Sergio F Sousa

List of Publications by Year
in descending order

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131	4,467	159585	114465
papers	citations	30 h-index	63 g-index

135	135	135	5513
all docs	docs citations	times ranked	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	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
4	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
5	The Carboxylate Shift in Zinc Enzymes: A Computational Study. Journal of the American Chemical Society, 2007, 129, 1378-1385.	13.7	133
6	Farnesyltransferase Inhibitors: A Detailed Chemical View on an Elusive Biological Problem. Current Medicinal Chemistry, 2008, 15, 1478-1492.	2.4	107
7	Receptor-based virtual screening protocol for drug discovery. Archives of Biochemistry and Biophysics, 2015, 582, 56-67.	3.0	98
8	Comparing AutoDock and Vina in Ligand/Decoy Discrimination for Virtual Screening. Applied Sciences (Switzerland), 2019, 9, 4538.	2.5	78
9	Analysis of zincâ€ligand bond lengths in metalloproteins: Trends and patterns. Proteins: Structure, Function and Bioinformatics, 2007, 69, 466-475.	2.6	71
10	The Zinc proteome: a tale of stability and functionality. Dalton Transactions, 2009, , 7946.	3.3	71
11	Virtual Screening in Drug Design and Development. Combinatorial Chemistry and High Throughput Screening, 2010, 13, 442-453.	1.1	71
12	Computational Alanine Scanning Mutagenesis: MM-PBSA vs TI. Journal of Chemical Theory and Computation, 2013, 9, 1311-1319.	5.3	67
13	PLP-dependent enzymes as important biocatalysts for the pharmaceutical, chemical and food industries: a structural and mechanistic perspective. Catalysis Science and Technology, 2019, 9, 4864-4876.	4.1	62
14	Farnesyltransferaseâ€”New Insights into the Zinc-Coordination Sphere Paradigm: Evidence for a Carboxylate-Shift Mechanism. Biophysical Journal, 2005, 88, 483-494.	0.5	61
15	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
16	Computational enzymatic catalysis â€“ clarifying enzymatic mechanisms with the help of computers. Physical Chemistry Chemical Physics, 2012, 14, 12431.	2.8	48
17	Perspectives on the Role of Enzymatic Biocatalysis for the Degradation of Plastic PET. International Journal of Molecular Sciences, 2021, 22, 11257.	4.1	46
18	VMD Storeâ€“A VMD Plugin to Browse, Discover, and Install VMD Extensions. Journal of Chemical Information and Modeling, 2019, 59, 4519-4523.	5.4	44

