

# Bernard R Brooks

## List of Publications by Citations

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133  
papers

26,205  
citations

39  
h-index

137  
g-index

137  
ext. papers

28,957  
ext. citations

4.6  
avg, IF

6.52  
L-index

#	Paper	IF	Citations
133	CHARMM: A program for macromolecular energy, minimization, and dynamics calculations. <i>Journal of Computational Chemistry</i> , <b>1983</b> , 4, 187-217	3.5	13044
132	Constant pressure molecular dynamics simulation: The Langevin piston method. <i>Journal of Chemical Physics</i> , <b>1995</b> , 103, 4613-4621	3.9	3093
131	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , <b>2015</b> , 113, 184-215	1.7	2068
130	New spherical-cutoff methods for long-range forces in macromolecular simulation. <i>Journal of Computational Chemistry</i> , <b>1994</b> , 15, 667-683	3.5	865
129	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. <i>PLoS Computational Biology</i> , <b>2017</b> , 13, e1005659	5	686
128	An analysis of the accuracy of Langevin and molecular dynamics algorithms. <i>Molecular Physics</i> , <b>1988</b> , 65, 1409-1419	1.7	668
127	Langevin dynamics of peptides: the frictional dependence of isomerization rates of N-acetylalanine-N-methylamide. <i>Biopolymers</i> , <b>1992</b> , 32, 523-35	2.2	663
126	Harmonic analysis of large systems. I. Methodology. <i>Journal of Computational Chemistry</i> , <b>1995</b> , 16, 1522-1542	3.5	430
125	Effect of Electrostatic Force Truncation on Interfacial and Transport Properties of Water. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 17011-17020		351
124	Self-guided Langevin dynamics simulation method. <i>Chemical Physics Letters</i> , <b>2003</b> , 381, 512-518	2.5	329
123	The effects of truncating long-range forces on protein dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1989</b> , 6, 32-45	4.2	224
122	Enzyme mechanisms with hybrid quantum and molecular mechanical potentials. I. Theoretical considerations. <i>International Journal of Quantum Chemistry</i> , <b>1996</b> , 60, 1189-1200	2.1	172
121	Dynamics of DNA oligomers. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>1983</b> , 1, 231-52	3.6	170
120	Optimization of quantum mechanical molecular mechanical partitioning schemes: Gaussian delocalization of molecular mechanical charges and the double link atom method. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 10534-10547	3.9	162
119	Psi4 1.4: Open-source software for high-throughput quantum chemistry. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 184108	3.9	158
118	Isotropic periodic sum: a method for the calculation of long-range interactions. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 44107	3.9	122
117	Molecular Dynamics of Staphylococcal Nuclease: Comparison of Simulation with <sup>15</sup> N and <sup>13</sup> C NMR Relaxation Data. <i>Journal of the American Chemical Society</i> , <b>1998</b> , 120, 5301-5311	16.4	114

