Jan Antosiewicz

List of Publications by Year
in descending order

93	4,191	172457 29	114465 63
papers	citations	h-index	g-index

108	108	108	2770
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Prediction of Ph-dependent Properties of Proteins. Journal of Molecular Biology, 1994, 238, 415-436.	4.2	807
2	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. Computer Physics Communications, 1995, 91, 57-95.	7.5	622
3	The Determinants of pKas in Proteins. Biochemistry, 1996, 35, 7819-7833.	2.5	439
4	Empirical relationships between protein structure and carboxyl pKa values in proteins. Proteins: Structure, Function and Bioinformatics, 2002, 48, 388-403.	2.6	191
5	UVâ€“Vis spectroscopy of tyrosine side-groups in studies of protein structure. Part 2: selected applications. Biophysical Reviews, 2016, 8, 163-177.	3.2	140
6	Computing ionization states of proteins with a detailed charge model. Journal of Computational Chemistry, 1996, 17, 1633-1644.	3.3	139
7	Chargeâ€“Charge Interactions are Key Determinants of the pK Values of Ionizable Groups in Ribonuclease Sa (pI=3.5) and a Basic Variant (pI=10.2). Journal of Molecular Biology, 2003, 325, 1077-1092.	4.2	96
8	Constant-pH molecular dynamics simulations: a test case of succinic acid. Chemical Physics, 2004, 302, 161-170.	1.9	76
9	Computation of the dipole moments of proteins. Biophysical Journal, 1995, 69, 1344-1354.	0.5	71
10	The nature of protein dipole moments: experimental and calculated permanent dipole of .alpha.-chymotrypsin. Biochemistry, 1989, 28, 10072-10078.	2.5	64
11	Simulation of charge-mutant acetylcholinesterases. Biochemistry, 1995, 34, 4211-4219.	2.5	63
12	Theoretical and Experimental Analysis of Ionization Equilibria in Ovomucoid Third Domainâ€. Biochemistry, 1998, 37, 8643-8652.	2.5	63
13	pKaMeasurements from Nuclear Magnetic Resonance for the B1 and B2 Immunoglobulin G-Binding Domains of Protein G:Â Comparison with Calculated Values for Nuclear Magnetic Resonance and X-ray Structuresâ€. Biochemistry, 1997, 36, 3580-3589.	2.5	62
14	Electrostatic and hydrodynamic orientational steering effects in enzyme-substrate association. Biophysical Journal, 1995, 69, 57-65.	0.5	60
15	Constant-pH molecular dynamics study of protonation-structure relationship in a heptapeptide derived from ovomucoid third domain. Physical Review E, 2004, 69, 021915.	2.1	58
16	Thermodynamic linkage between the binding of protons and inhibitors to HIVâ€1 protease. Protein Science, 1999, 8, 180-195.	7.6	55
17	Acetylcholinesterase: diffusional encounter rate constants for dumbbell models of ligand. Biophysical Journal, 1995, 68, 62-68.	0.5	54
18	On the Mechanism of Acetylcholinesterase Action:Â The Electrostatically Induced Acceleration of the Catalytic Acylation Step. Journal of the American Chemical Society, 1997, 119, 8159-8165.	13.7	53

