Christophe Chipot

List of Publications by Year
in descending order

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145 papers	24,779 citations	57752 44 h-index	9860 141 g-index
149 all docs	149 docs citations	149 times ranked	26874 citing authors

#	Article	IF	Citations
1	Scalable molecular dynamics with NAMD. Journal of Computational Chemistry, 2005, 26, 1781-1802.	3.3	15,208
2	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
3	Good Practices in Free-Energy Calculations. Journal of Physical Chemistry B, 2010, 114, 10235-10253.	2.6	509
4	Overcoming free energy barriers using unconstrained molecular dynamics simulations. Journal of Chemical Physics, 2004, 121, 2904-2914.	3.0	423
5	Exploring Multidimensional Free Energy Landscapes Using Time-Dependent Biases on Collective Variables. Journal of Chemical Theory and Computation, 2010, 6, 35-47.	5.3	366
6	The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask. Journal of Physical Chemistry B, 2015, 119, 1129-1151.	2.6	351
7	Benzene Dimer:Â A Good Model for Ï€âˆ'Ï€ Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. Journal of the American Chemical Society, 1996, 118, 11217-11224.	13.7	298
8	Standard Binding Free Energies from Computer Simulations: What Is the Best Strategy?. Journal of Chemical Theory and Computation, 2013, 9, 794-802.	5.3	298
9	Efficient Determination of Proteinâ€"Protein Standard Binding Free Energies from First Principles. Journal of Chemical Theory and Computation, 2013, 9, 3789-3798.	5.3	188
10	Cationâˆ'Ï€ Interactions in Proteins:Â Can Simple Models Provide an Accurate Description?. Journal of the American Chemical Society, 1999, 121, 10366-10372.	13.7	184
11	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	5.4	174
12	A Toolkit for the Analysis of Free-Energy Perturbation Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2606-2616.	5.3	153
13	Insights into the Recognition and Association of Transmembrane Î±-Helices. The Free Energy of Î±-Helix Dimerization in Glycophorin A. Journal of the American Chemical Society, 2005, 127, 8478-8484.	13.7	146
14	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	5.3	139
15	Frontiers in freeâ€energy calculations of biological systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 71-89.	14.6	135
16	Perturbations of Native Membrane Protein Structure in Alkyl Phosphocholine Detergents: A Critical Assessment of NMR and Biophysical Studies. Chemical Reviews, 2018, 118, 3559-3607.	47.7	132
17	Binding of ADP in the Mitochondrial ADP/ATP Carrier Is Driven by an Electrostatic Funnel. Journal of the American Chemical Society, 2008, 130, 12725-12733.	13.7	130
18	Conformational transitions of the serotonin 5-HT3 receptor. Nature, 2018, 563, 275-279.	27.8	128

