Charles L Brooks

List of Publications by Year in Descending Order

251 papers	31,053 citations	73 h-index	174 g-index
261 ext. papers	34,712 ext. citations	7.7 avg, IF	7.32 L-index

#	Paper	IF	Citations
251	Optimizing Multisite Dynamics Throughput with Charge Renormalization.. *Journal of Chemical Information and Modeling*, **2022**, 62, 1479-1488	6.1	1
250	Allostery in the dynamic coactivator domain KIX occurs through minor conformational micro-states.. *PLoS Computational Biology*, **2022**, 18, e1009977	5	
249	Flexible CDOCKER: Hybrid Searching Algorithm and Scoring Function with Side Chain Conformational Entropy. *Journal of Chemical Information and Modeling*, **2021**, 61, 5535-5549	6.1	1
248	BLaDE: A Basic Lambda Dynamics Engine for GPU-Accelerated Molecular Dynamics Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2021**, 17, 6799-6807	6.4	1
247	TMPRSS2 inhibitor discovery facilitated through an and biochemical screening platform **2021**,		4
246	Capturing the Catalytic Proton of Dihydrofolate Reductase: Implications for General Acid-Base Catalysis. *ACS Catalysis*, **2021**, 11, 5873-5884	13.1	0
245	A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. *Journal of Computational Chemistry*, **2021**, 42, 1088-1094	3.5	3
244	Norstictic Acid Is a Selective Allosteric Transcriptional Regulator. *Journal of the American Chemical Society*, **2021**, 143, 9297-9302	16.4	4
243	Generalizing the Discrete Gibbs Sampler-Based Dynamics Approach for Multisite Sampling of Many Ligands. *Journal of Chemical Theory and Computation*, **2021**, 17, 3895-3907	6.4	1
242	VIPERdb v3.0: a structure-based data analytics platform for viral capsids. *Nucleic Acids Research*, **2021**, 49, D809-D816	20.1	7
241	Accelerated CDOCKER with GPUs, Parallel Simulated Annealing, and Fast Fourier Transforms. *Journal of Chemical Theory and Computation*, **2020**, 16, 3910-3919	6.4	16
240	Exploring pH Dependent Host/Guest Binding Affinities. *Journal of Physical Chemistry B*, **2020**, 124, 6520-6528	3.4	2
239	Electrostatic Forces Control the Negative Allosteric Regulation in a Disordered Protein Switch. *Journal of Physical Chemistry Letters*, **2020**, 11, 864-868	6.4	8
238	M2 amphipathic helices facilitate pH-dependent conformational transition in influenza A virus. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 3583-3591	11.5	6
237	Accelerating the Generalized Born with Molecular Volume and Solvent Accessible Surface Area Implicit Solvent Model Using Graphics Processing Units. *Journal of Computational Chemistry*, **2020**, 41, 830-838	3.5	7
236	Automated, Accurate, and Scalable Relative Protein-Ligand Binding Free-Energy Calculations Using Lambda Dynamics. *Journal of Chemical Theory and Computation*, **2020**, 16, 7895-7914	6.4	16
235	Computational Studies of Catalytic Loop Dynamics in Protein Tyrosine Phosphatase Using Pathway Optimization Methods. *Journal of Physical Chemistry B*, **2019**, 123, 7840-7851	3.4	1

234	Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. *Journal of Physical Chemistry B*, **2019**, 123, 8065-8073	3.4	8
233	Enhanced Sampling Applied to Modeling Allosteric Regulation in Transcription. *Journal of Physical Chemistry Letters*, **2019**, 10, 5963-5968	6.4	9
232	Fast Solver for Large Scale Multistate Bennett Acceptance Ratio Equations. *Journal of Chemical Theory and Computation*, **2019**, 15, 799-802	6.4	16
231	Molecular Mechanisms of Interactions between Monolayered Transition Metal Dichalcogenides and Biological Molecules. *Journal of the American Chemical Society*, **2019**, 141, 9980-9988	16.4	18
230	Positioning-Group-Enabled Biocatalytic Oxidative Dearomatization. *ACS Central Science*, **2019**, 5, 1010-1016	10.8	6
229	Structural basis for selectivity in flavin-dependent monooxygenase-catalyzed oxidative dearomatization. *ACS Catalysis*, **2019**, 9, 3633-3640	13.1	17
228	Overcoming Challenging Substituent Perturbations with Multisite Dynamics: A Case Study Targeting Secretase 1. *Journal of Physical Chemistry Letters*, **2019**, 10, 4875-4880	6.4	10
227	Frustration and folding of a TIM barrel protein. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 16378-16383	11.5	11
226	Modeling pH-Dependent NMR Chemical Shift Perturbations in Peptides. *Biophysical Journal*, **2019**, 117, 258-268	2.9	1
225	Deciphering protein evolution and fitness landscapes with latent space models. *Nature Communications*, **2019**, 10, 5644	17.4	25
224	CDOCKER and dynamics for prospective prediction in DR Grand Challenge 2. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 89-102	4.2	5
223	Conservation of coactivator engagement mechanism enables small-molecule allosteric modulators. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 8960-8965	11.5	11
222	Molecular interactions between single layered MoS and biological molecules. *Chemical Science*, **2018**, 9, 1769-1773	9.4	20
221	Effect of immobilization site on the orientation and activity of surface-tethered enzymes. *Physical Chemistry Chemical Physics*, **2018**, 20, 1021-1029	3.6	29
220	Investigating the Effect of Two-Point Surface Attachment on Enzyme Stability and Activity. *Journal of the American Chemical Society*, **2018**, 140, 16560-16569	16.4	33
219	Reply to Misreading chaperone-substrate complexes from random noise *Nature Structural and Molecular Biology*, **2018**, 25, 990-991	17.6	1
218	VIPERdb: A Tool for Virus Research. *Annual Review of Virology*, **2018**, 5, 477-488	14.6	20
217	Ligand Modulates Cross-Coupling between Riboswitch Folding and Transcriptional Pausing. *Molecular Cell*, **2018**, 72, 541-552.e6	17.6	26

