Alan E Mark

List of Publications by Year in Descending Order

223 papers	35,808 citations	72 h-index	188 g-index
229 ext. papers	40,010 ext. citations	5.4 avg, IF	7.24 L-index

#	Paper	IF	Citations
223	Understanding the Effect of pH on the Solubility and Aggregation Extent of Humic Acid in Solution by Combining Simulation and the Experiment.. *Environmental Science & Technology*, **2022**,	10.3	1
222	Modelling of the dynamic polarizability of macromolecules for single-molecule optical biosensing.. *Scientific Reports*, **2022**, 12, 1995	4.9	3
221	Understanding the performance differences between solution and vacuum deposited OLEDs: A computational approach. *Journal of Chemical Physics*, **2022**, 156, 214703	3.9	0
220	Unraveling exciton processes in Ir(ppy):CBP OLED films upon photoexcitation. *Journal of Chemical Physics*, **2021**, 154, 164101	3.9	6
219	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bio-Molecular Systems: Overview and Perspective on Issues. *ChemPhysChem*, **2021**, 22, 264-282	3.2	2
218	Revealing the Interplay between Charge Transport, Luminescence Efficiency, and Morphology in Organic Light-Emitting Diode Blends. *Advanced Functional Materials*, **2020**, 30, 1907942	15.6	19
217	Curved or linear? Predicting the 3-dimensional structure of □helical antimicrobial peptides in an amphipathic environment. *FEBS Letters*, **2020**, 594, 1062-1080	3.8	1
216	Understanding the Activated Form of a Class-I Fusion Protein: Modeling the Interaction of the Ebola Virus Glycoprotein 2 with a Lipid Bilayer. *Biochemistry*, **2020**, 59, 4051-4058	3.2	0
215	Evolution and Morphology of Thin Films Formed by Solvent Evaporation: An Organic Semiconductor Case Study. *ACS Applied Materials & Interfaces*, **2020**, 12, 40548-40557	9.5	4
214	Effect of Triclosan and Chloroxylenol on Bacterial Membranes. *Journal of Physical Chemistry B*, **2019**, 123, 5291-5301	3.4	8
213	Response of microbial membranes to butanol: interdigitation vs. disorder. *Physical Chemistry Chemical Physics*, **2019**, 21, 11903-11915	3.6	11
212	Automated partial atomic charge assignment for drug-like molecules: a fast knapsack approach. *Algorithms for Molecular Biology*, **2019**, 14, 1	1.8	13
211	Effect of Surface Roughness on Light-Absorber Orientation in an Organic Photovoltaic Film. *Chemistry of Materials*, **2019**, 31, 6918-6924	9.6	2
210	Probing the Pharmacological Binding Sites of P-Glycoprotein Using Umbrella Sampling Simulations. *Journal of Chemical Information and Modeling*, **2019**, 59, 2287-2298	6.1	8
209	Effect of Binding on Enantioselectivity of Epoxide Hydrolase. *Journal of Chemical Information and Modeling*, **2018**, 58, 630-640	6.1	6
208	Developments in Glycopeptide Antibiotics. *ACS Infectious Diseases*, **2018**, 4, 715-735	5.5	112
207	Validierung von molekularen Simulationen: eine □bersicht verschiedener Aspekte. *Angewandte Chemie*, **2018**, 130, 894-915	3.6	3

