Mariusz Makowski

List of Publications by Year in Descending Order

102 papers	1,406 citations	21 h-index	32 g-index
105 ext. papers	1,586 ext. citations	3.8 avg, IF	4.47 L-index

#	Paper	IF	Citations
102	Sensors to the Diagnostic Assessment of Anticancer and Antimicrobial Therapies Effectiveness by Drugs a with Pyrazine Scaffold. *Chemosensors*, **2022**, 10, 24	4	
101	Modeling the Structure, Dynamics, and Transformations of Proteins with the UNRES Force Field. *Methods in Molecular Biology*, **2022**, 2376, 399-416	1.4	0
100	Study of the anticancer potential of Cd complexes of selenazoyl-hydrazones and their sulfur isosters.. *European Journal of Medicinal Chemistry*, **2022**, 238, 114449	6.8	0
99	Sulfonamides differing in the alkylamino substituent length Synthesis, electrochemical characteristic, acid-base profile and complexation properties. *Polyhedron*, **2022**, 221, 115868	2.7	1
98	Sulfonamides with hydroxyphenyl moiety: Synthesis, structure, physicochemical properties, and ability to form complexes with Rh(III) ion. *Polyhedron*, **2022**, 221, 115865	2.7	0
97	Recent advances in medicinal chemistry of ampicillin: Derivatives, metal complexes, and sensing approaches. *TrAC - Trends in Analytical Chemistry*, **2022**, 155, 116691	14.6	1
96	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,	6.3	3
95	What Can Electrochemical Methods Offer in Determining DNA-Drug Interactions?. *Molecules*, **2021**, 26,	4.8	5
94	Experimental and theoretical investigation of conformational states and noncovalent interactions in crystalline sulfonamides with a methoxyphenyl moiety. *CrystEngComm*, **2021**, 23, 6137-6162	3.3	7
93	Physicochemical and electrochemical characteristics of pyrazine-2-thiocarboxamide and its interaction ability against biomolecules. *Electrochimica Acta*, **2021**, 394, 139150	6.7	0
92	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	4	6
91	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	6	9
90	When biomolecules meet 2-hydrazinopyrazine: from theory through experiment to molecular levels using a wide spectrum of techniques.. *RSC Advances*, **2020**, 10, 40673-40688	3.7	0
89	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	6	
88	Influence of Ionic Strength on Hydrophobic Interactions in Water: Dependence on Solute Size and Shape. *Journal of Physical Chemistry B*, **2020**, 124, 10326-10336	3.4	8
87	Calculations of p Values of Selected Pyridinium and Its N-Oxide Ions in Water and Acetonitrile. *Journal of Physical Chemistry A*, **2020**, 124, 538-551	2.8	8
86	A comprehensive approach to the analysis of antibiotic-metal complexes. *TrAC - Trends in Analytical Chemistry*, **2020**, 123, 115771	14.6	14

85	Photosensitive and pH-dependent activity of pyrazine-functionalized carbazole derivative as promising antifungal and imaging agent. *Scientific Reports*, **2020**, 10, 11767	4.9	8
84	Influence of C–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	3.5	2
83	Introduction of Phosphorylated Residues into the UNRES Coarse-Grained Model: Toward Modeling of Signaling Processes. *Journal of Physical Chemistry B*, **2019**, 123, 5721-5729	3.4	9
82	Modern Approach to Medical Diagnostics - the Use of Separation Techniques in Microorganisms Detection. *Current Medicinal Chemistry*, **2019**, 26, 121-165	4.3	1
81	Physics-Based Modeling of Side Chain–Side Chain Interactions in the UNRES Force Field. *Springer Series on Bio- and Neurosystems*, **2019**, 89-115	0.5	2
80	Drug-like properties and complete physicochemical profile of pyrazine-2-amidoxime: A combined multi-experimental and computational studies. *Journal of Molecular Liquids*, **2019**, 276, 453-470	6	10
79	Metallopharmaceuticals in Therapy - A New Horizon for Scientific Research. *Current Medicinal Chemistry*, **2018**, 25, 1729-1791	4.3	13
78	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	2.8	3
77	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	3.9	31
76	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino Acid Side Chains in Water. VII. Charged-Hydrophobic/Polar and Polar-Hydrophobic/Polar Side Chains. *Journal of Physical Chemistry B*, **2017**, 121, 379-390	3.4	16
75	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	6	7
74	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	4.6	3
73	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	3.7	11
72	Experimental (FT-IR) and theoretical (DFT) studies on prototropy and H-bond formation for pyrazine-2-amidoxime. *Journal of Physical Organic Chemistry*, **2016**, 29, 326-335	2.1	8
71	Attractive S?□and □□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	3.4	15
70	Coordination chemistry of pyrazine derivatives analogues of PZA: design, synthesis, characterization and biological activity. *RSC Advances*, **2016**, 6, 52009-52025	3.7	15
69	Can Nitriles Be Stronger Bases Than Proton Sponges in the Gas Phase? A Computational Analysis. *Journal of Physical Chemistry A*, **2015**, 119, 8225-36	2.8	14
68	Theoretical Studies of Interactions between O-Phosphorylated and Standard Amino-Acid Side-Chain Models in Water. *Journal of Physical Chemistry B*, **2015**, 119, 8526-34	3.4	4

