Jacek Czub

List of Publications by Year
in descending order

61 papers	1,302 citations	361413 20 h-index	395702 33 g-index
65 all docs	65 docs citations	65 times ranked	1811 citing authors

#	Article	IF	Citations
1	Comparative Molecular Dynamics Study of Lipid Membranes Containing Cholesterol and Ergosterol. Biophysical Journal, 2006, 90, 2368-2382.	0.5	153
2	How Do Sterols Determine the Antifungal Activity of Amphotericin B? Free Energy of Binding between the Drug and Its Membrane Targets. Journal of the American Chemical Society, 2010, 132, 18266-18272.	13.7	71
3	Molecular modelling of membrane activity of amphotericin B, a polyene macrolide antifungal antibiotic.. Acta Biochimica Polonica, 2019, 52, 655-658.	0.5	69
4	Localization and Orientation of Xanthophylls in a Lipid Bilayer. Scientific Reports, 2017, 7, 9619.	3.3	66
5	Self-Association of Amphotericin B: Spontaneous Formation of Molecular Structures Responsible for the Toxic Side Effects of the Antibiotic. Journal of Physical Chemistry B, 2014, 118, 13821-13832.	2.6	53
6	Modulation of Amphotericin B Membrane Interaction by Cholesterol and ErgosterolA Molecular Dynamics Study. Journal of Physical Chemistry B, 2006, 110, 16743-16753.	2.6	46
7	Torsional elasticity and energetics of F ₁ -ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 7408-7413.	7.1	46
8	Interaction of amphotericin B and its selected derivatives with membranes: molecular modeling studies. Chemical Record, 2006, 6, 320-332.	5.8	45
9	Keep It Flexible: Driving Macromolecular Rotary Motions in Atomistic Simulations with GROMACS. Journal of Chemical Theory and Computation, 2011, 7, 1381-1393.	5.3	42
10	On the Possibility of the Amphotericin B-Sterol Complex Formation in Cholesterol- and Ergosterol-Containing Lipid Bilayers: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 15875-15885.	2.6	38
11	Molecular aspects of the interaction between amphotericin B and a phospholipid bilayer: molecular dynamics studies. Journal of Molecular Modeling, 2004, 10, 223-232.	1.8	34
12	The Effect of Sterols on Amphotericin B Self-Aggregation in a Lipid Bilayer as Revealed by Free Energy Simulations. Biophysical Journal, 2013, 104, 1485-1494.	0.5	34
13	A first-principles study of electron attachment to the fully hydrated bromonucleobases. Chemical Physics Letters, 2014, 595-596, 133-137.	2.6	32
14	Mechanism of Binding of Antifungal Antibiotic Amphotericin B to Lipid Membranes: An Insight from Combined Single-Membrane Imaging, Microspectroscopy, and Molecular Dynamics. Molecular Pharmaceutics, 2018, 15, 4202-4213.	4.6	31
15	Molecular dynamics simulations reveal the balance of forces governing the formation of a guanine tetradâ€"a common structural unit of G-quadruplex DNA. Nucleic Acids Research, 2016, 44, 3020-3030.	14.5	30
16	Influence of a lipid bilayer on the conformational behavior of amphotericin B derivatives â€" A molecular dynamics study. Biophysical Chemistry, 2009, 141, 105-116.	2.8	27
17	Why do G-quadruplexes dimerize through the 5â€™-ends? Driving forces for G4 DNA dimerization examined in atomic detail. PLoS Computational Biology, 2019, 15, e1007383.	3.2	26
18	Rotation Triggers Nucleotide-Independent Conformational Transition of the Empty Î² Subunit of F₁-ATPase. Journal of the American Chemical Society, 2014, 136, 6960-6968.	13.7	25

#	Article	IF	Citations
19	Thermodynamics and kinetics of amphotericin B self-association in aqueous solution characterized in molecular detail. Scientific Reports, 2016, 6, 19109.	3.3	25
20	Specific Binding of Cholesterol to the Amyloid Precursor Protein: Structure of the Complex and Driving Forces Characterized in Molecular Detail. Journal of Physical Chemistry Letters, 2015, 6, 784-790.	4.6	23
21	Mechanochemical Energy Transduction during the Main Rotary Step in the Synthesis Cycle of F₁-ATPase. Journal of the American Chemical Society, 2017, 139, 4025-4034.	13.7	23
22	Membrane Sterols Modulate the Binding Mode of Amphotericin B without Affecting Its Affinity for a Lipid Bilayer. Langmuir, 2016, 32, 3452-3461.	3.5	22
23	Hydration of amino acids: FTIR spectra and molecular dynamics studies. Amino Acids, 2015, 47, 2265-2278.	2.7	20
24	The Mechanism of Overcoming Multidrug Resistance (MDR) of Fungi by Amphotericin B and Its Derivatives. Journal of Antibiotics, 2007, 60, 436-446.	2.0	19
25	Molecular basis of the osmolyte effect on protein stability: a lesson from the mechanical unfolding of lysozyme. Biochemical Journal, 2016, 473, 3705-3724.	3.7	19
26	Ironâ€“Sulfur Cluster Biogenesis Chaperones: Evidence for Emergence of Mutational Robustness of a Highly Specific Proteinâ€“Protein Interaction. Molecular Biology and Evolution, 2016, 33, 643-656.	8.9	19
27	How proteins bind to DNA: target discrimination and dynamic sequence search by the telomeric protein TRF1. Nucleic Acids Research, 2017, 45, 7643-7654.	14.5	19
28	Effect of osmolytes on the thermal stability of proteins: replica exchange simulations of Trp-cage in urea and betaine solutions. Physical Chemistry Chemical Physics, 2018, 20, 11174-11182.	2.8	18
29	Two-step mechanism of J-domain action in driving Hsp70 function. PLoS Computational Biology, 2020, 16, e1007913.	3.2	18
30	Interactions of amphotericin B derivatives with lipid membranesâ€”A molecular dynamics study. Biochimica Et Biophysica Acta - Biomembranes, 2007, 1768, 2616-2626.	2.6	16
31	Molywood: streamlining the design and rendering of molecular movies. Bioinformatics, 2020, 36, 4660-4661.	4.1	16
32	Sequence-dependent structural properties of B-DNA: what have we learned in 40Âyears?. Biophysical Reviews, 2021, 13, 995-1005.	3.2	13
33	Monosaccharides as internal probes for the determination of the absolute configuration of 2-butanol. Magnetic Resonance in Chemistry, 2006, 44, 132-138.	1.9	12
34	Two Bacterial Small Heat Shock Proteins, IbpA and IbpB, Form a Functional Heterodimer. Journal of Molecular Biology, 2021, 433, 167054.	4.2	12
35	Mechanism of recognition of parallel G-quadruplexes by DEAH/RHAU helicase DHX36 explored by molecular dynamics simulations. Computational and Structural Biotechnology Journal, 2021, 19, 2526-2536.	4.1	12
36	Role of the disulfide bond in stabilizing and folding of the fimbrial protein DraE from uropathogenic Escherichia coli. Journal of Biological Chemistry, 2017, 292, 16136-16149.	3.4	9

