Jaime RodrÃ-guez-Guerra Pedregal

List of Publications by Year
in descending order

23 papers	427 citations	759233 12 h-index	752698 20 g-index
26 all docs	26 docs citations	26 times ranked	559 citing authors

#	Article	IF	Citations
1	Prediction of the interaction of metallic moieties with proteins: An update for proteinâ€ligand docking techniques. Journal of Computational Chemistry, 2018, 39, 42-51.	3.3	54
2	Toward the Computational Design of Artificial Metalloenzymes: From Proteinâ€“Ligand Docking to Multiscale Approaches. ACS Catalysis, 2015, 5, 2469-2480.	11.2	51
3	GaudiMM: A modular multiâ€objective platform for molecular modeling. Journal of Computational Chemistry, 2017, 38, 2118-2126.	3.3	37
4	Molecular Modeling for Artificial Metalloenzyme Design and Optimization. Accounts of Chemical Research, 2020, 53, 896-905.	15.6	29
5	Cerebral sex dimorphism and sexual orientation. Human Brain Mapping, 2018, 39, 1175-1186.	3.6	23
6	Elucidating the 3D structures of Al(<scp>iii</scp>)â€“Aî² complexes: a template free strategy based on the pre-organization hypothesis. Chemical Science, 2017, 8, 5041-5049.	7.4	21
7	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. Nature Communications, 2019, 10, 2222.	12.8	20
8	Simple Coordination Geometry Descriptors Allow to Accurately Predict Metal-Binding Sites in Proteins. ACS Omega, 2019, 4, 3726-3731.	3.5	20
9	ESIgen: Electronic Supporting Information Generator for Computational Chemistry Publications. Journal of Chemical Information and Modeling, 2018, 58, 561-564.	5.4	19
10	PyChimera: use UCSF Chimera modules in any Python 2.7 project. Bioinformatics, 2018, 34, 1784-1785.	4.1	18
11	Differential response to Cadmium exposure by expression of a two and a three-domain metallothionein isoform in the land winkle Pomatias elegans: Valuating the marine heritage of a land snail. Science of the Total Environment, 2019, 648, 561-571.	8.0	15
12	TeachOpenCADD-KNIME: A Teaching Platform for Computer-Aided Drug Design Using KNIME Workflows. Journal of Chemical Information and Modeling, 2019, 59, 4083-4086.	5.4	15
13	Theoretical Study of Radical Inactivation, LOX Inhibition, and Iron Chelation: The Role of Ferulic Acid in Skin Protection against UVA Induced Oxidative Stress. Antioxidants, 2021, 10, 1303.	5.1	15
14	GPathFinder: Identification of Ligand-Binding Pathways by a Multi-Objective Genetic Algorithm. International Journal of Molecular Sciences, 2019, 20, 3155.	4.1	14
15	Impact of the phenolic Oâ€“H vs. C-ring Câ€“H bond cleavage on the antioxidant potency of dihydrokaempferol. New Journal of Chemistry, 2021, 45, 7977-7986.	2.8	12
16	Computational insight into the interaction of oxaliplatin with insulin. Metallomics, 2019, 11, 765-773.	2.4	10
17	Integrated Computational Study of the Cu-Catalyzed Hydration of Alkenes in Water Solvent and into the Context of an Artificial Metallohydratase. ACS Catalysis, 2019, 9, 4616-4626.	11.2	10
18	The Effect of Cofactor Binding on the Conformational Plasticity of the Biological Receptors in Artificial Metalloenzymes: The Case Study of LmrR. Frontiers in Chemistry, 2019, 7, 211.	3.6	9

#	Article	IF	Citations
19	GARLEEK: Adding an extra flavor to ONIOM. Journal of Computational Chemistry, 2019, 40, 381-386.	3.3	6
20	TeachOpenCADD 2022: open source and FAIR Python pipelines to assist in structural bioinformatics and cheminformatics research. Nucleic Acids Research, 2022, 50, W753-W760.	14.5	6
21	OpenCADD-KLIFS: A Python package to fetch kinase data from the KLIFS database. Journal of Open Source Software, 2022, 7, 3951.	4.6	4
22	Teaching Computer-Aided Drug Design Using TeachOpenCADD. ACS Symposium Series, 0, , 135-158.	0.5	3
23	Chapter 15. Enzyme Design. RSC Theoretical and Computational Chemistry Series, 2016, , 481-521.	0.7	1