

# Jan Antosiewicz

## List of Publications by Year in descending order

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93  
papers

4,191  
citations

172207

29  
h-index

114278

63  
g-index

108  
all docs

108  
docs citations

108  
times ranked

2770  
citing authors

#	ARTICLE	IF	CITATIONS
1	Prediction of Ph-dependent Properties of Proteins. <i>Journal of Molecular Biology</i> , 1994, 238, 415-436.	2.0	807
2	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. <i>Computer Physics Communications</i> , 1995, 91, 57-95.	3.0	622
3	The Determinants of pKas in Proteins. <i>Biochemistry</i> , 1996, 35, 7819-7833.	1.2	439
4	Empirical relationships between protein structure and carboxyl pKa values in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 48, 388-403.	1.5	191
5	UV-Vis spectroscopy of tyrosine side-groups in studies of protein structure. Part 2: selected applications. <i>Biophysical Reviews</i> , 2016, 8, 163-177.	1.5	140
6	Computing ionization states of proteins with a detailed charge model. <i>Journal of Computational Chemistry</i> , 1996, 17, 1633-1644.	1.5	139
7	Charge-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). <i>Journal of Molecular Biology</i> , 2003, 325, 1077-1092.	2.0	96
8	Constant-pH molecular dynamics simulations: a test case of succinic acid. <i>Chemical Physics</i> , 2004, 302, 161-170.	0.9	76
9	Computation of the dipole moments of proteins. <i>Biophysical Journal</i> , 1995, 69, 1344-1354.	0.2	71
10	The nature of protein dipole moments: experimental and calculated permanent dipole of .alpha.-chymotrypsin. <i>Biochemistry</i> , 1989, 28, 10072-10078.	1.2	64
11	Simulation of charge-mutant acetylcholinesterases. <i>Biochemistry</i> , 1995, 34, 4211-4219.	1.2	63
12	Theoretical and Experimental Analysis of Ionization Equilibria in Ovomuroid Third Domain. <i>Biochemistry</i> , 1998, 37, 8643-8652.	1.2	63
13	pKa Measurements from Nuclear Magnetic Resonance for the B1 and B2 Immunoglobulin G-Binding Domains of Protein G: A Comparison with Calculated Values for Nuclear Magnetic Resonance and X-ray Structures. <i>Biochemistry</i> , 1997, 36, 3580-3589.	1.2	62
14	Electrostatic and hydrodynamic orientational steering effects in enzyme-substrate association. <i>Biophysical Journal</i> , 1995, 69, 57-65.	0.2	60
15	Constant-pH molecular dynamics study of protonation-structure relationship in a heptapeptide derived from ovomucoid third domain. <i>Physical Review E</i> , 2004, 69, 021915.	0.8	58
16	Thermodynamic linkage between the binding of protons and inhibitors to HIV-1 protease. <i>Protein Science</i> , 1999, 8, 180-195.	3.1	55
17	Acetylcholinesterase: diffusional encounter rate constants for dumbbell models of ligand. <i>Biophysical Journal</i> , 1995, 68, 62-68.	0.2	54
18	On the Mechanism of Acetylcholinesterase Action: The Electrostatically Induced Acceleration of the Catalytic Acylation Step. <i>Journal of the American Chemical Society</i> , 1997, 119, 8159-8165.	6.6	53