206	Validation of Molecular Simulation: An Overview of Issues. *Angewandte Chemie - International Edition*, **2018**, 57, 884-902	16.4	74
205	A potential new, stable state of the E-cadherin strand-swapped dimer in solution. *European Biophysics Journal*, **2018**, 47, 59-67	1.9	1
204	Predicting the Prevalence of Alternative Warfarin Tautomers in Solution. *Journal of Chemical Theory and Computation*, **2018**, 14, 4405-4415	6.4	6
203	Morphology of a Bulk Heterojunction Photovoltaic Cell with Low Donor Concentration. *ACS Applied Materials & Interfaces*, **2018**, 10, 32413-32419	9.5	16
202	The reliability of molecular dynamics simulations of the multidrug transporter P-glycoprotein in a membrane environment. *PLoS ONE*, **2018**, 13, e0191882	3.7	21
201	Could Cardiolipin Protect Membranes against the Action of Certain Antimicrobial Peptides? Aurein 1.2, a Case Study. *ACS Omega*, **2018**, 3, 16453-16464	3.9	10
200	Automated Topology Builder Version 3.0: Prediction of Solvation Free Enthalpies in Water and Hexane. *Journal of Chemical Theory and Computation*, **2018**, 14, 5834-5845	6.4	174
199	Do All X-ray Structures of Protein-Ligand Complexes Represent Functional States? EPOR, a Case Study. *Biophysical Journal*, **2017**, 112, 595-604	2.9	5
198	Elucidating the Spatial Arrangement of Emitter Molecules in Organic Light-Emitting Diode Films. *Angewandte Chemie - International Edition*, **2017**, 56, 8402-8406	16.4	33
197	Elucidating the Spatial Arrangement of Emitter Molecules in Organic Light-Emitting Diode Films. *Angewandte Chemie*, **2017**, 129, 8522-8526	3.6	1
196	Real Cost of Speed: The Effect of a Time-Saving Multiple-Time-Stepping Algorithm on the Accuracy of Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 2367-2372	6.4	36
195	The Molecular Origin of Anisotropic Emission in an Organic Light-Emitting Diode. *Nano Letters*, **2017**, 17, 6464-6468	11.5	30
194	Optimization of Empirical Force Fields by Parameter Space Mapping: A Single-Step Perturbation Approach. *Journal of Chemical Theory and Computation*, **2017**, 13, 6201-6212	6.4	16
193	Bestimmung von Strukturinformation aus experimentellen Messdaten f□ Biomolek□e. *Angewandte Chemie*, **2016**, 128, 16222-16244	3.6	7
192	Deriving Structural Information from Experimentally Measured Data on Biomolecules. *Angewandte Chemie - International Edition*, **2016**, 55, 15990-16010	16.4	21
191	The CC domain structure from the wheat stem rust resistance protein Sr33 challenges paradigms for dimerization in plant NLR proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 12856-12861	11.5	72
190	Interaction of Tarantula Venom Peptide ProTx-II with Lipid Membranes Is a Prerequisite for Its Inhibition of Human Voltage-gated Sodium Channel NaV1.7. *Journal of Biological Chemistry*, **2016**, 291, 17049-65	5.4	52
189	Validating lipid force fields against experimental data: Progress, challenges and perspectives. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1556-65	3.8	51

188	Understanding the accumulation of P-glycoprotein substrates within cells: The effect of cholesterol on membrane partitioning. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 776-82	3.8	12
187	Combination of Ambiguous and Unambiguous Data in the Restraint-driven Docking of Flexible Peptides with HADDOCK: The Binding of the Spider Toxin PcTx1 to the Acid Sensing Ion Channel (ASIC) 1a. *Journal of Chemical Information and Modeling*, **2016**, 56, 127-38	6.1	6
186	Revisiting the scissor-like mechanism of activation for the erythropoietin receptor. *FEBS Letters*, **2016**, 590, 3083-8	3.8	1
185	Membrane-binding properties of gating modifier and pore-blocking toxins: Membrane interaction is not a prerequisite for modification of channel gating. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 872-82	3.8	20
184	Binding of Starch Fragments to the Starch Branching Enzyme: Implications for Developing Slower-Digesting Starch. *Biomacromolecules*, **2015**, 16, 2475-81	6.9	5
183	A ring to rule them all: the effect of cyclopropane Fatty acids on the fluidity of lipid bilayers. *Journal of Physical Chemistry B*, **2015**, 119, 5487-95	3.4	80
182	Effect of Ring Size in Alicyclic Fatty Acids on the Structural and Dynamical Properties Associated with Fluidity in Lipid Bilayers. *Langmuir*, **2015**, 31, 11574-82	4	5
181	Molecular dynamics and functional studies define a hot spot of crystal contacts essential for PcTx1 inhibition of acid-sensing ion channel 1a. *British Journal of Pharmacology*, **2015**, 172, 4985-95	8.6	29
180	Identification of Possible Binding Sites for Morphine and Nicardipine on the Multidrug Transporter P-Glycoprotein Using Umbrella Sampling Techniques. *Journal of Chemical Information and Modeling*, **2015**, 55, 1202-17	6.1	23
179	The characterization of modified starch branching enzymes: toward the control of starch chain-length distributions. *PLoS ONE*, **2015**, 10, e0125507	3.7	18
178	Testing and validation of the Automated Topology Builder (ATB) version 2.0: prediction of hydration free enthalpies. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 221-33	4.2	334
177	Mechanism of activation of protein kinase JAK2 by the growth hormone receptor. *Science*, **2014**, 344, 1249783	33.3	269
176	Determining the structure of interfacial peptide films: comparing neutron reflectometry and molecular dynamics simulations. *Langmuir*, **2014**, 30, 10080-9	4	17
175	Activation of the epidermal growth factor receptor: a series of twists and turns. *Biochemistry*, **2014**, 53, 2710-21	3.2	11
174	The revised Penrose-Hameroff orchestrated objective-reduction proposal for human consciousness is not scientifically justified: comment on "Consciousness in the universe: a review of the Orch ORP theory" by Hameroff and Penrose. *Physics of Life Reviews*, **2014**, 11, 101-3; discussion 104-12	2.1	8
173	Structural characterization of two metastable ATP-bound states of P-glycoprotein. *PLoS ONE*, **2014**, 9, e91916	3.7	24
172	Small-Angle X-Ray Scattering for the Discerning Macromolecular Crystallographer. *Australian Journal of Chemistry*, **2014**, 67, 1786	1.2	2
171	Some Like It Hot: The Effect of Sterols and Hopanoids on Lipid Ordering at High Temperature. *Journal of Physical Chemistry Letters*, **2014**, 5, 3953-7	6.4	17

