

Josã© Malanho Silva

List of Publications by Year in descending order

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117
papers

4,689
citations

94433

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123
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123
docs citations

123
times ranked

5653
citing authors

#	ARTICLE	IF	CITATIONS
1	Solution Structure of Oxidized Horse Heart Cytochrome c. <i>Biochemistry</i> , 1997, 36, 9867-9877.	2.5	290
2	NMR Spectroscopy of Paramagnetic Metalloproteins. <i>ChemBioChem</i> , 2005, 6, 1536-1549.	2.6	289
3	Facing and Overcoming Sensitivity Challenges in Biomolecular NMR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9162-9185.	13.8	258
4	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
5	Carbonic anhydrase: An insight into the zinc binding site and into the active cavity through metal substitution. , 1982, , 45-92.		124
6	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
7	Bimodal Fluorescence-Magnetic Resonance Contrast Agent for Apoptosis Imaging. <i>Journal of the American Chemical Society</i> , 2019, 141, 6224-6233.	13.7	111
8	Partial Orientation of Oxidized and Reduced Cytochrome b5 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
9	Ultrafast MAS Solid-State NMR Permits Extensive ¹³ C and ¹ H Detection in Paramagnetic Metalloproteins. <i>Journal of the American Chemical Society</i> , 2010, 132, 5558-5559.	13.7	109
10	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
11	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
12	Solution Structure of the Paramagnetic Complex of the N-Terminal Domain of Calmodulin with Two Ce ³⁺ Ions by ¹ H NMR. <i>Biochemistry</i> , 1997, 36, 11605-11618.	2.5	93
13	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
14	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
15	Metabolomics in breast cancer: A decade in review. <i>Cancer Treatment Reviews</i> , 2018, 67, 88-96.	7.7	87
16	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
17	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
18	The CuA Center of a Soluble Domain from Thermus Cytochrome b ₃ . An NMR Investigation of the Paramagnetic Protein. <i>Journal of the American Chemical Society</i> , 1996, 118, 11658-11659.	13.7	78

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19	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
20	G-triplex structure and formation propensity. <i>Nucleic Acids Research</i> , 2014, 42, 13393-13404.	14.5	71
21	A critical assessment of methods to recover information from averaged data. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5686-5701.	2.8	70
22	A Serine → Cysteine Ligand Mutation in the High Potential Iron-Sulfur Protein from <i>Chromatium vinosum</i> Provides Insight into the Electronic Structure of the [4Fe-4S] Cluster. <i>Journal of the American Chemical Society</i> , 1996, 118, 75-80.	13.7	69
23	Solid-State NMR Crystallography through Paramagnetic Restraints. <i>Journal of the American Chemical Society</i> , 2012, 134, 5006-5009.	13.7	69
24	Examination of Matrix Metalloproteinase-1 in Solution. <i>Journal of Biological Chemistry</i> , 2013, 288, 30659-30671.	3.4	68
25	Analysis of the Temperature Dependence of the ¹ H 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
26	Nanodiamond-Gadolinium(III) Aggregates for Tracking Cancer Growth In Vivo at High Field. <i>Nano Letters</i> , 2016, 16, 7551-7564.	9.1	60
27	Magnetic susceptibility and paramagnetism-based NMR. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2019, 114-115, 211-236.	7.5	54
28	Basic facts and perspectives of Overhauser DNP NMR. <i>Journal of Magnetic Resonance</i> , 2016, 264, 78-87.	2.1	50
29	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
30	Local and Global Dynamics in Intrinsically Disordered Synuclein. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15262-15266.	13.8	49
31	NMR for sample quality assessment in metabolomics. <i>New Biotechnology</i> , 2019, 52, 25-34.	4.4	49
32	Solution Structure of the Oxidized Fe7S8 Ferredoxin from the Thermophilic Bacterium <i>Bacillus schlegelii</i> by ¹ H NMR Spectroscopy. <i>Biochemistry</i> , 1998, 37, 9812-9826.	2.5	48
33	Electronic and Geometric Structure of the CuA Site Studied by ¹ H 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
34	NMR crystallography on paramagnetic systems: solved and open issues. <i>CrystEngComm</i> , 2013, 15, 8639.	2.6	43
35	NMR and Spin Relaxation in Dimers. <i>Accounts of Chemical Research</i> , 1998, 31, 351-361.	15.6	42
36	Solid-State NMR of PEGylated Proteins. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2446-2449.	13.8	41