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19	UV-Vis spectroscopy of tyrosine side-groups in studies of protein structure. Part 1: basic principles and properties of tyrosine chromophore. <i>Biophysical Reviews</i> , 2016, 8, 151-161.	1.5	52
20	Volume correction for bead model simulations of rotational friction coefficients of macromolecules. <i>The Journal of Physical Chemistry</i> , 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. <i>Biophysical Chemistry</i> , 1989, 33, 19-30.	1.5	42
22	Stopped-flow and Brownian dynamics studies of electrostatic effects in the kinetics of binding of 7-methyl-GpppG to the protein eIF4E. <i>European Biophysics Journal</i> , 2000, 29, 487-498.	1.2	42
23	Prediction of titration properties of structures of a protein derived from molecular dynamics trajectories. <i>Protein Science</i> , 1997, 6, 373-382.	3.1	40
24	8-Azapurines as isosteric purine fluorescent probes for nucleic acid and enzymatic research. <i>Molecular BioSystems</i> , 2014, 10, 2756-2774.	2.9	40
25	Orientational steering in enzyme-substrate association: Ionic strength dependence of hydrodynamic torque effects. <i>European Biophysics Journal</i> , 1996, 24, 137-41.	1.2	37
26	pK Values of Histidine Residues in Ribonuclease Sa: Effect of Salt and Net Charge. <i>Journal of Molecular Biology</i> , 2003, 325, 1093-1105.	2.0	37
27	Langevin dynamics of proteins at constant pH. <i>Physical Review E</i> , 2002, 66, 051911.	0.8	34
28	Biophysical Approach to Studies of Cap-eIF4E Interaction by Synthetic Cap Analogs. <i>Methods in Enzymology</i> , 2007, 430, 209-245.	0.4	33
29	Acetylcholinesterase: Role of the enzyme's charge distribution in steering charged ligands toward the active site. <i>Biopolymers</i> , 1998, 39, 85-94.	1.2	31
30	Electrostatics of hemoglobins from measurements of the electric dichroism and computer simulations. <i>Biophysical Journal</i> , 1995, 68, 655-664.	0.2	28
31	Acetylcholinesterase: Role of the enzyme's charge distribution in steering charged ligands toward the active site. , 1996, 39, 85.		28
32	Methyl esterification of m7G5'p reversibly blocks its activity as an analog of eukaryotic mRNA 5'-caps. <i>Journal of Molecular Biology</i> , 1981, 153, 451-458.	2.0	26
33	Prediction of Secondary Ionization of the Phosphate Group in Phosphotyrosine Peptides. <i>Biophysical Journal</i> , 2003, 84, 750-756.	0.2	24
34	Structure of the Tet repressor and Tet repressor-operator complexes in solution from electrooptical measurements and hydrodynamic simulations. <i>Biochemistry</i> , 1988, 27, 4674-4679.	1.2	23
35	Structure and dynamics of curved DNA fragments in solution: Evidence for slow modes of configurational transitions. <i>Biophysical Chemistry</i> , 1993, 47, 179-191.	1.5	23
36	Poisson-Boltzmann continuum-solvation models: applications to pH-dependent properties of biomolecules. <i>Molecular BioSystems</i> , 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. <i>Journal of Biomolecular Structure and Dynamics</i> , 1988, 5, 819-837.	2.0	21
38	Acetylcholinesterase: Effects of Ionic Strength and Dimerization on the Rate Constants. <i>Israel Journal of Chemistry</i> , 1994, 34, 151-158.	1.0	21
39	Brownian dynamics simulation of electrooptical transients for complex macrodipoles. <i>The Journal of Physical Chemistry</i> , 1993, 97, 2767-2773.	2.9	20
40	Effects of Solute-Solvent Proton Exchange on Polypeptide Chain Dynamics: A Constant-pH Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 13777-13784.	1.2	19
41	Association of Aminoglycosidic Antibiotics with the Ribosomal A-Site Studied with Brownian Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 549-559.	2.3	19
42	Permanent dipole moment of tRNA's and variation of their structure in solution. <i>Biophysical Journal</i> , 1990, 58, 403-411.	0.2	17
43	Brownian dynamics simulation of electrooptical transients for solutions of rigid macromolecules. <i>Journal of Chemical Physics</i> , 1991, 95, 1354-1360.	1.2	16
44	Evaluation of Proteins' Rotational Diffusion Coefficients from Simulations of Their Free Brownian Motion in Volume-Occupied Environments. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 481-491.	2.3	16
45	Acetylcholinesterase: role of the enzyme's charge distribution in steering charged ligands toward the active site. <i>Biopolymers</i> , 1996, 39, 85-94.	1.2	16
46	Strong Effect of Hydrodynamic Coupling on the Electric Dichroism of Bent Rods. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1034-1038.	1.2	14
47	Toward an Accurate Modeling of Hydrodynamic Effects on the Translational and Rotational Dynamics of Biomolecules in Many-Body Systems. <i>Journal of Physical Chemistry B</i> , 2015, 119, 8425-8439.	1.2	14
48	Brownian Dynamics of the Polarization of Rodlike Polyelectrolytes. <i>The Journal of Physical Chemistry</i> , 1994, 98, 10881-10887.	2.9	13
49	Ultrasonic studies on hydration of pyrimidine nucleosides in aqueous ethanolic solutions. <i>The Journal of Physical Chemistry</i> , 1982, 86, 4831-4834.	2.9	12
50	Contributions of Far-Field Hydrodynamic Interactions to the Kinetics of Electrostatically Driven Molecular Association. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5437-5447.	1.2	12
51	Hydration of alcohols by ultrasonic velocity measurements in ternary systems. <i>Journal of Solution Chemistry</i> , 1984, 13, 493-503.	0.6	11
52	Towards the mechanism of trimeric purine nucleoside phosphorylases: Stopped-flow studies of binding of multisubstrate analogue inhibitor 2-amino-9-[2-(phosphonomethoxy)ethyl]-6-sulfanylpurine. <i>Biophysical Chemistry</i> , 2007, 125, 260-268.	1.5	11
53	Simulation of electrostatic and hydrodynamic properties of Serratia endonuclease. , 1997, 41, 443-450.		10
54	Poisson-Boltzmann model studies of molecular electrostatic properties of the cAMP-dependent protein kinase. <i>European Biophysics Journal</i> , 1999, 28, 457-467.	1.2	10

