Claudio Luchinat

List of Publications by Year
in descending order

616 papers	25,369 citations	7096 78 h-index	20358 116 g-index
651 all docs	651 docs citations	651 times ranked	18150 citing authors

#	Article	IF	Citations
1	Magnetic susceptibility in paramagnetic NMR. Progress in Nuclear Magnetic Resonance Spectroscopy, 2002, 40, 249-273.	7.5	431
2	Perspectives on NMR in drug discovery: a technique comes of age. Nature Reviews Drug Discovery, 2008, 7, 738-745.	46.4	373
3	Solution Structure of Oxidized Horse Heart Cytochrome câ€‚âŠ¥. Biochemistry, 1997, 36, 9867-9877.	2.5	290
4	NMR Spectroscopy of Paramagnetic Metalloproteins. ChemBioChem, 2005, 6, 1536-1549.	2.6	289
5	A New Structural Model of AÎ²₄₀ Fibrils. Journal of the American Chemical Society, 2011, 133, 16013-16022.	13.7	289
6	Standard operating procedures for pre-analytical handling of blood and urine for metabolomic studies and biobanks. Journal of Biomolecular NMR, 2011, 49, 231-243.	2.8	285
7	Facing and Overcoming Sensitivity Challenges in Biomolecular NMR Spectroscopy. Angewandte Chemie - International Edition, 2015, 54, 9162-9185.	13.8	258
8	Highâ€Throughput Metabolomics by 1D NMR. Angewandte Chemie - International Edition, 2019, 58, 968-994.	13.8	254
9	Evidence of different metabolic phenotypes in humans. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 1420-1424.	7.1	231
10	Lanthanide-Induced Pseudocontact Shifts for Solution Structure Refinements of Macromolecules in Shells up to 40 Ã... from the Metal Ion. Journal of the American Chemical Society, 2000, 122, 4154-4161.	13.7	212
11	From The Cover: Experimentally exploring the conformational space sampled by domain reorientation in calmodulin. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 6841-6846.	7.1	209
12	Accurate, Fully-Automated NMR Spectral Profiling for Metabolomics. PLoS ONE, 2015, 10, e0124219.	2.5	206
13	Standardizing the experimental conditions for using urine in NMR-based metabolomic studies with a particular focus on diagnostic studies: a review. Metabolomics, 2015, 11, 872-894.	3.0	196
14	Magnetic Susceptibility Tensor Anisotropies for a Lanthanide Ion Series in a Fixed Protein Matrix. Journal of the American Chemical Society, 2001, 123, 4181-4188.	13.7	183
15	Metabolomic NMR Fingerprinting to Identify and Predict Survival of Patients with Metastatic Colorectal Cancer. Cancer Research, 2012, 72, 356-364.	0.9	181
16	Protonless NMR Experiments for Sequence-Specific Assignment of Backbone Nuclei in Unfolded Proteins. Journal of the American Chemical Society, 2006, 128, 3918-3919.	13.7	176
17	The synthesis and in vitro testing of a zinc-activated MRI contrast agent. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 13881-13886.	7.1	172
18	Mechanistic Studies of a Calcium-Dependent MRI Contrast Agent. Inorganic Chemistry, 2002, 41, 4018-4024.	4.0	166

#	Article	IF	Citations
19	Solid-state NMR of proteins sedimented by ultracentrifugation. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 10396-10399.	7.1	163
20	Dynamic nuclear polarization at high magnetic fields in liquids. Progress in Nuclear Magnetic Resonance Spectroscopy, 2012, 64, 4-28.	7.5	162
21	The Metabonomic Signature of Celiac Disease. Journal of Proteome Research, 2009, 8, 170-177.	3.7	160
22	Conformational Space of Flexible Biological Macromolecules from Average Data. Journal of the American Chemical Society, 2010, 132, 13553-13558.	13.7	155
23	The iron-sulfur cluster (Fe4S4) centers in ferredoxins studied through proton and carbon hyperfine coupling. Sequence-specific assignments of cysteines in ferredoxins from Clostridium acidi urici and Clostridium pasteurianum. Journal of the American Chemical Society, 1994, 116, 651-660.	13.7	147
24	The crystal structure of yeast copper thionein: The solution of a long-lasting enigma. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 51-56.	7.1	146
25	Conformational variability of matrix metalloproteinases: Beyond a single 3D structure. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 5334-5339.	7.1	143
26	Albumin Binding, Relaxivity, and Water Exchange Kinetics of the Diastereoisomers of MS-325, a Gadolinium(III)-Based Magnetic Resonance Angiography Contrast Agent. Inorganic Chemistry, 2007, 46, 6632-6639.	4.0	143
27	Individual Human Phenotypes in Metabolic Space and Time. Journal of Proteome Research, 2009, 8, 4264-4271.	3.7	143
28	Proton NOE studies on dicopper(II) dicobalt(II) superoxide dismutase. Inorganic Chemistry, 1989, 28, 4650-4656.	4.0	140
29	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. Metabolomics, 2015, 11, 1587-1597.	3.0	140
30	Cobalt(II) as a probe of the structure and function of carbonic anhydrase. Accounts of Chemical Research, 1983, 16, 272-279.	15.6	139
31	The Gâ€Triplex DNA. Angewandte Chemie - International Edition, 2013, 52, 2269-2273.	13.8	133
32	A Modular System for the Synthesis of Multiplexed Magnetic Resonance Probes. Journal of the American Chemical Society, 2011, 133, 5329-5337.	13.7	126
33	Carbonic anhydrase: An insight into the zinc binding site and into the active cavity through metal substitution. , 1982, , 45-92.		124
34	Paramagnetism-Based NMR Restraints Provide Maximum Allowed Probabilities for the Different Conformations of Partially Independent Protein Domains. Journal of the American Chemical Society, 2007, 129, 12786-12794.	13.7	124
35	Recommendations and Standardization of Biomarker Quantification Using NMR-Based Metabolomics with Particular Focus on Urinary Analysis. Journal of Proteome Research, 2016, 15, 360-373.	3.7	122
36	Spectroscopic studies on Cu2Zn2SOD: a continuous advancement of investigation tools. Coordination Chemistry Reviews, 1990, 100, 67-103.	18.8	120

