Carme Rovira

List of Publications by Year in Descending Order

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	Computer Simulation to Rationalize "Rational" Engineering of Glycoside Hydrolases and Glycosyltransferases.. *Journal of Physical Chemistry B*, **2022**,	3.4	5
173	Enzymatic Hydrolysis of Human Milk Oligosaccharides. The Molecular Mechanism of Lacto--biosidase.. *ACS Catalysis*, **2022**, 12, 4737-4743	13.1	4
172	How Oxygen Binding Enhances Long-Range Electron Transfer: Lessons From Reduction of Lytic Polysaccharide Monooxygenases by Cellobiose Dehydrogenase. *Angewandte Chemie*, **2021**, 133, 2415-2422	3.6	0
171	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
170	O-/N-/S-Specificity in Glycosyltransferase Catalysis: From Mechanistic Understanding to Engineering. *ACS Catalysis*, **2021**, 11, 1810-1815	13.1	10
169	Cysteine Nucleophiles in Glycosidase Catalysis: Application of a Covalent -Arabinofuranosidase Inhibitor. *Angewandte Chemie - International Edition*, **2021**, 60, 5754-5758	16.4	5
168	Cysteine Nucleophiles in Glycosidase Catalysis: Application of a Covalent -Arabinofuranosidase Inhibitor. *Angewandte Chemie*, **2021**, 133, 5818-5822	3.6	0
167	Asparagine Tautomerization in Glycosyltransferase Catalysis. The Molecular Mechanism of Protein -Fucosyltransferase 1. *ACS Catalysis*, **2021**, 11, 9926-9932	13.1	3
166	Two distinct catalytic pathways for GH43 xylanolytic enzymes unveiled by X-ray and QM/MM simulations. *Nature Communications*, **2021**, 12, 367	17.4	9
165	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
164	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
163	Photocontrol of Endogenous Glycine Receptors In Vivo. *Cell Chemical Biology*, **2020**, 27, 1425-1433.e7	8.2	3
162	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
161	Mannosidase mechanism: at the intersection of conformation and catalysis. *Current Opinion in Structural Biology*, **2020**, 62, 79-92	8.1	13
160	Activation of O2 and H2O2 by Lytic Polysaccharide Monooxygenases. *ACS Catalysis*, **2020**, 10, 12760-12769	13.1	19
159	Substrate Engagement and Catalytic Mechanisms of N-Acetylglucosaminyltransferase V. *ACS Catalysis*, **2020**, 10, 8590-8596	13.1	12
158	The Catalytic Reaction Mechanism of the Galactocerebrosidase Enzyme Deficient in Krabbe Disease. *ACS Catalysis*, **2020**, 10, 12091-12097	13.1	7

157	An Epoxide Intermediate in Glycosidase Catalysis. *ACS Central Science*, **2020**, 6, 760-770	16.8	20
156	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
155	Dynamic and Functional Profiling of Xylan-Degrading Enzymes in Secretomes Using Activity-Based Probes. *ACS Central Science*, **2019**, 5, 1067-1078	16.8	23
154	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. *Nature Communications*, **2019**, 10, 2222	17.4	8
153	Conformational Itinerary of Sucrose During Hydrolysis by Retaining Amylosucrase. *Frontiers in Chemistry*, **2019**, 7, 269	5	6
152	Molecular Mechanisms of Oxygen Activation and Hydrogen Peroxide Formation in Lytic Polysaccharide Monooxygenases. *ACS Catalysis*, **2019**, 9, 4958-4969	13.1	51
151	A photoswitchable GABA receptor channel blocker. *British Journal of Pharmacology*, **2019**, 176, 2661-2678	8.6	10
150	Glucose transport via the pseudomonad porin OprB: implications for the design of Trojan Horse anti-infectives. *Physical Chemistry Chemical Physics*, **2019**, 21, 8457-8463	3.6	5
149	□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
148	Electrochemically Gated Long-Distance Charge Transport in Photosystem I. *Angewandte Chemie*, **2019**, 131, 13414-13418	3.6	
147	Electrochemically Gated Long-Distance Charge Transport in Photosystem I. *Angewandte Chemie - International Edition*, **2019**, 58, 13280-13284	16.4	7
146	Modeling catalytic reaction mechanisms in glycoside hydrolases. *Current Opinion in Chemical Biology*, **2019**, 53, 183-191	9.7	16
145	Deciphering the enzymatic mechanism of sugar ring contraction in UDP-apiose biosynthesis. *Nature Catalysis*, **2019**, 2, 1115-1123	36.5	8
144	Theory Uncovers the Role of the Methionine-Tyrosine-Tryptophan Radical Adduct in the Catalase Reaction of KatGs: O Release Mediated by Proton-Coupled Electron Transfer. *Chemistry - A European Journal*, **2018**, 24, 5388-5395	4.8	3
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	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
141	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
140	The Molecular Mechanism of Substrate Recognition and Catalysis of the Membrane Acyltransferase PatA from Mycobacteria. *ACS Chemical Biology*, **2018**, 13, 131-140	4.9	4

