

Sergio F Sousa

List of Publications by Year in Descending Order

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Version: 2024-04-11

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

107 papers	3,352 citations	26 h-index	56 g-index
135 ext. papers	3,936 ext. citations	4.5 avg, IF	5.55 L-index

#	Paper	IF	Citations
107	Drug Repurposing Targeting MvfR Using Docking, Virtual Screening, Molecular Dynamics, and Free-Energy Calculations.. <i>Antibiotics</i> , 2022 , 11,	4.9	1
106	Study of the anticancer potential of Cd complexes of selenazoyl-hydrazones and their sulfur isosters.. <i>European Journal of Medicinal Chemistry</i> , 2022 , 238, 114449	6.8	0
105	In Silico Identification of Protein Targets Associated to the Insecticide Activity of Eugenol Derivatives. <i>Chemistry Proceedings</i> , 2021 , 3, 138		
104	Assessing the effects of PMM2 variants on protein stability. <i>Molecular Genetics and Metabolism</i> , 2021 , 134, 344-344	3.7	0
103	New carvacrol and thymol derivatives as potential insecticides: synthesis, biological activity, computational studies and nanoencapsulation.. <i>RSC Advances</i> , 2021 , 11, 34024-34035	3.7	3
102	Perspectives on the Role of Enzymatic Biocatalysis for the Degradation of Plastic PET. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	4
101	In Silico Identification of Possible Inhibitors for Protein Kinase B (PknB) of. <i>Molecules</i> , 2021 , 26,	4.8	1
100	Amino Alcohols from Eugenol as Potential Semisynthetic Insecticides: Chemical, Biological, and Computational Insights. <i>Molecules</i> , 2021 , 26,	4.8	3
99	An Unusual Cys-Glu-Lys Catalytic Triad is Responsible for the Catalytic Mechanism of the Nitrilase Superfamily: A QM/MM Study on Nit2. <i>ChemPhysChem</i> , 2021 , 22, 796-804	3.2	0
98	Developing and Using BioSIMAR, an Augmented Reality Program to Visualize and Learn about Chemical Structures in a Virtual Environment on Any Internet-Connected Device. <i>Journal of Chemical Education</i> , 2021 , 98, 1789-1794	2.4	3
97	Identification of New Potential Inhibitors of Quorum Sensing through a Specialized Multi-Level Computational Approach. <i>Molecules</i> , 2021 , 26,	4.8	9
96	Compensatory epistasis explored by molecular dynamics simulations. <i>Human Genetics</i> , 2021 , 140, 1329-1342	13.42	1
95	New insights into the catalytic mechanism of the SARS-CoV-2 main protease: an ONIOM QM/MM approach. <i>Molecular Diversity</i> , 2021 , 1	3.1	4
94	A QM/MM Evaluation of the Missing Step in the Reduction Mechanism of HMG-CoA by Human HMG-CoA Reductase. <i>Processes</i> , 2021 , 9, 1085	2.9	
93	The complete catalytic mechanism of xanthine oxidase: a computational study. <i>Inorganic Chemistry Frontiers</i> , 2021 , 8, 405-416	6.8	4
92	Combined in silico and in vitro studies to identify novel antidiabetic flavonoids targeting glycogen phosphorylase. <i>Bioorganic Chemistry</i> , 2021 , 108, 104552	5.1	4
91	Selection of a new peptide homing SK-BR-3 breast cancer cells. <i>Chemical Biology and Drug Design</i> , 2021 , 97, 893-903	2.9	

