Daniel-Adriano Silva

List of Publications by Citations

34 papers	2,068 citations	22 h-index	35 g-index
35 ext. papers	2,745 ext. citations	15.2 avg, IF	4.5 L-index

#	Paper	IF	Citations
34	Monitoring and inhibition of insulin fibrillation by a small organic fluorogen with aggregation-induced emission characteristics. *Journal of the American Chemical Society*, **2012**, 134, 1680-9	16.4	293
33	Massively parallel de novo protein design for targeted therapeutics. *Nature*, **2017**, 550, 74-79	50.4	235
32	De novo design of potent and selective mimics of IL-2 and IL-15. *Nature*, **2019**, 565, 186-191	50.4	184
31	A role for both conformational selection and induced fit in ligand binding by the LAO protein. *PLoS Computational Biology*, **2011**, 7, e1002054	5	172
30	Macromolecular modeling and design in Rosetta: recent methods and frameworks. *Nature Methods*, **2020**, 17, 665-680	21.6	165
29	De novo design of potent and resilient hACE2 decoys to neutralize SARS-CoV-2. *Science*, **2020**, 370, 1208-1214	33.3	98
28	Comprehensive computational design of ordered peptide macrocycles. *Science*, **2017**, 358, 1461-1466	33.3	96
27	Millisecond dynamics of RNA polymerase II translocation at atomic resolution. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 7665-70	11.5	90
26	Principles for designing proteins with cavities formed by curved β sheets. *Science*, **2017**, 355, 201-206	33.3	82
25	De novo protein design by citizen scientists. *Nature*, **2019**, 570, 390-394	50.4	63
24	Simulating the T-jump-triggered unfolding dynamics of trpzip2 peptide and its time-resolved IR and two-dimensional IR signals using the Markov state model approach. *Journal of Physical Chemistry B*, **2011**, 115, 5415-24	3.4	59
23	Quantitatively characterizing the ligand binding mechanisms of choline binding protein using Markov state model analysis. *PLoS Computational Biology*, **2014**, 10, e1003767	5	55
22	Bridge helix bending promotes RNA polymerase II backtracking through a critical and conserved threonine residue. *Nature Communications*, **2016**, 7, 11244	17.4	54
21	Computationally designed high specificity inhibitors delineate the roles of BCL2 family proteins in cancer. *ELife*, **2016**, 5,	8.9	52
20	Initiation complex structure and promoter proofreading. *Science*, **2011**, 333, 633-7	33.3	48
19	De novo design of covalently constrained mesosize protein scaffolds with unique tertiary structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 10852-10857	11.5	44
18	Force field development for cofactors in the photosystem II. *Journal of Computational Chemistry*, **2012**, 33, 1969-80	3.5	40

17	Hierarchical Nyström methods for constructing Markov state models for conformational dynamics. *Journal of Chemical Physics*, **2013**, 138, 174106	3.9	37
16	Dynamic protein conformations preferentially drive energy transfer along the active chain of the photosystem II reaction centre. *Nature Communications*, **2014**, 5, 4170	17.4	33
15	Automatic state partitioning for multibody systems (APM): an efficient algorithm for constructing Markov state models to elucidate conformational dynamics of multibody systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 17-27	6.4	29
14	Motif-Driven Design of Protein-Protein Interfaces. *Methods in Molecular Biology*, **2016**, 1414, 285-304	1.4	26
13	Essentials of de novo protein design: Methods and applications. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1374	7.9	22
12	Application of Markov State Models to simulate long timescale dynamics of biological macromolecules. *Advances in Experimental Medicine and Biology*, **2014**, 805, 29-66	3.6	22
11	Conformational dynamics of L-lysine, L-arginine, L-ornithine binding protein reveals ligand-dependent plasticity. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2097-108	4.2	15
10	Analysis of the antimicrobial activities of a chemokine-derived peptide (CDAP-4) on Pseudomonas aeruginosa. *Biochemical and Biophysical Research Communications*, **2007**, 355, 352-8	3.4	13
9	Structural Model of RNA Polymerase II Elongation Complex with Complete Transcription Bubble Reveals NTP Entry Routes. *PLoS Computational Biology*, **2015**, 11, e1004354	5	9
8	On the molecular basis of the high affinity binding of basic amino acids to LAOBP, a periplasmic binding protein from Salmonella typhimurium. *Journal of Molecular Recognition*, **2015**, 28, 108-16	2.6	7
7	Structures and disulfide cross-linking of de novo designed therapeutic mini-proteins. *FEBS Journal*, **2018**, 285, 1783-1785	5.7	6
6	design of ACE2 protein decoys to neutralize SARS-CoV-2 **2020**,		6
5	The advent of de novo proteins for cancer immunotherapy. *Current Opinion in Chemical Biology*, **2020**, 56, 119-128	9.7	5
4	Bridging the Gap Between Optical Spectroscopic Experiments and Computer Simulations for Fast Protein Folding Dynamics. *Current Physical Chemistry*, **2012**, 2, 45-58	0.5	4
3	Computational design of mechanically coupled axle-rotor protein assemblies.. *Science*, **2022**, 376, 383-390	55.3	2
2	Super-enhancer-based identification of a BATF3/IL-2R-module reveals vulnerabilities in anaplastic large cell lymphoma. *Nature Communications*, **2021**, 12, 5577	17.4	1
1	An IL-2 Protein Therapeutic for Cancer that Gains Function on the Spot.. *Cancer Immunology Research*, **2022**, OF1	12.5	