216	Approaching protein design with multisite λdynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. *Protein Science*, **2018**, 27, 1910-1922	6.3	11
215	Predicting Binding Free Energies in a Large Combinatorial Chemical Space Using Multisite λ Dynamics. *Journal of Physical Chemistry Letters*, **2018**, 9, 3328-3332	6.4	17
214	Molecular Interactions between Graphene and Biological Molecules. *Journal of the American Chemical Society*, **2017**, 139, 1928-1936	16.4	77
213	Exploring Protein-Nanoparticle Interactions with Coarse-Grained Protein Folding Models. *Small*, **2017**, 13, 1603748	11	25
212	Adaptive Landscape Flattening Accelerates Sampling of Alchemical Space in Multisite λDynamics. *Journal of Physical Chemistry B*, **2017**, 121, 3626-3635	3.4	34
211	A rapid solvent accessible surface area estimator for coarse grained molecular simulations. *Journal of Computational Chemistry*, **2017**, 38, 1270-1274	3.5	7
210	Mechanism of Vps4 hexamer function revealed by cryo-EM. *Science Advances*, **2017**, 3, e1700325	14.3	40
209	Gibbs Sampler-Based λDynamics and Rao-Blackwell Estimator for Alchemical Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2017**, 13, 2501-2510	6.4	23
208	Tuning RNA folding and function through rational design of junction topology. *Nucleic Acids Research*, **2017**, 45, 9706-9715	20.1	6
207	Growth-incompetent monomers of human calcitonin lead to a noncanonical direct relationship between peptide concentration and aggregation lag time. *Journal of Biological Chemistry*, **2017**, 292, 14963-14976	5.4	10
206	Orientation Determination of a Hybrid Peptide Immobilized on CVD-Based Reactive Polymer Surfaces. *Journal of Physical Chemistry C*, **2016**, 120, 19078-19086	3.8	11
205	Nonuniform elastic properties of macromolecules and effect of prestrain on their continuum nature. *Physical Review E*, **2016**, 93, 012417	2.4	8
204	Capturing a Dynamic Chaperone-Substrate Interaction Using NMR-Informed Molecular Modeling. *Journal of the American Chemical Society*, **2016**, 138, 9826-39	16.4	23
203	Efficient implementation of constant pH molecular dynamics on modern graphics processors. *Journal of Computational Chemistry*, **2016**, 37, 2171-80	3.5	13
202	A Synthetic Loop Replacement Peptide That Blocks Canonical NF-ΒB Signaling. *Angewandte Chemie*, **2016**, 128, 15221-15225	3.6	4
201	A Synthetic Loop Replacement Peptide That Blocks Canonical NF-ΒB Signaling. *Angewandte Chemie - International Edition*, **2016**, 55, 14997-15001	16.4	11
200	Molecular Mechanism for Isoform-Selective Inhibition of Acyl Protein Thioesterases 1 and 2 (APT1 and APT2). *ACS Chemical Biology*, **2016**, 11, 3374-3382	4.9	44
199	Parallelization and improvements of the generalized born model with a simple sWitching function for modern graphics processors. *Journal of Computational Chemistry*, **2016**, 37, 927-39	3.5	21

