Carme Rovira

List of Publications by Citations

174 papers	6,121 citations	44 h-index	69 g-index
185 ext. papers	6,840 ext. citations	8.4 avg, IF	5.87 L-index

#	Paper	IF	Citations
174	Equilibrium Geometries and Electronic Structure of Iron Porphyrin Complexes: A Density Functional Study. *Journal of Physical Chemistry A*, **1997**, 101, 8914-8925	2.8	347
173	The molecular mechanism of the catalase reaction. *Journal of the American Chemical Society*, **2009**, 131, 11751-61	16.4	216
172	Privateer: software for the conformational validation of carbohydrate structures. *Nature Structural and Molecular Biology*, **2015**, 22, 833-4	17.6	215
171	Conformational analyses of the reaction coordinate of glycosidases. *Accounts of Chemical Research*, **2012**, 45, 308-16	24.3	184
170	The conformational free energy landscape of beta-D-glucopyranose. Implications for substrate preactivation in beta-glucoside hydrolases. *Journal of the American Chemical Society*, **2007**, 129, 10686-93	16.4	177
169	Reaction Mechanisms in Carbohydrate-Active Enzymes: Glycoside Hydrolases and Glycosyltransferases. Insights from ab Initio Quantum Mechanics/Molecular Mechanics Dynamic Simulations. *Journal of the American Chemical Society*, **2015**, 137, 7528-47	16.4	145
168	Structural basis for the high all-trans-retinaldehyde reductase activity of the tumor marker AKR1B10. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 20764-9	11.5	143
167	Do thiols merely passivate gold nanoclusters?. *Physical Review Letters*, **2000**, 85, 5250-1	7.4	142
166	Influence of the heme pocket conformation on the structure and vibrations of the Fe-CO bond in myoglobin: a QM/MM density functional study. *Biophysical Journal*, **2001**, 81, 435-45	2.9	120
165	The effect of a water molecule on the mechanism of formation of compound 0 in horseradish peroxidase. *Journal of the American Chemical Society*, **2007**, 129, 6346-7	16.4	90
164	QM/MM Studies into the H2O2-Dependent Activity of Lytic Polysaccharide Monooxygenases: Evidence for the Formation of a Caged Hydroxyl Radical Intermediate. *ACS Catalysis*, **2018**, 8, 1346-1351	13.1	87
163	Mechanism of cellulose hydrolysis by inverting GH8 endoglucanases: a QM/MM metadynamics study. *Journal of Physical Chemistry B*, **2009**, 113, 7331-9	3.4	87
162	The molecular mechanism of enzymatic glycosyl transfer with retention of configuration: evidence for a short-lived oxocarbenium-like species. *Angewandte Chemie - International Edition*, **2011**, 50, 10897-901	16.4	81
161	On the usefulness of the counterpoise method on hydrogen-bonded complexes: a numerical test using near complete basis sets on H2O HF, (H2O)2, (HF) 2 and CH4 H2O. *Chemical Physics Letters*, **1996**, 251, 33-46	2.5	79
160	Substrate distortion in the Michaelis complex of Bacillus 1,3-1,4-beta-glucanase. Insight from first principles molecular dynamics simulations. *Journal of Biological Chemistry*, **2006**, 281, 1432-41	5.4	76
159	On the role of water in peroxidase catalysis: a theoretical investigation of HRP compound I formation. *Journal of Physical Chemistry B*, **2010**, 114, 5161-9	3.4	75
158	Catalytic itinerary in 1,3-1,4- 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, 20301-9	16.4	74

157	Structural and electronic properties of Co-corrole, Co-corrin, and Co-porphyrin. *Inorganic Chemistry*, **2001**, 40, 11-7	5.1	74
156	Substrate-guided front-face reaction revealed by combined structural snapshots and metadynamics for the polypeptide N-acetylgalactosaminyltransferase 2. *Angewandte Chemie - International Edition*, **2014**, 53, 8206-10	16.4	73
