David S Cerutti

List of Publications by Year
in descending order

12	810	933447 10	1199594 12
papers	citations	h-index	g-index

13	13	13	1305
all docs	docs citations	times ranked	citing authors

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