Anna Pavlova

List of Publications by Year in Descending Order

21 papers	390 citations	10 h-index	19 g-index
25 ext. papers	549 ext. citations	5.8 avg, IF	3.7 L-index

#	Paper	IF	Citations
21	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations.. *Nature Protocols*, **2022**,	18.8	5
20	Tuning Proton Transfer Thermodynamics in SARS-CoV-2 Main Protease: Implications for Catalysis and Inhibitor Design. *Journal of Physical Chemistry Letters*, **2021**, 12, 4195-4202	6.4	11
19	Machine Learning Reveals the Critical Interactions for SARS-CoV-2 Spike Protein Binding to ACE2. *Journal of Physical Chemistry Letters*, **2021**, 12, 5494-5502	6.4	14
18	ACE2 glycans preferentially interact with SARS-CoV-2 over SARS-CoV. *Chemical Communications*, **2021**, 57, 5949-5952	5.8	6
17	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease.. *Chemical Science*, **2021**, 12, 1513-1527	9.4	29
16	Synergistic Biophysical Techniques Reveal Structural Mechanisms of Engineered Cationic Antimicrobial Peptides in Lipid Model Membranes. *Chemistry - A European Journal*, **2020**, 26, 6247-6256	4.8	2
15	Parameterization of a drug molecule with a halogen σhole particle using ffTK: Implementation, testing, and comparison. *Journal of Chemical Physics*, **2020**, 153, 164104	3.9	1
14	Tuning Proton Transfer Thermodynamics in SARS-Cov-2 Main Protease: Implications for Catalysis and Inhibitor Design. *ChemRxiv*, **2020**,	4.4	2
13	Accelerating Membrane Simulations with Hydrogen Mass Repartitioning. *Journal of Chemical Theory and Computation*, **2019**, 15, 4673-4686	6.4	33
12	Diverse Protein-Folding Pathways and Functions of βHairpins and βSheets **2018**, 1-20		
11	Development of CHARMM-Compatible Force-Field Parameters for Cobalamin and Related Cofactors from Quantum Mechanical Calculations. *Journal of Chemical Theory and Computation*, **2018**, 14, 784-798	6.4	14
10	Redox-Driven Conformational Dynamics in a Photosystem-II-Inspired βHairpin Maquette Determined through Spectroscopy and Simulation. *Journal of Physical Chemistry B*, **2017**, 121, 3536-3545	3.4	9
9	Toward the rational design of macrolide antibiotics to combat resistance. *Chemical Biology and Drug Design*, **2017**, 90, 641-652	2.9	6
8	Living on the edge: Simulations of bacterial outer-membrane proteins. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1753-9	3.8	25
7	Mechanistic Aspects of Using Formate as a Hydrogen Donor in Aqueous Transfer Hydrogenation. *ACS Catalysis*, **2016**, 6, 5350-5358	13.1	14
6	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. *Journal of Chemical Information and Modeling*, **2016**, 56, 721-33	6.1	127
5	Parametrization of macrolide antibiotics using the force field toolkit. *Journal of Computational Chemistry*, **2015**, 36, 2052-63	3.5	9

List of Publications

4	Clarifying the role of sodium in the silica oligomerization reaction. *Physical Chemistry Chemical Physics*, **2013**, 15, 1123-9	3.6	23
3	Understanding the role of water in aqueous ruthenium-catalyzed transfer hydrogenation of ketones. *ChemPhysChem*, **2012**, 13, 3492-6	3.2	57
2	Mechanism of action of HBV capsid assembly modulators predicted from binding to early assembly intermediates		2
1	Critical interactions for SARS-CoV-2 spike protein binding to ACE2 identified by machine learning		1