Pedro Alexandrino Fernandes

List of Publications by Year
in descending order

320 papers	11,144 citations	44069 48 h-index	46799 89 g-index

340 all docs	340 docs citations	340 times ranked	13132 citing authors

#	Article	IF	Citations
1	Engineering of PKS Megaenzymesâ€"A Promising Way to Biosynthesize High-Value Active Molecules. Topics in Catalysis, 2022, 65, 544-562.	2.8	2
2	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, 2022, 1864, 183838.	2.6	2
3	Evolution of Acridines and Xanthenes as a Core Structure for the Development of Antileishmanial Agents. Pharmaceuticals, 2022, 15, 148.	3.8	14
4	Inhibitory activity of flavonoids against human sucrase-isomaltase (Î±-glucosidase) activity in a Caco-2/TC7 cellular model. Food and Function, 2022, 13, 1108-1118.	4.6	9
5	The role of acetylated cyclooxygenase-2 in the biosynthesis of resolvin precursors derived from eicosapentaenoic acid. Organic and Biomolecular Chemistry, 2022, 20, 1260-1274.	2.8	3
6	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.	2.4	12
7	Pharmacological re-assessment of traditional medicinal plants-derived inhibitors as antidotes against snakebite envenoming: A critical review. Journal of Ethnopharmacology, 2022, 292, 115208.	4.1	13
8	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.	2.3	5
9	Towards the Accurate Thermodynamic Characterization of Enzyme Reaction Mechanisms. ChemPhysChem, 2022, 23, e202200159.	2.1	7
10	Transmembrane Protease Serine 2 Proteolytic Cleavage of the SARS-CoV-2 Spike Protein: A Mechanistic Quantum Mechanics/Molecular Mechanics Study to Inspire the Design of New Drugs To Fight the COVID-19 Pandemic. Journal of Chemical Information and Modeling, 2022, 62, 2510-2521.	5.4	8
11	The chemistry of snake venom and its medicinal potential. Nature Reviews Chemistry, 2022, 6, 451-469.	30.2	68
12	Different Enzyme Conformations Induce Different Mechanistic Traits in HIVâ€1 Protease. Chemistry - A European Journal, 2022, 28, .	3.3	4
13	Cover Feature: Different Enzyme Conformations Induce Different Mechanistic Traits in HIVâ€1 Protease (Chem. Eur. J. 42/2022). Chemistry - A European Journal, 2022, 28, .	3.3	0
14	Discovery of a multi-target compound for estrogen receptor-positive (ER+) breast cancer: Involvement of aromatase and ERs. Biochimie, 2021, 181, 65-76.	2.6	16
15	Alkyl vs. aryl modifications: a comparative study on modular modifications of triphenylphosphonium mitochondrial vectors. RSC Chemical Biology, 2021, 2, 1643-1650.	4.1	8
16	Unraveling the cGAS catalytic mechanism upon DNA activation through molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 9524-9531.	2.8	4
17	Structural, enzymatic and pharmacological profiles of AplTX-II - A basic sPLA2 (D49) isolated from the Agkistrodon piscivorus leucostoma snake venom. International Journal of Biological Macromolecules, 2021, 175, 572-585.	7.5	2
18	Thermophilic Enzymes. U Porto Journal of Engineering, 2021, 7, 13-23.	0.4	0

