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	General Performance of Density Functionals. Journal of Physical Chemistry A, 2007, 111, 10439-10452.	2.5	907
2	Protein-ligand docking: Current status and future challenges. Proteins: Structure, Function and Bioinformatics, 2006, 65, 15-26.	2.6	761
3	Hot spots-A review of the protein-protein interface determinant amino-acid residues. Proteins: Structure, Function and Bioinformatics, 2007, 68, 803-812.	2.6	639
4	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
5	Theoretical Insights into the Mechanism for Thiol/Disulfide Exchange. Chemistry - A European Journal, 2004, 10, 257-266.	3.3	257
6	Computational alanine scanning mutagenesisâ€”An improved methodological approach. Journal of Computational Chemistry, 2007, 28, 644-654.	3.3	230
7	Cholesterol Biosynthesis: A Mechanistic Overview. Biochemistry, 2016, 55, 5483-5506.	2.5	203
8	Protein-Ligand Docking in the New Millennium â€“ A Retrospective of 10 Years in the Field. Current Medicinal Chemistry, 2013, 20, 2296-2314.	2.4	197
9	Computational Enzymatic Catalysis. Accounts of Chemical Research, 2008, 41, 689-698.	15.6	152
10	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
11	The Carboxylate Shift in Zinc Enzymes: A Computational Study. Journal of the American Chemical Society, 2007, 129, 1378-1385.	13.7	133
12	Understanding Ribonucleotide Reductase Inactivation by Gemcitabine. Chemistry - A European Journal, 2007, 13, 8507-8515.	3.3	125
13	Farnesyltransferase Inhibitors: A Detailed Chemical View on an Elusive Biological Problem. Current Medicinal Chemistry, 2008, 15, 1478-1492.	2.4	107
14	Similarities and differences in the thioredoxin superfamily. Progress in Biophysics and Molecular Biology, 2006, 91, 229-248.	2.9	106
15	Overview of Ribonucleotide Reductase Inhibitors: An Appealing Target in Anti-Tumour Therapy. Current Medicinal Chemistry, 2005, 12, 1283-1294.	2.4	101
16	Proteinâ€“protein docking dealing with the unknown. Journal of Computational Chemistry, 2010, 31, 317-342.	3.3	100
17	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
18	Receptor-based virtual screening protocol for drug discovery. Archives of Biochemistry and Biophysics, 2015, 582, 56-67.	3.0	98

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19	Mechanism of Formation of the Internal Aldimine in Pyridoxal 5â€²-Phosphate-Dependent Enzymes. Journal of the American Chemical Society, 2011, 133, 15496-15505.	13.7	91
20	Vascular Endothelial Growth Factor (VEGF) Inhibition - A Critical Review. Anti-Cancer Agents in Medicinal Chemistry, 2007, 7, 223-245.	1.7	90
21	QM/MM Studies on the Î²-Galactosidase Catalytic Mechanism: Hydrolysis and Transglycosylation Reactions. Journal of Chemical Theory and Computation, 2010, 6, 421-433.	5.3	88
22	Gemcitabine: A Critical Nucleoside for Cancer Therapy. Current Medicinal Chemistry, 2012, 19, 1076-1087.	2.4	83
23	Ribonucleotide Reductase: A Critical Enzyme for Cancer Chemotherapy and Antiviral Agents. Recent Patents on Anti-Cancer Drug Discovery, 2007, 2, 11-29.	1.6	81
24	Molecular Dynamics Simulation of the Water/2-Heptanone Liquid-Liquid Interface. Journal of Physical Chemistry B, 1999, 103, 6290-6299.	2.6	74
25	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. ACS Catalysis, 2015, 5, 5617-5626.	11.2	72
26	Analysis of zincâ€ligand bond lengths in metalloproteins: Trends and patterns. Proteins: Structure, Function and Bioinformatics, 2007, 69, 466-475.	2.6	71
27	The Zinc proteome: a tale of stability and functionality. Dalton Transactions, 2009, , 7946.	3.3	71
28	Virtual Screening in Drug Design and Development. Combinatorial Chemistry and High Throughput Screening, 2010, 13, 442-453.	1.1	71
29	Mammalian Cytosolic Glutathione Transferases. Current Protein and Peptide Science, 2008, 9, 325-337.	1.4	70
30	Mechanism for ribonucleotide reductase inactivation by the anticancer drug gemcitabine. Journal of Computational Chemistry, 2004, 25, 1286-1294.	3.3	69
31	Benchmarking of DFT Functionals for the Hydrolysis of Phosphodiester Bonds. Journal of Chemical Theory and Computation, 2010, 6, 2281-2292.	5.3	69
32	The chemistry of snake venom and its medicinal potential. Nature Reviews Chemistry, 2022, 6, 451-469.	30.2	68
