Olle Edholm

List of Publications by Year in descending order

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52 papers	3,714 citations	185998 28 h-index	214527 47 g-index
52 all docs	52 docs citations	52 times ranked	3095 citing authors

#	Article	IF	Citations
1	Mesoscopic Undulations and Thickness Fluctuations in Lipid Bilayers from Molecular Dynamics Simulations. Biophysical Journal, 2000, 79, 426-433.	0.2	562
2	Molecular Dynamics Simulations of Phospholipid Bilayers with Cholesterol. Biophysical Journal, 2003, 84, 2192-2206.	0.2	452
3	Simulation of the Spontaneous Aggregation of Phospholipids into Bilayers. Journal of the American Chemical Society, 2001, 123, 8638-8639.	6.6	242
4	Spatial and energetic-entropic decomposition of surface tension in lipid bilayers from molecular dynamics simulations. Journal of Chemical Physics, 2000, 113, 3882-3893.	1.2	229
5	Areas of Molecules in Membranes Consisting of Mixtures. Biophysical Journal, 2005, 89, 1827-1832.	0.2	175
6	Molecular dynamics simulations of a sodium octanoate micelle in aqueous solution. Journal of Chemical Physics, 1986, 85, 2259-2271.	1.2	169
7	Effect of Ions on a Dipalmitoyl Phosphatidylcholine Bilayer. A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2008, 112, 1397-1408.	1.2	128
8	Free energy determination of polypeptide conformations generated by molecular dynamics. Macromolecules, 1984, 17, 2044-2050.	2.2	117
9	Interpretation of Fluctuation Spectra in Lipid Bilayer Simulations. Biophysical Journal, 2011, 100, 2104-2111.	0.2	117
10	Molecular dynamics simulation of NMR relaxation rates and slow dynamics in lipid bilayers. Journal of Chemical Physics, 2001, 115, 4938-4950.	1.2	109
11	Dynamics in atomistic simulations of phospholipid membranes: Nuclear magnetic resonance relaxation rates and lateral diffusion. Journal of Chemical Physics, 2006, 125, 204703.	1.2	109
12	Structure and Fluctuations of Bacteriorhodopsin in the Purple Membrane: A Molecular Dynamics Study. Journal of Molecular Biology, 1995, 250, 94-111.	2.0	103
13	Structure and Dynamics of Interfacial Water in an LÎ± Phase Lipid Bilayer from Molecular Dynamics Simulations. Biophysical Journal, 2003, 84, 102-115.	0.2	97
14	The Range and Shielding of Dipole-Dipole Interactions in Phospholipid Bilayers. Biophysical Journal, 2004, 87, 2433-2445.	0.2	83
15	Undulation Contributions to the Area Compressibility in Lipid Bilayer Simulations. Biophysical Journal, 2009, 97, 2754-2760.	0.2	82
16	Stretched exponentials and barrier distributions. Chemical Physics, 2000, 252, 221-225.	0.9	63
17	The structure of a membrane-spanning polypeptide studied by molecular dynamics. Biophysical Chemistry, 1988, 30, 279-292.	1.5	62
18	Phase Transitions in Coarse-Grained Lipid Bilayers Containing Cholesterol by Molecular Dynamics Simulations. Biophysical Journal, 2012, 103, 2125-2133.	0.2	55

