

Josã© Malanho Silva

List of Publications by Year in descending order

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117
papers

4,689
citations

94433

37
h-index

114465

63
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123
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123
docs citations

123
times ranked

5653
citing authors

#	ARTICLE	IF	CITATIONS
1	Using simple algebraic concepts to understand chemical composition problems. <i>International Journal of Mathematical Education in Science and Technology</i> , 2022, 53, 842-857.	1.4	1
2	Impact of the pre-examination phase on multicenter metabolomic studies. <i>New Biotechnology</i> , 2022, 68, 37-47.	4.4	10
3	Metabolite and lipoprotein profiles reveal sex-related oxidative stress imbalance in de novo drug-naïve Parkinson's disease patients. <i>Npj Parkinson's Disease</i> , 2022, 8, 14.	5.3	11
4	The early reduction of left ventricular mass after sleeve gastrectomy depends on the fall of branched-chain amino acid circulating levels. <i>EBioMedicine</i> , 2022, 76, 103864.	6.1	10
5	Interconversion between [2Fe-2S] and [4Fe-4S] cluster glutathione complexes. <i>Chemical Communications</i> , 2022, 58, 3533-3536.	4.1	7
6	Metabolomics Fingerprint Predicts Risk of Death in Dilated Cardiomyopathy and Heart Failure. <i>Frontiers in Cardiovascular Medicine</i> , 2022, 9, 851905.	2.4	3
7	An omics approach to study trace metals in sera of hemodialysis patients treated with erythropoiesis stimulating agents. <i>Metallomics</i> , 2022, 14, .	2.4	3
8	Profiling metabolites and lipoproteins in COMETA, an Italian cohort of COVID-19 patients. <i>PLoS Pathogens</i> , 2022, 18, e1010443.	4.7	30
9	Influence of ampelography on the molecular profile of Sangiovese and Cabernet Franc. <i>Flavour and Fragrance Journal</i> , 2022, 37, 219-233.	2.6	1
10	Paramagnetic effects in NMR for protein structures and ensembles: Studies of metalloproteins. <i>Current Opinion in Structural Biology</i> , 2022, 74, 102386.	5.7	9
11	Epitope Mapping and Binding Assessment by Solid-State NMR Provide a Way for the Development of Biologics under the Quality by Design Paradigm. <i>Journal of the American Chemical Society</i> , 2022, 144, 10006-10016.	13.7	9
12	A Quantum Chemistry View on Two Archetypical Paramagnetic Pentacoordinate Nickel(II) Complexes Offers a Fresh Look on Their NMR Spectra. <i>Inorganic Chemistry</i> , 2021, 60, 2068-2075.	4.0	18
13	Characterization of lanthanoid-binding proteins using NMR spectroscopy. <i>Methods in Enzymology</i> , 2021, 651, 103-137.	1.0	2
14	A geroscience approach for Parkinson's disease: Conceptual framework and design of PROPAG-AGEING project. <i>Mechanisms of Ageing and Development</i> , 2021, 194, 111426.	4.6	14
15	CXCR4 antagonism sensitizes cancer cells to novel indole-based MDM2/4 inhibitors in glioblastoma multiforme. <i>European Journal of Pharmacology</i> , 2021, 897, 173936.	3.5	11
16	A High-Resolution View of the Coordination Environment in a Paramagnetic Metalloprotein from its Magnetic Properties. <i>Angewandte Chemie</i> , 2021, 133, 15087-15093.	2.0	5
17	Exploration of Blood Lipoprotein and Lipid Fraction Profiles in Healthy Subjects through Integrated Univariate, Multivariate, and Network Analysis Reveals Association of Lipase Activity and Cholesterol Esterification with Sex and Age. <i>Metabolites</i> , 2021, 11, 326.	2.9	5
18	Unveiling protein dynamics in solution with field-cycling NMR relaxometry. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2021, 124-125, 85-98.	7.5	18

