Philippe H Hnenberger

List of Publications by Citations

124 papers	9,411 citations	48 h-index	96 g-index
128 ext. papers	10,238 ext. citations	4.3 avg, IF	6.3 L-index

#	Paper	IF	Citations
124	The GROMOS Biomolecular Simulation Program Package. *Journal of Physical Chemistry A*, **1999**, 103, 3596-3607	2.8	1220
123	A fast SHAKE algorithm to solve distance constraint equations for small molecules in molecular dynamics simulations. *Journal of Computational Chemistry*, **2001**, 22, 501-508	3.5	647
122	The GROMOS software for biomolecular simulation: GROMOS05. *Journal of Computational Chemistry*, **2005**, 26, 1719-51	3.5	514
121	Biomolecular modeling: Goals, problems, perspectives. *Angewandte Chemie - International Edition*, **2006**, 45, 4064-92	16.4	441
120	Thermostat Algorithms for Molecular Dynamics Simulations. *Advances in Polymer Science*, **2005**, 105-149	1.3	321
119	Comparison of four methods to compute the dielectric permittivity of liquids from molecular dynamics simulations. *Journal of Chemical Physics*, **2001**, 115, 1125-1136	3.9	303
118	Ewald artifacts in computer simulations of ionic solvation and ion–ion interaction: A continuum electrostatics study. *Journal of Chemical Physics*, **1999**, 110, 1856-1872	3.9	303
117	Martini Coarse-Grained Force Field: Extension to Carbohydrates. *Journal of Chemical Theory and Computation*, **2009**, 5, 3195-210	6.4	302
116	A new GROMOS force field for hexopyranose-based carbohydrates. *Journal of Computational Chemistry*, **2005**, 26, 1400-12	3.5	264
115	Molecular Dynamics Simulations of a Polyalanine Octapeptide under Ewald Boundary Conditions: Influence of Artificial Periodicity on Peptide Conformation. *Journal of Physical Chemistry B*, **2000**, 104, 3668-3675	3.4	255
114	Trehalose-protein interaction in aqueous solution. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 177-86	4.2	178
113	Computation of methodology-independent ionic solvation free energies from molecular simulations. II. The hydration free energy of the sodium cation. *Journal of Chemical Physics*, **2006**, 124, 224501	3.9	163
112	New Interaction Parameters for Charged Amino Acid Side Chains in the GROMOS Force Field. *Journal of Chemical Theory and Computation*, **2012**, 8, 3705-23	6.4	154
111	An improved nucleic acid parameter set for the GROMOS force field. *Journal of Computational Chemistry*, **2005**, 26, 725-37	3.5	147
110	Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: an accurate correction scheme for electrostatic finite-size effects. *Journal of Chemical Physics*, **2013**, 139, 184103	3.9	143
109	Interaction of the disaccharide trehalose with a phospholipid bilayer: a molecular dynamics study. *Biophysical Journal*, **2004**, 86, 2273-85	2.9	139
108	Computation of methodology-independent ionic solvation free energies from molecular simulations. I. The electrostatic potential in molecular liquids. *Journal of Chemical Physics*, **2006**, 124, 124106	3.9	130

107	A reoptimized GROMOS force field for hexopyranose-based carbohydrates accounting for the relative free energies of ring conformers, anomers, epimers, hydroxymethyl rotamers, and glycosidic linkage conformers. *Journal of Computational Chemistry*, **2011**, 32, 998-1032	3.5	128
106	Computation of methodology-independent single-ion solvation properties from molecular simulations. IV. Optimized Lennard-Jones interaction parameter sets for the alkali and halide ions in water. *Journal of Chemical Physics*, **2011**, 134, 144104	3.9	117
105	Influence of Artificial Periodicity and Ionic Strength in Molecular Dynamics Simulations of Charged Biomolecules Employing Lattice-Sum Methods. *Journal of Physical Chemistry B*, **2004**, 108, 774-788	3.4	117
104	Theoretical Investigation of Solvent Effects on Glycosylation Reactions: Stereoselectivity Controlled by Preferential Conformations of the Intermediate Oxacarbenium-Counterion Complex. *Journal of Chemical Theory and Computation*, **2010**, 6, 1783-97	6.4	114
103	Conformational properties of glucose-based disaccharides investigated using molecular dynamics simulations with local elevation umbrella sampling. *Carbohydrate Research*, **2010**, 345, 1781-801	2.9	111