170	Does tautomerization of FapyG influence its mutagenicity?. *ChemPhysChem*, **2014**, 15, 1779-84	3.2	10
169	The recognition of membrane-bound PtdIns3P by PX domains. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 2332-42	4.2	9
168	Effect of methyl-branched fatty acids on the structure of lipid bilayers. *Journal of Physical Chemistry B*, **2014**, 118, 13838-48	3.4	49
167	Study of Proteins and Peptides at Interfaces by Molecular Dynamics Simulation Techniques **2013**, 291-313		1
166	The relative effect of sterols and hopanoids on lipid bilayers: when comparable is not identical. *Journal of Physical Chemistry B*, **2013**, 117, 16129-40	3.4	39
165	Charge group partitioning in biomolecular simulation. *Journal of Computational Biology*, **2013**, 20, 188-98	1.7	120
164	Vancomycin: ligand recognition, dimerization and super-complex formation. *FEBS Journal*, **2013**, 280, 1294-307	5.7	29
163	Missing fragments: detecting cooperative binding in fragment-based drug design. *ACS Medicinal Chemistry Letters*, **2012**, 3, 322-6	4.3	21
162	Lipid Bilayers: The Effect of Force Field on Ordering and Dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 4807-17	6.4	66
161	Charge Group Partitioning in Biomolecular Simulation. *Lecture Notes in Computer Science*, **2012**, 29-43	0.9	5
160	Wilfred van Gunsteren: 35 Years of Biomolecular Simulation. *Journal of Chemical Theory and Computation*, **2012**, 8, 3425-9	6.4	0
159	Molecular dynamics simulations of the interactions of DMSO with DPPC and DOPC phospholipid membranes. *Journal of Physical Chemistry B*, **2012**, 116, 11911-23	3.4	53
158	Molecular dynamics unlocks atomic level self-assembly of the exopolysaccharide matrix of water-treatment granular biofilms. *Biomacromolecules*, **2012**, 13, 1965-72	6.9	16
157	Mimicking the action of folding chaperones by Hamiltonian replica-exchange molecular dynamics simulations: application in the refinement of de novo models. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1744-54	4.2	12
156	The Effect of Environment on the Structure of a Membrane Protein: P-Glycoprotein under Physiological Conditions. *Journal of Chemical Theory and Computation*, **2012**, 8, 3964-76	6.4	40
155	The effect of environment on the recognition and binding of vancomycin to native and resistant forms of lipid II. *Biophysical Journal*, **2011**, 101, 2684-92	2.9	28
154	Effect of high pressure on fully hydrated DPPC and POPC bilayers. *Journal of Physical Chemistry B*, **2011**, 115, 1038-44	3.4	26
153	A dynamic pharmacophore drives the interaction between Psalmotoxin-1 and the putative drug target acid-sensing ion channel 1a. *Molecular Pharmacology*, **2011**, 80, 796-808	4.3	78

