Zhixiong Lin

List of Publications by Year
in descending order

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Version: 2024-02-01

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	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
2	Refinement of the application of the GROMOS 54A7 force field to Î²-peptides. Journal of Computational Chemistry, 2013, 34, 2796-2805.	3.3	51
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	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
5	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
6	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
7	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
8	On the Use of Enveloping Distribution Sampling (EDS) to Compute Free Enthalpy Differences between Different Conformational States of Molecules: Application to 3₁₀-, Î±-, and Ï€-Helices. Journal of Chemical Theory and Computation, 2011, 7, 3884-3897.	5.3	18
9	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
10	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
11	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
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	A one-site polarizable model for liquid chloroform: COS/C. Molecular Physics, 2010, 108, 1749-1757.	1.7	12
14	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
15	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
16	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
17	Enhanced conformational sampling using enveloping distribution sampling. Journal of Chemical Physics, 2013, 139, 144105.	3.0	11
18	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

#	Article	IF	Citations
19	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
20	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
21	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
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 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
24	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
25	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
26	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
27	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
28	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
29	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
30	GROMOS polarizable charge-on-spring models for liquid urea: COS/U and COS/U2. Journal of Chemical Physics, 2015, 142, 094117.	3.0	3
31	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
32	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