33	Computational Alanine Scanning Mutagenesis: MM-PBSA vs TI. Journal of Chemical Theory and Computation, 2013, 9, 1311-1319.	5.3	67
34	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
35	Farnesyltransferaseâ€"New Insights into the Zinc-Coordination Sphere Paradigm: Evidence for a Carboxylate-Shift Mechanism. Biophysical Journal, 2005, 88, 483-494.	0.5	61
36	Unraveling the Importance of Proteinâ^'Protein Interaction:Â 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, 10962-10969.	2.6	60

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37	Glutathione Transferase: New Model for Glutathione Activation. Chemistry - A European Journal, 2008, 14, 9591-9598.	3.3	59
38	The Current Status of the NNRTI Family of Antiretrovirals Used Against HIV Infection. Current Medicinal Chemistry, 2008, 15, 1083-1095.	2.4	58
39	Studies on Î±-Glucosidase Inhibitors Development: Magic Molecules for the Treatment of Carbohydrate Mediated Diseases. Mini-Reviews in Medicinal Chemistry, 2012, 12, 713-720.	2.4	58
40	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
41	Theoretical Studies on the Mechanism of Inhibition of Ribonucleotide Reductase by (E)-2â€˜-Fluoromethylene-2â€˜-deoxycitidine-5â€˜-diphosphate. Journal of the American Chemical Society, 2003, 125, 6311-6322.	13.7	56
42	The Sulfur Shift: An Activation Mechanism for Periplasmic Nitrate Reductase and Formate Dehydrogenase. Inorganic Chemistry, 2013, 52, 10766-10772.	4.0	54
43	The Catalytic Mechanism of Carboxylesterases: A Computational Study. Biochemistry, 2014, 53, 5820-5829.	2.5	53
44	Glycosidase inhibitors: a patent review (2008 â€“ 2013). Expert Opinion on Therapeutic Patents, 2014, 24, 857-874.	5.0	52
45	Reaction Mechanism of the PET Degrading Enzyme PETase Studied with DFT/MM Molecular Dynamics Simulations. ACS Catalysis, 2021, 11, 11626-11638.	11.2	52
46	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, 2752-2763.	3.3	51
47	Inhibition of Pancreatic Elastase by Polyphenolic Compounds. Journal of Agricultural and Food Chemistry, 2010, 58, 10668-10676.	5.2	51
48	The Catalytic Mechanism of HIV-1 Integrase for DNA 3â€²-End Processing Established by QM/MM Calculations. Journal of the American Chemical Society, 2012, 134, 13436-13447.	13.7	51
49	Molecular Dynamics Study of the Transfer of Iodide across Two Liquid/Liquid Interfaces. Journal of Physical Chemistry B, 1999, 103, 8930-8939.	2.6	50
50	Aryl- and Heteroaryl-Thiosemicarbazone Derivatives and Their Metal Complexes: A Pharmacological Template. Recent Patents on Anti-Cancer Drug Discovery, 2013, 8, 168-182.	1.6	50
51	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
52	Dehydration of Ribonucleotides Catalyzed by Ribonucleotide Reductase: The Role of the Enzyme. Biophysical Journal, 2006, 90, 2109-2119.	0.5	48
53	Computational enzymatic catalysis â€“ clarifying enzymatic mechanisms with the help of computers. Physical Chemistry Chemical Physics, 2012, 14, 12431.	2.8	48
54	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

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55	Computational Mechanistic Studies Addressed to the Transimination Reaction Present in All Pyridoxal 5â€²-Phosphate-Requiring Enzymes. Journal of Chemical Theory and Computation, 2011, 7, 1356-1368.	5.3	46
56	Unique Triphenylphosphonium Derivatives for Enhanced Mitochondrial Uptake and Photodynamic Therapy. Bioconjugate Chemistry, 2017, 28, 590-599.	3.6	46
57	Accuracy of Density Functionals in the Prediction of Electronic Proton Affinities of Amino Acid Side Chains. Journal of Chemical Theory and Computation, 2011, 7, 3898-3908.	5.3	45
58	The Catalytic Mechanism of Protein Phosphataseâ€…5 Established by DFT Calculations. Chemistry - A European Journal, 2013, 19, 14081-14089.	3.3	44
59	Inhibition of protein tyrosine phosphatase 1B by flavonoids: A structure - activity relationship study. Food and Chemical Toxicology, 2018, 111, 474-481.	3.6	44
60	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
61	Farnesyltransferase Inhibitors: A Comprehensive Review Based on Quantitative Structural Analysis. Current Medicinal Chemistry, 2013, 20, 4888-4923.	2.4	44
62	The Catalytic Mechanism of RNA Polymerase II. Journal of Chemical Theory and Computation, 2011, 7, 1177-1188.	5.3	40