116	Albumin-chaperoned cyanine dye yields superbright NIR-II fluorophore with enhanced pharmacokinetics. <i>Science Advances</i> , <b>2019</b> , 5, eaaw0672	14.3	93
115	Exploring the quantum mechanical/molecular mechanical replica path method: a pathway optimization of the chorismate to prephenate Claisen rearrangement catalyzed by chorismate mutase. <i>Theoretical Chemistry Accounts</i> , <b>2003</b> , 109, 140-148	1.9	93
114	Pressure-Based Long-Range Correction for Lennard-Jones Interactions in Molecular Dynamics Simulations: Application to Alkanes and Interfaces. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 363-368	3.4	90
113	pH replica-exchange method based on discrete protonation states. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2011</b> , 79, 3420-36	4.2	89
112	Harmonic analysis of large systems. III. Comparison with molecular dynamics. <i>Journal of Computational Chemistry</i> , <b>1995</b> , 16, 1554-1566	3.5	81
111	Machine Learning Force Field Parameters from Ab Initio Data. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 4492-4503	6.4	73
110	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 499-511	6.4	70
109	Harmonic analysis of large systems. II. Comparison of different protein models. <i>Journal of Computational Chemistry</i> , <b>1995</b> , 16, 1543-1553	3.5	69
108	Direct observation of the folding and unfolding of a beta-hairpin in explicit water through computer simulation. <i>Journal of the American Chemical Society</i> , <b>2002</b> , 124, 5282-3	16.4	62
107	Recent advances in molecular dynamics simulation towards the realistic representation of biomolecules in solution. <i>Theoretical Chemistry Accounts</i> , <b>1998</b> , 99, 279-288	1.9	58
106	Absorption mode two-dimensional NOE spectroscopy of exchangeable protons in oligonucleotides. <i>FEBS Letters</i> , <b>1987</b> , 216, 249-52	3.8	58
105	Constant pH Molecular Dynamics in Explicit Solvent with Enveloping Distribution Sampling and Hamiltonian Exchange. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 2738-2750	6.4	54
104	Using the isotropic periodic sum method to calculate long-range interactions of heterogeneous systems. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 154115	3.9	54
103	Predicting hydration free energies with a hybrid QM/MM approach: an evaluation of implicit and explicit solvation models in SAMPL4. <i>Journal of Computer-Aided Molecular Design</i> , <b>2014</b> , 28, 245-57	4.2	53
102	Simulations of membranes and other interfacial systems using P2(1) and Pc periodic boundary conditions. <i>Biophysical Journal</i> , <b>2002</b> , 82, 2317-25	2.9	51
101	A parallel implementation of the analytic nuclear gradient for time-dependent density functional theory within the TammDancoff approximation. <i>Molecular Physics</i> , <b>2010</b> , 108, 2791-2800	1.7	49
100	A truncated Newton minimizer adapted for CHARMM and biomolecular applications. <i>Journal of Computational Chemistry</i> , <b>1994</b> , 15, 532-552	3.5	48
99	Backbone relaxation coupled to the ionization of internal groups in proteins: a self-guided Langevin dynamics study. <i>Biophysical Journal</i> , <b>2008</b> , 95, 4091-101	2.9	44

98	ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 2308-14	6.1	43
97	Modulation of Alzheimer's A $\beta$ -protofilament-membrane interactions by lipid headgroups. <i>ACS Chemical Neuroscience</i> , <b>2015</b> , 6, 446-55	5.7	42
96	An efficient algorithm for multipole energies and derivatives based on spherical harmonics and extensions to particle mesh Ewald. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 184101	3.9	41
95	Self-guided Langevin dynamics via generalized Langevin equation. <i>Journal of Computational Chemistry</i> , <b>2016</b> , 37, 595-601	3.5	40
94	Critical Sequence Hotspots for Binding of Novel Coronavirus to Angiotensin Converter Enzyme as Evaluated by Molecular Simulations. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 10034-10047	3.4	39
93	Numerical study on the partitioning of the molecular polarizability into fluctuating charge and induced atomic dipole contributions. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 5865-82	2.8	36
92	The ubiquitin ligase Ubr4 controls stability of podocin/MEC-2 supercomplexes. <i>Human Molecular Genetics</i> , <b>2016</b> , 25, 1328-44	5.6	36
91	Comparison of Methods To Reweight from Classical Molecular Simulations to QM/MM Potentials. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 1466-80	6.4	36
90	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 332-44	6.4	36
89	Correcting for the free energy costs of bond or angle constraints in molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - General Subjects</i> , <b>2015</b> , 1850, 932-943	4	35
88	Targeted conformational search with map-restrained self-guided Langevin dynamics: application to flexible fitting into electron microscopic density maps. <i>Journal of Structural Biology</i> , <b>2013</b> , 183, 429-440	3.4	35
87	Isotropic periodic sum of electrostatic interactions for polar systems. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 024107	3.9	35
86	Efficient treatment of induced dipoles. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 074115	3.9	34
85	Phosphoproteomic analysis reveals regulatory mechanisms at the kidney filtration barrier. <i>Journal of the American Society of Nephrology: JASN</i> , <b>2014</b> , 25, 1509-22	12.7	34
84	Self-guided Langevin dynamics study of regulatory interactions in NtrC. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2009</b> , 76, 1007-19	4.2	34
83	Toward canonical ensemble distribution from self-guided Langevin dynamics simulation. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 134108	3.9	33
82	Conformational dynamics and aggregation behavior of piezoelectric diphenylalanine peptides in an external electric field. <i>Biophysical Chemistry</i> , <b>2015</b> , 196, 16-24	3.5	32
81	Mapping the Drude polarizable force field onto a multipole and induced dipole model. <i>Journal of Chemical Physics</i> , <b>2017</b> , 147, 161702	3.9	32

