Christophe Chipot

List of Publications by Year
in descending order

145	24,779	66250	11282
papers	citations	44 h-index	141 g-index

149	149	149	30169
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Conformational transitions and ligand-binding to a muscle-type nicotinic acetylcholine receptor. Neuron, 2022, 110, 1358-1370.e5.	3.8	39
2	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.	2.3	14
3	Standard Binding Free Energy and Membrane Desorption Mechanism for a Phospholipase C. Journal of Chemical Information and Modeling, 2022, 62, 6602-6613.	2.5	8
4	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	5.5	56
5	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.	2.9	8
6	MLCV: Bridging Machine-Learning-Based Dimensionality Reduction and Free-Energy Calculation. Journal of Chemical Information and Modeling, 2022, 62, 1-8.	2.5	23
7	Hazardous Shortcuts in Standard Binding Free Energy Calculations. Journal of Physical Chemistry Letters, 2022, 13, 6250-6258.	2.1	10
8	Computational Assessment of Proteinâ€“Protein Binding Specificity within a Family of Synaptic Surface Receptors. Journal of Physical Chemistry B, 2022, 126, 7510-7527.	1.2	6
9	Avoiding non-equilibrium effects in adaptive biasing force calculations. Molecular Simulation, 2021, 47, 390-394.	0.9	8
10	Nanomachine-Assisted Ion Transport Across Membranes: From Mechanism to Rational Design and Applications. Journal of Physical Chemistry Letters, 2021, 12, 3281-3287.	2.1	11
11	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.	2.1	19
12	Structure of HIV-1 gp41 with its membrane anchors targeted by neutralizing antibodies. ELife, 2021, 10, .	2.8	15
13	BFEE2: Automated, Streamlined, and Accurate Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2116-2123.	2.5	35
14	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.	2.3	15
15	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.	2.3	12
16	Machine Learning Reveals the Critical Interactions for SARS-CoV-2 Spike Protein Binding to ACE2. Journal of Physical Chemistry Letters, 2021, 12, 5494-5502.	2.1	44
17	Correlation of membrane protein conformational and functional dynamics. Nature Communications, 2021, 12, 4363.	5.8	17
18	Cation-Ï€ Interactions and their Functional Roles in Membrane Proteins. Journal of Molecular Biology, 2021, 433, 167035.	2.0	59

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19	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	3.7	47
20	Repurposing Existing Molecular Machines through Accurate Regulation of Cooperative Motions. Journal of Physical Chemistry Letters, 2021, 12, 613-619.	2.1	12
21	Structure, substrate binding and symmetry of the mitochondrial ADP/ATP carrier in its matrix-open state. Biophysical Journal, 2021, 120, 5187-5195.	0.2	5
22	Modulation of membrane permeability by carbon dioxide. Journal of Computational Chemistry, 2020, 41, 421-426.	1.5	4
23	Cryo-EM and MD infer water-mediated proton transport and autoinhibition mechanisms of V _o complex. Science Advances, 2020, 6, .	4.7	51
24	The Binding of Palonosetron and Other Antiemetic Drugs to the Serotonin 5-HT3 Receptor. Structure, 2020, 28, 1131-1140.e4.	1.6	20
25	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
26	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.	2.3	23
27	Boosting Free-Energy Perturbation Calculations with GPU-Accelerated NAMD. Journal of Chemical Information and Modeling, 2020, 60, 5301-5307.	2.5	37
28	Finding an Optimal Pathway on a Multidimensional Free-Energy Landscape. Journal of Chemical Information and Modeling, 2020, 60, 5366-5374.	2.5	51
29	Free-Energy Landscape of Stepwise, Directional Motion in Multiple Molecular Switches. Journal of Physical Chemistry C, 2020, 124, 6448-6453.	1.5	3
30	Annexin-V stabilizes membrane defects by inducing lipid phase transition. Nature Communications, 2020, 11, 230.	5.8	58
31	Charge Transfer and Chemo-Mechanical Coupling in Respiratory Complex I. Journal of the American Chemical Society, 2020, 142, 9220-9230.	6.6	22
32	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.	2.5	52
33	Lysine Mutation of the Claw-Arm-Like Loop Accelerates Catalysis by Cellobiohydrolases. Journal of the American Chemical Society, 2019, 141, 14451-14459.	6.6	17
34	String Method for Proteinâ€“Protein Binding Free-Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 5829-5844.	2.3	33
35	Targeting G-quadruplexes with Organic Dyes: Chelerythrineâ€“DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. Antioxidants, 2019, 8, 472.	2.2	15
36	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.	2.1	19