139	Long distance electron transfer through the aqueous solution between redox partner proteins. *Nature Communications*, **2018**, 9, 5157	17.4	19
138	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
137	Palladium-mediated enzyme activation suggests multiphase initiation of glycogenesis. *Nature*, **2018**, 563, 235-240	50.4	31
136	Molecular-Scale Ligand Effects in Small Gold-Thiolate Nanoclusters. *Journal of the American Chemical Society*, **2018**, 140, 15430-15436	16.4	56
135	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
134	The molecular mechanism of the ligand exchange reaction of an antibody against a glutathione-coated gold cluster. *Nanoscale*, **2017**, 9, 3121-3127	7.7	10
133	The Catalase Activity of Catalase-Peroxidases Is Modulated by Changes in the pK of the Distal Histidine. *Biochemistry*, **2017**, 56, 2271-2281	3.2	9
132	Conformational Analysis of the Mannosidase Inhibitor Kifunensine: A Quantum Mechanical and Structural Approach. *ChemBioChem*, **2017**, 18, 1496-1501	3.8	8
131	Carba-cyclophellitols Are Neutral Retaining-Glucosidase Inhibitors. *Journal of the American Chemical Society*, **2017**, 139, 6534-6537	16.4	16
130	A front-face Ɓsi synthaseƦengineered from a retaining Ɓdouble-S2Ɓhydrolase. *Nature Chemical Biology*, **2017**, 13, 874-881	11.7	17
129	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
128	Contribution of Shape and Charge to the Inhibition of a Family GH99 endo-α-1,2-Mannanase. *Journal of the American Chemical Society*, **2017**, 139, 1089-1097	16.4	12
127	An atypical interaction explains the high-affinity of a non-hydrolyzable S-linked 1,6-α-mannanase inhibitor. *Chemical Communications*, **2017**, 53, 9238-9241	5.8	4
126	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
125	1,6-Cyclophellitol Cyclosulfates: A New Class of Irreversible Glycosidase Inhibitor. *ACS Central Science*, **2017**, 3, 784-793	16.8	33
124	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
123	A α-Mannanase with a Lysozyme-like Fold and a Novel Molecular Catalytic Mechanism. *ACS Central Science*, **2016**, 2, 896-903	16.8	33
122	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

121	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
120	Selective Derivatization of N-Terminal Cysteines Using Cyclopentenediones. *Organic Letters*, **2016**, 18, 4836-4839	6.2	8
119	The reaction mechanism of retaining glycosyltransferases. *Biochemical Society Transactions*, **2016**, 44, 51-60	5.1	34
118	The complete conformational free energy landscape of β-xylose reveals a two-fold catalytic itinerary for β-xylanases. *Chemical Science*, **2015**, 6, 1167-1177	9.4	35
117	Dynamic interplay between catalytic and lectin domains of GalNAc-transferases modulates protein O-glycosylation. *Nature Communications*, **2015**, 6, 6937	17.4	61
116	Binding of azole drugs to heme: A combined MS/MS and computational approach. *Polyhedron*, **2015**, 90, 245-251	2.7	6
115	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
114	Privateer: software for the conformational validation of carbohydrate structures. *Nature Structural and Molecular Biology*, **2015**, 22, 833-4	17.6	215
113	The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. *Journal of the American Chemical Society*, **2015**, 137, 11170-8	16.4	61
112	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
111	Computational Studies of Glycoside, Carboxylic Ester, and Thioester Hydrolase Mechanisms: A Review. *Industrial & Engineering Chemistry Research*, **2015**, 54, 10138-10161	3.9	5
110	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
109	Evidence for a Boat Conformation at the Transition State of GH76 α-1,6-Mannanases—Key Enzymes in Bacterial and Fungal Mannoprotein Metabolism. *Angewandte Chemie*, **2015**, 127, 5468-5472	3.6	1
108	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
107	Evidence for a boat conformation at the transition state of GH76 α-1,6-mannanases--key enzymes in bacterial and fungal mannoprotein metabolism. *Angewandte Chemie - International Edition*, **2015**, 54, 5378-82	16.4	33
106	Combined inhibitor free-energy landscape and structural analysis reports on the mannosidase conformational coordinate. *Angewandte Chemie - International Edition*, **2014**, 53, 1087-91	16.4	34
105	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
104	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