#	Article	IF	Citations
37	Self-assembly, stability and conductance of amphotericin B channels: bridging the gap between structure and function. Nanoscale, 2021, 13, 3686-3697.	5.6	9
38	Light-Modulated Sunscreen Mechanism in the Retina of the Human Eye. Journal of Physical Chemistry B, 2021, 125, 6090-6102.	2.6	9
39	Solvation of ionic liquids based on N-methyl-N-alkyl morpholinium cations in dimethylsulfoxide â€“ volumetric and compressibility studies. Journal of Chemical Thermodynamics, 2015, 88, 36-43.	2.0	8
40	Intercalation complex of imidazoacridinone C-1311, a potential anticancer drug, with DNA helix d(CGATCG)2: stereostructural studies by 2D NMR spectroscopy. Journal of Biomolecular Structure and Dynamics, 2016, 34, 653-663.	3.5	8
41	Effect of osmolytes of different type on DNA behavior in aqueous solution. Experimental and theoretical studies. Journal of Molecular Liquids, 2018, 271, 186-201.	4.9	8
42	Structure and evolution of the 4-helix bundle domain of Zuotin, a J-domain protein co-chaperone of Hsp70. PLoS ONE, 2019, 14, e0217098.	2.5	8
43	Defining a novel domain that provides an essential contribution to site-specific interaction of Rep protein with DNA. Nucleic Acids Research, 2021, 49, 3394-3408.	14.5	8
44	Molecular mechanism of proton-coupled ligand translocation by the bacterial efflux pump EmrE. PLoS Computational Biology, 2021, 17, e1009454.	3.2	8
45	Determinants of Directionality and Efficiency of the ATP Synthase F_o Motor at Atomic Resolution. Journal of Physical Chemistry Letters, 2022, 13, 387-392.	4.6	8
46	The Product of Matrix Metalloproteinase Cleavage of Doxorubicin Conjugate for Anticancer Drug Delivery: Calorimetric, Spectroscopic, and Molecular Dynamics Studies on Peptideâ€“Doxorubicin Binding to DNA. International Journal of Molecular Sciences, 2020, 21, 6923.	4.1	7
47	Dominant Pathways of Adenosyl Radical-Induced DNA Damage Revealed by QM/MM Metadynamics. Journal of Chemical Theory and Computation, 2017, 13, 6415-6423.	5.3	6
48	Intramolecular transformation of an antifungal antibiotic nystatin A₁ into its isomer, isoâ€nystatin A₁ â€“ structural and molecular modeling studies. Magnetic Resonance in Chemistry, 2016, 54, 953-961.	1.9	5
49	Effect of chemical structure on complexation efficiency of aromatic drugs with cyclodextrins: The example of dibenzazepine derivatives. Carbohydrate Polymers, 2020, 250, 116957.	10.2	5
50	Molecular Recognition in Complexes of TRF Proteins with Telomeric DNA. PLoS ONE, 2014, 9, e89460.	2.5	5
51	Correlation between the number of Proâ€“Ala repeats in the EmrA homologue of Acinetobacter baumannii and resistance to netilmicin, tobramycin, imipenem and ceftazidime. Journal of Global Antimicrobial Resistance, 2016, 7, 145-149.	2.2	4
52	Role of cholesterol in substrate recognition by $$gamma$$-secretase. Scientific Reports, 2021, 11, 15213.	3.3	4
53	Guanosine Dianions Hydrated by One to Four Water Molecules. Journal of Physical Chemistry Letters, 2022, , 3230-3236.	4.6	4
54	Telomere uncapping by common oxidative guanine lesions: Insights from atomistic models. Free Radical Biology and Medicine, 2020, 148, 162-169.	2.9	2

#	Article	IF	Citations
55	Spatial Distribution of Elasticity in the F1 Motor of ATP Synthase RevealsÂthe Microscopic Nature of the Coupling Between the Central Shaft and the Catalytic Subunit. Biophysical Journal, 2010, 98, 168a.	0.5	1
56	Title is missing!. , 2019, 15, e1007383.		0
57	Title is missing!. , 2019, 15, e1007383.		0
58	Title is missing!. , 2019, 15, e1007383.		0
59	Title is missing!. , 2019, 15, e1007383.		0
60	Title is missing!. , 2019, 15, e1007383.		0
61	Title is missing!. , 2019, 15, e1007383.		0