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19	Passive Diffusion of Ciprofloxacin and its Metalloantibiotic: A Computational and Experimental study. Journal of Molecular Biology, 2021, 433, 166911.	4.2	9
20	Chromeno[3,4-b]xanthones as First-in-Class AChE and AÎ² Aggregation Dual-Inhibitors. International Journal of Molecular Sciences, 2021, 22, 4145.	4.1	8
21	Animal Fatty Acid Synthase: A Chemical Nanofactory. Chemical Reviews, 2021, 121, 9502-9553.	47.7	32
22	Reaction Mechanism of MHETase, a PET Degrading Enzyme. ACS Catalysis, 2021, 11, 10416-10428.	11.2	36
23	Advances in the Therapeutic Application of Small-Molecule Inhibitors and Repurposed Drugs against Snakebite. Journal of Medicinal Chemistry, 2021, 64, 13938-13979.	6.4	10
24	Reaction Mechanism of the PET Degrading Enzyme PETase Studied with DFT/MM Molecular Dynamics Simulations. ACS Catalysis, 2021, 11, 11626-11638.	11.2	52
25	The Catalytic Mechanism of the Retaining Glycosyltransferase Mannosylglycerate Synthase. Chemistry - A European Journal, 2021, 27, 13998-14006.	3.3	5
26	The importance of intramolecular hydrogen bonds on the translocation of the small drug piracetam through a lipid bilayer. RSC Advances, 2021, 11, 899-908.	3.6	39
27	Computational Studies on the Mechanism of Farnesyltransferase. , 2021, , 1-7.		0
28	Structure based virtual screening of natural product molecules as glycosidase inhibitors. In Silico Pharmacology, 2021, 9, 56.	3.3	2
29	Modern Strategies for the Diversification of the Supply of Natural Compounds: The Case of Alkaloid Painkillers. ChemBioChem, 2021, , .	2.6	2
30	Catalytic Mechanism of Human Aldehyde Oxidase. ACS Catalysis, 2020, 10, 9276-9286.	11.2	20
31	Reaction Mechanism and Determinants for Efficient Catalysis by DszB, a Key Enzyme for Crude Oil Bio-desulfurization. ACS Catalysis, 2020, 10, 9545-9554.	11.2	44
32	A Computational and Modeling Study of the Reaction Mechanism of Staphylococcus aureus Monoglycosyltransferase Reveals New Insights on the GT51 Family of Enzymes. Journal of Chemical Information and Modeling, 2020, 60, 5513-5528.	5.4	3
33	Evolution of chromone-like compounds as potential antileishmanial agents, through the 21st century. Expert Opinion on Drug Discovery, 2020, 15, 1425-1439.	5.0	8
34	The bacterial 4S pathway â€“ an economical alternative for crude oil desulphurization thatÂreduces CO2 emissions. Green Chemistry, 2020, 22, 7604-7621.	9.0	7
35	Assessing the validity of <scp>DLPNOâ€CCSD</scp>(T) in the calculation of activation and reaction energies of ubiquitous enzymatic reactions. Journal of Computational Chemistry, 2020, 41, 2459-2468.	3.3	16
36	Structural Specificity of Flavonoids in the Inhibition of Human Fructose 1,6-Bisphosphatase. Journal of Natural Products, 2020, 83, 1541-1552.	3.0	14

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37	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.	11.2	22
38	How the Destabilization of a Reaction Intermediate Affects Enzymatic Efficiency: The Case of Human Transketolase. ACS Catalysis, 2020, 10, 2872-2881.	11.2	17
39	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.	2.9	21
40	Estrogen receptor-positive (ER+) breast cancer treatment: Are multi-target compounds the next promising approach?. Biochemical Pharmacology, 2020, 177, 113989.	4.4	35
41	Ribonucleotide-Diphosphate Reductase (RNR). , 2020, , 1-6.		0
42	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.	0.7	0
43	The dipeptidyl peptidase-4 inhibitory effect of flavonoids is hindered in protein rich environments. Food and Function, 2019, 10, 5718-5731.	4.6	19
44	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.	3.7	10
45	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.	11.2	9
46	The Catalytic Mechanism of Human Transketolase. ChemPhysChem, 2019, 20, 2881-2886.	2.1	12
47	Anandamide targets aromatase: A breakthrough on human decidualization. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2019, 1864, 158512.	2.4	13
48	Exploring the Identity of the General Base for a DNA Polymerase Catalyzed Reaction Using QM/MM: The Case Study of Human Translesion Synthesis Polymerase Î·. ACS Catalysis, 2019, 9, 2543-2551.	11.2	17
49	Benchmark of Density Functionals for the Calculation of the Redox Potential of Fe3+/Fe2+ Within Protein Coordination Shells. Frontiers in Chemistry, 2019, 7, 391.	3.6	14
50	A computational study on the redox properties and binding affinities of iron complexes of hydroxypyridinones. Journal of Molecular Modeling, 2019, 25, 172.	1.8	4
51	New insights about the monomer and homodimer structures of the human AOX1. Physical Chemistry Chemical Physics, 2019, 21, 13545-13554.	2.8	6
52	Enabling Mitochondrial Uptake of Lipophilic Dications Using Methylated Triphenylphosphonium Moieties. Inorganic Chemistry, 2019, 58, 8293-8299.	4.0	14
53	Conformational diversity induces nanosecond-timescale chemical disorder in the HIV-1 protease reaction pathway. Chemical Science, 2019, 10, 7212-7221.	7.4	20
54	Evaluation of a flavonoids library for inhibition of pancreatic Î±-amylase towards a structureâ€“activity relationship. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 577-588.	5.2	100