#	Article	IF	Citations
37	Paramagnetism-Based Restraints for Xplor-NIH. Journal of Biomolecular NMR, 2004, 28, 249-261.	2.8	119
38	High-Field Dynamic Nuclear Polarization with High-Spin Transition Metal Ions. Journal of the American Chemical Society, 2011, 133, 5648-5651.	13.7	119
39	Field Dependent Dynamic Nuclear Polarization with Radicals in Aqueous Solution. Journal of the American Chemical Society, 2008, 130, 3254-3255.	13.7	117
40	High-Resolution Solid-State NMR Structure of a 17.6 kDa Protein. Journal of the American Chemical Society, 2010, 132, 1032-1040.	13.7	117
41	A Computer Program for the Calculation of Paramagnetic Enhancements of Nuclear-Relaxation Rates in Slowly Rotating Systems. Journal of Magnetic Resonance Series A, 1995, 113, 151-158.	1.6	116
42	pKa of zinc-bound water and nucleophilicity of hydroxo-containing species. Ab initio calculations on models for zinc enzymes. Inorganic Chemistry, 1990, 29, 1460-1463.	4.0	114
43	Paramagnetic constraints: An aid for quick solution structure determination of paramagnetic metalloproteins. Concepts in Magnetic Resonance, 2002, 14, 259-286.	1.3	112
44	Proton NMR spectroscopy and the electronic structure of the high potential iron-sulfur protein from Chromatium vinosum. Journal of the American Chemical Society, 1991, 113, 1237-1245.	13.7	111
45	Bimodal Fluorescence-Magnetic Resonance Contrast Agent for Apoptosis Imaging. Journal of the American Chemical Society, 2019, 141, 6224-6233.	13.7	111
46	Partial Orientation of Oxidized and Reduced Cytochromeb5at High Magnetic Fields:Â Magnetic Susceptibility Anisotropy Contributions and Consequences for Protein Solution Structure Determination. Journal of the American Chemical Society, 1998, 120, 12903-12909.	13.7	110
47	Ultrafast MAS Solid-State NMR Permits Extensive ¹³C and ¹H Detection in Paramagnetic Metalloproteins. Journal of the American Chemical Society, 2010, 132, 5558-5559.	13.7	109
48	High Relaxivity Gd(III)â€“DNA Gold Nanostars: Investigation of Shape Effects on Proton Relaxation. ACS Nano, 2015, 9, 3385-3396.	14.6	108
49	Perspectives in paramagnetic NMR of metalloproteins. Dalton Transactions, 2008, , 3782.	3.3	107
50	High-Field NMR Studies of Oxidized Blue Copper Proteins:Â The Case of Spinach Plastocyanin. Journal of the American Chemical Society, 1999, 121, 2037-2046.	13.7	105
51	Structural Basis for Matrix Metalloproteinase 1-Catalyzed Collagenolysis. Journal of the American Chemical Society, 2012, 134, 2100-2110.	13.7	105
52	Uniqueness of the NMR approach to metabolomics. TrAC - Trends in Analytical Chemistry, 2019, 120, 115300.	11.4	103
53	Paramagnetism-based versus classical constraints: an analysis of the solution structure of Ca Ln calbindin D9k. Journal of Biomolecular NMR, 2001, 21, 85-98.	2.8	101
54	Accurate Solution Structures of Proteins from X-ray Data and a Minimal Set of NMR Data: Calmodulinâ^'Peptide Complexes As Examples. Journal of the American Chemical Society, 2009, 131, 5134-5144.	13.7	101

#	Article	IF	Citations
55	The three-dimensional structure in solution of the paramagnetic high-potential iron-sulfur protein I from Ectothiorhodospira halophila through nuclear magnetic resonance. FEBS Journal, 1994, 225, 715-725.	0.2	99
56	Pseudocontact shifts as constraints for energy minimization and molecular dynamics calculations on solution structures of paramagnetic metalloproteins. Proteins: Structure, Function and Bioinformatics, 1997, 29, 68-76.	2.6	99
57	Heme methyl 1H chemical shifts as structural parameters in some low-spin ferriheme proteins. Journal of Biological Inorganic Chemistry, 1999, 4, 515-519.	2.6	98
58	A Strategy for the NMR Characterization of Type II Copper(II) Proteins:Â the Case of the Copper Trafficking Protein CopC fromPseudomonasSyringae. Journal of the American Chemical Society, 2003, 125, 7200-7208.	13.7	98
59	Snapshots of the Reaction Mechanism of Matrix Metalloproteinases. Angewandte Chemie - International Edition, 2006, 45, 7952-7955.	13.8	98
60	Identification of the iron ions of high potential iron protein from Chromatium vinosum within the protein frame through two-dimensional NMR experiments. Journal of the American Chemical Society, 1992, 114, 3332-3340.	13.7	97
61	NMR and Electronic Relaxation in Paramagnetic Dicopper(II) Compounds. Journal of the American Chemical Society, 1997, 119, 2156-2162.	13.7	97
62	Tuning the Affinity for Lanthanides of Calcium Binding Proteins. Biochemistry, 2003, 42, 8011-8021.	2.5	96
63	Metabolomic fingerprint of severe obesity is dynamically affected by bariatric surgery in a procedure-dependent manner. American Journal of Clinical Nutrition, 2015, 102, 1313-1322.	4.7	96
64	Are true scalar protonâ€"proton connectivities ever measured in COSY spectra of paramagnetic macromolecules?. Chemical Physics Letters, 1993, 203, 445-449.	2.6	95
65	Structural Information through NMR Hyperfine Shifts in Blue Copper Proteins. Journal of the American Chemical Society, 2000, 122, 3701-3707.	13.7	95
66	Solution Structure of the Paramagnetic Complex of the N-Terminal Domain of Calmodulin with Two Ce3+Ions by1H NMRâ€,â€¡. Biochemistry, 1997, 36, 11605-11618.	2.5	93
67	Nuclear spin relaxation in paramagnetic complexes of S=1: Electron spin relaxation effects. Journal of Chemical Physics, 1999, 111, 5795-5807.	3.0	93
68	Paramagnetic shifts in solid-state NMR of proteins to elicit structural information. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 17284-17289.	7.1	93
69	The electronic structure of FeS centers in proteins and models a contribution to the understanding of their electron transfer properties. Structure and Bonding, 1995, , 1-53.	1.0	91
70	The 1H NMR parameters of magnetically coupled dimersâ€"The Fe2S2 proteins as an example. , 1990, , 113-136.		87
71	Metabolomics in breast cancer: A decade in review. Cancer Treatment Reviews, 2018, 67, 88-96.	7.7	87
72	The electronic structure of iron-sulfur [Fe4S4]3+ clusters in proteins. An investigation of the oxidized high-potential iron-sulfur protein II from Ectothiorhodospira vacuolata. Biochemistry, 1993, 32, 9387-9397.	2.5	86

#	Article	IF	Citations
73	Solution Structure of the Oxidized 2[4Fe-4S] Ferredoxin from Clostridium Pasteurianum. FEBS Journal, 1995, 232, 192-205.	0.2	86
74	Paramagnetically Induced Residual Dipolar Couplings for Solution Structure Determination of Lanthanide Binding Proteins. Journal of the American Chemical Society, 2002, 124, 5581-5587.	13.7	86
75	Paramagnetic Ions Provide Structural Restraints in Solid-State NMR of Proteins. Journal of the American Chemical Society, 2007, 129, 2218-2219.	13.7	85
76	Evidence of Reciprocal Reorientation of the Catalytic and Hemopexin-Like Domains of Full-Length MMP-12. Journal of the American Chemical Society, 2008, 130, 7011-7021.	13.7	84
77	Identification of a serum-detectable metabolomic fingerprint potentially correlated with the presence of micrometastatic disease in early breast cancer patients at varying risks of disease relapse by traditional prognostic methods. Annals of Oncology, 2011, 22, 1295-1301.	1.2	83
78	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. Molecular Oncology, 2015, 9, 128-139.	4.6	82
79	The three-dimensional solution structure of the reduced high-potential iron-sulfur protein from Chromatium vinosum through NMR. Biochemistry, 1995, 34, 206-219.	2.5	80
80	Plasma and urinary metabolomic profiles of Down syndrome correlate with alteration of mitochondrial metabolism. Scientific Reports, 2018, 8, 2977.	3.3	80
81	The CuA Center of a Soluble Domain from Thermus Cytochrome ba3. An NMR Investigation of the Paramagnetic Protein. Journal of the American Chemical Society, 1996, 118, 11658-11659.	13.7	78
82	Water 1H relaxation dispersion analysis on a nitroxide radical provides information on the maximal signal enhancement in Overhauser dynamic nuclear polarization experiments. Physical Chemistry Chemical Physics, 2010, 12, 5902.	2.8	78
83	Uncovering the metabolomic fingerprint of breast cancer. International Journal of Biochemistry and Cell Biology, 2011, 43, 1010-1020.	2.8	77
84	Long-Range Correlated Dynamics in Intrinsically Disordered Proteins. Journal of the American Chemical Society, 2014, 136, 16201-16209.	13.7	77
85	One-thousand-fold enhancement of high field liquid nuclear magnetic resonance signals at room temperature. Nature Chemistry, 2017, 9, 676-680.	13.6	77
86	Acyl positional distribution of glycerol tri-esters in vegetable oils: a 13C NMR study. Chemistry and Physics of Lipids, 1999, 103, 47-55.	3.2	76
87	Metabolomic/lipidomic profiling of COVID-19 and individual response to tocilizumab. PLoS Pathogens, 2021, 17, e1009243.	4.7	76
88	Interdomain Flexibility in Full-length Matrix Metalloproteinase-1 (MMP-1). Journal of Biological Chemistry, 2009, 284, 12821-12828.	3.4	73
89	Exploration of serum metabolomic profiles and outcomes in women with metastatic breast cancer: A pilot study. Molecular Oncology, 2012, 6, 437-444.	4.6	73
90	Exploring the Subtleties of Drugâ"Receptor Interactions:Â The Case of Matrix Metalloproteinases. Journal of the American Chemical Society, 2007, 129, 2466-2475.	13.7	72