80	Conformational relaxation and water penetration coupled to ionization of internal groups in proteins. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 4042-53	2.8	32
79	Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 948-958	6.4	31
78	On the convergence of multi-scale free energy simulations. <i>Molecular Simulation</i> , <b>2018</b> , 44, 1062-1081	2	30
77	Efficient and Unbiased Sampling of Biomolecular Systems in the Canonical Ensemble: A Review of Self-Guided Langevin Dynamics. <i>Advances in Chemical Physics</i> , <b>2012</b> , 150, 255-326		29
76	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 496-514	6.4	29
75	Enhancing constant-pH simulation in explicit solvent with a two-dimensional replica exchange method. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 2560-74	6.4	28
74	Probing the periplasmic-open state of lactose permease in response to sugar binding and proton translocation. <i>Journal of Molecular Biology</i> , <b>2010</b> , 404, 506-21	6.5	28
73	Hydrophobic hydration and the anomalous partial molar volumes in ethanol-water mixtures. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 064501	3.9	25
72	Predicting binding affinities of host-guest systems in the SAMPL3 blind challenge: the performance of relative free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , <b>2012</b> , 26, 543-50	4.2	25
71	Elastic molecular dynamics with self-consistent flexible constraints. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 7919-7929	3.9	25
70	Computational scheme for pH-dependent binding free energy calculation with explicit solvent. <i>Protein Science</i> , <b>2016</b> , 25, 231-43	6.3	25
69	Finding multiple reaction pathways via global optimization of action. <i>Nature Communications</i> , <b>2017</b> , 8, 15443	17.4	24
68	An empirical extrapolation scheme for efficient treatment of induced dipoles. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 164101	3.9	24
67	Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pK corrections. <i>Journal of Computer-Aided Molecular Design</i> , <b>2016</b> , 30, 1087-1100	4.2	24
66	Efficient Strategy for the Calculation of Solvation Free Energies in Water and Chloroform at the Quantum Mechanical/Molecular Mechanical Level. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 2476-2489	6.1	23
65	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. <i>Molecules</i> , <b>2018</b> , 23,	4.8	23
64	Mutations Decouple Proton Transfer from Phosphate Cleavage in the dUTPase Catalytic Reaction. <i>ACS Catalysis</i> , <b>2015</b> , 5, 3225-3237	13.1	22
63	Accurate high-throughput structure mapping and prediction with transition metal ion FRET. <i>Structure</i> , <b>2013</b> , 21, 9-19	5.2	21

