Ryan L Hayes

List of Publications by Year
in descending order

18 papers	749 citations	687363 13 h-index	839539 18 g-index
19 all docs	19 docs citations	19 times ranked	748 citing authors

#	Article	IF	Citations
1	Addressing Intersite Coupling Unlocks Large Combinatorial Chemical Spaces for Alchemical Free Energy Methods. Journal of Chemical Theory and Computation, 2022, 18, 2114-2123.	5.3	7
2	A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. Journal of Computational Chemistry, 2021, 42, 1088-1094.	3.3	12
3	Generalizing the Discrete Gibbs Sampler-Based Î»-Dynamics Approach for Multisite Sampling of Many Ligands. Journal of Chemical Theory and Computation, 2021, 17, 3895-3907.	5.3	7
4	BLaDE: A Basic Lambda Dynamics Engine for GPU-Accelerated Molecular Dynamics Free Energy Calculations. Journal of Chemical Theory and Computation, 2021, 17, 6799-6807.	5.3	23
5	Automated, Accurate, and Scalable Relative Proteinâ€“Ligand Binding Free-Energy Calculations Using Lambda Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 7895-7914.	5.3	43
6	Overcoming Challenging Substituent Perturbations with Multisite Î»-Dynamics: A Case Study Targeting Î²-Secretase 1. Journal of Physical Chemistry Letters, 2019, 10, 4875-4880.	4.6	17
7	Structure-Based Model of RNA Pseudoknot Captures Magnesium-Dependent Folding Thermodynamics. Journal of Physical Chemistry B, 2019, 123, 1505-1511.	2.6	6
8	CDOCKER and $$lambda$$-dynamics for prospective prediction in D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 89-102.	2.9	9
9	Approaching protein design with multisite Î» dynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. Protein Science, 2018, 27, 1910-1922.	7.6	26
10	Predicting Binding Free Energies in a Large Combinatorial Chemical Space Using Multisite Î» Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 3328-3332.	4.6	28
11	Adaptive Landscape Flattening Accelerates Sampling of Alchemical Space in Multisite Î» Dynamics. Journal of Physical Chemistry B, 2017, 121, 3626-3635.	2.6	54
12	Gibbs Sampler-Based Î»-Dynamics and Raoâ€“Blackwell Estimator for Alchemical Free Energy Calculation. Journal of Chemical Theory and Computation, 2017, 13, 2501-2510.	5.3	33
13	A magnesium-induced triplex pre-organizes the SAM-II riboswitch. PLoS Computational Biology, 2017, 13, e1005406.	3.2	24
14	SMOG 2: A Versatile Software Package for Generating Structure-Based Models. PLoS Computational Biology, 2016, 12, e1004794.	3.2	226
15	Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. Physical Review Letters, 2015, 114, 258105.	7.8	69
16	Reduced Model Captures Mg2+-RNA Interaction Free Energy of Riboswitches. Biophysical Journal, 2014, 106, 1508-1519.	0.5	46
17	Intercellular Stress Reconstitution from Traction Force Data. Biophysical Journal, 2014, 107, 548-554.	0.5	28
18	Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. Journal of the American Chemical Society, 2012, 134, 12043-12053.	13.7	91