155	A density functional study of iron-porphyrin complexes. *Chemical Physics Letters*, **1997**, 271, 247-250	2.5	66
154	A comparative study of O2, CO, and NO binding to iron porphyrin. *International Journal of Quantum Chemistry*, **1998**, 69, 31-35	2.1	66
153	Aldo-keto reductases from the AKR1B subfamily: retinoid specificity and control of cellular retinoic acid levels. *Chemico-Biological Interactions*, **2009**, 178, 171-7	5	65
152	Essential role of proximal histidine-asparagine interaction in mammalian peroxidases. *Journal of Biological Chemistry*, **2009**, 284, 25929-37	5.4	62
151	Dynamic interplay between catalytic and lectin domains of GalNAc-transferases modulates protein O-glycosylation. *Nature Communications*, **2015**, 6, 6937	17.4	61
150	The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. *Journal of the American Chemical Society*, **2015**, 137, 11170-8	16.4	61
149	Molecular mechanism of the glycosylation step catalyzed by Golgi alpha-mannosidase II: a QM/MM metadynamics investigation. *Journal of the American Chemical Society*, **2010**, 132, 8291-300	16.4	61
148	Structure of Helicobacter pylori catalase, with and without formic acid bound, at 1.6 A resolution. *Biochemistry*, **2004**, 43, 3089-103	3.2	61
147	Modulation of Abeta42 fibrillogenesis by glycosaminoglycan structure. *FASEB Journal*, **2010**, 24, 4250-61	10.9	60
146	Analysis of the reaction coordinate of alpha-L-fucosidases: a combined structural and quantum mechanical approach. *Journal of the American Chemical Society*, **2010**, 132, 1804-6	16.4	59
145	The Iron Sulfur Bond in Cytochrome c. *Journal of Physical Chemistry B*, **1999**, 103, 7031-7035	3.4	58
144	Molecular-Scale Ligand Effects in Small Gold-Thiolate Nanoclusters. *Journal of the American Chemical Society*, **2018**, 140, 15430-15436	16.4	56
143	Redesigning the Coumarin Scaffold into Small Bright Fluorophores with Far-Red to Near-Infrared Emission and Large Stokes Shifts Useful for Cell Imaging. *Journal of Organic Chemistry*, **2018**, 83, 1185-1195	4.2	55
142	The structures and electronic configuration of compound I intermediates of Helicobacter pylori and Penicillium vitale catalases determined by X-ray crystallography and QM/MM density functional theory calculations. *Journal of the American Chemical Society*, **2007**, 129, 4193-205	16.4	55
141	First-principles study of the neutral molecular metal Ni(tmdt)2. *Physical Review B*, **2002**, 65,	3.3	55
140	Ammonium recruitment and ammonia transport by E. coli ammonia channel AmtB. *Biophysical Journal*, **2006**, 91, 4401-12	2.9	54

139	Molecular Mechanisms of Oxygen Activation and Hydrogen Peroxide Formation in Lytic Polysaccharide Monooxygenases. *ACS Catalysis*, **2019**, 9, 4958-4969	13.1	51
138	The reaction coordinate of a bacterial GH47 -mannosidase: a combined quantum mechanical and structural approach. *Angewandte Chemie - International Edition*, **2012**, 51, 10997-1001	16.4	49
137	Factors Influencing Ligand-Binding Properties of Heme Models: A First Principles Study of Picket-Fence and Protoheme Complexes. *Chemistry - A European Journal*, **1999**, 5, 250-262	4.8	48
136	Hydroxide and proton migration in aquaporins. *Biophysical Journal*, **2005**, 89, 1744-59	2.9	47
135	Strength and Directionality of the S???S Intermolecular Interactions Present in TTF-Based Molecular Crystals. A Combined Statistical and Ab Initio Study. *Chemistry - A European Journal*, **1999**, 5, 3689-3697	4.8	45