102	Alternative schemes for the inclusion of a reaction-field correction into molecular dynamics simulations: Influence on the simulated energetic, structural, and dielectric properties of liquid water. *Journal of Chemical Physics*, **1998**, 108, 6117-6134	3.9	105
101	Molecular dynamics simulations of the hyperthermophilic protein sac7d from Sulfolobus acidocaldarius: contribution of salt bridges to thermostability. *Journal of Molecular Biology*, **1999**, 285, 1811-30	6.5	105
100	Explicit-solvent molecular dynamics simulation at constant pH: Methodology and application to small amines. *Journal of Chemical Physics*, **2001**, 114, 9706-9719	3.9	104
99	New Interaction Parameters for Oxygen Compounds in the GROMOS Force Field: Improved Pure-Liquid and Solvation Properties for Alcohols, Ethers, Aldehydes, Ketones, Carboxylic Acids, and Esters. *Journal of Chemical Theory and Computation*, **2011**, 7, 1016-31	6.4	93
98	Conformational and dynamical properties of disaccharides in water: a molecular dynamics study. *Biophysical Journal*, **2006**, 90, 4337-44	2.9	92
97	New functionalities in the GROMOS biomolecular simulation software. *Journal of Computational Chemistry*, **2012**, 33, 340-53	3.5	91
96	Using the local elevation method to construct optimized umbrella sampling potentials: calculation of the relative free energies and interconversion barriers of glucopyranose ring conformers in water. *Journal of Computational Chemistry*, **2010**, 31, 1-23	3.5	90
95	Interaction of the sugars trehalose, maltose and glucose with a phospholipid bilayer: a comparative molecular dynamics study. *Journal of Physical Chemistry B*, **2006**, 110, 15572-81	3.4	85
94	Determinants of ligand binding to cAMP-dependent protein kinase. *Biochemistry*, **1999**, 38, 2358-66	3.2	79
93	A GROMOS-Compatible Force Field for Small Organic Molecules in the Condensed Phase: The 2016H66 Parameter Set. *Journal of Chemical Theory and Computation*, **2016**, 12, 3825-50	6.4	75
92	Conformation, dynamics, solvation and relative stabilities of selected beta-hexopyranoses in water: a molecular dynamics study with the GROMOS 45A4 force field. *Carbohydrate Research*, **2007**, 342, 2097-124	2.9	71
91	Absolute Single-Molecule Entropies from Quasi-Harmonic Analysis of Microsecond Molecular Dynamics: Correction Terms and Convergence Properties. *Journal of Chemical Theory and Computation*, **2009**, 5, 3150-3160	6.4	68
90	Calculation of relative free energies for ligand-protein binding, solvation, and conformational transitions using the GROMOS software. *Journal of Physical Chemistry B*, **2011**, 115, 13570-7	3.4	66

89	Molecular dynamics simulations of a reversibly folding beta-heptapeptide in methanol: influence of the treatment of long-range electrostatic interactions. *Journal of Physical Chemistry B*, **2009**, 113, 3112-28	3.4	65
88	Molecular dynamics simulations of phospholipid bilayers: Influence of artificial periodicity, system size, and simulation time. *Journal of Physical Chemistry B*, **2005**, 109, 11643-52	3.4	65
87	Optimal charge-shaping functions for the particle□particle□particle□mesh (P3M) method for computing electrostatic interactions in molecular simulations. *Journal of Chemical Physics*, **2000**, 113, 10464-10476	3.9	65
86	Revision of the GROMOS 56A6(CARBO) force field: Improving the description of ring-conformational equilibria in hexopyranose-based carbohydrates chains. *Journal of Computational Chemistry*, **2016**, 37, 354-65	3.5	65
85	Car-Parrinello Molecular Dynamics Simulations of CaCl2 Aqueous Solutions. *Journal of Chemical Theory and Computation*, **2008**, 4, 779-89	6.4	63
84	Computation of methodology-independent single-ion solvation properties from molecular simulations. III. Correction terms for the solvation free energies, enthalpies, entropies, heat capacities, volumes, compressibilities, and expansivities of solvated ions. *Journal of Chemical*	3.9	60
83	Influence of cut-off truncation and artificial periodicity of electrostatic interactions in molecular simulations of solvated ions: A continuum electrostatics study. *Journal of Chemical Physics*, **2003**, 119, 9129-9144	3.9	60
