Fang-Yu Lin

List of Publications by Year
in descending order

15 papers	**553** citations	759233 **12** h-index	1058476 **14** g-index
15 all docs	**15** docs citations	**15** times ranked	**912** citing authors

#	Article	IF	Citations
1	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand–protein interactions. Bioorganic and Medicinal Chemistry, 2016, 24, 4812-4825.	3.0	168
2	Do Halogen–Hydrogen Bond Donor Interactions Dominate the Favorable Contribution of Halogens to Ligand–Protein Binding?. Journal of Physical Chemistry B, 2017, 121, 6813-6821.	2.6	85
3	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. Journal of Chemical Theory and Computation, 2020, 16, 3221-3239.	5.3	53
4	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	5.4	45
5	Polarizable Empirical Force Field for Halogen-Containing Compounds Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2018, 14, 1083-1098.	5.3	38
6	Force Fields for Small Molecules. Methods in Molecular Biology, 2019, 2022, 21-54.	0.9	29
7	Improved Modeling of Cation–π and Anion–Ring Interactions Using the Drude Polarizable Empirical Force Field for Proteins. Journal of Computational Chemistry, 2020, 41, 439-448.	3.3	27
8	Conformational dynamics of cathepsin D and binding to a small–molecule BACE1 inhibitor. Journal of Computational Chemistry, 2017, 38, 1260-1269.	3.3	24
9	Improved Modeling of Halogenated Ligand–Protein Interactions Using the Drude Polarizable and CHARMM Additive Empirical Force Fields. Journal of Chemical Information and Modeling, 2019, 59, 215-228.	5.4	23
10	Drude polarizable force field for aliphatic ketones and aldehydes, and their associated acyclic carbohydrates. Journal of Computer-Aided Molecular Design, 2017, 31, 349-363.	2.9	16
11	Combining the polarizable Drude force field with a continuum electrostatic Poisson–Boltzmann implicit solvation model. Journal of Computational Chemistry, 2018, 39, 1707-1719.	3.3	15
12	Structure-Based Fragment Hopping for Lead Optimization Using Predocked Fragment Database. Journal of Chemical Information and Modeling, 2011, 51, 1703-1715.	5.4	12
13	Species-Specific Endotoxin Stimulus Determines Toll-Like Receptor 4- and Caspase 11-Mediated Pathway Activation Characteristics. MSystems, 2021, 6, e0030621.	3.8	11
14	LeadOp+R: Structure-Based Lead Optimization With Synthetic Accessibility. Frontiers in Pharmacology, 2018, 9, 96.	3.5	5
15	CMOS-based Capacitive Micromachined Ultrasonic Transducers operating without external DC bias. , 2013, , .		2