Pedro Alexandrino Fernandes

List of Publications by Year in Descending Order

302 papers	8,795 citations	44 h-index	80 g-index
339 ext. papers	9,931 ext. citations	4.8 avg, IF	6.4 L-index

#	Paper	IF	Citations
302	Evolution of Acridines and Xanthenes as a Core Structure for the Development of Antileishmanial Agents.. *Pharmaceuticals*, **2022**, 15,	5.2	2
301	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
300	Pharmacological re-assessment of traditional medicinal plants-derived inhibitors as antidotes against snakebite envenoming: A critical review.. *Journal of Ethnopharmacology*, **2022**, 115208	5	1
299	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
298	Towards the Accurate Thermodynamic Characterization of Enzyme Reaction Mechanisms.. *ChemPhysChem*, **2022**, e202200159	3.2	0
297	MOLECULAR BIOINFORMATICS. *Revista De Ciência Elementar*, **2021**, 9,	0.3	2
296	Exploring the permeation of fluoroquinolone metalloantibiotics across outer membrane porins by combining molecular dynamics simulations and a porin-mimetic in vitro model.. *Biochimica Et Biophysica Acta - Biomembranes*, **2021**, 1864, 183838	3.8	1
295	Structure based virtual screening of natural product molecules as glycosidase inhibitors. *In Silico Pharmacology*, **2021**, 9, 56	4.3	1
294	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
293	Passive Diffusion of Ciprofloxacin and its Metalloantibiotic: A Computational and Experimental study. *Journal of Molecular Biology*, **2021**, 433, 166911	6.5	4
292	Chromeno[3,4-]xanthones as First-in-Class AChE and A Aggregation Dual-Inhibitors. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	3
291	Animal Fatty Acid Synthase: A Chemical Nanofactory. *Chemical Reviews*, **2021**, 121, 9502-9553	68.1	6
290	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
289	Alkyl aryl modifications: a comparative study on modular modifications of triphenylphosphonium mitochondrial vectors.. *RSC Chemical Biology*, **2021**, 2, 1643-1650	3	2
288	Unraveling the cGAS catalytic mechanism upon DNA activation through molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2021**, 23, 9524-9531	3.6	0
287	Reaction Mechanism of MHETase, a PET Degrading Enzyme. *ACS Catalysis*, **2021**, 11, 10416-10428	13.1	5
286	Advances in the Therapeutic Application of Small-Molecule Inhibitors and Repurposed Drugs against Snakebite. *Journal of Medicinal Chemistry*, **2021**, 64, 13938-13979	8.3	1

285	Reaction Mechanism of the PET Degrading Enzyme PETase Studied with DFT/MM Molecular Dynamics Simulations. *ACS Catalysis*, **2021**, 11, 11626-11638	13.1	4
284	The Catalytic Mechanism of the Retaining Glycosyltransferase Mannosylglycerate Synthase. *Chemistry - A European Journal*, **2021**, 27, 13998-14006	4.8	2
283	Structural Specificity of Flavonoids in the Inhibition of Human Fructose 1,6-Bisphosphatase. *Journal of Natural Products*, **2020**, 83, 1541-1552	4.9	8
282	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
281	How the Destabilization of a Reaction Intermediate Affects Enzymatic Efficiency: The Case of Human Transketolase. *ACS Catalysis*, **2020**, 10, 2872-2881	13.1	9
280	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
279	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	
278	Catalytic Mechanism of Human Aldehyde Oxidase. *ACS Catalysis*, **2020**, 10, 9276-9286	13.1	8
277	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
276	A Computational and Modeling Study of the Reaction Mechanism of Monoglycosyltransferase Reveals New Insights on the GT51 Family of Enzymes. *Journal of Chemical Information and Modeling*, **2020**, 60, 5513-5528	6.1	0
275	Evolution of chromone-like compounds as potential antileishmanial agents, through the 21 century. *Expert Opinion on Drug Discovery*, **2020**, 15, 1425-1439	6.2	3
274	The bacterial 4S pathway an economical alternative for crude oil desulphurization that reduces CO2 emissions. *Green Chemistry*, **2020**, 22, 7604-7621	10	2
273	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
272	Estrogen receptor-positive (ER) breast cancer treatment: Are multi-target compounds the next promising approach?. *Biochemical Pharmacology*, **2020**, 177, 113989	6	17
271	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
270	Anandamide targets aromatase: A breakthrough on human decidualization. *Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids*, **2019**, 1864, 158512	5	9
269	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
268	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