134	Formation of a covalent glycosyl-enzyme species in a retaining glycosyltransferase. *Chemistry - A European Journal*, **2013**, 19, 14018-23	4.8	44
133	Versatility of the electronic structure of compound I in catalase-peroxidases. *Journal of the American Chemical Society*, **2007**, 129, 13436-46	16.4	44
132	Harmonic and anharmonic dynamics of Fe-CO and Fe-O(2) in heme models. *Biophysical Journal*, **2000**, 78, 93-100	2.9	44
131	The reaction mechanisms of heme catalases: an atomistic view by ab initio molecular dynamics. *Archives of Biochemistry and Biophysics*, **2012**, 525, 121-30	4.1	42
130	First-principles molecular dynamics simulations of models for the myoglobin active center. *International Journal of Quantum Chemistry*, **2000**, 80, 1172-1180	2.1	42
129	The conformational free-energy landscape of -D-mannopyranose: evidence for a (1)S(5) -B(2,5) -o (O)S(2) catalytic itinerary in -mannosidases. *Journal of the American Chemical Society*, **2010**, 132, 16058-65	16.4	40
128	First principles study of coenzyme B12. Crystal packing forces effect on axial bond lengths. *Journal of Physical Chemistry B*, **2007**, 111, 3251-7	3.4	39
127	Structure, protonation state and dynamics of catalase compound II. *ChemPhysChem*, **2005**, 6, 1820-6	3.2	38
126	The Role of Hydrogen Bonds in the Stabilization of Silver-Mediated Cytosine Tetramers. *Journal of Physical Chemistry Letters*, **2015**, 6, 4061-6	6.4	37
125	Metal Complexes of Dithiolate Ligands: 5,6-Dihydro-1,4-dithiin-2,3-dithiolato (dddt(2-)), 5,7-Dihydro-1,4,6-trithiin-2,3-dithiolato (dtdt(2-)), and 2-Thioxo-1,3-dithiole-4,5-dithiolato (dmit(2-)). Synthesis, Electrochemical Studies, Crystal and Electronic Structures, and Conducting Properties. *Inorganic Chemistry*, **1996**, 35, 3856-3873	5.1	36
124	The complete conformational free energy landscape of -xylose reveals a two-fold catalytic itinerary for -xylanases. *Chemical Science*, **2015**, 6, 1167-1177	9.4	35
123	A Trapped Covalent Intermediate of a Glycoside Hydrolase on the Pathway to Transglycosylation. Insights from Experiments and Quantum Mechanics/Molecular Mechanics Simulations. *Journal of the American Chemical Society*, **2016**, 138, 3325-32	16.4	35
122	A neutral zwitterionic molecular solid. *Chemistry - A European Journal*, **2010**, 16, 14051-9	4.8	35

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120	The reaction mechanism of retaining glycosyltransferases. *Biochemical Society Transactions*, **2016**, 44, 51-60	5.1	34
119	A Mannanase with a Lysozyme-like Fold and a Novel Molecular Catalytic Mechanism. *ACS Central Science*, **2016**, 2, 896-903	16.8	33
118	1,6-Cyclophellitol Cyclosulfates: A New Class of Irreversible Glycosidase Inhibitor. *ACS Central Science*, **2017**, 3, 784-793	16.8	33
117	Evidence for a boat conformation at the transition state of GH76 1,6-mannanases--key enzymes in bacterial and fungal mannoprotein metabolism. *Angewandte Chemie - International Edition*, **2015**, 54, 5378-82	16.4	33
116	Structure-energy relations in methylcobalamin with and without bound axial base. *Inorganic Chemistry*, **2004**, 43, 6628-32	5.1	33
115	Hybrid DNA-gold nanostructured materials: anab initioapproach. *Nanotechnology*, **2001**, 12, 126-131	3.4	33
114	Interanionic (-)O-H...O(-) interactions: a solid-state and computational study of the ring and chain motifs. *Chemistry - A European Journal*, **2000**, 6, 4536-51	4.8	33