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37	A Mössbauer investigation of oxidized Fe ₄ S ₄ HiPIP II from <i>Ectothiorhodospira halophila</i> . <i>Journal of Inorganic Biochemistry</i> , 1993, 52, 227-234.	3.5	40
38	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
39	NMR metabolomic fingerprinting distinguishes milk from different farms. <i>Food Research International</i> , 2018, 113, 131-139.	6.2	39
40	Structural and Dynamical Properties of a Partially Unfolded Fe ₄ S ₄ Protein: A Role of the Cofactor in Protein Folding. <i>Biochemistry</i> , 1999, 38, 4669-4680.	2.5	38
41	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
42	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
43	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
44	Biosilica-Entrapped Enzymes Studied by Using Dynamic Nuclear Polarization-Enhanced High-Field NMR Spectroscopy. <i>ChemPhysChem</i> , 2015, 16, 2751-2754.	2.1	30
45	Profiling metabolites and lipoproteins in COMETA, an Italian cohort of COVID-19 patients. <i>PLoS Pathogens</i> , 2022, 18, e1010443.	4.7	30
46	Aggregation kinetics of the A β 1-40 peptide monitored by NMR. <i>Chemical Communications</i> , 2018, 54, 7601-7604.	4.1	29
47	Moving the frontiers in solution and solid-state bioNMR. <i>Coordination Chemistry Reviews</i> , 2011, 255, 649-663.	18.8	28
48	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
49	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
50	Paramagnetic ¹ H 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 [4Fe-4S] centers FA \cdot and FB \cdot . <i>Journal of Biological Inorganic Chemistry</i> , 2000, 5, 381-392.	2.6	26
51	A Metabolomic Perspective on Coeliac Disease. <i>Autoimmune Diseases</i> , 2014, 2014, 1-13.	0.6	26
52	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
53	Atomic structural details of a protein grafted onto gold nanoparticles. <i>Scientific Reports</i> , 2017, 7, 17934.	3.3	24
54	Characterization of the Unbound 2[Fe ₄ 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

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55	Plasma metabolome and cognitive skills in Down syndrome. <i>Scientific Reports</i> , 2020, 10, 10491.	3.3	23
56	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
57	NMR of sedimented, fibrillized, silica-entrapped and microcrystalline (metallo)proteins. <i>Journal of Magnetic Resonance</i> , 2015, 253, 60-70.	2.1	22
58	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
59	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
60	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
61	Perspectives on paramagnetic NMR from a life sciences infrastructure. <i>Journal of Magnetic Resonance</i> , 2017, 282, 154-169.	2.1	21
62	Simultaneous interpretation of Mössbauer, EPR and ⁵⁷ Fe ENDOR spectra of the [Fe ₄ 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
63	Water and Protein Dynamics in Sedimented Systems: A Relaxometric Investigation. <i>ChemPhysChem</i> , 2013, 14, 3156-3161.	2.1	20
64	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
65	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
66	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
67	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
68	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
69	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
70	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
71	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
72	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