267	A computational study on the redox properties and binding affinities of iron complexes of hydroxypyridinones. *Journal of Molecular Modeling*, **2019**, 25, 172	2	1
266	New insights about the monomer and homodimer structures of the human AOX1. *Physical Chemistry Chemical Physics*, **2019**, 21, 13545-13554	3.6	4
265	Enabling Mitochondrial Uptake of Lipophilic Dications Using Methylated Triphenylphosphonium Moieties. *Inorganic Chemistry*, **2019**, 58, 8293-8299	5.1	12
264	Conformational diversity induces nanosecond-timescale chemical disorder in the HIV-1 protease reaction pathway. *Chemical Science*, **2019**, 10, 7212-7221	9.4	10
263	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
262	The dipeptidyl peptidase-4 inhibitory effect of flavonoids is hindered in protein rich environments. *Food and Function*, **2019**, 10, 5718-5731	6.1	12
261	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
260	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
259	The Catalytic Mechanism of Human Transketolase. *ChemPhysChem*, **2019**, 20, 2881-2886	3.2	10
258	Glutamine synthetase structure-catalysis relationship: Recent advances and applications. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1399	7.9	2
257	Structural and mechanistic aspects of S-S bonds in the thioredoxin-like family of proteins. *Biological Chemistry*, **2019**, 400, 575-587	4.5	11
256	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
255	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
254	A Buried Water Molecule Influences Reactivity in α-Amylase on a Subnanosecond Time Scale. *ACS Catalysis*, **2018**, 8, 4055-4063	13.1	14
253	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
252	Parametrization of Molybdenum Cofactors for the AMBER Force Field. *Journal of Chemical Theory and Computation*, **2018**, 14, 2538-2548	6.4	5
251	Studies on neuraminidase inhibition. *International Journal of Quantum Chemistry*, **2018**, 118, e25592	2.1	1
250	Visualizing the Microscopic World. *Interdisciplinary Sciences, Computational Life Sciences*, **2018**, 10, 105-110	3.5	2

249	Mechanistic Pathway on Human □Glucosidase Maltase-Glucoamylase Unveiled by QM/MM Calculations. *Journal of Physical Chemistry B*, **2018**, 122, 3889-3899	3.4	18
248	Protocol for Computational Enzymatic Reactivity Based on Geometry Optimisation. *ChemPhysChem*, **2018**, 19, 669-689	3.2	14
247	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
246	Properties that rank protein:protein docking poses with high accuracy. *Physical Chemistry Chemical Physics*, **2018**, 20, 20927-20942	3.6	4
245	Understanding the Rate-Limiting Step of Glycogenolysis by Using QM/MM Calculations on Human Glycogen Phosphorylase. *ChemMedChem*, **2018**, 13, 1608-1616	3.7	4
244	Inhibition of protein tyrosine phosphatase 1B by flavonoids: A structure - activity relationship study. *Food and Chemical Toxicology*, **2018**, 111, 474-481	4.7	32
243	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
242	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
241	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
240	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. *Journal of Membrane Biology*, **2018**, 251, 609-631	2.3	26
239	Mechanistic Studies of a Flavin Monooxygenase: Sulfur Oxidation of Dibenzothiophenes by DszC. *ACS Catalysis*, **2018**, 8, 9298-9311	13.1	10
238	Determining the glycation site specificity of human holo-transferrin. *Journal of Inorganic Biochemistry*, **2018**, 186, 95-102	4.2	3
237	The binding of free and copper-complexed fluoroquinolones to OmpF porins: an experimental and molecular docking study. *RSC Advances*, **2017**, 7, 10009-10019	3.7	11
236	Revisiting Partition in Hydrated Bilayer Systems. *Journal of Chemical Theory and Computation*, **2017**, 13, 2290-2299	6.4	11
235	Clarifying the Catalytic Mechanism of Human Glutamine Synthetase: A QM/MM Study. *Journal of Physical Chemistry B*, **2017**, 121, 6313-6320	3.4	5
234	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
233	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
232	The mechanism of the Ser-(cis)Ser-Lys catalytic triad of peptide amidases. *Physical Chemistry Chemical Physics*, **2017**, 19, 12343-12354	3.6	9