103	Optical Control of Enzyme Enantioselectivity in Solid Phase. *ACS Catalysis*, **2014**, 4, 1004-1009	13.1	16
102	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
101	Enantioselective Preparation of -Valerolactones with Horse Liver Alcohol Dehydrogenase. *ChemCatChem*, **2014**, 6, 977-980	5.2	10
100	Combined Inhibitor Free-Energy Landscape and Structural Analysis Reports on the Mannosidase Conformational Coordinate. *Angewandte Chemie*, **2014**, 126, 1105-1109	3.6	4
99	Car-Parrinello Simulations of Chemical Reactions in Proteins **2014**, 51-70		
98	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
97	Molecular mechanism of a hotdog-fold acyl-CoA thioesterase. *Chemistry - A European Journal*, **2014**, 20, 9045-51	4.8	14
96	The description of electronic processes inside proteins from Car-Parrinello molecular dynamics: chemical transformations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 393-407	7.9	19
95	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
94	Formation of a covalent glycosyl-enzyme species in a retaining glycosyltransferase. *Chemistry - A European Journal*, **2013**, 19, 14018-23	4.8	44
93	Structural analysis and insights into the glycon specificity of the rice GH1 Os7BGlu26 -D-mannosidase. *Acta Crystallographica Section D: Biological Crystallography*, **2013**, 69, 2124-35		9
92	Innenrücktitelbild: The Reaction Coordinate of a Bacterial GH47 -Mannosidase: A Combined Quantum Mechanical and Structural Approach (Angew. Chem. 44/2012). *Angewandte Chemie*, **2012**, 124, 11333-11333	3.6	
91	Calcium-based functionalization of carbon nanostructures for peptide immobilization in aqueous media. *Journal of Materials Chemistry*, **2012**, 22, 19684		23
90	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
89	The Reaction Coordinate of a Bacterial GH47 -Mannosidase: A Combined Quantum Mechanical and Structural Approach. *Angewandte Chemie*, **2012**, 124, 11159-11163	3.6	9
88	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
87	Catalases versus peroxidases: DFT investigation of HOOH oxidation in models systems and implications for heme protein engineering. *Journal of Inorganic Biochemistry*, **2012**, 117, 292-7	4.2	29
86	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

85	Conformational analyses of the reaction coordinate of glycosidases. *Accounts of Chemical Research*, **2012**, 45, 308-16	24.3	184
84	Retinaldehyde is a substrate for human aldo-keto reductases of the 1C subfamily. *Biochemical Journal*, **2011**, 440, 335-44	3.8	26
83	Human and rodent aldo-keto reductases from the AKR1B subfamily and their specificity with retinaldehyde. *Chemico-Biological Interactions*, **2011**, 191, 199-205	5	22
82	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
81	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
80	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
79	Proton transfer drives protein radical formation in Helicobacter pylori catalase but not in Penicillium vitale catalase. *Journal of the American Chemical Society*, **2011**, 133, 4285-98	16.4	23
78	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
77	Catalytic itinerary in 1,3-1,4-β-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
76	Oxygen Binding to Catalase-Peroxidase. *Journal of Physical Chemistry Letters*, **2011**, 2, 196-200	6.4	16
75	Modulation of Abeta42 fibrillogenesis by glycosaminoglycan structure. *FASEB Journal*, **2010**, 24, 4250-61	10.9	60
74	Substrate conformational changes in glycoside hydrolase catalysis. A first-principles molecular dynamics study. *Biocatalysis and Biotransformation*, **2010**, 28, 33-40	2.5	11
73	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
72	Reductive cleavage mechanism of Co-C bond in cobalamin-dependent methionine synthase. *Journal of Physical Chemistry B*, **2010**, 114, 12965-71	3.4	26
71	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
70	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
69	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
68	The conformational free-energy landscape of β-D-mannopyranose: evidence for a (1)S(5) -> B(2,5) -> (O)S(2) catalytic itinerary in β-mannosidases. *Journal of the American Chemical Society*, **2010**, 132, 16058-65	16.4	40

