Alessandro Pandini

List of Publications by Citations

38 papers	1,171 citations	16 h-index	34 g-index
44 ext. papers	1,326 ext. citations	3.5 avg, IF	4.32 L-index

#	Paper	IF	Citations
38	Ligand binding and activation of the Ah receptor. *Chemico-Biological Interactions*, **2002**, 141, 3-24	5	342
37	Structural and functional characterization of the aryl hydrocarbon receptor ligand binding domain by homology modeling and mutational analysis. *Biochemistry*, **2007**, 46, 696-708	3.2	97
36	Detection of the TCDD binding-fingerprint within the Ah receptor ligand binding domain by structurally driven mutagenesis and functional analysis. *Biochemistry*, **2009**, 48, 5972-83	3.2	89
35	Detection of allosteric signal transmission by information-theoretic analysis of protein dynamics. *FASEB Journal*, **2012**, 26, 868-81	0.9	86
34	Predicting the accuracy of protein-ligand docking on homology models. *Journal of Computational Chemistry*, **2011**, 32, 81-98	3.5	57
33	Comparative analysis of homology models of the AH receptor ligand binding domain: verification of structure-function predictions by site-directed mutagenesis of a nonfunctional receptor. *Biochemistry*, **2013**, 52, 714-25	3.2	55
32	Structural alphabets derived from attractors in conformational space. *BMC Bioinformatics*, **2010**, 11, 97	3.6	41
31	GSATools: analysis of allosteric communication and functional local motions using a structural alphabet. *Bioinformatics*, **2013**, 29, 2053-5	7.2	38
30	Conformational and functional analysis of molecular dynamics trajectories by self-organising maps. *BMC Bioinformatics*, **2011**, 12, 158	3.6	33
29	Conservation and specialization in PAS domain dynamics. *Protein Engineering, Design and Selection*, **2005**, 18, 127-37	1.9	31
28	Specialized Dynamical Properties of Promiscuous Residues Revealed by Simulated Conformational Ensembles. *Journal of Chemical Theory and Computation*, **2013**, 9, 5127-5147	6.4	30
27	BCR-ABL residues interacting with ponatinib are critical to preserve the tumorigenic potential of the oncoprotein. *FASEB Journal*, **2014**, 28, 1221-36	0.9	25
26	The Gearbox of the Bacterial Flagellar Motor Switch. *Structure*, **2016**, 24, 1209-20	5.2	23
25	Detecting similarities among distant homologous proteins by comparison of domain flexibilities. *Protein Engineering, Design and Selection*, **2007**, 20, 285-99	1.9	19
24	Binding of Myomesin to Obscurin-Like-1 at the Muscle M-Band Provides a Strategy for Isoform-Specific Mechanical Protection. *Structure*, **2017**, 25, 107-120	5.2	17
23	The crystal structure of the human titin:obscurin complex reveals a conserved yet specific muscle M-band zipper module. *Journal of Molecular Biology*, **2015**, 427, 718-736	6.5	16
22	MinSet: a general approach to derive maximally representative database subsets by using fragment dictionaries and its application to the SCOP database. *Bioinformatics*, **2007**, 23, 515-6	7.2	16

21	Bridging topological and functional information in protein interaction networks by short loops profiling. *Scientific Reports*, **2015**, 5, 8540	4.9	14
20	Ligand-induced perturbation of the HIF-2ARNT dimer dynamics. *PLoS Computational Biology*, **2018**, 14, e1006021	5	14
19	Artificial neural networks for efficient clustering of conformational ensembles and their potential for medicinal chemistry. *Current Topics in Medicinal Chemistry*, **2013**, 13, 642-51	3	14
18	Machine Learning Prediction of Allosteric Drug Activity from Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2021**, 12, 3724-3732	6.4	14
17	Structure-based enzyme engineering improves donor-substrate recognition of Arabidopsis thaliana glycosyltransferases. *Biochemical Journal*, **2020**, 477, 2791-2805	3.8	13
16	Using Local States To Drive the Sampling of Global Conformations in Proteins. *Journal of Chemical Theory and Computation*, **2016**, 12, 1368-79	6.4	12
15	Functional annotation of the mesophilic-like character of mutants in a cold-adapted enzyme by self-organising map analysis of their molecular dynamics. *Molecular BioSystems*, **2012**, 8, 2680-91		11
14	The Phylogenetic Signature Underlying ATP Synthase c-Ring Compliance. *Biophysical Journal*, **2015**, 109, 975-87	2.9	9
13	Dynamic Profiling of Coronavirus 3CL M Protease Ligand-Binding Sites. *Journal of Chemical Information and Modeling*, **2021**, 61, 3058-3073	6.1	9
12	In silico identification of rescue sites by double force scanning. *Bioinformatics*, **2018**, 34, 207-214	7.2	8
11	Computational approaches to shed light on molecular mechanisms in biological processes. *Theoretical Chemistry Accounts*, **2007**, 117, 723-741	1.9	8
10	Coevolved Mutations Reveal Distinct Architectures for Two Core Proteins in the Bacterial Flagellar Motor. *PLoS ONE*, **2015**, 10, e0142407	3.7	7
9	Conformational coupling by trans-phosphorylation in calcium calmodulin dependent kinase II. *PLoS Computational Biology*, **2019**, 15, e1006796	5	5
8	Structure, Dynamics and Cellular Insight Into Novel Substrates of the Type II Secretion System. *Frontiers in Molecular Biosciences*, **2020**, 7, 112	5.6	4
7	Deep Autoencoders for Additional Insight into Protein Dynamics. *Lecture Notes in Computer Science* , **2018**, 79-89	0.9	4
6	Using Computational Intelligence Models for Additional Insight into Protein Structure **2017**, 62, 107-120		3
5	Reconstruction of ARNT PAS-B Unfolding Pathways by Steered Molecular Dynamics and Artificial Neural Networks. *Journal of Chemical Theory and Computation*, **2021**, 17, 2080-2089	6.4	3
4	Allosteric Priming of E.coli CheY by the Flagellar Motor Protein FliM. *Biophysical Journal*, **2020**, 119, 1108-1122	2.9	2

3	Allosteric priming ofE. coliCheY by the flagellar motor protein FliM		1
2	PathDetect-SOM: A Neural Network Approach for the Identification of Pathways in Ligand Binding Simulations.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	1
1	Detection of Allosteric Signal Transmission by Information-Theoretic Analysis of Protein Dynamics. *Biophysical Journal*, **2012**, 102, 225a	2.9	