Lingle Wang

List of Publications by Year
in descending order

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43 papers	7,533 citations	172457 29 h-index	254184 43 g-index
49 all docs	49 docs citations	49 times ranked	8805 citing authors

#	Article	IF	Citations
1	The Impact of Experimental and Calculated Error on the Performance of Affinity Predictions. Journal of Chemical Information and Modeling, 2022, 62, 703-717.	5.4	4
2	Novel Physics-Based Ensemble Modeling Approach That Utilizes 3D Molecular Conformation and Packing to Access Aqueous Thermodynamic Solubility: A Case Study of Orally Available Bromodomain and Extraterminal Domain Inhibitor Lead Optimization Series. Journal of Chemical Information and Modeling, 2021, 61, 1412-1426.	5.4	12
3	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. Journal of Chemical Theory and Computation, 2021, 17, 4291-4300.	5.3	582
4	General Theory of Fragment Linking in Molecular Design: Why Fragment Linking Rarely Succeeds and How to Improve Outcomes. Journal of Chemical Theory and Computation, 2021, 17, 450-462.	5.3	21
5	Enhancing Water Sampling in Free Energy Calculations with Grand Canonical Monte Carlo. Journal of Chemical Theory and Computation, 2020, 16, 6061-6076.	5.3	53
6	Is Structure-Based Drug Design Ready for Selectivity Optimization?. Journal of Chemical Information and Modeling, 2020, 60, 6211-6227.	5.4	25
7	Advancing Free-Energy Calculations of Metalloenzymes in Drug Discovery via Implementation of LFMM Potentials. Journal of Chemical Theory and Computation, 2020, 16, 6926-6937.	5.3	8
8	Evaluation of Free Energy Calculations for the Prioritization of Macrocycle Synthesis. Journal of Chemical Information and Modeling, 2020, 60, 3489-3498.	5.4	13
9	Improving the Accuracy of Protein Thermostability Predictions for Single Point Mutations. Biophysical Journal, 2020, 119, 115-127.	0.5	37
10	Toward Atomistic Modeling of Irreversible Covalent Inhibitor Binding Kinetics. Journal of Chemical Information and Modeling, 2019, 59, 3955-3967.	5.4	23
11	Relative Binding Affinity Prediction of Charge-Changing Sequence Mutations with FEP in Proteinâ€“Protein Interfaces. Journal of Molecular Biology, 2019, 431, 1481-1493.	4.2	68
12	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1863-1874.	5.3	698
13	Rigorous Free Energy Perturbation Approach to Estimating Relative Binding Affinities between Ligands with Multiple Protonation and Tautomeric States. Journal of Chemical Theory and Computation, 2019, 15, 424-435.	5.3	36
14	Proteinâ€“Ligand Binding Free Energy Calculations with FEP+. Methods in Molecular Biology, 2019, 2022, 201-232.	0.9	43
15	Modeling the value of predictive affinity scoring in preclinical drug discovery. Current Opinion in Structural Biology, 2018, 52, 103-110.	5.7	14
16	Accurate Calculation of Relative Binding Free Energies between Ligands with Different Net Charges. Journal of Chemical Theory and Computation, 2018, 14, 6346-6358.	5.3	77
17	Predicting resistance of clinical Abl mutations to targeted kinase inhibitors using alchemical free-energy calculations. Communications Biology, 2018, 1, 70.	4.4	66
18	Conformational Free Energy Changes via an Alchemical Path without Reaction Coordinates. Journal of Physical Chemistry Letters, 2018, 9, 4428-4435.	4.6	11

