Tai-Sung Lee

List of Publications by Year
in descending order

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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	A pseudobond approach to combining quantum mechanical and molecular mechanical methods. Journal of Chemical Physics, 1999, 110, 46-54.	3.0	460
2	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
3	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
4	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
5	Using AMBER18 for Relative Free Energy Calculations. Journal of Chemical Information and Modeling, 2019, 59, 3128-3135.	5.4	138
6	Solvent Structure and Hammerhead RibozymeÂCatalysis. Chemistry and Biology, 2008, 15, 332-342.	6.0	104
7	Role of Mg²⁺ in Hammerhead Ribozyme Catalysis from Molecular Simulation. Journal of the American Chemical Society, 2008, 130, 3053-3064.	13.7	102
8	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
9	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
10	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
11	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
12	Quantum Mechanical Study of Aqueous Polarization Effects on Biological Macromolecules. Journal of the American Chemical Society, 1996, 118, 10940-10941.	13.7	61
13	Roadmaps through Free Energy Landscapes Calculated Using the Multidimensional vFEP Approach. Journal of Chemical Theory and Computation, 2014, 10, 24-34.	5.3	58
14	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
15	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
16	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
17	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
18	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

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19	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. Journal of Chemical Theory and Computation, 2020, 16, 5512-5525.	5.3	35
20	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
21	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
22	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
23	QCRNA 1.0: A database of quantum calculations for RNA catalysis. Journal of Molecular Graphics and Modelling, 2006, 25, 423-433.	2.4	26
24	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
25	A Two-Metal-Ion-Mediated Conformational Switching Pathway for HDV Ribozyme Activation. ACS Catalysis, 2016, 6, 1853-1869.	11.2	24
26	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
27	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
28	Computational Mutagenesis Studies of Hammerhead Ribozyme Catalysis. Journal of the American Chemical Society, 2010, 132, 13505-13518.	13.7	19
29	Validation of Free Energy Methods in AMBER. Journal of Chemical Information and Modeling, 2020, 60, 5296-5300.	5.4	19
30	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
31	Reverse Conservation Analysis Reveals the Specificity Determining Residues of Cytochrome P450 Family 2 (CYP 2). Evolutionary Bioinformatics, 2008, 4, EBO.S291.	1.2	16
32	Multiscale Methods for Computational RNA Enzymology. Methods in Enzymology, 2015, 553, 335-374.	1.0	16
33	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
34	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
35	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
36	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

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37	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
38	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
39	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
40	Identification of dynamical hinge points of the L1 ligase molecular switch. Rna, 2010, 16, 769-780.	3.5	7
41	Mapping L1 Ligase Ribozyme Conformational Switch. Journal of Molecular Biology, 2012, 423, 106-122.	4.2	6
42	RepEx: A Flexible Framework for Scalable Replica Exchange Molecular Dynamics Simulations. , 2016, , .		6
43	On the Regulation and Activation of JAK2: A Novel Hypothetical Model. Molecular Cancer Research, 2013, 11, 811-814.	3.4	3
44	A framework for flexible and scalable replica-exchange on production distributed CI. , 2013, , .		3
45	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
46	Unraveling the Mechanisms of Ribozyme Catalysis with Multiscale Simulations. Challenges and Advances in Computational Chemistry and Physics, 2009, , 377-408.	0.6	1
47	A Common but Overlooked Mechanism of BCR-ABL1 Kinase Inhibitor Resistance in Chronic Myeloid Leukemia.. Blood, 2009, 114, 2179-2179.	1.4	1
48	Multiple property tolerance analysis for the evaluation of missense mutations. Evolutionary Bioinformatics, 2007, 2, 321-32.	1.2	1