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55	Drug Permeation Across the Bacterial Membrane: Combining Theoretical and Experimental Approaches. Biophysical Journal, 2019, 116, 206a.	0.5	0
56	Glutamine synthetase structureâ€¢catalysis relationshipâ€"Recent advances and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1399.	14.6	4
57	Structural and mechanistic aspects of S-S bonds in the thioredoxin-like family of proteins. Biological Chemistry, 2019, 400, 575-587.	2.5	22
58	A novel synthetic peptide inspired on Lys49 phospholipase A 2 from Crotalus oreganus abyssus snake venom active against multidrug-resistant clinical isolates. European Journal of Medicinal Chemistry, 2018, 149, 248-256.	5.5	31
59	A QM/MM approach on the structural and stereoelectronic factors governing glycosylation by GTF-SI fromStreptococcus mutans. Organic and Biomolecular Chemistry, 2018, 16, 2438-2447.	2.8	14
60	A Buried Water Molecule Influences Reactivity in Î±-Amylase on a Subnanosecond Time Scale. ACS Catalysis, 2018, 8, 4055-4063.	11.2	21
61	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.	11.2	24
62	Parametrization of Molybdenum Cofactors for the AMBER Force Field. Journal of Chemical Theory and Computation, 2018, 14, 2538-2548.	5.3	8
63	Studies on neuraminidase inhibition. International Journal of Quantum Chemistry, 2018, 118, e25592.	2.0	1
64	Visualizing the Microscopic World. Interdisciplinary Sciences, Computational Life Sciences, 2018, 10, 105-110.	3.6	2
65	Mechanistic Pathway on Human Î±-Glucosidase Maltase-Glucoamylase Unveiled by QM/MM Calculations. Journal of Physical Chemistry B, 2018, 122, 3889-3899.	2.6	24
66	Protocol for Computational Enzymatic Reactivity Based on Geometry Optimisation. ChemPhysChem, 2018, 19, 669-689.	2.1	18
67	Inhibition of protein tyrosine phosphatase 1B by flavonoids: A structure - activity relationship study. Food and Chemical Toxicology, 2018, 111, 474-481.	3.6	44
68	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.	2.6	17
69	Mechanistic Insights on Human Phosphoglucomutase Revealed by Transition Path Sampling and Molecular Dynamics Calculations. Chemistry - A European Journal, 2018, 24, 1978-1987.	3.3	11
70	Structure, Dynamics, and Energetics of ATP Hydrolysis by ABC Transporters. ACS Central Science, 2018, 4, 1300-1302.	11.3	1
71	QM/MM Study of the Reaction Mechanism of the Dehydratase Domain from Mammalian Fatty Acid Synthase. ACS Catalysis, 2018, 8, 10267-10278.	11.2	34
72	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. Journal of Membrane Biology, 2018, 251, 609-631.	2.1	33