#	Article	IF	Citations
91	Paramagnetic relaxation as a tool for solution structure determination:Clostridium pasteurianum ferredoxin as an example. , 1997, 29, 348-358.		71
92	Liquid state DNP of water at 9.2 T: an experimental access to saturation. Physical Chemistry Chemical Physics, 2013, 15, 6049.	2.8	71
93	G-triplex structure and formation propensity. Nucleic Acids Research, 2014, 42, 13393-13404.	14.5	71
94	Evidence of the breaking of the copper-imidazolate bridge in copper/cobalt-substituted superoxide dismutase upon reduction of the copper(II) centers. Journal of the American Chemical Society, 1985, 107, 2178-2179.	13.7	70
95	Proton NMR spectra of oxidized high-potential iron-sulfur protein (HiPIP) from Rhodocyclus gelatinosus. A model for oxidized HiPIPs. Inorganic Chemistry, 1991, 30, 4517-4524.	4.0	70
96	Bond-Mediated Electron Tunneling in Ruthenium-Modified High-Potential Ironâ^'Sulfur Protein. Journal of the American Chemical Society, 2000, 122, 4532-4533.	13.7	70
97	Mechanistic Investigation of Î²-Galactosidase-Activated MR Contrast Agents. Inorganic Chemistry, 2008, 47, 56-68.	4.0	70
98	Entropic Contribution to the Linking Coefficient in Fragment Based Drug Design: A Case Study. Journal of Medicinal Chemistry, 2010, 53, 4285-4289.	6.4	70
99	A critical assessment of methods to recover information from averaged data. Physical Chemistry Chemical Physics, 2016, 18, 5686-5701.	2.8	70
100	The iron-sulfur cluster in the oxidized high-potential iron protein from Ectothiorhodospira halophila. Journal of the American Chemical Society, 1993, 115, 3431-3440.	13.7	69
101	A Serine â†' Cysteine Ligand Mutation in the High Potential Ironâ^'Sulfur Protein fromChromatium vinosumProvides Insight into the Electronic Structure of the [4Feâ^'4S] Cluster. Journal of the American Chemical Society, 1996, 118, 75-80.	13.7	69
102	The Solution Structure Refinement of the Paramagnetic Reduced High-Potential Iron-Sulfur Protein I from Ectothiorhodospira Halophila by Using Stable Isotope Labeling and Nuclear Relaxation. FEBS Journal, 1996, 241, 440-452.	0.2	69
103	1H NMRD PROFILES OF PARAMAGNETIC COMPLEXES AND METALLOPROTEINS. Advances in Inorganic Chemistry, 2005, 57, 105-172.	1.0	69
104	The Cardiovascular Risk of Healthy Individuals Studied by NMR Metabonomics of Plasma Samples. Journal of Proteome Research, 2011, 10, 4983-4992.	3.7	69
105	Solid-State NMR Crystallography through Paramagnetic Restraints. Journal of the American Chemical Society, 2012, 134, 5006-5009.	13.7	69
106	Paramagnetic Probes in Metalloproteins. Methods in Enzymology, 2001, 339, 314-340.	1.0	68
107	Examination of Matrix Metalloproteinase-1 in Solution. Journal of Biological Chemistry, 2013, 288, 30659-30671.	3.4	68
108	Paramagnetic NMR spectroscopy and coordination structure of cobalt(II) Cys112Asp azurin. Inorganic Chemistry, 1995, 34, 737-742.	4.0	67

#	Article	IF	Citations
109	Quality assurance multicenter comparison of different MR scanners for quantitative diffusion-weighted imaging. Journal of Magnetic Resonance Imaging, 2016, 43, 213-219.	3.4	67
110	The solution structure of paramagnetic metalloproteins. Progress in Biophysics and Molecular Biology, 1996, 66, 43-80.	2.9	66
111	Characterization of a Partially Unfolded High Potential Iron Protein. Biochemistry, 1997, 36, 9332-9339.	2.5	66
112	Locating the Metal Ion in Calcium-Binding Proteins by Using Cerium(III) as a Probe. ChemBioChem, 2001, 2, 550-558.	2.6	66
113	Phenotyping COPD by 1H NMR metabolomics of exhaled breath condensate. Metabolomics, 2014, 10, 302-311.	3.0	66
114	Evidence of a DHA Signature in the Lipidome and Metabolome of Human Hepatocytes. International Journal of Molecular Sciences, 2017, 18, 359.	4.1	66
115	Age and Sex Effects on Plasma Metabolite Association Networks in Healthy Subjects. Journal of Proteome Research, 2018, 17, 97-107.	3.7	66
116	NMR-based metabolomics identifies patients at high risk of death within two years after acute myocardial infarction in the AMI-Florence II cohort. BMC Medicine, 2019, 17, 3.	5.5	66
117	PSEUDYANA for NMR structure calculation of paramagnetic metalloproteins using torsion angle molecular dynamics. Journal of Biomolecular NMR, 1998, 12, 553-557.	2.8	65
118	The First Solution Structure of a Paramagnetic Copper(II) Protein:Â The Case of Oxidized Plastocyanin from the CyanobacteriumSynechocystisPCC6803. Journal of the American Chemical Society, 2001, 123, 2405-2413.	13.7	65
119	Serum Metabolomic Profiles Identify ER-Positive Early Breast Cancer Patients at Increased Risk of Disease Recurrence in a Multicenter Population. Clinical Cancer Research, 2017, 23, 1422-1431.	7.0	65
120	Three-Dimensional Solution Structure of the Oxidized High Potential Iron-Sulfur Protein from Chromatium vinosum through NMR. Comparative Analysis with the Solution Structure of the Reduced Species. Biochemistry, 1995, 34, 9851-9858.	2.5	64
121	Analysis of the Temperature Dependence of the1H and13C Isotropic Shifts of Horse Heart Ferricytochromec:Â Explanation of Curie and Anti-Curie Temperature Dependence and Nonlinear Pseudocontact Shifts in a Common Two-Level Framework. Journal of the American Chemical Society, 1998, 120, 8472-8479.	13.7	64
122	Sulfonamide-Functionalized Gadolinium DTPA Complexes as Possible Contrast Agents for MRI: A Relaxometric Investigation. , 2000, 2000, 625-630.		64
123	Are Patients with Potential Celiac Disease Really Potential? The Answer of Metabonomics. Journal of Proteome Research, 2011, 10, 714-721.	3.7	64
124	Dynamic Nuclear Polarization of ¹H, ¹³C, and ⁵⁹Co in a Tris(ethylenediamine)cobalt(III) Crystalline Lattice Doped with Cr(III). Journal of the American Chemical Society, 2014, 136, 11716-11727.	13.7	64
125	Regulation of HuR structure and function by dihydrotanshinone-I. Nucleic Acids Research, 2017, 45, 9514-9527.	14.5	64
126	Structural Basis of Serine/Threonine Phosphatase Inhibition by the Archetypal Small Molecules Cantharidin and Norcantharidin. Journal of Medicinal Chemistry, 2009, 52, 4838-4843.	6.4	62

