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	SMOG 2: A Versatile Software Package for Generating Structure-Based Models. PLoS Computational Biology, 2016, 12, e1004794.	3.2	226
2	Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. Journal of the American Chemical Society, 2012, 134, 12043-12053.	13.7	91
3	Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. Physical Review Letters, 2015, 114, 258105.	7.8	69
4	Adaptive Landscape Flattening Accelerates Sampling of Alchemical Space in Multisite Î» Dynamics. Journal of Physical Chemistry B, 2017, 121, 3626-3635.	2.6	54
5	Reduced Model Captures Mg2+-RNA Interaction Free Energy of Riboswitches. Biophysical Journal, 2014, 106, 1508-1519.	0.5	46
6	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
7	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
8	Intercellular Stress Reconstitution from Traction Force Data. Biophysical Journal, 2014, 107, 548-554.	0.5	28
9	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
10	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
11	A magnesium-induced triplex pre-organizes the SAM-II riboswitch. PLoS Computational Biology, 2017, 13, e1005406.	3.2	24
12	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
13	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
14	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
15	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
16	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
17	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
18	Structure-Based Model of RNA Pseudoknot Captures Magnesium-Dependent Folding Thermodynamics. Journal of Physical Chemistry B, 2019, 123, 1505-1511.	2.6	6