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73	Mechanistic Studies of a Flavin Monooxygenase: Sulfur Oxidation of Dibenzothiophenes by DszC. ACS Catalysis, 2018, 8, 9298-9311.	11.2	17
74	Determining the glycation site specificity of human holo-transferrin. Journal of Inorganic Biochemistry, 2018, 186, 95-102.	3.5	4
75	Membrane partition of bis-(3-hydroxy-4-pyridinonato) zinc(ii) complexes revealed by molecular dynamics simulations. RSC Advances, 2018, 8, 27081-27090.	3.6	4
76	Properties that rank protein:protein docking poses with high accuracy. Physical Chemistry Chemical Physics, 2018, 20, 20927-20942.	2.8	7
77	Understanding the Rateâ€Limiting Step of Glycogenolysis by Using QM/MM Calculations on Human Glycogen Phosphorylase. ChemMedChem, 2018, 13, 1608-1616.	3.2	5
78	The binding of free and copper-complexed fluoroquinolones to OmpF porins: an experimental and molecular docking study. RSC Advances, 2017, 7, 10009-10019.	3.6	14
79	Revisiting Partition in Hydrated Bilayer Systems. Journal of Chemical Theory and Computation, 2017, 13, 2290-2299.	5.3	13
80	Clarifying the Catalytic Mechanism of Human Glutamine Synthetase: A QM/MM Study. Journal of Physical Chemistry B, 2017, 121, 6313-6320.	2.6	9
81	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.	7.1	49
82	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.	2.0	37
83	The mechanism of the Ser-(cis)Ser-Lys catalytic triad of peptide amidases. Physical Chemistry Chemical Physics, 2017, 19, 12343-12354.	2.8	17
84	Diffusion of the small, very polar, drug piracetam through a lipid bilayer: an MD simulation study. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	20
85	Unique Triphenylphosphonium Derivatives for Enhanced Mitochondrial Uptake and Photodynamic Therapy. Bioconjugate Chemistry, 2017, 28, 590-599.	3.6	46
86	New Parameters for Higher Accuracy in the Computation of Binding Free Energy Differences upon Alanine Scanning Mutagenesis on Proteinâ€“Protein Interfaces. Journal of Chemical Information and Modeling, 2017, 57, 60-72.	5.4	47
87	Improving the Catalytic Power of the DszD Enzyme for the Biodesulfurization of Crude Oil and Derivatives. Chemistry - A European Journal, 2017, 23, 17231-17241.	3.3	19
88	Î±-Glucosidase inhibition by flavonoids: an in vitro and in silico structureâ€“activity relationship study. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 1216-1228.	5.2	274
89	Influence of Frozen Residues on the Exploration of the PES of Enzyme Reaction Mechanisms. Journal of Chemical Theory and Computation, 2017, 13, 5486-5495.	5.3	28
90	A QM/MM study of the reaction mechanism of human Î²-ketoacyl reductase. Physical Chemistry Chemical Physics, 2017, 19, 347-355.	2.8	17

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91	Amino acid deprivation using enzymes as a targeted therapy for cancer and viral infections. Expert Opinion on Therapeutic Patents, 2017, 27, 283-297.	5.0	63
92	Binding free energy calculations on Eâ€selectin complexes with <scp>sL</scp>e^x oligosaccharide analogs. Chemical Biology and Drug Design, 2017, 89, 114-123.	3.2	8
93	Application of quantum mechanics/molecular mechanics methods in the study of enzymatic reaction mechanisms. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1281.	14.6	137
94	Molecular motion regulates the activity of the Mitochondrial Serine Protease HtrA2. Cell Death and Disease, 2017, 8, e3119-e3119.	6.3	21
95	Cancer therapies based on enzymatic amino acid depletion. , 2017, , 623-651.		2
96	Glutamine Synthetase Drugability beyond Its Active Site: Exploring Oligomerization Interfaces and Pockets. Molecules, 2016, 21, 1028.	3.8	12
97	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.	4.1	21
98	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, 5300-5306.	2.5	24
99	Binding mode of conformations and structure-based pharmacophore development for farnesyltransferase inhibitors. Medicinal Chemistry Research, 2016, 25, 1340-1357.	2.4	0
100	Insights into the reaction mechanism of 3-O-sulfotransferase through QM/MM calculations. Physical Chemistry Chemical Physics, 2016, 18, 11488-11496.	2.8	11
101	Cholesterol Biosynthesis: A Mechanistic Overview. Biochemistry, 2016, 55, 5483-5506.	2.5	203
102	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.	2.9	5
103	The Catalytic Mechanism of the Marineâ€Derived Macrocyclase PatGmac. Chemistry - A European Journal, 2016, 22, 13089-13097.	3.3	16
104	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.	5.0	19
105	Reaction Mechanism of Mycobacterium Tuberculosis Glutamine Synthetase Using Quantum Mechanics/Molecular Mechanics Calculations. Chemistry - A European Journal, 2016, 22, 9218-9225.	3.3	19
106	Unveiling the Catalytic Mechanism of NADP⁺-Dependent Isocitrate Dehydrogenase with QM/MM Calculations. ACS Catalysis, 2016, 6, 357-368.	11.2	23
107	Molecular dynamic simulations and structure-based pharmacophore development for farnesyltransferase inhibitors discovery. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 1428-1442.	5.2	6
108	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.	0.8	7