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19	Efficient sampling of puckering states of monosaccharides through replica exchange with solute tempering and bond softening. Journal of Chemical Physics, 2018, 149, 072306.	3.0	12
20	Prospective Evaluation of Free Energy Calculations for the Prioritization of Cathepsin L Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 2485-2497.	6.4	110
21	Free Energy Perturbation Calculation of Relative Binding Free Energy between Broadly Neutralizing Antibodies and the gp120 Glycoprotein of HIV-1. Journal of Molecular Biology, 2017, 429, 930-947.	4.2	82
22	Predicting the Effect of Amino Acid Single-Point Mutations on Protein Stabilityâ€"Large-Scale Validation of MD-Based Relative Free Energy Calculations. Journal of Molecular Biology, 2017, 429, 948-963.	4.2	89
23	Accurate and Reliable Prediction of the Binding Affinities of Macrocycles to Their Protein Targets. Journal of Chemical Theory and Computation, 2017, 13, 6290-6300.	5.3	39
24	Advancing Drug Discovery through Enhanced Free Energy Calculations. Accounts of Chemical Research, 2017, 50, 1625-1632.	15.6	211
25	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. Journal of Chemical Theory and Computation, 2017, 13, 42-54.	5.3	103
26	A Critical Review of Validation, Blind Testing, and Real- World Use of Alchemical Protein-Ligand Binding Free Energy Calculations. Current Topics in Medicinal Chemistry, 2017, 17, 2577-2585.	2.1	88
27	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. ACS Omega, 2016, 1, 293-304.	3.5	108
28	Sensitivity in Binding Free Energies Due to Protein Reorganization. Journal of Chemical Theory and Computation, 2016, 12, 4620-4631.	5.3	65
29	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. Journal of Chemical Theory and Computation, 2016, 12, 281-296.	5.3	2,349
30	How To Deal with Multiple Binding Poses in Alchemical Relative Proteinâ€"Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2670-2679.	5.3	54
31	Accurate and Reliable Prediction of Relative Ligand Binding Potency in Prospective Drug Discovery by Way of a Modern Free-Energy Calculation Protocol and Force Field. Journal of the American Chemical Society, 2015, 137, 2695-2703.	13.7	931
32	Is Ring Breaking Feasible in Relative Binding Free Energy Calculations?. Journal of Chemical Information and Modeling, 2015, 55, 727-735.	5.4	42
33	Accurate Binding Free Energy Predictions in Fragment Optimization. Journal of Chemical Information and Modeling, 2015, 55, 2411-2420.	5.4	119
34	Docking and Free Energy Perturbation Studies of Ligand Binding in the Kappa Opioid Receptor. Journal of Physical Chemistry B, 2015, 119, 824-835.	2.6	26
35	Modeling Local Structural Rearrangements Using FEP/REST: Application to Relative Binding Affinity Predictions of CDK2 Inhibitors. Journal of Chemical Theory and Computation, 2013, 9, 1282-1293.	5.3	179
36	On achieving high accuracy and reliability in the calculation of relative proteinâ€"ligand binding affinities. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 1937-1942.	7.1	204

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37	Replica Exchange with Solute Scaling: A More Efficient Version of Replica Exchange with Solute Tempering (REST2). Journal of Physical Chemistry B, 2011, 115, 9431-9438.	2.6	595
38	Ligand binding to protein-binding pockets with wet and dry regions. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 1326-1330.	7.1	178
39	Competition of Electrostatic and Hydrophobic Interactions between Small Hydrophobes and Model Enclosures. Journal of Physical Chemistry B, 2010, 114, 7294-7301.	2.6	32
40	A Displaced-Solvent Functional Analysis of Model Hydrophobic Enclosures. Journal of Chemical Theory and Computation, 2010, 6, 2924-2934.	5.3	31
41	Hydrophobic interactions in model enclosures from small to large length scales: non-additivity in explicit and implicit solvent models. Faraday Discussions, 2010, 146, 247.	3.2	31
42	Thermodynamic Properties of Liquid Water: An Application of a Nonparametric Approach to Computing the Entropy of a Neat Fluid. Journal of Chemical Theory and Computation, 2009, 5, 1462-1473.	5.3	47
43	Impacting Drug Discovery Projects with Large-Scale Enumerations, Machine Learning Strategies, and Free-Energy Predictions. ACS Symposium Series, 0, , 205-226.	0.5	5