Maria J. Ramos

List of Publications by Citations

377 papers	10,540 citations	47 h-index	85 g-index
410 ext. papers	11,882 ext. citations	4.6 avg, IF	6.56 L-index

#	Paper	IF	Citations
377	General performance of density functionals. *Journal of Physical Chemistry A*, **2007**, 111, 10439-52	2.8	810
376	Protein-ligand docking: current status and future challenges. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 15-26	4.2	597
375	Hot spots--a review of the protein-protein interface determinant amino-acid residues. *Proteins: Structure, Function and Bioinformatics*, **2007**, 68, 803-12	4.2	537
374	The adaptive evolution of the mammalian mitochondrial genome. *BMC Genomics*, **2008**, 9, 119	4.5	234
373	Theoretical insights into the mechanism for thiol/disulfide exchange. *Chemistry - A European Journal*, **2004**, 10, 257-66	4.8	218
372	Computational alanine scanning mutagenesis--an improved methodological approach. *Journal of Computational Chemistry*, **2007**, 28, 644-54	3.5	190
371	Protein-ligand docking in the new millennium--a retrospective of 10 years in the field. *Current Medicinal Chemistry*, **2013**, 20, 2296-314	4.3	160
370	□Glucosidase inhibition by flavonoids: an in vitro and in silico structure-activity relationship study. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2017**, 32, 1216-1228	5.6	153
369	AutoDock4(Zn): an improved AutoDock force field for small-molecule docking to zinc metalloproteins. *Journal of Chemical Information and Modeling*, **2014**, 54, 2371-9	6.1	152
368	Computational enzymatic catalysis. *Accounts of Chemical Research*, **2008**, 41, 689-98	24.3	130
367	The carboxylate shift in zinc enzymes: a computational study. *Journal of the American Chemical Society*, **2007**, 129, 1378-85	16.4	120
366	NF-kappaB in human disease: current inhibitors and prospects for de novo structure based design of inhibitors. *Current Medicinal Chemistry*, **2005**, 12, 357-74	4.3	119
365	Cholesterol Biosynthesis: A Mechanistic Overview. *Biochemistry*, **2016**, 55, 5483-5506	3.2	116
364	Understanding ribonucleotide reductase inactivation by gemcitabine. *Chemistry - A European Journal*, **2007**, 13, 8507-15	4.8	105
363	Application of quantum mechanics/molecular mechanics methods in the study of enzymatic reaction mechanisms. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1281	7.9	104
362	Farnesyltransferase inhibitors: a detailed chemical view on an elusive biological problem. *Current Medicinal Chemistry*, **2008**, 15, 1478-92	4.3	101
361	Similarities and differences in the thioredoxin superfamily. *Progress in Biophysics and Molecular Biology*, **2006**, 91, 229-48	4.7	94

360	Muonium substituted organic free radicals in liquids. Muonium–electron hyperfine, coupling constants of alkyl and allyl radicals. *Chemical Physics*, **1982**, 67, 275-285	2.3	90
359	Protein-protein docking dealing with the unknown. *Journal of Computational Chemistry*, **2010**, 31, 317-42	3.5	85
358	Overview of ribonucleotide reductase inhibitors: an appealing target in anti-tumour therapy. *Current Medicinal Chemistry*, **2005**, 12, 1283-94	4.3	85
357	Vascular endothelial growth factor (VEGF) inhibition--a critical review. *Anti-Cancer Agents in Medicinal Chemistry*, **2007**, 7, 223-45	2.2	83
356	The first mammalian aldehyde oxidase crystal structure: insights into substrate specificity. *Journal of Biological Chemistry*, **2012**, 287, 40690-702	5.4	79
355	Receptor-based virtual screening protocol for drug discovery. *Archives of Biochemistry and Biophysics*, **2015**, 582, 56-67	4.1	74
354	Mechanism of formation of the internal aldimine in pyridoxal 5'-phosphate-dependent enzymes. *Journal of the American Chemical Society*, **2011**, 133, 15496-505	16.4	71
353	QM/MM Studies on the β-Galactosidase Catalytic Mechanism: Hydrolysis and Transglycosylation Reactions. *Journal of Chemical Theory and Computation*, **2010**, 6, 421-33	6.4	69
352	Ribonucleotide reductase: a critical enzyme for cancer chemotherapy and antiviral agents. *Recent Patents on Anti-Cancer Drug Discovery*, **2007**, 2, 11-29	2.6	67
351	Benchmarking of DFT Functionals for the Hydrolysis of Phosphodiester Bonds. *Journal of Chemical Theory and Computation*, **2010**, 6, 2281-92	6.4	62
350	Analysis of zinc-ligand bond lengths in metalloproteins: trends and patterns. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 466-75	4.2	62
349	Gemcitabine: a critical nucleoside for cancer therapy. *Current Medicinal Chemistry*, **2012**, 19, 1076-87	4.3	61
348	The Zinc proteome: a tale of stability and functionality. *Dalton Transactions*, **2009**, 7946-56	4.3	59
347	Mammalian cytosolic glutathione transferases. *Current Protein and Peptide Science*, **2008**, 9, 325-37	2.8	59
346	Mechanism for ribonucleotide reductase inactivation by the anticancer drug gemcitabine. *Journal of Computational Chemistry*, **2004**, 25, 1286-94	3.5	59
345	Nuclear factor kappa B: a potential target for anti-HIV chemotherapy. *Current Medicinal Chemistry*, **2003**, 10, 1603-15	4.3	58
344	Definition of an electronic profile of compounds with inhibitory activity against hematin aggregation in malaria parasite. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 3313-21	3.4	57
343	The current status of the NNRTI family of antiretrovirals used in the HAART regime against HIV infection. *Current Medicinal Chemistry*, **2008**, 15, 1083-95	4.3	56