113	Unravelling the intrinsic features of NO binding to iron(II)- and iron(III)-hemes. *Inorganic Chemistry*, **2008**, 47, 7792-801	5.1	31
112	The synthesis and characterization of radical cation salts of bis(ethylenedithio)tetraselenafulvalene. *Synthetic Metals*, **1993**, 56, 2090-2095	3.6	31
111	Palladium-mediated enzyme activation suggests multiphase initiation of glycogenesis. *Nature*, **2018**, 563, 235-240	50.4	31
110	Factors governing the charge density wave patterns of layered transition-metal compounds of octahedral coordination with d2 and d3 electron counts. *Inorganic Chemistry*, **1993**, 32, 4094-4097	5.1	30
109	Catalases versus peroxidases: DFT investigation of HDDoxidation in models systems and implications for heme protein engineering. *Journal of Inorganic Biochemistry*, **2012**, 117, 292-7	4.2	29
108	The Proximal Hydrogen-Bonded Residue Controls the Stability of the CompoundIIIIntermediate of Peroxidases and Catalases. *Journal of Physical Chemistry B*, **2003**, 107, 5300-5305	3.4	29
107	Strength and directionality of the C(sp3)?H?S(sp3) interaction. An ab initio study using the H2S?CH4 model complex. *Chemical Physics Letters*, **1997**, 279, 140-150	2.5	28
106	A density functional study of crystalline acetic acid and its proton transfer polymorphic forms. *Journal of Chemical Physics*, **2000**, 113, 9208-9216	3.9	28
105	Characterisation of the Fermi surface and phase transitions of (BEDO-TTF)2 ReO4(H2O) by physical property measurements and electronic band structure calculations. *European Physical Journal B*, **1994**, 94, 39-47	1.2	28
104	Structural and Mechanistic Insights into the Catalytic-Domain-Mediated Short-Range Glycosylation Preferences of GalNAc-T4. *ACS Central Science*, **2018**, 4, 1274-1290	16.8	28

103	Retinaldehyde is a substrate for human aldo-keto reductases of the 1C subfamily. *Biochemical Journal*, **2011**, 440, 335-44	3.8	26
102	Reductive cleavage mechanism of Co-C bond in cobalamin-dependent methionine synthase. *Journal of Physical Chemistry B*, **2010**, 114, 12965-71	3.4	26
101	Role of the Axial Base in the Modulation of the Cob(I)alamin Electronic Properties: Insight from QM/MM, DFT, and CASSCF Calculations. *Journal of Chemical Theory and Computation*, **2011**, 7, 1541-51	6.4	26
100	20 K crystal structure, electrical transport, electronic band structure, scanning tunnelling microscopy and pressure□RF impedance studies on the organic conducting salt □(BEDT□TSF)2Cu[N(CN)2]Br. *Journal of Materials Chemistry*, **1995**, 5, 1659-1669		24
99	Dynamic and Functional Profiling of Xylan-Degrading Enzymes in Secretomes Using Activity-Based Probes. *ACS Central Science*, **2019**, 5, 1067-1078	16.8	23
98	An ionizable active-site tryptophan imparts catalase activity to a peroxidase core. *Journal of the American Chemical Society*, **2014**, 136, 7249-52	16.4	23
97	Calcium-based functionalization of carbon nanostructures for peptide immobilization in aqueous media. *Journal of Materials Chemistry*, **2012**, 22, 19684		23
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95	Protonated heme. *Chemistry - A European Journal*, **2007**, 13, 776-85	4.8	23
94	Binding of the antitubercular pro-drug isoniazid in the heme access channel of catalase-peroxidase (KatG). A combined structural and metadynamics investigation. *Journal of Physical Chemistry B*, **2014**, 118, 2924-31	3.4	22
93	Human and rodent aldo-keto reductases from the AKR1B subfamily and their specificity with retinaldehyde. *Chemico-Biological Interactions*, **2011**, 191, 199-205	5	22
