Wojciech Plazinski

List of Publications by Year in Descending Order

87 papers	2,310 citations	21 h-index	46 g-index
93 ext. papers	2,669 ext. citations	4.8 avg, IF	5.69 L-index

#	Paper	IF	Citations
87	Adsorption of hyaluronan saccharides on the surface of a single walled carbon nanotube. A computational study. *Applied Surface Science*, **2022**, 584, 152599	6.7	0
86	The Val34Met, Thr164Ile and Ser220Cys Polymorphisms of the β2-Adrenergic Receptor and Their Consequences on the Receptor Conformational Features: A Molecular Dynamics Simulation Study. *International Journal of Molecular Sciences*, **2022**, 23, 5449	6.3	
85	Chitosan characteristics in electrolyte solutions: Combined molecular dynamics modeling and slender body hydrodynamics. *Carbohydrate Polymers*, **2022**, 119676	10.3	0
84	Aggregation and weak gel formation by pectic polysaccharide homogalacturonan. *Carbohydrate Polymers*, **2021**, 256, 117566	10.3	6
83	Comparison of Carbohydrate Force Fields in Molecular Dynamics Simulations of Protein-Carbohydrate Complexes. *Journal of Chemical Theory and Computation*, **2021**, 17, 2575-2585	6.4	4
82	Polymers Sorption Properties towards Photosynthetic Pigments and Fungicides. *Materials*, **2021**, 14,	3.5	1
81	Combinations of Piperine with Hydroxypropyl-β-Cyclodextrin as a Multifunctional System. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
80	Macroion molecule properties from slender body hydrodynamics. *Polymers for Advanced Technologies*, **2021**, 32, 3900-3908	3.2	1
79	Effect of the dichloro-substitution on antiproliferative activity of phthalimide-thiazole derivatives. Rational design, synthesis, elastase, caspase 3/7, and EGFR tyrosine kinase activity and molecular modeling study. *Bioorganic Chemistry*, **2021**, 110, 104819	5.1	7
78	Molecular Structure of Cefuroxime Axetil Complexes with α-, β-, γ- and 2-Hydroxypropyl-β-Cyclodextrins: Molecular Simulations and Raman Spectroscopic and Imaging Studies. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	6
77	Tautomers of N-acetyl-d-allosamine: an NMR and computational chemistry study. *Organic and Biomolecular Chemistry*, **2021**, 19, 7190-7201	3.9	2
76	Novel 2-(Adamantan-1-ylamino)Thiazol-4(5)-One Derivatives and Their Inhibitory Activity towards 11β-HSD1-Synthesis, Molecular Docking and In Vitro Studies. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
75	Conformational Properties of Glycosaminoglycan Disaccharides: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2021**, 125, 10900-10916	3.4	6
74	Carrageenan molecule conformations and electrokinetic properties in electrolyte solutions: Modeling and experimental measurements. *Food Hydrocolloids*, **2021**, 121, 107033	10.6	1
73	Efficient sampling of high-energy states by machine learning force fields. *Physical Chemistry Chemical Physics*, **2020**, 22, 14364-14374	3.6	2
72	Conformational properties of inulin, levan and arabinan studied by molecular dynamics simulations. *Carbohydrate Polymers*, **2020**, 240, 116266	10.3	3
71	Tedizolid-Cyclodextrin System as Delayed-Release Drug Delivery with Antibacterial Activity. *International Journal of Molecular Sciences*, **2020**, 22,	6.3	6

