Maria J. Ramos

List of Publications by Year in Descending Order

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	Lessons from a Single Amino Acid Substitution: Anticancer and Antibacterial Properties of Two Phospholipase A2-Derived Peptides. *Current Issues in Molecular Biology*, **2022**, 44, 46-62	2.9	3
376	Necessity is the Mother of Invention: A Remote Molecular Bioinformatics Practical Course in the COVID-19 Era.. *Journal of Chemical Education*, **2022**, 99, 2147-2153	2.4	1
375	Towards the Accurate Thermodynamic Characterization of Enzyme Reaction Mechanisms.. *ChemPhysChem*, **2022**, e202200159	3.2	0
374	A combined experimental and computational study to discover novel tyrosinase inhibitors. *Journal of Inorganic Biochemistry*, **2022**, 111879	4.2	
373	MOLECULAR BIOINFORMATICS. *Revista De Ciência Elementar*, **2021**, 9,	0.3	2
372	Structure based virtual screening of natural product molecules as glycosidase inhibitors. *In Silico Pharmacology*, **2021**, 9, 56	4.3	1
371	Novel Pet-Degrading Enzymes: Structure-Function from a Computational Perspective. *ChemBioChem*, **2021**, 22, 2032-2050	3.8	6
370	Structural, enzymatic and pharmacological profiles of AplTX-II - A basic sPLA (D49) isolated from the Agkistrodon piscivorus leucostoma snake venom. *International Journal of Biological Macromolecules*, **2021**, 175, 572-585	7.9	1
369	Passive Diffusion of Ciprofloxacin and its Metalloantibiotic: A Computational and Experimental study. *Journal of Molecular Biology*, **2021**, 433, 166911	6.5	4
368	Chromeno[3,4-]xanthones as First-in-Class AChE and A Aggregation Dual-Inhibitors. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	3
367	Animal Fatty Acid Synthase: A Chemical Nanofactory. *Chemical Reviews*, **2021**, 121, 9502-9553	68.1	6
366	Combined in silico and in vitro studies to identify novel antidiabetic flavonoids targeting glycogen phosphorylase. *Bioorganic Chemistry*, **2021**, 108, 104552	5.1	4
365	Discovery of a multi-target compound for estrogen receptor-positive (ER) breast cancer: Involvement of aromatase and ERs. *Biochimie*, **2021**, 181, 65-76	4.6	6
364	Alkyl aryl modifications: a comparative study on modular modifications of triphenylphosphonium mitochondrial vectors.. *RSC Chemical Biology*, **2021**, 2, 1643-1650	3	2
363	Unraveling the cGAS catalytic mechanism upon DNA activation through molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2021**, 23, 9524-9531	3.6	0
362	Reaction Mechanism of MHETase, a PET Degrading Enzyme. *ACS Catalysis*, **2021**, 11, 10416-10428	13.1	5
361	Reaction Mechanism of the PET Degrading Enzyme PETase Studied with DFT/MM Molecular Dynamics Simulations. *ACS Catalysis*, **2021**, 11, 11626-11638	13.1	4

360	The Catalytic Mechanism of the Retaining Glycosyltransferase Mannosylglycerate Synthase. *Chemistry - A European Journal*, **2021**, 27, 13998-14006	4.8	2
359	Structural Specificity of Flavonoids in the Inhibition of Human Fructose 1,6-Bisphosphatase. *Journal of Natural Products*, **2020**, 83, 1541-1552	4.9	8
358	Activation Free Energy, Substrate Binding Free Energy, and Enzyme Efficiency Fall in a Very Narrow Range of Values for Most Enzymes. *ACS Catalysis*, **2020**, 10, 8444-8453	13.1	5
357	How the Destabilization of a Reaction Intermediate Affects Enzymatic Efficiency: The Case of Human Transketolase. *ACS Catalysis*, **2020**, 10, 2872-2881	13.1	9
356	Cannabidiol (CBD) but not tetrahydrocannabinol (THC) dysregulate in vitro decidualization of human endometrial stromal cells by disruption of estrogen signaling. *Reproductive Toxicology*, **2020** , 93, 75-82	3.4	14
355	Binding Mode Prediction and Identification of New Lead Compounds from Natural Products as 3-OST Enzyme Inhibitors. *Letters in Drug Design and Discovery*, **2020**, 17, 1186-1196	0.8	
354	Catalytic Mechanism of Human Aldehyde Oxidase. *ACS Catalysis*, **2020**, 10, 9276-9286	13.1	8
353	Reaction Mechanism and Determinants for Efficient Catalysis by DszB, a Key Enzyme for Crude Oil Bio-desulfurization. *ACS Catalysis*, **2020**, 10, 9545-9554	13.1	17
352	The bacterial 4S pathway an economical alternative for crude oil desulphurization that reduces CO2 emissions. *Green Chemistry*, **2020**, 22, 7604-7621	10	2
351	Assessing the validity of DLPNO-CCSD(T) in the calculation of activation and reaction energies of ubiquitous enzymatic reactions. *Journal of Computational Chemistry*, **2020**, 41, 2459-2468	3.5	7
350	Solving the Catalytic Mechanism of Tryptophan Synthase: an Emergent Drug Target in the Treatment of Tuberculosis. *ChemCatChem*, **2020**, 12, 227-237	5.2	4
349	Estrogen receptor-positive (ER) breast cancer treatment: Are multi-target compounds the next promising approach?. *Biochemical Pharmacology*, **2020**, 177, 113989	6	17
348	The importance of intramolecular hydrogen bonds on the translocation of the small drug piracetam through a lipid bilayer.. *RSC Advances*, **2020**, 11, 899-908	3.7	9
347	The interaction of aluminum with catecholamine-based neurotransmitters: can the formation of these species be considered a potential risk factor for neurodegenerative diseases?. *Dalton Transactions*, **2019**, 48, 6003-6018	4.3	8
346	Exploring the Identity of the General Base for a DNA Polymerase Catalyzed Reaction Using QM/MM: The Case Study of Human Translesion Synthesis Polymerase *ACS Catalysis*, **2019**, 9, 2543-2551	13.1	10
345	Benchmark of Density Functionals for the Calculation of the Redox Potential of Fe/Fe Within Protein Coordination Shells. *Frontiers in Chemistry*, **2019**, 7, 391	5	6
344	A computational study on the redox properties and binding affinities of iron complexes of hydroxypyridinones. *Journal of Molecular Modeling*, **2019**, 25, 172	2	1
343	New insights about the monomer and homodimer structures of the human AOX1. *Physical Chemistry Chemical Physics*, **2019**, 21, 13545-13554	3.6	4