#	Article	IF	Citations
127	SedNMR: On the Edge between Solution and Solid-State NMR. Accounts of Chemical Research, 2013, 46, 2059-2069.	15.6	62
128	Sarcolab pilot study into skeletal muscleâ€™s adaptation to long-term spaceflight. Npj Microgravity, 2018, 4, 18.	3.7	62
129	13C Direct Detected NMR Increases the Detectability of Residual Dipolar Couplings. Journal of the American Chemical Society, 2006, 128, 15042-15043.	13.7	61
130	1H NMRD profiles of diamagnetic proteins: a model-free analysis. Magnetic Resonance in Chemistry, 2000, 38, 543-550.	1.9	60
131	Nanodiamondâ€“Gadolinium(III) Aggregates for Tracking Cancer Growth In Vivo at High Field. Nano Letters, 2016, 16, 7551-7564.	9.1	60
132	An investigation of superoxide dismutase Lys-143, Ile-143, and Glu-143 mutants: Cu2Co2SOD derivatives. Journal of the American Chemical Society, 1988, 110, 3629-3633.	13.7	59
133	Metabolomic fingerprint of heart failure in humans: A nuclear magnetic resonance spectroscopy analysis. International Journal of Cardiology, 2013, 168, e113-e115.	1.7	59
134	Allostasis and Resilience of the Human Individual Metabolic Phenotype. Journal of Proteome Research, 2015, 14, 2951-2962.	3.7	58
135	Thermotoga maritima IscU. Structural Characterization and Dynamics of a New Class of Metallochaperone. Journal of Molecular Biology, 2003, 331, 907-924.	4.2	57
136	¹H and ¹³C Dynamic Nuclear Polarization in Aqueous Solution with a Two-Field (0.35 T/14 T) Shuttle DNP Spectrometer. Journal of the American Chemical Society, 2009, 131, 15086-15087.	13.7	57
137	EF-hand protein dynamics and evolution of calcium signal transduction: an NMR view. Journal of Biological Inorganic Chemistry, 2006, 11, 949-962.	2.6	56
138	Dynamic Nuclear Polarization of Sedimented Solutes. Journal of the American Chemical Society, 2013, 135, 1641-1644.	13.7	56
139	The epr spectra of the inhibitor derivatives of cobalt carbonic anhydrase. Journal of Inorganic Biochemistry, 1981, 14, 81-93.	3.5	55
140	Browsing gene banks for Fe2S2 ferredoxins and structural modeling of 88 plant-type sequences: An analysis of fold and function. Proteins: Structure, Function and Bioinformatics, 2002, 46, 110-127.	2.6	55
141	In vitro fermentation of potential prebiotic flours from natural sources: Impact on the human colonic microbiota and metabolome. Molecular Nutrition and Food Research, 2012, 56, 1342-1352.	3.3	55
142	1H-NMR studies on partially and fully reduced 2(4Fe-4S) ferredoxin from Clostridium pasteurianum. FEBS Journal, 1992, 204, 831-839.	0.2	54
143	Paramagnetic Metal Ions in Ligand Screening: The CoII Matrix Metalloproteinase 12. Angewandte Chemie - International Edition, 2004, 43, 2254-2256.	13.8	54
144	Magnetic susceptibility and paramagnetism-based NMR. Progress in Nuclear Magnetic Resonance Spectroscopy, 2019, 114-115, 211-236.	7.5	54

#	Article	IF	Citations
145	Hydrogen-1 NMR spectra of the coordination sphere of cobalt-substituted carbonic anhydrase. Journal of the American Chemical Society, 1981, 103, 7784-7788.	13.7	53
146	Water Exchange at the Active Site of Carbonic Anhydrase. Biophysical Journal, 1983, 41, 179-187.	0.5	53
147	A Heteronuclear Direct-Detection NMR Spectroscopy Experiment for Protein-Backbone Assignment. Angewandte Chemie - International Edition, 2004, 43, 2257-2259.	13.8	52
148	Persistent contrast enhancement by sterically stabilized paramagnetic liposomes in murine melanoma. Magnetic Resonance in Medicine, 2004, 52, 669-672.	3.0	52
149	Unraveling Hidden Regulatory Sites in Structurally Homologous Metalloproteases. Journal of Molecular Biology, 2013, 425, 2330-2346.	4.2	52
150	Recognition Pliability Is Coupled to Structural Heterogeneity: A Calmodulin Intrinsically Disordered Binding Region Complex. Structure, 2012, 20, 522-533.	3.3	51
151	Pseudoâ€Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMPâ€12 from First Principles. Angewandte Chemie - International Edition, 2016, 55, 14713-14717.	13.8	51
152	Identification of productive and futile encounters in an electron transfer protein complex. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E1840-E1847.	7.1	51
153	Backbone Dynamics of Plastocyanin in Both Oxidation States. Journal of Biological Chemistry, 2001, 276, 47217-47226.	3.4	50
154	Gd(III)-Labeled Peptide Nanofibers for Reporting on Biomaterial Localization in Vivo. ACS Nano, 2014, 8, 7325-7332.	14.6	50
155	Basic facts and perspectives of Overhauser DNP NMR. Journal of Magnetic Resonance, 2016, 264, 78-87.	2.1	50
156	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. Analytical Chemistry, 2018, 90, 649-656.	6.5	50
157	High resolution solution structure of the protein part of Cu7 metallothionein. FEBS Journal, 2000, 267, 1008-1018.	0.2	49
158	Crystal Structure of the Catalytic Domain of Human Matrix Metalloproteinase 10. Journal of Molecular Biology, 2004, 336, 707-716.	4.2	49
159	Local and Global Dynamics in Intrinsically Disordered Synuclein. Angewandte Chemie - International Edition, 2018, 57, 15262-15266.	13.8	49
160	NMR for sample quality assessment in metabolomics. New Biotechnology, 2019, 52, 25-34.	4.4	49
161	Proton NMR studies of the cobalt(II)-metallothionein system. Journal of the American Chemical Society, 1989, 111, 7296-7300.	13.7	48
162	Solution Structure of the Oxidized Fe7S8Ferredoxin from the Thermophilic BacteriumBacillusschlegeliiby1H NMR Spectroscopyâ€,â€¡. Biochemistry, 1998, 37, 9812-9826.	2.5	48