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19	Not only manganese, but fruit component effects dictate the efficiency of fruit juice as an oral magnetic resonance imaging contrast agent. <i>NMR in Biomedicine</i> , 2021, , e4623.	2.8	2
20	Origin of the MRI Contrast in Natural and Hydrogel Formulation of Pineapple Juice. <i>Bioinorganic Chemistry and Applications</i> , 2021, 2021, 1-12.	4.1	3
21	Fecal metabolomic profiles: A comparative study of patients with colorectal cancer <i>vs</i> adenomatous polyps. <i>World Journal of Gastroenterology</i> , 2021, 27, 6430-6441.	3.3	11
22	A framework for validating AI in precision medicine: considerations from the European ITFoC consortium. <i>BMC Medical Informatics and Decision Making</i> , 2021, 21, 274.	3.0	28
23	Exploring Serum NMR-Based Metabolomic Fingerprint of Colorectal Cancer Patients: Effects of Surgery and Possible Associations with Cancer Relapse. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 11120.	2.5	3
24	Orientation of immobilized antigens on common surfaces by a simple computational model: Exposition of SARS-CoV-2 Spike protein RBD epitopes. <i>Biophysical Chemistry</i> , 2020, 265, 106441.	2.8	9
25	Maximizing Magnetic Resonance Contrast in Gd(III) Nanoconjugates: Investigation of Proton Relaxation in Zirconium Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 41157-41166.	8.0	20
26	Nuclear Magnetic Resonance-Based Metabolomic Comparison of Breast Milk and Organic and Traditional Formula Milk Brands for Infants and Toddlers. <i>OMICS A Journal of Integrative Biology</i> , 2020, 24, 424-436.	2.0	5
27	Plasma metabolome and cognitive skills in Down syndrome. <i>Scientific Reports</i> , 2020, 10, 10491.	3.3	23
28	The Photocatalyzed Thiol-ene reaction: A New Tag to Yield Fast, Selective and reversible Paramagnetic Tagging of Proteins. <i>ChemPhysChem</i> , 2020, 21, 863-869.	2.1	11
29	The NMR tube bioreactor. <i>Methods in Enzymology</i> , 2020, 633, 71-101.	1.0	3
30	¹ H NMR Relaxometric Study of Chitosan-Based Nanogels Containing Mono- and Bis-Hydrated Gd(III) Chelates: Clues for MRI Probes of Improved Sensitivity. <i>ACS Applied Bio Materials</i> , 2020, 3, 9065-9072.	4.6	16
31	Hochdurchsatz-Metabolomik mit 1D-NMR. <i>Angewandte Chemie</i> , 2019, 131, 980-1007.	2.0	8
32	What are the methodological and theoretical prospects for paramagnetic NMR in structural biology? A glimpse into the crystal ball. <i>Journal of Magnetic Resonance</i> , 2019, 306, 173-179.	2.1	16
33	Assessing Structural Preferences of Unstructured Protein Regions by NMR. <i>Biophysical Journal</i> , 2019, 117, 1948-1953.	0.5	4
34	Magnetic susceptibility and paramagnetism-based NMR. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2019, 114-115, 211-236.	7.5	54
35	How Do Nuclei Couple to the Magnetic Moment of a Paramagnetic Center? A New Theory at the Gauntlet of the Experiments. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3610-3614.	4.6	18
36	NMR for sample quality assessment in metabolomics. <i>New Biotechnology</i> , 2019, 52, 25-34.	4.4	49

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37	Bimodal Fluorescence-Magnetic Resonance Contrast Agent for Apoptosis Imaging. <i>Journal of the American Chemical Society</i> , 2019, 141, 6224-6233.	13.7	111
38	Metal centers in biomolecular solid-state NMR. <i>Journal of Structural Biology</i> , 2019, 206, 99-109.	2.8	10
39	Non-crystallographic symmetry in proteins: Jahn-Teller-like and Butterfly-like effects?. <i>Journal of Biological Inorganic Chemistry</i> , 2019, 24, 91-101.	2.6	2
40	Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry. <i>Molecular Physics</i> , 2019, 117, 888-897.	1.7	15
41	Interfering with HuR-RNA Interaction: Design, Synthesis and Biological Characterization of Tanshinone Mimics as Novel, Effective HuR Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 1483-1498.	6.4	39
42	Metabolomics in breast cancer: A decade in review. <i>Cancer Treatment Reviews</i> , 2018, 67, 88-96.	7.7	87
43	Effect of Magnetic Coupling on Water Proton Relaxivity in a Series of Transition Metal Gd ^{III} Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 5810-5819.	4.0	11
44	Enriching the biological space of natural products and charting drug metabolites, through real time biotransformation monitoring: The NMR tube bioreactor. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2018, 1862, 1-8.	2.4	8
45	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. <i>Analytical Chemistry</i> , 2018, 90, 649-656.	6.5	50
46	Long-range paramagnetic NMR data can provide a closer look on metal coordination in metalloproteins. <i>Journal of Biological Inorganic Chemistry</i> , 2018, 23, 71-80.	2.6	22
47	¹ H NMR Spectroscopy of [FeFe] Hydrogenase: Insight into the Electronic Structure of the Active Site. <i>Journal of the American Chemical Society</i> , 2018, 140, 131-134.	13.7	9
48	Protein Glycosylation through Sulfur Fluoride Exchange (SuFEx) Chemistry: The Key Role of a Fluorosulfate Thiolactoside. <i>Chemistry - A European Journal</i> , 2018, 24, 18981-18987.	3.3	17
49	Local and Global Dynamics in Intrinsically Disordered Synuclein. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15262-15266.	13.8	49
50	Lokale und globale Dynamik im ungeordneten Synuclein-Protein. <i>Angewandte Chemie</i> , 2018, 130, 15482-15486.	2.0	0
51	NMR Spectroscopy and Metal Ions in Life Sciences. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 4752-4770.	2.0	9
52	Aggregation kinetics of the A β 1-40 peptide monitored by NMR. <i>Chemical Communications</i> , 2018, 54, 7601-7604.	4.1	29
53	NMR metabolomic fingerprinting distinguishes milk from different farms. <i>Food Research International</i> , 2018, 113, 131-139.	6.2	39
54	Paradoxically, Most Flexible Ligand Binds Most Entropy-Favored: Intriguing Impact of Ligand Flexibility and Solvation on Drug-Kinase Binding. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 5922-5933.	6.4	36

