Stefan M Kast

List of Publications by Year
in descending order

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Version: 2024-02-01

56 papers	1,481 citations	279798 23 h-index	330143 37 g-index
59 all docs	59 docs citations	59 times ranked	1458 citing authors

#	Article	IF	Citations
1	Quantumâ€“mechanical property prediction of solvated drug molecules: what have we learned from a decade of SAMPL blind prediction challenges?. Journal of Computer-Aided Molecular Design, 2021, 35, 453-472.	2.9	9
2	Evaluation of logÂP, pKa, and logÂD predictions from the SAMPL7 blind challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 771-802.	2.9	42
3	SAMPL7 physical property prediction from EC-RISM theory. Journal of Computer-Aided Molecular Design, 2021, 35, 933-941.	2.9	5
4	Chemically Stabilized DNA Barcodes for DNAâ€Encoded Chemistry. Angewandte Chemie - International Edition, 2021, 60, 19744-19749.	13.8	15
5	Chemisch stabilisierte DNAâ€Codes fÃ¼r DNAâ€kodierte Chemie. Angewandte Chemie, 2021, 133, 19897-19902.	2.0	0
6	A Joint Venture of Ab Initio Molecular Dynamics, Coupled Cluster Electronic Structure Methods, and Liquid-State Theory to Compute Accurate Isotropic Hyperfine Constants of Nitroxide Probes in Water. Journal of Chemical Theory and Computation, 2021, 17, 6366-6386.	5.3	11
7	Asymmetric Interplay Between K+ and Blocker and Atomistic Parameters From Physiological Experiments Quantify K+ Channel Blocker Release. Frontiers in Physiology, 2021, 12, 737834.	2.8	1
8	Pressure-dependent electronic structure calculations using integral equation-based solvation models. Biophysical Chemistry, 2020, 257, 106258.	2.8	14
9	Tautomeric Equilibria of Nucleobases in the Hachimoji Expanded Genetic Alphabet. Journal of Chemical Theory and Computation, 2020, 16, 2766-2777.	5.3	22
10	The SAMPL6 challenge on predicting octanolâ€“water partition coefficients from EC-RISM theory. Journal of Computer-Aided Molecular Design, 2020, 34, 453-461.	2.9	16
11	Structure and thermodynamics of aqueous urea solutions from ambient to kilobar pressures: From thermodynamic modeling, experiments, and first principles simulations to an accurate force field description. Biophysical Chemistry, 2019, 254, 106260.	2.8	10
12	High pressure response of 1H NMR chemical shifts of purine nucleotides. Biophysical Chemistry, 2019, 254, 106261.	2.8	1
13	pKa calculations for tautomerizable and conformationally flexible molecules: partition function vs. state transition approach. Journal of Molecular Modeling, 2019, 25, 139.	1.8	9
14	Overcoming EGFRG724S-mediated osimertinib resistance through unique binding characteristics of second-generation EGFR inhibitors. Nature Communications, 2018, 9, 4655.	12.8	107
15	The SAMPL6 challenge on predicting aqueous pKa values from EC-RISM theory. Journal of Computer-Aided Molecular Design, 2018, 32, 1151-1163.	2.9	28
16	Identification of Intrahelical Bifurcated H-Bonds as a New Type of Gate in K⁺ Channels. Journal of the American Chemical Society, 2017, 139, 7494-7503.	13.7	17
17	Thermodynamic Characterization of Hydration Sites from Integral Equation-Derived Free Energy Densities: Application to Protein Binding Sites and Ligand Series. Journal of Chemical Information and Modeling, 2017, 57, 1652-1666.	5.4	17
18	Drugging the catalytically inactive state of RET kinase in RET-rearranged tumors. Science Translational Medicine, 2017, 9, .	12.4	55