342	Unraveling the importance of protein-protein interaction: application of a computational alanine-scanning mutagenesis to the study of the IgG1 streptococcal protein G (C2 fragment) complex. *Journal of Physical Chemistry B*, **2006**, 110, 10962-9	3.4	56
341	Farnesyltransferase--new insights into the zinc-coordination sphere paradigm: evidence for a carboxylate-shift mechanism. *Biophysical Journal*, **2005**, 88, 483-94	2.9	55
340	Computational Alanine Scanning Mutagenesis: MM-PBSA vs TI. *Journal of Chemical Theory and Computation*, **2013**, 9, 1311-9	6.4	54
339	Evaluation of a flavonoids library for inhibition of pancreatic □amylase towards a structure-activity relationship. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 577-588	5.6	53
338	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. *ACS Catalysis*, **2015**, 5, 5617-5626	10.6	53
337	Theoretical studies on the mechanism of inhibition of Ribonucleotide Reductase by (E)-2'-Fluoromethylene-2'-deoxycitidine-5'-diphosphate. *Journal of the American Chemical Society*, **2003**, 125, 6311-22	16.4	53
336	Glutathione transferase: new model for glutathione activation. *Chemistry - A European Journal*, **2008**, 14, 9591-8	4.8	51
335	Structural characterization of inclusion complexes between cyanidin-3-O-glucoside and □cyclodextrin. *Carbohydrate Polymers*, **2014**, 102, 269-77	10.3	50
334	Studies on □glucosidase inhibitors development: magic molecules for the treatment of carbohydrate mediated diseases. *Mini-Reviews in Medicinal Chemistry*, **2012**, 12, 713-20	3.2	49
333	Discovery of a large number of previously unrecognized mitochondrial pseudogenes in fish genomes. *Genomics*, **2005**, 86, 708-17	4.3	48
332	Glycosidase inhibitors: a patent review (2008-2013). *Expert Opinion on Therapeutic Patents*, **2014**, 24, 857-74	6.8	47
331	The catalytic mechanism of HIV-1 integrase for DNA 3'-end processing established by QM/MM calculations. *Journal of the American Chemical Society*, **2012**, 134, 13436-47	16.4	47
330	Unraveling the enigmatic mechanism of L-asparaginase II with QM/QM calculations. *Journal of the American Chemical Society*, **2013**, 135, 7146-58	16.4	45
329	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for zinc complexes. *Journal of Computational Chemistry*, **2009**, 30, 2752-63	3.5	45
328	Dehydration of ribonucleotides catalyzed by ribonucleotide reductase: the role of the enzyme. *Biophysical Journal*, **2006**, 90, 2109-19	2.9	45
327	Amino acid deprivation using enzymes as a targeted therapy for cancer and viral infections. *Expert Opinion on Therapeutic Patents*, **2017**, 27, 283-297	6.8	44
326	Computational enzymatic catalysis--clarifying enzymatic mechanisms with the help of computers. *Physical Chemistry Chemical Physics*, **2012**, 14, 12431-41	3.6	44
325	The sulfur shift: an activation mechanism for periplasmic nitrate reductase and formate dehydrogenase. *Inorganic Chemistry*, **2013**, 52, 10766-72	5.1	42