342	Enabling Mitochondrial Uptake of Lipophilic Dications Using Methylated Triphenylphosphonium Moieties. *Inorganic Chemistry*, **2019**, 58, 8293-8299	5.1	12
341	Conformational diversity induces nanosecond-timescale chemical disorder in the HIV-1 protease reaction pathway. *Chemical Science*, **2019**, 10, 7212-7221	9.4	10
340	Evaluation of a flavonoids library for inhibition of pancreatic α-amylase towards a structure-activity relationship. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 577-588	5.6	53
339	Human Fatty Acid Synthase: A Computational Study of the Transfer of the Acyl Moieties from MAT to the ACP Domain. *ChemCatChem*, **2019**, 11, 3853-3864	5.2	7
338	Complexities of the Reaction Mechanisms of CC Double Bond Reduction in Mammalian Fatty Acid Synthase Studied with Quantum Mechanics/Molecular Mechanics Calculations. *ACS Catalysis*, **2019**, 9, 11404-11412	13.1	8
337	The Catalytic Mechanism of Human Transketolase. *ChemPhysChem*, **2019**, 20, 2881-2886	3.2	10
336	Structural and mechanistic aspects of S-S bonds in the thioredoxin-like family of proteins. *Biological Chemistry*, **2019**, 400, 575-587	4.5	11
335	A novel synthetic peptide inspired on Lys49 phospholipase A from Crotalus oreganus abyssus snake venom active against multidrug-resistant clinical isolates. *European Journal of Medicinal Chemistry*, **2018**, 149, 248-256	6.8	16
334	A QM/MM approach on the structural and stereoelectronic factors governing glycosylation by GTF-SI from Streptococcus mutans. *Organic and Biomolecular Chemistry*, **2018**, 16, 2438-2447	3.9	7
333	A Buried Water Molecule Influences Reactivity in α-Amylase on a Subnanosecond Time Scale. *ACS Catalysis*, **2018**, 8, 4055-4063	13.1	14
332	Understanding the Catalytic Machinery and the Reaction Pathway of the Malonyl-Acetyl Transferase Domain of Human Fatty Acid Synthase. *ACS Catalysis*, **2018**, 8, 4860-4872	13.1	20
331	Parametrization of Molybdenum Cofactors for the AMBER Force Field. *Journal of Chemical Theory and Computation*, **2018**, 14, 2538-2548	6.4	5
330	Studies on neuraminidase inhibition. *International Journal of Quantum Chemistry*, **2018**, 118, e25592	2.1	1
329	Visualizing the Microscopic World. *Interdisciplinary Sciences, Computational Life Sciences*, **2018**, 10, 105-110	3.5	2
328	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	2.9	6
327	Mechanistic Pathway on Human α-Glucosidase Maltase-Glucoamylase Unveiled by QM/MM Calculations. *Journal of Physical Chemistry B*, **2018**, 122, 3889-3899	3.4	18
326	Protocol for Computational Enzymatic Reactivity Based on Geometry Optimisation. *ChemPhysChem* , **2018**, 19, 669-689	3.2	14
325	Membrane partition of bis-(3-hydroxy-4-pyridinonato) zinc(ii) complexes revealed by molecular dynamics simulations.. *RSC Advances*, **2018**, 8, 27081-27090	3.7	4

324	Properties that rank protein:protein docking poses with high accuracy. *Physical Chemistry Chemical Physics*, **2018**, 20, 20927-20942	3.6	4
323	Understanding the Rate-Limiting Step of Glycogenolysis by Using QM/MM Calculations on Human Glycogen Phosphorylase. *ChemMedChem*, **2018**, 13, 1608-1616	3.7	4
322	Tuning the affinity of catechols and salicylic acids towards Al(iii): characterization of Al-chelator interactions. *Dalton Transactions*, **2018**, 47, 9592-9607	4.3	8
321	Modeling of Human Fatty Acid Synthase and in Silico Docking of Acyl Carrier Protein Domain and Its Partner Catalytic Domains. *Journal of Physical Chemistry B*, **2018**, 122, 77-85	3.4	14
320	Mechanistic Insights on Human Phosphoglucomutase Revealed by Transition Path Sampling and Molecular Dynamics Calculations. *Chemistry - A European Journal*, **2018**, 24, 1978-1987	4.8	7
319	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
318	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. *Journal of Membrane Biology*, **2018**, 251, 609-631	2.3	26
317	Mechanistic Studies of a Flavin Monooxygenase: Sulfur Oxidation of Dibenzothiophenes by DszC. *ACS Catalysis*, **2018**, 8, 9298-9311	13.1	10
316	Catalytic Mechanism of the Serine Hydroxymethyltransferase: A Computational ONIOM QM/MM Study. *ACS Catalysis*, **2018**, 8, 10096-10110	13.1	19
315	Determining the glycation site specificity of human holo-transferrin. *Journal of Inorganic Biochemistry*, **2018**, 186, 95-102	4.2	3
314	Transport Properties of Light Gases in Nanochannels of L□eu-L-Ser Dipeptide Crystals: A Comparative Study by Molecular Dynamics Simulations. *ChemistrySelect*, **2018**, 3, 5517-5525	1.8	1
313	Revisiting Partition in Hydrated Bilayer Systems. *Journal of Chemical Theory and Computation*, **2017**, 13, 2290-2299	6.4	11
312	Clarifying the Catalytic Mechanism of Human Glutamine Synthetase: A QM/MM Study. *Journal of Physical Chemistry B*, **2017**, 121, 6313-6320	3.4	5
311	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
310	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
309	The Catalytic Mechanism of the Pyridoxal-5'-phosphate-Dependent Enzyme, Histidine Decarboxylase: A Computational Study. *Chemistry - A European Journal*, **2017**, 23, 9162-9173	4.8	19
308	The mechanism of the Ser-(cis)Ser-Lys catalytic triad of peptide amidases. *Physical Chemistry Chemical Physics*, **2017**, 19, 12343-12354	3.6	9
307	Diffusion of the small, very polar, drug piracetam through a lipid bilayer: an MD simulation study. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	12