90	, and Models for Monitoring SARS-CoV-2 Spike/Human ACE2 Complex, Viral Entry and Cell Fusion. <i>Viruses</i> , 2021 , 13,	6.2	5
89	AlDecreases Neprilysin-Mediated Alzheimer's Amyloid- β Peptide Degradation. <i>ACS Chemical Neuroscience</i> , 2021 , 12, 3708-3718	5.7	0
88	The milk-derived lactoferrin inhibits V-ATPase activity by targeting its V1 domain. <i>International Journal of Biological Macromolecules</i> , 2021 , 186, 54-70	7.9	2
87	LegionellaDB - A Database on Legionella Outbreaks. <i>Trends in Microbiology</i> , 2021 , 29, 863-866	12.4	3
86	Databases for the study of biofilms: current status and potential applications. <i>Biofouling</i> , 2021 , 37, 96-108	9.3	0
85	Current Status of the Use of Multifunctional Enzymes as Anti-Cancer Drug Targets.. <i>Pharmaceutics</i> , 2021 , 14,	6.4	2
84	The Biofilms Structural Database. <i>Trends in Biotechnology</i> , 2020 , 38, 937-940	15.1	3
83	In silico development of quorum sensing inhibitors 2020 , 329-357		
82	Activation Free Energy, Substrate Binding Free Energy, and Enzyme Efficiency Fall in a Very Narrow Range of Values for Most Enzymes. <i>ACS Catalysis</i> , 2020 , 10, 8444-8453	13.1	5
81	Modelling Enzymatic Mechanisms with QM/MM Approaches: Current Status and Future Challenges. <i>Israel Journal of Chemistry</i> , 2020 , 60, 655-666	3.4	19
80	A Molecular Perspective on Sirtuin Activity. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	10
79	Reaction Mechanism and Determinants for Efficient Catalysis by DszB, a Key Enzyme for Crude Oil Bio-desulfurization. <i>ACS Catalysis</i> , 2020 , 10, 9545-9554	13.1	17
78	An Atomic-Level Perspective of HMG-CoA-Reductase: The Target Enzyme to Treat Hypercholesterolemia. <i>Molecules</i> , 2020 , 25,	4.8	9
77	Solving the Catalytic Mechanism of Tryptophan Synthase: an Emergent Drug Target in the Treatment of Tuberculosis. <i>ChemCatChem</i> , 2020 , 12, 227-237	5.2	4
76	Structural Characterization of Membrane Protein Dimers. <i>Methods in Molecular Biology</i> , 2019 , 1958, 403-436	14.6	0
75	PLP-dependent enzymes as important biocatalysts for the pharmaceutical, chemical and food industries: a structural and mechanistic perspective. <i>Catalysis Science and Technology</i> , 2019 , 9, 4864-4876	5.5	32
74	Human Fatty Acid Synthase: A Computational Study of the Transfer of the Acyl Moieties from MAT to the ACP Domain. <i>ChemCatChem</i> , 2019 , 11, 3853-3864	5.2	7
73	Formation of Unstable and very Reactive Chemical Species Catalyzed by Metalloenzymes: A Mechanistic Overview. <i>Molecules</i> , 2019 , 24,	4.8	11

72	VMD Store-A VMD Plugin to Browse, Discover, and Install VMD Extensions. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4519-4523	6.1	10
71	Comparing AutoDock and Vina in Ligand/Decoy Discrimination for Virtual Screening. <i>Applied Sciences (Switzerland)</i> , 2019 , 9, 4538	2.6	36
70	Tailoring Specialized Scoring Functions For More Efficient Virtual Screening 2019 , 2,		4
69	Enzymatic Amino Acid Deprivation Therapies Targeting Cancer 2019 , 311-347		
68	Structural and mechanistic aspects of S-S bonds in the thioredoxin-like family of proteins. <i>Biological Chemistry</i> , 2019 , 400, 575-587	4.5	11
67	Understanding the Catalytic Machinery and the Reaction Pathway of the Malonyl-Acetyl Transferase Domain of Human Fatty Acid Synthase. <i>ACS Catalysis</i> , 2018 , 8, 4860-4872	13.1	20
66	Study of human salivary proline-rich proteins interaction with food tannins. <i>Food Chemistry</i> , 2018 , 243, 175-185	8.5	30
65	Analyzing PEGylation through Molecular Dynamics Simulations. <i>ChemistrySelect</i> , 2018 , 3, 8415-8427	1.8	11
64	Mechanistic Studies of a Flavin Monooxygenase: Sulfur Oxidation of Dibenzothiophenes by DszC. <i>ACS Catalysis</i> , 2018 , 8, 9298-9311	13.1	10
63	Transport Properties of Light Gases in Nanochannels of LLeu-L-Ser Dipeptide Crystals: A Comparative Study by Molecular Dynamics Simulations. <i>ChemistrySelect</i> , 2018 , 3, 5517-5525	1.8	1
62	Improving the Catalytic Power of the DszD Enzyme for the Biodesulfurization of Crude Oil and Derivatives. <i>Chemistry - A European Journal</i> , 2017 , 23, 17231-17241	4.8	15
61	Application of quantum mechanics/molecular mechanics methods in the study of enzymatic reaction mechanisms. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017 , 7, e1281	7.9	104
60	HMG-CoA Reductase inhibitors: an updated review of patents of novel compounds and formulations (2011-2015). <i>Expert Opinion on Therapeutic Patents</i> , 2016 , 26, 1257-1272	6.8	16
59	Molecular dynamic simulations and structure-based pharmacophore development for farnesyltransferase inhibitors discovery. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016 , 31, 1428-42	5.6	5
58	A Flow Cytometric and Computational Approaches to Carbapenems Affinity to the Different Types of Carbapenemases. <i>Frontiers in Microbiology</i> , 2016 , 7, 1259	5.7	3
57	Improving the Biodesulfurization of Crude Oil and Derivatives: A QM/MM Investigation of the Catalytic Mechanism of NADH-FMN Oxidoreductase (DszD). <i>Journal of Physical Chemistry A</i> , 2016 , 120, 5300-6	2.8	22
56	Binding mode of conformations and structure-based pharmacophore development for farnesyltransferase inhibitors. <i>Medicinal Chemistry Research</i> , 2016 , 25, 1340-1357	2.2	
55	Molecular Dynamics Analysis of FAAH Complexed with Anandamide. <i>Progress in Theoretical Chemistry and Physics</i> , 2015 , 115-131	0.6	