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19	Effect of Force Field Parameters on Sodium and Potassium Ion Binding to Dipalmitoyl Phosphatidylcholine Bilayers. Journal of Chemical Theory and Computation, 2009, 5, 2125-2134.	2.3	54
20	Molecular dynamics study of zinc binding to cysteines in a peptide mimic of the alcohol dehydrogenase structural zinc site. Physical Chemistry Chemical Physics, 2009, 11, 975-983.	1.3	54
21	Determination of Electron Density Profiles and Area from Simulations of Undulating Membranes. Biophysical Journal, 2011, 100, 2112-2120.	0.2	54
22	Nonlinear response effects in continuum models of the hydration of ions. Journal of Chemical Physics, 2002, 116, 2936-2944.	1.2	52
23	A fast and simple method to calculate protonation states in proteins. , 1999, 36, 474-483.		51
24	Modeling of the structure of bacteriorhodopsin. Journal of Molecular Biology, 1992, 226, 837-850.	2.0	47
25	Calculated Hydration Free Energies of Small Organic Molecules Using a Nonlinear Dielectric Continuum Model. Journal of Physical Chemistry B, 2002, 106, 7889-7897.	1.2	39
26	Theoretical studies of Rhizomucor miehei lipase activation. Protein Engineering, Design and Selection, 1993, 6, 855-863.	1.0	32
27	Reparameterized United Atom Model for Molecular Dynamics Simulations of Gel and Fluid Phosphatidylcholine Bilayers. Journal of Chemical Theory and Computation, 2014, 10, 5706-5715.	2.3	32
28	A comparison between two prokaryotic potassium channels (KirBac1.1 and KcsA) in a molecular dynamics (MD) simulation study. Biophysical Chemistry, 2006, 120, 1-9.	1.5	31
29	Quantum Corrections to Classical Molecular Dynamics Simulations of Water and Ice. Journal of Chemical Theory and Computation, 2011, 7, 2903-2909.	2.3	30
30	Effect of different treatments of long-range interactions and sampling conditions in molecular dynamic simulations of rhodopsin embedded in a dipalmitoyl phosphatidylcholine bilayer. Journal of Computational Chemistry, 2007, 28, 1017-1030.	1.5	29
31	Stretched exponential dynamics in lipid bilayer simulations. Journal of Chemical Physics, 2010, 133, 115101.	1.2	26
32	pKa calculations along a bacteriorhodopsin molecular dynamics trajectory. Biophysical Chemistry, 1997, 65, 189-204.	1.5	24
33	Dynamic Structure Factors from Lipid Membrane Molecular Dynamics Simulations. Biophysical Journal, 2009, 96, 1828-1838.	0.2	23
34	Calculated Solvation Free Energies of Amino Acids in a Dipolar Approximation. Journal of Physical Chemistry B, 2001, 105, 273-281.	1.2	20
35	Dispersion Corrections to the Surface Tension at Planar Surfaces. Journal of Chemical Theory and Computation, 2016, 12, 4025-4032.	2.3	19
36	Conformation and aggregation of M13 coat protein studied by molecular dynamics. Biophysical Chemistry, 1991, 41, 193-202.	1.5	17

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37	Chapter 3 Time and Length Scales in Lipid Bilayer Simulations. Current Topics in Membranes, 2008, 60, 91-110.	0.5	17
38	Molecular dynamics simulations of Zn2+ coordination in protein binding sites. Journal of Chemical Physics, 2010, 132, 205101.	1.2	17
39	Solvent diffusion outside macromolecular surfaces. Physical Review E, 1998, 57, 791-796.	0.8	16
40	Order parameters in hydrocarbon chains. Chemical Physics, 1982, 65, 259-270.	0.9	14
41	Hydrocarbon chain dynamics in lipid bilayers. Chemistry and Physics of Lipids, 1981, 29, 213-224.	1.5	13
42	Can the structure of proteins be calculated?. European Physical Journal B, 1990, 78, 137-143.	0.6	10
43	Molecular dynamics simulation of a binary mixture near the lower critical point. Journal of Chemical Physics, 2016, 145, 014501.	1.2	10
44	Molecular dynamics study of the binding of phenylalanine stereoisomers to thermolysin. Biophysical Chemistry, 1994, 50, 237-248.	1.5	8
45	Biomolecular dynamics: A report from a workshop in Gysinge, Sweden, October 4â€“7, 1982. Quarterly Reviews of Biophysics, 1984, 17, 125-151.	2.4	7
46	Investigation of the Proton Release Channel of Bacteriorhodopsin in Different Intermediates of the Photo Cycle. A Molecular Dynamics Study. Biochemistry, 1997, 36, 2875-2883.	1.2	7
47	Hysteresis and Statistical Errors in Free Energy Perturbation L to D Amino Acid Conversion. Molecular Simulation, 1993, 10, 241-253.	0.9	6
48	The shape and free energy of a lipid bilayer surrounding a membrane inclusion. Chemistry and Physics of Lipids, 2013, 169, 2-8.	1.5	1
49	Response to ?a fast and simple method to calculate protonation states in proteins?. , 2000, 40, 4-5.		0
50	Studies of Phase Transition(s) in Phospholipid/Cholesterol Systems by Molecular Dynamics Simulations. Biophysical Journal, 2011, 100, 491a.	0.2	0
51	Molecular Dynamics Studies of Model Membranes with Alfa Helices. Springer Series in Biophysics, 1987, , 285-288.	0.4	0
52	Structure and Dynamics of Membrane Proteins. NATO ASI Series Series B: Physics, 1994, , 229-237.	0.2	0