306	Unique Triphenylphosphonium Derivatives for Enhanced Mitochondrial Uptake and Photodynamic Therapy. *Bioconjugate Chemistry*, **2017**, 28, 590-599	6.3	36
305	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
304	Improving the Catalytic Power of the DszD Enzyme for the Biodesulfurization of Crude Oil and Derivatives. *Chemistry - A European Journal*, **2017**, 23, 17231-17241	4.8	15
303	-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
302	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
301	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
300	Binding free energy calculations on E-selectin complexes with sLe oligosaccharide analogs. *Chemical Biology and Drug Design*, **2017**, 89, 114-123	2.9	6
299	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
298	Molecular motion regulates the activity of the Mitochondrial Serine Protease HtrA2. *Cell Death and Disease*, **2017**, 8, e3119	9.8	11
297	Cancer therapies based on enzymatic amino acid depletion **2017**, 623-651		2
296	HMG-CoA Reductase inhibitors: an updated review of patents of novel compounds and formulations (2011-2015). *Expert Opinion on Therapeutic Patents*, **2016**, 26, 1257-1272	6.8	16
295	Reaction Mechanism of Mycobacterium Tuberculosis Glutamine Synthetase Using Quantum Mechanics/Molecular Mechanics Calculations. *Chemistry - A European Journal*, **2016**, 22, 9218-25	4.8	17
294	Unveiling the Catalytic Mechanism of NADP+-Dependent Isocitrate Dehydrogenase with QM/MM Calculations. *ACS Catalysis*, **2016**, 6, 357-368	13.1	18
293	Molecular dynamic simulations and structure-based pharmacophore development for farnesyltransferase inhibitors discovery. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 1428-42	5.6	5
292	Structure of a truncated form of leucine zipper II of JIP3 reveals an unexpected antiparallel coiled-coil arrangement. *Acta Crystallographica Section F, Structural Biology Communications*, **2016**, 72, 198-206	1.1	2
291	Synthesis and structural characterization, by spectroscopic and computational methods, of two fluorescent 3-hydroxy-4-pyridinone chelators bearing sulphorhodamine B and naphthalene. *RSC Advances*, **2016**, 6, 4200-4211	3.7	5
290	A QM/MM study of the reaction mechanism of human -ketoacyl reductase. *Physical Chemistry Chemical Physics*, **2016**, 19, 347-355	3.6	14
289	Glutamine Synthetase Drugability beyond Its Active Site: Exploring Oligomerization Interfaces and Pockets. *Molecules*, **2016**, 21,	4.8	11

288	QM/MM study of the mechanism of reduction of 3-hydroxy-3-methylglutaryl coenzyme A catalyzed by human HMG-CoA reductase. *Catalysis Science and Technology*, **2016**, 6, 7172-7185	5.5	14
287	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
286	Binding mode of conformations and structure-based pharmacophore development for farnesyltransferase inhibitors. *Medicinal Chemistry Research*, **2016**, 25, 1340-1357	2.2	
285	Insights into the reaction mechanism of 3-O-sulfotransferase through QM/MM calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 11488-96	3.6	10
284	Cholesterol Biosynthesis: A Mechanistic Overview. *Biochemistry*, **2016**, 55, 5483-5506	3.2	116
283	Calculation of distribution coefficients in the SAMPL5 challenge from atomic solvation parameters and surface areas. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 1079-1086	4.2	3
282	The Catalytic Mechanism of the Marine-Derived Macrocyclase PatGmac. *Chemistry - A European Journal*, **2016**, 22, 13089-97	4.8	15
281	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
280	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
279	Molecular Dynamics Analysis of FAAH Complexed with Anandamide. *Progress in Theoretical Chemistry and Physics*, **2015**, 115-131	0.6	
278	Receptor-based virtual screening protocol for drug discovery. *Archives of Biochemistry and Biophysics*, **2015**, 582, 56-67	4.1	74
277	Synthesis and Hydrolytic Studies on the Air-Stable [(4-CN-PhO)(E)P(□N(t)Bu)]2 (E = O, S, and Se) Cyclodiphosphazanes. *Inorganic Chemistry*, **2015**, 54, 6423-32	5.1	20
276	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
275	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. *ACS Catalysis*, **2015**, 5, 5617-5626	9.1	53
274	Relationship between Enzyme/Substrate Properties and Enzyme Efficiency in Hydrolases. *ACS Catalysis*, **2015**, 5, 5877-5887	13.1	20
273	Ligand based analysis on HMG-CoA reductase inhibitors. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 140, 102-116	3.8	15
272	A new scoring function for protein-protein docking that identifies native structures with unprecedented accuracy. *Physical Chemistry Chemical Physics*, **2015**, 17, 2378-87	3.6	12
271	Dynamics of excited clusters of □alanine in the gas phase. *Journal of Physics: Conference Series*, **2015**, 635, 032089	0.3	

270	Re(I) and Tc(I) complexes for targeting nitric oxide synthase: influence of the chelator in the affinity for the enzyme. *Chemical Biology and Drug Design*, **2015**, 86, 1072-86	2.9	6
269	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
268	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
267	PLP undergoes conformational changes during the course of an enzymatic reaction. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 596-606		20
266	Discovery of new druggable sites in the anti-cholesterol target HMG-CoA reductase by computational alanine scanning mutagenesis. *Journal of Molecular Modeling*, **2014**, 20, 2178	2	11
265	CHEM-PATH-TRACKER: An automated tool to analyze chemical motifs in molecular structures. *Chemical Biology and Drug Design*, **2014**, 84, 44-53	2.9	1
264	Structural characterization of inclusion complexes between cyanidin-3-O-glucoside and Ecyclodextrin. *Carbohydrate Polymers*, **2014**, 102, 269-77	10.3	50
263	Catalytic Mechanism of Retroviral Integrase for the Strand Transfer Reaction Explored by QM/MM Calculations. *Journal of Chemical Theory and Computation*, **2014**, 10, 5458-66	6.4	4
262	Enzymatic Bricks Carboxylate shift and sulfur shift. *International Journal of Quantum Chemistry*, **2014**, 114, 1253-1256	2.1	11
261	Discovery of new sites for drug binding to the hypertension-related renin-angiotensinogen complex. *Chemical Biology and Drug Design*, **2014**, 83, 427-39	2.9	2
260	Protein Ligand Docking in Drug Discovery **2014**, 249-286		5
259	Reaction Mechanism of Human Renin Studied by Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations. *ACS Catalysis*, **2014**, 4, 3869-3876	13.1	28
258	Are hot-spots occluded from water?. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 186-97	3.6	8
257	Biomolecular structure manipulation using tailored electromagnetic radiation: a proof of concept on a simplified model of the active site of bacterial DNA topoisomerase. *Physical Chemistry Chemical Physics*, **2014**, 16, 21768-77	3.6	3
256	Binding mode prediction and identification of new lead compounds from natural products as renin and angiotensin converting enzyme inhibitors. *RSC Advances*, **2014**, 4, 19550-19568	3.7	6
255	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
254	The catalytic mechanism of carboxylesterases: a computational study. *Biochemistry*, **2014**, 53, 5820-9	3.2	37
253	Isomerization of 5-androstene-3,17-dione into 4-androstene-3,17-dione catalyzed by human glutathione transferase A3-3: a computational study identifies a dual role for glutathione. *Journal of Physical Chemistry A*, **2014**, 118, 5790-800	2.8	11