63	Unraveling the mechanism of the farnesyltransferase enzyme. Journal of Biological Inorganic Chemistry, 2005, 10, 3-10.	2.6	39
64	Theoretical studies on farnesyltransferase: The distances paradox explained. Proteins: Structure, Function and Bioinformatics, 2006, 66, 205-218.	2.6	39
65	Theoretical studies on farnesyl transferase: Evidence for thioether product coordination to the active-site zinc sphere. Journal of Computational Chemistry, 2007, 28, 1160-1168.	3.3	39
66	Understanding the Binding of Procyanidins to Pancreatic Elastase by Experimental and Computational Methods. Biochemistry, 2010, 49, 5097-5108.	2.5	39
67	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
68	Influence of Ion Size and Charge in Ion Transfer Processes Across a Liquid|Liquid Interface. Journal of Physical Chemistry B, 2000, 104, 2278-2286.	2.6	38
69	The Accuracy of Density Functional Theory in the Description of Cationâ‹¯Ï€ and Ï€â€“Hydrogen Bond Interactions. Journal of Chemical Theory and Computation, 2011, 7, 2059-2067.	5.3	38
70	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
71	Mechanistic studies on the formation of glycosidaseâ€“substrate and glycosidaseâ€“inhibitor covalent intermediates. Journal of Computational Chemistry, 2008, 29, 2565-2574.	3.3	37
72	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

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73	Reaction Mechanism of MHETase, a PET Degrading Enzyme. ACS Catalysis, 2021, 11, 10416-10428.	11.2	36
74	Unravelling Hot Spots: a comprehensive computational mutagenesis study. Theoretical Chemistry Accounts, 2006, 117, 99-113.	1.4	35
75	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, 2511-2523.	2.6	35
76	Estrogen receptor-positive (ER+) breast cancer treatment: Are multi-target compounds the next promising approach?. Biochemical Pharmacology, 2020, 177, 113989.	4.4	35
77	Determination of the Î”pKa between the active site cysteines of thioredoxin and DsbA. Journal of Computational Chemistry, 2006, 27, 966-975.	3.3	34
78	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
79	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
80	Parameters for Molecular Dynamics Simulations of Manganese-Containing Metalloproteins. Journal of Chemical Theory and Computation, 2013, 9, 2718-2732.	5.3	33
81	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
82	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. Journal of Membrane Biology, 2018, 251, 609-631.	2.1	33
83	Ribonucleotide activation by enzyme ribonucleotide reductase: Understanding the role of the enzyme. Journal of Computational Chemistry, 2004, 25, 2031-2037.	3.3	32
84	Comparative Assessment of Theoretical Methods for the Determination of Geometrical Properties in Biological Zinc Complexes. Journal of Physical Chemistry B, 2007, 111, 9146-9152.	2.6	32
85	The Search for the Mechanism of the Reaction Catalyzed by Farnesyltransferase. Chemistry - A European Journal, 2009, 15, 4243-4247.	3.3	32
86	Reaction Mechanism of Human Renin Studied by Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations. ACS Catalysis, 2014, 4, 3869-3876.	11.2	32
87	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
88	Animal Fatty Acid Synthase: A Chemical Nanofactory. Chemical Reviews, 2021, 121, 9502-9553.	47.7	32
89	Hot Spot Occlusion from Bulk Water:Â a Comprehensive Study of the Complex between the Lysozyme HEL and the Antibody FVD1.3. Journal of Physical Chemistry B, 2007, 111, 2697-2706.	2.6	31
90	MADAMM: A multistaged docking with an automated molecular modeling protocol. Proteins: Structure, Function and Bioinformatics, 2009, 74, 192-206.	2.6	31

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91	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
92	Relationship between Enzyme/Substrate Properties and Enzyme Efficiency in Hydrolases. ACS Catalysis, 2015, 5, 5877-5887.	11.2	31
93	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
94	Aryl- and Heteroaryl-Thiosemicarbazone Derivatives and Their Metal Complexes: A Pharmacological Template. Recent Patents on Anti-Cancer Drug Discovery, 2013, 8, 168-182.	1.6	30
95	Accuracy of the numerical solution of the Poissonâ€“Boltzmann equation. Computational and Theoretical Chemistry, 2005, 729, 11-18.	1.5	29
