Piotr Setny

List of Publications by Year in descending order

35 papers	926 citations	623574 14 h-index	477173 29 g-index
44 all docs	44 docs citations	44 times ranked	1098 citing authors

#	Article	IF	Citations
1	Membrane-Bound Configuration and Lipid Perturbing Effects of Hemagglutinin Subunit 2 N-Terminus Investigated by Computer Simulations. Frontiers in Molecular Biosciences, 2022, 9, 826366.	1.6	2
2	Granger Causality Analysis of Chignolin Folding. Journal of Chemical Theory and Computation, 2022, 18, 1936-1944.	2.3	5
3	Transient Excursions to Membrane Core as Determinants of Influenza Virus Fusion Peptide Activity. International Journal of Molecular Sciences, 2021, 22, 5301.	1.8	5
4	Entropyâ€based distance cutoff for protein internal contact networks. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1333-1339.	1.5	2
5	Conserved internal hydration motifs in protein kinases. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1578-1591.	1.5	6
6	GridSolvate: A Web Server for the Prediction of Biomolecular Hydration Properties. Journal of Chemical Information and Modeling, 2020, 60, 5907-5911.	2.5	2
7	Restriction of S-adenosylmethionine conformational freedom by knotted protein binding sites. PLoS Computational Biology, 2020, 16, e1007904.	1.5	13
8	Restriction of S-adenosylmethionine conformational freedom by knotted protein binding sites. , 2020, 16, e1007904.		0
9	Restriction of S-adenosylmethionine conformational freedom by knotted protein binding sites. , 2020, 16, e1007904.		0
10	Restriction of S-adenosylmethionine conformational freedom by knotted protein binding sites. , 2020, 16, e1007904.		0
11	Restriction of S-adenosylmethionine conformational freedom by knotted protein binding sites. , 2020, 16, e1007904.		0
12	Restriction of S-adenosylmethionine conformational freedom by knotted protein binding sites. , 2020, 16, e1007904.		0
13	Restriction of S-adenosylmethionine conformational freedom by knotted protein binding sites. , 2020, 16, e1007904.		0
14	Quick temperature-sweep pure-shift NMR: the case of solvent effects in atorvastatin. Physical Chemistry Chemical Physics, 2019, 21, 19209-19215.	1.3	10
15	Water-mediated conformational preselection mechanism in substrate binding cooperativity to protein kinase A. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3852-3857.	3.3	17
16	Affinity, kinetics, and pathways of anisotropic ligands binding to hydrophobic model pockets. Journal of Chemical Physics, 2018, 149, 094902.	1.2	1
17	Charged N-terminus of Influenza Fusion Peptide Facilitates Membrane Fusion. International Journal of Molecular Sciences, 2018, 19, 578.	1.8	8
18	Explicit Solvent Hydration Benchmark for Proteins with Application to the PBSA Method. Journal of Chemical Theory and Computation, 2017, 13, 2762-2776.	2.3	1

#	Article	IF	Citations
19	Principles for Tuning Hydrophobic Ligandâ€“Receptor Binding Kinetics. Journal of Chemical Theory and Computation, 2017, 13, 3012-3019.	2.3	13
20	Three conserved C-terminal residues of influenza fusion peptide alter its behavior at the membrane interface. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 97-105.	1.1	16
21	Solvent Fluctuations Induce Non-Markovian Kinetics in Hydrophobic Pocket-Ligand Binding. Journal of Physical Chemistry B, 2016, 120, 8127-8136.	1.2	8
22	Hydration in Discrete Water (II): From Neutral to Charged Solutes. Journal of Physical Chemistry B, 2015, 119, 5970-5978.	1.2	6
23	Prediction of Water Binding to Protein Hydration Sites with a Discrete, Semiexplicit Solvent Model. Journal of Chemical Theory and Computation, 2015, 11, 5961-5972.	2.3	14
24	Solvent fluctuations in hydrophobic cavityâ€“ligand binding kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 1197-1202.	3.3	86
25	Protein-DNA docking with a coarse-grained force field. BMC Bioinformatics, 2012, 13, 228.	1.2	31
26	A coarse-grained force field for Proteinâ€“RNA docking. Nucleic Acids Research, 2011, 39, 9118-9129.	6.5	55
27	How Can Hydrophobic Association Be Enthalpy Driven?. Journal of Chemical Theory and Computation, 2010, 6, 2866-2871.	2.3	205
28	Hydration in Discrete Water. A Mean Field, Cellular Automata Based Approach to Calculating Hydration Free Energies. Journal of Physical Chemistry B, 2010, 114, 8667-8675.	1.2	18
29	Water in Cavityâ^'Ligand Recognition. Journal of the American Chemical Society, 2010, 132, 12091-12097.	6.6	236
30	Interfaces and hydrophobic interactions in receptor-ligand systems: A level-set variational implicit solvent approach. Journal of Chemical Physics, 2009, 131, 144102.	1.2	40
31	Search for Novel Aminoglycosides by Combining Fragment-Based Virtual Screening and 3D-QSAR Scoring. Journal of Chemical Information and Modeling, 2009, 49, 390-400.	2.5	26
32	Hydrophobic interactions between methane and a nanoscopic pocket: Three dimensional distribution of potential of mean force revealed by computer simulations. Journal of Chemical Physics, 2008, 128, 125105.	1.2	20
33	Water properties and potential of mean force for hydrophobic interactions of methane and nanoscopic pockets studied by computer simulations. Journal of Chemical Physics, 2007, 127, 054505.	1.2	25
34	Water properties inside nanoscopic hydrophobic pocket studied by computer simulations. Journal of Chemical Physics, 2006, 125, 144717.	1.2	35
35	Refinement of X-ray data on dual cosubstrate specificity of CK2 kinase by free energy calculations based on molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2004, 58, 511-517.	1.5	6