Richard T Bradshaw

List of Publications by Year
in descending order

13	314	1307594 7	1125743 13
papers	citations	h-index	g-index

21	21	21	536
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interpreting hydrogen-deuterium exchange experiments with molecular simulations: Tutorials and applications of the HDXer ensemble reweighting software [Article v1.0]. Living Journal of Computational Molecular Science, 2022, 3, .	6.4	3
2	Chloride-dependent conformational changes in the GlyT1 glycine transporter. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	16
3	Testing the Limitations of MD-Based Local Electric Fields Using the Vibrational Stark Effect in Solution: Penicillin G as a Test Case. Journal of Physical Chemistry B, 2021, 125, 4415-4427.	2.6	8
4	Modeling the native ensemble of PhuS using enhanced sampling MD and HDX-ensemble reweighting. Biophysical Journal, 2021, 120, 5141-5157.	0.5	7
5	Interpretation of HDX Data by Maximum-Entropy Reweighting of Simulated Structural Ensembles. Biophysical Journal, 2020, 118, 1649-1664.	0.5	28
6	The Role of Electrostatics in Enzymes: Do Biomolecular Force Fields Reflect Protein Electric Fields?. Journal of Chemical Information and Modeling, 2020, 60, 3131-3144.	5.4	29
7	Structural predictions of the functions of membrane proteins from HDX-MS. Biochemical Society Transactions, 2020, 48, 971-979.	3.4	7
8	Evaluating Anti-CD32b F(ab) Conformation Using Molecular Dynamics and Small-Angle X-Ray Scattering. Biophysical Journal, 2018, 115, 289-299.	0.5	4
9	Advanced Potential Energy Surfaces for Molecular Simulation. Journal of Physical Chemistry B, 2016, 120, 9811-9832.	2.6	77
10	Evaluating Parametrization Protocols for Hydration Free Energy Calculations with the AMOEBA Polarizable Force Field. Journal of Chemical Theory and Computation, 2016, 12, 3871-3883.	5.3	27
11	Evaluation of solvation free energies for small molecules with the AMOEBA polarizable force field. Journal of Computational Chemistry, 2016, 37, 2749-2758.	3.3	31
12	Mutational Locally Enhanced Sampling (MULES) for quantitative prediction of the effects of mutations at proteinâ€“protein interfaces. Chemical Science, 2012, 3, 1503.	7.4	2
13	Comparing experimental and computational alanine scanning techniques for probing a prototypical proteinâ€“protein interaction. Protein Engineering, Design and Selection, 2011, 24, 197-207.	2.1	73