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55	One-thousand-fold enhancement of high field liquid nuclear magnetic resonance signals at room temperature. <i>Nature Chemistry</i> , 2017, 9, 676-680.	13.6	77
56	Paramagnetic Properties of a Crystalline Iron-Sulfur Protein by Magic-Angle Spinning NMR Spectroscopy. <i>Inorganic Chemistry</i> , 2017, 56, 6624-6629.	4.0	19
57	Characterization of the Conjugation Pattern in Large Polysaccharide-Protein Conjugates by NMR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14997-15001.	13.8	21
58	Characterization of the Conjugation Pattern in Large Polysaccharide-Protein Conjugates by NMR Spectroscopy. <i>Angewandte Chemie</i> , 2017, 129, 15193-15197.	2.0	3
59	De-escalating and escalating treatment beyond endocrine therapy in patients with luminal breast cancer. <i>Breast</i> , 2017, 34, S13-S18.	2.2	6
60	Atomic structural details of a protein grafted onto gold nanoparticles. <i>Scientific Reports</i> , 2017, 7, 17934.	3.3	24
61	Perspectives on paramagnetic NMR from a life sciences infrastructure. <i>Journal of Magnetic Resonance</i> , 2017, 282, 154-169.	2.1	21
62	Solid-State NMR of PEGylated Proteins. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2446-2449.	13.8	41
63	Solid-State NMR of PEGylated Proteins. <i>Angewandte Chemie</i> , 2016, 128, 2492-2495.	2.0	12
64	Basic facts and perspectives of Overhauser DNP NMR. <i>Journal of Magnetic Resonance</i> , 2016, 264, 78-87.	2.1	50
65	Active-Site Targeting Paramagnetic Probe for Matrix Metalloproteinases. <i>ChemPlusChem</i> , 2016, 81, 1333-1338.	2.8	2
66	Nanodiamond-Gadolinium(III) Aggregates for Tracking Cancer Growth In Vivo at High Field. <i>Nano Letters</i> , 2016, 16, 7551-7564.	9.1	60
67	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP12 from First Principles. <i>Angewandte Chemie</i> , 2016, 128, 14933-14937.	2.0	14
68	How to tackle protein structural data from solution and solid state: An integrated approach. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2016, 92-93, 54-70.	7.5	27
69	Exploring the conformational heterogeneity of biomolecules: theory and experiments. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5684-5685.	2.8	4
70	Improved Accuracy from Joint X-ray and NMR Refinement of a Protein-RNA Complex Structure. <i>Journal of the American Chemical Society</i> , 2016, 138, 1601-1610.	13.7	22
71	A critical assessment of methods to recover information from averaged data. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5686-5701.	2.8	70
72	Inter-helical conformational preferences of HIV-1 TAR-RNA from maximum occurrence analysis of NMR data and molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5743-5752.	2.8	15