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55	Effects of pH on kinetics of binding of mRNA-cap analogs by translation initiation factor eIF4E. <i>European Biophysics Journal</i> , 2003, 31, 608-616.	1.2	10
56	Brownian Dynamics Simulations of Binding mRNA Cap Analogues to eIF4E Protein. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13107-13115.	1.2	10
57	Hydrodynamic Effects on the Relative Rotational Velocity of Associating Proteins. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6165-6174.	1.2	10
58	Simulation of pH-Dependent Properties of Proteins Using Mesoscopic Models. <i>Reviews in Computational Chemistry</i> , 2007, , 249-311.	1.5	9
59	Multiple Protonation Equilibria in Electrostatics of Protein-Protein Binding. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15074-15085.	1.2	9
60	Brownian Dynamics of the Polarization of Rodlike Polyelectrolytes: Anisotropy and the Effect of Hydrodynamic Interactions. <i>Journal of Physical Chemistry B</i> , 1997, 101, 4478-4484.	1.2	8
61	Ultrasonic Velocity Studies on Carbohydrates in Aqueous Ethanolic Solutions. <i>Zeitschrift Fur Physikalische Chemie</i> , 1986, 148, 185-195.	1.4	7
62	Helix-coil dynamics of a Z-helix hairpin. <i>Biopolymers</i> , 1988, 27, 1319-1327.	1.2	7
63	A procedure for analysis of stopped-flow transients for protein-ligand association. <i>Journal of Proteomics</i> , 2002, 51, 179-193.	2.4	7
64	Protonation free energy levels in complex molecular systems. <i>Biopolymers</i> , 2008, 89, 262-269.	1.2	7
65	Effects of Hydrodynamic Coupling on Electro-Optical Transients. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13988-13992.	1.2	7
66	Effects of Hydrodynamic Interactions on the Near-Surface Diffusion of Spheroidal Molecules. <i>ACS Omega</i> , 2019, 4, 17016-17030.	1.6	7
67	Constant-pH Brownian Dynamics Simulations of a Protein near a Charged Surface. <i>ACS Omega</i> , 2020, 5, 30282-30298.	1.6	7
68	Dependence of ultrasonic velocity on structure in a homologous series of nonelectrolytes in aqueous medium. <i>Journal of Solution Chemistry</i> , 1983, 12, 123-133.	0.6	6
69	Hydration of alcohols in aqueous methanol solutions from ultrasonic velocity measurements. <i>Journal of Solution Chemistry</i> , 1983, 12, 783-789.	0.6	6
70	Electric moments of rodlike molecules due to asymmetry of ligand binding induced by electric fields. <i>The Journal of Physical Chemistry</i> , 1991, 95, 5983-5988.	2.9	6
71	Modes of rotational motion of wormlike chains and the effect of charges on electrooptical transients. <i>Macromolecules</i> , 1992, 25, 6500-6504.	2.2	6
72	Stopped-flow studies of guanine binding by calf spleen purine nucleoside phosphorylase. <i>Biophysical Chemistry</i> , 2005, 115, 67-76.	1.5	6

