Bernard R Brooks

List of Publications by Year
in descending order

136 papers	31,555 citations	61945 43 h-index	11303 136 g-index
137 all docs	137 docs citations	137 times ranked	24521 citing authors

#	Article	IF	Citations
1	Protein pK_a Prediction by Tree-Based Machine Learning. Journal of Chemical Theory and Computation, 2022, 18, 2673-2686.	2.3	13
2	CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. Journal of Chemical Theory and Computation, 2022, 18, 479-493.	2.3	53
3	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
4	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
5	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
6	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
7	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
8	A compression strategy for particle mesh Ewald theory. Journal of Chemical Physics, 2021, 154, 054112.	1.2	18
9	Analytical Hessians for Ewald and particle mesh Ewald electrostatics. Journal of Chemical Physics, 2021, 154, 104101.	1.2	8
10	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
11	The Extended Eighthâ€Shell method for periodic boundary conditions with rotational symmetry. Journal of Computational Chemistry, 2021, 42, 1373-1383.	1.5	2
12	Replica Exchange Molecular Dynamics of Diphenylalanine Amyloid Peptides in Electric Fields. Journal of Physical Chemistry B, 2021, 125, 5233-5242.	1.2	5
13	Improving the speed of volumetric density map generation via cubic spline interpolation. Journal of Molecular Graphics and Modelling, 2021, 104, 107832.	1.3	6
14	Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2. Biophysical Journal, 2021, 120, 2902-2913.	0.2	22
15	Determinants of conductance of a bacterial voltage-gated sodium channel. Biophysical Journal, 2021, 120, 3050-3069.	0.2	4
16	Variational embedding of protein folding simulations using Gaussian mixture variational autoencoders. Journal of Chemical Physics, 2021, 155, 194108.	1.2	11
17	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
18	A protocol for preparing explicitly solvated systems for stable molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 054123.	1.2	37

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19	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
20	Reformulation of the self-guided molecular simulation method. Journal of Chemical Physics, 2020, 153, 094112.	1.2	2
21	Membrane permeability of small molecules from unbiased molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 124107.	1.2	42
22	Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. International Journal of Molecular Sciences, 2020, 21, 6222.	1.8	4
23	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
24	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
25	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
26	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
27	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 495-510.	1.3	11
28	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
29	A double exponential potential for van der Waals interaction. AIP Advances, 2019, 9, 065304.	0.6	11
30	Albumin-chaperoned cyanine dye yields superbright NIR-II fluorophore with enhanced pharmacokinetics. Science Advances, 2019, 5, eaaw0672.	4.7	171
31	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
32	Structural Modulation of Human Amylin Protofilaments by Naturally Occurring Mutations. Journal of Physical Chemistry B, 2018, 122, 5657-5665.	1.2	11
33	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
34	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
35	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
36	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

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37	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
38	Amyloid Fibril Design: Limiting Structural Polymorphism in Alzheimerâ€™s AÎ² Protofilaments. Journal of Physical Chemistry B, 2018, 122, 11535-11545.	1.2	7
39	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
40	Reservoir pH replica exchange. Journal of Chemical Physics, 2018, 149, 072321.	1.2	22
41	Conformational analysis of replica exchange MD: Temperature-dependent Markov networks for FF amyloid peptides. Journal of Chemical Physics, 2018, 149, 072323.	1.2	7
42	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
43	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
44	On the convergence of multi-scale free energy simulations. Molecular Simulation, 2018, 44, 1062-1081.	0.9	42
45	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
46	Absolute binding free energies for octa-acids and guests in SAMPL5. Journal of Computer-Aided Molecular Design, 2017, 31, 107-118.	1.3	16
47	Finding multiple reaction pathways via global optimization of action. Nature Communications, 2017, 8, 15443.	5.8	29
48	Inverse Resolution Limit of Partition Density and Detecting Overlapping Communities by Link-Surprise. Scientific Reports, 2017, 7, 12399.	1.6	8
49	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
50	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
51	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	2.3	105
52	Mapping the Drude polarizable force field onto a multipole and induced dipole model. Journal of Chemical Physics, 2017, 147, 161702.	1.2	42
53	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
54	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

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55	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. PLoS Computational Biology, 2017, 13, e1005659.	1.5	1,561
56	An empirical extrapolation scheme for efficient treatment of induced dipoles. Journal of Chemical Physics, 2016, 145, 164101.	1.2	27
57	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
58	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
59	Computational scheme for pHâ€dependent binding free energy calculation with explicit solvent. Protein Science, 2016, 25, 231-243.	3.1	29
60	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
61	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
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. Journal of Computer-Aided Molecular Design, 2016, 30, 989-1006.	1.3	24
63	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
64	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
65	The ubiquitin ligase Ubr4 controls stability of podocin/MEC-2 supercomplexes. Human Molecular Genetics, 2016, 25, 1328-1344.	1.4	45
66	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
67	Molecular Multipole Potential Energy Functions for Water. Journal of Physical Chemistry B, 2016, 120, 1833-1842.	1.2	10
68	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
69	Efficient treatment of induced dipoles. Journal of Chemical Physics, 2015, 143, 074115.	1.2	38
70	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
71	Mutations Decouple Proton Transfer from Phosphate Cleavage in the dUTPase Catalytic Reaction. ACS Catalysis, 2015, 5, 3225-3237.	5.5	28
72	Modulation of Alzheimerâ€™s AÎ² Protofilament-Membrane Interactions by Lipid Headgroups. ACS Chemical Neuroscience, 2015, 6, 446-455.	1.7	55