198	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand-protein interactions. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4812-4825	3.4	95
197	Visualizing chaperone-assisted protein folding. *Nature Structural and Molecular Biology*, **2016**, 23, 691-7	17.6	34
196	Coupled folding and binding with 2D Window-Exchange Umbrella Sampling. *Journal of Computational Chemistry*, **2016**, 37, 587-94	3.5	19
195	Flexible CDOCKER: Development and application of a pseudo-explicit structure-based docking method within CHARMM. *Journal of Computational Chemistry*, **2016**, 37, 753-62	3.5	61
194	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. *Journal of Chemical Theory and Computation*, **2016**, 12, 405-13	6.4	1303
193	Secondary structure encodes a cooperative tertiary folding funnel in the Azoarcus ribozyme. *Nucleic Acids Research*, **2016**, 44, 402-12	20.1	3
192	Probing Site-Specific Structural Information of Peptides at Model Membrane Interface In Situ. *Journal of the American Chemical Society*, **2015**, 137, 10190-8	16.4	41
191	Noncanonical secondary structure stabilizes mitochondrial tRNA(Ser(UCN)) by reducing the entropic cost of tertiary folding. *Journal of the American Chemical Society*, **2015**, 137, 3592-9	16.4	11
190	CapsidMaps: protein-protein interaction pattern discovery platform for the structural analysis of virus capsids using Google Maps. *Journal of Structural Biology*, **2015**, 190, 47-55	3.4	4
189	Stability and orientation of cecropin P1 on maleimide self-assembled monolayer (SAM) surfaces and suggested functional mutations. *Chinese Chemical Letters*, **2015**, 26, 485-490	8.1	9
188	Accurate modeling of ionic surfactants at high concentration. *Journal of Physical Chemistry B*, **2015**, 119, 6217-24	3.4	15
187	Membrane environment modulates the pKa values of transmembrane helices. *Journal of Physical Chemistry B*, **2015**, 119, 4601-7	3.4	35
186	Effects of Peptide Immobilization Sites on the Structure and Activity of Surface-Tethered Antimicrobial Peptides. *Journal of Physical Chemistry C*, **2015**, 119, 7146-7155	3.8	48
185	Regulation of calreticulin-major histocompatibility complex (MHC) class I interactions by ATP. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E5608-17	11.5	13
184	Protein-Protein Interfaces in Viral Capsids Are Structurally Unique. *Journal of Molecular Biology*, **2015**, 427, 3613-3624	6.5	3
183	Interfacial Behaviors of Antimicrobial Peptide Cecropin P1 Immobilized on Different Self-Assembled Monolayers. *Journal of Physical Chemistry C*, **2015**, 119, 22542-22551	3.8	20
182	Predicting protein backbone chemical shifts from C□coordinates: extracting high resolution experimental observables from low resolution models. *Journal of Chemical Theory and Computation* , **2015**, 11, 325-31	6.4	10
181	Frequent side chain methyl carbon-oxygen hydrogen bonding in proteins revealed by computational and stereochemical analysis of neutron structures. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 403-410	4.2	31

180	PCalign: a method to quantify physicochemical similarity of protein-protein interfaces. *BMC Bioinformatics*, **2015**, 16, 33	3.6	13
179	Molecular-Level Insights into Orientation-Dependent Changes in the Thermal Stability of Enzymes Covalently Immobilized on Surfaces. *Langmuir*, **2015**, 31, 6145-53	4	34
178	Residue-level resolution of alphavirus envelope protein interactions in pH-dependent fusion. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 2034-9	11.5	21
177	Biasing Potential Replica Exchange Multisite λ-Dynamics for Efficient Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 1267-77	6.4	25
176	pH-dependent transient conformational states control optical properties in cyan fluorescent protein. *Journal of the American Chemical Society*, **2015**, 137, 2892-900	16.4	14
175	Multiscale modeling of a conditionally disordered pH-sensing chaperone. *Journal of Molecular Biology*, **2015**, 427, 1670-80	6.5	23
174	Prepaying the entropic cost for allosteric regulation in KIX. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 12067-72	11.5	50
173	Topological constraints are major determinants of tRNA tertiary structure and dynamics and provide basis for tertiary folding cooperativity. *Nucleic Acids Research*, **2014**, 42, 11792-804	20.1	18
172	Hamiltonian Mapping Revisited: Calibrating Minimalist Models to Capture Molecular Recognition by Intrinsically Disordered Proteins. *Journal of Physical Chemistry Letters*, **2014**, 5, 3441-3444	6.4	10
171	WExplore: hierarchical exploration of high-dimensional spaces using the weighted ensemble algorithm. *Journal of Physical Chemistry B*, **2014**, 118, 3532-42	3.4	62
170	A simple and fast approach for predicting (1)H and (13)C chemical shifts: toward chemical shift-guided simulations of RNA. *Journal of Physical Chemistry B*, **2014**, 118, 12168-75	3.4	23
169	Constant pH molecular dynamics of proteins in explicit solvent with proton tautomerism. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1319-31	4.2	73
168	pH-induced stability switching of the bacteriophage HK97 maturation pathway. *Journal of the American Chemical Society*, **2014**, 136, 3097-107	16.4	16
167	Hierarchy of RNA functional dynamics. *Annual Review of Biochemistry*, **2014**, 83, 441-66	29.1	110
166	PCASSO: a fast and efficient Cα-based method for accurately assigning protein secondary structure elements. *Journal of Computational Chemistry*, **2014**, 35, 1757-61	3.5	19
165	Modulation of frustration in folding by sequence permutation. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 10562-7	11.5	19
164	Coarse grained models reveal essential contributions of topological constraints to the conformational free energy of RNA bulges. *Journal of Physical Chemistry B*, **2014**, 118, 2615-27	3.4	43
163	Uncovering pH-dependent transient states of proteins with buried ionizable residues. *Journal of the American Chemical Society*, **2014**, 136, 8496-9	16.4	33