67	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
66	A neutral zwitterionic molecular solid. *Chemistry - A European Journal*, **2010**, 16, 14051-9	4.8	35
65	Essential role of proximal histidine-asparagine interaction in mammalian peroxidases. *Journal of Biological Chemistry*, **2009**, 284, 25929-37	5.4	62
64	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
63	The molecular mechanism of the catalase reaction. *Journal of the American Chemical Society*, **2009**, 131, 11751-61	16.4	216
62	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
61	Electronic state of the molecular oxygen released by catalase. *Journal of Physical Chemistry A*, **2008**, 112, 12842-8	2.8	12
60	Unravelling the intrinsic features of NO binding to iron(II)- and iron(III)-hemes. *Inorganic Chemistry*, **2008**, 47, 7792-801	5.1	31
59	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
58	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
57	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
56	Versatility of the electronic structure of compound I in catalase-peroxidases. *Journal of the American Chemical Society*, **2007**, 129, 13436-46	16.4	44
55	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
54	Protonated heme. *Chemistry - A European Journal*, **2007**, 13, 776-85	4.8	23
53	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
52	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
51	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
50	Structure and dynamics of dioxygen bound to cobalt and iron heme. *Biophysical Journal*, **2006**, 91, 2024-34	3.9	20

49	Ammonium recruitment and ammonia transport by E. coli ammonia channel AmtB. *Biophysical Journal*, **2006**, 91, 4401-12	2.9	54
48	Electronic structure and charge transfer in the ternary intercalated graphite beta-KS0.25C3. *Inorganic Chemistry*, **2006**, 45, 9387-93	5.1	
47	A first principles study of the binding of formic acid in catalase complementing high resolution X-ray structures. *Chemical Physics*, **2006**, 323, 129-137	2.3	11
46	Hydroxide and proton migration in aquaporins. *Biophysical Journal*, **2005**, 89, 1744-59	2.9	47
45	Structure, protonation state and dynamics of catalase compound II. *ChemPhysChem*, **2005**, 6, 1820-6	3.2	38
44	Study of ligand-protein interactions by means of density functional theory and first-principles molecular dynamics. *Methods in Molecular Biology*, **2005**, 305, 517-54	1.4	3
43	Concerning the origin of superstructures in hydrogen molybdenum bronzes HxMoO3. *Solid State Ionics*, **2004**, 168, 291-298	3.3	6
42	Structure of Helicobacter pylori catalase, with and without formic acid bound, at 1.6 A resolution. *Biochemistry*, **2004**, 43, 3089-103	3.2	61
41	Structure-energy relations in methylcobalamin with and without bound axial base. *Inorganic Chemistry*, **2004**, 43, 6628-32	5.1	33
40	The structure and dynamics of the Fe□CO bond in myoglobin. *Journal of Physics Condensed Matter*, **2003**, 15, S1809-S1822	1.8	22
39	Role of the His64 residue on the properties of the Fe□O and Fe□2 bonds in myoglobin. A CHARMM/DFT study. *Computational and Theoretical Chemistry*, **2003**, 632, 309-321		21
38	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
37	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
36	First-principles study of the neutral molecular metal Ni(tmdt)2. *Physical Review B*, **2002**, 65,	3.3	55
35	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
34	Structural and electronic properties of Co-corrole, Co-corrin, and Co-porphyrin. *Inorganic Chemistry*, **2001**, 40, 11-7	5.1	74
33	Hybrid DNA-gold nanostructured materials: anab initioapproach. *Nanotechnology*, **2001**, 12, 126-131	3.4	33
32	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

31	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
30	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
29	First-principles molecular dynamics simulations of models for the myoglobin active center. *International Journal of Quantum Chemistry*, **2000**, 80, 1172-1180	2.1	42
28	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
27	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
26	Harmonic and anharmonic dynamics of Fe-CO and Fe-O(2) in heme models. *Biophysical Journal*, **2000**, 78, 93-100	2.9	44
25	Do thiols merely passivate gold nanoclusters?. *Physical Review Letters*, **2000**, 85, 5250-1	7.4	142
24	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
23	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
22	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
21	Structural Properties, Electron Localization and Magnetic Behavior of Copper Hydroxonitrate: A Density Functional Study. *Journal of Physical Chemistry B*, **1999**, 103, 9387-9391	3.4	18
20	The Iron−Sulfur Bond in Cytochrome c. *Journal of Physical Chemistry B*, **1999**, 103, 7031-7035	3.4	58
19	Factors Influencing Ligand-Binding Properties of Heme Models: A First Principles Study of Picket-Fence and Protoheme Complexes **1999**, 5, 250		2
18	A comparative study of O2, CO, and NO binding to iron−porphyrin. *International Journal of Quantum Chemistry*, **1998**, 69, 31-35	2.1	66
17	Oxygen binding to iron−porphyrin: A density functional study using both LSD and LSD+GC schemes **1998**, 70, 387-394		19
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