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73	Biosilica-Entrapped Enzymes Studied by Using Dynamic Nuclear Polarization-Enhanced High-Field NMR Spectroscopy. <i>ChemPhysChem</i> , 2015, 16, 2751-2754.	2.1	30
74	Differences in Dynamics between Crosslinked and Non-Crosslinked Hyaluronates Measured by using Fast Field-Cycling Relaxometry. <i>ChemPhysChem</i> , 2015, 16, 2803-2809.	2.1	19
75	Facing and Overcoming Sensitivity Challenges in Biomolecular NMR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9162-9185.	13.8	258
76	Serum metabolomic profiles evaluated after surgery may identify patients with oestrogen receptor negative early breast cancer at increased risk of disease recurrence. Results from a retrospective study. <i>Molecular Oncology</i> , 2015, 9, 128-139.	4.6	82
77	NMR of sedimented, fibrillized, silica-entrapped and microcrystalline (metallo)proteins. <i>Journal of Magnetic Resonance</i> , 2015, 253, 60-70.	2.1	22
78	High Relaxivity Gd(III)-DNA Gold Nanostars: Investigation of Shape Effects on Proton Relaxation. <i>ACS Nano</i> , 2015, 9, 3385-3396.	14.6	108
79	Metabolomic fingerprint of severe obesity is dynamically affected by bariatric surgery in a procedure-dependent manner. <i>American Journal of Clinical Nutrition</i> , 2015, 102, 1313-1322.	4.7	96
80	Of Monkeys and Men: A Metabolomic Analysis of Static and Dynamic Urinary Metabolic Phenotypes in Two Species. <i>PLoS ONE</i> , 2014, 9, e106077.	2.5	22
81	G-triplex structure and formation propensity. <i>Nucleic Acids Research</i> , 2014, 42, 13393-13404.	14.5	71
82	The competitive world of RAS biology. <i>Nature Chemical Biology</i> , 2014, 10, 173-174.	8.0	1
83	A Metabolomic Perspective on Coeliac Disease. <i>Autoimmune Diseases</i> , 2014, 2014, 1-13.	0.6	26
84	Telomerase activated thymidine analogue pro-drug is a new molecule targeting hepatocellular carcinoma. <i>Journal of Hepatology</i> , 2014, 61, 1064-1072.	3.7	10
85	Practical considerations over spectral quality in solid state NMR spectroscopy of soluble proteins. <i>Journal of Biomolecular NMR</i> , 2013, 57, 155-166.	2.8	36
86	NMR crystallography on paramagnetic systems: solved and open issues. <i>CrystEngComm</i> , 2013, 15, 8639.	2.6	43
87	Discovery of a New Class of Potent MMP Inhibitors by Structure-Based Optimization of the Arylsulfonamide Scaffold. <i>ACS Medicinal Chemistry Letters</i> , 2013, 4, 565-569.	2.8	18
88	Examination of Matrix Metalloproteinase-1 in Solution. <i>Journal of Biological Chemistry</i> , 2013, 288, 30659-30671.	3.4	68
89	Water and Protein Dynamics in Sedimented Systems: A Relaxometric Investigation. <i>ChemPhysChem</i> , 2013, 14, 3156-3161.	2.1	20
90	Metabolomics for the future of personalized medicine through information and communication technologies. <i>Personalized Medicine</i> , 2012, 9, 133-136.	1.5	4

