

# Emilia P Barros

## List of Publications by Year in descending order

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7  
papers

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1683934  
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1717  
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#	ARTICLE	IF	CITATIONS
1	Recent developments in multiscale free energy simulations. <i>Current Opinion in Structural Biology</i> , 2022, 72, 55-62.	2.6	5
2	Relative free-energy calculations for scaffold hopping-type transformations with an automated RE-EDS sampling procedure. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 117-130.	1.3	10
3	Replica-Exchange Enveloping Distribution Sampling Using Generalized AMBER Force-Field Topologies: Application to Relative Hydration Free-Energy Calculations for Large Sets of Molecules. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3043-3056.	2.5	5
4	Markov state models and NMR uncover an overlooked allosteric loop in p53. <i>Chemical Science</i> , 2021, 12, 1891-1900.	3.7	22
5	AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. <i>International Journal of High Performance Computing Applications</i> , 2021, 35, 432-451.	2.4	91
6	An integrated view of p53 dynamics, function, and reactivation. <i>Current Opinion in Structural Biology</i> , 2021, 67, 187-194.	2.6	21
7	Beyond Shielding: The Roles of Glycans in the SARS-CoV-2 Spike Protein. <i>ACS Central Science</i> , 2020, 6, 1722-1734.	5.3	727