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37	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	13.5	122
38	Taming Rugged Free Energy Landscapes Using an Average Force. Accounts of Chemical Research, 2019, 52, 3254-3264.	7.6	98
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.	5.1	56
40	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. Journal of Physical Chemistry Letters, 2019, 10, 7133-7140.	2.1	14
41	Mechanism of the allosteric activation of the ClpP protease machinery by substrates and active-site inhibitors. Science Advances, 2019, 5, eaaw3818.	4.7	41
42	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.	2.3	7
43	Triggering Tautomerization of Curcumin by Confinement into Liposomes. ChemPhotoChem, 2019, 3, 1034-1041.	1.5	14
44	Hepatitis C virus sequence divergence preserves p7 viroporin structural and dynamic features. Scientific Reports, 2019, 9, 8383.	1.6	13
45	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.	2.3	27
46	Rotational Mechanism Model of the Bacterial V1 Motor Based on Structural and Computational Analyses. Frontiers in Physiology, 2019, 10, 46.	1.3	7
47	pH-Controlled Fluorescence Probes for Rotaxane Isomerization. Journal of Physical Chemistry C, 2019, 123, 11304-11309.	1.5	9
48	Enthalpyâ€“Entropy Interplay in Ï€-Stacking Interaction of Benzene Dimer in Water. Journal of Chemical Theory and Computation, 2019, 15, 1538-1545.	2.3	16
49	Changes in Microenvironment Modulate the B- to A-DNA Transition. Journal of Chemical Information and Modeling, 2019, 59, 2324-2330.	2.5	11
50	Enzyme-mimetic self-catalyzed polymerization of polypeptide helices. Nature Communications, 2019, 10, 5470.	5.8	46
51	Curvature of Buckybowl Corannulene Enhances Its Binding to Proteins. Journal of Physical Chemistry C, 2019, 123, 922-930.	1.5	8
52	Perturbations of Native Membrane Protein Structure in Alkyl Phosphocholine Detergents: A Critical Assessment of NMR and Biophysical Studies. Chemical Reviews, 2018, 118, 3559-3607.	23.0	132
53	Water-Controlled Switching in Rotaxanes. Journal of Physical Chemistry C, 2018, 122, 9229-9234.	1.5	16
54	How Detergent Impacts Membrane Proteins: Atomic-Level Views of Mitochondrial Carriers in Dodecylphosphocholine. Journal of Physical Chemistry Letters, 2018, 9, 933-938.	2.1	41

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55	Î±-Helix Unwinding as Force Buffer in Spectrins. ACS Nano, 2018, 12, 2719-2727.	7.3	37
56	BFEE: A User-Friendly Graphical Interface Facilitating Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2018, 58, 556-560.	2.5	51
57	Enhanced configurational sampling with hybrid non-equilibrium molecular dynamicsâ€“Monte Carlo propagator. Journal of Chemical Physics, 2018, 148, 014101.	1.2	26
58	Modeling induction phenomena in amino acid cationâ€“ $$pi $$ Ï€ interactions. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	14
59	Re-evaluating the p7 viroporin structure. Nature, 2018, 562, E8-E18.	13.7	14
60	Conformational transitions of the serotonin 5-HT3 receptor. Nature, 2018, 563, 275-279.	13.7	128
61	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. Molecules, 2018, 23, 228.	1.7	85
62	Dynamics and interactions of AAC3 in DPC are not functionally relevant. Nature Structural and Molecular Biology, 2018, 25, 745-747.	3.6	8
63	Link between Membrane Composition and Permeability to Drugs. Journal of Chemical Theory and Computation, 2018, 14, 2895-2909.	2.3	35
64	Zooming across the Free-Energy Landscape: Shaving Barriers, and Flooding Valleys. Journal of Physical Chemistry Letters, 2018, 9, 4738-4745.	2.1	100
65	Conformational changes of DNA induced by a trans-azobenzene derivative via non-covalent interactions. Physical Chemistry Chemical Physics, 2018, 20, 22645-22651.	1.3	5
66	ELF: An Extended-Lagrangian Free Energy Calculation Module for Multiple Molecular Dynamics Engines. Journal of Chemical Information and Modeling, 2018, 58, 1315-1318.	2.5	12
67	The Extended Generalized Adaptive Biasing Force Algorithm for Multidimensional Free-Energy Calculations. Journal of Chemical Theory and Computation, 2017, 13, 1566-1576.	2.3	44
68	Tribute to Klaus Schulten. Journal of Physical Chemistry B, 2017, 121, 3203-3205.	1.2	0
69	The lubricating role of water in the shuttling of rotaxanes. Chemical Science, 2017, 8, 5087-5094.	3.7	35
70	Permeability of a Fluid Lipid Bilayer to Short-Chain Alcohols from First Principles. Journal of Chemical Theory and Computation, 2017, 13, 2523-2532.	2.3	33
71	Chemomechanical Coupling in Hexameric Proteinâ€“Protein Interfaces Harnesses Energy within V-Type ATPases. Journal of the American Chemical Society, 2017, 139, 293-310.	6.6	44
72	New Coarse Variables for the Accurate Determination of Standard Binding Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 5173-5178.	2.3	49

