

Fang-Yu Lin

List of Publications by Year in descending order

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15
papers

553
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759233

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times ranked

912
citing authors

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