

David S Cerutti

List of Publications by Year in descending order

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12
papers

810
citations

933447

10
h-index

1199594

12
g-index

13
all docs

13
docs citations

13
times ranked

1305
citing authors

#	ARTICLE	IF	CITATIONS
1	GPU-Accelerated Molecular Dynamics and Free Energy Methods in Amber18: Performance Enhancements and New Features. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2043-2050.	5.4	293
2	Further along the Road Less Traveled: AMBER ff15ipq, an Original Protein Force Field Built on a Self-Consistent Physical Model. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3926-3947.	5.3	161
3	Derivation of Fixed Partial Charges for Amino Acids Accommodating a Specific Water Model and Implicit Polarization. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2328-2338.	2.6	95
4	ff14ipq: A Self-Consistent Force Field for Condensed-Phase Simulations of Proteins. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4515-4534.	5.3	87
5	Simulations of a Protein Crystal with a High Resolution X-ray Structure: Evaluation of Force Fields and Water Models. <i>Journal of Physical Chemistry B</i> , 2010, 114, 12811-12824.	2.6	77
6	Multi-Level Ewald: A Hybrid Multigrid/Fast Fourier Transform Approach to the Electrostatic Particle-Mesh Problem. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 443-458.	5.3	26
7	Molecular dynamics simulations of macromolecular crystals. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1402.	14.6	25
8	A twist in the road less traveled: The AMBER ff15ipq-m force field for protein mimetics. <i>Journal of Chemical Physics</i> , 2020, 153, .	3.0	16
9	Histidine protonation controls structural heterogeneity in the cyanobacteriochrome AnPixJg2. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7359-7367.	2.8	14
10	Fast Implementation of the Nudged Elastic Band Method in AMBER. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4699-4707.	5.3	12
11	Links between the charge model and bonded parameter force constants in biomolecular force fields. <i>Journal of Chemical Physics</i> , 2017, 147, 161730.	3.0	3
12	Molecular Dynamics of Oxazole Yellow Dye in its Ground and First Excited Electronic States in Solution and when Intercalated in dsDNA. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10242-10248.	2.6	0