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73	Kinetics of binding the mRNA cap analogues to the translation initiation factor eIF4E under second-order reaction conditions. <i>Biophysical Chemistry</i> , 2007, 129, 289-297.	1.5	6
74	Transient Effects of Excluded Volume Interactions on the Translational Diffusion of Hydrodynamically Anisotropic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2583-2590.	2.3	6
75	The impact of protonation equilibria on protein structure. <i>Journal of Physics Condensed Matter</i> , 2005, 17, S1607-S1616.	0.7	5
76	Poisson-Boltzmann model analysis of binding mRNA cap analogues to the translation initiation factor eIF4E. <i>Biophysical Chemistry</i> , 2009, 140, 16-23.	1.5	5
77	Anisotropic Diffusion Effects on the Barnase-Barstar Encounter Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1667-1677.	2.3	5
78	Binding of Cations and Protons in the Active Site of Acetylcholinesterase. <i>Jerusalem Symposia on Quantum Chemistry and Biochemistry</i> , 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. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15662-15669.	1.2	4
80	Effects of Spatially Dependent Mobilities on the Kinetics of the Diffusion-Controlled Association Derived from the First-Passage-Time Approach. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7114-7127.	1.2	4
81	Does Ionic Screening Lower Activation Barriers for Conformational Transitions in Proteins?. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11817-11826.	1.2	4
82	Circular Dichroism Spectra of $\hat{\pm}$ -Chymotrypsin SDS Solutions Depend on the Procedure of Their Preparation. <i>ACS Omega</i> , 2022, 7, 23782-23789.	1.6	4
83	Hydrodynamic Steering in Protein Association Revisited: Surprisingly Minuscule Effects of Considerable Torques. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8475-8491.	1.2	3
84	Resolving Differences in Substrate Specificities between Human and Parasite Phosphoribosyltransferases via Analysis of Functional Groups of Substrates and Receptors. <i>Current Pharmaceutical Design</i> , 2013, 19, 4226-4240.	0.9	3
85	Quasichemical interpretation of the ultrasonic velocity in ternary aqueous systems. <i>Journal of Solution Chemistry</i> , 1987, 16, 285-294.	0.6	2
86	$pK_a$ 's of Ionizable Groups and Energetics of Protein Conformational Transitions. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1393-1406.	1.2	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. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9328-9342.	1.2	2
88	Searching for Hydrodynamic Orienting Effects in the Association of Tri-N-acetylglucosamine with Hen Egg-White Lysozyme. <i>Journal of Physical Chemistry B</i> , 2021, 125, 10701-10709.	1.2	2
89	Prediction of pKas of Titratable Residues in Proteins Using a Poisson-Boltzmann Model of the Solute-Solvent System. <i>Lecture Notes in Computational Science and Engineering</i> , 1999, , 176-196.	0.1	2
90	Kinetics of Binding of Multisubstrate Analogue Inhibitor (2-Amino-9-[2-(Phosphonomethoxy)Ethyl]-6-Sulfanylpurine) with Trimeric Purine Nucleoside Phosphorylase. <i>Nucleosides, Nucleotides and Nucleic Acids</i> , 2007, 26, 969-974.	0.4	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.	1.6	0