152	Effect of poly(ethylene glycol) (PEG) spacers on the conformational properties of small peptides: a molecular dynamics study. *Langmuir*, **2011**, 27, 296-303	4	28
151	An Automated Force Field Topology Builder (ATB) and Repository: Version 1.0. *Journal of Chemical Theory and Computation*, **2011**, 7, 4026-37	6.4	1030
150	Challenges in the determination of the binding modes of non-standard ligands in X-ray crystal complexes. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 1-12	4.2	23
149	The effect of membrane curvature on the conformation of antimicrobial peptides: implications for binding and the mechanism of action. *European Biophysics Journal*, **2011**, 40, 545-53	1.9	46
148	Definition and testing of the GROMOS force-field versions 54A7 and 54B7. *European Biophysics Journal*, **2011**, 40, 843-56	1.9	1326
147	Protein □Turns Recreated in Structurally Stable Small Molecules. *Angewandte Chemie*, **2011**, 123, 11303-11307	3.6	8
146	Protein □turns recreated in structurally stable small molecules. *Angewandte Chemie - International Edition*, **2011**, 50, 11107-11	16.4	19
145	Using Theory to Reconcile Experiment: The Structural and Thermodynamic Basis of Ligand Recognition by Phenylethanolamine N-Methyltransferase (PNMT). *Journal of Chemical Theory and Computation*, **2011**, 7, 1458-68	6.4	13
144	Comparison of enveloping distribution sampling and thermodynamic integration to calculate binding free energies of phenylethanolamine N-methyltransferase inhibitors. *Journal of Chemical Physics*, **2011**, 135, 024105	3.9	36
143	Activating the Prolactin Receptor: Effect of the Ligand on the Conformation of the Extracellular Domain. *Journal of Chemical Theory and Computation*, **2010**, 6, 3274-83	6.4	2
142	On the Validation of Molecular Dynamics Simulations of Saturated and cis-Monounsaturated Phosphatidylcholine Lipid Bilayers: A Comparison with Experiment. *Journal of Chemical Theory and Computation*, **2010**, 6, 325-36	6.4	232
141	Basic ingredients of free energy calculations: a review. *Journal of Computational Chemistry*, **2010**, 31, 1569-82	3.5	225
140	On the relative merits of equilibrium and non-equilibrium simulations for the estimation of free-energy differences. *ChemPhysChem*, **2010**, 11, 3734-43	3.2	9
139	A new force field for simulating phosphatidylcholine bilayers. *Journal of Computational Chemistry*, **2010**, 31, 1117-25	3.5	261
138	Turning the growth hormone receptor on: evidence that hormone binding induces subunit rotation. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1163-74	4.2	17
137	Weak, strong, and coherent regimes of Fr□lich condensation and their applications to terahertz medicine and quantum consciousness. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 4219-24	11.5	74
136	Probing the free energy landscape of the FBP28WW domain using multiple techniques. *Journal of Computational Chemistry*, **2009**, 30, 1059-68	3.5	6
135	Calcium binding to the purple membrane: A molecular dynamics study. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 669-81	4.2	5

134	Inclusion of ionization states of ligands in affinity calculations. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 138-50	4.2	9
133	Binding and enantiomeric selectivity of threonyl-tRNA synthetase. *Journal of the American Chemical Society*, **2009**, 131, 3848-9	16.4	13
132	Factors that affect the degree of twist in beta-sheet structures: a molecular dynamics simulation study of a cross-beta filament of the GNNQQNY peptide. *Journal of Physical Chemistry B*, **2009**, 113, 1728-37	3.4	54
131	Disturb or stabilize? A molecular dynamics study of the effects of resorcinolic lipids on phospholipid bilayers. *Biophysical Journal*, **2009**, 96, 3140-53	2.9	18
130	Alternative mechanisms for the interaction of the cell-penetrating peptides penetratin and the TAT peptide with lipid bilayers. *Biophysical Journal*, **2009**, 97, 40-9	2.9	143
129	Penrose-Hameroff orchestrated objective-reduction proposal for human consciousness is not biologically feasible. *Physical Review E*, **2009**, 80, 021912	2.4	48
128	Molecular simulation as an aid to experimentalists. *Current Opinion in Structural Biology*, **2008**, 18, 149-53	8.1	150
127	The structure of a two-disulfide intermediate assists in elucidating the oxidative folding pathway of a cyclic cystine knot protein. *Structure*, **2008**, 16, 842-51	5.2	34
126	Application of mean field boundary potentials in simulations of lipid vesicles. *Journal of Physical Chemistry B*, **2008**, 112, 7438-47	3.4	57
125	The Cys3-Cys4 loop of the hydrophobin EAS is not required for rodlet formation and surface activity. *Journal of Molecular Biology*, **2008**, 382, 708-20	6.5	60
124	Toroidal pores formed by antimicrobial peptides show significant disorder. *Biochimica Et Biophysica Acta - Biomembranes*, **2008**, 1778, 2308-17	3.8	364
123	Histidine protonation and the activation of viral fusion proteins. *Biochemical Society Transactions*, **2008**, 36, 43-5	5.1	51
122	The conformation of the extracellular binding domain of Death Receptor 5 in the presence and absence of the activating ligand TRAIL: a molecular dynamics study. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 333-43	4.2	14
121	Refining homology models by combining replica-exchange molecular dynamics and statistical potentials. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 1171-88	4.2	65
120	Electrophoretic mobility does not always reflect the charge on an oil droplet. *Journal of Colloid and Interface Science*, **2008**, 318, 477-86	9.3	45
119	How sensitive are nanosecond molecular dynamics simulations of proteins to changes in the force field?. *Journal of Physical Chemistry B*, **2007**, 111, 6015-25	3.4	16
118	On the characterization of host-guest complexes: surface tension, calorimetry, and molecular dynamics of cyclodextrins with a non-ionic surfactant. *Journal of Physical Chemistry B*, **2007**, 111, 4383-92	3.4	89
117	Molecular dynamics simulations from putative transition states of alpha-spectrin SH3 domain. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 536-50	4.2	13