162	Efficient in silico exploration of RNA interhelical conformations using Euler angles and WExplore. *Nucleic Acids Research*, **2014**, 42, 12126-37	20.1	20
161	Role of the essential light chain in the activation of smooth muscle myosin by regulatory light chain phosphorylation. *Journal of Structural Biology*, **2014**, 185, 375-82	3.4	25
160	Flipping of the ribosomal A-site adenines provides a basis for tRNA selection. *Journal of Molecular Biology*, **2014**, 426, 3201-3213	6.5	26
159	Conformational dynamics of a regulator of G-protein signaling protein reveals a mechanism of allosteric inhibition by a small molecule. *ACS Chemical Biology*, **2013**, 8, 2778-84	4.9	30
158	Native states of fast-folding proteins are kinetic traps. *Journal of the American Chemical Society*, **2013**, 135, 4729-34	16.4	43
157	Towards Accurate Prediction of Protonation Equilibrium of Nucleic Acids. *Journal of Physical Chemistry Letters*, **2013**, 4, 760-766	6.4	26
156	Assessing the quality of absolute hydration free energies among CHARMM-compatible ligand parameterization schemes. *Journal of Computational Chemistry*, **2013**, 34, 893-903	3.5	30
155	Ordering a dynamic protein via a small-molecule stabilizer. *Journal of the American Chemical Society* , **2013**, 135, 3363-6	16.4	61
154	Deconstructing activation events in rhodopsin. *Journal of the American Chemical Society*, **2013**, 135, 10906-9	16.4	15
153	Binding and folding of the small bacterial chaperone HdeA. *Journal of Physical Chemistry B*, **2013**, 117, 13219-25	3.4	15
152	pH-dependent dynamics of complex RNA macromolecules. *Journal of Chemical Theory and Computation*, **2013**, 9, 935-943	6.4	47
151	Quantifying chaperone-mediated transitions in the proteostasis network of E. coli. *PLoS Computational Biology*, **2013**, 9, e1003324	5	5
150	Viral capsid proteins are segregated in structural fold space. *PLoS Computational Biology*, **2013**, 9, e1002905	5	38
149	Chaperone activation by unfolding. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, E1254-62	11.5	57
148	pH-sensitive residues in the p19 RNA silencing suppressor protein from carnation Italian ringspot virus affect siRNA binding stability. *Protein Science*, **2013**, 22, 595-604	6.3	13
147	Single transcriptional and translational preQ1 riboswitches adopt similar pre-folded ensembles that follow distinct folding pathways into the same ligand-bound structure. *Nucleic Acids Research*, **2013**, 41, 10462-75	20.1	64
146	MATCH: an atom-typing toolset for molecular mechanics force fields. *Journal of Computational Chemistry*, **2012**, 33, 189-202	3.5	115
145	Sekikaic acid and lobaric acid target a dynamic interface of the coactivator CBP/p300. *Angewandte Chemie - International Edition*, **2012**, 51, 11258-62	16.4	47

144	Constant pH Molecular Dynamics Simulations of Nucleic Acids in Explicit Solvent. *Journal of Chemical Theory and Computation*, **2012**, 8, 36-46	6.4	73
143	From Molecular Phylogenetics to Quantum Chemistry: Discovering Enzyme Design Principles through Computation. *Computational and Structural Biotechnology Journal*, **2012**, 2, e201209018	6.8	2
142	On the morphology of viral capsids: elastic properties and buckling transitions. *Journal of Physical Chemistry B*, **2012**, 116, 8604-9	3.4	33
141	Quantifying hub-like behavior in protein folding networks. *Journal of Chemical Theory and Computation*, **2012**, 8, 3044-3052	6.4	21
140	Exploring the symmetry and mechanism of virus capsid maturation via an ensemble of pathways. *Biophysical Journal*, **2012**, 102, 606-12	2.9	35
139	Unraveling the structural complexity in a single-stranded RNA tail: implications for efficient ligand binding in the prequeuosine riboswitch. *Nucleic Acids Research*, **2012**, 40, 1345-55	20.1	46
138	Mechanics of bacteriophage maturation. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 2342-7	11.5	91
137	New insights into the fundamental role of topological constraints as a determinant of two-way junction conformation. *Nucleic Acids Research*, **2012**, 40, 892-904	20.1	31
136	Multiscale Modeling of Virus Structure, Assembly, and Dynamics **2012**, 167-189		
135	Viral capsid equilibrium dynamics reveals nonuniform elastic properties. *Biophysical Journal*, **2011**, 100, L59-61	2.9	30
134	Probing pH-dependent dissociation of HdeA dimers. *Journal of the American Chemical Society*, **2011**, 133, 19393-8	16.4	37
133	Multi-Site dynamics for simulated Structure-Activity Relationship studies. *Journal of Chemical Theory and Computation*, **2011**, 7, 2728-2739	6.4	51
132	Topological constraints: using RNA secondary structure to model 3D conformation, folding pathways, and dynamic adaptation. *Current Opinion in Structural Biology*, **2011**, 21, 296-305	8.1	53
131	Predicting extreme pKa shifts in staphylococcal nuclease mutants with constant pH molecular dynamics. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 3276-86	4.2	39
130	A Mechanism for Evolving Novel Plant Sesquiterpene Synthase Function. *Molecular Informatics*, **2011**, 30, 896-906	3.8	6
129	Surveying implicit solvent models for estimating small molecule absolute hydration free energies. *Journal of Computational Chemistry*, **2011**, 32, 2909-23	3.5	58
128	Applying efficient implicit nongeometric constraints in alchemical free energy simulations. *Journal of Computational Chemistry*, **2011**, 32, 3423-32	3.5	32
127	Cooperative and directional folding of the preQ1 riboswitch aptamer domain. *Journal of the American Chemical Society*, **2011**, 133, 4196-9	16.4	50