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73	Mitochondrial ADP/ATP Carrier in Dodecylphosphocholine Binds Cardiolipins with Non-native Affinity. Biophysical Journal, 2017, 113, 2311-2315.	0.2	18
74	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	2.3	139
75	Methodology for the Simulation of Molecular Motors at Different Scales. Journal of Physical Chemistry B, 2017, 121, 3502-3514.	1.2	20
76	Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. Physical Chemistry Chemical Physics, 2016, 18, 33180-33186.	1.3	10
77	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	2.5	174
78	AlaScan: A Graphical User Interface for Alanine Scanning Free-Energy Calculations. Journal of Chemical Information and Modeling, 2016, 56, 1122-1126.	2.5	22
79	Decrypting protein insertion through the translocon with free-energy calculations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1663-1671.	1.4	15
80	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.	1.4	9
81	Complex Movements in Rotaxanes: Shuttling Coupled with Conformational Transition of Cyclodextrins. Journal of Physical Chemistry C, 2016, 120, 19479-19486.	1.5	18
82	Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. Journal of Physical Chemistry B, 2016, 120, 8733-8742.	1.2	14
83	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.	2.3	113
84	Subdiffusion in Membrane Permeation of Small Molecules. Scientific Reports, 2016, 6, 35913.	1.6	63
85	High-speed atomic force microscopy shows that annexin V stabilizes membranes on the second timescale. Nature Nanotechnology, 2016, 11, 783-790.	15.6	96
86	The true nature of rotary movements in rotaxanes. Chemical Science, 2016, 7, 457-462.	3.7	25
87	Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2234-2244.	2.3	11
88	Why do the structural properties of complexes formed by glucans and carbon nanotubes differ so much?. RSC Advances, 2015, 5, 95682-95689.	1.7	4
89	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.	1.2	351
90	Achieving ergodic sampling using replica-exchange free-energy calculations. Molecular Simulation, 2014, 40, 218-228.	0.9	23

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91	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.	2.3	66
92	Thermodynamics of Deca-alanine Folding in Water. Journal of Chemical Theory and Computation, 2014, 10, 2836-2844.	2.3	44
93	Unveiling the Underlying Mechanism for Compression and Decompression Strokes of a Molecular Engine. Journal of Physical Chemistry C, 2014, 118, 12562-12567.	1.5	4
94	From Material Science to Avant-Garde Cuisine. The Art of Shaping Liquids into Spheres. Journal of Physical Chemistry B, 2014, 118, 11747-11756.	1.2	32
95	Calculation of Lipid-Bilayer Permeabilities Using an Average Force. Journal of Chemical Theory and Computation, 2014, 10, 554-564.	2.3	57
96	Diffusive Models of Membrane Permeation with Explicit Orientational Freedom. Journal of Chemical Theory and Computation, 2014, 10, 2710-2718.	2.3	43
97	Frontiers in freeâ€energy calculations of biological systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 71-89.	6.2	135
98	Efficient Determination of Proteinâ€“Protein Standard Binding Free Energies from First Principles. Journal of Chemical Theory and Computation, 2013, 9, 3789-3798.	2.3	188
99	How Do Membrane Transporters Sense pH? The Case of the Mitochondrial ADPâ€“ATP Carrier. Journal of Physical Chemistry Letters, 2013, 4, 3787-3791.	2.1	9
100	Dangerous Liaisons between Detergents and Membrane Proteins. The Case of Mitochondrial Uncoupling Protein 2. Journal of the American Chemical Society, 2013, 135, 15174-15182.	6.6	86
101	The substrate specificity of the human ADP/ATP carrier AAC1. Molecular Membrane Biology, 2013, 30, 160-168.	2.0	50
102	Calculating Position-Dependent Diffusivity in Biased Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 876-882.	2.3	64
103	Standard Binding Free Energies from Computer Simulations: What Is the Best Strategy?. Journal of Chemical Theory and Computation, 2013, 9, 794-802.	2.3	298
104	Water Conduction through a Peptide Nanotube. Journal of Physical Chemistry C, 2013, 117, 26797-26803.	1.5	30
105	The p7 Protein of Hepatitis C Virus Forms Structurally Plastic, Minimalist Ion Channels. PLoS Computational Biology, 2012, 8, e1002702.	1.5	60
106	Solvent-Controlled Shuttling in a Molecular Switch. Journal of Physical Chemistry C, 2012, 116, 4471-4476.	1.5	21
107	A Toolkit for the Analysis of Free-Energy Perturbation Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2606-2616.	2.3	153
108	Molecular Basis of Drug Resistance in A/H1N1 Virus. Journal of Chemical Information and Modeling, 2012, 52, 2650-2656.	2.5	23