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91	Solid-State NMR Crystallography through Paramagnetic Restraints. <i>Journal of the American Chemical Society</i> , 2012, 134, 5006-5009.	13.7	69
92	Moving the frontiers in solution and solid-state bioNMR. <i>Coordination Chemistry Reviews</i> , 2011, 255, 649-663.	18.8	28
93	High-Resolution Solid-State NMR Structure of a 17.6 kDa Protein. <i>Journal of the American Chemical Society</i> , 2010, 132, 1032-1040.	13.7	117
94	Ultrafast MAS Solid-State NMR Permits Extensive ^{13}C and ^1H Detection in Paramagnetic Metalloproteins. <i>Journal of the American Chemical Society</i> , 2010, 132, 5558-5559.	13.7	109
95	Paramagnetic shifts in solid-state NMR of proteins to elicit structural information. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 17284-17289.	7.1	93
96	Paramagnetic Ions Provide Structural Restraints in Solid-State NMR of Proteins. <i>Journal of the American Chemical Society</i> , 2007, 129, 2218-2219.	13.7	85
97	NMR Spectroscopy of Paramagnetic Metalloproteins. <i>ChemBioChem</i> , 2005, 6, 1536-1549.	2.6	289
98	Magnetic Susceptibility Tensor Anisotropies for a Lanthanide Ion Series in a Fixed Protein Matrix. <i>Journal of the American Chemical Society</i> , 2001, 123, 4181-4188.	13.7	183
99	Hyperfine Shifts in Low-Spin Iron(III) Hemes: A Ligand Field Analysis. <i>European Journal of Inorganic Chemistry</i> , 2000, 2000, 2473-2480.	2.0	25
100	Paramagnetic ^1H NMR spectroscopy of the reduced, unbound Photosystem I subunit PsaC: sequence-specific assignment of contact-shifted resonances and identification of mixed- and equal-valence Fe-Fe pairs in $[\text{4Fe-4S}]$ centers FA a'' and FB a'' . <i>Journal of Biological Inorganic Chemistry</i> , 2000, 5, 381-392.	2.6	26
101	Simultaneous interpretation of Mössbauer, EPR and ^{57}Fe ENDOR spectra of the $[\text{Fe}_4\text{S}_4]$ cluster in the high-potential iron protein I <i>Ectothiorhodospira halophila</i> . <i>Journal of Biological Inorganic Chemistry</i> , 1999, 4, 727-741.	2.6	20
102	Structural and Dynamical Properties of a Partially Unfolded Fe_4S_4 Protein: A Role of the Cofactor in Protein Folding. <i>Biochemistry</i> , 1999, 38, 4669-4680.	2.5	38
103	NMR and Spin Relaxation in Dimers. <i>Accounts of Chemical Research</i> , 1998, 31, 351-361.	15.6	42
104	Accurate Determination of Deuterium/Hydrogen Ratios in Natural Organic Compounds through a Nuclear Magnetic Resonance Time-Domain Reference Convolution Method: Application to Ethanol from Three Botanical Sources and Critical Analysis of Systematic Inaccuracies in Previous Methods. <i>Journal of Agricultural and Food Chemistry</i> , 1998, 46, 3943-3946.	5.2	5
105	Solution Structure of the Oxidized Fe_7S_8 Ferredoxin from the Thermophilic Bacterium <i>Bacillus schlegelii</i> by ^1H NMR Spectroscopy. <i>Biochemistry</i> , 1998, 37, 9812-9826.	2.5	48
106	Analysis of the Temperature Dependence of the ^1H and ^{13}C Isotropic Shifts of Horse Heart Ferricytochrome c: A Explanation of Curie and Anti-Curie Temperature Dependence and Nonlinear Pseudocontact Shifts in a Common Two-Level Framework. <i>Journal of the American Chemical Society</i> , 1998, 120, 8472-8479.	13.7	64
107	Partial Orientation of Oxidized and Reduced Cytochrome b_5 at High Magnetic Fields: A Magnetic Susceptibility Anisotropy Contributions and Consequences for Protein Solution Structure Determination. <i>Journal of the American Chemical Society</i> , 1998, 120, 12903-12909.	13.7	110
108	An NMR Study of the ^7Fe - ^8S Ferredoxin from <i>Rhodospseudomonas palustris</i> and Reinterpretation of Data on Similar Systems. <i>Biochemistry</i> , 1997, 36, 3570-3579.	2.5	37

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109	Electronic and Geometric Structure of the CuA Site Studied by ^1H NMR in a Soluble Domain of Cytochrome c Oxidase from <i>Paracoccus denitrificans</i> . <i>Journal of the American Chemical Society</i> , 1997, 119, 11023-11027.	13.7	45
110	Characterization of the Unbound $2[\text{Fe}_4\text{S}_4]$ -Ferredoxin-Like Photosystem I Subunit PsaC from the Cyanobacterium <i>Synechococcus elongatus</i> . <i>Biochemistry</i> , 1997, 36, 13629-13637.	2.5	23
111	Solution Structure of the Paramagnetic Complex of the N-Terminal Domain of Calmodulin with Two Ce^{3+} Ions by ^1H NMR. <i>Biochemistry</i> , 1997, 36, 11605-11618.	2.5	93
112	Solution Structure of Oxidized Horse Heart Cytochrome c . <i>Biochemistry</i> , 1997, 36, 9867-9877.	2.5	290
113	A Serine \rightarrow Cysteine Ligand Mutation in the High Potential Iron-Sulfur Protein from <i>Chromatium vinosum</i> Provides Insight into the Electronic Structure of the $[\text{Fe}_4\text{S}_4]$ Cluster. <i>Journal of the American Chemical Society</i> , 1996, 118, 75-80.	13.7	69
114	The CuA Center of a Soluble Domain from <i>Thermus</i> Cytochrome ba_3 . An NMR Investigation of the Paramagnetic Protein. <i>Journal of the American Chemical Society</i> , 1996, 118, 11658-11659.	13.7	78
115	The electronic structure of FeS centers in proteins and models a contribution to the understanding of their electron transfer properties. <i>Structure and Bonding</i> , 1995, , 1-53.	1.0	91
116	A Mössbauer investigation of oxidized Fe_4S_4 HiPIP II from <i>Ectothiorhodospira halophila</i> . <i>Journal of Inorganic Biochemistry</i> , 1993, 52, 227-234.	3.5	40
117	Carbonic anhydrase: An insight into the zinc binding site and into the active cavity through metal substitution. , 1982, , 45-92.		124