126	Determination of viral capsid elastic properties from equilibrium thermal fluctuations. *Physical Review Letters*, **2011**, 106, 188101	7.4	36
125	3D maps of RNA interhelical junctions. *Nature Protocols*, **2011**, 6, 1536-45	18.8	38
124	Periodic table of virus capsids: implications for natural selection and design. *PLoS ONE*, **2010**, 5, e9423	3.7	57
123	Hexameric helicase deconstructed: interplay of conformational changes and substrate coupling. *Biophysical Journal*, **2010**, 98, 1449-57	2.9	14
122	Topological frustration in beta alpha-repeat proteins: sequence diversity modulates the conserved folding mechanisms of alpha/beta/alpha sandwich proteins. *Journal of Molecular Biology*, **2010**, 398, 332-50	6.5	27
121	Steric and thermodynamic limits of design for the incorporation of large unnatural amino acids in aminoacyl-tRNA synthetase enzymes. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1926-38	4.2	3
120	FoldGPCR: structure prediction protocol for the transmembrane domain of G protein-coupled receptors from class A. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2189-201	4.2	31
119	The flexible C-terminal arm of the Lassa arenavirus Z-protein mediates interactions with multiple binding partners. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2251-64	4.2	9
118	VIPERdb2: an enhanced and web API enabled relational database for structural virology. *Nucleic Acids Research*, **2009**, 37, D436-42	20.1	317
117	Geometric considerations in virus capsid size specificity, auxiliary requirements, and buckling. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 8531-6	11.5	26
116	CHARMM: the biomolecular simulation program. *Journal of Computational Chemistry*, **2009**, 30, 1545-614	3.5	5515
115	Lambda-dynamics free energy simulation methods. *Journal of Computational Chemistry*, **2009**, 30, 1692-700	3.5	138
114	Predicting structurally conserved contacts for homologous proteins using sequence conservation filters. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 448-53	4.2	10
113	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. *Nature Reviews Drug Discovery*, **2009**, 8, 455-63	64.1	236
112	Functionally important conformations of the Met20 loop in dihydrofolate reductase are populated by rapid thermal fluctuations. *Journal of the American Chemical Society*, **2009**, 131, 5642-7	16.4	52
111	Invariant polymorphism in virus capsid assembly. *Journal of the American Chemical Society*, **2009**, 131, 2606-14	16.4	94
110	Insights from coarse-grained Gō models for protein folding and dynamics. *International Journal of Molecular Sciences*, **2009**, 10, 889-905	6.3	198
109	Validating CHARMM parameters and exploring charge distribution rules in structure-based drug design. *Journal of Chemical Theory and Computation*, **2009**, 5, 1680-1691	6.4	10

108	Recent advances in implicit solvent-based methods for biomolecular simulations. *Current Opinion in Structural Biology*, **2008**, 18, 140-8	8.1	266
107	Coevolution of function and the folding landscape: correlation with density of native contacts. *Biophysical Journal*, **2008**, 95, L57-9	2.9	17
106	Subdomain competition, cooperativity, and topological frustration in the folding of CheY. *Journal of Molecular Biology*, **2008**, 382, 485-95	6.5	48
105	Tilable nature of virus capsids and the role of topological constraints in natural capsid design. *Physical Review E*, **2008**, 77, 051902	2.4	28
104	De novo prediction of the structures of M. tuberculosis membrane proteins. *Journal of the American Chemical Society*, **2008**, 130, 5384-5	16.4	10
103	Improved model building and assessment of the Calcium-sensing receptor transmembrane domain. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 215-26	4.2	26
102	A novel method to map and compare protein-protein interactions in spherical viral capsids. *Proteins: Structure, Function and Bioinformatics*, **2008**, 73, 644-55	4.2	10
101	Prediction of protein loop conformations using multiscale modeling methods with physical energy scoring functions. *Journal of Computational Chemistry*, **2008**, 29, 820-31	3.5	37
100	Implicit modeling of nonpolar solvation for simulating protein folding and conformational transitions. *Physical Chemistry Chemical Physics*, **2008**, 10, 471-81	3.6	116
99	Folding intermediate in the villin headpiece domain arises from disruption of a N-terminal hydrogen-bonded network. *Journal of the American Chemical Society*, **2007**, 129, 3056-7	16.4	33
98	Membrane assembly of simple helix homo-oligomers studied via molecular dynamics simulations. *Biophysical Journal*, **2007**, 92, 854-63	2.9	74
97	Can molecular dynamics simulations provide high-resolution refinement of protein structure?. *Proteins: Structure, Function and Bioinformatics*, **2007**, 67, 922-30	4.2	116
96	Conformational change of the methionine 20 loop of Escherichia coli dihydrofolate reductase modulates pKa of the bound dihydrofolate. *Protein Science*, **2007**, 16, 1087-100	6.3	34
95	Deprotonation by dehydration: the origin of ammonium sensing in the AmtB channel. *PLoS Computational Biology*, **2007**, 3, e22	5	38
94	Chapter 1 Molecular Simulations of pH-Mediated Biological Processes. *Annual Reports in Computational Chemistry*, **2007**, 3-13	1.8	7
93	Linking folding with aggregation in Alzheimer's beta-amyloid peptides. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 16880-5	11.5	133
92	Large-scale allosteric conformational transitions of adenylate kinase appear to involve a population-shift mechanism. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 18496-501	11.5	216
91	Electrostatic properties of cowpea chlorotic mottle virus and cucumber mosaic virus capsids. *Biopolymers*, **2006**, 82, 106-20	2.2	50

