Bernard R Brooks

List of Publications by Year
in descending order

136 papers	31,555 citations	61857 43 h-index	11288 136 g-index
137 all docs	137 docs citations	137 times ranked	24521 citing authors

#	Article	IF	Citations
1	CHARMM: A program for macromolecular energy, minimization, and dynamics calculations. Journal of Computational Chemistry, 1983, 4, 187-217.	1.5	14,316
2	Constant pressure molecular dynamics simulation: The Langevin piston method. Journal of Chemical Physics, 1995, 103, 4613-4621.	1.2	3,818
3	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
4	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. PLoS Computational Biology, 2017, 13, e1005659.	1.5	1,561
5	New spherical-cutoff methods for long-range forces in macromolecular simulation. Journal of Computational Chemistry, 1994, 15, 667-683.	1.5	1,002
6	Langevin dynamics of peptides: The frictional dependence of isomerization rates ofN-acetylalanyl-N?-methylamide. Biopolymers, 1992, 32, 523-535.	1.2	922
7	An analysis of the accuracy of Langevin and molecular dynamics algorithms. Molecular Physics, 1988, 65, 1409-1419.	0.8	865
8	Harmonic analysis of large systems. I. Methodology. Journal of Computational Chemistry, 1995, 16, 1522-1542.	1.5	470
9	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
10	Self-guided Langevin dynamics simulation method. Chemical Physics Letters, 2003, 381, 512-518.	1.2	398
11	Effect of Electrostatic Force Truncation on Interfacial and Transport Properties of Water. The Journal of Physical Chemistry, 1996, 100, 17011-17020.	2.9	369
12	The effects of truncating long-range forces on protein dynamics. Proteins: Structure, Function and Bioinformatics, 1989, 6, 32-45.	1.5	237
13	Dynamics of DNA Oligomers. Journal of Biomolecular Structure and Dynamics, 1983, 1, 231-252.	2.0	188
14	Enzyme mechanisms with hybrid quantum and molecular mechanical potentials. I. Theoretical considerations. International Journal of Quantum Chemistry, 1996, 60, 1189-1200.	1.0	185
15	Optimization of quantum mechanical molecular mechanical partitioning schemes: Gaussian delocalization of molecular mechanical charges and the double link atom method. Journal of Chemical Physics, 2002, 117, 10534-10547.	1.2	173
16	Albumin-chaperoned cyanine dye yields superbright NIR-II fluorophore with enhanced pharmacokinetics. Science Advances, 2019, 5, eaaw0672.	4.7	171
17	Isotropic periodic sum: A method for the calculation of long-range interactions. Journal of Chemical Physics, 2005, 122, 044107.	1.2	127
18	Molecular Dynamics of Staphylococcal Nuclease:Â Comparison of Simulation with15N and13C NMR Relaxation Data. Journal of the American Chemical Society, 1998, 120, 5301-5311.	6.6	121

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19	pH replicaâ€exchange method based on discrete protonation states. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3420-3436.	1.5	112
20	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	2.3	105
21	Exploring the quantum mechanical/molecular mechanical replica path method: a pathway optimization of the chorismate to prephenate Claisen rearrangement catalyzed by chorismate mutase. Theoretical Chemistry Accounts, 2003, 109, 140-148.	0.5	100
22	Pressure-Based Long-Range Correction for Lennard-Jones Interactions in Molecular Dynamics Simulations:Â Application to Alkanes and Interfaces. Journal of Physical Chemistry B, 2004, 108, 363-368.	1.2	96
23	Harmonic analysis of large systems. III. Comparison with molecular dynamics. Journal of Computational Chemistry, 1995, 16, 1554-1566.	1.5	87
24	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. Journal of Chemical Theory and Computation, 2016, 12, 499-511.	2.3	78
25	Harmonic analysis of large systems. II. Comparison of different protein models. Journal of Computational Chemistry, 1995, 16, 1543-1553.	1.5	76
26	Constant pH Molecular Dynamics in Explicit Solvent with Enveloping Distribution Sampling and Hamiltonian Exchange. Journal of Chemical Theory and Computation, 2014, 10, 2738-2750.	2.3	68
27	Absorption mode two-dimensional NOE spectroscopy of exchangeable protons in oligonucleotides. FEBS Letters, 1987, 216, 249-252.	1.3	67
28	Simulations of Membranes and Other Interfacial Systems Using P21 and Pc Periodic Boundary Conditions. Biophysical Journal, 2002, 82, 2317-2325.	0.2	66
29	Direct Observation of the Folding and Unfolding of a Î²-Hairpin in Explicit Water through Computer Simulation. Journal of the American Chemical Society, 2002, 124, 5282-5283.	6.6	63
30	Recent advances in molecular dynamics simulation towards the realistic representation of biomolecules in solution. Theoretical Chemistry Accounts, 1998, 99, 279-288.	0.5	61
31	Selfâ€guided <scp>L</scp>angevin dynamics via generalized <scp>L</scp>angevin equation. Journal of Computational Chemistry, 2016, 37, 595-601.	1.5	60
32	Predicting hydration free energies with a hybrid QM/MM approach: an evaluation of implicit and explicit solvation models in SAMPL4. Journal of Computer-Aided Molecular Design, 2014, 28, 245-257.	1.3	59
33	Using the isotropic periodic sum method to calculate long-range interactions of heterogeneous systems. Journal of Chemical Physics, 2008, 129, 154115.	1.2	58
34	A parallel implementation of the analytic nuclear gradient for time-dependent density functional theory within the Tammâ€“Dancoff approximation. Molecular Physics, 2010, 108, 2791-2800.	0.8	58
35	Modulation of Alzheimerâ€™s AÎ² Protofilament-Membrane Interactions by Lipid Headgroups. ACS Chemical Neuroscience, 2015, 6, 446-455.	1.7	55
36	ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. Journal of Chemical Information and Modeling, 2015, 55, 2308-2314.	2.5	54