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19	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
20	Farnesyltransferase Inhibitors: A Comprehensive Review Based on Quantitative Structural Analysis. Current Medicinal Chemistry, 2013, 20, 4888-4923.	2.4	44
21	Study of human salivary proline-rich proteins interaction with food tannins. Food Chemistry, 2018, 243, 175-185.	8.2	43
22	Modelling Enzymatic Mechanisms with QM/MM Approaches: Current Status and Future Challenges. Israel Journal of Chemistry, 2020, 60, 655-666.	2.3	40
23	Unraveling the mechanism of the farnesyltransferase enzyme. Journal of Biological Inorganic Chemistry, 2005, 10, 3-10.	2.6	39
24	Theoretical studies on farnesyltransferase: The distances paradox explained. Proteins: Structure, Function and Bioinformatics, 2006, 66, 205-218.	2.6	39
25	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
26	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
27	Chemically Modified Tetracyclines as Inhibitors of MMP-2 Matrix Metalloproteinase: A Molecular and Structural Study. Journal of Physical Chemistry B, 2012, 116, 13644-13654.	2.6	35
28	Parameters for Molecular Dynamics Simulations of Manganese-Containing Metalloproteins. Journal of Chemical Theory and Computation, 2013, 9, 2718-2732.	5.3	33
29	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
30	The Search for the Mechanism of the Reaction Catalyzed by Farnesyltransferase. Chemistry - A European Journal, 2009, 15, 4243-4247.	3.3	32
31	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
32	Relationship between Enzyme/Substrate Properties and Enzyme Efficiency in Hydrolases. ACS Catalysis, 2015, 5, 5877-5887.	11.2	31
33	Direct Covalent Modification as a Strategy to Inhibit Nuclear Factor-Kappa B. Current Medicinal Chemistry, 2009, 16, 4261-4273.	2.4	28
34	Molecular dynamics simulations on the critical states of the farnesyltransferase enzyme. Bioorganic and Medicinal Chemistry, 2009, 17, 3369-3378.	3.0	28
35	A Molecular Perspective on Sirtuin Activity. International Journal of Molecular Sciences, 2020, 21, 8609.	4.1	28
36	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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37	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
38	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
39	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
40	Structural and mechanistic aspects of S-S bonds in the thioredoxin-like family of proteins. Biological Chemistry, 2019, 400, 575-587.	2.5	22
41	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
42	An Atomic-Level Perspective of HMG-CoA-Reductase: The Target Enzyme to Treat Hypercholesterolemia. Molecules, 2020, 25, 3891.	3.8	21
43	Identification of New Potential Inhibitors of Quorum Sensing through a Specialized Multi-Level Computational Approach. Molecules, 2021, 26, 2600.	3.8	21
44	New carvacrol and thymol derivatives as potential insecticides: synthesis, biological activity, computational studies and nanoencapsulation. RSC Advances, 2021, 11, 34024-34035.	3.6	20
45	Enzyme Flexibility and the Catalytic Mechanism of Farnesyltransferase: Targeting the Relation. Journal of Physical Chemistry B, 2008, 112, 8681-8691.	2.6	19
46	Structural feature study of benzofuran derivatives as farnesyltransferase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2011, 26, 777-791.	5.2	19
47	Comparative assessment of computational methods for the determination of solvation free energies in alcoholâ€based molecules. Journal of Computational Chemistry, 2013, 34, 1354-1362.	3.3	19
48	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
49	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
50	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
51	Detailed Atomistic Analysis of the HIV-1 Protease Interface. Journal of Physical Chemistry B, 2011, 115, 7045-7057.	2.6	18
52	Mechanistic Studies of a Flavin Monooxygenase: Sulfur Oxidation of Dibenzothiophenes by DszC. ACS Catalysis, 2018, 8, 9298-9311.	11.2	17
53	New insights into the catalytic mechanism of the SARS-CoV-2 main protease: an ONIOM QM/MM approach. Molecular Diversity, 2022, 26, 1373-1381.	3.9	17
54	In Silicoâ€“Based Structural Analysis of Arylthiophene Derivatives for FTase Inhibitory Activity, hERG, and Other Toxic Effects. Journal of Biomolecular Screening, 2011, 16, 1037-1046.	2.6	16