82	A GROMOS Parameter Set for Vicinal Diether Functions: Properties of Polyethyleneoxide and Polyethyleneglycol. *Journal of Chemical Theory and Computation*, **2012**, 8, 3943-63	6.4	56
81	Absolute proton hydration free energy, surface potential of water, and redox potential of the hydrogen electrode from first principles: QM/MM MD free-energy simulations of sodium and potassium hydration. *Journal of Chemical Physics*, **2018**, 148, 222814	3.9	55
80	Comparison of atomic-level and coarse-grained models for liquid hydrocarbons from molecular dynamics configurational entropy estimates. *Journal of Physical Chemistry B*, **2006**, 110, 8464-73	3.4	55
79	Configurational entropies of lipids in pure and mixed bilayers from atomic-level and coarse-grained molecular dynamics simulations. *Journal of Physical Chemistry B*, **2006**, 110, 15602-14	3.4	55
78	Explicit-solvent molecular dynamics simulations of the polysaccharide schizophyllan in water. *Biophysical Journal*, **2007**, 93, 442-55	2.9	50
77	pH-Dependent Stability of a Decalysine □Helix Studied by Explicit-Solvent Molecular Dynamics Simulations at Constant pH. *Journal of Physical Chemistry B*, **2004**, 108, 13551-13559	3.4	49
76	Comparison of different schemes to treat long-range electrostatic interactions in molecular dynamics simulations of a protein crystal. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 509-19	4.2	48
75	Free Energies of Transfer of Trp Analogs from Chloroform to Water: Comparison of Theory and Experiment and the Importance of Adequate Treatment of Electrostatic and Internal Interactions. *Journal of the American Chemical Society*, **1996**, 118, 6285-6294	16.4	47
74	A fast pairlist-construction algorithm for molecular simulations under periodic boundary conditions. *Journal of Computational Chemistry*, **2004**, 25, 1474-86	3.5	45
73	Combining the lattice-sum and reaction-field approaches for evaluating long-range electrostatic interactions in molecular simulations. *Journal of Chemical Physics*, **2005**, 123, 34107	3.9	44
72	Molecular dynamics simulations of the native and partially folded states of ubiquitin: influence of methanol cosolvent, pH, and temperature on the protein structure and dynamics. *Protein Science*, **2007**, 16, 1101-18	6.3	43

71	Intramolecular hydrogen-bonding in aqueous carbohydrates as a cause or consequence of conformational preferences: a molecular dynamics study of cellobiose stereoisomers. *European Biophysics Journal*, **2013**, 42, 521-37	1.9	40
70	Effect of trehalose on a phospholipid membrane under mechanical stress. *Biophysical Journal*, **2008**, 95, 3525-34	2.9	40
69	Calculation of the group-based pressure in molecular simulations. I. A general formulation including Ewald and particle-particle□particle-mesh electrostatics. *Journal of Chemical Physics*, **2002**, 116, 6880-6897	3.9	39
68	The transition between the B and Z conformations of DNA investigated by targeted molecular dynamics simulations with explicit solvation. *Biophysical Journal*, **2006**, 91, 2976-90	2.9	38
67	Molecular dynamics simulation of highly charged proteins: comparison of the particle-particle particle-mesh and reaction field methods for the calculation of electrostatic interactions. *Protein Science*, **2003**, 12, 2161-72	6.3	37
66	Lattice-sum methods for computing electrostatic interactions in molecular simulations **1999**,		35
65	Computational analysis of PKA-balanol interactions. *Journal of Medicinal Chemistry*, **2001**, 44, 1530-9	8.3	32
64	The influence of polyhydroxylated compounds on a hydrated phospholipid bilayer: a molecular dynamics study. *Molecular Simulation*, **2008**, 34, 403-420	2	31
63	Polarization around an ion in a dielectric continuum with truncated electrostatic interactions. *Journal of Chemical Physics*, **1999**, 110, 10679-10692	3.9	31
62	Origin of Asymmetric Solvation Effects for Ions in Water and Organic Solvents Investigated Using Molecular Dynamics Simulations: The Swain Acity-Basity Scale Revisited. *Journal of Physical Chemistry B*, **2016**, 120, 8485-517	3.4	31