70	Conformations of saturated five-membered heterocycles evaluated by MP2 calculations. *Chemistry of Heterocyclic Compounds*, **2020**, 56, 1599-1604	1.4	4
69	The endo- and exo-Anomeric Effects in Furanosides. A Computational Study. *European Journal of Organic Chemistry*, **2020**, 2020, 674-679	3.2	8
68	Resolving the nanostructure of sodium carbonate extracted pectins (DASP) from apple cell walls with atomic force microscopy and molecular dynamics. *Food Hydrocolloids*, **2020**, 104, 105726	10.6	17
67	Sorption of Heavy Metal Ions of Chromium, Manganese, Selenium, Nickel, Cobalt, Iron from Aqueous Acidic Solutions in Batch and Dynamic Conditions on Natural and Synthetic Aluminosilicate Sorbents. *Materials*, **2020**, 13,	3.5	10
66	Tropinone-Derived Alkaloids as Potent Anticancer Agents: Synthesis, Tyrosinase Inhibition, Mechanism of Action, DFT Calculation, and Molecular Docking Studies. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	5
65	Chirality Effects in Biomolecular Systems: Calculation of the Relative Free Energies by Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2020**, 60, 5424-5436	6.1	1
64	Dissipative particle dynamics model of homogalacturonan based on molecular dynamics simulations. *Scientific Reports*, **2020**, 10, 14691	4.9	8
63	Deciphering the conformational preferences of furanosides. A molecular dynamics study. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 3359-3370	3.6	3
62	Thermodynamic study of new antiepileptic compounds by combining chromatography on the phosphatidylcholine biomimetic stationary phase and differential scanning calorimetry. *Journal of Separation Science*, **2019**, 42, 2628-2639	3.4	3
61	HPLC-DAD Determination of Nitrite and Nitrate in Human Saliva Utilizing a Phosphatidylcholine Column. *Molecules*, **2019**, 24,	4.8	11
60	Synthesis of the N-methyl Derivatives of 2-Aminothiazol-4(5H)-one and Their Interactions with 11βHSD1-Molecular Modeling and in Vitro Studies. *Chemistry and Biodiversity*, **2019**, 16, e1900065	2.5	3
59	Relation between the NMR data and the pseudorotational free-energy profile for oxolane. *Journal of Theoretical and Computational Chemistry*, **2019**, 18, 1950012	1.8	2
58	The systematic influence of solvent on the conformational features of furanosides. *Organic and Biomolecular Chemistry*, **2019**, 17, 2479-2485	3.9	10
57	Benzo[b]thiophene-thiazoles as potent anti-Toxoplasma gondii agents: Design, synthesis, tyrosinase/tyrosine hydroxylase inhibitors, molecular docking study, and antioxidant activity. *European Journal of Medicinal Chemistry*, **2019**, 184, 111765	6.8	15
56	Tautomeric and epimeric equilibria of aldo- and ketohexoses studied by the MD simulations and QM calculations. *Carbohydrate Research*, **2019**, 474, 8-15	2.9	2
55	A GROMOS Force Field for Furanose-Based Carbohydrates. *Journal of Chemical Theory and Computation*, **2019**, 15, 1168-1186	6.4	18
54	A novel derivatives of thiazol-4(5H)-one and their activity in the inhibition of 11βhydroxysteroid dehydrogenase type 1. *Bioorganic Chemistry*, **2018**, 79, 115-121	5.1	7
53	Extension of the GROMOS 56a6 Force Field for Charged, Protonated, and Esterified Uronates. *Journal of Physical Chemistry B*, **2018**, 122, 3696-3710	3.4	14