92	The structure and dynamics of the Fe□CO bond in myoglobin. *Journal of Physics Condensed Matter*, **2003**, 15, S1809-S1822	1.8	22
91	Density Functional Study of 17O NMR Chemical Shift and Nuclear Quadrupole Coupling Tensors in Oxyheme Model Complexes. *Journal of Physical Chemistry B*, **2000**, 104, 5200-5208	3.4	22
90	Transfer of a Proton between N Atoms in Excited Electronic States of 1,5-Diaza-1,3-pentadiene. *The Journal of Physical Chemistry*, **1995**, 99, 9854-9861		22
89	Fenton-Derived OH Radicals Enable the MPnS Enzyme to Convert 2-Hydroxyethylphosphonate to Methylphosphonate: Insights from Ab Initio QM/MM MD Simulations. *Journal of the American Chemical Society*, **2019**, 141, 9284-9291	16.4	21
88	Role of the His64 residue on the properties of the Fe□CO and Fe□O2 bonds in myoglobin. A CHARMM/DFT study. *Computational and Theoretical Chemistry*, **2003**, 632, 309-321		21
87	Bis(ethylenethio)tetrathiafulvalene (BET-TTF), an organic donor with high electrical conductivity. *Advanced Materials*, **1995**, 7, 1023-1027	24	21
86	Oxazoline or Oxazolinium Ion? The Protonation State and Conformation of the Reaction Intermediate of Chitinase Enzymes Revisited. *Chemistry - A European Journal*, **2018**, 24, 19258-19265	4.8	21

85	Rational Design of Mechanism-Based Inhibitors and Activity-Based Probes for the Identification of Retaining □-Arabinofuranosidases. *Journal of the American Chemical Society*, **2020**, 142, 4648-4662	16.4	20
84	Precise Probing of Residue Roles by Post-Translational □C,N Aza-Michael Mutagenesis in Enzyme Active Sites. *ACS Central Science*, **2017**, 3, 1168-1173	16.8	20
83	Structure and dynamics of dioxygen bound to cobalt and iron heme. *Biophysical Journal*, **2006**, 91, 2024-34	2.9	20
82	An Epoxide Intermediate in Glycosidase Catalysis. *ACS Central Science*, **2020**, 6, 760-770	16.8	20
81	How do Water Solvent and Glutathione Ligands Affect the Structure and Electronic Properties of Au25(SR)18(-)?. *Journal of Physical Chemistry Letters*, **2015**, 6, 3859-65	6.4	19
80	The description of electronic processes inside proteins from Car□Parrinello molecular dynamics: chemical transformations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 393-407	7.8	19
79	Staple motifs, initial steps in the formation of thiolate-protected gold nanoparticles: how do they form?. *Inorganic Chemistry*, **2012**, 51, 11422-9	5.1	19
78	Oxygen binding to iron□porphyrin: A density functional study using both LSD and LSD+GC schemes **1998**, 70, 387-394		19
77	Hydrogen bonding and collective proton modes in clusters and periodic layers of squaric acid: A density functional study. *Journal of Chemical Physics*, **2001**, 115, 6406-6417	3.9	19
76	Activation of O2 and H2O2 by Lytic Polysaccharide Monooxygenases. *ACS Catalysis*, **2020**, 10, 12760-12769	13.1	19
75	Long distance electron transfer through the aqueous solution between redox partner proteins. *Nature Communications*, **2018**, 9, 5157	17.4	19
74	A Single Glycosidase Harnesses Different Pyranoside Ring Transition State Conformations for Hydrolysis of Mannosides and Glucosides. *ACS Catalysis*, **2015**, 5, 6041-6051	13.1	18
73	Interdependence of redox state, hydrogen bonding, anion recognition and charge partition in crystals of (EDT-TTF-CONHMe)6 [Re6Se8(CN)6] (CH3CN)2(CH2Cl2)2. *Chemical Communications*, **2003**, 1820-1	5.8	18
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71	Enzymatic Cleavage of Glycosidic Bonds: Strategies on How to Set Up and Control a QM/MM Metadynamics Simulation. *Methods in Enzymology*, **2016**, 577, 159-83	1.7	18