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19	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	28.9	122
20	NMR Structure and Ion Channel Activity of the p7 Protein from Hepatitis C Virus. Journal of Biological Chemistry, 2010, 285, 31446-31461.	3.4	119
21	Exploring the free-energy landscape of a short peptide using an average force. Journal of Chemical Physics, 2005, 123, 244906.	3.0	113
22	Extended Adaptive Biasing Force Algorithm. An On-the-Fly Implementation for Accurate Free-Energy Calculations. Journal of Chemical Theory and Computation, 2016, 12, 3506-3513.	5.3	113
23	Can Absolute Free Energies of Association Be Estimated from Molecular Mechanical Simulations? The Biotinâ˜Streptavidin System Revisited. Journal of Physical Chemistry A, 2001, 105, 9795-9799.	2.5	104
24	Zooming across the Free-Energy Landscape: Shaving Barriers, and Flooding Valleys. Journal of Physical Chemistry Letters, 2018, 9, 4738-4745.	4.6	100
25	Diffusion of Glycerol through Escherichia coli Aquaglyceroporin GlpF. Biophysical Journal, 2008, 94, 832-839.	0.5	98
26	Taming Rugged Free Energy Landscapes Using an Average Force. Accounts of Chemical Research, 2019, 52, 3254-3264.	15.6	98
27	High-speed atomic force microscopy shows that annexin V stabilizes membranes on the second timescale. Nature Nanotechnology, 2016, 11, 783-790.	31.5	96
28	Molecular Dynamics Potential of Mean Force Calculations:â€‰ A Study of the Tolueneâ˜Ammonium Ï€-Cation Interactions. Journal of the American Chemical Society, 1996, 118, 2998-3005.	13.7	91
29	Dangerous Liaisons between Detergents and Membrane Proteins. The Case of Mitochondrial Uncoupling Protein 2. Journal of the American Chemical Society, 2013, 135, 15174-15182.	13.7	86
30	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. Molecules, 2018, 23, 228.	3.8	85
31	Free-energy cost for translocon-assisted insertion of membrane proteins. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3596-3601.	7.1	74
32	Multiple-Replica Strategies for Free-Energy Calculations in NAMD: Multiple-Walker Adaptive Biasing Force and Walker Selection Rules. Journal of Chemical Theory and Computation, 2014, 10, 5276-5285.	5.3	66
33	Calculating Position-Dependent Diffusivity in Biased Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 876-882.	5.3	64
34	Subdiffusion in Membrane Permeation of Small Molecules. Scientific Reports, 2016, 6, 35913.	3.3	63
35	The p7 Protein of Hepatitis C Virus Forms Structurally Plastic, Minimalist Ion Channels. PLoS Computational Biology, 2012, 8, e1002702.	3.2	60
36	Cation-Ï€ Interactions and their Functional Roles in Membrane Proteins. Journal of Molecular Biology, 2021, 433, 167035.	4.2	59

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37	Annexin-V stabilizes membrane defects by inducing lipid phase transition. Nature Communications, 2020, 11, 230.	12.8	58
38	Calculation of Lipid-Bilayer Permeabilities Using an Average Force. Journal of Chemical Theory and Computation, 2014, 10, 554-564.	5.3	57
39	Structural Basis for Broad HIV-1 Neutralization by the MPER-Specific Human Broadly Neutralizing Antibody LN01. Cell Host and Microbe, 2019, 26, 623-637.e8.	11.0	56
40	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	12.0	56
41	Can free energy calculations be fast and accurate at the same time? Binding of low-affinity, non-peptide inhibitors to the SH2 domain of the src protein. Journal of Computer-Aided Molecular Design, 2005, 19, 765-770.	2.9	53
42	Computing Relative Binding Affinity of Ligands to Receptor: An Effective Hybrid Single-Dual-Topology Free-Energy Perturbation Approach in NAMD. Journal of Chemical Information and Modeling, 2019, 59, 3794-3802.	5.4	52
43	BFEE: A User-Friendly Graphical Interface Facilitating Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2018, 58, 556-560.	5.4	51
44	Cryo-EM and MD infer water-mediated proton transport and autoinhibition mechanisms of V _o complex. Science Advances, 2020, 6, .	10.3	51
45	Finding an Optimal Pathway on a Multidimensional Free-Energy Landscape. Journal of Chemical Information and Modeling, 2020, 60, 5366-5374.	5.4	51
46	The substrate specificity of the human ADP/ATP carrier AAC1. Molecular Membrane Biology, 2013, 30, 160-168.	2.0	50
47	New Coarse Variables for the Accurate Determination of Standard Binding Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 5173-5178.	5.3	49
48	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	7.4	47
49	Enzyme-mimetic self-catalyzed polymerization of polypeptide helices. Nature Communications, 2019, 10, 5470.	12.8	46
50	Conformational Equilibria of Terminally Blocked Single Amino Acids at the Waterâ^'Hexane Interface. A Molecular Dynamics Study. Journal of Physical Chemistry B, 1998, 102, 281-290.	2.6	44
51	Thermodynamics of Deca-alanine Folding in Water. Journal of Chemical Theory and Computation, 2014, 10, 2836-2844.	5.3	44
52	The Extended Generalized Adaptive Biasing Force Algorithm for Multidimensional Free-Energy Calculations. Journal of Chemical Theory and Computation, 2017, 13, 1566-1576.	5.3	44
53	Chemomechanical Coupling in Hexameric Proteinâ€“Protein Interfaces Harnesses Energy within V-Type ATPases. Journal of the American Chemical Society, 2017, 139, 293-310.	13.7	44
54	Machine Learning Reveals the Critical Interactions for SARS-CoV-2 Spike Protein Binding to ACE2. Journal of Physical Chemistry Letters, 2021, 12, 5494-5502.	4.6	44