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109	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.	2.3	29
110	Impaired Transport of Nucleotides in a Mitochondrial Carrier Explains Severe Human Genetic Diseases. ACS Chemical Biology, 2012, 7, 1164-1169.	1.6	13
111	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.	6.6	13
112	Free Energy of Nascent-Chain Folding in the Translocon. Journal of the American Chemical Society, 2011, 133, 7602-7607.	6.6	36
113	Enhanced Sampling of Multidimensional Free-Energy Landscapes Using Adaptive Biasing Forces. SIAM Journal on Applied Mathematics, 2011, 71, 1673-1695.	0.8	31
114	Free Energy Calculations for Cyclodextrin Inclusion Complexes. Current Organic Chemistry, 2011, 15, 839-847.	0.9	13
115	Polarization effects in molecular interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 844-854.	6.2	28
116	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.	0.7	0
117	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.	3.3	74
118	Good Practices in Free-Energy Calculations. Journal of Physical Chemistry B, 2010, 114, 10235-10253.	1.2	509
119	NMR Structure and Ion Channel Activity of the p7 Protein from Hepatitis C Virus. Journal of Biological Chemistry, 2010, 285, 31446-31461.	1.6	119
120	Thermodynamic Insights into the Dynamic Switching of a Cyclodextrin in a Bistable Molecular Shuttle. Journal of Physical Chemistry Letters, 2010, 1, 1776-1780.	2.1	16
121	Exploring Multidimensional Free Energy Landscapes Using Time-Dependent Biases on Collective Variables. Journal of Chemical Theory and Computation, 2010, 6, 35-47.	2.3	366
122	Polarizable Intermolecular Potentials for Water and Benzene Interacting with Halide and Metal Ions. Journal of Chemical Theory and Computation, 2009, 5, 3022-3031.	2.3	34
123	High-Chloride Concentrations Abolish the Binding of Adenine Nucleotides in the Mitochondrial ADP/ATP Carrier Family. Biophysical Journal, 2009, 97, L25-L27.	0.2	20
124	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.	6.6	130
125	Diffusion of Glycerol through Escherichia coli Aquaglyceroporin GlpF. Biophysical Journal, 2008, 94, 832-839.	0.2	98
126	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913.	2.3	41

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127	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. Journal of Chemical Theory and Computation, 2007, 3, 1914-1926.	2.3	34
128	Modeling Lipid Membranes. , 2005, , 929-958.		5
129	Scalable molecular dynamics with NAMD. Journal of Computational Chemistry, 2005, 26, 1781-1802.	1.5	15,208
130	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.	1.3	53
131	Exploring the free-energy landscape of a short peptide using an average force. Journal of Chemical Physics, 2005, 123, 244906.	1.2	113
132	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.	6.6	146
133	Modeling Lipid Membranes. , 2005, , 929-958.		2
134	Overcoming free energy barriers using unconstrained molecular dynamics simulations. Journal of Chemical Physics, 2004, 121, 2904-2914.	1.2	423
135	OPEP: A tool for the optimal partitioning of electric properties. Journal of Computational Chemistry, 2003, 24, 997-1008.	1.5	39
136	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.	1.1	104
137	Alternative Approaches for the Calculation of Induction Energies:Â Characterization, Effectiveness, and Pitfalls. Journal of Physical Chemistry A, 2001, 105, 11505-11514.	1.1	23
138	Distributed polarizabilities derived from induction energies: A finite perturbation approach. Journal of Chemical Physics, 2000, 112, 2709-2717.	1.2	40
139	Cationâ˜Ï€ Interactions in Proteins:Â Can Simple Models Provide an Accurate Description?. Journal of the American Chemical Society, 1999, 121, 10366-10372.	6.6	184
140	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.	1.2	44
141	Statistical analysis of distributed multipoles derived from molecular electrostatic potentials. Molecular Physics, 1998, 94, 881-895.	0.8	35
142	Concentrations of anesthetics across the waterâ€“membrane interface; the Meyerâ€“Overton hypothesis revisited. Toxicology Letters, 1998, 100-101, 421-430.	0.4	32
143	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.	6.6	91
144	Benzene Dimer:Â A Good Model for Ï€â˜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.	6.6	298

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145	Free Energy Methods in Drug Discoveryâ€"Introduction. ACS Symposium Series, 0, , 1-38.	0.5	24