252	Structural and dynamics analysis of matrix metalloproteinases MMP-2 complexed with chemically modified tetracyclines (CMTs). *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1907-18	3.6	5
251	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
250	Analyses of cobalt-ligand and potassium-ligand bond lengths in metalloproteins: trends and patterns. *Journal of Molecular Modeling*, **2014**, 20, 2271	2	2
249	Glycosidase inhibitors: a patent review (2008-2013). *Expert Opinion on Therapeutic Patents*, **2014**, 24, 857-74	6.8	47
248	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
247	The glycation site specificity of human serum transferrin is a determinant for transferrin's functional impairment under elevated glycaemic conditions. *Biochemical Journal*, **2014**, 461, 33-42	3.8	16
246	QM/MM Study and MD Simulations on the Hypertension Regulator Angiotensin-Converting Enzyme. *ACS Catalysis*, **2014**, 4, 2587-2597	13.1	20
245	Divalent metal ion-based catalytic mechanism of the Nudix hydrolase Orf153 (YmfB) from Escherichia coli. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 1297-310		5
244	Biomembrane simulations of 12 lipid types using the general amber force field in a tensionless ensemble. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 88-103	3.6	7
243	Predictive QSAR models development and validation for human ether-a-go-go related gene (hERG) blockers using newer tools. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2014**, 29, 317-24	5.6	9
242	Relevant interactions of antimicrobial iron chelators and membrane models revealed by nuclear magnetic resonance and molecular dynamics simulations. *Journal of Physical Chemistry B*, **2014**, 118, 14590-601	3.4	10
241	Influence of the environment on protein bond energies. *Chemical Physics Letters*, **2014**, 615, 75-82	2.5	
240	Classification study of solvation free energies of organic molecules using machine learning techniques. *RSC Advances*, **2014**, 4, 61624-61630	3.7	10
239	Molecular dynamics studies on both bound and unbound renin protease. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 351-63	3.6	10
238	Fused aryl-phenazines: scaffold for the development of bioactive molecules. *Current Drug Targets*, **2014**, 15, 681-8	3	11
237	CompASM: an Amber-VMD alanine scanning mutagenesis plug-in. *Highlights in Theoretical Chemistry*, **2014**, 81-87		1
236	Computational Alanine Scanning Mutagenesis: MM-PBSA vs TI. *Journal of Chemical Theory and Computation*, **2013**, 9, 1311-9	6.4	54
235	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

234	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
233	Theoretical studies on the binding of rhenium(I) complexes to inducible nitric oxide synthase. *Journal of Molecular Graphics and Modelling*, **2013**, 45, 13-25	2.8	12
232	A DFT study of the applicability of the charge balance model in two-metal enzymes: The case of cAMP-dependent protein kinase. *Chemical Physics Letters*, **2013**, 571, 66-70	2.5	7
231	Combined ligand and structure based binding mode analysis of oxidosqualene cyclase inhibitors. *RSC Advances*, **2013**, 3, 23409	3.7	5
230	Molecular dynamics analysis of a series of 22 potential farnesyltransferase substrates containing a CaaX-motif. *Journal of Molecular Modeling*, **2013**, 19, 673-88	2	8
229	Parameters for molecular dynamics simulations of iron-sulfur proteins. *Journal of Computational Chemistry*, **2013**, 34, 1540-8	3.5	27
228	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
227	Insights into the structural determinants for selective inhibition of nitric oxide synthase isoforms. *Journal of Molecular Modeling*, **2013**, 19, 1537-51	2	12
226	Parameters for Molecular Dynamics Simulations of Manganese-Containing Metalloproteins. *Journal of Chemical Theory and Computation*, **2013**, 9, 2718-32	6.4	30
225	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
224	Mechanism of glutathione transferase P1-1-catalyzed activation of the prodrug canfosfamide (TLK286, TELCYTA). *Biochemistry*, **2013**, 52, 8069-78	3.2	23
223	The sulfur shift: an activation mechanism for periplasmic nitrate reductase and formate dehydrogenase. *Inorganic Chemistry*, **2013**, 52, 10766-72	5.1	42
222	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
221	Structural features of copigmentation of oenin with different polyphenol copigments. *Journal of Agricultural and Food Chemistry*, **2013**, 61, 6942-8	5.7	38
220	The catalytic mechanism of protein phosphatase 5 established by DFT calculations. *Chemistry - A European Journal*, **2013**, 19, 14081-9	4.8	42
219	QSAR and pharmacophore analysis of a series of piperidinyl urea derivatives as HERG blockers and H3 antagonists. *Current Drug Discovery Technologies*, **2013**, 10, 47-58	1.5	3
218	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
217	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

216	Farnesyltransferase inhibitors: a comprehensive review based on quantitative structural analysis. *Current Medicinal Chemistry*, **2013**, 20, 4888-923	4.3	33
215	Development of ribonucleotide reductase inhibitors: a review on structure activity relationships. *Mini-Reviews in Medicinal Chemistry*, **2013**, 13, 1862-72	3.2	22
214	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
213	Improving the study of proton transfers between amino acid side chains in solution: choosing appropriate DFT functionals and avoiding hidden pitfalls. *Highlights in Theoretical Chemistry*, **2013**, 199-205		
212	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
211	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
210	Virtual screening and QSAR study of some pyrrolidine derivatives as β-mannosidase inhibitors for binding feature analysis. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 6945-59	3.4	7
209	Computational enzymatic catalysis--clarifying enzymatic mechanisms with the help of computers. *Physical Chemistry Chemical Physics*, **2012**, 14, 12431-41	3.6	44
208	The catalytic mechanism of mouse renin studied with QM/MM calculations. *Physical Chemistry Chemical Physics*, **2012**, 14, 12605-13	3.6	20
207	The extracellular subunit interface of the 5-HT3 receptors: a computational alanine scanning mutagenesis study. *Journal of Biomolecular Structure and Dynamics*, **2012**, 30, 280-98	3.6	6
206	Influence of a flavan-3-ol substituent on the affinity of anthocyanins (pigments) toward vinylcatechin dimers and proanthocyanidins (copigments). *Journal of Physical Chemistry B*, **2012**, 116, 14089-99	3.4	24
205	Multidimensional epistasis and fitness landscapes in enzyme evolution. *Biochemical Journal*, **2012**, 445, 39-46	3.8	25
204	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
203	Structural analysis of structurally diverse β-glucosidase inhibitors for active site feature analysis. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2012**, 27, 649-57	5.6	5
202	CompASM: an Amber-VMD alanine scanning mutagenesis plug-in. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	13
201	Analysis of van der Waals surface area properties for human ether-a-go-go-related gene blocking activity: computational study on structurally diverse compounds. *SAR and QSAR in Environmental Research*, **2012**, 23, 521-36	3.5	20
200	Comparative structural analysis of β-glucosidase inhibitors on difference species: a computational study. *Archiv Der Pharmazie*, **2012**, 345, 265-74	4.3	10
199	QSAR and pharmacophore analysis of thiosemicarbazone derivatives as ribonucleotide reductase inhibitors. *Medicinal Chemistry Research*, **2012**, 21, 739-746	2.2	8