#	Article	IF	Citations
163	On the use of ultracentrifugal devices for sedimented solute NMR. Journal of Biomolecular NMR, 2012, 54, 123-127.	2.8	48
164	Extreme Hypoxic Conditions Induce Selective Molecular Responses and Metabolic Reset in Detached Apple Fruit. Frontiers in Plant Science, 2016, 7, 146.	3.6	48
165	Deconvoluting interrelationships between concentrations and chemical shifts in urine provides a powerful analysis tool. Nature Communications, 2017, 8, 1662.	12.8	48
166	Nuclear and electron relaxation of hexaaquairon(3+). The Journal of Physical Chemistry, 1993, 97, 1134-1137.	2.9	47
167	Electron self-exchange in high-potential iron-sulfur proteins. Characterization of protein I from Ectothiorhodospira vacuolata. Biochemistry, 1993, 32, 12887-12893.	2.5	47
168	NMR properties of sedimented solutes. Physical Chemistry Chemical Physics, 2012, 14, 439-447.	2.8	47
169	Nuclear Magnetic Relaxation Dispersion Studies of Hexaaquo Mn(II) Ions in Water-Glycerol Mixtures. Journal of Magnetic Resonance Series A, 1993, 101, 198-201.	1.6	46
170	Individual Reduction Potentials of the Iron Ions in Fe2S2and High-Potential Fe4S4Ferredoxins. Inorganic Chemistry, 1996, 35, 4248-4253.	4.0	46
171	Collective Relaxation of Protein Protons at Very Low Magnetic Field:Â A New Window on Protein Dynamics and Aggregation. Journal of the American Chemical Society, 2007, 129, 1055-1064.	13.7	46
172	Metabolomic profile of term infants of gestational diabetic mothers. Journal of Maternal-Fetal and Neonatal Medicine, 2014, 27, 537-542.	1.5	46
173	Electronic and Geometric Structure of the CuA Site Studied by 1H NMR in a Soluble Domain of Cytochrome c Oxidase from Paracoccus denitrificans. Journal of the American Chemical Society, 1997, 119, 11023-11027.	13.7	45
174	The Magnetic Properties of Myoglobin as Studied by NMR Spectroscopy. Chemistry - A European Journal, 2003, 9, 2316-2322.	3.3	45
175	Combining in Silico Tools and NMR Data To Validate Proteinâ^'Ligand Structural Models:Â Application to Matrix Metalloproteinases. Journal of Medicinal Chemistry, 2005, 48, 7544-7559.	6.4	45
176	The catalytic domain of MMPâ€1 studied through tagged lanthanides. FEBS Letters, 2012, 586, 557-567.	2.8	45
177	Simultaneous use of solution NMR and X-ray data inREFMAC5 for joint refinement/detection of structural differences. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 958-967.	2.5	45
178	Probabilistic Networks of Blood Metabolites in Healthy Subjects As Indicators of Latent Cardiovascular Risk. Journal of Proteome Research, 2015, 14, 1101-1111.	3.7	45
179	2D1H NMR studies of oxidized 2(Fe4S4) ferredoxin fromClostridium pasteurianum. FEBS Letters, 1991, 289, 253-256.	2.8	44
180	X-Ray, NMR and Molecular Dynamics Studies on Reduced Bovine Superoxide Dismutase: Implications for the Mechanism. Biochemical and Biophysical Research Communications, 1994, 202, 1088-1095.	2.1	44

#	Article	IF	Citations
181	Coordination sphere versus protein environment as determinants of electronic and functional properties of iron-sulfur proteins. Structure and Bonding, 1998, , 127-160.	1.0	44
182	Non-ionic bulky Gd(III) DTPA-bisamide complexes as potential contrast agents for magnetic resonance imaging. Magnetic Resonance in Medicine, 1999, 41, 767-773.	3.0	44
183	Solution Structure Calculations through Self-Orientation in a Magnetic Field of a Cerium(III) Substituted Calcium-Binding Protein. Journal of Magnetic Resonance, 2001, 148, 23-30.	2.1	44
184	Cross Correlation between the Dipoleâ€“Dipole Interaction and the Curie Spin Relaxation: The Effect of Anisotropic Magnetic Susceptibility. Journal of Magnetic Resonance, 2001, 152, 103-108.	2.1	43
185	NMR crystallography on paramagnetic systems: solved and open issues. CrystEngComm, 2013, 15, 8639.	2.6	43
186	Plasma and Serum Metabolite Association Networks: Comparability within and between Studies Using NMR and MS Profiling. Journal of Proteome Research, 2017, 16, 2547-2559.	3.7	43
187	NMR and Spin Relaxation in Dimers. Accounts of Chemical Research, 1998, 31, 351-361.	15.6	42
188	Narrowing the conformational space sampled by two-domain proteins with paramagnetic probes in both domains. Journal of Biomolecular NMR, 2011, 51, 253-263.	2.8	42
189	Experimental Determination of Microsecond Reorientation Correlation Times in Protein Solutions. Journal of Physical Chemistry B, 2013, 117, 3548-3553.	2.6	42
190	Metabolomics to Assess Response to Immune Checkpoint Inhibitors in Patients with Non-Small-Cell Lung Cancer. Cancers, 2020, 12, 3574.	3.7	42
191	An investigation of a human erythrocyte SOD modified at position 137. Journal of the American Chemical Society, 1989, 111, 714-719.	13.7	41
192	A Calix[4]arene GdIII Complex Endowed with High Stability, Relaxivity, and Binding Affinity to Serum Albumin. Angewandte Chemie - International Edition, 2001, 40, 4737-4739.	13.8	41
193	X-ray Structures of Binary and Ternary Enzyme-Product-Inhibitor Complexes of Matrix Metalloproteinases. Angewandte Chemie - International Edition, 2003, 42, 2673-2676.	13.8	41
194	Conformational freedom of metalloproteins revealed by paramagnetism-assisted NMR. Coordination Chemistry Reviews, 2013, 257, 2652-2667.	18.8	41
195	Solidâ€State NMR of PEGylated Proteins. Angewandte Chemie - International Edition, 2016, 55, 2446-2449.	13.8	41
196	Interaction of anions with the active site of carboxypeptidase A. Biochemistry, 1988, 27, 1050-1057.	2.5	40
197	Proton NMR studies of the oxidized and partially reduced 2(4Fe-4S) ferredoxin from Clostridium pasteurianum. Inorganic Chemistry, 1990, 29, 1874-1880.	4.0	40
198	A mÃ¶ssbauer investigation of oxidized Fe4S4 HiPIP II from Ectothiorhodospira halophila. Journal of Inorganic Biochemistry, 1993, 52, 227-234.	3.5	40

#	Article	IF	Citations
199	Influence of Surface Charges on Redox Properties in High Potential Iron-Sulfur Proteins. Biochemical and Biophysical Research Communications, 1994, 203, 436-442.	2.1	40
200	Sequence-Specific Assignment of Ligand Cysteine Protons of Oxidized, Recombinant HiPIP I from Ectothiorhodospira halophila. Inorganic Chemistry, 1995, 34, 2516-2523.	4.0	40
201	Concentration dependence of13C NMR spectra of triglycerides: implications for the NMR analysis of olive oils. Magnetic Resonance in Chemistry, 2000, 38, 886-890.	1.9	40
202	Nuclear Spin Relaxation in Paramagnetic Systems:Â Electron Spin Relaxation Effects under Near-Redfield Limit Conditions and Beyond. Journal of Physical Chemistry A, 2002, 106, 7376-7382.	2.5	40
203	Cross correlation rates between Curie spin and dipole-dipole relaxation in paramagnetic proteins: the case of cerium substituted calbindin D9k. Journal of Biomolecular NMR, 2002, 23, 115-125.	2.8	40
204	Solid-State NMR of Matrix Metalloproteinase 12: An Approach Complementary to Solution NMR. ChemBioChem, 2007, 8, 486-489.	2.6	40
205	Paramagnetic relaxation enhancement for the characterization of the conformational heterogeneity in two-domain proteins. Physical Chemistry Chemical Physics, 2012, 14, 9149.	2.8	40
206	Topical Developments in Highâ€Field Dynamic Nuclear Polarization. Israel Journal of Chemistry, 2014, 54, 207-221.	2.3	40
207	Knowledge discovery by accuracy maximization. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5117-5122.	7.1	40
208	SSNMR of biosilica-entrapped enzymes permits an easy assessment of preservation of native conformation in atomic detail. Chemical Communications, 2014, 50, 421-423.	4.1	40
209	COSY spectra of paramagnetic macromolecules: Observability, scalar effects, cross-correlation effects, relaxation-allowed coherence transfer. Concepts in Magnetic Resonance, 1994, 6, 307-335.	1.3	39
210	New applications of paramagnetic NMR in chemical biology. Current Opinion in Chemical Biology, 1999, 3, 145-151.	6.1	39
211	Effects of Intra- and Post-Operative Ischemia on the Metabolic Profile of Clinical Liver Tissue Specimens Monitored by NMR. Journal of Proteome Research, 2013, 12, 5723-5729.	3.7	39
212	High-field liquid state NMR hyperpolarization: a combined DNP/NMRD approach. Physical Chemistry Chemical Physics, 2014, 16, 18781-18787.	2.8	39
213	Insights into Domainâ€“Domain Motions in Proteins and RNA from Solution NMR. Accounts of Chemical Research, 2014, 47, 3118-3126.	15.6	39
214	FANTEN: a new web-based interface for the analysis of magnetic anisotropy-induced NMR data. Journal of Biomolecular NMR, 2015, 61, 21-34.	2.8	39
215	NMR metabolomic fingerprinting distinguishes milk from different farms. Food Research International, 2018, 113, 131-139.	6.2	39
216	Mixing AÎ²(1â€“40) and AÎ²(1â€“42) peptides generates unique amyloid fibrils. Chemical Communications, 2020, 56, 8830-8833.	4.1	39