67	Geometric and energetic consequences of prototropy for adenine and its structural models review. *RSC Advances*, **2015**, 5, 36587-36604	3.7	39
66	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	1.6	6
65	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	2.1	10
64	Theoretical studies on the anionic association of phenol and its derivatives in acetonitrile. *Journal of Molecular Structure*, **2014**, 1076, 165-173	3.4	4
63	A unified coarse-grained model of biological macromolecules based on mean-field multipole-multipole interactions. *Journal of Molecular Modeling*, **2014**, 20, 2306	2	83
62	Geometric consequences of electron delocalization for adenine tautomers in aqueous solution. *Journal of Molecular Modeling*, **2014**, 20, 2234	2	11
61	Fluorescence quenching of fluoroquinolone antibiotics by 4-hydroxy-TEMPO in aqueous solution. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 133, 887-91	4.4	13
60	Coordination mode and reactivity of nickel(II) with vitamin B6. *Journal of Coordination Chemistry*, **2014**, 67, 2885-2897	1.6	6
59	Physics-Based Modeling of Side Chain - Side Chain Interactions in the UNRES Force Field. *Springer Series in Bio-/neuroinformatics*, **2014**, 81-107		1
58	Quantum-chemical studies on the favored and rare tautomers of neutral and redox adenine. *Journal of Physical Chemistry A*, **2013**, 117, 1548-59	2.8	41
57	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, 6844-53	3.4	7
56	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, 6130-7	3.4	29
55	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, 6119-29	3.4	23
54	Coarse-Grained Models of Proteins: Theory and Applications **2011**, 35-83		10
53	Potential of mean force of association of large hydrophobic particles: toward the nanoscale limit. *Journal of Physical Chemistry B*, **2010**, 114, 993-1003	3.4	73
52	Change of the favored routes of EI MS fragmentation when proceeding from N1, N1-dimethyl-N2-arylformamidines to 1,1,3,3-tetraalkyl-2-arylguanidines: substituent effects. *Journal of Mass Spectrometry*, **2010**, 45, 762-71	2.2	1
51	Importance of CH tautomers in the tautomeric mixture of uric acid. *Computational and Theoretical Chemistry*, **2010**, 947, 83-91		10
50	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, 547-52	1.9	20

49	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/oxamate–guanidinium cation) and neutral adducts (pyruvic/oxamic acids–guanidine). *Journal of Physical Organic Chemistry*, **2009**, 22, 77-88	2.1	2
48	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, 11385-95	3.4	34
47	Determination of protolytic equilibria for methyl 3-azido-6-iodo-2,3,6-trideoxy-α-d-arabino-hexopyranoside by ab initio and spectrophotometric methods. *Journal of Molecular Structure*, **2008**, 892, 140-145	3.4	
46	Simulation of Protein Structure and Dynamics with the Coarse-Grained UNRES Force Field **2008**, 107-122		4
45	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, 2910-6	3.4	21
44	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, 2925-31	3.4	30
43	Further evidence for the absence of polyproline II stretch in the XAO peptide. *Biophysical Journal*, **2007**, 92, 2904-17	2.9	49
42	Potential of mean force of hydrophobic association: dependence on solute size. *Journal of Physical Chemistry B*, **2007**, 111, 10765-74	3.4	54
41	Potentials of Mean Force of Two Hydrophobic Amino-Acid Side Chain Models Dependent on Orientation. *AIP Conference Proceedings*, **2007**,	0	1
40	Molecular Heteroconjugation Equilibria in (n-Butylamine + Acetic Acid) Systems in Binary (Dimethyl Sulfoxide + 1,4-Dioxane) Solvent Mixtures. *International Journal of Thermophysics*, **2007**, 28, 865-875	2.1	2
39	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	2.9	4
38	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	2.9	3
37	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, 2917-24	3.4	25
36	Potentiometric studies of acid–base interactions in substituted 4-nitropyridine N-oxide systems. *Journal of Chemical Thermodynamics*, **2006**, 38, 554-558	2.9	4
35	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	2.9	7
34	Assessment of two theoretical methods to estimate potentiometric titration curves of peptides: comparison with experiment. *Journal of Physical Chemistry B*, **2006**, 110, 4451-8	3.4	15
33	Potentiometric and ab initio studies of acid–base interactions of substituted 4-halo(Cl, Br)pyridine N-oxide systems. *Journal of Chemical Thermodynamics*, **2006**, 38, 1584-1591	2.9	8
32	Determination of the protonation and deprotonation centres for isomers of methyl 3-azido-2,3-dideoxyhexopyranosides. *Computational and Theoretical Chemistry*, **2005**, 714, 1-6		9