324	The catalytic mechanism of protein phosphatase 5 established by DFT calculations. *Chemistry - A European Journal*, **2013**, 19, 14081-9	4.8	42
323	Virtual screening in drug design and development. *Combinatorial Chemistry and High Throughput Screening*, **2010**, 13, 442-53	1.3	42
322	Aryl- and heteroaryl-thiosemicarbazone derivatives and their metal complexes: a pharmacological template. *Recent Patents on Anti-Cancer Drug Discovery*, **2013**, 8, 168-82	2.6	41
321	Inhibition of pancreatic elastase by polyphenolic compounds. *Journal of Agricultural and Food Chemistry*, **2010**, 58, 10668-76	5.7	39
320	Computational Mechanistic Studies Addressed to the Transimination Reaction Present in All Pyridoxal 5'-Phosphate-Requiring Enzymes. *Journal of Chemical Theory and Computation*, **2011**, 7, 1356-68	6.4	39
319	Structural features of copigmentation of oenin with different polyphenol copigments. *Journal of Agricultural and Food Chemistry*, **2013**, 61, 6942-8	5.7	38
318	The catalytic mechanism of carboxylesterases: a computational study. *Biochemistry*, **2014**, 53, 5820-9	3.2	37
317	The Catalytic Mechanism of RNA Polymerase II. *Journal of Chemical Theory and Computation*, **2011**, 7, 1177-88	6.4	37
316	Molecular recognition of 15-deoxy-delta(12,14)-prostaglandin J2 by nuclear factor-kappa B and other cellular proteins. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 4057-63	2.9	37
315	Unraveling the mechanism of the farnesyltransferase enzyme. *Journal of Biological Inorganic Chemistry*, **2005**, 10, 3-10	3.7	37
314	Unique Triphenylphosphonium Derivatives for Enhanced Mitochondrial Uptake and Photodynamic Therapy. *Bioconjugate Chemistry*, **2017**, 28, 590-599	6.3	36
313	Structural basis for the GSK-3beta binding affinity and selectivity against CDK-2 of 1-(4-aminofurazan-3yl)-5-dialkylaminomethyl-1H-[1,2,3] triazole-4-carboxylic acid derivatives. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 5129-35	2.9	36
312	Accuracy of Density Functionals in the Prediction of Electronic Proton Affinities of Amino Acid Side Chains. *Journal of Chemical Theory and Computation*, **2011**, 7, 3898-908	6.4	35
311	The Accuracy of Density Functional Theory in the Description of Cation-π and π-Hydrogen Bond Interactions. *Journal of Chemical Theory and Computation*, **2011**, 7, 2059-67	6.4	35
310	Mechanistic studies on the formation of glycosidase-substrate and glycosidase-inhibitor covalent intermediates. *Journal of Computational Chemistry*, **2008**, 29, 2565-74	3.5	35
309	Theoretical studies on farnesyltransferase: the distances paradox explained. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 205-18	4.2	35
308	Theoretical quantitative structure-activity relationships of flavone ligands interacting with cytochrome P450 1A1 and 1A2 isozymes. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 4366-74	3.4	35
307	Theoretical study of arginine–carboxylate interactions. *Computational and Theoretical Chemistry*, **1999**, 463, 81-90		35