90	Harmonic Fourier beads method for studying rare events on rugged energy surfaces. *Journal of Chemical Physics*, **2006**, 125, 174108	3.9	37
89	Antibody evolution constrains conformational heterogeneity by tailoring protein dynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 13722-7	11.5	101
88	Exploring atomistic details of pH-dependent peptide folding. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 18546-50	11.5	79
87	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. *Molecular Simulation*, **2006**, 32, 231-249	2	101
86	Symmetry, form, and shape: guiding principles for robustness in macromolecular machines. *Annual Review of Biophysics and Biomolecular Structure*, **2006**, 35, 115-33		228
85	Balancing solvation and intramolecular interactions: toward a consistent generalized Born force field. *Journal of the American Chemical Society*, **2006**, 128, 3728-36	16.4	290
84	Toward the accurate first-principles prediction of ionization equilibria in proteins. *Biochemistry*, **2006**, 45, 9363-73	3.2	150
83	Model of the toxic complex of anthrax: responsive conformational changes in both the lethal factor and the protective antigen heptamer. *Protein Science*, **2006**, 15, 2190-200	6.3	21
82	Diversity and identity of mechanical properties of icosahedral viral capsids studied with elastic network normal mode analysis. *Journal of Molecular Biology*, **2005**, 345, 299-314	6.5	157
81	Constant pH molecular dynamics with proton tautomerism. *Biophysical Journal*, **2005**, 89, 141-57	2.9	223
80	Receptor rigidity and ligand mobility in trypsin-ligand complexes. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 407-17	4.2	21
79	A nonadditive methanol force field: bulk liquid and liquid-vapor interfacial properties via molecular dynamics simulations using a fluctuating charge model. *Journal of Chemical Physics*, **2005**, 122, 024508	3.9	61
78	Detailed considerations for a balanced and broadly applicable force field: a study of substituted benzenes modeled with OPLS-AA. *Journal of Computational Chemistry*, **2005**, 26, 1529-41	3.5	25
77	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. *Journal of Computational Chemistry*, **2005**, 26, 1565-78	3.5	63
76	Generation of native-like protein structures from limited NMR data, modern force fields and advanced conformational sampling. *Journal of Biomolecular NMR*, **2005**, 31, 59-64	3	35
75	Exploring Mechanical, Physical and Chemical Aspects of Virus Swelling and Assembly Using Elastic Network Normal Mode Analysis. *Journal of Theoretical Medicine*, **2005**, 6, 135-135		
74	Integrating folding kinetics and protein function: biphasic kinetics and dual binding specificity in a WW domain. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 3432-7	11.5	61
73	Recent advances in the development and application of implicit solvent models in biomolecule simulations. *Current Opinion in Structural Biology*, **2004**, 14, 217-24	8.1	485