116	Applications of Free Energy Calculations to Chemistry and Biology. *Springer Series in Chemical Physics*, **2007**, 463-501	0.3	11
115	Convergence and sampling efficiency in replica exchange simulations of peptide folding in explicit solvent. *Journal of Chemical Physics*, **2007**, 126, 014903	3.9	105
114	Does isoprene protect plant membranes from thermal shock? A molecular dynamics study. *Biochimica Et Biophysica Acta - Biomembranes*, **2007**, 1768, 198-206	3.8	81
113	Ion transport across transmembrane pores. *Biophysical Journal*, **2007**, 92, 4209-15	2.9	80
112	The Role of histidine residues in low-pH-mediated viral membrane fusion. *Structure*, **2006**, 14, 1481-7	5.2	120
111	The effect of box shape on the dynamic properties of proteins simulated under periodic boundary conditions. *Journal of Computational Chemistry*, **2006**, 27, 316-25	3.5	28
110	Antimicrobial peptides in action. *Journal of the American Chemical Society*, **2006**, 128, 12156-61	16.4	372
109	Phase behavior of a phospholipid/fatty acid/water mixture studied in atomic detail. *Journal of the American Chemical Society*, **2006**, 128, 2030-4	16.4	43
108	Conformational polymorphism of the PrP106-126 peptide in different environments: a molecular dynamics study. *Journal of Physical Chemistry B*, **2006**, 110, 1423-8	3.4	34
107	Molecular dynamics simulations of the hydrophobin SC3 at a hydrophobic/hydrophilic interface. *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 863-73	4.2	27
106	Mimicking the action of GroEL in molecular dynamics simulations: application to the refinement of protein structures. *Protein Science*, **2006**, 15, 441-8	6.3	8
105	Molecular structure of the lecithin ripple phase. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 5392-6	11.5	146
104	A molecular dynamics study of the formation, stability, and oligomerization state of two designed coiled coils: possibilities and limitations. *Biophysical Journal*, **2005**, 89, 3701-13	2.9	23
103	A molecular dynamics study of the structural stability of HIV-1 protease under physiological conditions: the role of Na+ ions in stabilizing the active site. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 450-8	4.2	19
102	Advanced approaches for the characterization of a de novo designed antiparallel coiled coil peptide. *Organic and Biomolecular Chemistry*, **2005**, 3, 1189-94	3.9	22
101	Incorporating the effect of ionic strength in free energy calculations using explicit ions. *Journal of Computational Chemistry*, **2005**, 26, 115-22	3.5	35
100	GROMACS: fast, flexible, and free. *Journal of Computational Chemistry*, **2005**, 26, 1701-18	3.5	10273
99	Stability of SIV gp32 fusion-peptide single-layer protofibrils as monitored by molecular-dynamics simulations. *Angewandte Chemie - International Edition*, **2005**, 44, 1065-1067	16.4	21

98	Stability of SIV gp32 Fusion-Peptide Single-Layer Protofibrils as Monitored by Molecular-Dynamics Simulations. *Angewandte Chemie*, **2005**, 117, 1089-1091	3.6	4
97	Calculation of the redox potential of the protein azurin and some mutants. *ChemBioChem*, **2005**, 6, 738-46	3.8	46
96	Simulation of gel phase formation and melting in lipid bilayers using a coarse grained model. *Chemistry and Physics of Lipids*, **2005**, 135, 223-44	3.7	261
95	Comparative study of generalized Born models: protein dynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6760-4	11.5	63
94	Simulation studies of pore and domain formation in a phospholipid monolayer. *Journal of Chemical Physics*, **2005**, 122, 024704	3.9	48
93	Electrofreezing of confined water. *Journal of Chemical Physics*, **2004**, 120, 7123-30	3.9	99
92	Mimicking the action of folding chaperones in molecular dynamics simulations: Application to the refinement of homology-based protein structures. *Protein Science*, **2004**, 13, 992-9	6.3	15
91	A biomolecular force field based on the free enthalpy of hydration and solvation: the GROMOS force-field parameter sets 53A5 and 53A6. *Journal of Computational Chemistry*, **2004**, 25, 1656-76	3.5	2844
90	Photoactivation of the photoactive yellow protein: why photon absorption triggers a trans-to-cis Isomerization of the chromophore in the protein. *Journal of the American Chemical Society*, **2004**, 126, 4228-33	16.4	246
89	Refinement of homology-based protein structures by molecular dynamics simulation techniques. *Protein Science*, **2004**, 13, 211-20	6.3	154
88	Molecular view of hexagonal phase formation in phospholipid membranes. *Biophysical Journal*, **2004**, 87, 3894-900	2.9	167
87	Molecular dynamics simulation of the spontaneous formation of a small DPPC vesicle in water in atomistic detail. *Journal of the American Chemical Society*, **2004**, 126, 4488-9	16.4	150
86	Coarse Grained Model for Semiquantitative Lipid Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 750-760	3.4	1767
85	The Binary Mixing Behavior of Phospholipids in a Bilayer: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2004**, 108, 2454-2463	3.4	104
84	Molecular dynamics simulations of hydrophilic pores in lipid bilayers. *Biophysical Journal*, **2004**, 86, 2156-64	2.9	248
83	Sampling and convergence in free energy calculations of protein-ligand interactions: the binding of triphenoxypyridine derivatives to factor Xa and trypsin. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 673-86	4.2	21
82	Relative stability of protein structures determined by X-ray crystallography or NMR spectroscopy: a molecular dynamics simulation study. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 111-20	4.2	44
81	Monolayer ice. *Physical Review Letters*, **2003**, 91, 025502	7.4	195