54	Receptor-based virtual screening protocol for drug discovery. <i>Archives of Biochemistry and Biophysics</i> , 2015 , 582, 56-67	4.1	74
53	Relationship between Enzyme/Substrate Properties and Enzyme Efficiency in Hydrolases. <i>ACS Catalysis</i> , 2015 , 5, 5877-5887	13.1	20
52	Enzymatic Bricks—Carboxylate shift and sulfur shift. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 1253-1256	2.1	11
51	Protein Ligand Docking in Drug Discovery 2014 , 249-286		5
50	Prediction of Solvation Free Energies with Thermodynamic Integration Using the General Amber Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3570-7	6.4	25
49	Structural and dynamics analysis of matrix metalloproteinases MMP-2 complexed with chemically modified tetracyclines (CMTs). <i>Journal of Biomolecular Structure and Dynamics</i> , 2014 , 32, 1907-18	3.6	5
48	Biomembrane simulations of 12 lipid types using the general amber force field in a tensionless ensemble. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014 , 32, 88-103	3.6	7
47	Classification study of solvation free energies of organic molecules using machine learning techniques. <i>RSC Advances</i> , 2014 , 4, 61624-61630	3.7	10
46	Computational Alanine Scanning Mutagenesis: MM-PBSA vs TI. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 1311-9	6.4	54
45	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. <i>Journal of Computational Chemistry</i> , 2013 , 34, 2079-90	3.5	27
44	Molecular dynamics analysis of a series of 22 potential farnesyltransferase substrates containing a CaaX-motif. <i>Journal of Molecular Modeling</i> , 2013 , 19, 673-88	2	8
43	Comparative assessment of computational methods for the determination of solvation free energies in alcohol-based molecules. <i>Journal of Computational Chemistry</i> , 2013 , 34, 1354-62	3.5	17
42	Parameters for Molecular Dynamics Simulations of Manganese-Containing Metalloproteins. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2718-32	6.4	30
41	Protein-ligand docking in the new millennium--a retrospective of 10 years in the field. <i>Current Medicinal Chemistry</i> , 2013 , 20, 2296-314	4.3	160
40	Farnesyltransferase inhibitors: a comprehensive review based on quantitative structural analysis. <i>Current Medicinal Chemistry</i> , 2013 , 20, 4888-923	4.3	33
39	Chemically modified tetracyclines as inhibitors of MMP-2 matrix metalloproteinase: a molecular and structural study. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 13644-54	3.4	26
38	Dehydration of a polyether type extraction agent and of the corresponding K ⁺ complex: insights into liquid-liquid extraction mechanisms by quantum chemical methods. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4909-15	2	1
37	Computational enzymatic catalysis--clarifying enzymatic mechanisms with the help of computers. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 12431-41	3.6	44