306	Mechanism of thioredoxin-catalyzed disulfide reduction. Activation of the buried thiol and role of the variable active-site residues. *Journal of Physical Chemistry B*, **2008**, 112, 2511-23	3.4	34
305	Theoretical studies on farnesyl transferase: evidence for thioether product coordination to the active-site zinc sphere. *Journal of Computational Chemistry*, **2007**, 28, 1160-8	3.5	34
304	Unravelling Hot Spots: a comprehensive computational mutagenesis study. *Theoretical Chemistry Accounts*, **2006**, 117, 99-113	1.9	34
303	Understanding the binding of procyanidins to pancreatic elastase by experimental and computational methods. *Biochemistry*, **2010**, 49, 5097-108	3.2	33
302	Determination of the DeltapKa between the active site cysteines of thioredoxin and DsbA. *Journal of Computational Chemistry*, **2006**, 27, 966-75	3.5	33
301	Farnesyltransferase inhibitors: a comprehensive review based on quantitative structural analysis. *Current Medicinal Chemistry*, **2013**, 20, 4888-923	4.3	33
300	Atomistic details of the Catalytic Mechanism of Fe(III)-Zn(II) Purple Acid Phosphatase. *Journal of Chemical Theory and Computation*, **2010**, 6, 2424-33	6.4	32
299	Receptor-drug association studies in the inhibition of the hematin aggregation process of malaria. *FEBS Letters*, **2003**, 547, 217-22	3.8	32
298	Muon spin rotation spectra for muonium isotopically substituted ethyl radicals. *Journal of the Chemical Society Faraday Transactions I*, **1984**, 80, 255		32
297	Mechanistic insights on the reduction of glutathione disulfide by protein disulfide isomerase. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E4724-E4733	11.5	31
296	Comparative assessment of theoretical methods for the determination of geometrical properties in biological zinc complexes. *Journal of Physical Chemistry B*, **2007**, 111, 9146-52	3.4	31
295	The barriers to internal rotation for muonic-substituted ethyl radicals. *Journal of the Chemical Society Faraday Transactions I*, **1984**, 80, 267		31
294	Parameters for Molecular Dynamics Simulations of Manganese-Containing Metalloproteins. *Journal of Chemical Theory and Computation*, **2013**, 9, 2718-32	6.4	30
293	New Parameters for Higher Accuracy in the Computation of Binding Free Energy Differences upon Alanine Scanning Mutagenesis on Protein-Protein Interfaces. *Journal of Chemical Information and Modeling*, **2017**, 57, 60-72	6.1	29
292	Hot spot occlusion from bulk water: a comprehensive study of the complex between the lysozyme HEL and the antibody FVD1.3. *Journal of Physical Chemistry B*, **2007**, 111, 2697-706	3.4	29
291	A molecular modeling study of inhibitors of nuclear factor kappa-B (p50)--DNA binding. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 825-36	4.2	29
290	Reaction Mechanism of Human Renin Studied by Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations. *ACS Catalysis*, **2014**, 4, 3869-3876	13.1	28
289	Insight into Enzymatic Nitrile Reduction: QM/MM Study of the Catalytic Mechanism of QueF Nitrile Reductase. *ACS Catalysis*, **2015**, 5, 3740-3751	13.1	28

288	Anchoring effects in a wide binding pocket: the molecular basis of regioselectivity in engineered cytochrome P450 monooxygenase from B. megaterium. *Proteins: Structure, Function and Bioinformatics*, **2008**, 73, 597-607	4.2	28
287	Molecular dynamics simulations of the enzyme Cu, Zn superoxide dismutase. *Journal of Physical Chemistry B*, **2006**, 110, 16754-62	3.4	28
286	Accuracy of the numerical solution of the PoissonBoltzmann equation. *Computational and Theoretical Chemistry*, **2005**, 729, 11-18		28
285	Establishing the catalytic mechanism of human pancreatic amylase with QM/MM methods. *Journal of Chemical Theory and Computation*, **2015**, 11, 2508-16	6.4	27
284	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. *Journal of Computational Chemistry*, **2013**, 34, 2079-90	3.5	27
283	Structural characterization of a A-type linked trimeric anthocyanin derived pigment occurring in a young Port wine. *Food Chemistry*, **2013**, 141, 1987-96	8.5	27
282	Parameters for molecular dynamics simulations of iron-sulfur proteins. *Journal of Computational Chemistry*, **2013**, 34, 1540-8	3.5	27
281	Understanding the importance of the aromatic amino-acid residues as hot-spots. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2013**, 1834, 404-14	4	27
280	MADAMM: a multistaged docking with an automated molecular modeling protocol. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 192-206	4.2	27
279	Molecular determinants of ligand specificity in family 11 carbohydrate binding modules: an NMR, X-ray crystallography and computational chemistry approach. *FEBS Journal*, **2008**, 275, 2524-35	5.7	27
278	Ribonucleotide activation by enzyme ribonucleotide reductase: understanding the role of the enzyme. *Journal of Computational Chemistry*, **2004**, 25, 2031-7	3.5	27
277	Prediction of the Raman spectrum of the aqueous formate anion by a combined density functional theory and self-consistent-reaction-field study. *Theoretical Chemistry Accounts*, **2000**, 105, 68-76	1.9	27
276	Benchmarking of Density Functionals for the Accurate Description of Thiol-Disulfide Exchange. *Journal of Chemical Theory and Computation*, **2014**, 10, 4842-56	6.4	26
275	Chemically modified tetracyclines as inhibitors of MMP-2 matrix metalloproteinase: a molecular and structural study. *Journal of Physical Chemistry B*, **2012**, 116, 13644-54	3.4	26
274	The search for the mechanism of the reaction catalyzed by farnesyltransferase. *Chemistry - A European Journal*, **2009**, 15, 4243-7	4.8	26
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272	Effective tailor-made force field parameterization of the several Zn coordination environments in the puzzling FTase enzyme: opening the door to the full understanding of its elusive catalytic mechanism. *Theoretical Chemistry Accounts*, **2006**, 117, 171-181	1.9	26
271	Structural divergence and adaptive evolution in mammalian cytochromes P450 2C. *Gene*, **2007**, 387, 58-68	3.5	26