61	Interaction of the disaccharides trehalose and gentiobiose with lipid bilayers: a comparative molecular dynamics study. *Journal of Molecular Graphics and Modelling*, **2010**, 29, 331-46	2.8	30
60	Explicit-Solvent Molecular Dynamics Simulations of the □(1-3)- and □(1-6)-Linked Disaccharides □Laminarabiose and □Gentiobiose in Water. *Journal of Physical Chemistry B*, **2004**, 108, 5815-5826	3.4	30
59	Conformation, dynamics and ion-binding properties of single-chain polyuronates: a molecular dynamics study. *Molecular Simulation*, **2008**, 34, 421-446	2	29
58	Biomolekulare Modellierung: Ziele, Probleme, Perspektiven. *Angewandte Chemie*, **2006**, 118, 4168-4198	3.6	29
57	Use of molecular dynamics in the design and structure determination of a photoinducible beta-hairpin. *Journal of the American Chemical Society*, **2005**, 127, 4935-42	16.4	29
56	A fast-Fourier transform method to solve continuum-electrostatics problems with truncated electrostatic interactions: Algorithm and application to ionic solvation and ion□ion interaction. *Journal of Chemical Physics*, **2003**, 119, 12205-12223	3.9	29
55	Ball-and-Stick Local Elevation Umbrella Sampling: Molecular Simulations Involving Enhanced Sampling within Conformational or Alchemical Subspaces of Low Internal Dimensionalities, Minimal Irrelevant Volumes, and Problem-Adapted Geometries. *Journal of Chemical Theory and Computation*, **2010**, 6, 2622-46	6.4	28
54	Experimental and Theoretical Approach to Hydrogen-Bonded Diastereomeric Interactions in a Model Complex. *Journal of the American Chemical Society*, **1997**, 119, 7533-7544	16.4	26

53	Simulating the Transition between Gel and Liquid-Crystal Phases of Lipid Bilayers: Dependence of the Transition Temperature on the Hydration Level. *Journal of Chemical Theory and Computation*, **2010**, 6, 2488-500	6.4	25
52	Interaction of alginate single-chain polyguluronate segments with mono- and divalent metal cations: a comparative molecular dynamics study. *Molecular Simulation*, **2010**, 36, 778-795	2	24
51	Enhanced Conformational Sampling in Molecular Dynamics Simulations of Solvated Peptides: Fragment-Based Local Elevation Umbrella Sampling. *Journal of Chemical Theory and Computation*, **2010**, 6, 2598-621	6.4	24
50	Solving the Poisson equation for solute□olvent systems using fast Fourier transforms. *Journal of Chemical Physics*, **2002**, 116, 7434-7451	3.9	24
49	Molecular dynamics simulations of a double unit cell in a protein crystal: volume relaxation at constant pressure and correlation of motions between the two unit cells. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 327-40	4.2	21
48	Influence of the Treatment of Nonbonded Interactions on the Thermodynamic and Transport Properties of Pure Liquids Calculated Using the 2016H66 Force Field. *Journal of Chemical Theory and Computation*, **2019**, 15, 1806-1826	6.4	17
47	Temperature dependence of the dielectric permittivity of acetic acid, propionic acid and their methyl esters: a molecular dynamics simulation study. *ChemPhysChem*, **2012**, 13, 1182-90	3.2	17
46	Local Elevation Umbrella Sampling Applied to the Calculation of Alchemical Free-Energy Changes via □Dynamics: The □LEUS Scheme. *Journal of Chemical Theory and Computation*, **2014**, 10, 3006-22	6.4	16
45	Efficient Combination of Environment Change and Alchemical Perturbation within the Enveloping Distribution Sampling (EDS) Scheme: Twin-System EDS and Application to the Determination of Octanol-Water Partition Coefficients. *Journal of Chemical Theory and Computation*, **2013**, 9, 1334-46	6.4	14
44	Alchemical Free-Energy Calculations by Multiple-Replica □Dynamics: The Conveyor Belt Thermodynamic Integration Scheme. *Journal of Chemical Theory and Computation*, **2019**, 15, 2392-2419	6.4	13
43	Multistate □ocal-elevation umbrella-sampling (MS-□LEUS): method and application to the complexation of cations by crown ethers. *Journal of Chemical Theory and Computation*, **2015**, 11, 2575-88	6.4	13
42	Evaluating Classical Force Fields against Experimental Cross-Solvation Free Energies. *Journal of Chemical Theory and Computation*, **2020**, 16, 7556-7580	6.4	13