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55	Diffusive Models of Membrane Permeation with Explicit Orientational Freedom. Journal of Chemical Theory and Computation, 2014, 10, 2710-2718.	5.3	43
56	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913.	5.3	41
57	How Detergent Impacts Membrane Proteins: Atomic-Level Views of Mitochondrial Carriers in Dodecylphosphocholine. Journal of Physical Chemistry Letters, 2018, 9, 933-938.	4.6	41
58	Mechanism of the allosteric activation of the ClpP protease machinery by substrates and active-site inhibitors. Science Advances, 2019, 5, eaaw3818.	10.3	41
59	Distributed polarizabilities derived from induction energies: A finite perturbation approach. Journal of Chemical Physics, 2000, 112, 2709-2717.	3.0	40
60	OPEP: A tool for the optimal partitioning of electric properties. Journal of Computational Chemistry, 2003, 24, 997-1008.	3.3	39
61	Conformational transitions and ligand-binding to a muscle-type nicotinic acetylcholine receptor. Neuron, 2022, 110, 1358-1370.e5.	8.1	39
62	Î±-Helix Unwinding as Force Buffer in Spectrins. ACS Nano, 2018, 12, 2719-2727.	14.6	37
63	Boosting Free-Energy Perturbation Calculations with GPU-Accelerated NAMD. Journal of Chemical Information and Modeling, 2020, 60, 5301-5307.	5.4	37
64	Free Energy of Nascent-Chain Folding in the Translocon. Journal of the American Chemical Society, 2011, 133, 7602-7607.	13.7	36
65	Statistical analysis of distributed multipoles derived from molecular electrostatic potentials. Molecular Physics, 1998, 94, 881-895.	1.7	35
66	The lubricating role of water in the shuttling of rotaxanes. Chemical Science, 2017, 8, 5087-5094.	7.4	35
67	Link between Membrane Composition and Permeability to Drugs. Journal of Chemical Theory and Computation, 2018, 14, 2895-2909.	5.3	35
68	BFEE2: Automated, Streamlined, and Accurate Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2116-2123.	5.4	35
69	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. Journal of Chemical Theory and Computation, 2007, 3, 1914-1926.	5.3	34
70	Polarizable Intermolecular Potentials for Water and Benzene Interacting with Halide and Metal Ions. Journal of Chemical Theory and Computation, 2009, 5, 3022-3031.	5.3	34
71	Permeability of a Fluid Lipid Bilayer to Short-Chain Alcohols from First Principles. Journal of Chemical Theory and Computation, 2017, 13, 2523-2532.	5.3	33
72	String Method for Proteinâ€“Protein Binding Free-Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 5829-5844.	5.3	33

