives. Journal of Physical Chemistry A, 2001, 105, 6743-6749.	1.1	24
24	Metallopharmaceuticals in Therapy - A New Horizon for Scientific Research. Current Medicinal Chemistry, 2018, 25, 1729-1791.	1.2	23
25	Calculations of pKaValues of Selected Pyridinium and Its N-Oxide Ions in Water and Acetonitrile. Journal of Physical Chemistry A, 2020, 124, 538-551.	1.1	22
26	Experimental and Theoretical Studies of Acidâ^'Base Equilibria of Substituted 4-Nitropyridine N-Oxides. Journal of Physical Chemistry A, 2003, 107, 6293-6300.	1.1	21
27	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force for the Interaction of Amino Acid Side Chains in Water. 1. Approximate Expression for the Free Energy of Hydrophobic Association Based on a Gaussian-Overlap Model. Journal of Physical Chemistry B, 2007, 111, 2910-2916.	1.2	21
28	Coordination chemistry of pyrazine derivatives analogues of PZA: design, synthesis, characterization and biological activity. RSC Advances, 2016, 6, 52009-52025.	1.7	21
29	What Can Electrochemical Methods Offer in Determining DNAâ€“Drug Interactions?. Molecules, 2021, 26, 3478.	1.7	21
30	A potentiometric study of acidâ€“base properties of the (phenol+phenolate) systems in acetonitrile and, (acetonitrile+cyclohexane) solvent system. Journal of Chemical Thermodynamics, 2003, 35, 77-89.	1.0	20
31	Towards temperature-dependent coarse-grained potentials of side-chain interactions for protein folding simulations. I: Molecular dynamics study of a pair of methane molecules in water at various temperatures. Protein Engineering, Design and Selection, 2009, 22, 547-552.	1.0	20
32	Scale-consistent approach to the derivation of coarse-grained force fields for simulating structure, dynamics, and thermodynamics of biopolymers. Progress in Molecular Biology and Translational Science, 2020, 170, 73-122.	0.9	20
33	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino Acid Side Chains in Water. VII. Chargedâ€“Hydrophobic/Polar and Polarâ€“Hydrophobic/Polar Side Chains. Journal of Physical Chemistry B, 2017, 121, 379-390.	1.2	19
34	New benzothiazole based copper(II) hydrazone Schiff base complexes for selective and environmentally friendly oxidation of benzylic alcohols: The importance of the bimetallic species tuned by the choice of the counterion. Journal of Molecular Liquids, 2020, 302, 112590.	2.3	19
35	Fluorescence quenching of fluoroquinolone antibiotics by 4-hydroxy-TEMPO in aqueous solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 887-891.	2.0	18
36	Attractive Sâ‹¯Ï€ and Ï€-Ï€ interactions in the pyrazine-2-thiocarboxamide structure: Experimental and computational studies in the context of crystal engineering and microbiological properties. Journal of Molecular Structure, 2016, 1105, 96-104.	1.8	17

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37	Assessment of Two Theoretical Methods to Estimate Potentiometric Titration Curves of Peptides:Â Comparison with Experiment. Journal of Physical Chemistry B, 2006, 110, 4451-4458.	1.2	16
38	Photosensitive and pH-dependent activity of pyrazine-functionalized carbazole derivative as promising antifungal and imaging agent. Scientific Reports, 2020, 10, 11767.	1.6	16
39	Theoretical Calculations of Heteroconjugation Equilibrium Constants in Systems Modeling Acidâ^'Base Interactions in Side Chains of Biomolecules Using the Potential of Mean Force. Journal of Physical Chemistry B, 2004, 108, 12222-12230.	1.2	15
40	Can Nitriles Be Stronger Bases Than Proton Sponges in the Gas Phase? A Computational Analysis. Journal of Physical Chemistry A, 2015, 119, 8225-8236.	1.1	15
41	Crystalline pyrazine-2-amidoxime isolated by diffusion method and its structural and behavioral analysis in the context of crystal engineering and microbiological activity. RSC Advances, 2016, 6, 64499-64512.	1.7	15
42	Modeling the Structure, Dynamics, and Transformations of Proteins with the UNRES Force Field. Methods in Molecular Biology, 2022, 2376, 399-416.	0.4	14