41	Explicit-solvent molecular dynamics simulations of a DNA tetradecanucleotide duplex: lattice-sum versus reaction-field electrostatics. *Molecular Simulation*, **2008**, 34, 491-499	2	13
40	Overcoming Orthogonal Barriers in Alchemical Free Energy Calculations: On the Relative Merits of □Variations, □Extrapolations, and Biasing. *Journal of Chemical Theory and Computation*, **2020**, 16, 1630-1645	6.4	12
39	Reoptimized interaction parameters for the peptide-backbone model compound N-methylacetamide in the GROMOS force field: influence on the folding properties of two beta-peptides in methanol. *Journal of Computational Chemistry*, **2012**, 33, 1907-17	3.5	12
38	Development of a lattice-sum method emulating nonperiodic boundary conditions for the treatment of electrostatic interactions in molecular simulations: a continuum-electrostatics study. *Journal of Chemical Physics*, **2006**, 124, 124108	3.9	12
37	Flexible Boundaries for Multiresolution Solvation: An Algorithm for Spatial Multiscaling in Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 5447-63	6.4	11
36	Calculation of Derivative Thermodynamic Hydration and Aqueous Partial Molar Properties of Ions Based on Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2012**, 8, 3542-64	6.4	11

35	Enantiomeric segregation in the gel phase of lipid bilayers. *Journal of the American Chemical Society* , **2011**, 133, 8464-6	16.4	11
34	Communication: estimating the initial biasing potential for local-elevation umbrella-sampling (LEUS) simulations via slow growth. *Journal of Chemical Physics*, **2014**, 141, 201101	3.9	10
33	Orthogonal sampling in free-energy calculations of residue mutations in a tripeptide: TI versus LEUS. *Journal of Computational Chemistry*, **2015**, 36, 1686-97	3.5	10
32	Effect of the cosolutes trehalose and methanol on the equilibrium and phase-transition properties of glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulations. *European Biophysics Journal*, **2014**, 43, 517-44	1.9	10
31	Phase-transition properties of glycerol-monopalmitate lipid bilayers investigated by molecular dynamics simulation: influence of the system size and force-field parameters. *Molecular Simulation*, **2013**, 39, 563-583	2	10
30	Calculation of the group-based pressure in molecular simulations. II. Numerical tests and application to liquid water. *Journal of Chemical Physics*, **2002**, 116, 6898-6909	3.9	10
29	An Alternative to Conventional Intermediate States in Alchemical Free Energy Calculations: Enveloping Distribution Sampling. *Journal of Chemical Information and Modeling*, **2020**, 60, 5407-5423	6.1	10
28	Simulating Bilayers of Nonionic Surfactants with the GROMOS-Compatible 2016H66 Force Field. *Langmuir*, **2017**, 33, 10225-10238	4	9
27	Systematic Optimization of a Fragment-Based Force Field against Experimental Pure-Liquid Properties Considering Large Compound Families: Application to Saturated Haloalkanes. *Journal of Chemical Theory and Computation*, **2020**, 16, 7525-7555	6.4	9
26	Single-Ion Thermodynamics from First Principles: Calculation of the Absolute Hydration Free Energy and Single-Electrode Potential of Aqueous Li Using ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 6443-6450	6.4	9
25	Effect of methanol on the phase-transition properties of glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulations: in quest of the biphasic effect. *Journal of Molecular Graphics and Modelling*, **2015**, 55, 85-104	2.8	8
24	Reaction-field electrostatics in molecular dynamics simulations: development of a conservative scheme compatible with an atomic cutoff. *Physical Chemistry Chemical Physics*, **2020**, 22, 26419-26437	3.6	8
23	Interfacial solvation can explain attraction between like-charged objects in aqueous solution. *Journal of Chemical Physics*, **2020**, 152, 104713	3.9	7
22	Solvent-Modulated Influence of Intramolecular Hydrogen-Bonding on the Conformational Properties of the Hydroxymethyl Group in Glucose and Galactose: A Molecular Dynamics Simulation Study. *Helvetica Chimica Acta*, **2017**, 100, e1600158	2	7