72	A modified TIP3P water potential for simulation with Ewald summation. *Journal of Chemical Physics* , **2004**, 121, 10096-103	3.9	715
71	Constant-pH molecular dynamics using continuous titration coordinates. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 738-52	4.2	267
70	An electrostatic basis for the stability of thermophilic proteins. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 128-41	4.2	108
69	The coupling of structural fluctuations to hydride transfer in dihydrofolate reductase. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 444-57	4.2	47
68	Ribosome motions modulate electrostatic properties. *Biopolymers*, **2004**, 74, 423-31	2.2	40
67	Studying protein folding on the Grid: experiences using CHARMM on NPACI resources under Legion. *Concurrency Computation Practice and Experience*, **2004**, 16, 385-397	1.4	6
66	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. *Journal of Computational Chemistry*, **2004**, 25, 1-15	3.5	414
65	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. *Journal of Computational Chemistry*, **2004**, 25, 265-84	3.5	465
64	Efficient approximate all-atom solvent accessible surface area method parameterized for folded and denatured protein conformations. *Journal of Computational Chemistry*, **2004**, 25, 1005-14	3.5	21
63	Extending the treatment of backbone energetics in protein force fields: limitations of gas-phase quantum mechanics in reproducing protein conformational distributions in molecular dynamics simulations. *Journal of Computational Chemistry*, **2004**, 25, 1400-15	3.5	2792
62	CHARMM fluctuating charge force field for proteins: II protein/solvent properties from molecular dynamics simulations using a nonadditive electrostatic model. *Journal of Computational Chemistry*, **2004**, 25, 1504-14	3.5	371
61	MMTSB Tool Set: enhanced sampling and multiscale modeling methods for applications in structural biology. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 377-95	2.8	709
60	Improved treatment of the protein backbone in empirical force fields. *Journal of the American Chemical Society*, **2004**, 126, 698-9	16.4	773
59	Implicit solvation based on generalized Born theory in different dielectric environments. *Journal of Chemical Physics*, **2004**, 120, 903-11	3.9	124
58	Refinement of NMR structures using implicit solvent and advanced sampling techniques. *Journal of the American Chemical Society*, **2004**, 126, 16038-47	16.4	53
57	Assessing scoring functions for protein-ligand interactions. *Journal of Medicinal Chemistry*, **2004**, 47, 3032-47	8.3	433
56	The structural basis for biphasic kinetics in the folding of the WW domain from a formin-binding protein: lessons for protein design?. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 3954-9	11.5	119
55	Comparative study of several algorithms for flexible ligand docking. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 755-63	4.2	245

54	Temperature-dependent behavior of protein-chromophore interactions: a theoretical study of a blue fluorescent antibody. *ChemPhysChem*, **2003**, 4, 848-55	3.2	5
53	New analytic approximation to the standard molecular volume definition and its application to generalized Born calculations. *Journal of Computational Chemistry*, **2003**, 24, 1348-56	3.5	435
52	Detailed analysis of grid-based molecular docking: A case study of CDOCKER-A CHARMm-based MD docking algorithm. *Journal of Computational Chemistry*, **2003**, 24, 1549-62	3.5	1032
51	Generalized born model with a simple smoothing function. *Journal of Computational Chemistry*, **2003**, 24, 1691-702	3.5	578
50	The importance of explicit chain representation in protein folding models: an examination of Ising-like models. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 740-7	4.2	30
49	Barriers to Hydride Transfer in Wild Type and Mutant Dihydrofolate Reductase from E. coli. *Journal of Physical Chemistry B*, **2003**, 107, 14042-14051	3.4	57
48	Force Field Influence on the Observation of □Helical Protein Structures in Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2003**, 107, 2831-2836	3.4	186
47	Improved G□like models demonstrate the robustness of protein folding mechanisms towards non-native interactions. *Journal of Molecular Biology*, **2003**, 334, 309-25	6.5	175
46	How dihydrofolate reductase facilitates protonation of dihydrofolate. *Journal of the American Chemical Society*, **2003**, 125, 8718-9	16.4	42
45	An implicit membrane generalized born theory for the study of structure, stability, and interactions of membrane proteins. *Biophysical Journal*, **2003**, 85, 2900-18	2.9	346
44	Correlated motion and the effect of distal mutations in dihydrofolate reductase. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 6980-5	11.5	202
43	The origins of asymmetry in the folding transition states of protein L and protein G. *Protein Science*, **2002**, 11, 2351-61	6.3	313
42	Modern protein force fields behave comparably in molecular dynamics simulations. *Journal of Computational Chemistry*, **2002**, 23, 1045-57	3.5	92
41	Evaluating CASP4 predictions with physical energy functions. *Proteins: Structure, Function and Bioinformatics*, **2002**, 49, 232-45	4.2	75
40	Protein and peptide folding explored with molecular simulations. *Accounts of Chemical Research*, **2002**, 35, 447-54	24.3	118
39	Novel generalized Born methods. *Journal of Chemical Physics*, **2002**, 116, 10606-10614	3.9	391
38	Viewing protein folding from many perspectives. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 1099-100	11.5	16
37	Modeling of the metallo-beta-lactamase from B. fragilis: structural and dynamic effects of inhibitor binding. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 448-59	4.2	41