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19	UVâ€“Vis spectroscopy of tyrosine side-groups in studies of protein structure. Part 1: basic principles and properties of tyrosine chromophore. Biophysical Reviews, 2016, 8, 151-161.	3.2	52
20	Volume correction for bead model simulations of rotational friction coefficients of macromolecules. The Journal of Physical Chemistry, 1989, 93, 5301-5305.	2.9	44
21	An unusual electrooptical effect observed for DNA fragments and its apparent relation to a permanent electric moment associated with bent DNA. Biophysical Chemistry, 1989, 33, 19-30.	2.8	42
22	Stopped-flow and Brownian dynamics studies of electrostatic effects in the kinetics of binding of 7-methyl-GpppG to the protein eIF4E. European Biophysics Journal, 2000, 29, 487-498.	2.2	42
23	Prediction of titration properties of structures of a protein derived from molecular dynamics trajectories. Protein Science, 1997, 6, 373-382.	7.6	40
24	8-Azapurines as isosteric purine fluorescent probes for nucleic acid and enzymatic research. Molecular BioSystems, 2014, 10, 2756-2774.	2.9	40
25	Orientational steering in enzyme-substrate association: Ionic strength dependence of hydrodynamic torque effects. European Biophysics Journal, 1996, 24, 137-41.	2.2	37
26	pK Values of Histidine Residues in Ribonuclease Sa: Effect of Salt and Net Charge. Journal of Molecular Biology, 2003, 325, 1093-1105.	4.2	37
27	Langevin dynamics of proteins at constantpH. Physical Review E, 2002, 66, 051911.	2.1	34
28	Biophysical Approach to Studies of Capâ€“eIF4E Interaction by Synthetic Cap Analogs. Methods in Enzymology, 2007, 430, 209-245.	1.0	33
29	Acetylcholinesterase: Role of the enzyme's charge distribution in steering charged ligands toward the active site. Biopolymers, 1996, 39, 85-94.	2.4	31
30	Electrostatics of hemoglobins from measurements of the electric dichroism and computer simulations. Biophysical Journal, 1995, 68, 655-664.	0.5	28
31	Acetylcholinesterase: Role of the enzyme's charge distribution in steering charged ligands toward the active site. Biopolymers, 1996, 39, 85-94.	2.4	28
32	Methyl esterification of m7G5â€²p reversibly blocks its activity as an analog of eukaryotic mRNA 5â€²-caps. Journal of Molecular Biology, 1981, 153, 451-458.	4.2	26
33	Prediction of Secondary Ionization of the Phosphate Group in Phosphotyrosine Peptides. Biophysical Journal, 2003, 84, 750-756.	0.5	24
34	Structure of the Tet repressor and Tet repressor-operator complexes in solution from electrooptical measurements and hydrodynamic simulations. Biochemistry, 1988, 27, 4674-4679.	2.5	23
35	Structure and dynamics of curved DNA fragments in solution: Evidence for slow modes of configurational transitions. Biophysical Chemistry, 1993, 47, 179-191.	2.8	23
36	Poissonâ€“Boltzmann continuum-solvation models: applications to pH-dependent properties of biomolecules. Molecular BioSystems, 2011, 7, 2923.	2.9	23

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37	Turn of Promotor DNA by cAMP Receptor Protein Characterized by Bead Model Simulation of Rotational Diffusion. Journal of Biomolecular Structure and Dynamics, 1988, 5, 819-837.	3.5	21
38	Acetylcholinesterase: Effects of Ionic Strength and Dimerization on the Rate Constants. Israel Journal of Chemistry, 1994, 34, 151-158.	2.3	21
39	Brownian dynamics simulation of electrooptical transients for complex macrodipoles. The Journal of Physical Chemistry, 1993, 97, 2767-2773.	2.9	20
40	Effects of Soluteâ˜'Solvent Proton Exchange on Polypeptide Chain Dynamics:Â A Constant-pH Molecular Dynamics Study. Journal of Physical Chemistry B, 2005, 109, 13777-13784.	2.6	19
41	Association of Aminoglycosidic Antibiotics with the Ribosomal A-Site Studied with Brownian Dynamics. Journal of Chemical Theory and Computation, 2008, 4, 549-559.	5.3	19
42	Permanent dipole moment of tRNA's and variation of their structure in solution. Biophysical Journal, 1990, 58, 403-411.	0.5	17
43	Brownian dynamics simulation of electrooptical transients for solutions of rigid macromolecules. Journal of Chemical Physics, 1991, 95, 1354-1360.	3.0	16
44	Evaluation of Proteinsâ€™ Rotational Diffusion Coefficients from Simulations of Their Free Brownian Motion in Volume-Occupied Environments. Journal of Chemical Theory and Computation, 2014, 10, 481-491.	5.3	16
45	Acetylcholinesterase: role of the enzyme's charge distribution in steering charged ligands toward the active site. Biopolymers, 1996, 39, 85-94.	2.4	16
46	Strong Effect of Hydrodynamic Coupling on the Electric Dichroism of Bent Rods. Journal of Physical Chemistry B, 2005, 109, 1034-1038.	2.6	14
47	Toward an Accurate Modeling of Hydrodynamic Effects on the Translational and Rotational Dynamics of Biomolecules in Many-Body Systems. Journal of Physical Chemistry B, 2015, 119, 8425-8439.	2.6	14
48	Brownian Dynamics of the Polarization of Rodlike Polyelectrolytes. The Journal of Physical Chemistry, 1994, 98, 10881-10887.	2.9	13
49	Ultrasonic studies on hydration of pyrimidine nucleosides in aqueous ethanolic solutions. The Journal of Physical Chemistry, 1982, 86, 4831-4834.	2.9	12
50	Contributions of Far-Field Hydrodynamic Interactions to the Kinetics of Electrostatically Driven Molecular Association. Journal of Physical Chemistry B, 2012, 116, 5437-5447.	2.6	12
51	Hydration of alcohols by ultrasonic velocity measurements in ternary systems. Journal of Solution Chemistry, 1984, 13, 493-503.	1.2	11
52	Towards the mechanism of trimeric purine nucleoside phosphorylases: Stopped-flow studies of binding of multisubstrate analogue inhibitor â€" 2-amino-9-[2-(phosphonomethoxy)ethyl]-6-sulfanylpurine. Biophysical Chemistry, 2007, 125, 260-268.	2.8	11
53	Simulation of electrostatic and hydrodynamic properties ofSerratia endonuclease. , 1997, 41, 443-450.		10
54	Poisson-Boltzmann model studies of molecular electrostatic properties of the cAMP-dependent protein kinase. European Biophysics Journal, 1999, 28, 457-467.	2.2	10