21	On the relative stabilities of the alkali cations 222 cryptates in the gas phase and in water-methanol solution. *Journal of Molecular Modeling*, **2007**, 13, 1017-25	2	7
20	Effect of mutations involving charged residues on the stability of staphylococcal nuclease: a continuum electrostatics study. *Protein Engineering, Design and Selection*, **2003**, 16, 831-40	1.9	7
19	Long-timescale motions in glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulation. *Journal of Molecular Graphics and Modelling*, **2015**, 55, 48-64	2.8	6
18	Molecular dynamics simulations of the interaction between polyhydroxylated compounds and Lennard-Jones walls: preferential affinity/exclusion effects and their relevance for bioprotection. *Molecular Simulation*, **2010**, 36, 708-728	2	6

17	Residual structure in a peptide fragment of the outer membrane protein X under denaturing conditions: a molecular dynamics study. *European Biophysics Journal*, **2010**, 39, 1421-32	1.9	6
16	Empirical Classical Force Fields for Molecular Systems. *Lecture Notes in Quantum Chemistry II*, **1999**, 177-214	2.4	6
15	A multiple time step algorithm compatible with a large number of distance classes and an arbitrary distance dependence of the time step size for the fast evaluation of nonbonded interactions in molecular simulations. *Journal of Computational Chemistry*, **2006**, 27, 1163-76	3.5	5
14	On the ambiguity of conformational states: A B&S-LEUS simulation study of the helical conformations of decaalanine in water. *Journal of Chemical Physics*, **2015**, 142, 165102	3.9	4
13	Vase-Kite Equilibrium of Resorcin[4]arene Cavitands Investigated Using Molecular Dynamics Simulations with Ball-and-Stick Local Elevation Umbrella Sampling. *Helvetica Chimica Acta*, **2019**, 102, e1900060	2	3
12	Preferential affinity of the components of liquid mixtures at a rigid non-polar surface: enthalpic and entropic driving forces. *ChemPhysChem*, **2011**, 12, 3214-23	3.2	3
11	Measuring 1H-1H and 1H-13C RDCs in methyl groups: example of pulse sequences with numerically optimized coherence transfer schemes. *Journal of Magnetic Resonance*, **2005**, 172, 36-47	3	3
10	Evaluation of nine condensed-phase force fields of the GROMOS, CHARMM, OPLS, AMBER, and OpenFF families against experimental cross-solvation free energies. *Physical Chemistry Chemical Physics*, **2021**, 23, 13055-13074	3.6	3
9	Phase-transition properties of glycerol-dipalmitate lipid bilayers investigated using molecular dynamics simulation. *Journal of Molecular Graphics and Modelling*, **2015**, 59, 136-47	2.8	2
8	In the eye of the beholder: Inhomogeneous distribution of high-resolution shapes within the random-walk ensemble. *Journal of Chemical Physics*, **2009**, 130, 214904	3.9	2
7	Efficient Alchemical Intermediate States in Free Energy Calculations Using Enveloping Distribution Sampling. *Journal of Chemical Theory and Computation*, **2021**, 17, 5805-5815	6.4	2
6	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bio-Molecular Systems: Overview and Perspective on Issues. *ChemPhysChem*, **2021**, 22, 264-282	3.2	2
5	The Conveyor Belt Umbrella Sampling (CBUS) Scheme: Principle and Application to the Calculation of the Absolute Binding Free Energies of Alkali Cations to Crown Ethers. *Journal of Chemical Theory and Computation*, **2020**, 16, 2474-2493	6.4	1
4	Systematic optimization of a fragment-based force field against experimental pure-liquid properties considering large compound families: application to oxygen and nitrogen compounds. *Physical Chemistry Chemical Physics*, **2021**, 23, 17774-17793	3.6	1
3	Solvent-scaling as an alternative to coarse-graining in adaptive-resolution simulations: The adaptive solvent-scaling (AdSoS) scheme. *Journal of Chemical Physics*, **2021**, 155, 094107	3.9	1
2	Wilfred van Gunsteren: 35 Years of Biomolecular Simulation. *Journal of Chemical Theory and Computation*, **2012**, 8, 3425-9	6.4	0
1	RestraintMaker: a graph-based approach to select distance restraints in free-energy calculations with dual topology.. *Journal of Computer-Aided Molecular Design*, **2022**, 36, 175	4.2	0