Antonia Mey

List of Publications by Year in Descending Order

26 papers	770 citations	12 h-index	27 g-index
31 ext. papers	971 ext. citations	5.2 avg, IF	4.3 L-index

#	Paper	IF	Citations
26	Implementation of the QUBE Force Field in SOMD for High-Throughput Alchemical Free-Energy Calculations. *Journal of Chemical Information and Modeling*, **2021**, 61, 2124-2130	6.1	0
25	Dynamic Profiling of Coronavirus 3CL M Protease Ligand-Binding Sites. *Journal of Chemical Information and Modeling*, **2021**, 61, 3058-3073	6.1	9
24	Self-organized emergence of folded protein-like network structures from geometric constraints. *PLoS ONE*, **2020**, 15, e0229230	3.7	1
23	Hybrid Alchemical Free Energy/Machine-Learning Methodology for the Computation of Hydration Free Energies. *Journal of Chemical Information and Modeling*, **2020**, 60, 5331-5339	6.1	11
22	Dynamic design: manipulation of millisecond timescale motions on the energy landscape of cyclophilin A. *Chemical Science*, **2020**, 11, 2670-2680	9.4	10
21	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. *Living Journal of Computational Molecular Science*, **2020**, 2,	10.1	38
20	Assessment of Binding Affinity via Alchemical Free-Energy Calculations. *Journal of Chemical Information and Modeling*, **2020**, 60, 3120-3130	6.1	47
19	Effect of set up protocols on the accuracy of alchemical free energy calculation over a set of ACK1 inhibitors. *PLoS ONE*, **2019**, 14, e0213217	3.7	10
18	Allosteric effects in cyclophilin mutants may be explained by changes in nano-microsecond time scale motions. *Communications Chemistry*, **2019**, 2,	6.3	10
17	BioSimSpace: An interoperable Python framework for biomolecular simulation. *Journal of Open Source Software*, **2019**, 4, 1831	5.2	12
16	Impact of domain knowledge on blinded predictions of binding energies by alchemical free energy calculations. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 199-210	4.2	12
15	Blinded predictions of host-guest standard free energies of binding in the SAMPL5 challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 61-70	4.2	22
14	Blinded predictions of binding modes and energies of HSP90- ligands for the 2015 D3R grand challenge. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4890-4899	3.4	21
13	Blinded predictions of distribution coefficients in the SAMPL5 challenge. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 1101-1114	4.2	12
12	Elucidation of Nonadditive Effects in Protein-Ligand Binding Energies: Thrombin as a Case Study. *Journal of Physical Chemistry B*, **2016**, 120, 5340-50	3.4	22
11	Analytical methods for structural ensembles and dynamics of intrinsically disordered proteins. *Biophysical Reviews*, **2016**, 8, 429-439	3.7	10
10	Shedding Light on the Dock-Lock Mechanism in Amyloid Fibril Growth Using Markov State Models. *Journal of Physical Chemistry Letters*, **2015**, 6, 1076-81	6.4	28

9	Dynamic properties of force fields. *Journal of Chemical Physics*, **2015**, 142, 084101	3.9	60
8	Variational Approach to Molecular Kinetics. *Journal of Chemical Theory and Computation*, **2014**, 10, 1739-52	6.4	193
7	Statistically optimal analysis of state-discretized trajectory data from multiple thermodynamic states. *Journal of Chemical Physics*, **2014**, 141, 214106	3.9	62
6	Rare-event trajectory ensemble analysis reveals metastable dynamical phases in lattice proteins. *Physical Review E*, **2014**, 89, 032109	2.4	22
5	xTRAM: Estimating Equilibrium Expectations from Time-Correlated Simulation Data at Multiple Thermodynamic States. *Physical Review X*, **2014**, 4,	9.1	23
4	EMMA: A Software Package for Markov Model Building and Analysis. *Journal of Chemical Theory and Computation*, **2012**, 8, 2223-38	6.4	123
3	Thermodynamics of trajectories of the one-dimensional Ising model. *Journal of Statistical Mechanics: Theory and Experiment*, **2011**, 2011, P12011	1.9	8
2	Impact of domain knowledge on blinded predictions of binding energies by alchemical free energy calculations		1
1	Structural dynamics of the Coronavirus Mpro protease ligand binding sites		2