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37	Critical Sequence Hotspots for Binding of Novel Coronavirus to Angiotensin Converter Enzyme as Evaluated by Molecular Simulations. Journal of Physical Chemistry B, 2020, 124, 10034-10047.	1.2	54
38	CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. Journal of Chemical Theory and Computation, 2022, 18, 479-493.	2.3	53
39	A truncated Newton minimizer adapted for CHARMM and biomolecular applications. Journal of Computational Chemistry, 1994, 15, 532-552.	1.5	52
40	Targeted conformational search with map-restrained self-guided Langevin dynamics: Application to flexible fitting into electron microscopic density maps. Journal of Structural Biology, 2013, 183, 429-440.	1.3	50
41	Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. Journal of Chemical Theory and Computation, 2018, 14, 948-958.	2.3	50
42	Backbone Relaxation Coupled to the Ionization of Internal Groups in Proteins: A Self-Guided Langevin Dynamics Study. Biophysical Journal, 2008, 95, 4091-4101.	0.2	49
43	The ubiquitin ligase Ubr4 controls stability of podocin/MEC-2 supercomplexes. Human Molecular Genetics, 2016, 25, 1328-1344.	1.4	45
44	CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Phosphatidylethanolamine, Phosphatidylglycerol, and Ether Lipids. Journal of Chemical Theory and Computation, 2021, 17, 1581-1595.	2.3	45
45	Numerical Study on the Partitioning of the Molecular Polarizability into Fluctuating Charge and Induced Atomic Dipole Contributions. Journal of Physical Chemistry A, 2015, 119, 5865-5882.	1.1	44
46	An efficient algorithm for multipole energies and derivatives based on spherical harmonics and extensions to particle mesh Ewald. Journal of Chemical Physics, 2014, 140, 184101.	1.2	43
47	Comparison of Methods To Reweight from Classical Molecular Simulations to QM/MM Potentials. Journal of Chemical Theory and Computation, 2016, 12, 1466-1480.	2.3	42
48	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. Journal of Chemical Theory and Computation, 2016, 12, 332-344.	2.3	42
49	Mapping the Drude polarizable force field onto a multipole and induced dipole model. Journal of Chemical Physics, 2017, 147, 161702.	1.2	42
50	On the convergence of multi-scale free energy simulations. Molecular Simulation, 2018, 44, 1062-1081.	0.9	42
51	Membrane permeability of small molecules from unbiased molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 124107.	1.2	42
52	Conformational Relaxation and Water Penetration Coupled to Ionization of Internal Groups in Proteins. Journal of Physical Chemistry A, 2011, 115, 4042-4053.	1.1	41
53	Conformational dynamics and aggregation behavior of piezoelectric diphenylalanine peptides in an external electric field. Biophysical Chemistry, 2015, 196, 16-24.	1.5	41
54	Isotropic periodic sum of electrostatic interactions for polar systems. Journal of Chemical Physics, 2009, 131, 024107.	1.2	40