270	Theoretical study of the unusual protonation properties of the active site cysteines in thioredoxin. *Journal of Physical Chemistry B*, **2006**, 110, 5758-61	3.4	26
269	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. *Journal of Membrane Biology*, **2018**, 251, 609-631	2.3	26
268	Prediction of Solvation Free Energies with Thermodynamic Integration Using the General Amber Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 3570-7	6.4	25
267	QSAR analysis of 2-benzoxazolyl hydrazone derivatives for anticancer activity and its possible target prediction. *Medicinal Chemistry Research*, **2012**, 21, 133-144	2.2	25
266	Multidimensional epistasis and fitness landscapes in enzyme evolution. *Biochemical Journal*, **2012**, 445, 39-46	3.8	25
265	Structural analysis of □-glucosidase inhibitors by validated QSAR models using topological and hydrophobicity based descriptors. *Chemometrics and Intelligent Laboratory Systems*, **2011**, 109, 101-112	3.8	25
264	vsLab□An implementation for virtual high-throughput screening using AutoDock and VMD. *International Journal of Quantum Chemistry*, **2011**, 111, 1208-1212	2.1	25
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262	Farnesyltransferase: Theoretical studies on peptide substrate entrance□thiol or thiolate coordination?. *Computational and Theoretical Chemistry*, **2005**, 729, 125-129		25
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260	Volarea - a bioinformatics tool to calculate the surface area and the volume of molecular systems. *Chemical Biology and Drug Design*, **2013**, 82, 743-55	2.9	24
259	Mitochondrial introgressions into the nuclear genome of the domestic cat. *Journal of Heredity*, **2007**, 98, 414-20	2.4	24
258	Benchmarking of density functionals for the kinetics and thermodynamics of the hydrolysis of glycosidic bonds catalyzed by glycosidases. *International Journal of Quantum Chemistry*, **2017**, 117, e25409	2.1	23
257	Periplasmic nitrate reductase and formate dehydrogenase: similar molecular architectures with very different enzymatic activities. *Accounts of Chemical Research*, **2015**, 48, 2875-84	24.3	23
256	Mechanism of glutathione transferase P1-1-catalyzed activation of the prodrug canfosfamide (TLK286, TELCYTA). *Biochemistry*, **2013**, 52, 8069-78	3.2	23
255	Chemical behavior of methylpyranomalvidin-3-O-glucoside in aqueous solution studied by NMR and UV-visible spectroscopy. *Journal of Physical Chemistry B*, **2011**, 115, 1538-45	3.4	23
254	The reduction of ribonucleotides catalyzed by the enzyme ribonucleotide reductase. *Theoretical Chemistry Accounts*, **2002**, 108, 352-364	1.9	23
253	Theoretical studies on the mode of inhibition of ribonucleotide reductase by 2'-substituted substrate analogues. *Chemistry - A European Journal*, **2003**, 9, 5916-25	4.8	23