31	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		7
30	Theoretical studies on acid-base interactions in the substituted 4-nitropyridines and their N-oxides systems. *Computational and Theoretical Chemistry*, **2005**, 731, 193-199		3
29	Ab initio studies of acid–base reactions in the substituted 4-nitropyridine N-oxide systems. *Computational and Theoretical Chemistry*, **2005**, 756, 1-9		4
28	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, 235-42	3.5	8
27	Potentiometric investigations of molecular heteroconjugation equilibria of substituted phenol+n-butylamine systems in dimethyl sulfoxide. *Journal of Chemical Thermodynamics*, **2005**, 37, 778-782	2.9	2
26	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	2.9	3
25	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	6.3	38
24	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, 7547-52	11.5	120
23	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		2
22	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		4
21	Ab Initio Studies on Acid–Base Equilibria of Substituted Phenols. *Journal of Physical Chemistry A*, **2004**, 108, 10354-10358	2.8	12
20	Theoretical Calculations of Heteroconjugation Equilibrium Constants in Systems Modeling Acid–Base Interactions in Side Chains of Biomolecules Using the Potential of Mean Force. *Journal of Physical Chemistry B*, **2004**, 108, 12222-12230	3.4	13
19	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	3.4	29
18	A potentiometric study of acid–base properties of the (phenol+phenolate) systems in acetonitrile and, (acetonitrile+cyclohexane) solvent system. *Journal of Chemical Thermodynamics*, **2003**, 35, 77-89	2.9	19
17	Potentiometric investigation of acid dissociation and anionic homoconjugation equilibria of substituted phenols in dimethyl sulfoxide. *Journal of Chemical Thermodynamics*, **2003**, 35, 1645-1655	2.9	10
16	A study of the energetics of asymmetric OHN+/NHO+ hydrogen bridge formation using ab initio methods. *Computational and Theoretical Chemistry*, **2003**, 621, 149-155		
15	Ab initio study 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	2.1	28
14	Experimental and Theoretical Studies of Acid–Base Equilibria of Substituted 4-Nitropyridine N-Oxides. *Journal of Physical Chemistry A*, **2003**, 107, 6293-6300	2.8	20

13	An ab initio study of the energetics of protonation of some N-□-glucopyranosylamine derivatives. *Computational and Theoretical Chemistry*, **2002**, 579, 247-256		1
12	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	2.9	12
11	Ab initio study of the energetics of asymmetric hydrogen bridge formation in substituted pyridines. *Computational and Theoretical Chemistry*, **2002**, 587, 147-157		1
10	Tautomerism of neutral and monoprotonated histamine□ comparison of semi-empirical and ab initio quantum mechanical predictions for □essential□and □scorpio□conformations. *Journal of Physical Organic Chemistry*, **2001**, 14, 770-777	2.1	9
9	The Azatriquinenamine Trimer-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*	16.4	8
8	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		3
7	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	2.8	8
6	A study of the tendency of organic bases towards cationic heteroconjugation in polar non-aqueous solvents. *Perkin Transactions II RSC*, **2001**, 1844-1849		7
5	Ab Initio Study of Possible and Preferred Basic Site(s) in Polyfunctional N1,N1-Dimethyl-N2-cyanoformamidine. *Journal of Physical Chemistry A*, **2001**, 105, 869-874	2.8	27
4	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	2.8	24
3	Acid□Base equilibria in systems involving substituted pyridines in polar aprotic protophobic media and in the amphiprotic methanol. *Analytica Chimica Acta*, **2000**, 418, 233-240	6.6	30
2	Acid□Base and hydrogen-bonding equilibria in aliphatic amine and carboxylic acid systems in non-aqueous solutions. *Analytica Chimica Acta*, **1999**, 401, 317-321	6.6	33
1	Ab Initio Study of Energetics of Protonation and Hydrogen Bonding of Pyridine N-Oxide and Its Derivatives. *Journal of Physical Chemistry A*, **1999**, 103, 11104-11108	2.8	25