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55	The Biofilms Structural Database. Trends in Biotechnology, 2020, 38, 937-940.	9.3	16
56	Analyzing PEGylation through Molecular Dynamics Simulations. ChemistrySelect, 2018, 3, 8415-8427.	1.5	14
57	Formation of Unstable and very Reactive Chemical Species Catalyzed by Metalloenzymes: A Mechanistic Overview. Molecules, 2019, 24, 2462.	3.8	14
58	The complete catalytic mechanism of xanthine oxidase: a computational study. Inorganic Chemistry Frontiers, 2021, 8, 405-416.	6.0	14
59	Drug Repurposing Targeting Pseudomonas aeruginosa MvfR Using Docking, Virtual Screening, Molecular Dynamics, and Free-Energy Calculations. Antibiotics, 2022, 11, 185.	3.7	14
60	Virtual Screening of Compound Libraries. Methods in Molecular Biology, 2010, 572, 57-70.	0.9	13
61	Antimicrobial Susceptibility of Persister Biofilm Cells of Bacillus cereus and Pseudomonas fluorescens. Microorganisms, 2022, 10, 160.	3.6	13
62	New designs for MRI contrast agents. Journal of Computer-Aided Molecular Design, 2003, 17, 463-473.	2.9	12
63	Molecular Dynamics Simulations: Difficulties, Solutions and Strategies for Treating Metalloenzymes. Challenges and Advances in Computational Chemistry and Physics, 2010, , 299-330.	0.6	12
64	Classification study of solvation free energies of organic molecules using machine learning techniques. RSC Advances, 2014, 4, 61624-61630.	3.6	12
65	Enzymatic â€œtricksâ€: Carboxylate shift and sulfur shift. International Journal of Quantum Chemistry, 2014, 114, 1253-1256.	2.0	12
66	In Silico, In Vitro and In Cellulo Models for Monitoring SARS-CoV-2 Spike/Human ACE2 Complex, Viral Entry and Cell Fusion. Viruses, 2021, 13, 365.	3.3	12
67	Developing and Using BioSIM^{AR}, an Augmented Reality Program to Visualize and Learn about Chemical Structures in a Virtual Environment on Any Internet-Connected Device. Journal of Chemical Education, 2021, 98, 1789-1794.	2.3	12
68	Amino Alcohols from Eugenol as Potential Semisynthetic Insecticides: Chemical, Biological, and Computational Insights. Molecules, 2021, 26, 6616.	3.8	12
69	Identification of novel candidates for inhibition ofLasR, a quorum-sensing receptor of multidrug resistantPseudomonas aeruginosa, through a specialized multi-levelin silicoapproach. Molecular Systems Design and Engineering, 2022, 7, 434-446.	3.4	12
70	Crown-Ether Type Podands as Alkali Metal Cation Extractants: Influence of the Number of Oxygens inÂtheÂChain. Journal of Solution Chemistry, 2010, 39, 1230-1242.	1.2	11
71	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
72	Protein Ligand DockingDocking in Drug DiscoveryDrug Discovery. , 2014, , 249-286.		11

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73	Molecular dynamics analysis of farnesyltransferase: A closer look into the amino acid behavior. International Journal of Quantum Chemistry, 2008, 108, 1939-1950.	2.0	10
74	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
75	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
76	Current Status of the Use of Multifunctional Enzymes as Anti-Cancer Drug Targets. Pharmaceutics, 2022, 14, 10.	4.5	10
77	A comparative molecular dynamics study on the complexation of alkali metal cations by a poly-ethylene-glycol type podand in water and in dichloromethane. Computational and Theoretical Chemistry, 2010, 946, 77-82.	1.5	9
78	Transfer of the K⁺ Cation Across a Water/Dichloromethane Interface: A Steered Molecular Dynamics Study with Implications in Cation Extraction. Journal of Physical Chemistry B, 2012, 116, 1843-1849.	2.6	9
79	Solving the Catalytic Mechanism of Tryptophan Synthase: an Emergent Drug Target in the Treatment of Tuberculosis. ChemCatChem, 2020, 12, 227-237.	3.7	9
80	Selection of Bis-Indolyl Pyridines and Triphenylamines as New Inhibitors of SARS-CoV-2 Cellular Entry by Modulating the Spike Protein/ACE2 Interfaces. Antimicrobial Agents and Chemotherapy, 2022, 66, .	3.2	9
81	Computational Studies Devoted to the Catalytic Mechanism of Threonine Aldolase, a Critical Enzyme in the Pharmaceutical Industry to Synthesize Î²-Hydroxy-Î±-amino Acids. ACS Catalysis, 2022, 12, 4990-4999.	11.2	8
82	Study of the anticancer potential of Cd complexes of selenazoyl-hydrazones and their sulfur isosters. European Journal of Medicinal Chemistry, 2022, 238, 114449.	5.5	8
83	Detection of Farnesyltransferase Interface Hot Spots through Computational Alanine Scanning Mutagenesis. Journal of Physical Chemistry B, 2011, 115, 15339-15354.	2.6	7
84	Complexation of alkali metal cations by crown-ether type podands with applications in solvent extraction: insights from quantum chemical calculations. Journal of Molecular Modeling, 2011, 17, 3275-3288.	1.8	7
85	Combined in silico and in vitro studies to identify novel antidiabetic flavonoids targeting glycogen phosphorylase. Bioorganic Chemistry, 2021, 108, 104552.	4.1	7
86	An Unsual Cysâ€Gluâ€Lys Catalytic Triad is Responsible for the Catalytic Mechanism of the Nitrilase Superfamily: A QM/MM Study on Nit2. ChemPhysChem, 2021, 22, 796-804.	2.1	7
87	The milk-derived lactoferrin inhibits V-ATPase activity by targeting its V1 domain. International Journal of Biological Macromolecules, 2021, 186, 54-70.	7.5	7
88	Multifunctional Enzymes as Targets for the Treatment of Tuberculosis: Paving the Way for New Anti-TB Drugs. Current Medicinal Chemistry, 2021, 28, 5847-5882.	2.4	7
89	LegionellaDB â€“ A Database on Legionella Outbreaks. Trends in Microbiology, 2021, 29, 863-866.	7.7	7
90	Development of Neuropeptide Y and Cell-Penetrating Peptide MAP Adsorbed onto Lipid Nanoparticle Surface. Molecules, 2022, 27, 2734.	3.8	7