62	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2016</b> , 30, 989-1006	4.2	20
61	Structural Characterization of Arginine Fingers: Identification of an Arginine Finger for the Pyrophosphatase dUTPases. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 15035-15045	16.4	20
60	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3854-3867	6.4	19
59	Theoretical studies of relaxation of a monomeric subunit of HIV-1 protease in water using molecular dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1993</b> , 15, 374-84	4.2	19
58	Force-momentum-based self-guided Langevin dynamics: a rapid sampling method that approaches the canonical ensemble. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 204101	3.9	18
57	Open science grid study of the coupling between conformation and water content in the interior of a protein. <i>Journal of Chemical Information and Modeling</i> , <b>2008</b> , 48, 2021-9	6.1	18
56	Sigma-RF: prediction of the variability of spatial restraints in template-based modeling by random forest. <i>BMC Bioinformatics</i> , <b>2015</b> , 16, 94	3.6	16
55	Origin of pK Shifts of Internal Lysine Residues in SNase Studied Via Equal-Molar VMMS Simulations in Explicit Water. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 3318-3330	3.4	16
54	Enhanced Sampling in Free Energy Calculations: Combining SGLD with the Bennett's Acceptance Ratio and Enveloping Distribution Sampling Methods. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 3650-62	6.4	16
53	Absolute binding free energies for octa-acids and guests in SAMPL5 : Evaluating binding free energies for octa-acid and guest complexes in the SAMPL5 blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2017</b> , 31, 107-118	4.2	15
52	Applications of Molecular Dynamics for Structural Analysis of Proteins and Peptides. <i>ACS Symposium Series</i> , <b>1987</b> , 123-145	0.4	15
51	Membrane permeability of small molecules from unbiased molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 124107	3.9	15
50	Force matching as a stepping stone to QM/MM CB[8] host/guest binding free energies: a SAMPL6 cautionary tale. <i>Journal of Computer-Aided Molecular Design</i> , <b>2018</b> , 32, 983-999	4.2	15
49	An explicit-solvent hybrid QM and MM approach for predicting pKa of small molecules in SAMPL6 challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2018</b> , 32, 1191-1201	4.2	15
48	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 679-695	6.4	14
47	An efficient protocol for obtaining accurate hydration free energies using quantum chemistry and reweighting from molecular dynamics simulations. <i>Bioorganic and Medicinal Chemistry</i> , <b>2016</b> , 24, 4988-4997	3.4	14
46	Absolute and relative pK predictions via a DFT approach applied to the SAMPL6 blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2018</b> , 32, 1179-1189	4.2	14
45	Comparison of the umbrella sampling and the double decoupling method in binding free energy predictions for SAMPL6 octa-acid host-guest challenges. <i>Journal of Computer-Aided Molecular Design</i> , <b>2018</b> , 32, 1075-1086	4.2	14



44	Computing the Free Energy along a Reaction Coordinate Using Rigid Body Dynamics. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 4198-4207	6.4	13
43	Protein structure determination by conformational space annealing using NMR geometric restraints. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2015</b> , 83, 2251-62	4.2	13
42	A Virtual Mixture Approach to the Study of Multistate Equilibrium: Application to Constant pH Simulation in Explicit Water. <i>PLoS Computational Biology</i> , <b>2015</b> , 11, e1004480	5	13
41	Reservoir pH replica exchange. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 072321	3.9	13
40	The Atomistic Mechanism of Conformational Transition of Adenylate Kinase Investigated by Lorentzian Structure-Based Potential. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 3211-24	6.4	12
39	Conformational states of a TT mismatch from molecular dynamics simulation of duplex d (CGCGATTCGCG). <i>Biopolymers</i> , <b>1992</b> , 32, 783-94	2.2	11
38	Computer simulations of a tumor surface octapeptide epitope. <i>Biopolymers</i> , <b>1989</b> , 28, 525-30	2.2	11
37	A protocol for preparing explicitly solvated systems for stable molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 054123	3.9	11
36	A deep learning approach for the blind logP prediction in SAMPL6 challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2020</b> , 34, 535-542	4.2	10
35	Structural Modulation of Human Amylin Protofilaments by Naturally Occurring Mutations. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 5657-5665	3.4	10
34	Prediction of CB[8] host-guest binding free energies in SAMPL6 using the double-decoupling method. <i>Journal of Computer-Aided Molecular Design</i> , <b>2018</b> , 32, 1059-1073	4.2	10
33	CHARMM Force Field Parameters for Nitroalkanes and Nitroarenes. <i>Journal of Chemical Theory and Computation</i> , <b>2008</b> , 4, 107-15	6.4	10
32	Molecular Multipole Potential Energy Functions for Water. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 1833-42	3.4	9
31	Absolute binding free energy calculations of CBClip host-guest systems in the SAMPL5 blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2017</b> , 31, 71-85	4.2	9
30	Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2. <i>Biophysical Journal</i> , <b>2021</b> , 120, 2902-2913	2.9	9
29	CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Phosphatidylethanolamine, Phosphatidylglycerol, and Ether Lipids. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1581-1595	6.4	8
28	Conformational analysis of replica exchange MD: Temperature-dependent Markov networks for FF amyloid peptides. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 072323	3.9	7
27	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. <i>Journal of Computer-Aided Molecular Design</i> , <b>2020</b> , 34, 495-510	4.2	7