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19	The hpCADD NDDO Hamiltonian: Parametrization. Journal of Chemical Information and Modeling, 2017, 57, 1907-1922.	5.4	11
20	Signatures of Solvation Thermodynamics in Spectra of Intermolecular Vibrations. Journal of Chemical Theory and Computation, 2017, 13, 4467-4481.	5.3	52
21	Die Basislinie der chemischen Verschiebung in Hochdruckâ€NMRâ€Spektren von Proteinen. Angewandte Chemie, 2016, 128, 8900-8904.	2.0	3
22	The Chemical Shift Baseline for Highâ€Pressure NMR Spectra of Proteins. Angewandte Chemie - International Edition, 2016, 55, 8757-8760.	13.8	23
23	Design principles for highâ€“pressure force fields: Aqueous TMAO solutions from ambient to kilobar pressures. Journal of Chemical Physics, 2016, 144, 144104.	3.0	79
24	Structure and thermodynamics of nondipolar molecular liquids and solutions from integral equation theory. Molecular Physics, 2016, 114, 2461-2476.	1.7	5
25	Toward Extreme Biophysics: Deciphering the Infrared Response of Biomolecular Solutions at High Pressures. Angewandte Chemie, 2016, 128, 9686-9690.	2.0	4
26	The SAMPL5 challenge for embedded-cluster integral equation theory: solvation free energies, aqueous pK a, and cyclohexaneâ€“water log D. Journal of Computer-Aided Molecular Design, 2016, 30, 1035-1044.	2.9	28
27	Toward Extreme Biophysics: Deciphering the Infrared Response of Biomolecular Solutions at High Pressures. Angewandte Chemie - International Edition, 2016, 55, 9534-9538.	13.8	47
28	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
29	3D RISM theory with fast reciprocal-space electrostatics. Journal of Chemical Physics, 2015, 142, 114107.	3.0	23
30	Targeting Drug Resistance in EGFR with Covalent Inhibitors: A Structure-Based Design Approach. Journal of Medicinal Chemistry, 2015, 58, 6844-6863.	6.4	92
31	Bridge function of the repulsive Weeksâ€“Chandlerâ€“Andersen (WCA) fluid. Chemical Physics Letters, 2014, 591, 237-242.	2.6	5
32	Solvation Effects on Chemical Shifts by Embedded Cluster Integral Equation Theory. Journal of Physical Chemistry A, 2014, 118, 11620-11628.	2.5	26
33	Acidity in DMSO from the embedded cluster integral equation quantum solvation model. Journal of Molecular Modeling, 2014, 20, 2161.	1.8	13
34	Viral potassium channels as a robust model system for studies of membraneâ€“protein interaction. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1096-1103.	2.6	28
35	Three-Dimensional RISM Integral Equation Theory for Polarizable Solute Models. Journal of Chemical Theory and Computation, 2013, 9, 4718-4726.	5.3	18
36	Thermally induced polarizabilities and dipole moments of small tin clusters. Journal of Chemical Physics, 2012, 136, 134320.	3.0	10

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37	Communication: An exact bound on the bridge function in integral equation theories. Journal of Chemical Physics, 2012, 137, 171102.	3.0	2
38	Minimal art: Or why small viral K+ channels are good tools for understanding basic structure and function relations. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 580-588.	2.6	35
39	A minimalist model for ion partitioning and competition in a K+ channel selectivity filter. Journal of General Physiology, 2011, 138, 371-373.	1.9	9
40	Prediction of tautomer ratios by embedded-cluster integral equation theory. Journal of Computer-Aided Molecular Design, 2010, 24, 343-353.	2.9	34
41	Model Development for the Viral Kcv Potassium Channel. Biophysical Journal, 2009, 96, 485-498.	0.5	35
42	Chlorella virus ATCV-1 encodes a functional potassium channel of 82 amino acids. Biochemical Journal, 2009, 420, 295-305.	3.7	38
43	Closed-form expressions of the chemical potential for integral equation closures with certain bridge functions. Journal of Chemical Physics, 2008, 129, 236101.	3.0	76
44	Quantum Chemistry in Solution by Combining 3D Integral Equation Theory with a Cluster Embedding Approach. Journal of Physical Chemistry B, 2008, 112, 4337-4343.	2.6	69
45	Molecular Dynamics Simulation of the Cytosolic Mouth in Kcv-Type Potassium Channels. Biochemistry, 2007, 46, 4826-4839.	2.5	40
46	Addendum to â€œFree energies from integral equation theories: Enforcing path independenceâ€• Physical Review E, 2006, 73, 012201.	2.1	5
47	Long Distance Interactions within the Potassium Channel Pore Are Revealed by Molecular Diversity of Viral Proteins. Journal of Biological Chemistry, 2004, 279, 28443-28449.	3.4	38
48	Hybrid Integral-Equation/Simulation Models: From Complexation Thermodynamics to Direct Free Energies. ChemPhysChem, 2004, 5, 449-455.	2.1	8
49	Integral equation theory for correcting truncation errors in molecular simulations. Chemical Physics Letters, 2003, 367, 398-404.	2.6	18
50	Parametrization Strategy for the MolFESD Concept:â€‰ Quantitative Surface Representation of Local Hydrophobicity. Journal of Chemical Information and Computer Sciences, 2003, 43, 237-247.	2.8	14
51	Binary Phases of AliphaticN-Oxides and Water:Â Force Field Development and Molecular Dynamics Simulation. Journal of Physical Chemistry A, 2003, 107, 5342-5351.	2.5	123
52	Free energies from integral equation theories: Enforcing path independence. Physical Review E, 2003, 67, 041203.	2.1	19
53	Hybrid Integral Equation/Monte Carlo Approach to Complexation Thermodynamics. Journal of Physical Chemistry B, 2002, 106, 6289-6297.	2.6	16
54	Combinations of simulation and integral equation theory. Physical Chemistry Chemical Physics, 2001, 3, 5087-5092.	2.8	48

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55	Fast prediction of hydration free energies from molecular interaction fields. Journal of Molecular Graphics and Modelling, 2001, 20, 123-131.	2.4	3
56	Investigations Into Chemically Stabilized Four-Letter DNA for DNA-Encoded Chemistry. Frontiers in Chemistry, 0, 10, .	3.6	1