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55	Phosphoproteomic Analysis Reveals Regulatory Mechanisms at the Kidney Filtration Barrier. Journal of the American Society of Nephrology: JASN, 2014, 25, 1509-1522.	3.0	40
56	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. Journal of Chemical Theory and Computation, 2021, 17, 1562-1580.	2.3	39
57	Efficient treatment of induced dipoles. Journal of Chemical Physics, 2015, 143, 074115.	1.2	38
58	Correcting for the free energy costs of bond or angle constraints in molecular dynamics simulations. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 932-943.	1.1	38
59	Selfâ€guided Langevin dynamics study of regulatory interactions in NtrC. Proteins: Structure, Function and Bioinformatics, 2009, 76, 1007-1019.	1.5	37
60	Toward canonical ensemble distribution from self-guided Langevin dynamics simulation. Journal of Chemical Physics, 2011, 134, 134108.	1.2	37
61	A protocol for preparing explicitly solvated systems for stable molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 054123.	1.2	37
62	Enhancing Constant-pH Simulation in Explicit Solvent with a Two-Dimensional Replica Exchange Method. Journal of Chemical Theory and Computation, 2015, 11, 2560-2574.	2.3	33
63	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. Journal of Chemical Theory and Computation, 2011, 7, 496-514.	2.3	32
64	Efficient and Unbiased Sampling of Biomolecular Systems in the Canonical Ensemble: A Review of Selfâ€Guided Langevin Dynamics. Advances in Chemical Physics, 2012, 150, 255-326.	0.3	32
65	Structural Characterization of Arginine Fingers: Identification of an Arginine Finger for the Pyrophosphatase dUTPases. Journal of the American Chemical Society, 2016, 138, 15035-15045.	6.6	32
66	Accurate High-Throughput Structure Mapping and Prediction with Transition Metal Ion FRET. Structure, 2013, 21, 9-19.	1.6	31
67	Probing the Periplasmic-Open State of Lactose Permease in Response to Sugar Binding and Proton Translocation. Journal of Molecular Biology, 2010, 404, 506-521.	2.0	30
68	Hydrophobic hydration and the anomalous partial molar volumes in ethanol-water mixtures. Journal of Chemical Physics, 2015, 142, 064501.	1.2	29
69	Computational scheme for pHâ€dependent binding free energy calculation with explicit solvent. Protein Science, 2016, 25, 231-243.	3.1	29
70	Finding multiple reaction pathways via global optimization of action. Nature Communications, 2017, 8, 15443.	5.8	29
71	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. Molecules, 2018, 23, 2695.	1.7	29
72	Mutations Decouple Proton Transfer from Phosphate Cleavage in the dUTPase Catalytic Reaction. ACS Catalysis, 2015, 5, 3225-3237.	5.5	28

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73	Efficient Strategy for the Calculation of Solvation Free Energies in Water and Chloroform at the Quantum Mechanical/Molecular Mechanical Level. Journal of Chemical Information and Modeling, 2017, 57, 2476-2489.	2.5	28
74	Elastic molecular dynamics with self-consistent flexible constraints. Journal of Chemical Physics, 2000, 112, 7919-7929.	1.2	27
75	Predicting binding affinities of host-guest systems in the SAMPL3 blind challenge: the performance of relative free energy calculations. Journal of Computer-Aided Molecular Design, 2012, 26, 543-550.	1.3	27
76	An empirical extrapolation scheme for efficient treatment of induced dipoles. Journal of Chemical Physics, 2016, 145, 164101.	1.2	27
77	Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pK a corrections. Journal of Computer-Aided Molecular Design, 2016, 30, 1087-1100.	1.3	27
78	An explicit-solvent hybrid QM and MM approach for predicting pKa of small molecules in SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 1191-1201.	1.3	25
79	Absolute and relative pKa predictions via a DFT approach applied to the SAMPL6 blind challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 1179-1189.	1.3	25
80	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. Journal of Chemical Theory and Computation, 2019, 15, 3854-3867.	2.3	25
81	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. Journal of Computer-Aided Molecular Design, 2016, 30, 989-1006.	1.3	24
82	Force-momentum-based self-guided Langevin dynamics: A rapid sampling method that approaches the canonical ensemble. Journal of Chemical Physics, 2011, 135, 204101.	1.2	22
83	Reservoir pH replica exchange. Journal of Chemical Physics, 2018, 149, 072321.	1.2	22
84	Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2. Biophysical Journal, 2021, 120, 2902-2913.	0.2	22
85	Force matching as a stepping stone to QM/MM CB[8] host/guest binding free energies: a SAMPL6 cautionary tale. Journal of Computer-Aided Molecular Design, 2018, 32, 983-999.	1.3	21
86	Theoretical studies of relaxation of a monomeric subunit of HIV-1 protease in water using molecular dynamics. Proteins: Structure, Function and Bioinformatics, 1993, 15, 374-384.	1.5	20
87	Open Science Grid Study of the Coupling between Conformation and Water Content in the Interior of a Protein. Journal of Chemical Information and Modeling, 2008, 48, 2021-2029.	2.5	19
88	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. Journal of Chemical Theory and Computation, 2017, 13, 679-695.	2.3	19
89	A deep learning approach for the blind logP prediction in SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 535-542.	1.3	19
90	Enhanced Sampling in Free Energy Calculations: Combining SGLD with the Bennettâ€™s Acceptance Ratio and Enveloping Distribution Sampling Methods. Journal of Chemical Theory and Computation, 2012, 8, 3650-3662.	2.3	18