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55	Effects of pH on kinetics of binding of mRNA-cap analogs by translation initiation factor eIF4E. European Biophysics Journal, 2003, 31, 608-616.	2.2	10
56	Brownian Dynamics Simulations of Binding mRNA Cap Analogues to eIF4E Protein. Journal of Physical Chemistry B, 2007, 111, 13107-13115.	2.6	10
57	Hydrodynamic Effects on the Relative Rotational Velocity of Associating Proteins. Journal of Physical Chemistry B, 2013, 117, 6165-6174.	2.6	10
58	Simulation of pH-Dependent Properties of Proteins Using Mesoscopic Models. Reviews in Computational Chemistry, 2007, , 249-311.	1.5	9
59	Multiple Protonation Equilibria in Electrostatics of Proteinâ^'Protein Binding. Journal of Physical Chemistry B, 2008, 112, 15074-15085.	2.6	9
60	Brownian Dynamics of the Polarization of Rodlike Polyelectrolytes:â€‰ Anisotropy and the Effect of Hydrodynamic Interactions. Journal of Physical Chemistry B, 1997, 101, 4478-4484.	2.6	8
61	Ultrasonic Velocity Studies on Carbohydrates in Aqueous Ethanolic Solutions. Zeitschrift Fur Physikalische Chemie, 1986, 148, 185-195.	2.8	7
62	Helix-coil dynamics of a Z-helix hairpin. Biopolymers, 1988, 27, 1319-1327.	2.4	7
63	A procedure for analysis of stopped-flow transients for proteinâ€“ligand association. Journal of Proteomics, 2002, 51, 179-193.	2.4	7
64	Protonation free energy levels in complex molecular systems. Biopolymers, 2008, 89, 262-269.	2.4	7
65	Effects of Hydrodynamic Coupling on Electro-Optical Transients. Journal of Physical Chemistry B, 2009, 113, 13988-13992.	2.6	7
66	Effects of Hydrodynamic Interactions on the Near-Surface Diffusion of Spheroidal Molecules. ACS Omega, 2019, 4, 17016-17030.	3.5	7
67	Constant-pH Brownian Dynamics Simulations of a Protein near a Charged Surface. ACS Omega, 2020, 5, 30282-30298.	3.5	7
68	Dependence of ultrasonic velocity on structure in a homologous series of nonelectrolytes in aqueous medium. Journal of Solution Chemistry, 1983, 12, 123-133.	1.2	6
69	Hydration of alcohols in aqueous methanol solutions from ultrasonic velocity measurements. Journal of Solution Chemistry, 1983, 12, 783-789.	1.2	6
70	Electric moments of rodlike molecules due to asymmetry of ligand binding induced by electric fields. The Journal of Physical Chemistry, 1991, 95, 5983-5988.	2.9	6
71	Modes of rotational motion of wormlike chains and the effect of charges on electrooptical transients. Macromolecules, 1992, 25, 6500-6504.	4.8	6
72	Stopped-flow studies of guanine binding by calf spleen purine nucleoside phosphorylase. Biophysical Chemistry, 2005, 115, 67-76.	2.8	6