#	Article	IF	Citations
217	Three-Dimensional Structure of the Reduced C77S Mutant of theChromatium vinosumHigh-Potential Ironâ^'Sulfur Protein through Nuclear Magnetic Resonance:Â Comparison with the Solution Structure of the Wild-Type Proteinâ€,â€¡. Biochemistry, 1996, 35, 5928-5936.	2.5	38
218	Structural and Dynamical Properties of a Partially Unfolded Fe4S4Protein:Â Role of the Cofactor in Protein Foldingâ€. Biochemistry, 1999, 38, 4669-4680.	2.5	38
219	Solvent 1H NMRD study of biotinylated paramagnetic liposomes containing Gd-bis-SDA-DTPA or Gd-DMPE-DTPA. Inorganica Chimica Acta, 2002, 331, 151-157.	2.4	38
220	Direct Carbon Detection in Paramagnetic Metalloproteins To Further Exploit Pseudocontact Shift Restraints. Journal of the American Chemical Society, 2004, 126, 10496-10497.	13.7	38
221	Formation Kinetics and Structural Features of Betaâ€Amyloid Aggregates by Sedimented Solute NMR. ChemBioChem, 2013, 14, 1891-1897.	2.6	38
222	Individual Human Metabolic Phenotype Analyzed by ¹H NMR of Saliva Samples. Journal of Proteome Research, 2016, 15, 1787-1793.	3.7	38
223	1H NMRD studies of solutions of paramagnetic metal ions in ethyleneglycol. Inorganica Chimica Acta, 1985, 100, 173-181.	2.4	37
224	An NMR Study of the 7Fe-8S Ferredoxin fromRhodopseudomonas palustrisand Reinterpretation of Data on Similar Systemsâ€. Biochemistry, 1997, 36, 3570-3579.	2.5	37
225	Are unit charges always negligible?. Journal of Biological Inorganic Chemistry, 1997, 2, 114-118.	2.6	37
226	Molecular Determinants of a Selective Matrix Metalloprotease-12 Inhibitor: Insights from Crystallography and Thermodynamic Studies. Journal of Medicinal Chemistry, 2013, 56, 1149-1159.	6.4	37
227	Copper-zinc superoxide dismutase: A paramagnetic protein that provides a unique frame for the NMR investigation. Progress in Nuclear Magnetic Resonance Spectroscopy, 1994, 26, 91-139.	7.5	36
228	Ab initio solution and refinement of two high-potential iron protein structures at atomic resolution. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1773-1784.	2.5	36
229	Probing Structural and Electronic Properties of the Oxidized [Fe4S4]3+Cluster ofEctothiorhodospirahalophilaiso-II High-Potential Ironâ^'Sulfur Protein by ENDOR Spectroscopy. Journal of the American Chemical Society, 1999, 121, 1925-1935.	13.7	36
230	MaxOcc: a web portal for maximum occurrence analysis. Journal of Biomolecular NMR, 2012, 53, 271-280.	2.8	36
231	Practical considerations over spectral quality in solid state NMR spectroscopy of soluble proteins. Journal of Biomolecular NMR, 2013, 57, 155-166.	2.8	36
232	DNP-Enhanced MAS NMR of Bovine Serum Albumin Sediments and Solutions. Journal of Physical Chemistry B, 2014, 118, 2957-2965.	2.6	36
233	Paradoxically, Most Flexible Ligand Binds Most Entropy-Favored: Intriguing Impact of Ligand Flexibility and Solvation on Drugâ€"Kinase Binding. Journal of Medicinal Chemistry, 2018, 61, 5922-5933.	6.4	36
234	The metabolic fingerprints of HCV and HBV infections studied by Nuclear Magnetic Resonance Spectroscopy. Scientific Reports, 2019, 9, 4128.	3.3	36

#	Article	IF	Citations
235	A multinuclear ligand NMR investigation of cyanide, cyanate, and thiocyanate binding to zinc and cobalt carbonic anhydrase. Inorganic Chemistry, 1992, 31, 3975-3979.	4.0	35
236	One- and two-dimensional NMR characterization of oxidized and reduced cytochrome c' from Rhodocyclus gelatinosus. Biochemistry, 1993, 32, 776-783.	2.5	35
237	Bioinformatic Comparison of Structures and Homology-Models of Matrix Metalloproteinases. Journal of Proteome Research, 2004, 3, 21-31.	3.7	35
238	NMR in structural proteomics and beyond. Progress in Nuclear Magnetic Resonance Spectroscopy, 2010, 56, 247-266.	7.5	35
239	Hydrogen-1 NOE and ligand field studies of copper-cobalt superoxide dismutase with anions. Inorganic Chemistry, 1990, 29, 4867-4873.	4.0	34
240	13C-13C NOESY: A constructive use of 13C-13C spin-diffusion. Journal of Biomolecular NMR, 2004, 30, 245-251.	2.8	34
241	NMR Spectroscopic Detection of Protein Protons and Longitudinal Relaxation Rates between 0.01 and 50 MHz. Angewandte Chemie - International Edition, 2005, 44, 2223-2225.	13.8	34
242	Efficient determination of the most favoured orientations of protein domains from paramagnetic NMR data. Inverse Problems, 2006, 22, 1485-1502.	2.0	34
243	Nuclear Relaxometry Helps Designing Systems for Solution DNP on Proteins. Applied Magnetic Resonance, 2008, 34, 379.	1.2	34
244	Electronic relaxation of a copper(II) dimer in a macromolecular complex as evaluated from solvent proton relaxation. Inorganic Chemistry, 1988, 27, 951-953.	4.0	33
245	Molecular dynamics simulations on HiPIP from Chromatium vinosum and comparison with NMR data. Journal of the American Chemical Society, 1992, 114, 10683-10689.	13.7	33
246	1H-NMR investigation of oxidized and reduced high-potential iron-sulfur protein from Rhodopseudomonas globiformis. FEBS Journal, 1993, 212, 69-78.	0.2	33
247	Binding of Gadobenate Dimeglumine to Proteins Extravasated into Interstitial Space Enhances Conspicuity of Reperfused Infarcts. Investigative Radiology, 1994, 29, S50-S53.	6.2	33
248	Structural and Dynamic Information on Double-Decker Yb3+and Dy3+Porphyrin Complexes in Solution through1H NMR. Inorganic Chemistry, 1996, 35, 6308-6315.	4.0	33
249	â€œFour-Dimensionalâ€•Protein Structures:â€‰ Examples from Metalloproteins. Accounts of Chemical Research, 2006, 39, 909-917.	15.6	33
250	KODAMA: an R package for knowledge discovery and data mining. Bioinformatics, 2017, 33, 621-623.	4.1	33
251	Water in the coordination sphere of metallocarbonic anhydrases: A solvent proton longitudinal relaxation study at several frequencies. Inorganica Chimica Acta, 1981, 56, 99-107.	2.4	32
252	Magnetic relaxation of solvent protons by copper(2+)- and dioxovanadium(2+)-substituted transferrin: theoretical analysis and biochemical implications. Biochemistry, 1985, 24, 6287-6290.	2.5	32