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73	Concentrations of anesthetics across the waterâ€“membrane interface; the Meyerâ€“Overton hypothesis revisited. Toxicology Letters, 1998, 100-101, 421-430.	0.8	32
74	From Material Science to Avant-Garde Cuisine. The Art of Shaping Liquids into Spheres. Journal of Physical Chemistry B, 2014, 118, 11747-11756.	2.6	32
75	Enhanced Sampling of Multidimensional Free-Energy Landscapes Using Adaptive Biasing Forces. SIAM Journal on Applied Mathematics, 2011, 71, 1673-1695.	1.8	31
76	Water Conduction through a Peptide Nanotube. Journal of Physical Chemistry C, 2013, 117, 26797-26803.	3.1	30
77	Insight into the Properties of Cardiolipin Containing Bilayers from Molecular Dynamics Simulations, Using a Hybrid All-Atom/United-Atom Force Field. Journal of Chemical Theory and Computation, 2012, 8, 1765-1773.	5.3	29
78	Polarization effects in molecular interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 844-854.	14.6	28
79	Affordable Membrane Permeability Calculations: Permeation of Short-Chain Alcohols through Pure-Lipid Bilayers and a Mammalian Cell Membrane. Journal of Chemical Theory and Computation, 2019, 15, 2913-2924.	5.3	27
80	Enhanced configurational sampling with hybrid non-equilibrium molecular dynamicsâ€“Monte Carlo propagator. Journal of Chemical Physics, 2018, 148, 014101.	3.0	26
81	The true nature of rotary movements in rotaxanes. Chemical Science, 2016, 7, 457-462.	7.4	25
82	Free Energy Methods in Drug Discoveryâ€”Introduction. ACS Symposium Series, 0, , 1-38.	0.5	24
83	Alternative Approaches for the Calculation of Induction Energies:Â Characterization, Effectiveness, and Pitfalls. Journal of Physical Chemistry A, 2001, 105, 11505-11514.	2.5	23
84	Molecular Basis of Drug Resistance in A/H1N1 Virus. Journal of Chemical Information and Modeling, 2012, 52, 2650-2656.	5.4	23
85	Achieving ergodic sampling using replica-exchange free-energy calculations. Molecular Simulation, 2014, 40, 218-228.	2.0	23
86	Accurate Description of Cationâ^Ï€ Interactions in Proteins with a Nonpolarizable Force Field at No Additional Cost. Journal of Chemical Theory and Computation, 2020, 16, 6397-6407.	5.3	23
87	MLCV: Bridging Machine-Learning-Based Dimensionality Reduction and Free-Energy Calculation. Journal of Chemical Information and Modeling, 2022, 62, 1-8.	5.4	23
88	AlaScan: A Graphical User Interface for Alanine Scanning Free-Energy Calculations. Journal of Chemical Information and Modeling, 2016, 56, 1122-1126.	5.4	22
89	Charge Transfer and Chemo-Mechanical Coupling in Respiratory Complex I. Journal of the American Chemical Society, 2020, 142, 9220-9230.	13.7	22
90	Solvent-Controlled Shuttling in a Molecular Switch. Journal of Physical Chemistry C, 2012, 116, 4471-4476.	3.1	21

