Tai-Sung Lee

List of Publications by Year
in descending order

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Version: 2024-02-01

48 papers	2,553 citations	279798 23 h-index	233421 45 g-index
49 all docs	49 docs citations	49 times ranked	2452 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	CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER. Journal of Chemical Information and Modeling, 2021, 61, 4145-4151.	5.4	24
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	A fast and high-quality charge model for the next generation general AMBER force field. Journal of Chemical Physics, 2020, 153, 114502.	3.0	195
5	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. Journal of Chemical Information and Modeling, 2020, 60, 5595-5623.	5.4	177
6	Validation of Free Energy Methods in AMBER. Journal of Chemical Information and Modeling, 2020, 60, 5296-5300.	5.4	19
7	Fast, Accurate, and Reliable Protocols for Routine Calculations of Proteinâ€“Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. ACS Omega, 2020, 5, 4611-4619.	3.5	74
8	Using AMBER18 for Relative Free Energy Calculations. Journal of Chemical Information and Modeling, 2019, 59, 3128-3135.	5.4	138
9	GPU-Accelerated Molecular Dynamics and Free Energy Methods in Amber18: Performance Enhancements and New Features. Journal of Chemical Information and Modeling, 2018, 58, 2043-2050.	5.4	293
10	Toward Fast and Accurate Binding Affinity Prediction with pmemdGTI: An Efficient Implementation of GPU-Accelerated Thermodynamic Integration. Journal of Chemical Theory and Computation, 2017, 13, 3077-3084.	5.3	93
11	A Multidimensional B-Spline Correction for Accurate Modeling Sugar Puckering in QM/MM Simulations. Journal of Chemical Theory and Computation, 2017, 13, 3975-3984.	5.3	12
12	The importance of protonation and tautomerization in relative binding affinity prediction: a comparison of AMBER TI and SchrÃ¶dinger FEP. Journal of Computer-Aided Molecular Design, 2016, 30, 533-539.	2.9	25
13	RepEx: A Flexible Framework for Scalable Replica Exchange Molecular Dynamics Simulations. , 2016, , .		6
14	A Two-Metal-Ion-Mediated Conformational Switching Pathway for HDV Ribozyme Activation. ACS Catalysis, 2016, 6, 1853-1869.	11.2	24
15	Assessment of metal-assisted nucleophile activation in the hepatitis delta virus ribozyme from molecular simulation and 3D-RISM. Rna, 2015, 21, 1566-1577.	3.5	18
16	Characterization of the Three-Dimensional Free Energy Manifold for the Uracil Ribonucleoside from Asynchronous Replica Exchange Simulations. Journal of Chemical Theory and Computation, 2015, 11, 373-377.	5.3	10
17	Multiscale Methods for Computational RNA Enzymology. Methods in Enzymology, 2015, 553, 335-374.	1.0	16
18	Improvement of DNA and RNA Sugar Pucker Profiles from Semiempirical Quantum Methods. Journal of Chemical Theory and Computation, 2014, 10, 1538-1545.	5.3	50