96	Molecular determinants of ligand specificity in family 11 carbohydrate binding modules â€“ an NMR, Xâ€ray crystallography and computational chemistry approach. FEBS Journal, 2008, 275, 2524-2535.	4.7	29
97	Multidimensional epistasis and fitness landscapes in enzyme evolution. Biochemical Journal, 2012, 445, 39-46.	3.7	29
98	QSAR analysis of 2-benzoxazolyl hydrazone derivatives for anticancer activity and its possible target prediction. Medicinal Chemistry Research, 2012, 21, 133-144.	2.4	29
99	Mechanism of Glutathione Transferase P1-1-Catalyzed Activation of the Prodrug Canfosfamide (TLK286,) Tj ETQq1 1 0.784314 rgBT /Ov	2.5	29
100	Molecular Dynamics Simulations of the Enzyme Cu, Zn Superoxide Dismutase. Journal of Physical Chemistry B, 2006, 110, 16754-16762.	2.6	28
101	Molecular dynamics simulations on the critical states of the farnesyltransferase enzyme. Bioorganic and Medicinal Chemistry, 2009, 17, 3369-3378.	3.0	28
102	Chemical Behavior of Methylpyranomalvidin-3-O-glucoside in Aqueous Solution Studied by NMR and UVâ^'Visible Spectroscopy. Journal of Physical Chemistry B, 2011, 115, 1538-1545.	2.6	28
103	Structural analysis of Î±-glucosidase inhibitors by validated QSAR models using topological and hydrophobicity based descriptors. Chemometrics and Intelligent Laboratory Systems, 2011, 109, 101-112.	3.5	28
104	vsLabâ€"An implementation for virtual highâ€throughput screening using AutoDock and VMD. International Journal of Quantum Chemistry, 2011, 111, 1208-1212.	2.0	28
105	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
106	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
107	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
108	Farnesyltransferase: Theoretical studies on peptide substrate entranceâ€"thiol or thiolate coordination?. Computational and Theoretical Chemistry, 2005, 729, 125-129.	1.5	27

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109	Theoretical Study of the Unusual Protonation Properties of the Active Site Cysteines in Thioredoxin. Journal of Physical Chemistry B, 2006, 110, 5758-5761.	2.6	27
110	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.	1.4	26
111	Comparative evolutionary genomics of the HADH2 gene encoding AÎ²-binding alcohol dehydrogenase/17Î²-hydroxysteroid dehydrogenase type 10 (ABAD/HSD10). BMC Genomics, 2006, 7, 202.	2.8	26
112	Volarea â€“ A Bioinformatics Tool to Calculate the Surface Area and the Volume of Molecular Systems. Chemical Biology and Drug Design, 2013, 82, 743-755.	3.2	26
113	Development of Ribonucleotide Reductase Inhibitors: A Review on Structure Activity Relationships. Mini-Reviews in Medicinal Chemistry, 2013, 13, 1862-1872.	2.4	26
114	Theoretical Studies on the Mode of Inhibition of Ribonucleotide Reductase by 2â€²-Substituted Substrate Analogues. Chemistry - A European Journal, 2003, 9, 5916-5925.	3.3	25
115	PLP undergoes conformational changes during the course of an enzymatic reaction. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 596-606.	2.5	25
116	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
117	The reduction of ribonucleotides catalyzed by the enzyme ribonucleotide reductase. Theoretical Chemistry Accounts, 2002, 108, 352-364.	1.4	24
118	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
119	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
120	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
121	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
122	QM/MM Study and MD Simulations on the Hypertension Regulator Angiotensin-Converting Enzyme. ACS Catalysis, 2014, 4, 2587-2597.	11.2	23
123	Unveiling the Catalytic Mechanism of NADP⁺-Dependent Isocitrate Dehydrogenase with QM/MM Calculations. ACS Catalysis, 2016, 6, 357-368.	11.2	23
124	Theoretical study of ribonucleotide reductase mechanism-based inhibition by 2?-azido-2?-deoxyribonucleoside 5?-diphosphates. Journal of Computational Chemistry, 2004, 25, 227-237.	3.3	22
125	DFT studies on the Î²-glycosidase catalytic mechanism: The deglycosylation step. Computational and Theoretical Chemistry, 2010, 946, 125-133.	1.5	22
126	Structural and mechanistic aspects of S-S bonds in the thioredoxin-like family of proteins. Biological Chemistry, 2019, 400, 575-587.	2.5	22

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127	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