80	The mechanism of vesicle fusion as revealed by molecular dynamics simulations. *Journal of the American Chemical Society*, **2003**, 125, 11144-5	16.4	278
79	The Influence of Trifluoromethyl Groups on the Miscibility of Fluorinated Alcohols with Water: A Molecular Dynamics Simulation Study of 1,1,1-Trifluoropropan-2-ol in Aqueous Solution. *Journal of Physical Chemistry B*, **2003**, 107, 4855-4861	3.4	11
78	Understanding binding affinity: a combined isothermal titration calorimetry/molecular dynamics study of the binding of a series of hydrophobically modified benzamidinium chloride inhibitors to trypsin. *Journal of the American Chemical Society*, **2003**, 125, 10570-9	16.4	90
77	Simulation of MscL gating in a bilayer under stress. *Biophysical Journal*, **2003**, 84, 2331-7	2.9	67
76	Simulation of pore formation in lipid bilayers by mechanical stress and electric fields. *Journal of the American Chemical Society*, **2003**, 125, 6382-3	16.4	363
75	Molecular dynamics simulation of the formation, structure, and dynamics of small phospholipid vesicles. *Journal of the American Chemical Society*, **2003**, 125, 15233-42	16.4	263
74	Bilayer ice and alternate liquid phases of confined water. *Journal of Chemical Physics*, **2003**, 119, 1694-1700	3.0	114
73	Computation of Free Energy. *Helvetica Chimica Acta*, **2002**, 85, 3113-3129	2	85
72	Calculation of the free energy of solvation for neutral analogs of amino acid side chains. *Journal of Computational Chemistry*, **2002**, 23, 548-53	3.5	157
71	Entropy calculations on the molten globule state of a protein: side-chain entropies of alpha-lactalbumin. *Proteins: Structure, Function and Bioinformatics*, **2002**, 46, 215-24	4.2	55
70	Folding and stability of the three-stranded beta-sheet peptide Betanova: insights from molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2002**, 46, 380-92	4.2	45
69	Signal transduction in the photoactive yellow protein. II. Proton transfer initiates conformational changes. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 212-9	4.2	36
68	Signal transduction in the photoactive yellow protein. I. Photon absorption and the isomerization of the chromophore. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 202-11	4.2	61
67	A comparison of methods for calculating NMR cross-relaxation rates (NOESY and ROESY intensities) in small peptides. *Journal of Biomolecular NMR*, **2002**, 23, 181-94	3	28
66	Mechanism by which 2,2,2-trifluoroethanol/water mixtures stabilize secondary-structure formation in peptides: a molecular dynamics study. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 12179-84	11.5	406
65	The Effect of the Neglect of Electronic Polarization in Peptide Folding Simulations. *Journal of Physical Chemistry B*, **2002**, 106, 12830-12833	3.4	16
64	Molecular dynamics simulations of mixed micelles modeling human bile. *Biochemistry*, **2002**, 41, 5375-82	3.2	81
63	Dynamic Conformations of Flavin Adenine Dinucleotide: Simulated Molecular Dynamics of the Flavin Cofactor Related to the Time-Resolved Fluorescence Characteristics. *Journal of Physical Chemistry B*, **2002**, 106, 8858-8869	3.4	113