36	Transfer of the K ⁺ cation across a water/dichloromethane interface: a steered molecular dynamics study with implications in cation extraction. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 1843-9	3.4	8
35	Decomplexation and complexation of alkali metal cations by a crown-ether-type podand in dichloromethane: a steered molecular dynamics study. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	5
34	In silico based structural analysis of some piperidine analogs as farnesyltransferase inhibitors. <i>Medicinal Chemistry</i> , 2012 , 8, 853-64	1.8	1
33	Detailed atomistic analysis of the HIV-1 protease interface. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 7045-57	3.4	15
32	In silico-based structural analysis of arylthiophene derivatives for FTase inhibitory activity, hERG, and other toxic effects. <i>Journal of Biomolecular Screening</i> , 2011 , 16, 1037-46		14
31	Complexation of alkali metal cations by crown-ether type podands with applications in solvent extraction: insights from quantum chemical calculations. <i>Journal of Molecular Modeling</i> , 2011 , 17, 3275-88		7
30	Detection of farnesyltransferase interface hot spots through computational alanine scanning mutagenesis. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 15339-54	3.4	7
29	Structural feature study of benzofuran derivatives as farnesyltransferase inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2011 , 26, 777-91	5.6	15
28	Molecular Dynamics Simulations: Difficulties, Solutions and Strategies for Treating Metalloenzymes. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010 , 299-330	0.7	10
27	Virtual screening in drug design and development. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2010 , 13, 442-53	1.3	42
26	Factors influencing the binding of a potassium cation to a polyethylene glycol type podand in liquid-liquid extraction—molecular dynamics study. <i>Theoretical Chemistry Accounts</i> , 2010 , 127, 681-687	1.9	5
25	Crown-Ether Type Podands as Alkali Metal Cation Extractants: Influence of the Number of Oxygens in the Chain. <i>Journal of Solution Chemistry</i> , 2010 , 39, 1230-1242	1.8	11
24	A comparative molecular dynamics study on the complexation of alkali metal cations by a poly-ethylene-glycol type podand in water and in dichloromethane. <i>Computational and Theoretical Chemistry</i> , 2010 , 946, 77-82		8
23	Direct covalent modification as a strategy to inhibit nuclear factor-kappa B. <i>Current Medicinal Chemistry</i> , 2009 , 16, 4261-73	4.3	25
22	Gas-phase geometry optimization of biological molecules as a reasonable alternative to a continuum environment description: fact, myth, or fiction?. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 14231-6	2.8	17
21	The search for the mechanism of the reaction catalyzed by farnesyltransferase. <i>Chemistry - A European Journal</i> , 2009 , 15, 4243-7	4.8	26
20	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for zinc complexes. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2752-63	3.5	45
19	Molecular dynamics simulations on the critical states of the farnesyltransferase enzyme. <i>Bioorganic and Medicinal Chemistry</i> , 2009 , 17, 3369-78	3.4	26

18	The Zinc proteome: a tale of stability and functionality. <i>Dalton Transactions</i> , 2009 , 7946-56	4.3	59
17	Virtual screening of compound libraries. <i>Methods in Molecular Biology</i> , 2009 , 572, 57-70	1.4	9
16	Enzyme flexibility and the catalytic mechanism of farnesyltransferase: targeting the relation. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 8681-91	3.4	17
15	Farnesyltransferase inhibitors: a detailed chemical view on an elusive biological problem. <i>Current Medicinal Chemistry</i> , 2008 , 15, 1478-92	4.3	101
14	Molecular dynamics analysis of farnesyltransferase: A closer look into the amino acid behavior. <i>International Journal of Quantum Chemistry</i> , 2008 , 108, 1939-1950	2.1	10
13	Comparative assessment of theoretical methods for the determination of geometrical properties in biological zinc complexes. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 9146-52	3.4	31
12	The carboxylate shift in zinc enzymes: a computational study. <i>Journal of the American Chemical Society</i> , 2007 , 129, 1378-85	16.4	120
11	Theoretical studies on farnesyl transferase: evidence for thioether product coordination to the active-site zinc sphere. <i>Journal of Computational Chemistry</i> , 2007 , 28, 1160-8	3.5	34
10	Analysis of zinc-ligand bond lengths in metalloproteins: trends and patterns. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 69, 466-75	4.2	62
9	General performance of density functionals. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 10439-52	2.8	810
8	Theoretical studies on farnesyltransferase: the distances paradox explained. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 66, 205-18	4.2	35
7	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. <i>Theoretical Chemistry Accounts</i> , 2006 , 117, 171-181	1.9	26
6	Protein-ligand docking: current status and future challenges. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006 , 65, 15-26	4.2	597
5	Farnesyltransferase--new insights into the zinc-coordination sphere paradigm: evidence for a carboxylate-shift mechanism. <i>Biophysical Journal</i> , 2005 , 88, 483-94	2.9	55
4	Farnesyltransferase: Theoretical studies on peptide substrate entrance: thiol or thiolate coordination?. <i>Computational and Theoretical Chemistry</i> , 2005 , 729, 125-129		25
3	Unraveling the mechanism of the farnesyltransferase enzyme. <i>Journal of Biological Inorganic Chemistry</i> , 2005 , 10, 3-10	3.7	37
2	New designs for MRI contrast agents. <i>Journal of Computer-Aided Molecular Design</i> , 2003 , 17, 463-73	4.2	12
1	Computational Studies Devoted to the Catalytic Mechanism of Threonine Aldolase, a Critical Enzyme in the Pharmaceutical Industry to Synthesize β -Hydroxy- α -Amino Acids. <i>ACS Catalysis</i> , 2009 , 9, 4990-4999	13.1	0