198	Improving the study of proton transfers between amino acid side chains in solution: choosing appropriate DFT functionals and avoiding hidden pitfalls. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	5
197	Gemcitabine: a critical nucleoside for cancer therapy. *Current Medicinal Chemistry*, **2012**, 19, 1076-87	4.3	61
196	The first mammalian aldehyde oxidase crystal structure: insights into substrate specificity. *Journal of Biological Chemistry*, **2012**, 287, 40690-702	5.4	79
195	In silico based structural analysis of some piperidine analogs as farnesyltransferase inhibitors. *Medicinal Chemistry*, **2012**, 8, 853-64	1.8	1
194	Structural analysis of 2-piperidin-4-yl-actamide derivatives for hERG blocking and MCH R1 antagonistic activities. *Current Drug Discovery Technologies*, **2012**, 9, 25-38	1.5	8
193	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
192	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
191	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
190	The Catalytic Mechanism of RNA Polymerase II. *Journal of Chemical Theory and Computation*, **2011**, 7, 1177-88	6.4	37
189	Detailed atomistic analysis of the HIV-1 protease interface. *Journal of Physical Chemistry B*, **2011**, 115, 7045-57	3.4	15
188	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
187	In silico-based structural analysis of arylthiophene derivatives for FTase inhibitory activity, hERG, and other toxic effects. *Journal of Biomolecular Screening*, **2011**, 16, 1037-46		14
186	Metals in proteins: cluster analysis studies. *Journal of Molecular Modeling*, **2011**, 17, 429-42	2	8
185	Theoretical insights into the catalytic mechanism of □hexosaminidase. *Theoretical Chemistry Accounts*, **2011**, 129, 119-129	1.9	11
184	Conformational study of two diasteroisomers of vinylcatechin dimers in a methanol solution. *International Journal of Quantum Chemistry*, **2011**, 111, 1498-1510	2.1	3
183	Computational insights into the photochemical step of the reaction catalyzed by protochlorophylide oxidoreductase. *International Journal of Quantum Chemistry*, **2011**, 111, 1472-1479	2.1	5
182	vsLab□An implementation for virtual high-throughput screening using AutoDock and VMD. *International Journal of Quantum Chemistry*, **2011**, 111, 1208-1212	2.1	25
181	Prediction of the relationship between the structural features of andrographolide derivatives and □glucosidase inhibitory activity: a quantitative structure-activity relationship (QSAR) study. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2011**, 26, 78-87	5.6	12

180	hERG binding feature analysis of structurally diverse compounds by QSAR and fragmental analysis. *RSC Advances*, **2011**, 1, 1126	3.7	18
179	Detection of farnesyltransferase interface hot spots through computational alanine scanning mutagenesis. *Journal of Physical Chemistry B*, **2011**, 115, 15339-54	3.4	7
178	Topological, hydrophobicity, and other descriptors on -glucosidase inhibition: a QSAR study on xanthone derivatives. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2011**, 26, 755-66	5.6	11
177	QM/MM study of the catalytic mechanism of GalNAc removal from GM2 ganglioside catalyzed by human -hexosaminidaseA. *Journal of Physical Chemistry B*, **2011**, 115, 14751-9	3.4	14
176	The Accuracy of Density Functional Theory in the Description of Cation- and -Hydrogen Bond Interactions. *Journal of Chemical Theory and Computation*, **2011**, 7, 2059-67	6.4	35
175	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
174	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
173	Computational characterization of the substrate-binding mode in coproporphyrinogen III oxidase. *Journal of Physical Chemistry B*, **2011**, 115, 1903-10	3.4	5
172	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
171	QSAR Analysis of Isosteviol Derivatives as α-Glucosidase Inhibitors with Element Count and Other Descriptors. *Letters in Drug Design and Discovery*, **2011**, 8, 14-25	0.8	12
170	Structural feature study of benzofuran derivatives as farnesyltransferase inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2011**, 26, 777-91	5.6	15
169	Analysis of the -glucosidase inhibitory activity of chromenone derivatives based on their molecular features: a computational study. *Medicinal Chemistry*, **2011**, 7, 526-33	1.8	11
168	Ribonucleotide reductase: a mechanistic portrait of substrate analogues inhibitors. *Current Medicinal Chemistry*, **2010**, 17, 2854-72	4.3	12
167	Inhibition of pancreatic elastase by polyphenolic compounds. *Journal of Agricultural and Food Chemistry*, **2010**, 58, 10668-76	5.7	39
166	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
165	A tale of two acids: when arginine is a more appropriate acid than H3O+. *Journal of Physical Chemistry B*, **2010**, 114, 8994-9001	3.4	14
164	Glutathione transferase classes alpha, pi, and mu: GSH activation mechanism. *Journal of Physical Chemistry B*, **2010**, 114, 12972-80	3.4	14
163	Substrate recognition in HIV-1 protease: a computational study. *Journal of Physical Chemistry B*, **2010**, 114, 2525-32	3.4	19

162	Vinylcatechin dimers are much better copigments for anthocyanins than catechin dimer procyanidin b3. *Journal of Agricultural and Food Chemistry*, **2010**, 58, 3159-66	5.7	18
161	Benchmarking of DFT Functionals for the Hydrolysis of Phosphodiester Bonds. *Journal of Chemical Theory and Computation*, **2010**, 6, 2281-92	6.4	62
160	Glutathione transferase A1-1: catalytic importance of arginine 15. *Journal of Physical Chemistry B*, **2010**, 114, 1690-7	3.4	16
159	Understanding the binding of procyanidins to pancreatic elastase by experimental and computational methods. *Biochemistry*, **2010**, 49, 5097-108	3.2	33
158	Molecular Dynamics Simulations: Difficulties, Solutions and Strategies for Treating Metalloenzymes. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 299-330	0.7	10
157	Understanding the Mechanism for Ribonucleotide Reductase Inactivation by 2'-Deoxy-2'-methylenecytidine-5'-diphosphate. *Journal of Chemical Theory and Computation*, **2010**, 6, 2770-81	6.4	8
156	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
155	Protein-protein docking dealing with the unknown. *Journal of Computational Chemistry*, **2010**, 31, 317-42	3.5	85
154	Virtual screening in drug design and development. *Combinatorial Chemistry and High Throughput Screening*, **2010**, 13, 442-53	1.3	42
153	DFT studies on the β-glycosidase catalytic mechanism: The deglycosylation step. *Computational and Theoretical Chemistry*, **2010**, 946, 125-133		21
152	Computational analysis of ligand recognition sites of homo- and heteropentameric 5-HT3 receptors. *European Journal of Medicinal Chemistry*, **2010**, 45, 4746-60	6.8	14
151	Structural analysis of ABAD point mutations causing 2-methyl-3-hydroxylbutyryl-coA deficiency. *International Journal of Quantum Chemistry*, **2010**, 110, 148-160	2.1	
150	ABAD: a potential therapeutic target for Abeta-induced mitochondrial dysfunction in Alzheimer's disease. *Mini-Reviews in Medicinal Chemistry*, **2009**, 9, 1002-8	3.2	5
149	Direct covalent modification as a strategy to inhibit nuclear factor-kappa B. *Current Medicinal Chemistry*, **2009**, 16, 4261-73	4.3	25
148	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
147	The search for the mechanism of the reaction catalyzed by farnesyltransferase. *Chemistry - A European Journal*, **2009**, 15, 4243-7	4.8	26
146	Role of the variable active site residues in the function of thioredoxin family oxidoreductases. *Journal of Computational Chemistry*, **2009**, 30, 710-24	3.5	11
145	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