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109	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.	3.6	5
110	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, 1072-1086.	3.2	8
111	Insight into Enzymatic Nitrile Reduction: QM/MM Study of the Catalytic Mechanism of QueF Nitrile Reductase. ACS Catalysis, 2015, 5, 3740-3751.	11.2	28
112	Insights into the structural determinants of substrate specificity and activity in mouse aldehyde oxidases. Journal of Biological Inorganic Chemistry, 2015, 20, 209-217.	2.6	19
113	Establishing the Catalytic Mechanism of Human Pancreatic Î±-Amylase with QM/MM Methods. Journal of Chemical Theory and Computation, 2015, 11, 2508-2516.	5.3	32
114	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, 107-115.	3.0	24
115	Molecular Dynamics Analysis of FAAH Complexed with Anandamide. Progress in Theoretical Chemistry and Physics, 2015, , 115-131.	0.2	0
116	Receptor-based virtual screening protocol for drug discovery. Archives of Biochemistry and Biophysics, 2015, 582, 56-67.	3.0	98
117	Synthesis and Hydrolytic Studies on the Air-Stable [(4-CN-PhO)(E)P(Î¼-N^tBu)]₂ (E = O, S, and Se) Cyclodiphosphazanes. Inorganic Chemistry, 2015, 54, 6423-6432.	4.0	25
118	Periplasmic Nitrate Reductase and Formate Dehydrogenase: Similar Molecular Architectures with Very Different Enzymatic Activities. Accounts of Chemical Research, 2015, 48, 2875-2884.	15.6	28
119	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. ACS Catalysis, 2015, 5, 5617-5626.	11.2	72
120	Relationship between Enzyme/Substrate Properties and Enzyme Efficiency in Hydrolases. ACS Catalysis, 2015, 5, 5877-5887.	11.2	31
121	Ligand based analysis on HMG-CoA reductase inhibitors. Chemometrics and Intelligent Laboratory Systems, 2015, 140, 102-116.	3.5	15
122	A new scoring function for proteinâ€“protein docking that identifies native structures with unprecedented accuracy. Physical Chemistry Chemical Physics, 2015, 17, 2378-2387.	2.8	14
123	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, 14590-14601.	2.6	11
124	Influence of the environment on protein bond energies. Chemical Physics Letters, 2014, 615, 75-82.	2.6	0
125	Classification study of solvation free energies of organic molecules using machine learning techniques. RSC Advances, 2014, 4, 61624-61630.	3.6	12
126	Molecular dynamics studies on both bound and unbound renin protease. Journal of Biomolecular Structure and Dynamics, 2014, 32, 351-363.	3.5	12