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19	Roadmaps through Free Energy Landscapes Calculated Using the Multidimensional vFEP Approach. Journal of Chemical Theory and Computation, 2014, 10, 24-34.	5.3	58
20	On the Regulation and Activation of JAK2: A Novel Hypothetical Model. Molecular Cancer Research, 2013, 11, 811-814.	3.4	3
21	A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. Journal of Chemical Theory and Computation, 2013, 9, 153-164.	5.3	76
22	Bridging the Gap Between Theory and Experiment to Derive a Detailed Understanding of Hammerhead Ribozyme Catalysis. Progress in Molecular Biology and Translational Science, 2013, 120, 25-91.	1.7	8
23	A framework for flexible and scalable replica-exchange on production distributed CI. , 2013, , .		3
24	Mapping L1 Ligase Ribozyme Conformational Switch. Journal of Molecular Biology, 2012, 423, 106-122.	4.2	6
25	Characterization of the Structure and Dynamics of the HDV Ribozyme in Different Stages Along the Reaction Path. Journal of Physical Chemistry Letters, 2011, 2, 2538-2543.	4.6	30
26	Active Participation of the Mg²⁺ Ion in the Reaction Coordinate of RNA Self-Cleavage Catalyzed by the Hammerhead Ribozyme. Journal of Chemical Theory and Computation, 2011, 7, 1-3.	5.3	50
27	Effects of Clinically Relevant MPL Mutations in the Transmembrane Domain Revealed at the Atomic Level through Computational Modeling. PLoS ONE, 2011, 6, e23396.	2.5	12
28	Insights into the Role of Conformational Transitions and Metal Ion Binding in RNA Catalysis from Molecular Simulations. Annual Reports in Computational Chemistry, 2010, 6, 168-200.	1.7	1
29	Identification of dynamical hinge points of the L1 ligase molecular switch. Rna, 2010, 16, 769-780.	3.5	7
30	Computational Mutagenesis Studies of Hammerhead Ribozyme Catalysis. Journal of the American Chemical Society, 2010, 132, 13505-13518.	13.7	19
31	Mechanisms of constitutive activation of Janus kinase 2â€V617F revealed at the atomic level through molecular dynamics simulations. Cancer, 2009, 115, 1692-1700.	4.1	30
32	Structural effects of clinically observed mutations in JAK2 exons 13-15: comparison with V617F and exon 12 mutations. BMC Structural Biology, 2009, 9, 58.	2.3	32
33	Threshold Occupancy and Specific Cation Binding Modes in the Hammerhead Ribozyme Active Site are Required for Active Conformation. Journal of Molecular Biology, 2009, 388, 195-206.	4.2	43
34	Basis for Resistance to Imatinib in 16 BCR-ABL Mutants as Determined Using Molecular Dynamics. Recent Patents on Anti-Cancer Drug Discovery, 2009, 4, 164-173.	1.6	7
35	Unraveling the Mechanisms of Ribozyme Catalysis with Multiscale Simulations. Challenges and Advances in Computational Chemistry and Physics, 2009, , 377-408.	0.6	1
36	A Common but Overlooked Mechanism of BCR-ABL1 Kinase Inhibitor Resistance in Chronic Myeloid Leukemia.. Blood, 2009, 114, 2179-2179.	1.4	1

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37	Molecular basis explanation for imatinib resistance of BCRâ€ABL due to T315I and Pâ€loop mutations from molecular dynamics simulations. Cancer, 2008, 112, 1744-1753.	4.1	46
38	Solvent Structure and Hammerhead RibozymeÂCatalysis. Chemistry and Biology, 2008, 15, 332-342.	6.0	104
39	Role of Mg²⁺ in Hammerhead Ribozyme Catalysis from Molecular Simulation. Journal of the American Chemical Society, 2008, 130, 3053-3064.	13.7	102
40	Origin of Mutational Effects at the C3 and G8 Positions on Hammerhead Ribozyme Catalysis from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2008, 130, 7168-7169.	13.7	19
41	BCR-ABLalternative splicing as a common mechanism for imatinib resistance: evidence from molecular dynamics simulations. Molecular Cancer Therapeutics, 2008, 7, 3834-3841.	4.1	63
42	Reverse Conservation Analysis Reveals the Specificity Determining Residues of Cytochrome P450 Family 2 (CYP 2). Evolutionary Bioinformatics, 2008, 4, EBO.S291.	1.2	16
43	Insight into the Role of Mg2+ in Hammerhead Ribozyme Catalysis from X-ray Crystallography and Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2007, 3, 325-327.	5.3	38
44	Multiple property tolerance analysis for the evaluation of missense mutations. Evolutionary Bioinformatics, 2007, 2, 321-32.	1.2	1
45	QCRNA 1.0: A database of quantum calculations for RNA catalysis. Journal of Molecular Graphics and Modelling, 2006, 25, 423-433.	2.4	26
46	A pseudobond approach to combining quantum mechanical and molecular mechanical methods. Journal of Chemical Physics, 1999, 110, 46-54.	3.0	460
47	Quantum Mechanical Study of Aqueous Polarization Effects on Biological Macromolecules. Journal of the American Chemical Society, 1996, 118, 10940-10941.	13.7	61
48	Robust, Efficient and Automated Methods for Accurate Prediction of Protein-Ligand Binding Affinities in AMBER Drug Discovery Boost. ACS Symposium Series, 0, , 161-204.	0.5	9