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73	¹ H NMR Relaxometric Study of Chitosan-Based Nanogels Containing Mono- and Bis-Hydrated Gd(III) Chelates: Clues for MRI Probes of Improved Sensitivity. ACS Applied Bio Materials, 2020, 3, 9065-9072.	4.6	16
74	Inter-helical conformational preferences of HIV-1 TAR-RNA from maximum occurrence analysis of NMR data and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2016, 18, 5743-5752.	2.8	15
75	Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry. Molecular Physics, 2019, 117, 888-897.	1.7	15
76	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP1.2 from First Principles. Angewandte Chemie, 2016, 128, 14933-14937.	2.0	14
77	A geroscience approach for Parkinson's disease: Conceptual framework and design of PROPAG-AGEING project. Mechanisms of Ageing and Development, 2021, 194, 111426.	4.6	14
78	Solid-State NMR of PEGylated Proteins. Angewandte Chemie, 2016, 128, 2492-2495.	2.0	12
79	Effect of Magnetic Coupling on Water Proton Relaxivity in a Series of Transition Metal Gd ^{III} Complexes. Inorganic Chemistry, 2018, 57, 5810-5819.	4.0	11
80	The Photocatalyzed Thiol-ene reaction: A New Tag to Yield Fast, Selective and reversible Paramagnetic Tagging of Proteins. ChemPhysChem, 2020, 21, 863-869.	2.1	11
81	CXCR4 antagonism sensitizes cancer cells to novel indole-based MDM2/4 inhibitors in glioblastoma multiforme. European Journal of Pharmacology, 2021, 897, 173936.	3.5	11
82	Fecal metabolomic profiles: A comparative study of patients with colorectal cancer <i>vs</i> adenomatous polyps. World Journal of Gastroenterology, 2021, 27, 6430-6441.	3.3	11
83	Metabolite and lipoprotein profiles reveal sex-related oxidative stress imbalance in de novo drug-naive Parkinson's disease patients. Npj Parkinson's Disease, 2022, 8, 14.	5.3	11
84	Telomerase activated thymidine analogue pro-drug is a new molecule targeting hepatocellular carcinoma. Journal of Hepatology, 2014, 61, 1064-1072.	3.7	10
85	Metal centers in biomolecular solid-state NMR. Journal of Structural Biology, 2019, 206, 99-109.	2.8	10
86	Impact of the pre-examination phase on multicenter metabolomic studies. New Biotechnology, 2022, 68, 37-47.	4.4	10
87	The early reduction of left ventricular mass after sleeve gastrectomy depends on the fall of branched-chain amino acid circulating levels. EBioMedicine, 2022, 76, 103864.	6.1	10
88	¹ H NMR Spectroscopy of [FeFe] Hydrogenase: Insight into the Electronic Structure of the Active Site. Journal of the American Chemical Society, 2018, 140, 131-134.	13.7	9
89	NMR Spectroscopy and Metal Ions in Life Sciences. European Journal of Inorganic Chemistry, 2018, 2018, 4752-4770.	2.0	9
90	Orientation of immobilized antigens on common surfaces by a simple computational model: Exposition of SARS-CoV-2 Spike protein RBD epitopes. Biophysical Chemistry, 2020, 265, 106441.	2.8	9

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91	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
92	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
93	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
94	Hochdurchsatz-Metabolomik mit 1D-NMR. <i>Angewandte Chemie</i> , 2019, 131, 980-1007.	2.0	8
95	Interconversion between [2Fe-2S] and [4Fe-4S] cluster glutathione complexes. <i>Chemical Communications</i> , 2022, 58, 3533-3536.	4.1	7
96	De-escalating and escalating treatment beyond endocrine therapy in patients with luminal breast cancer. <i>Breast</i> , 2017, 34, S13-S18.	2.2	6
97	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
98	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
99	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
100	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
101	Metabolomics for the future of personalized medicine through information and communication technologies. <i>Personalized Medicine</i> , 2012, 9, 133-136.	1.5	4
102	Exploring the conformational heterogeneity of biomolecules: theory and experiments. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5684-5685.	2.8	4
103	Assessing Structural Preferences of Unstructured Protein Regions by NMR. <i>Biophysical Journal</i> , 2019, 117, 1948-1953.	0.5	4
104	Characterization of the Conjugation Pattern in Large Polysaccharide-Protein Conjugates by NMR Spectroscopy. <i>Angewandte Chemie</i> , 2017, 129, 15193-15197.	2.0	3
105	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
106	The NMR tube bioreactor. <i>Methods in Enzymology</i> , 2020, 633, 71-101.	1.0	3
107	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
108	Metabolomics Fingerprint Predicts Risk of Death in Dilated Cardiomyopathy and Heart Failure. <i>Frontiers in Cardiovascular Medicine</i> , 2022, 9, 851905.	2.4	3

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109	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
110	Active-Site Targeting Paramagnetic Probe for Matrix Metalloproteinases. <i>ChemPlusChem</i> , 2016, 81, 1333-1338.	2.8	2
111	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
112	Characterization of lanthanoid-binding proteins using NMR spectroscopy. <i>Methods in Enzymology</i> , 2021, 651, 103-137.	1.0	2
113	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
114	The competitive world of RAS biology. <i>Nature Chemical Biology</i> , 2014, 10, 173-174.	8.0	1
115	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
116	Influence of in-ampthorae vinification on the molecular profile of Sangiovese and Cabernet Franc. <i>Flavour and Fragrance Journal</i> , 2022, 37, 219-233.	2.6	1
117	Lokale und globale Dynamik im ungeordneten Synuklein-Protein. <i>Angewandte Chemie</i> , 2018, 130, 15482-15486.	2.0	0