43	Potentials of mean force for hydrophobic interactions between hydrocarbons in water solution: dependence on temperature, solute shape, and solute size. Journal of Physical Organic Chemistry, 2015, 28, 10-16.	0.9	13
44	Drug-like properties and complete physicochemical profile of pyrazineâ€'2â€'amidoxime: A combined multi-experimental and computational studies. Journal of Molecular Liquids, 2019, 276, 453-470.	2.3	13
45	Experimental and theoretical investigation of conformational states and noncovalent interactions in crystalline sulfonamides with a methoxyphenyl moiety. CrystEngComm, 2021, 23, 6137-6162.	1.3	13
46	Potentiometric studies of cationic heteroconjugation equilibria in systems involving free and protonated pyridine derivatives in dimethyl sulfoxide. Journal of Chemical Thermodynamics, 2002, 34, 391-400.	1.0	12
47	Ab Initio Studies on Acidâ^'Base Equilibria of Substituted Phenols. Journal of Physical Chemistry A, 2004, 108, 10354-10358.	1.1	12
48	Importance of CH tautomers in the tautomeric mixture of uric acid. Computational and Theoretical Chemistry, 2010, 947, 83-91.	1.5	12
49	Geometric consequences of electron delocalization for adenine tautomers in aqueous solution. Journal of Molecular Modeling, 2014, 20, 2234.	0.8	12
50	Coarse-Grained Models of Proteins: Theory and Applications. , 2011, , 35-83.		12
51	The Azatriquinenamine Trimerâ€" A Novel Proton Chelate Azatriquinanes, Part 3. This work was financially supported by the University of Nottingham and the Polish State Committee for Scientific Research (grant DS/8231-4-0097-1). We also thank the EPSRC National Crystallography Service, University of Southampton, for data collection. Part 2: Ref [4].. Angewandte Chemie - International Edition, 2001, 40, 3696.	7.2	11
52	Potentiometric investigation of acid dissociation and anionic homoconjugation equilibria of substituted phenols in dimethyl sulfoxide. Journal of Chemical Thermodynamics, 2003, 35, 1645-1655.	1.0	11
53	Experimental (FTâ€IR) and theoretical (DFT) studies on prototropy and Hâ€bond formation for pyrazineâ€2â€amidoxime. Journal of Physical Organic Chemistry, 2016, 29, 326-335.	0.9	11
54	Recent advances in medicinal chemistry of ampicillin: Derivatives, metal complexes, and sensing approaches. TrAC - Trends in Analytical Chemistry, 2022, 155, 116691.	5.8	11

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55	Introduction of Phosphorylated Residues into the UNRES Coarse-Grained Model: Toward Modeling of Signaling Processes. Journal of Physical Chemistry B, 2019, 123, 5721-5729.	1.2	10
56	Tautomerism of neutral and monoprotonated histamine?a comparison of semi-empirical andab initio quantum mechanical predictions for ?essential? and ?scorpio? conformations. Journal of Physical Organic Chemistry, 2001, 14, 770-777.	0.9	9
57	Determination of the protonation and deprotonation centres for isomers of methyl 3-azido-2,3-dideoxyhexopyranosides. Computational and Theoretical Chemistry, 2005, 714, 1-6.	1.5	9
58	Multi-analytical studies about physico-chemical properties of Ni(II)-vitamin B6 coordination compounds and their CT-DNA interactions. Journal of Molecular Liquids, 2017, 243, 771-780.	2.3	9
59	Ab Initio Study of Energetics of Cationic Heteroconjugation in Pyridine N-Oxide and Its Derivatives Systems. Journal of Physical Chemistry A, 2001, 105, 7381-7390.	1.1	8
60	Theoretical calculations of homoconjugation equilibrium constants in systems modeling acid-base interactions in side chains of biomolecules using the potential of mean force. Journal of Computational Chemistry, 2005, 26, 235-242.	1.5	8
61	Potentiometric and ab initio studies of acidâ€“base interactions of substituted 4-halo(Cl,Br)pyridine N-oxide systems. Journal of Chemical Thermodynamics, 2006, 38, 1584-1591.	1.0	8
62	Stimulation of Sulfonamides Antibacterial Drugs Activity as a Result of Complexation with Ru(III): Physicochemical and Biological Study. International Journal of Molecular Sciences, 2021, 22, 13482.	1.8	8
