Pilar Cossio

List of Publications by Year in descending order

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DILAD COSSIO

#	Article	IF	CITATIONS
1	<i>Ab initio</i> metadynamics determination of temperature-dependent free-energy landscape in ultrasmall silver clusters. Journal of Chemical Physics, 2022, 156, 154301.	3.0	4
2	Computational Evolution Protocol for Peptide Design. Methods in Molecular Biology, 2022, 2405, 335-359.	0.9	3
3	Multiple-Allele MHC Class II Epitope Engineering by a Molecular Dynamics-Based Evolution Protocol. Frontiers in Immunology, 2022, 13, 862851.	4.8	7
4	PARCE: Protocol for Amino acid Refinement through Computational Evolution. Computer Physics Communications, 2021, 260, 107716.	7.5	12
5	PepFun: Open Source Protocols for Peptide-Related Computational Analysis. Molecules, 2021, 26, 1664.	3.8	11
6	Impact of Structural Observables From Simulations to Predict the Effect of Single-Point Mutations in MHC Class II Peptide Binders. Frontiers in Molecular Biosciences, 2021, 8, 636562.	3.5	3
7	Editorial: Integrating Timescales From Molecules Up. Frontiers in Chemistry, 2021, 9, 680533.	3.6	0
8	A Bayesian approach to extracting free-energy profiles from cryo-electron microscopy experiments. Scientific Reports, 2021, 11, 13657.	3.3	27
9	Application of ensemble pharmacophore-based virtual screening to the discovery of novel antimitotic tubulin inhibitors. Computational and Structural Biotechnology Journal, 2021, 19, 4360-4372.	4.1	14
10	Cardiolipin prevents pore formation in phosphatidylglycerol bacterial membrane models. FEBS Letters, 2021, 595, 2701-2714.	2.8	9
11	Flexi-pharma: a molecule-ranking strategy for virtual screening using pharmacophores from ligand-free conformational ensembles. Journal of Computer-Aided Molecular Design, 2020, 34, 1063-1077.	2.9	9
12	Validation tests for cryo-EM maps using an independent particle set. Journal of Structural Biology: X, 2020, 4, 100032.	1.3	1
13	In silico discovery and biological validation of ligands of FAD synthase, a promising new antimicrobial target. PLoS Computational Biology, 2020, 16, e1007898.	3.2	11
14	Need for Cross-Validation of Single Particle Cryo-EM. Journal of Chemical Information and Modeling, 2020, 60, 2413-2418.	5.4	5
15	Computational Design of Peptides Bound to the Major Histocompatibility Complex Class II. Biophysical Journal, 2020, 118, 359a.	0.5	0
16	An automated protocol for modelling peptide substrates to proteases. BMC Bioinformatics, 2020, 21, 586.	2.6	7
17	Title is missing!. , 2020, 16, e1007898.		0

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19	Title is missing!. , 2020, 16, e1007898.		Ο
20	Title is missing!. , 2020, 16, e1007898.		0
21	Predicting the Affinity of Peptides to Major Histocompatibility Complex Class II by Scoring Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2019, 59, 3464-3473.	5.4	34
22	Molecular free energy profiles from force spectroscopy experiments by inversion of observed committors. Journal of Chemical Physics, 2019, 151, 154115.	3.0	14
23	Exponential consensus ranking improves the outcome in docking and receptor ensemble docking. Scientific Reports, 2019, 9, 5142.	3.3	89
24	Transition paths in single-molecule force spectroscopy. Journal of Chemical Physics, 2018, 148, 123309.	3.0	47
25	Discovery of antimicrobial compounds targeting bacterial type FAD synthetases. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 241-254.	5.2	23
26	Likelihood-based structural analysis of electron microscopy images. Current Opinion in Structural Biology, 2018, 49, 162-168.	5.7	15
27	Assessing the capability of <i>in silico</i> mutation protocols for predicting the finite temperature conformation of amino acids. Physical Chemistry Chemical Physics, 2018, 20, 25901-25909.	2.8	18
28	The Dimer-of-Trimers Assembly Prevents Catalysis at the Transferase Site of Prokaryotic FAD Synthase. Biophysical Journal, 2018, 115, 988-995.	0.5	11
29	Bayesian inference of rotor ring stoichiometry from electron microscopy images of archaeal ATP synthase. Microscopy (Oxford, England), 2018, 67, 266-273.	1.5	8
30	BioEM: GPU-accelerated computing of Bayesian inference of electron microscopy images. Computer Physics Communications, 2017, 210, 163-171.	7.5	27
31	Kinetic Ductility and Force-Spike Resistance of Proteins from Single-Molecule Force Spectroscopy. Biophysical Journal, 2016, 111, 832-840.	0.5	27
32	On artifacts in single-molecule force spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14248-14253.	7.1	89
33	Effects of a disulfide bridge prior to amyloid formation of the ABRI peptide. RSC Advances, 2014, 4, 36923-36928.	3.6	3
34	Bayesian analysis of individual electron microscopy images: Towards structures of dynamic and heterogeneous biomolecular assemblies. Journal of Structural Biology, 2013, 184, 427-437.	2.8	66
35	The Molecular Mechanism of Substrate Engagement and Immunosuppressant Inhibition of Calcineurin. PLoS Biology, 2013, 11, e1001492.	5.6	123
36	A simple and efficient statistical potential for scoring ensembles of protein structures. Scientific Reports, 2012, 2, .	3.3	48

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37	Protein Folding and Ligand-Enzyme Binding from Bias-Exchange Metadynamics Simulations. Current Physical Chemistry, 2012, 2, 79-91.	0.2	6
38	Conformations of the Huntingtin N-term in aqueous solution from atomistic simulations. FEBS Letters, 2011, 585, 3086-3089.	2.8	24
39	Which similarity measure is better for analyzing protein structures in a molecular dynamics trajectory?. Physical Chemistry Chemical Physics, 2011, 13, 10421.	2.8	25
40	Exploring the Universe of Protein Structures beyond the Protein Data Bank. PLoS Computational Biology, 2010, 6, e1000957.	3.2	62
41	Optimizing the Performance of Bias-Exchange Metadynamics: Folding a 48-Residue LysM Domain Using a Coarse-Grained Model. Journal of Physical Chemistry B, 2010, 114, 3259-3265.	2.6	40