70	A front-face □Si synthase□engineered from a retaining □double-S2□hydrolase. *Nature Chemical Biology*, **2017**, 13, 874-881	11.7	17
69	X-ray diffraction and electronic band structure study of the organic superconductor ?-(ET)2Cu[N(CN)2]. *Physica C: Superconductivity and Its Applications*, **1994**, 234, 300-306	1.3	17
68	Carba-cyclophellitols Are Neutral Retaining-Glucosidase Inhibitors. *Journal of the American Chemical Society*, **2017**, 139, 6534-6537	16.4	16

67	Modeling catalytic reaction mechanisms in glycoside hydrolases. *Current Opinion in Chemical Biology*, **2019**, 53, 183-191	9.7	16
66	Optical Control of Enzyme Enantioselectivity in Solid Phase. *ACS Catalysis*, **2014**, 4, 1004-1009	13.1	16
65	The dynamic role of distal side residues in heme hydroperoxidase catalysis. Interplay between X-ray crystallography and ab initio MD simulations. *Archives of Biochemistry and Biophysics*, **2010**, 500, 37-44	4.1	16
64	Oxygen Binding to Catalase-Peroxidase. *Journal of Physical Chemistry Letters*, **2011**, 2, 196-200	6.4	16
63	A Single Point Mutation Converts GH84 -GlcNAc Hydrolases into Phosphorylases: Experimental and Theoretical Evidence. *Journal of the American Chemical Society*, **2020**, 142, 2120-2124	16.4	16
62	Sequential Uncaging with Green Light can be Achieved by Fine-Tuning the Structure of a Dicyanocoumarin Chromophore. *ChemistryOpen*, **2017**, 6, 375-384	2.3	15
61	Molecular mechanism of a hotdog-fold acyl-CoA thioesterase. *Chemistry - A European Journal*, **2014**, 20, 9045-51	4.8	14
60	Structures of the substrate-free and product-bound forms of HmuO, a heme oxygenase from corynebacterium diphtheriae: x-ray crystallography and molecular dynamics investigation. *Journal of Biological Chemistry*, **2013**, 288, 34443-58	5.4	13
59	Mannosidase mechanism: at the intersection of conformation and catalysis. *Current Opinion in Structural Biology*, **2020**, 62, 79-92	8.1	13
58	Contribution of Shape and Charge to the Inhibition of a Family GH99 endo-α1,2-Mannanase. *Journal of the American Chemical Society*, **2017**, 139, 1089-1097	16.4	12
57	Re-engineering specificity in 1,3-1, 4-β-glucanase to accept branched xyloglucan substrates. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 365-75	4.2	12
56	Substrate recognition in the Escherichia coli ammonia channel AmtB: a QM/MM investigation. *Journal of Physical Chemistry B*, **2010**, 114, 11859-65	3.4	12
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54	Substrate Engagement and Catalytic Mechanisms of N-Acetylglucosaminyltransferase V. *ACS Catalysis*, **2020**, 10, 8590-8596	13.1	12
53	Computational Design of Experiment Unveils the Conformational Reaction Coordinate of GH125 α-Mannosidases. *Journal of the American Chemical Society*, **2017**, 139, 1085-1088	16.4	11
52	Structural and kinetic features of aldehyde dehydrogenase 1A (ALDH1A) subfamily members, cancer stem cell markers active in retinoic acid biosynthesis. *Archives of Biochemistry and Biophysics*, **2020**, 681, 108256	4.1	11
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48	A photoswitchable GABA receptor channel blocker. *British Journal of Pharmacology*, **2019**, 176, 2661-2678	8.6	10
47	Substrate-Guided Front-Face Reaction Revealed by Combined Structural Snapshots and Metadynamics for the Polypeptide N-Acetylgalactosaminyltransferase 2. *Angewandte Chemie*, **2014**, 126, 8345-8349	3.6	10