63	Study of the anticancer potential of Cd complexes of selenazoyl-hydrazones and their sulfur isosters. European Journal of Medicinal Chemistry, 2022, 238, 114449.	2.6	8
64	A study of the tendency of organic bases towards cationic heteroconjugation in polar non-aqueous solvents. Perkin Transactions II RSC, 2001, , 1844-1849.	1.1	7
65	Ab initio study of the energetics of protonation and deprotonation of the methyl 3-amino-2,3-dideoxyhexopyranosides isomers. Computational and Theoretical Chemistry, 2005, 718, 87-92.	1.5	7
66	A potentiometric study of molecular heteroconjugation equilibria in (n-butylamine+acetic acid) systems in binary (acetonitrile +1,4-dioxane) solvent mixtures. Journal of Chemical Thermodynamics, 2006, 38, 606-610.	1.0	7
67	Toward Temperature-Dependent Coarse-Grained Potentials of Side-Chain Interactions for Protein Folding Simulations. II. Molecular Dynamics Study of Pairs of Different Types of Interactions in Water at Various Temperatures. Journal of Physical Chemistry B, 2012, 116, 6844-6853.	1.2	7
68	Coordination mode and reactivity of nickel(II) with vitamin B6. Journal of Coordination Chemistry, 2014, 67, 2885-2897.	0.8	7
69	Spectrophotometric, potentiometric, and conductometric studies of binary complex formation between copper(II) and three forms of vitamin B₆ in aqueous solutions. Journal of Coordination Chemistry, 2015, 68, 3761-3775.	0.8	6
70	Effects of Positive and Negative Ionization on Prototropy in Pyrimidine Bases: An Unusual Case of Isocytosine. Journal of Physical Chemistry A, 2018, 122, 7863-7879.	1.1	6
71	Theoretical studies on the anionic association of phenol and its derivatives in acetonitrile. Journal of Molecular Structure, 2014, 1076, 165-173.	1.8	5
72	Ab initio study of the energetics of protonation, deprotonation and homocomplexed cations and anions formation in systems modeling side chains of biomolecules. Computational and Theoretical Chemistry, 2004, 674, 61-67.	1.5	4

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73	Ab initio studies of acidâ€“base reactions in the substituted 4-nitropyridine N-oxide systems. Computational and Theoretical Chemistry, 2005, 756, 1-9.	1.5	4
74	Potentiometric studies of acidâ€“base interactions in substituted 4-nitropyridine N-oxide systems. Journal of Chemical Thermodynamics, 2006, 38, 554-558.	1.0	4
75	A potentiometric study of (acid+base) equilibria in substituted 4-nitropyridine N-oxide systems in methanol and dimethyl sulfoxide. Journal of Chemical Thermodynamics, 2007, 39, 309-315.	1.0	4
76	Experimental and theoretical studies of solvent effects on the hydrogen bonds in homoconjugated cations of substituted 4-halo (Cl,Br) pyridine N-oxide derivatives. Journal of Chemical Thermodynamics, 2007, 39, 1272-1278.	1.0	4
77	Theoretical Studies of Interactions between O-Phosphorylated and Standard Amino-Acid Side-Chain Models in Water. Journal of Physical Chemistry B, 2015, 119, 8526-8534.	1.2	4
78	Stable cationic coordination polymers of the Cu(II)-vitamin B 6 type: Structural analysis, application abilities and physicochemical properties in the solid state and solutions. Dyes and Pigments, 2017, 136, 278-291.	2.0	4
79	Simulation of Protein Structure and Dynamics with the Coarse-Grained UNRES Force Field. , 2008, , 107-122.		4
80	Sulfonamides differing in the alkylamino substituent length â€“ Synthesis, electrochemical characteristic, acid-base profile and complexation properties. Polyhedron, 2022, 221, 115868.	1.0	4
81	A study of energetics of formation of heterocomplexed cations of trimethylamine N-oxide by using ab initio methods. Computational and Theoretical Chemistry, 2001, 544, 159-171.	1.5	3
82	Theoretical studies on acid-base interactions in the substituted 4-nitropyridines and their N-oxides systems. Computational and Theoretical Chemistry, 2005, 731, 193-199.	1.5	3
83	Potentiometric investigations of (acid+base) equilibria in (n-butylamine+acetic acid) systems in binary (acetone+cyclohexane) solvent mixtures. Journal of Chemical Thermodynamics, 2005, 37, 783-790.	1.0	3