#	Article	IF	Citations
253	Solution structure of the unbound, oxidized Photosystem I subunit PsaC, containing [4Fe-4S] clusters FA and FB: a conformational change occurs upon binding to Photosystem I. Journal of Biological Inorganic Chemistry, 2002, 7, 461-472.	2.6	32
254	Paramagnetism-Based Refinement Strategy for the Solution Structure of Human Î±-Parvalbuminâ€. Biochemistry, 2004, 43, 5562-5573.	2.5	32
255	Characterization of PEGylated Asparaginase: New Opportunities from NMR Analysis of Large PEGylated Therapeutics. Chemistry - A European Journal, 2019, 25, 1984-1991.	3.3	32
256	Fingerprinting Alzheimerâ€™s Disease by ¹H Nuclear Magnetic Resonance Spectroscopy of Cerebrospinal Fluid. Journal of Proteome Research, 2020, 19, 1696-1705.	3.7	32
257	Evidence of exchangeable protons in the donor groups of the acidic form of cobalt bovine carbonic anhydrase B. Biochemical and Biophysical Research Communications, 1977, 78, 158-160.	2.1	31
258	pH-Dependent properties of a CoN4(OH2) chromophore: a spectroscopic model of cobalt carbonic anhydrase. Inorganic Chemistry, 1981, 20, 1670-1673.	4.0	31
259	Mechanism and Inhibition of Matrix Metalloproteinases. Current Medicinal Chemistry, 2019, 26, 2609-2633.	2.4	31
260	The acid-base equilibria of carbonic anhydrase. Inorganica Chimica Acta, 1980, 46, 85-89.	2.4	30
261	NMR proton relaxation in bimetallic complexes of zinc(II), nickel(II), and copper(II). Journal of the American Chemical Society, 1986, 108, 3298-3303.	13.7	30
262	Investigation of copper-zinc superoxide dismutase Ser-137 and Ala-137 mutants. Inorganic Chemistry, 1990, 29, 2398-2403.	4.0	30
263	A comment on the proton NMR spectra of cobalt(II)-substituted superoxide dismutases with histidines deuteriated in the .epsilon.1-position. Inorganic Chemistry, 1990, 29, 1438-1440.	4.0	30
264	The Solution Structure of Oxidized HiPIP I from Ectothiorhodospira halophila; Can NMR Spectroscopy Be Used to Probe Rearrangements Associated with Electron Transfer Processes?. Chemistry - A European Journal, 1995, 1, 598-607.	3.3	30
265	ePHOGSY experiments on a paramagnetic protein: location of the catalytic water molecule in the heme crevice of the oxidized form of horse heart cytochrome c. FEBS Letters, 1997, 415, 45-48.	2.8	30
266	Backbone-Only Protein Solution Structures with a Combination of Classical and Paramagnetism-Based Constraints: A Method that Can Be Scaled to Large Molecules. ChemPhysChem, 2004, 5, 797-806.	2.1	30
267	Structure-based approach to nanomolar, water soluble matrix metalloproteinases inhibitors (MMPIs). European Journal of Medicinal Chemistry, 2010, 45, 5919-5925.	5.5	30
268	Biosilicaâ€Entrapped Enzymes Studied by Using Dynamic Nuclearâ€Polarizationâ€Enhanced Highâ€Field NMR Spectroscopy. ChemPhysChem, 2015, 16, 2751-2754.	2.1	30
269	Dependence of apparent diffusion coefficient measurement on diffusion gradient direction and spatial position â€“ A quality assurance intercomparison study of forty-four scanners for quantitative diffusion-weighted imaging. Physica Medica, 2018, 55, 135-141.	0.7	30
270	Solution structure of reduced Clostridium pasteurianum rubredoxin. Journal of Biological Inorganic Chemistry, 1998, 3, 401.	2.6	30

#	Article	IF	Citations
271	Profiling metabolites and lipoproteins in COMETA, an Italian cohort of COVID-19 patients. PLoS Pathogens, 2022, 18, e1010443.	4.7	30
272	Water in the active cavity of copper/zinc superoxide dismutase. A water 1H-nuclear-magnetic-relaxation-dispersion study. FEBS Journal, 1989, 184, 125-129.	0.2	29
273	1H NOE studies of oxidized high potential iron sulfur protein II from Ectothiorhodospira halophila. Inorganica Chimica Acta, 1991, 180, 171-175.	2.4	29
274	NMR is a unique and necessary step in the investigation of iron sulfur proteins: the HiPIP from R. gelatinosus as an example. Inorganica Chimica Acta, 1992, 198-200, 483-491.	2.4	29
275	Solution Structure of Human Î²-Parvalbumin and Structural Comparison with Its Paralog Î±-Parvalbumin and with Their Rat Orthologsâ€,â€¡. Biochemistry, 2004, 43, 16076-16085.	2.5	29
276	The impact of free or standardized lifestyle and urine sampling protocol on metabolome recognition accuracy. Genes and Nutrition, 2015, 10, 441.	2.5	29
277	Aggregation kinetics of the AÎ²1â€“40 peptide monitored by NMR. Chemical Communications, 2018, 54, 7601-7604.	4.1	29
278	Binding affinity of bicarboxylate ions for cobalt(II) bovine carbonic anhydrase. Bioinorganic Chemistry, 1978, 9, 93-100.	1.1	28
279	Two-dimensional proton NMR studies of the paramagnetic metalloenzyme copper-nickel superoxide dismutase. Inorganic Chemistry, 1992, 31, 4433-4435.	4.0	28
280	[17] Two-dimensional nuclear magnetic resonance spectra of paramagnetic systems. Methods in Enzymology, 1994, 239, 485-514.	1.0	28
281	Protein Hydration and Location of Water Molecules in Oxidized Horse Heart Cytochrome c by 1H NMR. Journal of Magnetic Resonance, 2000, 147, 1-8.	2.1	28
282	Principal Component Analysis of the Conformational Freedom within the EF-Hand Superfamily. Journal of Proteome Research, 2005, 4, 1961-1971.	3.7	28
283	A High-Affinity Carbohydrate-Containing Inhibitor of Matrix Metalloproteinases. ChemMedChem, 2006, 1, 598-601.	3.2	28
284	Moving the frontiers in solution and solid-state bioNMR. Coordination Chemistry Reviews, 2011, 255, 649-663.	18.8	28
285	The effect of Gd on trityl-based dynamic nuclear polarisation in solids. Physical Chemistry Chemical Physics, 2015, 17, 26969-26978.	2.8	28
286	Metabolomics in Breast Cancer: Current Status and Perspectives. Advances in Experimental Medicine and Biology, 2016, 882, 217-234.	1.6	28
287	NMR-based metabolomic approach to study urine samples of chronic inflammatory rheumatic disease patients. Analytical and Bioanalytical Chemistry, 2017, 409, 1405-1413.	3.7	28
288	Solution of a Puzzle: High-Level Quantum-Chemical Treatment of Pseudocontact Chemical Shifts Confirms Classic Semiempirical Theory. Journal of Physical Chemistry Letters, 2020, 11, 8735-8744.	4.6	28