52	Force-induced structural changes in non-sulfated carrageenan based oligosaccharides - a theoretical study. *Soft Matter*, **2018**, 14, 6264-6277	3.6	4
51	Solid-phase extraction using octadecyl-bonded silica modified with photosynthetic pigments from Spinacia oleracea L. for the preconcentration of lead(II) ions from aqueous samples. *Journal of Separation Science*, **2018**, 41, 3129-3142	3.4	6
50	Pyranose ring puckering in aldopentoses, ketohexoses and deoxyaldohexoses. A molecular dynamics study. *Carbohydrate Research*, **2018**, 455, 62-70	2.9	10
49	Molecular dynamics simulations of hexopyranose ring distortion in different force fields. *Pure and Applied Chemistry*, **2017**, 89, 1283-1294	2.1	12
48	Stereoselective binding of agonists to the □adrenergic receptor: insights into molecular details and thermodynamics from molecular dynamics simulations. *Molecular BioSystems*, **2017**, 13, 910-920		6
47	Pyranose ring conformations in mono- and oligosaccharides: a combined MD and DFT approach. *Physical Chemistry Chemical Physics*, **2017**, 19, 20760-20772	3.6	12
46	Ligand-induced action of the W286 rotamer toggle switch in the □adrenergic receptor. *Physical Chemistry Chemical Physics*, **2017**, 20, 581-594	3.6	2
45	Acyclic forms of aldohexoses and ketohexoses in aqueous and DMSO solutions: conformational features studied using molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 9626-35	3.6	15
44	Ring inversion properties of 1-□, 1-□ and 1-□-linked hexopyranoses and their correlation with the conformation of glycosidic linkages. *Carbohydrate Research*, **2016**, 423, 43-8	2.9	9
43	Revision of the GROMOS 56A6(CARBO) force field: Improving the description of ring-conformational equilibria in hexopyranose-based carbohydrates chains. *Journal of Computational Chemistry*, **2016**, 37, 354-65	3.5	65
42	Binding of bivalent metal cations by □L-guluronate: insights from the DFT-MD simulations. *New Journal of Chemistry*, **2015**, 39, 3987-3994	3.6	14
41	The water-catalyzed mechanism of the ring-opening reaction of glucose. *Physical Chemistry Chemical Physics*, **2015**, 17, 21622-9	3.6	15
40	Agonist binding by the □-adrenergic receptor: an effect of receptor conformation on ligand association-dissociation characteristics. *European Biophysics Journal*, **2015**, 44, 149-63	1.9	9
39	Kinetic characteristics of conformational changes in the hexopyranose rings. *Carbohydrate Research* , **2015**, 416, 41-50	2.9	8
38	The influence of the hexopyranose ring geometry on the conformation of glycosidic linkages investigated using molecular dynamics simulations. *Carbohydrate Research*, **2015**, 415, 17-27	2.9	22
37	Fast, metadynamics-based method for prediction of the stereochemistry-dependent relative free energies of ligand-receptor interactions. *Journal of Computational Chemistry*, **2014**, 35, 876-82	3.5	10
36	The dynamics of the conformational changes in the hexopyranose ring: a transition path sampling approach. *RSC Advances*, **2014**, 4, 25028-25039	3.7	14
35	Binding of heavy metals by algal biosorbents. Theoretical models of kinetics, equilibria and thermodynamics. *Advances in Colloid and Interface Science*, **2013**, 197-198, 58-67	14.3	45

34	Calcium-L-guluronate complexes: Ca2+ binding modes from DFT-MD simulations. *Journal of Physical Chemistry B*, **2013**, 117, 12105-12	3.4	22
33	Modeling of sorption kinetics: the pseudo-second order equation and the sorbate intraparticle diffusivity. *Adsorption*, **2013**, 19, 1055-1064	2.6	151
32	Equilibrium and kinetic modeling of metal ion biosorption: on the ways of model generalization for the case of multicomponent systems. *Adsorption*, **2013**, 19, 659-666	2.6	6
31	The 'order-to-disorder' conformational transition in CD44 protein: an umbrella sampling analysis. *Journal of Molecular Graphics and Modelling*, **2013**, 45, 122-7	2.8	8
30	Sorption of metal cations by alginate-based biosorbents. On the correct determination of the thermodynamic parameters. *Journal of Colloid and Interface Science*, **2012**, 368, 547-51	9.3	10
29	Sorption of lead, copper, and cadmium by calcium alginate. Metal binding stoichiometry and the pH effect. *Environmental Science and Pollution Research*, **2012**, 19, 3516-24	5.1	25
28	Conformational properties of acidic oligo- and disaccharides and their ability to bind calcium: a molecular modeling study. *Carbohydrate Research*, **2012**, 357, 111-7	2.9	10
27	Interactions between CD44 protein and hyaluronan: insights from the computational study. *Molecular BioSystems*, **2012**, 8, 543-7		21
26	Thermodynamic aspects of calcium binding by poly(L-guluronate) chains. A molecular simulation study. *Applied Surface Science*, **2012**, 262, 153-155	6.7	9
25	Molecular modeling of Ca2+-oligo(L-guluronate) complexes: toward the understanding of the junction zone structure in calcium alginate gels. *Structural Chemistry*, **2012**, 23, 1409-1415	1.8	22
24	The dynamics of the calcium-induced chain-chain association in the polyuronate systems. *Journal of Computational Chemistry*, **2012**, 33, 1709-15	3.5	10
23	Molecular basis of calcium binding by polyguluronate chains. Revising the egg-box model. *Journal of Computational Chemistry*, **2011**, 32, 2988-95	3.5	72
22	Molecular dynamics study of the interactions between phenolic compounds and alginate/alginic acid chains. *New Journal of Chemistry*, **2011**, 35, 1607	3.6	10
21	Biosorption of Heavy Metal Ions: Ion-Exchange versus Adsorption and the Heterogeneity of Binding Sites. *Adsorption Science and Technology*, **2011**, 29, 479-486	3.6	5
20	Statistical Rate Theory Approach to Description of the pH-Dependent Kinetics of Metal Ion Adsorption. *Journal of Physical Chemistry C*, **2010**, 114, 9952-9954	3.8	5
19	A novel two-resistance model for description of the adsorption kinetics onto porous particles. *Langmuir*, **2010**, 26, 802-8	4	19
18	Heavy metals binding to biosorbents. Insights into Non-competitive models from a simple pH-dependent model. *Colloids and Surfaces B: Biointerfaces*, **2010**, 80, 133-7	6	5
17	How does mechanism of biosorption determine the differences between the initial and equilibrium adsorption states?. *Adsorption*, **2010**, 16, 351-357	2.6	11