84	Change of the favored routes of EI MS fragmentation when proceeding from N¹, N¹â€dimethylâ€N²â€arylformamidines to 1,1,3,3â€tetraalkylâ€2â€arylguanidines: substituent effects. Journal of Mass Spectrometry, 2010, 45, 762-771.	0.7	3
85	Influence of Câ€“H/X (X = S, Cl, N, Pt/Pd) Interactions on the Molecular and Crystal Structures of Pt(II) and Pd(II) Complexes with Thiomorpholine-4-carbonitrile: Crystallographic, Thermal, and DFT Study. Crystal Growth and Design, 2020, 20, 3018-3033.	1.4	3
86	Sulfonamides with hydroxyphenyl moiety: Synthesis, structure, physicochemical properties, and ability to form complexes with Rh(III) ion. Polyhedron, 2022, 221, 115865.	1.0	3
87	Ab initio study of the energetics of molecular heteroconjugation reactions in systems modeling side chains of biomolecules. Computational and Theoretical Chemistry, 2004, 672, 183-190.	1.5	2
88	Potentiometric investigations of molecular heteroconjugation equilibria of substituted phenol+n-butylamine systems in dimethyl sulfoxide. Journal of Chemical Thermodynamics, 2005, 37, 778-782.	1.0	2
89	Molecular Heteroconjugation Equilibria in (n-ButylamineÂ+ÂAcetic Acid) Systems in Binary (Dimethyl) Tj ETQq1 1 0.784314 rgBT /Overlock 1.0	1.0	2
90	Computational (MP2 and DFT) modeling of the substrate/inhibitor interaction with the LDH active pocket in the gas phase and aqueous solution: bimolecular charged (pyruvate/oxamateâ€“guanidinium) Tj ETQq0 0 0 rgBT /Overlock 10 Chemistry, 2009, 22, 77-88.	0.9	2

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91	Physicochemical and electrochemical characteristics of pyrazine-2-thiocarboxamide and its interaction ability against biomolecules. Electrochimica Acta, 2021, 394, 139150.	2.6	2
92	Physics-Based Modeling of Side Chainâ€"Side Chain Interactions in the UNRES Force Field. Springer Series on Bio- and Neurosystems, 2019, , 89-115.	0.2	2
93	Modern Approach to Medical Diagnostics - the Use of Separation Techniques in Microorganisms Detection. Current Medicinal Chemistry, 2019, 26, 121-165.	1.2	2
94	Sensors to the Diagnostic Assessment of Anticancer and Antimicrobial Therapies Effectiveness by Drugs a with Pyrazine Scaffold. Chemosensors, 2022, 10, 24.	1.8	2
95	Influence of Temperature and Salt Concentration on the Hydrophobic Interactions of Adamantane and Hexane. Journal of Physical Chemistry B, 2022, 126, 634-642.	1.2	2
96	Low-Molecular Pyrazine-Based DNA Binders: Physicochemical and Antimicrobial Properties. Molecules, 2022, 27, 3704.	1.7	2
97	An ab initio study of the energetics of protonation of some N-Î²-d-glucopyranosylamine derivatives. Computational and Theoretical Chemistry, 2002, 579, 247-256.	1.5	1
98	Ab initio study of the energetics of asymmetric hydrogen bridge formation in substituted pyridines. Computational and Theoretical Chemistry, 2002, 587, 147-157.	1.5	1
99	Potentials of Mean Force of Two Hydrophobic Amino-Acid Side Chain Models Dependent on Orientation. AIP Conference Proceedings, 2007, , .	0.3	1
100	Physics-Based Modeling of Side Chain - Side Chain Interactions in the UNRES Force Field. Springer Series in Bio-/neuroinformatics, 2014, , 81-107.	0.1	1
101	When biomolecules meet 2-hydrazinopyrazine: from theory through experiment to molecular levels using a wide spectrum of techniques. RSC Advances, 2020, 10, 40673-40688.	1.7	1
102	A study of the energetics of asymmetric OHN+/NHO+ hydrogen bridge formation using ab initio methods. Computational and Theoretical Chemistry, 2003, 621, 149-155.	1.5	0
103	Determination of protolytic equilibria for methyl 3-azido-6-iodo-2,3,6-trideoxy-Î±-d-arabino-hexopyranoside by ab initio and spectrophotometric methods. Journal of Molecular Structure, 2008, 892, 140-145.	1.8	0
104	On the acid-base properties of pyrazine-2-thiocarboxamide and its complexes with Fe(II), Cu(II), Zn(II) and Ni(II) in polar solvents. Journal of Molecular Liquids, 2020, 311, 113349.	2.3	0