Javier Iglesias-Fernandez

List of Publications by Year
in descending order

30 papers	1,229 citations	471371 17 h-index	395590 33 g-index
37 all docs	37 docs citations	37 times ranked	2335 citing authors

#	Article	IF	Citations
1	Privateer: software for the conformational validation of carbohydrate structures. Nature Structural and Molecular Biology, 2015, 22, 833-834.	3.6	301
2	Role of conformational dynamics in the evolution of novel enzyme function. Chemical Communications, 2018, 54, 6622-6634.	2.2	123
3	Catalytic Itinerary in 1,3-1,4-Î²-Glucanase Unraveled by QM/MM Metadynamics. Charge Is Not Yet Fully Developed at the Oxocarbenium Ion-like Transition State. Journal of the American Chemical Society, 2011, 133, 20301-20309.	6.6	86
4	Substrateâ€Guided Frontâ€Face Reaction Revealed by Combined Structural Snapshots and Metadynamics for the Polypeptide Nâ€Acetylgalactosaminyltransferaseâ€…2. Angewandte Chemie - International Edition, 2014, 53, 8206-8210.	7.2	80
5	Dynamic interplay between catalytic and lectin domains of GalNAc-transferases modulates protein O-glycosylation. Nature Communications, 2015, 6, 6937.	5.8	77
6	The Reaction Coordinate of a Bacterial GH47 Î±â€Mannosidase: A Combined Quantum Mechanical and Structural Approach. Angewandte Chemie - International Edition, 2012, 51, 10997-11001.	7.2	57
7	Deciphering the Allosterically Driven Conformational Ensemble in Tryptophan Synthase Evolution. Journal of the American Chemical Society, 2019, 141, 13049-13056.	6.6	49
8	The reaction mechanism of retaining glycosyltransferases. Biochemical Society Transactions, 2016, 44, 51-60.	1.6	45
9	The complete conformational free energy landscape of Î²-xylose reveals a two-fold catalytic itinerary for Î²-xylanases. Chemical Science, 2015, 6, 1167-1177.	3.7	44
10	Palladium-mediated enzyme activation suggests multiphase initiation of glycogenesis. Nature, 2018, 563, 235-240.	13.7	42
11	Evidence for a Boat Conformation at the Transition State of GH76 Î±â€1,6â€Mannanasesâ€”Key Enzymes in Bacterial and Fungal Mannoprotein Metabolism. Angewandte Chemie - International Edition, 2015, 54, 5378-5382.	7.2	40
12	Combined Inhibitor Freeâ€Energy Landscape and Structural Analysis Reports on the Mannosidase Conformational Coordinate. Angewandte Chemie - International Edition, 2014, 53, 1087-1091.	7.2	39
13	In Silico Identification and Experimental Validation of Distal Activity-Enhancing Mutations in Tryptophan Synthase. ACS Catalysis, 2021, 11, 13733-13743.	5.5	30
14	Molecular Dynamics Simulations and Neutron Reflectivity as an Effective Approach To Characterize Biological Membranes and Related Macromolecular Assemblies. Journal of Chemical Theory and Computation, 2015, 11, 4875-4884.	2.3	22
15	A Single Glycosidase Harnesses Different Pyranoside Ring Transition State Conformations for Hydrolysis of Mannosides and Glucosides. ACS Catalysis, 2015, 5, 6041-6051.	5.5	22
16	A front-face 'SNi synthase' engineered from a retaining 'double-SN2' hydrolase. Nature Chemical Biology, 2017, 13, 874-881.	3.9	22
17	Hidden Conformations in Aspergillus niger Monoamine Oxidase are Key for Catalytic Efficiency. Angewandte Chemie - International Edition, 2019, 58, 3097-3101.	7.2	18
18	Surfactin at the Water/Air Interface and in Solution. Langmuir, 2015, 31, 11097-11104.	1.6	16

#	Article	IF	Citations
19	Enantioselective Preparation of Î´â€Valerolactones with Horse Liver Alcohol Dehydrogenase. ChemCatChem, 2014, 6, 977-980.	1.8	15
20	Multivalent Ligands with Tailorâ€Made Anion Binding Motif as Stabilizers of Proteinâ€“Protein Interactions. ChemBioChem, 2019, 20, 2921-2926.	1.3	13
21	Membrane Phase-Dependent Occlusion of Intramolecular GLUT1 Cavities Demonstrated by Simulations. Biophysical Journal, 2017, 112, 1176-1184.	0.2	12
22	Structural analysis and insights into the glycon specificity of the rice GH1 Os7BGlu26 Î²-<scp>D</scp>-mannosidase. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 2124-2135.	2.5	11
23	Conformational Landscapes of Halohydrin Dehalogenases and Their Accessible Active Site Tunnels. Catalysts, 2020, 10, 1403.	1.6	9
24	Binding of azole drugs to heme: A combined MS/MS and computational approach. Polyhedron, 2015, 90, 245-251.	1.0	7
25	Insights into the molecular determinants of thermal stability in halohydrin dehalogenase HheD2. FEBS Journal, 2021, 288, 4683-4701.	2.2	5
26	Exploring the Conversion of a <scp>d</scp>â€Sialic Acid Aldolase into a <scp>l</scp>â€KDO Aldolase. European Journal of Organic Chemistry, 2018, 2018, 2603-2608.	1.2	4
27	Mutational Analysis of Linalool Dehydratase Isomerase Suggests That Alcohol and Alkene Transformations Are Catalyzed Using Noncovalent Mechanisms. ACS Catalysis, 2020, 10, 11136-11146.	5.5	4
28	A Multiperspective Approach to Solvent Regulation of Enzymatic Activity: HMGâ€CoA Reductase. ChemBioChem, 2018, 19, 153-158.	1.3	3
29	InnenrÃ¼cktitelbild: The Reaction Coordinate of a Bacterial GH47 Î±-Mannosidase: A Combined Quantum Mechanical and Structural Approach (Angew. Chem. 44/2012). Angewandte Chemie, 2012, 124, 11333-11333.	1.6	0
30	Hidden Conformations in Aspergillus niger Monoamine Oxidase are Key for Catalytic Efficiency. Angewandte Chemie, 2019, 131, 3129-3133.	1.6	0