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91	Zn(<scp>ii</scp>) complexes with thiazolylâ€“hydrazones: structure, intermolecular interactions, photophysical properties, computational study and anticancer activity. CrystEngComm, 2022, 24, 5194-5214.	2.6	7
92	Structural and dynamics analysis of matrix metalloproteinases MMP-2 complexed with chemically modified tetracyclines (CMTs). Journal of Biomolecular Structure and Dynamics, 2014, 32, 1907-1918.	3.5	6
93	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
94	Compensatory epistasis explored by molecular dynamics simulations. Human Genetics, 2021, 140, 1329-1342.	3.8	6
95	Tailoring Specialized Scoring Functions For More Efficient Virtual Screening. Frontiers in Drug Chemistry and Clinical Research, 2019, 2, .	0.6	6
96	In Silico Identification of Possible Inhibitors for Protein Kinase B (PknB) of Mycobacterium tuberculosis. Molecules, 2021, 26, 6162.	3.8	6
97	Factors influencing the binding of a potassium cation to a polyethylene glycol type podand in liquidâ€“liquid extractionâ€”a molecular dynamics study. Theoretical Chemistry Accounts, 2010, 127, 681-687.	1.4	5
98	Decomplexation and complexation of alkali metal cations by a crown-ether-type podand in dichloromethane: a steered molecular dynamics study. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
99	A Flow Cytometric and Computational Approaches to Carbapenems Affinity to the Different Types of Carbapenemases. Frontiers in Microbiology, 2016, 7, 1259.	3.5	5
100	Identification of tripeptides against tyrosine kinase domain of EGFR for lung cancer cell inhibition by in silico and in vitro studies. Chemical Biology and Drug Design, 2022, 99, 456-469.	3.2	5
101	AÎ²_{31â€“35} Decreases Neprilysin-Mediated Alzheimerâ€™s Amyloid-Î² Peptide Degradation. ACS Chemical Neuroscience, 2021, 12, 3708-3718.	3.5	4
102	Identification of novel aptamers targeting cathepsin B-overexpressing prostate cancer cells. Molecular Systems Design and Engineering, 2022, 7, 637-650.	3.4	4
103	The critical role of Asp206 stabilizing residues on the catalytic mechanism of the Ideonella sakaiensis PETase. Catalysis Science and Technology, 2022, 12, 3474-3483.	4.1	4
104	Transport Properties of Light Gases in Nanochannels of Lâ€“Leuâ€“Lâ€“Ser Dipeptide Crystals: A Comparative Study by Molecular Dynamics Simulations. ChemistrySelect, 2018, 3, 5517-5525.	1.5	3
105	The catalytic mechanism of Pdx2 glutamine driven by a Cysâ€“Hisâ€“Glu triad: a computational study. ChemBioChem, 2021, , .	2.6	3
106	In silico Based Structural Analysis of Some Piperidine Analogs as Farnesyltransferase Inhibitors. Medicinal Chemistry, 2012, 8, 853-864.	1.5	2
107	Selection of a new peptide homing SKâ€“BRâ€“3 breast cancer cells. Chemical Biology and Drug Design, 2021, 97, 893-903.	3.2	2
108	Databases for the study of biofilms: current status and potential applications. Biofouling, 2021, 37, 96-108.	2.2	2