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91	High-Chloride Concentrations Abolish the Binding of Adenine Nucleotides in the Mitochondrial ADP/ATP Carrier Family. Biophysical Journal, 2009, 97, L25-L27.	0.5	20
92	Methodology for the Simulation of Molecular Motors at Different Scales. Journal of Physical Chemistry B, 2017, 121, 3502-3514.	2.6	20
93	The Binding of Palonosetron and Other Antiemetic Drugs to the Serotonin 5-HT3 Receptor. Structure, 2020, 28, 1131-1140.e4.	3.3	20
94	Molecular Bases of DNA Packaging in Bacteria Revealed by All-Atom Molecular Dynamics Simulations: The Case of Histone-Like Proteins inBorrelia burgdorferi. Journal of Physical Chemistry Letters, 2019, 10, 7200-7207.	4.6	19
95	Tuning Proton Transfer Thermodynamics in SARS-CoV-2 Main Protease: Implications for Catalysis and Inhibitor Design. Journal of Physical Chemistry Letters, 2021, 12, 4195-4202.	4.6	19
96	Complex Movements in Rotaxanes: Shuttling Coupled with Conformational Transition of Cyclodextrins. Journal of Physical Chemistry C, 2016, 120, 19479-19486.	3.1	18
97	Mitochondrial ADP/ATP Carrier in Dodecylphosphocholine Binds Cardiolipins with Non-native Affinity. Biophysical Journal, 2017, 113, 2311-2315.	0.5	18
98	Lysine Mutation of the Claw-Arm-Like Loop Accelerates Catalysis by Cellobiohydrolases. Journal of the American Chemical Society, 2019, 141, 14451-14459.	13.7	17
99	Correlation of membrane protein conformational and functional dynamics. Nature Communications, 2021, 12, 4363.	12.8	17
100	Thermodynamic Insights into the Dynamic Switching of a Cyclodextrin in a Bistable Molecular Shuttle. Journal of Physical Chemistry Letters, 2010, 1, 1776-1780.	4.6	16
101	Water-Controlled Switching in Rotaxanes. Journal of Physical Chemistry C, 2018, 122, 9229-9234.	3.1	16
102	Enthalpyâ€“Entropy Interplay in Ï€-Stacking Interaction of Benzene Dimer in Water. Journal of Chemical Theory and Computation, 2019, 15, 1538-1545.	5.3	16
103	Decrypting protein insertion through the translocon with free-energy calculations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1663-1671.	2.6	15
104	Targeting G-quadruplexes with Organic Dyes: Chelerythrineâ€“DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. Antioxidants, 2019, 8, 472.	5.1	15
105	Structure of HIV-1 gp41 with its membrane anchors targeted by neutralizing antibodies. ELife, 2021, 10, .	6.0	15
106	Overcoming Free-Energy Barriers with a Seamless Combination of a Biasing Force and a Collective Variable-Independent Boost Potential. Journal of Chemical Theory and Computation, 2021, 17, 3886-3894.	5.3	15
107	Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. Journal of Physical Chemistry B, 2016, 120, 8733-8742.	2.6	14
108	Modeling induction phenomena in amino acid cationâ€“ $$pi $$ Ï€ interactions. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	14

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109	Re-evaluating the p7 viroporin structure. Nature, 2018, 562, E8-E18.	27.8	14
110	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. Journal of Physical Chemistry Letters, 2019, 10, 7133-7140.	4.6	14
111	Triggering Tautomerization of Curcumin by Confinement into Liposomes. ChemPhotoChem, 2019, 3, 1034-1041.	3.0	14
112	A Companion Guide to the String Method with Swarms of Trajectories: Characterization, Performance, and Pitfalls. Journal of Chemical Theory and Computation, 2022, 18, 1406-1422.	5.3	14
113	Oligomerization State of Photosynthetic Core Complexes Is Correlated with the Dimerization Affinity of a Transmembrane Helix. Journal of the American Chemical Society, 2011, 133, 14071-14081.	13.7	13
114	Free Energy Calculations for Cyclodextrin Inclusion Complexes. Current Organic Chemistry, 2011, 15, 839-847.	1.6	13
115	Impaired Transport of Nucleotides in a Mitochondrial Carrier Explains Severe Human Genetic Diseases. ACS Chemical Biology, 2012, 7, 1164-1169.	3.4	13
116	Hepatitis C virus sequence divergence preserves p7 viroporin structural and dynamic features. Scientific Reports, 2019, 9, 8383.	3.3	13
117	ELF: An Extended-Lagrangian Free Energy Calculation Module for Multiple Molecular Dynamics Engines. Journal of Chemical Information and Modeling, 2018, 58, 1315-1318.	5.4	12
118	Accuracy of Alternate Nonpolarizable Force Fields for the Determination of Proteinâ€“Ligand Binding Affinities Dominated by Cationâ^Ï€ Interactions. Journal of Chemical Theory and Computation, 2021, 17, 3908-3915.	5.3	12
119	Repurposing Existing Molecular Machines through Accurate Regulation of Cooperative Motions. Journal of Physical Chemistry Letters, 2021, 12, 613-619.	4.6	12
120	Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2234-2244.	5.3	11
121	Changes in Microenvironment Modulate the B- to A-DNA Transition. Journal of Chemical Information and Modeling, 2019, 59, 2324-2330.	5.4	11
122	Nanomachine-Assisted Ion Transport Across Membranes: From Mechanism to Rational Design and Applications. Journal of Physical Chemistry Letters, 2021, 12, 3281-3287.	4.6	11
123	Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. Physical Chemistry Chemical Physics, 2016, 18, 33180-33186.	2.8	10
124	Hazardous Shortcuts in Standard Binding Free Energy Calculations. Journal of Physical Chemistry Letters, 2022, 13, 6250-6258.	4.6	10
125	How Do Membrane Transporters Sense pH? The Case of the Mitochondrial ADPâ€“ATP Carrier. Journal of Physical Chemistry Letters, 2013, 4, 3787-3791.	4.6	9
126	Assessing the physiological relevance of alternate architectures of the p7 protein of hepatitis C virus in different environments. Bioorganic and Medicinal Chemistry, 2016, 24, 4920-4927.	3.0	9