144	Docking and molecular dynamics studies on the stereoselectivity in the enzymatic synthesis of carbohydrates. *Theoretical Chemistry Accounts*, **2009**, 122, 283-296	1.9	15
143	Glutathione transferase A1-1: catalytic role of water. *Theoretical Chemistry Accounts*, **2009**, 124, 71-83	1.9	6
142	MADAMM: a multistaged docking with an automated molecular modeling protocol. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 192-206	4.2	27
141	Modelling beta-1,3-exoglucanase-saccharide interactions: structure of the enzyme-substrate complex and enzyme binding to the cell wall. *Journal of Molecular Graphics and Modelling*, **2009**, 27, 908-20	2.8	8
140	Molecular dynamics simulations on the critical states of the farnesyltransferase enzyme. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 3369-78	3.4	26
139	Synthesis and structural characterization of two diasteroisomers of vinylcatechin dimers. *Journal of Agricultural and Food Chemistry*, **2009**, 57, 10341-8	5.7	11
138	Computational studies on the reactivity of substituted 1,2-dihydro-1,2-azaborines. *Journal of Organic Chemistry*, **2009**, 74, 6120-9	4.2	17
137	The Zinc proteome: a tale of stability and functionality. *Dalton Transactions*, **2009**, 7946-56	4.3	59
136	Virtual screening of compound libraries. *Methods in Molecular Biology*, **2009**, 572, 57-70	1.4	9
135	The adaptive evolution of the mammalian mitochondrial genome. *BMC Genomics*, **2008**, 9, 119	4.5	234
134	Computational enzymatic catalysis. *Accounts of Chemical Research*, **2008**, 41, 689-98	24.3	130
133	Enzyme flexibility and the catalytic mechanism of farnesyltransferase: targeting the relation. *Journal of Physical Chemistry B*, **2008**, 112, 8681-91	3.4	17
132	Structural insight on the activity of type 1 angiotensin II peptide antagonists using MD simulations. *Journal of Physical Chemistry B*, **2008**, 112, 13620-8	3.4	
131	Comparative density functional study of models for the reaction mechanism of uroporphyrinogen III synthase. *Journal of Physical Chemistry B*, **2008**, 112, 3144-8	3.4	11
130	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
129	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
128	Farnesyltransferase inhibitors: a detailed chemical view on an elusive biological problem. *Current Medicinal Chemistry*, **2008**, 15, 1478-92	4.3	101
127	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

126	Mammalian cytosolic glutathione transferases. *Current Protein and Peptide Science*, **2008**, 9, 325-37	2.8	59
125	Protein–protein recognition: a computational mutagenesis study of the MDM2–p53 complex. *Theoretical Chemistry Accounts*, **2008**, 120, 533-542	1.9	20
124	Molecular dynamics analysis of farnesyltransferase: A closer look into the amino acid behavior. *International Journal of Quantum Chemistry*, **2008**, 108, 1939-1950	2.1	10
123	Computational optimization of AG18051 inhibitor for amyloid-β binding alcohol dehydrogenase enzyme. *International Journal of Quantum Chemistry*, **2008**, 108, 1982-1991	2.1	2
122	Carbohydrate-binding modules from family 11: Understanding the binding mode of polysaccharides. *International Journal of Quantum Chemistry*, **2008**, 108, 2030-2040	2.1	20
121	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
120	Glutathione transferase: new model for glutathione activation. *Chemistry - A European Journal*, **2008**, 14, 9591-8	4.8	51
119	Mechanistic studies on the formation of glycosidase-substrate and glycosidase-inhibitor covalent intermediates. *Journal of Computational Chemistry*, **2008**, 29, 2565-74	3.5	35
118	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
117	Molecular dynamics simulations of the amyloid-beta binding alcohol dehydrogenase (ABAD) enzyme. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 9511-8	3.4	10
116	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
115	Reaction mechanism of the vitamin K-dependent glutamate carboxylase: a computational study. *Journal of Physical Chemistry B*, **2007**, 111, 12883-7	3.4	8
114	Backbone Importance for Protein-Protein Binding. *Journal of Chemical Theory and Computation*, **2007**, 3, 885-93	6.4	12
113	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
112	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
111	The carboxylate shift in zinc enzymes: a computational study. *Journal of the American Chemical Society*, **2007**, 129, 1378-85	16.4	120
110	Understanding ribonucleotide reductase inactivation by gemcitabine. *Chemistry - A European Journal*, **2007**, 13, 8507-15	4.8	105
109	Computational alanine scanning mutagenesis--an improved methodological approach. *Journal of Computational Chemistry*, **2007**, 28, 644-54	3.5	190

108	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
107	Microscopic detail provided for the adsorption of protected amino-cyclopentene on Si(100). *Chemical Physics Letters*, **2007**, 448, 111-114	2.5	
106	Drug design: new inhibitors for HIV-1 protease based on Nelfinavir as lead. *Journal of Molecular Graphics and Modelling*, **2007**, 26, 634-42	2.8	10
105	Parameterization of AZT□A widely used nucleoside inhibitor of HIV-1 reverse transcriptase. *International Journal of Quantum Chemistry*, **2007**, 107, 292-298	2.1	6
104	Hot spot computational identification: Application to the complex formed between the hen egg white lysozyme (HEL) and the antibody HyHEL-10. *International Journal of Quantum Chemistry*, **2007** , 107, 299-310	2.1	20
103	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
102	Analysis of zinc-ligand bond lengths in metalloproteins: trends and patterns. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 466-75	4.2	62
101	Isolation and characterization of microsatellite markers in pangolins (Mammalia, Pholidota, Manis spp.). *Molecular Ecology Notes*, **2007**, 7, 269-272		9
100	Structural and functional implications of positive selection at the primate angiogenin gene. *BMC Evolutionary Biology*, **2007**, 7, 167	3	10
99	Vascular endothelial growth factor (VEGF) inhibition--a critical review. *Anti-Cancer Agents in Medicinal Chemistry*, **2007**, 7, 223-45	2.2	83
98	Effect of the tert-butiloxycarbonyl protecting group on the adsorption of protected amino-cyclopentene on the Si(100) surface. *Physical Review B*, **2007**, 75,	3.3	2
97	The excision mechanism in reverse transcriptase: pyrophosphate leaving and fingers opening are uncoupled events with the analogues AZT and d4T. *Journal of Physical Chemistry B*, **2007**, 111, 12032-9	3.4	5
96	Mitochondrial introgressions into the nuclear genome of the domestic cat. *Journal of Heredity*, **2007**, 98, 414-20	2.4	24
95	Gathering Computational Genomics and Proteomics to Unravel Adaptive Evolution. *Evolutionary Bioinformatics*, **2007**, 3, 117693430700300	1.9	4
94	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
93	Structural divergence and adaptive evolution in mammalian cytochromes P450 2C. *Gene*, **2007**, 387, 58-66	3.68	26
92	General performance of density functionals. *Journal of Physical Chemistry A*, **2007**, 111, 10439-52	2.8	810
91	Theoretical studies on farnesyltransferase: the distances paradox explained. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 205-18	4.2	35

