Bettina G Keller

List of Publications by Year in Descending Order

41 papers	1,863 citations	20 h-index	43 g-index
47 ext. papers	2,173 ext. citations	5.4 avg, IF	4.96 L-index

#	Paper	IF	Citations
41	Path probability ratios for Langevin dynamics-Exact and approximate. *Journal of Chemical Physics*, **2021**, 154, 094102	3.9	6
40	The molecular basis for the pH-dependent calcium affinity of the pattern recognition receptor langerin. *Journal of Biological Chemistry*, **2021**, 296, 100718	5.4	3
39	Markov models from the square root approximation of the Fokker-Planck equation: calculating the grid-dependent flux. *Journal of Physics Condensed Matter*, **2021**, 33, 115902	1.8	4
38	Iodine-Mediated Tryptathionine Formation Facilitates the Synthesis of Amanitins. *Journal of the American Chemical Society*, **2021**, 143, 14322-14331	16.4	2
37	Dynamical reweighting methods for Markov models. *Current Opinion in Structural Biology*, **2020**, 61, 124-131	8.1	10
36	Allostery in C-type lectins. *Current Opinion in Structural Biology*, **2020**, 62, 31-38	8.1	17
35	Total Synthesis of the Death Cap Toxin Phalloidin: Atropoisomer Selectivity Explained by Molecular-Dynamics Simulations. *Chemistry - A European Journal*, **2019**, 25, 8030-8034	4.8	12
34	Rationalization of the Membrane Permeability Differences in a Series of Analogue Cyclic Decapeptides. *Journal of Chemical Information and Modeling*, **2019**, 59, 294-308	6.1	38
33	Trendbericht Theoretische Chemie 2017: Molekü in Bewegung. *Nachrichten Aus Der Chemie*, **2018**, 66, 325-326	0.1	
32	Multiply Intercalator-Substituted Cu(II) Cyclen Complexes as DNA Condensers and DNA/RNA Synthesis Inhibitors. *Inorganic Chemistry*, **2018**, 57, 5004-5012	5.1	13
31	An Automatic Adaptive Importance Sampling Algorithm for Molecular Dynamics in Reaction Coordinates. *SIAM Journal of Scientific Computing*, **2018**, 40, A653-A670	2.6	8
30	The vibrational spectrum of the hydrated alanine-leucine peptide in the amide region from IR experiments and first principles calculations. *Chemical Physics Letters*, **2018**, 698, 227-233	2.5	4
29	Common Nearest Neighbor Clustering—A Benchmark. *Algorithms*, **2018**, 11, 19	1.8	16
28	Girsanov reweighting for metadynamics simulations. *Journal of Chemical Physics*, **2018**, 149, 072335	3.9	29
27	Markov State Models in Drug Design. *Methods and Principles in Medicinal Chemistry*, **2018**, 67-86	0.4	2
26	Exploring Rigid and Flexible Core Trivalent Sialosides for Influenza Virus Inhibition. *Chemistry - A European Journal*, **2018**, 24, 19373-19385	4.8	9
25	Estimation of the infinitesimal generator by square-root approximation. *Journal of Physics Condensed Matter*, **2018**, 30, 425201	1.8	9

24	Broad substrate tolerance of tubulin tyrosine ligase enables one-step site-specific enzymatic protein labeling. *Chemical Science*, **2017**, 8, 3471-3478	9.4	24
23	Girsanov reweighting for path ensembles and Markov state models. *Journal of Chemical Physics*, **2017**, 146, 244112	3.9	26
22	Single-molecule FRET reveals the energy landscape of the full-length SAM-I riboswitch. *Nature Chemical Biology*, **2017**, 13, 1172-1178	11.7	31
21	Interconversion Rates between Conformational States as Rationale for the Membrane Permeability of Cyclosporines. *ChemPhysChem*, **2017**, 18, 3309-3314	3.2	36
20	Intradomain Allosteric Network Modulates Calcium Affinity of the C-Type Lectin Receptor Langerin. *Journal of the American Chemical Society*, **2016**, 138, 12176-86	16.4	33
19	Kinetic Models of Cyclosporin A in Polar and Apolar Environments Reveal Multiple Congruent Conformational States. *Journal of Chemical Information and Modeling*, **2016**, 56, 1547-62	6.1	68
18	Molecular dynamics simulations data of the twenty encoded amino acids in different force fields. *Data in Brief*, **2016**, 7, 582-90	1.2	10
17	Publishers Note: "Density-based cluster algorithms for the identification of core sets" [J. Chem. Phys. 145, 164104 (2016)]. *Journal of Chemical Physics*, **2016**, 145, 199902	3.9	
16	Density-based cluster algorithms for the identification of core sets. *Journal of Chemical Physics*, **2016**, 145, 164104	3.9	42
15	Dynamic properties of force fields. *Journal of Chemical Physics*, **2015**, 142, 084101	3.9	60
14	A Basis Set for Peptides for the Variational Approach to Conformational Kinetics. *Journal of Chemical Theory and Computation*, **2015**, 11, 3992-4004	6.4	23
13	Computational close up on protein–protein interactions: how to unravel the invisible using molecular dynamics simulations?. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 345-359	7.9	27
12	Variational Approach to Molecular Kinetics. *Journal of Chemical Theory and Computation*, **2014**, 10, 1739-52	6.4	193
11	Complex RNA folding kinetics revealed by single-molecule FRET and hidden Markov models. *Journal of the American Chemical Society*, **2014**, 136, 4534-43	16.4	69
10	Modulation of a ligands energy landscape and kinetics by the chemical environment. *Journal of Physical Chemistry B*, **2012**, 116, 13597-607	3.4	1
9	Markov models and dynamical fingerprints: Unraveling the complexity of molecular kinetics. *Chemical Physics*, **2012**, 396, 92-107	2.3	48
8	An Analysis of the Validity of Markov State Models for Emulating the Dynamics of Classical Molecular Systems and Ensembles. *Journal of Chemical Theory and Computation*, **2011**, 7, 1032-44	6.4	25
7	Probing molecular kinetics with Markov models: metastable states, transition pathways and spectroscopic observables. *Physical Chemistry Chemical Physics*, **2011**, 13, 16912-27	3.6	86

6	Markov models of molecular kinetics: generation and validation. *Journal of Chemical Physics*, **2011**, 134, 174105	3.9	738
5	Comparing geometric and kinetic cluster algorithms for molecular simulation data. *Journal of Chemical Physics*, **2010**, 132, 074110	3.9	93
4	What stabilizes the 3(14)-helix in beta3-peptides? A conformational analysis using molecular simulation. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1677-90	4.2	9
3	On using oscillating time-dependent restraints in MD simulation. *Journal of Biomolecular NMR*, **2007**, 37, 1-14	3	14
2	Biomolecular structure refinement based on adaptive restraints using local-elevation simulation. *Journal of Biomolecular NMR*, **2007**, 39, 265-73	3	20
1	Molecular mechanism of the pH-dependent calcium affinity in langerin		1