Payal Chatterjee

List of Publications by Year
in descending order

13	255	840776 11	1125743 13
papers	citations	h-index	g-index

13	13	13	446
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Can Relative Binding Free Energy Predict Selectivity of Reversible Covalent Inhibitors?. Journal of the American Chemical Society, 2017, 139, 17945-17952.	13.7	44
2	Molecular Mechanism of Resveratrolâ€™s Lipid Membrane Protection. Scientific Reports, 2018, 8, 1587.	3.3	37
3	Ranking Reversible Covalent Drugs: From Free Energy Perturbation to Fragment Docking. Journal of Chemical Information and Modeling, 2019, 59, 2093-2102.	5.4	35
4	<scp>CHARMMâ€GUI</scp> Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. Journal of Computational Chemistry, 2022, 43, 359-375.	3.3	24
5	Toward Prediction of Electrostatic Parameters for Force Fields That Explicitly Treat Electronic Polarization. Journal of Chemical Theory and Computation, 2019, 15, 2460-2469.	5.3	21
6	Effects of bioactive constituents in the Traditional Chinese Medicinal formula Siâ€“Wuâ€“Tang on Nrf2 signaling and neoplastic cellular transformation. Phytomedicine, 2018, 40, 1-9.	5.3	17
7	Harnessing Deep Learning for Optimization of Lennard-Jones Parameters for the Polarizable Classical Drude Oscillator Force Field. Journal of Chemical Theory and Computation, 2022, 18, 2388-2407.	5.3	17
8	Polymodal allosteric regulation of Type 1 Serine/Threonine Kinase Receptors via a conserved electrostatic lock. PLoS Computational Biology, 2017, 13, e1005711.	3.2	16
9	The connexin26 human mutation N14K disrupts cytosolic intersubunit interactions and promotes channel opening. Journal of General Physiology, 2019, 151, 328-341.	1.9	16
10	Deep Neural Network Model to Predict the Electrostatic Parameters in the Polarizable Classical Drude Oscillator Force Field. Journal of Chemical Theory and Computation, 2022, 18, 1711-1725.	5.3	13
11	Solvation dynamics: improved reproduction of the time-dependent Stokes shift with polarizable empirical force field chromophore models. Physical Chemistry Chemical Physics, 2019, 21, 17703-17710.	2.8	12
12	Cancer Cell Metabolism Featuring Nrf2. Current Drug Discovery Technologies, 2020, 17, 263-271.	1.2	2
13	Overlapping structure features selection in linear and non-linear QSAR. Journal of Pharmacy Research, 2013, 6, 183-187.	0.4	1