231	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
230	Unique Triphenylphosphonium Derivatives for Enhanced Mitochondrial Uptake and Photodynamic Therapy. *Bioconjugate Chemistry*, **2017**, 28, 590-599	6.3	36
229	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
228	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
227	-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
226	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
225	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
224	Binding free energy calculations on E-selectin complexes with sLe oligosaccharide analogs. *Chemical Biology and Drug Design*, **2017**, 89, 114-123	2.9	6
223	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
222	Molecular motion regulates the activity of the Mitochondrial Serine Protease HtrA2. *Cell Death and Disease*, **2017**, 8, e3119	9.8	11
221	Cancer therapies based on enzymatic amino acid depletion **2017**, 623-651		2
220	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
219	Reaction Mechanism of Mycobacterium Tuberculosis Glutamine Synthetase Using Quantum Mechanics/Molecular Mechanics Calculations. *Chemistry - A European Journal*, **2016**, 22, 9218-25	4.8	17
218	Unveiling the Catalytic Mechanism of NADP+-Dependent Isocitrate Dehydrogenase with QM/MM Calculations. *ACS Catalysis*, **2016**, 6, 357-368	13.1	18
217	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
216	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
215	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
214	A QM/MM study of the reaction mechanism of human -ketoacyl reductase. *Physical Chemistry Chemical Physics*, **2016**, 19, 347-355	3.6	14

213	Glutamine Synthetase Drugability beyond Its Active Site: Exploring Oligomerization Interfaces and Pockets. *Molecules*, **2016**, 21,	4.8	11
212	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
211	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
210	Binding mode of conformations and structure-based pharmacophore development for farnesyltransferase inhibitors. *Medicinal Chemistry Research*, **2016**, 25, 1340-1357	2.2	
209	Insights into the reaction mechanism of 3-O-sulfotransferase through QM/MM calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 11488-96	3.6	10
208	Cholesterol Biosynthesis: A Mechanistic Overview. *Biochemistry*, **2016**, 55, 5483-5506	3.2	116
207	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
206	The Catalytic Mechanism of the Marine-Derived Macrocyclase PatGmac. *Chemistry - A European Journal*, **2016**, 22, 13089-97	4.8	15
205	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
204	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
203	Molecular Dynamics Analysis of FAAH Complexed with Anandamide. *Progress in Theoretical Chemistry and Physics*, **2015**, 115-131	0.6	
202	Receptor-based virtual screening protocol for drug discovery. *Archives of Biochemistry and Biophysics*, **2015**, 582, 56-67	4.1	74
201	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
200	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
199	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. *ACS Catalysis*, **2015**, 5, 5617-5626	10.1	53
198	Relationship between Enzyme/Substrate Properties and Enzyme Efficiency in Hydrolases. *ACS Catalysis*, **2015**, 5, 5877-5887	13.1	20
197	Ligand based analysis on HMG-CoA reductase inhibitors. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 140, 102-116	3.8	15
196	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

195	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
194	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
193	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
192	PLP undergoes conformational changes during the course of an enzymatic reaction. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 596-606		20
191	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
190	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
189	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
188	Enzymatic "tricks" Carboxylate shift and sulfur shift. *International Journal of Quantum Chemistry*, **2014**, 114, 1253-1256	2.1	11
187	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
186	Protein Ligand Docking in Drug Discovery **2014**, 249-286		5
185	Reaction Mechanism of Human Renin Studied by Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations. *ACS Catalysis*, **2014**, 4, 3869-3876	13.1	28
184	Are hot-spots occluded from water?. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 186-97	3.6	8
183	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
182	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
181	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
180	The catalytic mechanism of carboxylesterases: a computational study. *Biochemistry*, **2014**, 53, 5820-9	3.2	37
179	Isomerization of Δ5-androstene-3,17-dione into Δ4-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
178	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

