Gonzalo A JaÃ±a

List of Publications by Year
in descending order

18 papers	138 citations	1306789 7 h-index	1372195 10 g-index
18 all docs	18 docs citations	18 times ranked	117 citing authors

#	Article	IF	Citations
1	QM/MM Study of a VIM-1 Metallo-Î²-Lactamase Enzyme: The Catalytic Reaction Mechanism. ACS Catalysis, 2022, 12, 36-47.	5.5	9
2	Glucosylation mechanism of resveratrol through the mutant Q345F sucrose phosphorylase from the organism Bifidobacterium adolescentis: a computational study. Organic and Biomolecular Chemistry, 2022, 20, 5270-5283.	1.5	5
3	New Insights into the Determinants of Specificity in Human Type I Arginase: Generation of a Mutant That Is Only Active with Agmatine as Substrate. International Journal of Molecular Sciences, 2022, 23, 6438.	1.8	2
4	The inverting mechanism of the metal ion-independent LanGT2: the first step to understand the glycosylation of natural product antibiotic precursors through QM/MM simulations. Organic and Biomolecular Chemistry, 2021, 19, 5888-5898.	1.5	4
5	Catalytic Role of Gln202 in the Carboligation Reaction Mechanism of Yeast AHAS: A QM/MM Study. Journal of Chemical Information and Modeling, 2020, 60, 915-922.	2.5	6
6	Unveiling the Dynamical and Structural Features That Determine the Orientation of the Acceptor Substrate in the Landomycin Glycosyltransferase LanGT2 and Its Variant with C-Glycosylation Activity. Journal of Chemical Information and Modeling, 2020, 60, 933-943.	2.5	9
7	Mechanism-Based Rational Discovery and In Vitro Evaluation of Novel Microtubule Stabilizing Agents with Non-Taxol-Competitive Activity. Journal of Chemical Information and Modeling, 2020, 60, 3204-3213.	2.5	6
8	The role of conserved arginine in the GH70 family: a computational study of the structural features and their implications on the catalytic mechanism of GTF-SI from Streptoccocus mutans. Organic and Biomolecular Chemistry, 2019, 17, 6269-6276.	1.5	7
9	Molecular modeling study on the differential microtubuleâ€stabilizing effect in singlyâ€•and doublyâ€bonded complexes with peloruside A and paclitaxel. Proteins: Structure, Function and Bioinformatics, 2019, 87, 668-678.	1.5	6
10	Modulation of glucanâ€enzyme interactions by domain V in GTFâ€SI from Streptococcus mutans. Proteins: Structure, Function and Bioinformatics, 2019, 87, 74-80.	1.5	7
11	A QM/MM approach on the structural and stereoelectronic factors governing glycosylation by GTF-SI fromStreptococcus mutans. Organic and Biomolecular Chemistry, 2018, 16, 2438-2447.	1.5	14
12	Modulation of lateral and longitudinal interdimeric interactions in microtubule models by Laulimalide and Peloruside A association: A molecular modeling approach on the mechanism of microtubule stabilizing agents. Chemical Biology and Drug Design, 2018, 91, 1042-1055.	1.5	7
13	Structural insight into the role of Gln293Met mutation on the Peloruside A/Laulimalide association with Î±Î²-tubulin from molecular dynamics simulations, binding free energy calculations and weak interactions analysis. Journal of Computer-Aided Molecular Design, 2017, 31, 643-652.	1.3	11
14	A QM/MM study on the reaction pathway leading to 2â€Acetoâ€2â€hydroxybutyrate in the catalytic cycle of AHAS. Journal of Computational Chemistry, 2014, 35, 488-494.	1.5	8
15	Electron density reactivity indexes of the tautomeric/ionization forms of thiamin diphosphate. Journal of Molecular Modeling, 2013, 19, 3799-3803.	0.8	7
16	On the inhibition of AHAS by chlorimuron ethyl: A theoretical study. Chemical Physics Letters, 2011, 516, 239-243.	1.2	3
17	A QM/MM study on the last two steps of the catalytic cycle of acetohydroxyacid synthase. Computational and Theoretical Chemistry, 2011, 966, 159-166.	1.1	11
18	Computational study on the carboligation reaction of acetohidroxyacid synthase: New approach on the role of the HEThDP^{â^’} intermediate. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1774-1788.	1.5	16