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127	pH-Controlled Fluorescence Probes for Rotaxane Isomerization. Journal of Physical Chemistry C, 2019, 123, 11304-11309.	3.1	9
128	Dynamics and interactions of AAC3 in DPC are not functionally relevant. Nature Structural and Molecular Biology, 2018, 25, 745-747.	8.2	8
129	Curvature of Buckybowl Corannulene Enhances Its Binding to Proteins. Journal of Physical Chemistry C, 2019, 123, 922-930.	3.1	8
130	Avoiding non-equilibrium effects in adaptive biasing force calculations. Molecular Simulation, 2021, 47, 390-394.	2.0	8
131	Standard Binding Free Energy and Membrane Desorption Mechanism for a Phospholipase C. Journal of Chemical Information and Modeling, 2022, 62, 6602-6613.	5.4	8
132	The Mechanism of Action of Hepatitis B Virus Capsid Assembly Modulators Can Be Predicted from Binding to Early Assembly Intermediates. Journal of Medicinal Chemistry, 2022, 65, 4854-4864.	6.4	8
133	Addressing Polarization Phenomena in Molecular Machines Containing Transition Metal Ions with an Additive Force Field. Journal of Chemical Theory and Computation, 2019, 15, 1841-1847.	5.3	7
134	Rotational Mechanism Model of the Bacterial V1 Motor Based on Structural and Computational Analyses. Frontiers in Physiology, 2019, 10, 46.	2.8	7
135	Computational Assessment of Proteinâ€“Protein Binding Specificity within a Family of Synaptic Surface Receptors. Journal of Physical Chemistry B, 2022, 126, 7510-7527.	2.6	6
136	Modeling Lipid Membranes. , 2005, , 929-958.		5
137	Conformational changes of DNA induced by a trans-azobenzene derivative via non-covalent interactions. Physical Chemistry Chemical Physics, 2018, 20, 22645-22651.	2.8	5
138	Structure, substrate binding and symmetry of the mitochondrial ADP/ATP carrier in its matrix-open state. Biophysical Journal, 2021, 120, 5187-5195.	0.5	5
139	Unveiling the Underlying Mechanism for Compression and Decompression Strokes of a Molecular Engine. Journal of Physical Chemistry C, 2014, 118, 12562-12567.	3.1	4
140	Why do the structural properties of complexes formed by glucans and carbon nanotubes differ so much?. RSC Advances, 2015, 5, 95682-95689.	3.6	4
141	Modulation of membrane permeability by carbon dioxide. Journal of Computational Chemistry, 2020, 41, 421-426.	3.3	4
142	Free-Energy Landscape of Stepwise, Directional Motion in Multiple Molecular Switches. Journal of Physical Chemistry C, 2020, 124, 6448-6453.	3.1	3
143	Modeling Lipid Membranes. , 2005, , 929-958.		2
144	Reconciling alternate methods for the determination of charge distributions: a probabilistic approach to high-dimensional least-squares approximations. Journal of Mathematical Chemistry, 2011, 49, 296-324.	1.5	0

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145	Tribute to Klaus Schulten. Journal of Physical Chemistry B, 2017, 121, 3203-3205.	2.6	0