36	From folding theories to folding proteins: a review and assessment of simulation studies of protein folding and unfolding. *Annual Review of Physical Chemistry*, **2001**, 52, 499-535	15.7	447
35	Virus Particle Explorer (VIPER), a website for virus capsid structures and their computational analyses. *Journal of Virology*, **2001**, 75, 11943-7	6.6	163
34	Ligand-protein database: linking protein-ligand complex structures to binding data. *Journal of Medicinal Chemistry*, **2001**, 44, 3592-8	8.3	114
33	Application of Multiple Topology Dynamics to a Host Guest System: Cyclodextrin with Substituted Benzenes. *Journal of Physical Chemistry B*, **2001**, 105, 9316-9322	3.4	25
32	Statistical thermodynamics. Taking a walk on a landscape. *Science*, **2001**, 293, 612-3	33.3	143
31	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. *Proteins: Structure, Function and Bioinformatics*, **2000**, 41, 86-97	4.2	80
30	Energetic frustration and the nature of the transition state in protein folding. *Journal of Chemical Physics*, **2000**, 113, 7663-7671	3.9	75
29	Free energy screening of small ligands binding to an artificial protein cavity. *Journal of Chemical Physics*, **2000**, 113, 3423-3433	3.9	19
28	Efficient Sampling of Ligand Orientations and Conformations in Free Energy Calculations Using the Dynamics Method. *Journal of Physical Chemistry B*, **2000**, 104, 6903-6910	3.4	37
27	Protein Dynamics in Enzymatic Catalysis: Exploration of Dihydrofolate Reductase. *Journal of the American Chemical Society*, **2000**, 122, 225-231	16.4	269
26	Are Many-Body Effects Important in Protein Folding?. *Journal of Physical Chemistry B*, **2000**, 104, 9554-9563	3.4	60
25	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models **2000**, 41, 86		3
24	Correlation between knowledge-based and detailed atomic potentials: Application to the unfolding of the GCN4 leucine zipper. *Proteins: Structure, Function and Bioinformatics*, **1999**, 35, 447-452	4.2	29
23	Methodology for protein-ligand binding studies: application to a model for drug resistance, the HIV/FIV protease system. *Proteins: Structure, Function and Bioinformatics*, **1999**, 36, 318-31	4.2	17
22	Development of a Generalized Born Model Parametrization for Proteins and Nucleic Acids. *Journal of Physical Chemistry B*, **1999**, 103, 3765-3773	3.4	342
21	Do active site conformations of small ligands correspond to low free-energy solution structures?. *Journal of Computer-Aided Molecular Design*, **1998**, 12, 563-72	4.2	82
20	Assessing energy functions for flexible docking. *Journal of Computational Chemistry*, **1998**, 19, 1612-1622	3.5	132
19	Assessing search strategies for flexible docking. *Journal of Computational Chemistry*, **1998**, 19, 1623-1631	3.5	102

18	Rapid Screening of Binding Affinities: Application of the Dynamics Method to a Trypsin-Inhibitor System. *Journal of the American Chemical Society*, **1998**, 120, 1920-1921	16.4	35
17	Calculations on folding of segment B1 of streptococcal protein G. *Journal of Molecular Biology*, **1998**, 278, 439-56	6.5	178
16	Exploring the space of protein folding Hamiltonians: The balance of forces in a minimalist barrel model. *Journal of Chemical Physics*, **1998**, 109, 2895-2903	3.9	89
15	Multireference Configuration Interaction Calculations of Electronic States of N-Methylformamide, Acetamide, and N-Methylacetamide. *Journal of Physical Chemistry A*, **1997**, 101, 4821-4827	2.8	60
14	A reexamination of the hydrophobic effect: Exploring the role of the solvent model in computing the methanethane potential of mean force. *Journal of Chemical Physics*, **1997**, 106, 9265-9269	3.9	64
13	Curious structure in "canonical" alanine-based peptides. *Proteins: Structure, Function and Bioinformatics*, **1997**, 28, 59-71	4.2	53
12	A molecular dynamics simulation study of segment B1 of protein G. *Proteins: Structure, Function and Bioinformatics*, **1997**, 29, 193-202	4.2	39
11	Thermodynamics of protein folding: a statistical mechanical study of a small all-beta protein. *Biopolymers*, **1997**, 42, 745-57	2.2	103
10	dynamics: A new approach to free energy calculations. *Journal of Chemical Physics*, **1996**, 105, 2414-2423	3.9	267
9	Charge Screening and the Dielectric Constant of Proteins: Insights from Molecular Dynamics. *Journal of the American Chemical Society*, **1996**, 118, 8452-8458	16.4	320
8	Statistical clustering techniques for the analysis of long molecular dynamics trajectories: analysis of 2.2-ns trajectories of YPGDV. *Biochemistry*, **1993**, 32, 412-20	3.2	199
7	Constant-temperature free energy surfaces for physical and chemical processes. *The Journal of Physical Chemistry*, **1993**, 97, 4509-4513		145
6	A method for predicting protein structure from sequence. *Current Biology*, **1993**, 3, 414-23	6.3	73
5	Conformational flexibility in free energy simulations. *Chemical Physics Letters*, **1989**, 156, 256-260	2.5	26
4	Thermodynamics of aqueous solvation: Solution properties of alcohols and alkanes. *Journal of Chemical Physics*, **1987**, 87, 3029-3037	3.9	118
3	Stochastic boundary conditions for molecular dynamics simulations of ST2 water. *Chemical Physics Letters*, **1984**, 105, 495-500	2.5	484
2	Exploring the Functional Landscape of Biomolecular Machines via Elastic Network Normal Mode Analysis	59-77	2
1	Implicit Solvent Force-Field Optimization	167-190	1