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91	Sigma-RF: prediction of the variability of spatial restraints in template-based modeling by random forest. BMC Bioinformatics, 2015, 16, 94.	1.2	18
92	Origin of pK_a Shifts of Internal Lysine Residues in SNase Studied Via Equal-Molar VMMS Simulations in Explicit Water. Journal of Physical Chemistry B, 2017, 121, 3318-3330.	1.2	18
93	Comparison of the umbrella sampling and the double decoupling method in binding free energy predictions for SAMPL6 octa-acid hostâ€“guest challenges. Journal of Computer-Aided Molecular Design, 2018, 32, 1075-1086.	1.3	18
94	A compression strategy for particle mesh Ewald theory. Journal of Chemical Physics, 2021, 154, 054112.	1.2	18
95	GraphVAMPNet, using graph neural networks and variational approach to Markov processes for dynamical modeling of biomolecules. Journal of Chemical Physics, 2022, 156, 184103.	1.2	18
96	Applications of Molecular Dynamics for Structural Analysis of Proteins and Peptides. ACS Symposium Series, 1987, , 123-145.	0.5	16
97	Protein structure determination by conformational space annealing using <scp>NMR</scp> geometric restraints. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2251-2262.	1.5	16
98	Absolute binding free energies for octa-acids and guests in SAMPL5. Journal of Computer-Aided Molecular Design, 2017, 31, 107-118.	1.3	16
99	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. Journal of Chemical Theory and Computation, 2021, 17, 1086-1097.	2.3	16
100	The Atomistic Mechanism of Conformational Transition of Adenylate Kinase Investigated by Lorentzian Structure-Based Potential. Journal of Chemical Theory and Computation, 2015, 11, 3211-3224.	2.3	15
101	An efficient protocol for obtaining accurate hydration free energies using quantum chemistry and reweighting from molecular dynamics simulations. Bioorganic and Medicinal Chemistry, 2016, 24, 4988-4997.	1.4	15
102	Computing the Free Energy along a Reaction Coordinate Using Rigid Body Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 4198-4207.	2.3	14
103	A Virtual Mixture Approach to the Study of Multistate Equilibrium: Application to Constant pH Simulation in Explicit Water. PLoS Computational Biology, 2015, 11, e1004480.	1.5	14
104	Absolute binding free energy calculations of CBClip hostâ€“guest systems in the SAMPL5 blind challenge. Journal of Computer-Aided Molecular Design, 2017, 31, 71-85.	1.3	13
105	Prediction of CB[8] hostâ€“guest binding free energies in SAMPL6 using the double-decoupling method. Journal of Computer-Aided Molecular Design, 2018, 32, 1059-1073.	1.3	13
106	Quantum chemical predictions of waterâ€“octanol partition coefficients applied to the SAMPL6 logP blind challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 485-493.	1.3	13
107	Protein pK_a Prediction by Tree-Based Machine Learning. Journal of Chemical Theory and Computation, 2022, 18, 2673-2686.	2.3	13
108	Computer simulations of a tumor surface octapeptide epitope. Biopolymers, 1989, 28, 525-530.	1.2	12