16	Binding stoichiometry in sorption of divalent metal ions: a theoretical analysis based on the ion-exchange model. *Journal of Colloid and Interface Science*, **2010**, 344, 165-70	9.3	10
15	Applicability of the film-diffusion model for description of the adsorption kinetics at the solid/solution interfaces. *Applied Surface Science*, **2010**, 256, 5157-5163	6.7	25
14	On the applicability of the pseudo-second order equation to represent the kinetics of adsorption at solid/solution interfaces: a theoretical analysis based on the statistical rate theory. *Adsorption*, **2009**, 15, 181-192	2.6	87
13	Theoretical models of sorption kinetics including a surface reaction mechanism: a review. *Advances in Colloid and Interface Science*, **2009**, 152, 2-13	14.3	589
12	Modeling the effect of surface heterogeneity in equilibrium of heavy metal ion biosorption by using the ion exchange model. *Environmental Science & Technology*, **2009**, 43, 7465-71	10.3	38
11	Modeling the effect of pH on kinetics of heavy metal ion biosorption. A theoretical approach based on the statistical rate theory. *Langmuir*, **2009**, 25, 298-304	4	21
10	Kinetics of Adsorption at Solid/Solution Interfaces Controlled by Intraparticle Diffusion: A Theoretical Analysis. *Journal of Physical Chemistry C*, **2009**, 113, 12495-12501	3.8	47
9	Kinetics of dyes adsorption at the solid-solution interfaces: a theoretical description based on the two-step kinetic model. *Environmental Science & Technology*, **2008**, 42, 2470-5	10.3	56
8	Kinetics of solute adsorption at solid/aqueous interfaces: searching for the theoretical background of the modified pseudo-first-order kinetic equation. *Langmuir*, **2008**, 24, 5393-9	4	44
7	Kinetics of solute adsorption at solid/solution interfaces: on the special features of the initial adsorption kinetics. *Langmuir*, **2008**, 24, 6738-44	4	38
6	Kinetics of metal ions adsorption at heterogeneous solid/solution interfaces: A theoretical treatment based on statistical rate theory. *Journal of Colloid and Interface Science*, **2008**, 327, 36-43	9.3	17
5	Studies of the Kinetics of Solute Adsorption at Solid/Solution Interfaces: On the Possibility of Distinguishing between the Diffusional and the Surface Reaction Kinetic Models by Studying the Pseudo-First-order Kinetics. *Journal of Physical Chemistry C*, **2007**, 111, 15100-15110	3.8	97
4	Reply to Comment on Kinetics of Solute Adsorption at Solid/Solution Interfaces: A Theoretical Development of the Empirical Pseudo-First and Pseudo-Second Order Kinetic Rate Equations, Based on Applying the Statistical Rate Theory of Interfacial Transport *Journal of Physical Chemistry B*, **2007**, 111, 319-319	3.4	3
3	Theoretical description of the kinetics of solute adsorption at heterogeneous solid/solution interfaces. *Applied Surface Science*, **2007**, 253, 5827-5840	6.7	88
2	Kinetics of solute adsorption at solid/solution interfaces: a theoretical development of the empirical pseudo-first and pseudo-second order kinetic rate equations, based on applying the statistical rate theory of interfacial transport. *Journal of Physical Chemistry B*, **2006**, 110, 16514-25	3.4	240
1	Kinetics of isothermal gas adsorption on heterogeneous solid surfaces: equations based on generalization of the statistical rate theory of interfacial transport. *Journal of Physical Chemistry B*, **2005**, 109, 21868-78	3.4	14