177	Analyses of cobalt-ligand and potassium-ligand bond lengths in metalloproteins: trends and patterns. *Journal of Molecular Modeling*, **2014**, 20, 2271	2	2
176	Glycosidase inhibitors: a patent review (2008-2013). *Expert Opinion on Therapeutic Patents*, **2014**, 24, 857-74	6.8	47
175	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
174	QM/MM Study and MD Simulations on the Hypertension Regulator Angiotensin-Converting Enzyme. *ACS Catalysis*, **2014**, 4, 2587-2597	13.1	20
173	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
172	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
171	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
170	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
169	Influence of the environment on protein bond energies. *Chemical Physics Letters*, **2014**, 615, 75-82	2.5	
168	Classification study of solvation free energies of organic molecules using machine learning techniques. *RSC Advances*, **2014**, 4, 61624-61630	3.7	10
167	Molecular dynamics studies on both bound and unbound renin protease. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 351-63	3.6	10
166	Fused aryl-phenazines: scaffold for the development of bioactive molecules. *Current Drug Targets*, **2014**, 15, 681-8	3	11
165	CompASM: an Amber-VMD alanine scanning mutagenesis plug-in. *Highlights in Theoretical Chemistry*, **2014**, 81-87		1
164	Computational Alanine Scanning Mutagenesis: MM-PBSA vs TI. *Journal of Chemical Theory and Computation*, **2013**, 9, 1311-9	6.4	54
163	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
162	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
161	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
160	Combined ligand and structure based binding mode analysis of oxidosqualene cyclase inhibitors. *RSC Advances*, **2013**, 3, 23409	3.7	5

159	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
158	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
157	Insights into the structural determinants for selective inhibition of nitric oxide synthase isoforms. *Journal of Molecular Modeling*, **2013**, 19, 1537-51	2	12
156	Parameters for Molecular Dynamics Simulations of Manganese-Containing Metalloproteins. *Journal of Chemical Theory and Computation*, **2013**, 9, 2718-32	6.4	30
155	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
154	Mechanism of glutathione transferase P1-1-catalyzed activation of the prodrug canfosfamide (TLK286, TELCYTA). *Biochemistry*, **2013**, 52, 8069-78	3.2	23
153	The sulfur shift: an activation mechanism for periplasmic nitrate reductase and formate dehydrogenase. *Inorganic Chemistry*, **2013**, 52, 10766-72	5.1	42
152	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
151	The catalytic mechanism of protein phosphatase 5 established by DFT calculations. *Chemistry - A European Journal*, **2013**, 19, 14081-9	4.8	42
150	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
149	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
148	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
147	Farnesyltransferase inhibitors: a comprehensive review based on quantitative structural analysis. *Current Medicinal Chemistry*, **2013**, 20, 4888-923	4.3	33
146	Development of ribonucleotide reductase inhibitors: a review on structure activity relationships. *Mini-Reviews in Medicinal Chemistry*, **2013**, 13, 1862-72	3.2	22
145	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
144	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		
143	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
142	Virtual screening and QSAR study of some pyrrolidine derivatives as □mannosidase inhibitors for binding feature analysis. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 6945-59	3.4	7

141	Computational enzymatic catalysis--clarifying enzymatic mechanisms with the help of computers. *Physical Chemistry Chemical Physics*, **2012**, 14, 12431-41	3.6	44
140	The catalytic mechanism of mouse renin studied with QM/MM calculations. *Physical Chemistry Chemical Physics*, **2012**, 14, 12605-13	3.6	20
139	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
138	Multidimensional epistasis and fitness landscapes in enzyme evolution. *Biochemical Journal*, **2012**, 445, 39-46	3.8	25
137	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
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