62	Molecular dynamics study of the folding of hydrophobin SC3 at a hydrophilic/hydrophobic interface. *Biophysical Journal*, **2002**, 83, 112-24	2.9	44
61	Folding study of an Aib-rich peptide in DMSO by molecular dynamics simulations. *Chemical Biology and Drug Design*, **2001**, 57, 107-18		36
60	Free energy barrier estimation of unfolding the alpha-helical surfactant-associated polypeptide C. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 395-402	4.2	9
59	Entropy calculations on a reversibly folding peptide: changes in solute free energy cannot explain folding behavior. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 45-56	4.2	85
58	Further investigation on the validity of StokesEinstein behaviour at the molecular level. *Chemical Physics Letters*, **2001**, 334, 337-342	2.5	22
57	Model of 1,1,1,3,3,3-Hexafluoro-propan-2-ol for Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2001**, 105, 10967-10975	3.4	66
56	Essential dynamics of reversible peptide folding: memory-free conformational dynamics governed by internal hydrogen bonds. *Journal of Molecular Biology*, **2001**, 309, 299-313	6.5	119
55	Investigation of the mechanism of domain closure in citrate synthase by molecular dynamics simulation. *Journal of Molecular Biology*, **2001**, 310, 1039-53	6.5	44
54	Effect of Undulations on Surface Tension in Simulated Bilayers. *Journal of Physical Chemistry B*, **2001**, 105, 6122-6127	3.4	237
53	Simulation of the spontaneous aggregation of phospholipids into bilayers. *Journal of the American Chemical Society*, **2001**, 123, 8638-9	16.4	223
52	Entropy calculations on a reversibly folding peptide: Changes in solute free energy cannot explain folding behavior **2001**, 43, 45		1
51	The GROMOS96 benchmarks for molecular simulation. *Computer Physics Communications*, **2000**, 128, 550-557	4.2	26
50	On the temperature and pressure dependence of a range of properties of a type of water model commonly used in high-temperature protein unfolding simulations. *Biophysical Journal*, **2000**, 78, 2752-60	2.9	39
49	Molecular Dynamics Simulation of the Kinetics of Spontaneous Micelle Formation. *Journal of Physical Chemistry B*, **2000**, 104, 12165-12173	3.4	248
48	A New 2,2,2-Trifluoroethanol Model for Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2000**, 104, 12347-12354	3.4	99
47	Absolute entropies from molecular dynamics simulation trajectories. *Journal of Chemical Physics*, **2000**, 113, 7809-7817	3.9	158
46	The effect of force-field parameters on properties of liquids: Parametrization of a simple three-site model for methanol. *Journal of Chemical Physics*, **2000**, 112, 10450-10459	3.9	120
45	On the validity of StokesPlaw at the molecular level. *Chemical Physics Letters*, **1999**, 303, 583-586	2.5	43

44	Peptide folding simulations: no solvent required?. *Computer Physics Communications*, **1999**, 123, 97-102	4.2	32
43	Estimating relative free energies from a single ensemble: Hydration free energies. *Journal of Computational Chemistry*, **1999**, 20, 1604-1617	3.5	55
42	Folding-unfolding thermodynamics of a beta-heptapeptide from equilibrium simulations. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 269-80	4.2	330
41	The effect of motional averaging on the calculation of NMR-derived structural properties **1999**, 36, 542-555		83
40	Peptidfaltung: Wenn die Simulation das Experiment erreicht. *Angewandte Chemie*, **1999**, 111, 249-253	3.6	51
39	Peptide Folding: When Simulation Meets Experiment. *Angewandte Chemie - International Edition*, **1999**, 38, 236-240	16.4	1258
38	The GROMOS Biomolecular Simulation Program Package. *Journal of Physical Chemistry A*, **1999**, 103, 3596-3607	2.8	1220
37	Estimating Relative Free Energies from a Single Simulation of the Initial State. *Lecture Notes in Computational Science and Engineering*, **1999**, 149-162	0.3	1
36	Peptide Folding: When Simulation Meets Experiment **1999**, 38, 236		54
35	On using time-averaging restraints in molecular dynamics simulation. *Journal of Biomolecular NMR*, **1998**, 12, 501-8	3	25
34	Parametrization of aliphatic CHn united atoms of GROMOS96 force field **1998**, 19, 535-547		335
33	Reversible peptide folding in solution by molecular dynamics simulation. *Journal of Molecular Biology*, **1998**, 280, 925-32	6.5	340
32	Molecular dynamics simulations of peptide fragments from hen lysozyme: insight into non-native protein conformations. *Journal of Molecular Biology*, **1998**, 280, 703-19	6.5	12
31	Validation of molecular dynamics simulation. *Journal of Chemical Physics*, **1998**, 108, 6109-6116	3.9	139
30	Solvent structure at a hydrophobic protein surface. *Proteins: Structure, Function and Bioinformatics*, **1997**, 27, 395-404	4.2	42
29	Free Energies of Transfer of Trp Analogs from Chloroform to Water: Comparison of Theory and Experiment and the Importance of Adequate Treatment of Electrostatic and Internal Interactions. *Journal of the American Chemical Society*, **1996**, 118, 6285-6294	16.4	47
28	Estimating the Relative Free Energy of Different Molecular States with Respect to a Single Reference State. *The Journal of Physical Chemistry*, **1996**, 100, 9485-9494		146
27	Computational approaches to study protein unfolding: hen egg white lysozyme as a case study. *Proteins: Structure, Function and Bioinformatics*, **1995**, 21, 196-213	4.2	89