26	Inverse Resolution Limit of Partition Density and Detecting Overlapping Communities by Link-Surprise. <i>Scientific Reports</i> , <b>2017</b> , 7, 12399	4.9	6
25	Quantum chemical predictions of water-octanol partition coefficients applied to the SAMPL6 logP blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2020</b> , 34, 485-493	4.2	6
24	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1562-1580	6.4	6
23	Amyloid Fibril Design: Limiting Structural Polymorphism in Alzheimer's A $\beta$ Protofilaments. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 11535-11545	3.4	6
22	Multi-phase Boltzmann weighting: accounting for local inhomogeneity in molecular simulations of water-octanol partition coefficients in the SAMPL6 challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2020</b> , 34, 471-483	4.2	5
21	A double exponential potential for van der Waals interaction. <i>AIP Advances</i> , <b>2019</b> , 9, 065304	1.5	5
20	Web-based computational chemistry education with CHARMMing II: Coarse-grained protein folding. <i>PLoS Computational Biology</i> , <b>2014</b> , 10, e1003738	5	5
19	Web-based computational chemistry education with CHARMMing III: Reduction potentials of electron transfer proteins. <i>PLoS Computational Biology</i> , <b>2014</b> , 10, e1003739	5	5
18	Isotropic periodic sum for multipole interactions and a vector relation for calculation of the Cartesian multipole tensor. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 164110	3.9	5
17	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1086-1097	6.4	5
16	Hydronium Ions Accompanying Buried Acidic Residues Lead to High Apparent Dielectric Constants in the Interior of Proteins. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 6215-6223	3.4	5
15	Global organization of a binding site network gives insight into evolution and structure-function relationships of proteins. <i>Scientific Reports</i> , <b>2017</b> , 7, 11652	4.9	4
14	Protonation state of the selectivity filter of bacterial voltage-gated sodium channels is modulated by ions. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2020</b> , 88, 527-539	4.2	4
13	The homogeneity condition: A simple way to derive isotropic periodic sum potentials for efficient calculation of long-range interactions in molecular simulation. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 214109	3.9	3
12	Variational embedding of protein folding simulations using Gaussian mixture variational autoencoders. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 194108	3.9	3
11	Protein-Protein Docking Using EMAP in CHARMM and Support Vector Machine: Application to Ab/Ag Complexes. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 4186-94	6.4	2
10	Analytical Hessians for Ewald and particle mesh Ewald electrostatics. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 104101	3.9	2
9	A compression strategy for particle mesh Ewald theory. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 054112	3.9	2



8	GraphVAMPNet, using graph neural networks and variational approach to Markov processes for dynamical modeling of biomolecules.. <i>Journal of Chemical Physics</i> , <b>2022</b> , 156, 184103	3.9	2
7	Reformulation of the self-guided molecular simulation method. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 094112	3.9	1
6	Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. <i>International Journal of Molecular Sciences</i> , <b>2020</b> , 21,	6.3	1
5	A replica exchange umbrella sampling (REUS) approach to predict host-guest binding free energies in SAMPL8 challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2021</b> , 35, 667-677	4.2	1
4	The Extended Eighth-Shell method for periodic boundary conditions with rotational symmetry. <i>Journal of Computational Chemistry</i> , <b>2021</b> , 42, 1373-1383	3.5	1
3	Replica Exchange Molecular Dynamics of Diphenylalanine Amyloid Peptides in Electric Fields. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 5233-5242	3.4	1
2	Improving the speed of volumetric density map generation via cubic spline interpolation. <i>Journal of Molecular Graphics and Modelling</i> , <b>2021</b> , 104, 107832	2.8	1
1	Determinants of conductance of a bacterial voltage-gated sodium channel. <i>Biophysical Journal</i> , <b>2021</b> , 120, 3050-3069	2.9	0