90	Gathering computational genomics and proteomics to unravel adaptive evolution. *Evolutionary Bioinformatics*, **2007**, 3, 207-9	1.9	4
89	Computational Determination of the Relative Free Energy of Binding Application to Alanine Scanning Mutagenesis. *Challenges and Advances in Computational Chemistry and Physics*, **2007**, 305-339	0.7	5
88	Computational studies on class I ribonucleotide reductase: understanding the mechanisms of action and inhibition of a cornerstone enzyme for the treatment of cancer. *European Biophysics Journal*, **2006**, 35, 125-35	1.9	10
87	Cu, Zn Superoxide dismutase: distorted active site binds substrate without significant energetic cost. *Theoretical Chemistry Accounts*, **2006**, 115, 27-31	1.9	12
86	Unravelling Hot Spots: a comprehensive computational mutagenesis study. *Theoretical Chemistry Accounts*, **2006**, 117, 99-113	1.9	34
85	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
84	Similarities and differences in the thioredoxin superfamily. *Progress in Biophysics and Molecular Biology*, **2006**, 91, 229-48	4.7	94
83	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
82	Determination of the DeltapKa between the active site cysteines of thioredoxin and DsbA. *Journal of Computational Chemistry*, **2006**, 27, 966-75	3.5	33
81	QM/QM study of the coverage effects on the adsorption of amino-cyclopentene at the Si(100) surface. *Journal of Computational Chemistry*, **2006**, 27, 1892-7	3.5	4
80	Molecular insights into the mechanisms of HIV-1 reverse transcriptase resistance to nucleoside analogs. *Mini-Reviews in Medicinal Chemistry*, **2006**, 6, 549-55	3.2	5
79	Molecular dynamics simulations of the enzyme Cu, Zn superoxide dismutase. *Journal of Physical Chemistry B*, **2006**, 110, 16754-62	3.4	28
78	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
77	Protein-ligand docking: current status and future challenges. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 15-26	4.2	597
76	Dehydration of ribonucleotides catalyzed by ribonucleotide reductase: the role of the enzyme. *Biophysical Journal*, **2006**, 90, 2109-19	2.9	45
75	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
74	Insights on resistance to reverse transcriptase: the different patterns of interaction of the nucleoside reverse transcriptase inhibitors in the deoxyribonucleotide triphosphate binding site relative to the normal substrate. *Journal of Medicinal Chemistry*, **2006**, 49, 7675-82	8.3	5
73	Enzyme ribonucleotide reductase: unraveling an enigmatic paradigm of enzyme inhibition by furanone derivatives. *Journal of Physical Chemistry B*, **2006**, 110, 21272-81	3.4	14

72	Atomic-Level Rational Drug Design. *Current Computer-Aided Drug Design*, **2006**, 2, 57-81	1.4	4
71	Molecular dynamics model of unliganded HIV-1 reverse transcriptase. *Medicinal Chemistry*, **2006**, 2, 491-8	1.8	2
70	Computational study of some benzamidine-based inhibitors of thrombin-like snake venom proteinases. *International Journal of Quantum Chemistry*, **2006**, 106, 2107-2121	2.1	5
69	Detailed microscopic study of the full zipA:FtsZ interface. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 811-21	4.2	18
68	Biological evaluation, chelation, and molecular modeling studies of novel metal-chelating inhibitors of NF-kappaB-DNA binding: structure activity relationships. *Journal of Medicinal Chemistry*, **2006**, 49, 3595-601	8.3	17
67	Mechanism of a soluble fumarate reductase from Shewanella frigidimarina: a theoretical study. *Journal of Physical Chemistry B*, **2006**, 110, 10550-6	3.4	4
66	Molecular interactions between human cytochrome P450 1A2 and flavone derivatives. *Medicinal Chemistry*, **2006**, 2, 401-6	1.8	
65	Density-functional study of mechanisms for the cofactor-free decarboxylation performed by uroporphyrinogen III decarboxylase. *Journal of Physical Chemistry B*, **2005**, 109, 18195-200	3.4	13
64	Theoretical study of the suicide inhibition mechanism of the enzyme pyruvate formate lyase by methacrylate. *Journal of the American Chemical Society*, **2005**, 127, 6902-9	16.4	7
63	Theoretical study on the inhibition of ribonucleotide reductase by 2'-mercapto-2'-deoxyribonucleoside-5'-diphosphates. *Journal of the American Chemical Society*, **2005**, 127, 5174-9	16.4	16
62	Discovery of a large number of previously unrecognized mitochondrial pseudogenes in fish genomes. *Genomics*, **2005**, 86, 708-17	4.3	48
61	Farnesyltransferase--new insights into the zinc-coordination sphere paradigm: evidence for a carboxylate-shift mechanism. *Biophysical Journal*, **2005**, 88, 483-94	2.9	55
60	Computer Modeling and Research in the Classroom. *Journal of Chemical Education*, **2005**, 82, 1021	2.4	3
59	Molecular dynamics simulations of angiotensin II in aqueous and dimethyl sulfoxide environments. *Journal of Physical Chemistry B*, **2005**, 109, 17743-51	3.4	17
58	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
57	Density-functional calculations of the Cu, Zn superoxide dismutase redox potential: The influence of active site distortion. *Computational and Theoretical Chemistry*, **2005**, 729, 141-146		11
56	Accuracy of the numerical solution of the Poisson–Boltzmann equation. *Computational and Theoretical Chemistry*, **2005**, 729, 11-18		28
55	Farnesyltransferase: Theoretical studies on peptide substrate entrance—thiol or thiolate coordination?. *Computational and Theoretical Chemistry*, **2005**, 729, 125-129		25