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73	Kinetics of binding the mRNA cap analogues to the translation initiation factor eIF4E under second-order reaction conditions. Biophysical Chemistry, 2007, 129, 289-297.	2.8	6
74	Transient Effects of Excluded Volume Interactions on the Translational Diffusion of Hydrodynamically Anisotropic Molecules. Journal of Chemical Theory and Computation, 2014, 10, 2583-2590.	5.3	6
75	The impact of protonation equilibria on protein structure. Journal of Physics Condensed Matter, 2005, 17, S1607-S1616.	1.8	5
76	Poissonâ€“Boltzmann model analysis of binding mRNA cap analogues to the translation initiation factor eIF4E. Biophysical Chemistry, 2009, 140, 16-23.	2.8	5
77	Anisotropic Diffusion Effects on the Barnaseâ€“Barstar Encounter Kinetics. Journal of Chemical Theory and Computation, 2013, 9, 1667-1677.	5.3	5
78	Binding of Cations and Protons in the Active Site of Acetylcholinesterase. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1995, , 25-37.	0.2	5
79	pH-Dependent Association of Proteins. The Test Case of Monoclonal Antibody HyHEL-5 and Its Antigen Hen Egg White Lysozyme. Journal of Physical Chemistry B, 2009, 113, 15662-15669.	2.6	4
80	Effects of Spatially Dependent Mobilities on the Kinetics of the Diffusion-Controlled Association Derived from the First-Passage-Time Approach. Journal of Physical Chemistry B, 2016, 120, 7114-7127.	2.6	4
81	Does Ionic Screening Lower Activation Barriers for Conformational Transitions in Proteins?. Journal of Physical Chemistry B, 2018, 122, 11817-11826.	2.6	4
82	Circular Dichroism Spectra of Î±-Chymotrypsinâ€“SDS Solutions Depend on the Procedure of Their Preparation. ACS Omega, 2022, 7, 23782-23789.	3.5	4
83	Hydrodynamic Steering in Protein Association Revisited: Surprisingly Minuscule Effects of Considerable Torques. Journal of Physical Chemistry B, 2017, 121, 8475-8491.	2.6	3
84	Resolving Differences in Substrate Specificities between Human and Parasite Phosphoribosyltransferases via Analysis of Functional Groups of Substrates and Receptors. Current Pharmaceutical Design, 2013, 19, 4226-4240.	1.9	3
85	Quasichemical interpretation of the ultrasonic velocity in ternary aqueous systems. Journal of Solution Chemistry, 1987, 16, 285-294.	1.2	2
86	pK_aâ€™s of Ionizable Groups and Energetics of Protein Conformational Transitions. Journal of Physical Chemistry B, 2010, 114, 1393-1406.	2.6	2
87	Diffusional Encounter Rate Constants for Xanthone and 2-Naphthoic Acid by Flash Photolysis Experiments and Brownian Dynamics Simulations: Substantial Effects of Polarizability of the Triplet State. Journal of Physical Chemistry B, 2019, 123, 9328-9342.	2.6	2
88	Searching for Hydrodynamic Orienting Effects in the Association of Tri-N-acetylglucosamine with Hen Egg-White Lysozyme. Journal of Physical Chemistry B, 2021, 125, 10701-10709.	2.6	2
89	Prediction of pKas of Titratable Residues in Proteins Using a Poisson-Boltzmann Model of the Solute-Solvent System. Lecture Notes in Computational Science and Engineering, 1999, , 176-196.	0.3	2
90	Kinetics of Binding of Multisubstrate Analogue Inhibitor (2-Amino-9-[2-(Phosphonomethoxy)Ethyl]-6-Sulfanylpurine) with Trimeric Purine Nucleoside Phosphorylase. Nucleosides, Nucleotides and Nucleic Acids, 2007, 26, 969-974.	1.1	0

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91	On the analysis of fluorimetric titration curves of purine nucleoside phosphorylase. Nucleic Acids Symposium Series, 2008, 52, 671-672.	0.3	0
92	HIV-1 Protease and its Inhibitors. , 1997, , 237-254.		0
93	Editorial: Intracellular Molecular Processes Affected by pH. Frontiers in Molecular Biosciences, 2022, 9, 891533.	3.5	0