Zhixiong Lin

List of Publications by Year
in descending order

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32	592	759233 12	642732 23
papers	citations	h-index	g-index

34	34	34	695
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Scaffold Hopping Transformations Using Auxiliary Restraints for Calculating Accurate Relative Binding Free Energies. Journal of Chemical Theory and Computation, 2021, 17, 3710-3726.	5.3	12
2	A Cloud Computing Platform for Scalable Relative and Absolute Binding Free Energy Predictions: New Opportunities and Challenges for Drug Discovery. Journal of Chemical Information and Modeling, 2021, 61, 2720-2732.	5.4	23
3	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. Journal of Chemical Theory and Computation, 2020, 16, 5512-5525.	5.3	35
4	Accounting for the Central Role of Interfacial Water in Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2020, 16, 7883-7894.	5.3	24
5	A comparison of pathwayâ€independent and pathwayâ€dependent methods in the calculation of conformational free enthalpy differences. Protein Science, 2016, 25, 184-191.	7.6	1
6	GROMOS polarizable charge-on-spring models for liquid urea: COS/U and COS/U2. Journal of Chemical Physics, 2015, 142, 094117.	3.0	3
7	Effects of Polarizable Solvent Models upon the Relative Stability of an Î±-Helical and a Î²-Hairpin Structure of an Alanine Decapeptide. Journal of Chemical Theory and Computation, 2015, 11, 1983-1986.	5.3	8
8	Using enveloping distribution sampling to compute the folding free enthalpy of a Î²-peptide with a very unstable folded conformation in solution: The advantage of focused sampling using EDS. Chemical Physics, 2014, 428, 156-163.	1.9	3
9	On the use of one-step perturbation to investigate the dependence of NOE-derived atomâ€“atom distance bound violations of peptides upon a variation of force-field parameters. European Biophysics Journal, 2014, 43, 113-119.	2.2	7
10	On the Sensitivity of Peptide Nucleic Acid Duplex Formation and Crystal Dissolution to a Variation of Force-Field Parameters. Journal of Chemical Theory and Computation, 2014, 10, 391-400.	5.3	3
11	Use of Enveloping Distribution Sampling to Evaluate Important Characteristics of Biomolecular Force Fields. Journal of Physical Chemistry B, 2014, 118, 6424-6430.	2.6	4
12	Free Enthalpy Differences between Î±-, Ï€-, and 3₁₀-Helices of an Atomic Level Fine-Grained Alanine Deca-Peptide Solvated in Supramolecular Coarse-Grained Water. Journal of Chemical Theory and Computation, 2013, 9, 1328-1333.	5.3	13
13	The effect of branched side chains on the relative stability of Î±- and Ï€-helices: a combination of the enveloping distribution sampling and one-step perturbation methods^{â€}. Molecular Physics, 2013, 111, 2126-2130.	1.7	5
14	On the choice of a reference state for oneâ€step perturbation calculations between polar and nonpolar molecules in a polar environment. Journal of Computational Chemistry, 2013, 34, 387-393.	3.3	5
15	Combination of Enveloping Distribution Sampling (EDS) of a Soft-Core Reference-State Hamiltonian with One-Step Perturbation to Predict the Effect of Side Chain Substitution on the Relative Stability of Right- and Left-Helical Folds of Î²-Peptides. Journal of Chemical Theory and Computation, 2013, 9, 126-134.	5.3	8
16	Refinement of the application of the GROMOS 54A7 force field to Î²-peptides. Journal of Computational Chemistry, 2013, 34, 2796-2805.	3.3	51
17	Influence of variation of a side chain on the folding equilibrium of a Î²â€peptide: Limitations of oneâ€step perturbation. Journal of Computational Chemistry, 2013, 34, 1899-1906.	3.3	1
18	Enhanced conformational sampling using enveloping distribution sampling. Journal of Chemical Physics, 2013, 139, 144105.	3.0	11

#	Article	IF	Citations
19	Using enveloping distribution sampling to compute the free enthalpy difference between right- and left-handed helices of a Î²-peptide in solution. Journal of Chemical Physics, 2012, 137, 064108.	3.0	12
20	Reoptimized interaction parameters for the peptideâ€backbone model compound Nâ€methylacetamide in the GROMOS force field: Influence on the folding properties of two betaâ€peptides in methanol. Journal of Computational Chemistry, 2012, 33, 1907-1917.	3.3	13
21	Helical Content of a Î²³â€Octapeptide in Methanol: Molecular Dynamics Simulations Explain a Seeming Discrepancy between Conclusions Derived from CD and NMR Data. Chemistry - A European Journal, 2012, 18, 586-593.	3.3	14
22	Exploring the Effect of Side-Chain Substitutions upon the Secondary Structure Preferences of Î²-Peptides. Journal of Physical Chemistry B, 2011, 115, 12984-12992.	2.6	7
23	On the Use of Enveloping Distribution Sampling (EDS) to Compute Free Enthalpy Differences between Different Conformational States of Molecules: Application to 3₁₀-, Î±-, and Î€-Helices. Journal of Chemical Theory and Computation, 2011, 7, 3884-3897.	5.3	18
24	Validation of the GROMOS 54A7 Force Field with Respect to Î²-Peptide Folding. Journal of Chemical Theory and Computation, 2011, 7, 1237-1243.	5.3	184
25	Influence of Variation of a Side Chain on the Folding Equilibrium of a Î²â€Peptide. Helvetica Chimica Acta, 2011, 94, 597-610.	1.6	5
26	Conformational stateâ€specific free energy differences by oneâ€step perturbation: Protein secondary structure preferences of the GROMOS 43A1 and 53A6 force fields. Journal of Computational Chemistry, 2011, 32, 2290-2297.	3.3	12
27	The effect of using a polarizable solvent model upon the folding equilibrium of different Î²-peptides. Molecular Physics, 2011, 109, 493-506.	1.7	18
28	Using oneâ€step perturbation to predict the effect of changing forceâ€field parameters on the simulated folding equilibrium of a Î²â€peptide in solution. Journal of Computational Chemistry, 2010, 31, 2419-2427.	3.3	9
29	A one-site polarizable model for liquid chloroform: COS/C. Molecular Physics, 2010, 108, 1749-1757.	1.7	12
30	Prediction of Folding Equilibria of Differently Substituted Peptides Using One-Step Perturbation. Journal of the American Chemical Society, 2010, 132, 7276-7278.	13.7	19
31	Using one-step perturbation to predict the folding equilibrium of differently stereochemically substituted Î²-peptides. Physical Chemistry Chemical Physics, 2010, 12, 15442.	2.8	8
32	Refining the description of peptide backbone conformations improves protein simulations using the GROMOS 53A6 force field. Journal of Computational Chemistry, 2009, 30, 645-660.	3.3	34