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109	Conformational states of a TT mismatch from molecular dynamics simulation of duplex d(CGCGATTCGCG). Biopolymers, 1992, 32, 783-794.	1.2	11
110	CHARMM Force Field Parameters for Nitroalkanes and Nitroarenes. Journal of Chemical Theory and Computation, 2008, 4, 107-115.	2.3	11
111	Structural Modulation of Human Amylin Protofilaments by Naturally Occurring Mutations. Journal of Physical Chemistry B, 2018, 122, 5657-5665.	1.2	11
112	A double exponential potential for van der Waals interaction. AIP Advances, 2019, 9, 065304.	0.6	11
113	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 495-510.	1.3	11
114	Variational embedding of protein folding simulations using Gaussian mixture variational autoencoders. Journal of Chemical Physics, 2021, 155, 194108.	1.2	11
115	Web-Based Computational Chemistry Education with CHARMMing III: Reduction Potentials of Electron Transfer Proteins. PLoS Computational Biology, 2014, 10, e1003739.	1.5	10
116	Molecular Multipole Potential Energy Functions for Water. Journal of Physical Chemistry B, 2016, 120, 1833-1842.	1.2	10
117	Web-Based Computational Chemistry Education with CHARMMing II: Coarse-Grained Protein Folding. PLoS Computational Biology, 2014, 10, e1003738.	1.5	8
118	Inverse Resolution Limit of Partition Density and Detecting Overlapping Communities by Link-Surprise. Scientific Reports, 2017, 7, 12399.	1.6	8
119	Protonation state of the selectivity filter of bacterial voltageâ€gated sodium channels is modulated by ions. Proteins: Structure, Function and Bioinformatics, 2020, 88, 527-539.	1.5	8
120	Analytical Hessians for Ewald and particle mesh Ewald electrostatics. Journal of Chemical Physics, 2021, 154, 104101.	1.2	8
121	Amyloid Fibril Design: Limiting Structural Polymorphism in Alzheimerâ€™s AÎ² Protofilaments. Journal of Physical Chemistry B, 2018, 122, 11535-11545.	1.2	7
122	Conformational analysis of replica exchange MD: Temperature-dependent Markov networks for FF amyloid peptides. Journal of Chemical Physics, 2018, 149, 072323.	1.2	7
123	Multi-phase Boltzmann weighting: accounting for local inhomogeneity in molecular simulations of waterâ€“octanol partition coefficients in the SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 471-483.	1.3	7
124	Proteinâ€“Protein Docking Using EMAP in CHARMM and Support Vector Machine: Application to Ab/Ag Complexes. Journal of Chemical Theory and Computation, 2013, 9, 4186-4194.	2.3	6
125	Isotropic periodic sum for multipole interactions and a vector relation for calculation of the Cartesian multipole tensor. Journal of Chemical Physics, 2016, 145, 164110.	1.2	6
126	Hydronium Ions Accompanying Buried Acidic Residues Lead to High Apparent Dielectric Constants in the Interior of Proteins. Journal of Physical Chemistry B, 2018, 122, 6215-6223.	1.2	6

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127	Improving the speed of volumetric density map generation via cubic spline interpolation. Journal of Molecular Graphics and Modelling, 2021, 104, 107832.	1.3	6
128	The homogeneity condition: A simple way to derive isotropic periodic sum potentials for efficient calculation of long-range interactions in molecular simulation. Journal of Chemical Physics, 2019, 150, 214109.	1.2	5
129	A replica exchange umbrella sampling (REUS) approach to predict hostâ€“guest binding free energies in SAMPL8 challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 667-677.	1.3	5
130	Replica Exchange Molecular Dynamics of Diphenylalanine Amyloid Peptides in Electric Fields. Journal of Physical Chemistry B, 2021, 125, 5233-5242.	1.2	5
131	Global organization of a binding site network gives insight into evolution and structure-function relationships of proteins. Scientific Reports, 2017, 7, 11652.	1.6	4
132	Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. International Journal of Molecular Sciences, 2020, 21, 6222.	1.8	4
133	Determinants of conductance of a bacterial voltage-gated sodium channel. Biophysical Journal, 2021, 120, 3050-3069.	0.2	4
134	Obtaining QM/MM binding free energies in the SAMPL8 drugs of abuse challenge: indirect approaches. Journal of Computer-Aided Molecular Design, 2022, 36, 263-277.	1.3	4
135	Reformulation of the self-guided molecular simulation method. Journal of Chemical Physics, 2020, 153, 094112.	1.2	2
136	The Extended Eighthâ€Shell method for periodic boundary conditions with rotational symmetry. Journal of Computational Chemistry, 2021, 42, 1373-1383.	1.5	2