46	Enantioselective Preparation of δ-Valerolactones with Horse Liver Alcohol Dehydrogenase. *ChemCatChem*, **2014**, 6, 977-980	5.2	10
45	A First-Principles Computation of the Low-Energy Polymorphic Forms of the Acetic Acid Crystal. A Test of the Atom−Atom Force Field Predictions. *Journal of Physical Chemistry B*, **2001**, 105, 1710-1719	3.4	10
44	O-/N-/S-Specificity in Glycosyltransferase Catalysis: From Mechanistic Understanding to Engineering. *ACS Catalysis*, **2021**, 11, 1810-1815	13.1	10
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42	Can an Alcohol Act As an Acid/Base Catalyst in Water Solution? An Experimental and Theoretical Study of Imidazole Catalysis of the Aqueous Morita−Baylis−Hillman Reaction. *ACS Catalysis*, **2018**, 8, 1703-1714	13.1	9
41	The Reaction Coordinate of a Bacterial GH47 α-Mannosidase: A Combined Quantum Mechanical and Structural Approach. *Angewandte Chemie*, **2012**, 124, 11159-11163	3.6	9
40	Structural analysis and insights into the glycon specificity of the rice GH1 Os7BGlu26 β-D-mannosidase. *Acta Crystallographica Section D: Biological Crystallography*, **2013**, 69, 2124-35		9
39	The Molecular Mechanism of Enzymatic Glycosyl Transfer with Retention of Configuration: Evidence for a Short-Lived Oxocarbenium-Like Species. *Angewandte Chemie*, **2011**, 123, 11089-11093	3.6	9
38	Density-functional molecular dynamics studies of biologically relevant iron and cobalt complexes with macrocyclic ligands. *Coordination Chemistry Reviews*, **2008**, 252, 1497-1513	23.2	9
37	Theoretical study of the structure and vibrational spectra of the (H2O)2−HF and H2O−(HF)2 molecular complexes. *International Journal of Quantum Chemistry*, **1994**, 52, 177-189	2.1	9
36	How Oxygen Binding Enhances Long-Range Electron Transfer: Lessons From Reduction of Lytic Polysaccharide Monooxygenases by Cellobiose Dehydrogenase. *Angewandte Chemie - International Edition*, **2021**, 60, 2385-2392	16.4	9
35	Two distinct catalytic pathways for GH43 xylanolytic enzymes unveiled by X-ray and QM/MM simulations. *Nature Communications*, **2021**, 12, 367	17.4	9
34	Conformational Analysis of the Mannosidase Inhibitor Kifunensine: A Quantum Mechanical and Structural Approach. *ChemBioChem*, **2017**, 18, 1496-1501	3.8	8
33	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. *Nature Communications*, **2019**, 10, 2222	17.4	8
32	Protonation state of the equatorial ligands and dynamics of the OH...O units in a cobaloxime biomimetic. *Inorganic Chemistry*, **2002**, 41, 4810-4	5.1	8

31	Selective Derivatization of N-Terminal Cysteines Using Cyclopentenediones. *Organic Letters*, **2016**, 18, 4836-4839	6.2	8
30	Deciphering the enzymatic mechanism of sugar ring contraction in UDP-apiose biosynthesis. *Nature Catalysis*, **2019**, 2, 1115-1123	36.5	8
29	-D-Gal-cyclophellitol cyclosulfamidate is a Michaelis complex analog that stabilizes therapeutic lysosomal -galactosidase A in Fabry disease. *Chemical Science*, **2019**, 10, 9233-9243	9.4	7
28	Electrochemically Gated Long-Distance Charge Transport in Photosystem I. *Angewandte Chemie - International Edition*, **2019**, 58, 13280-13284	16.4	7
27	Low temperature crystal and electronic band structure of the (BEDO-TTF)2Cl1.28(H3O)0.282.44H2O stable organic metal. *Journal of Materials Chemistry*, **1998**, 8, 1151-1156		7
26	The Catalytic Reaction Mechanism of the -Galactocerebrosidase Enzyme Deficient in Krabbe Disease. *ACS Catalysis*, **2020**, 10, 12091-12097	13.1	7
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