54	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
53	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
52	Inhibitory activity of polyhydroxycarboxylate chelators against recombinant NF-kappaB p50 protein-DNA binding. *Bioorganic Chemistry*, **2005**, 33, 67-81	5.1	10
51	New designs for inhibitors of the NF-B: DNA binding. *Theoretical Chemistry Accounts*, **2005**, 113, 197-204	1.9	1
50	A new strategy to model the Si(100) surface. *Comptes Rendus Chimie*, **2005**, 8, 1461-1468	2.7	8
49	Unraveling the mechanism of the farnesyltransferase enzyme. *Journal of Biological Inorganic Chemistry*, **2005**, 10, 3-10	3.7	37
48	Overview of ribonucleotide reductase inhibitors: an appealing target in anti-tumour therapy. *Current Medicinal Chemistry*, **2005**, 12, 1283-94	4.3	85
47	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
46	Adsorption of protected and unprotected amino-cyclopentene at the Si(100) surface modeled with a hybrid quantum mechanical cluster technique. *Physical Review B*, **2005**, 72,	3.3	6
45	Computational insight into anti-mutagenic properties of CYP1A flavonoid ligands. *Medicinal Chemistry*, **2005**, 1, 355-60	1.8	
44	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
43	Mechanism for ribonucleotide reductase inactivation by the anticancer drug gemcitabine. *Journal of Computational Chemistry*, **2004**, 25, 1286-94	3.5	59
42	Ribonucleotide activation by enzyme ribonucleotide reductase: understanding the role of the enzyme. *Journal of Computational Chemistry*, **2004**, 25, 2031-7	3.5	27
41	Theoretical insights into the mechanism for thiol/disulfide exchange. *Chemistry - A European Journal*, **2004**, 10, 257-66	4.8	218
40	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
39	New insights into a critical biological control step of the mechanism of Ribonucleotide reductase. *Computational and Theoretical Chemistry*, **2004**, 709, 53-65		13
38	Design of 2-cyclopentenone derivatives with enhanced NF-B: DNA binding inhibitory properties. *Computational and Theoretical Chemistry*, **2004**, 685, 73-82		3
37	Evans Blue is an inhibitor of nuclear factor-kappa B (NF-kappaB)-DNA binding. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 6123-7	2.9	13

36	Modeling Chemical and Biological Systems: A Successful Course for Undergraduate Students. *Journal of Chemical Education*, **2004**, 81, 72	2.4	7
35	On the modeling of snake venom serine proteinase interactions with benzamidine-based thrombin inhibitors. *Protein Science*, **2004**, 13, 2355-69	6.3	9
34	Modelling the metabolic action of human and rat CYP1A2 and its relationship with the carcinogenicity of heterocyclic amines. *Molecular Physics*, **2003**, 101, 2731-2741	1.7	3
33	Nuclear factor kappa B: a potential target for anti-HIV chemotherapy. *Current Medicinal Chemistry*, **2003**, 10, 1603-15	4.3	58
32	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
31	New designs for MRI contrast agents. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 463-73	4.2	12
30	Computational studies of new potential antimalarial compounds--stereoelectronic complementarity with the receptor. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 583-95	4.2	7
29	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
28	A theoretical study of radical-only and combined radical/carbocationic mechanisms of arachidonic acid cyclooxygenation by prostaglandin H synthase. *Theoretical Chemistry Accounts*, **2003**, 110, 345-351	1.9	15
27	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
26	Studies of inclusion complexes between cyclodextrins and polyazamacrocyclic chelates of lanthanide (III) ions. *Journal of Chemical Thermodynamics*, **2003**, 35, 1717-1735	2.9	6
25	Parametrization of Synthetic Amino Acids. *Journal of Physical Chemistry B*, **2003**, 107, 14556-14562	3.4	9
24	Pyruvate Formate Lyase: A New Perspective. *Journal of Physical Chemistry B*, **2003**, 107, 5751-5757	3.4	14
23	Receptor-drug association studies in the inhibition of the hematin aggregation process of malaria. *FEBS Letters*, **2003**, 547, 217-22	3.8	32
22	Modelling studies in aqueous solution of lanthanide (III) chelates designed for nuclear magnetic resonance biomedical applications. *Molecular Physics*, **2003**, 101, 2319-2333	1.7	14
21	Theoretical study of the amino acid interactions in the binding region of the trypsin□pancreatic trypsin inhibitor complex. *Computational and Theoretical Chemistry*, **2002**, 580, 251-262		2
20	The reduction of ribonucleotides catalyzed by the enzyme ribonucleotide reductase. *Theoretical Chemistry Accounts*, **2002**, 108, 352-364	1.9	23
19	The search for a new model structure of beta-factor XIIa. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 309-22	4.2	5

18	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
17	Byte structure variable length coding (BS-VLC): a new specific algorithm applied in the compression of trajectories generated by molecular dynamics. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 559-66		1
16	Theoretical study of arginine□carboxylate interactions. *Computational and Theoretical Chemistry*, **1999**, 463, 81-90		35
15	A new partitioning scheme for molecular interacting systems within a multiconfigurational or monoconfigurational Hartree□ock formalism. *International Journal of Quantum Chemistry*, **1999**, 72, 157-176	2.1	6
14	Computational approaches to the study of some lanthanide (III)□olyazamacrocyclic chelates for magnetic resonance imaging. *International Journal of Quantum Chemistry*, **1999**, 73, 237-248	2.1	23
13	Modeling enzyme□nhibitor interactions in serine proteases **1999**, 74, 299-314		16
12	The nature of trypsin-pancreatic trypsin inhibitor binding: free energy calculation of Tyr39-->Phe39 mutation in trypsin. *Chemical Biology and Drug Design*, **1997**, 50, 382-7		6
11	Interactions in the model system □yclodextrin□lycerol. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 2061-2067		10
10	Inclusion of conserved buried water molecules in the model structure of rat submaxillary kallikrein. *Journal of Computer-Aided Molecular Design*, **1997**, 11, 547-56	4.2	6
9	Proton transfer in arginine-carboxylate interactions. *Chemical Physics Letters*, **1995**, 245, 498-502	2.5	13
8	Model structure for the human blood coagulation agent beta-factor XIIa. *Journal of Molecular Graphics*, **1991**, 9, 91-3, 99		3
7	Calculation of hyperfine coupling constants of muonated radicals. *Chemical Physics Letters*, **1990**, 165, 528-534	2.5	8
6	The inclusion of d-type Gaussian functions in the analytic method for the calculation of electrostatic molecular potentials. Interaction of a proton or a positive muon with carbon monoxide. *Journal of the Chemical Society, Faraday Transactions 2*, **1985**, 81, 1761		5
5	Muon spin rotation spectra for muonium isotopically substituted ethyl radicals. *Journal of the Chemical Society Faraday Transactions I*, **1984**, 80, 255		32
4	The barriers to internal rotation for muonic-substituted ethyl radicals. *Journal of the Chemical Society Faraday Transactions I*, **1984**, 80, 267		31
3	An analytic method for the calculation of electrostatic molecular potentials. *Journal of the Chemical Society, Faraday Transactions 2*, **1983**, 79, 1389		10
2	Muonium substituted organic free radicals in liquids. Muonium□lectron hyperfine, coupling constants of alkyl and allyl radicals. *Chemical Physics*, **1982**, 67, 275-285	2.3	90
1	Engineering of PKS Megaenzymes□ Promising Way to Biosynthesize High-Value Active Molecules. *Topics in Catalysis*,1	2.3	1