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73	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
74	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
75	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
76	Hydrophobic hydration and the anomalous partial molar volumes in ethanol-water mixtures. Journal of Chemical Physics, 2015, 142, 064501.	1.2	29
77	Sigma-RF: prediction of the variability of spatial restraints in template-based modeling by random forest. BMC Bioinformatics, 2015, 16, 94.	1.2	18
78	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
79	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
80	Conformational dynamics and aggregation behavior of piezoelectric diphenylalanine peptides in an external electric field. Biophysical Chemistry, 2015, 196, 16-24.	1.5	41
81	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
82	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
83	Web-Based Computational Chemistry Education with CHARMMing II: Coarse-Grained Protein Folding. PLoS Computational Biology, 2014, 10, e1003738.	1.5	8
84	Web-Based Computational Chemistry Education with CHARMMing III: Reduction Potentials of Electron Transfer Proteins. PLoS Computational Biology, 2014, 10, e1003739.	1.5	10
85	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
86	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
87	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
88	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
89	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
90	Accurate High-Throughput Structure Mapping and Prediction with Transition Metal Ion FRET. Structure, 2013, 21, 9-19.	1.6	31

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91	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
92	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
93	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
94	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
95	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
96	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
97	Toward canonical ensemble distribution from self-guided Langevin dynamics simulation. Journal of Chemical Physics, 2011, 134, 134108.	1.2	37
98	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
99	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. Journal of Chemical Theory and Computation, 2011, 7, 496-514.	2.3	32
100	pH replicaâ€exchange method based on discrete protonation states. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3420-3436.	1.5	112
101	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
102	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
103	Isotropic periodic sum of electrostatic interactions for polar systems. Journal of Chemical Physics, 2009, 131, 024107.	1.2	40
104	Selfâ€guided Langevin dynamics study of regulatory interactions in NtrC. Proteins: Structure, Function and Bioinformatics, 2009, 76, 1007-1019.	1.5	37
105	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
106	CHARMM Force Field Parameters for Nitroalkanes and Nitroarenes. Journal of Chemical Theory and Computation, 2008, 4, 107-115.	2.3	11
107	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
108	Using the isotropic periodic sum method to calculate long-range interactions of heterogeneous systems. Journal of Chemical Physics, 2008, 129, 154115.	1.2	58

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109	Isotropic periodic sum: A method for the calculation of long-range interactions. Journal of Chemical Physics, 2005, 122, 044107.	1.2	127
110	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
111	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
112	Self-guided Langevin dynamics simulation method. Chemical Physics Letters, 2003, 381, 512-518.	1.2	398
113	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
114	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
115	Simulations of Membranes and Other Interfacial Systems Using P21 and Pc Periodic Boundary Conditions. Biophysical Journal, 2002, 82, 2317-2325.	0.2	66
116	Elastic molecular dynamics with self-consistent flexible constraints. Journal of Chemical Physics, 2000, 112, 7919-7929.	1.2	27
117	Recent advances in molecular dynamics simulation towards the realistic representation of biomolecules in solution. Theoretical Chemistry Accounts, 1998, 99, 279-288.	0.5	61
118	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
119	Effect of Electrostatic Force Truncation on Interfacial and Transport Properties of Water. The Journal of Physical Chemistry, 1996, 100, 17011-17020.	2.9	369
120	Enzyme mechanisms with hybrid quantum and molecular mechanical potentials. I. Theoretical considerations. International Journal of Quantum Chemistry, 1996, 60, 1189-1200.	1.0	185
121	Harmonic analysis of large systems. I. Methodology. Journal of Computational Chemistry, 1995, 16, 1522-1542.	1.5	470
122	Harmonic analysis of large systems. II. Comparison of different protein models. Journal of Computational Chemistry, 1995, 16, 1543-1553.	1.5	76
123	Harmonic analysis of large systems. III. Comparison with molecular dynamics. Journal of Computational Chemistry, 1995, 16, 1554-1566.	1.5	87
124	Constant pressure molecular dynamics simulation: The Langevin piston method. Journal of Chemical Physics, 1995, 103, 4613-4621.	1.2	3,818
125	A truncated Newton minimizer adapted for CHARMM and biomolecular applications. Journal of Computational Chemistry, 1994, 15, 532-552.	1.5	52
126	New spherical-cutoff methods for long-range forces in macromolecular simulation. Journal of Computational Chemistry, 1994, 15, 667-683.	1.5	1,002

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127	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
128	Langevin dynamics of peptides: The frictional dependence of isomerization rates ofN-acetylalanyl-N?-methylamide. Biopolymers, 1992, 32, 523-535.	1.2	922
129	Conformational states of a TT mismatch from molecular dynamics simulation of duplex d(CGCGATTCGCG). Biopolymers, 1992, 32, 783-794.	1.2	11
130	Computer simulations of a tumor surface octapeptide epitope. Biopolymers, 1989, 28, 525-530.	1.2	12
131	The effects of truncating long-range forces on protein dynamics. Proteins: Structure, Function and Bioinformatics, 1989, 6, 32-45.	1.5	237
132	An analysis of the accuracy of Langevin and molecular dynamics algorithms. Molecular Physics, 1988, 65, 1409-1419.	0.8	865
133	Applications of Molecular Dynamics for Structural Analysis of Proteins and Peptides. ACS Symposium Series, 1987, , 123-145.	0.5	16
134	Absorption mode two-dimensional NOE spectroscopy of exchangeable protons in oligonucleotides. FEBS Letters, 1987, 216, 249-252.	1.3	67
135	CHARMM: A program for macromolecular energy, minimization, and dynamics calculations. Journal of Computational Chemistry, 1983, 4, 187-217.	1.5	14,316
136	Dynamics of DNA Oligomers. Journal of Biomolecular Structure and Dynamics, 1983, 1, 231-252.	2.0	188