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109	Assessing the effects of PMM2 variants on protein stability. Molecular Genetics and Metabolism, 2021, 134, 344-352.	1.1	2
110	Dehydration of a polyether type extraction agent and of the corresponding K+ complex: insights into liquid-liquid extraction mechanisms by quantum chemical methods. Journal of Molecular Modeling, 2012, 18, 4909-4915.	1.8	1
111	Structural Characterization of Membrane Protein Dimers. Methods in Molecular Biology, 2019, 1958, 403-436.	0.9	1
112	Editorial: The Chemistry of Biofilms and Their Inhibitors. Frontiers in Chemistry, 2020, 8, 746.	3.6	1
113	In silico development of quorum sensing inhibitors. , 2020, , 329-357.		1
114	Creation of a Structural Database for Inhibition of Biofilm Formation. , 0, , .		1
115	Transformation of a Chiral Glycolic Acid to an Isoaurone: Stereochemical Assignment of a Benzilic Acid Rearrangment Product. Asian Journal of Organic Chemistry, 0, , .	2.7	1
116	Targeting Pseudomonas aeruginosa MvfR in the battle against biofilm formation: a multi-level computational approach. Molecular Systems Design and Engineering, 2022, 7, 1294-1306.	3.4	1
117	Molecular Dynamics Analysis of FAAH Complexed with Anandamide. Progress in Theoretical Chemistry and Physics, 2015, , 115-131.	0.2	0
118	Binding mode of conformations and structure-based pharmacophore development for farnesyltransferase inhibitors. Medicinal Chemistry Research, 2016, 25, 1340-1357.	2.4	0
119	Frontispiece: Improving the Catalytic Power of the DszD Enzyme for the Biodesulfurization of Crude Oil and Derivatives. Chemistry - A European Journal, 2017, 23, .	3.3	0
120	Evaluation of Scoring Functions for Large Scale Application of Virtual Screening in the Identification of Novel Beta-Lactamase Inhibitors. , 2019, , .		0
121	Molecular dynamic simulations and QM/MM studies addressed to build an active Tryptophan Synthase model. A critical enzyme to treat tuberculosis. , 2019, , .		0
122	A QM/MM Evaluation of the Missing Step in the Reduction Mechanism of HMG-CoA by Human HMG-CoA Reductase. Processes, 2021, 9, 1085.	2.8	0
123	Special Issue on â€œThe Application of Quantum Mechanics in Reactivity of Moleculesâ€. Applied Sciences (Switzerland), 2021, 11, 1132.	2.5	0
124	Computational proteomics: from methodological developments to biological applications. , 2011, , 181-220.		0
125	DNA (QuÃmica BiolÃ³gica). Revista De CiÃªncia Elementar, 2013, 1, .	0.0	0
126	Combined experimental and computational studies devoted to the synthesis of 1,4-lactones. , 0, , .		0

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127	Is the 5,10-methylenetetrahydrofolate cofactor synthesized through a non-enzymatic or enzymatic mechanism?. , 0, , .		0
128	Unraveling the catalytic mechanism of Tryptophan synthase, a drug target against Mycobacterium tuberculosis. , 0, , .		0
129	In Silico Identification of Protein Targets Associated to the Insecticide Activity of Eugenol Derivatives. Chemistry Proceedings, 2020, 3, .	0.1	0
130	Development and Validation of a Multi-Level Computational Protocol for Drug Repurposing in the Treatment of Bacterial Infections. , 2021, 8, .		0
131	Synthesis and In Silico Evaluation of Potential Insecticide Activity of Benzamides. , 0, , .		0