## **Emilia P Barros**

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Beyond Shielding: The Roles of Glycans in the SARS-CoV-2 Spike Protein. ACS Central Science, 2020, 6, 1722-1734.	5.3	727
2	Al-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. International Journal of High Performance Computing Applications, 2021, 35, 432-451.	2.4	91
3	Markov state models and NMR uncover an overlooked allosteric loop in p53. Chemical Science, 2021, 12, 1891-1900.	3.7	22
4	An integrated view of p53 dynamics, function, and reactivation. Current Opinion in Structural Biology, 2021, 67, 187-194.	2.6	21
5	Relative free-energy calculations for scaffold hopping-type transformations with an automated RE-EDS sampling procedure. Journal of Computer-Aided Molecular Design, 2022, 36, 117-130.	1.3	10
6	Recent developments in multiscale free energy simulations. Current Opinion in Structural Biology, 2022, 72, 55-62.	2.6	5
7	Replica-Exchange Enveloping Distribution Sampling Using Generalized AMBER Force-Field Topologies: Application to Relative Hydration Free-Energy Calculations for Large Sets of Molecules. Journal of Chemical Information and Modeling, 2022, 62, 3043-3056.	2.5	5