Gerhard KÃ¶nig

List of Publications by Year
in descending order

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41 papers	1,121 citations	394421 19 h-index	414414 32 g-index
41 all docs	41 docs citations	41 times ranked	995 citing authors

#	Article	IF	Citations
1	Comparative Performance of PETase as a Function of Reaction Conditions, Substrate Properties, and Product Accumulation. ChemSusChem, 2022, 15, .	6.8	42
2	Mechanistic details of the actinobacterial lyase-catalyzed degradation reaction of 2-hydroxyisobutyryl-CoA. Journal of Biological Chemistry, 2022, 298, 101522.	3.4	2
3	Relative free-energy calculations for scaffold hopping-type transformations with an automated RE-EDS sampling procedure. Journal of Computer-Aided Molecular Design, 2022, 36, 117-130.	2.9	10
4	Ensembler: A Simple Package for Fast Prototyping and Teaching Molecular Simulations. Journal of Chemical Information and Modeling, 2021, 61, 560-564.	5.4	4
5	Effect of Flexibility, Lipophilicity, and the Location of Polar Residues on the Passive Membrane Permeability of a Series of Cyclic Decapeptides. Journal of Medicinal Chemistry, 2021, 64, 12761-12773.	6.4	22
6	Efficient Alchemical Intermediate States in Free Energy Calculations Using Î»-Enveloping Distribution Sampling. Journal of Chemical Theory and Computation, 2021, 17, 5805-5815.	5.3	8
7	nâ€Butanol: An Ecologically and Economically Viable Extraction Solvent for Isolating Polar Products from Aqueous Solutions. European Journal of Organic Chemistry, 2021, 2021, 6224-6228.	2.4	5
8	Rational prioritization strategy allows the design of macrolide derivatives that overcome antibiotic resistance. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, e2113632118.	7.1	7
9	An Alternative to Conventional Î»-Intermediate States in Alchemical Free Energy Calculations: Î»-Enveloping Distribution Sampling. Journal of Chemical Information and Modeling, 2020, 60, 5407-5423.	5.4	18
10	On the faithfulness of molecular mechanics representations of proteins towards quantum-mechanical energy surfaces. Interface Focus, 2020, 10, 20190121.	3.0	13
11	Overcoming Orthogonal Barriers in Alchemical Free Energy Calculations: On the Relative Merits of Î»-Variations, Î»-Extrapolations, and Biasing. Journal of Chemical Theory and Computation, 2020, 16, 1630-1645.	5.3	20
12	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.	3.8	29
13	On the convergence of multi-scale free energy simulations. Molecular Simulation, 2018, 44, 1062-1081.	2.0	42
14	1-Butanol as a Solvent for Efficient Extraction of Polar Compounds from Aqueous Medium: Theoretical and Practical Aspects. Journal of Physical Chemistry B, 2018, 122, 6975-6988.	2.6	24
15	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.	5.3	19
16	Absolute binding free energies for octa-acids and guests in SAMPL5. Journal of Computer-Aided Molecular Design, 2017, 31, 107-118.	2.9	16
17	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.	2.9	13
18	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.	2.9	27

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19	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.	3.0	15
20	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.	2.9	24
21	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. Journal of Chemical Theory and Computation, 2016, 12, 499-511.	5.3	78
22	Comparison of Methods To Reweight from Classical Molecular Simulations to QM/MM Potentials. Journal of Chemical Theory and Computation, 2016, 12, 1466-1480.	5.3	42
23	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.	5.3	42
24	Multiple Environment Single System Quantum Mechanical/Molecular Mechanical (MESS-QM/MM) Calculations. 1. Estimation of Polarization Energies. Journal of Physical Chemistry A, 2015, 119, 1511-1523.	2.5	23
25	Quantum Mechanical Molecular Mechanical Calculations using AMOEBA Force Fields. Biophysical Journal, 2015, 108, 158a.	0.5	1
26	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.	2.4	38
27	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.	2.9	59
28	Computing the Free Energy along a Reaction Coordinate Using Rigid Body Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 4198-4207.	5.3	14
29	Multiscale Free Energy Simulations: An Efficient Method for Connecting Classical MD Simulations to QM or QM/MM Free Energies Using Non-Boltzmann Bennett Reweighting Schemes. Journal of Chemical Theory and Computation, 2014, 10, 1406-1419.	5.3	111
30	Simulation and the Problem of Simplification. Philosophy and Technology, 2013, 26, 81-91.	4.3	1
31	Absolute Hydration Free Energies of Blocked Amino Acids: Implications for Protein Solvation and Stability. Biophysical Journal, 2013, 104, 453-462.	0.5	52
32	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.	5.3	18
33	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.	2.9	27
34	Computing eigenvectors of block tridiagonal matrices based on twisted block factorizations. Journal of Computational and Applied Mathematics, 2012, 236, 3696-3703.	2.0	6
35	Nonâ€Boltzmann sampling and Bennett's acceptance ratio method: How to profit from bending the rules. Journal of Computational Chemistry, 2011, 32, 1082-1090.	3.3	63
36	On twisted factorizations of block tridiagonal matrices. Procedia Computer Science, 2010, 1, 279-287.	2.0	2

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37	Unorthodox uses of Bennett's acceptance ratio method. Journal of Computational Chemistry, 2009, 30, 1712-1718.	3.3	38
38	Hydration Free Energies of Amino Acids: Why Side Chain Analog Data Are Not Enough. Journal of Physical Chemistry B, 2009, 113, 8967-8974.	2.6	57
39	Hydrophobic moments as physicochemical descriptors in structure-activity relationship studies of P-glycoprotein inhibitors. Monatshefte FÃ¼r Chemie, 2008, 139, 401-405.	1.8	7
40	Synthesis and structure activity relationships of novel small molecule cathepsin D inhibitors. Bioorganic and Medicinal Chemistry Letters, 1999, 9, 2531-2536.	2.2	79
41	Testing and Optimizing the Drude Polarizable Force Field for Blocked Amino Acids Based on High-Level Quantum-Mechanical Energy Surfaces. Journal of Computational Biophysics and Chemistry, 0, , 1-9.	1.7	3