Bettina G Keller

List of Publications by Year
in descending order

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42	2,473	361413 20	254184 43
papers	citations	h-index	g-index

47	47	47	2302
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Markov models of molecular kinetics: Generation and validation. Journal of Chemical Physics, 2011, 134, 174105.	3.0	968
2	Variational Approach to Molecular Kinetics. Journal of Chemical Theory and Computation, 2014, 10, 1739-1752.	5.3	256
3	Comparing geometric and kinetic cluster algorithms for molecular simulation data. Journal of Chemical Physics, 2010, 132, 074110.	3.0	110
4	Probing molecular kinetics with Markov models: metastable states, transition pathways and spectroscopic observables. Physical Chemistry Chemical Physics, 2011, 13, 16912.	2.8	106
5	Kinetic Models of Cyclosporin A in Polar and Apolar Environments Reveal Multiple Congruent Conformational States. Journal of Chemical Information and Modeling, 2016, 56, 1547-1562.	5.4	95
6	Complex RNA Folding Kinetics Revealed by Single-Molecule FRET and Hidden Markov Models. Journal of the American Chemical Society, 2014, 136, 4534-4543.	13.7	84
7	Dynamic properties of force fields. Journal of Chemical Physics, 2015, 142, 084101.	3.0	70
8	Density-based cluster algorithms for the identification of core sets. Journal of Chemical Physics, 2016, 145, 164104.	3.0	60
9	Rationalization of the Membrane Permeability Differences in a Series of Analogue Cyclic Decapeptides. Journal of Chemical Information and Modeling, 2019, 59, 294-308.	5.4	55
10	Interconversion Rates between Conformational States as Rationale for the Membrane Permeability of Cyclosporines. ChemPhysChem, 2017, 18, 3309-3314.	2.1	53
11	Markov models and dynamical fingerprints: Unraveling the complexity of molecular kinetics. Chemical Physics, 2012, 396, 92-107.	1.9	52
12	Single-molecule FRET reveals the energy landscape of the full-length SAM-I riboswitch. Nature Chemical Biology, 2017, 13, 1172-1178.	8.0	47
13	Girsanov reweighting for metadynamics simulations. Journal of Chemical Physics, 2018, 149, 072335.	3.0	46
14	Computational close up on proteinâ€“protein interactions: how to unravel the invisible using molecular dynamics simulations?. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 345-359.	14.6	45
15	Intradomain Allosteric Network Modulates Calcium Affinity of the C-Type Lectin Receptor Langerin. Journal of the American Chemical Society, 2016, 138, 12176-12186.	13.7	40
16	Girsanov reweighting for path ensembles and Markov state models. Journal of Chemical Physics, 2017, 146, 244112.	3.0	36
17	Broad substrate tolerance of tubulin tyrosine ligase enables one-step site-specific enzymatic protein labeling. Chemical Science, 2017, 8, 3471-3478.	7.4	31
18	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, 1032-1044.	5.3	25

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19	A Basis Set for Peptides for the Variational Approach to Conformational Kinetics. Journal of Chemical Theory and Computation, 2015, 11, 3992-4004.	5.3	25
20	Biomolecular structure refinement based on adaptive restraints using local-elevation simulation. Journal of Biomolecular NMR, 2007, 39, 265-273.	2.8	22
21	Common Nearest Neighbor Clusteringâ€"A Benchmark. Algorithms, 2018, 11, 19.	2.1	22
22	Allostery in C-type lectins. Current Opinion in Structural Biology, 2020, 62, 31-38.	5.7	22
23	Dynamical reweighting methods for Markov models. Current Opinion in Structural Biology, 2020, 61, 124-131.	5.7	22
24	Molecular dynamics simulations data of the twenty encoded amino acids in different force fields. Data in Brief, 2016, 7, 582-590.	1.0	17
25	Multiply Intercalator-Substituted Cu(II) Cyclen Complexes as DNA Condensers and DNA/RNA Synthesis Inhibitors. Inorganic Chemistry, 2018, 57, 5004-5012.	4.0	17
26	On using oscillating time-dependent restraints in MD simulation. Journal of Biomolecular NMR, 2007, 37, 1-14.	2.8	15
27	Estimation of the infinitesimal generator by square-root approximation. Journal of Physics Condensed Matter, 2018, 30, 425201.	1.8	15
28	Total Synthesis of the Death Cap Toxin Phalloidin: Atropoisomer Selectivity Explained by Molecularâ€Đynamics Simulations. Chemistry - A European Journal, 2019, 25, 8030-8034.	3.3	15
29	Exploring Rigid and Flexible Core Trivalent Sialosides for Influenza Virus Inhibition. Chemistry - A European Journal, 2018, 24, 19373-19385.	3.3	14
30	Markov models from the square root approximation of the Fokkerâ€"Planck equation: calculating the grid-dependent flux. Journal of Physics Condensed Matter, 2021, 33, 115902.	1.8	12
31	Path probability ratios for Langevin dynamicsâ€"Exact and approximate. Journal of Chemical Physics, 2021, 154, 094102.	3.0	12
32	The molecular basis for the pH-dependent calcium affinity of the pattern recognition receptor langerin. Journal of Biological Chemistry, 2021, 296, 100718.	3.4	11
33	What stabilizes the 3₁₄â€helix in Î²³â€peptides? A conformational analysis using molecular simulation. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1677-1690.	2.6	10
34	An Automatic Adaptive Importance Sampling Algorithm for Molecular Dynamics in Reaction Coordinates. SIAM Journal of Scientific Computing, 2018, 40, A653-A670.	2.8	9
35	Fluorine-induced polarity increases inhibitory activity of BPTI towards chymotrypsin. RSC Chemical Biology, 2022, 3, 773-782.	4.1	8
36	Iodine-Mediated Tryptathionine Formation Facilitates the Synthesis of Amanitins. Journal of the American Chemical Society, 2021, 143, 14322-14331.	13.7	7

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37	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.	2.6	6
38	Pentafluorophosphatoâ€Phenylalanines:ÂAmphiphilic Phosphotyrosine Mimetics Displaying Fluorineâ€Specific Protein Interactions. Angewandte Chemie - International Edition, 2022, , .	13.8	3
39	Target Recognition in Tandem WW Domains: Complex Structures for Parallel and Antiparallel Ligand Orientation in h-FBP21 Tandem WW. Journal of Chemical Information and Modeling, 2022, 62, 6586-6601.	5.4	3
40	Modulation of a Ligandâ€™s Energy Landscape and Kinetics by the Chemical Environment. Journal of Physical Chemistry B, 2012, 116, 13597-13607.	2.6	1
41	Publisherâ€™s Note: â€œDensity-based cluster algorithms for the identification of core setsâ€•[J. Chem. Phys. 145, 164104 (2016)]. Journal of Chemical Physics, 2016, 145, 199902.	3.0	1
42	Trendbericht Theoretische Chemie 2017: MolekÃ¼le in Bewegung. Nachrichten Aus Der Chemie, 2018, 66, 325-326.	0.0	0