252	Computational approaches to the study of some lanthanide (III)–polyazamacrocyclic chelates for magnetic resonance imaging. *International Journal of Quantum Chemistry*, **1999**, 73, 237-248	2.1	23
251	Theoretical study of ribonucleotide reductase mechanism-based inhibition by 2'-azido-2'-deoxyribonucleoside 5'-diphosphates. *Journal of Computational Chemistry*, **2004**, 25, 227-37	3.5	22
250	Development of ribonucleotide reductase inhibitors: a review on structure activity relationships. *Mini-Reviews in Medicinal Chemistry*, **2013**, 13, 1862-72	3.2	22
249	Improving the Biodesulfurization of Crude Oil and Derivatives: A QM/MM Investigation of the Catalytic Mechanism of NADH-FMN Oxidoreductase (DszD). *Journal of Physical Chemistry A*, **2016**, 120, 5300-6	2.8	22
248	DFT studies on the β-glycosidase catalytic mechanism: The deglycosylation step. *Computational and Theoretical Chemistry*, **2010**, 946, 125-133		21
247	Comparative evolutionary genomics of the HADH2 gene encoding Abeta-binding alcohol dehydrogenase/17beta-hydroxysteroid dehydrogenase type 10 (ABAD/HSD10). *BMC Genomics*, **2006**, 7, 202	4.5	21
246	Influence of Frozen Residues on the Exploration of the PES of Enzyme Reaction Mechanisms. *Journal of Chemical Theory and Computation*, **2017**, 13, 5486-5495	6.4	20
245	Synthesis and Hydrolytic Studies on the Air-Stable [(4-CN-PhO)(E)P(μ-N(t)Bu)]2 (E = O, S, and Se) Cyclodiphosphazanes. *Inorganic Chemistry*, **2015**, 54, 6423-32	5.1	20
244	Relationship between Enzyme/Substrate Properties and Enzyme Efficiency in Hydrolases. *ACS Catalysis*, **2015**, 5, 5877-5887	13.1	20
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238	Successes and failures of DFT functionals in acid/base and redox reactions of organic and biochemical interest. *Computational and Theoretical Chemistry*, **2011**, 966, 120-126	2	20
237	The Protein kinase inhibitor balanol: structure-activity relationships and structure-based computational studies. *Anti-Cancer Agents in Medicinal Chemistry*, **2008**, 8, 638-45	2.2	20
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235	Protein–protein recognition: a computational mutagenesis study of the MDM2–P53 complex. *Theoretical Chemistry Accounts*, **2008**, 120, 533-542	1.9	20

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232	New insights in the catalytic mechanism of tyrosine ammonia-lyase given by QM/MM and QM cluster models. *Archives of Biochemistry and Biophysics*, **2015**, 582, 107-15	4.1	19
231	Substrate recognition in HIV-1 protease: a computational study. *Journal of Physical Chemistry B*, **2010**, 114, 2525-32	3.4	19
230	QM/MM Study of the Reaction Mechanism of the Dehydratase Domain from Mammalian Fatty Acid Synthase. *ACS Catalysis*, **2018**, 8, 10267-10278	13.1	19
229	Catalytic Mechanism of the Serine Hydroxymethyltransferase: A Computational ONIOM QM/MM Study. *ACS Catalysis*, **2018**, 8, 10096-10110	13.1	19
228	Mechanistic Pathway on Human □Glucosidase Maltase-Glucoamylase Unveiled by QM/MM Calculations. *Journal of Physical Chemistry B*, **2018**, 122, 3889-3899	3.4	18
227	Unveiling the Catalytic Mechanism of NADP+-Dependent Isocitrate Dehydrogenase with QM/MM Calculations. *ACS Catalysis*, **2016**, 6, 357-368	13.1	18
226	Human ether-a-go-go-related gene channel blockers and its structural analysis for drug design. *Current Drug Targets*, **2013**, 14, 102-13	3	18
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223	Detailed microscopic study of the full zipA:FtsZ interface. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 811-21	4.2	18
222	Reaction Mechanism of Mycobacterium Tuberculosis Glutamine Synthetase Using Quantum Mechanics/Molecular Mechanics Calculations. *Chemistry - A European Journal*, **2016**, 22, 9218-25	4.8	17
221	Insights into the structural determinants of substrate specificity and activity in mouse aldehyde oxidases. *Journal of Biological Inorganic Chemistry*, **2015**, 20, 209-17	3.7	17
220	Gas-phase geometry optimization of biological molecules as a reasonable alternative to a continuum environment description: fact, myth, or fiction?. *Journal of Physical Chemistry A*, **2009**, 113, 14231-6	2.8	17
219	Computational studies on the reactivity of substituted 1,2-dihydro-1,2-azaborines. *Journal of Organic Chemistry*, **2009**, 74, 6120-9	4.2	17
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217	A comparative density-functional study of the reaction mechanism of the O2-dependent coproporphyrinogen III oxidase. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 2726-33	3.4	17

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