Paul S Nerenberg

List of Publications by Year
in descending order

20 papers	1,065 citations	623734 14 h-index	794594 19 g-index
22 all docs	22 docs citations	22 times ranked	1410 citing authors

#	Article	IF	Citations
1	Phosphoserine inhibits neighboring arginine methylation in the RKS motif of histone H3. Archives of Biochemistry and Biophysics, 2021, 698, 108716.	3.0	4
2	Development and Validation of AMBER-FB15-Compatible Force Field Parameters for Phosphorylated Amino Acids. Journal of Physical Chemistry B, 2021, 125, 11927-11942.	2.6	8
3	Benchmarking Electronic Structure Methods for Accurate Fixed-Charge Electrostatic Models. Journal of Chemical Information and Modeling, 2020, 60, 249-258.	5.4	12
4	Building capacity for undergraduate education and training in computational molecular science: A collaboration between the MERCURY consortium and the Molecular Sciences Software Institute. International Journal of Quantum Chemistry, 2020, 120, e26359.	2.0	9
5	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). Communications Chemistry, 2020, 3, .	4.5	98
6	Systematic Optimization of Water Models Using Liquid/Vapor Surface Tension Data. Journal of Physical Chemistry B, 2019, 123, 7061-7073.	2.6	31
7	New developments in force fields for biomolecular simulations. Current Opinion in Structural Biology, 2018, 49, 129-138.	5.7	181
8	Disordered Structural Ensembles of Vasopressin and Oxytocin and Their Mutants. Journal of Physical Chemistry B, 2015, 119, 896-905.	2.6	32
9	Optimizing Proteinâ€“Protein van der Waals Interactions for the AMBER ff9x/ff12 Force Field. Journal of Chemical Theory and Computation, 2014, 10, 273-281.	5.3	23
10	Embedding AÎ²42 in Heterogeneous Membranes Depends on Cholesterol Asymmetries. Biophysical Journal, 2013, 105, 899-910.	0.5	18
11	Optimizing Soluteâ€“Water van der Waals Interactions To Reproduce Solvation Free Energies. Journal of Physical Chemistry B, 2012, 116, 4524-4534.	2.6	145
12	Homogeneous and Heterogeneous Tertiary Structure Ensembles of Amyloid-Î² Peptides. Biochemistry, 2011, 50, 7612-7628.	2.5	130
13	Optimizing Proteinâ˜Solvent Force Fields to Reproduce Intrinsic Conformational Preferences of Model Peptides. Journal of Chemical Theory and Computation, 2011, 7, 1220-1230.	5.3	149
14	Perturbing the folding energy landscape of the bacterial immunity protein Im7 by site-specific N-linked glycosylation. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 22528-22533.	7.1	72
15	Cleavage Site Specificity and Conformational Selection in Type I Collagen Degradation. Biochemistry, 2010, 49, 4147-4158.	2.5	34
16	The Contribution of Interchain Salt Bridges to Triple-Helical Stability inÂCollagen. Biophysical Journal, 2010, 98, 2634-2643.	0.5	32
17	Physical Basis of Metal-Binding Specificity in Escherichia coli NikR. Journal of the American Chemical Society, 2009, 131, 10220-10228.	13.7	14
18	Metal Preference At The Second Metal Binding Site Of E. coli NikR. Biophysical Journal, 2009, 96, 58a.	0.5	0

#	Article	IF	Citations
19	Do collagenases unwind tripleâ€helical collagen before peptide bond hydrolysis? Reinterpreting experimental observations with mathematical models. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1154-1161.	2.6	36
20	Differential Unfolding of Î±1 and Î±2 Chains in Type I Collagen and Collagenolysis. Journal of Molecular Biology, 2008, 382, 246-256.	4.2	37