26	Comparison of MD simulations and NMR experiments for hen lysozyme. Analysis of local fluctuations, cooperative motions, and global changes. *Biochemistry*, **1995**, 34, 10918-31	3.2	120
25	Fluctuation and cross-correlation analysis of protein motions observed in nanosecond molecular dynamics simulations. *Journal of Molecular Biology*, **1995**, 252, 492-503	6.5	332
24	The effect of environment on the stability of an integral membrane helix: molecular dynamics simulations of surfactant protein C in chloroform, methanol and water. *Journal of Molecular Biology* , **1995**, 247, 808-22	6.5	34
23	Computer simulation of protein motion. *Computer Physics Communications*, **1995**, 91, 305-319	4.2	48
22	Fundamentals of drug design from a biophysical viewpoint. *Quarterly Reviews of Biophysics*, **1994**, 27, 435-81	7	20
21	Avoiding singularities and numerical instabilities in free energy calculations based on molecular simulations. *Chemical Physics Letters*, **1994**, 222, 529-539	2.5	819
20	Convergence Properties of Free Energy Calculations: .alpha.-Cyclodextrin Complexes as a Case Study. *Journal of the American Chemical Society*, **1994**, 116, 6293-6302	16.4	150
19	Decomposition of the free energy of a system in terms of specific interactions. Implications for theoretical and experimental studies. *Journal of Molecular Biology*, **1994**, 240, 167-76	6.5	289
18	Investigation of shape variations in the antibody binding site by molecular dynamics computer simulation. *Journal of Molecular Biology*, **1994**, 236, 1186-95	6.5	15
17	Solvent-dependent conformation and hydrogen-bonding capacity of cyclosporin A: evidence from partition coefficients and molecular dynamics simulations. *Journal of Medicinal Chemistry*, **1993**, 36, 3757-64	8.3	169
16	Can the stability of protein mutants be predicted by free energy calculations?. *Protein Engineering, Design and Selection*, **1993**, 6, 289-95	1.9	72
15	Dielectric properties of trypsin inhibitor and lysozyme calculated from molecular dynamics simulations. *The Journal of Physical Chemistry*, **1993**, 97, 2009-2014		167
14	An approximate but efficient method to calculate free energy trends by computer simulation: application to dihydrofolate reductase-inhibitor complexes. *Journal of Computer-Aided Molecular Design*, **1993**, 7, 305-23	4.2	38
13	On the interpretation of biochemical data by molecular dynamics computer simulation **1993**, 63-77		
12	Simulation of the thermal denaturation of hen egg white lysozyme: trapping the molten globule state. *Biochemistry*, **1992**, 31, 7745-8	3.2	141
11	Prediction of the activity and stability effects of site-directed mutagenesis on a protein core. *Journal of Molecular Biology*, **1992**, 227, 389-95	6.5	39
10	Construction and molecular dynamics simulation of calmodulin in the extended and in a bent conformation. *FEBS Journal*, **1992**, 204, 931-7		24
9	On the interpretation of biochemical data by molecular dynamics computer simulation. *FEBS Journal*, **1992**, 204, 947-61		105

8	Conformational flexibility of aqueous monomeric and dimeric insulin: a molecular dynamics study. *Biochemistry*, **1991**, 30, 10866-72	3.2	39
7	Calculation of relative free energy via indirect pathways. *Journal of Chemical Physics*, **1991**, 94, 3808-3816	3.9	70
6	The self-association of zinc-free bovine insulin. Four model patterns and their significance. *Biological Chemistry Hoppe-Seyler*, **1990**, 371, 1165-74		21
5	The binding of an indefinitely associating ligand to acceptor: consideration of monovalent ligand species binding to a multivalent acceptor. *Journal of Theoretical Biology*, **1988**, 131, 137-49	2.3	4
4	The self-association of zinc-free bovine insulin. A single model based on interactions in the crystal that describes the association pattern in solution at pH 2, 7 and 10. *Biophysical Chemistry*, **1987**, 27, 103-17	3.5	25
3	Interaction of analogs of nicotinamide adenine dinucleotide phosphate with dihydrofolate reductase from Escherichia coli. *Biochemistry*, **1984**, 23, 4340-4346	3.2	13
2	Free Energy Perturbation Calculations		4
1	GROMOS Force Field		14