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127	PLP undergoes conformational changes during the course of an enzymatic reaction. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 596-606.	2.5	25
128	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.	1.8	11
129	<scp>chemâ€pathâ€tracker</scp>: An Automated Tool to Analyze Chemical Motifs in Molecular Structures. Chemical Biology and Drug Design, 2014, 84, 44-53.	3.2	1
130	Catalytic Mechanism of Retroviral Integrase for the Strand Transfer Reaction Explored by QM/MM Calculations. Journal of Chemical Theory and Computation, 2014, 10, 5458-5466.	5.3	6
131	Enzymatic â€œtricksâ€: Carboxylate shift and sulfur shift. International Journal of Quantum Chemistry, 2014, 114, 1253-1256.	2.0	12
132	Discovery of New Sites for Drug Binding to the Hypertensionâ€Related Reninâ€“Angiotensinogen Complex. Chemical Biology and Drug Design, 2014, 83, 427-439.	3.2	4
133	Protein Ligand DockingDocking in Drug DiscoveryDrug Discovery. , 2014, , 249-286.		11
134	Reaction Mechanism of Human Renin Studied by Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations. ACS Catalysis, 2014, 4, 3869-3876.	11.2	32
135	Are hot-spots occluded from water?. Journal of Biomolecular Structure and Dynamics, 2014, 32, 186-197.	3.5	11
136	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, 21768-21777.	2.8	3
137	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.	3.6	7
138	Prediction of Solvation Free Energies with Thermodynamic Integration Using the General Amber Force Field. Journal of Chemical Theory and Computation, 2014, 10, 3570-3577.	5.3	31
139	The Catalytic Mechanism of Carboxylesterases: A Computational Study. Biochemistry, 2014, 53, 5820-5829.	2.5	53
140	Isomerization of Î”⁵-Androstene-3,17-dione into Î”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, 5790-5800.	2.5	14
141	Benchmarking of Density Functionals for the Accurate Description of Thiolâ€“Disulfide Exchange. Journal of Chemical Theory and Computation, 2014, 10, 4842-4856.	5.3	33
142	Analyses of cobaltâ€“ligand and potassiumâ€“ligand bond lengths in metalloproteins: trends and patterns. Journal of Molecular Modeling, 2014, 20, 2271.	1.8	4
143	Glycosidase inhibitors: a patent review (2008 â€“ 2013). Expert Opinion on Therapeutic Patents, 2014, 24, 857-874.	5.0	52
144	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.	3.7	17

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145	QM/MM Study and MD Simulations on the Hypertension Regulator Angiotensin-Converting Enzyme. ACS Catalysis, 2014, 4, 2587-2597.	11.2	23
146	Divalent metal ion-based catalytic mechanism of the Nudix hydrolase Orf153 (YmfB) fromEscherichia coli. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1297-1310.	2.5	5
147	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.	3.5	10
148	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, 317-324.	5.2	10
149	CompASM: an Amber-VMD alanine scanning mutagenesis plug-in. Highlights in Theoretical Chemistry, 2014, , 81-87.	0.0	1
150	Fused Aryl-Phenazines: Scaffold for the Development of Bioactive Molecules. Current Drug Targets, 2014, 15, 681-688.	2.1	16
151	Computational Alanine Scanning Mutagenesis: MM-PBSA vs TI. Journal of Chemical Theory and Computation, 2013, 9, 1311-1319.	5.3	67
152	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, 2079-2090.	3.3	38
153	Are Hot-Spots Occluded from Water?. Biophysical Journal, 2013, 104, 505a.	0.5	0
154	Theoretical studies on the binding of rhenium(I) complexes to inducible nitric oxide synthase. Journal of Molecular Graphics and Modelling, 2013, 45, 13-25.	2.4	13
155	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.	2.6	7
156	Combined ligand and structure based binding mode analysis of oxidosqualene cyclase inhibitors. RSC Advances, 2013, 3, 23409.	3.6	5
157	Molecular dynamics analysis of a series of 22 potential farnesyltransferase substrates containing a CaaX-motif. Journal of Molecular Modeling, 2013, 19, 673-688.	1.8	11
158	Unraveling the Enigmatic Mechanism of <scp>l</scp>-Asparaginase II with QM/QM Calculations. Journal of the American Chemical Society, 2013, 135, 7146-7158.	13.7	57
159	Insights into the structural determinants for selective inhibition of nitric oxide synthase isoforms. Journal of Molecular Modeling, 2013, 19, 1537-1551.	1.8	14
160	Parameters for Molecular Dynamics Simulations of Manganese-Containing Metalloproteins. Journal of Chemical Theory and Computation, 2013, 9, 2718-2732.	5.3	33
161	Understanding the importance of the aromatic amino-acid residues as hot-spots. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 404-414.	2.3	34
162	Mechanism of Glutathione Transferase P1-1-Catalyzed Activation of the Prodrug Canfosfamide (TLK286,) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	29

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