128	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.	2.0	21
129	Proteinâ€“protein recognition: a computational mutagenesis study of the MDM2â€“P53 complex. Theoretical Chemistry Accounts, 2008, 120, 533-542.	1.4	21
130	The catalytic mechanism of mouse renin studied with QM/MM calculations. Physical Chemistry Chemical Physics, 2012, 14, 12605.	2.8	21
131	Human Ether-a-Go-Go-Related Gene Channel Blockers and its Structural Analysis for Drug Design. Current Drug Targets, 2013, 14, 102-113.	2.1	21
132	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
133	Molecular motion regulates the activity of the Mitochondrial Serine Protease HtrA2. Cell Death and Disease, 2017, 8, e3119-e3119.	6.3	21
134	A Buried Water Molecule Influences Reactivity in Î±-Amylase on a Subnanosecond Time Scale. ACS Catalysis, 2018, 8, 4055-4063.	11.2	21
135	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
136	Carbohydrateâ€binding modules from family 11: Understanding the binding mode of polysaccharides. International Journal of Quantum Chemistry, 2008, 108, 2030-2040.	2.0	20
137	Ribonucleotide Reductase: A Mechanistic Portrait of Substrate Analogues Inhibitors. Current Medicinal Chemistry, 2010, 17, 2854-2872.	2.4	20
138	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, 521-536.	2.2	20
139	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
140	Conformational diversity induces nanosecond-timescale chemical disorder in the HIV-1 protease reaction pathway. Chemical Science, 2019, 10, 7212-7221.	7.4	20
141	Catalytic Mechanism of Human Aldehyde Oxidase. ACS Catalysis, 2020, 10, 9276-9286.	11.2	20
142	Molecular Simulation of the Interface between Two Immiscible Electrolyte Solutions. Journal of Physical Chemistry B, 2001, 105, 981-993.	2.6	19
143	Detailed microscopic study of the full zipA:FtsZ interface. Proteins: Structure, Function and Bioinformatics, 2006, 63, 811-821.	2.6	19
144	Enzyme Flexibility and the Catalytic Mechanism of Farnesyltransferase: Targeting the Relation. Journal of Physical Chemistry B, 2008, 112, 8681-8691.	2.6	19

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145	Substrate Recognition in HIV-1 Protease: A Computational Study. Journal of Physical Chemistry B, 2010, 114, 2525-2532.	2.6	19
146	Glutathione Transferase A1-1: Catalytic Importance of Arginine 15. Journal of Physical Chemistry B, 2010, 114, 1690-1697.	2.6	19
147	Structural feature study of benzofuran derivatives as farnesyltransferase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2011, 26, 777-791.	5.2	19
148	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
149	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
150	Reaction Mechanism of Mycobacterium Tuberculosis Glutamine Synthetase Using Quantum Mechanics/Molecular Mechanics Calculations. Chemistry - A European Journal, 2016, 22, 9218-9225.	3.3	19
151	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
152	The dipeptidyl peptidase-4 inhibitory effect of flavonoids is hindered in protein rich environments. Food and Function, 2019, 10, 5718-5731.	4.6	19
153	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.	1.4	18
154	Theoretical Study on the Inhibition of Ribonucleotide Reductase by 2â€˜-Mercapto-2â€˜-deoxyribonucleoside-5â€˜-diphosphates. Journal of the American Chemical Society, 2005, 127, 5174-5179.	13.7	18
155	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, 125-135.	2.2	18
156	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, 14231-14236.	2.5	18
157	hERG binding feature analysis of structurally diverse compounds by QSAR and fragmental analysis. RSC Advances, 2011, 1, 1126.	3.6	18
158	Detailed Atomistic Analysis of the HIV-1 Protease Interface. Journal of Physical Chemistry B, 2011, 115, 7045-7057.	2.6	18
159	Protocol for Computational Enzymatic Reactivity Based on Geometry Optimisation. ChemPhysChem, 2018, 19, 669-689.	2.1	18
160	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
161	The mechanism of the Ser-(cis)Ser-Lys catalytic triad of peptide amidases. Physical Chemistry Chemical Physics, 2017, 19, 12343-12354.	2.8	17
162	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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163	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
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