#	Article	IF	Citations
289	Investigation of the system copper(II) carbonic anhydrase and HCO3â¯1/CO2. Journal of Inorganic Biochemistry, 1983, 18, 221-229.	3.5	27
290	1H and 13C NMR Studies of an Oxidized HiPIP. Inorganic Chemistry, 1997, 36, 4798-4803.	4.0	27
291	Lanthanide induced residual dipolar couplings for the conformational investigation of peripheral 15NH2 moieties. Journal of Biomolecular NMR, 2000, 18, 347-355.	2.8	27
292	Chemical shift-based constraints for solution structure determination of paramagnetic low-spin heme proteins with bis-His and His-CN axial ligands: the cases of oxidized cytochrome b 5 and Met80Ala cyano-cytochrome c. Journal of Biological Inorganic Chemistry, 2002, 7, 416-426.	2.6	27
293	Efficiency of paramagnetism-based constraints to determine the spatial arrangement of alpha-helical secondary structure elements. Journal of Biomolecular NMR, 2002, 22, 123-136.	2.8	27
294	How to tackle protein structural data from solution and solid state: An integrated approach. Progress in Nuclear Magnetic Resonance Spectroscopy, 2016, 92-93, 54-70.	7.5	27
295	Differential Network Analysis Reveals Metabolic Determinants Associated with Mortality in Acute Myocardial Infarction Patients and Suggests Potential Mechanisms Underlying Different Clinical Scores Used To Predict Death. Journal of Proteome Research, 2020, 19, 949-961.	3.7	27
296	Relaxation of the electronic spin moment of copper(II)-macromolecular complexes in solution. Journal of the American Chemical Society, 1989, 111, 3532-3536.	13.7	26
297	Proton NMR spectra of the Co4S11 cluster in metallothioneins: a theoretical model. Journal of the American Chemical Society, 1989, 111, 7300-7303.	13.7	26
298	Electronic structure of the [Fe4Se4]3+ clusters in C. vinosum HiPIP and Ectothiorhodospiza halophila HiPIP II through NMR and EPR studies. Journal of the American Chemical Society, 1993, 115, 12020-12028.	13.7	26
299	A theoretical analysis of the 1H nuclear magnetic relaxation dispersion profiles of diferric transferrin. The Journal of Physical Chemistry, 1995, 99, 14217-14222.	2.9	26
300	The solution structure of parsley [2Fe-2S]ferredoxin. FEBS Journal, 1998, 258, 465-477.	0.2	26
301	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 [4Fe-4S] centers FA â˚ and FB â˚. Journal of Biological Inorganic Chemistry, 2000, 5, 381-392.	2.6	26
302	A use of Ramachandran potentials in protein solution structure determinations. Journal of Biomolecular NMR, 2003, 26, 355-366.	2.8	26
303	Towards a Protocol for Solution Structure Determination of Copper(II) Proteins: the Case of CuIIZnII Superoxide Dismutase. ChemBioChem, 2007, 8, 1422-1429.	2.6	26
304	A Metabolomic Perspective on Coeliac Disease. Autoimmune Diseases, 2014, 2014, 1-13.	0.6	26
305	Exploring Regions of Conformational Space Occupied by Two-Domain Proteins. Journal of Physical Chemistry B, 2014, 118, 10576-10587.	2.6	26
306	Metabolic Signature of Primary Biliary Cholangitis and Its Comparison with Celiac Disease. Journal of Proteome Research, 2019, 18, 1228-1236.	3.7	26

#	Article	IF	Citations
307	Assignment of active-site protons in the 1H-NMR spectrum of reduced human Cu/Zn superoxide dismutase. FEBS Journal, 1991, 197, 691-697.	0.2	25
308	Strategies of Signal Assignments in Paramagnetic Metalloproteins. An NMR Investigation of the Thiocyanate Adduct of the Cobalt(II)-Substituted Human Carbonic Anhydrase II. Journal of Magnetic Resonance Series B, 1994, 104, 230-239.	1.6	25
309	Sequence-specific assignment of the 1H and 15N nuclear magnetic resonance spectra of the reduced recombinant high-potential iron-sulfur protein I from Ectothiorhodospira halophila. FEBS Journal, 1994, 225, 703-714.	0.2	25
310	Hyperfine Shifts in Low-Spin Iron(III) Hemes: A Ligand Field Analysis. European Journal of Inorganic Chemistry, 2000, 2000, 2473-2480.	2.0	25
311	Solvent 1H NMRD Study of Hexaaquochromium(III):â€‰ Inferences on Hydration and Electron Relaxation. Inorganic Chemistry, 2001, 40, 4030-4035.	4.0	25
312	Solution structure and dynamics of S100A5 in the apo and Ca2+-bound states. Journal of Biological Inorganic Chemistry, 2009, 14, 1097-1107.	2.6	25
313	Intra- and Interdomain Flexibility in Matrix Metalloproteinases: Functional Aspects and Drug Design. Current Pharmaceutical Design, 2009, 15, 3592-3605.	1.9	25
314	Overhauser DNP with¹⁵N labelled FrÃ©my's salt at 0.35 Tesla. Physical Chemistry Chemical Physics, 2012, 14, 502-510.	2.8	25
315	Mechanisms of Gadographene-Mediated Proton Spin Relaxation. Journal of Physical Chemistry C, 2013, 117, 16263-16273.	3.1	25
316	Atomicâ€Level Quality Assessment of Enzymes Encapsulated in Bioinspired Silica. Chemistry - A European Journal, 2016, 22, 425-432.	3.3	25
317	Breathomics for Assessing the Effects of Treatment and Withdrawal With Inhaled Beclomethasone/Formoterol in Patients With COPD. Frontiers in Pharmacology, 2018, 9, 258.	3.5	25
318	Dissecting the Interactions between Human Serum Albumin and Î±-Synuclein: New Insights on the Factors Influencing Î±-Synuclein Aggregation in Biological Fluids. Journal of Physical Chemistry B, 2019, 123, 4380-4386.	2.6	25
319	Serum or Plasma (and Which Plasma), That Is the Question. Journal of Proteome Research, 2022, 21, 1061-1072.	3.7	25
320	Application of 2D NMR techniques to paramagnetic systems. Inorganic Chemistry, 1990, 29, 4351-4353.	4.0	24
321	Transient versus steady state NOE in paramagnetic molecules Cu2Co2SOD as an example. FEBS Letters, 1990, 272, 175-180.	2.8	24
322	Chapter 8 considerations on high resolution solid state NMR in paramagnetic molecules. Coordination Chemistry Reviews, 1996, 150, 221-242.	18.8	24
323	1H NMR studies of the Fe7S8 ferredoxin from Bacillus schlegelii: a further attempt to understand Fe3S4 clusters. Journal of Biological Inorganic Chemistry, 1996, 1, 523-528.	2.6	24
324	Paramagnetic NMR Analysis of the Seven-Iron Ferredoxin from the Hyperthermoacidophilic Archaeon Desulfurolobus ambivalens Reveals Structural Similarity to other Dicluster Ferredoxins. FEBS Journal, 1996, 236, 92-99.	0.2	24

#	Article	IF	Citations
325	Iron-sulfur interconversions in the anaerobic ribonucleotide reductase from Escherichia coli. Journal of Biological Inorganic Chemistry, 1999, 4, 614-620.	2.6	24
326	A paramagnetic probe to localize residues next to carboxylates on protein surfaces. Journal of Biological Inorganic Chemistry, 2002, 7, 617-622.	2.6	24
327	NMR-validated structural model for oxidized Rhodopseudomonas palustris cytochrome c 556. Journal of Biological Inorganic Chemistry, 2004, 9, 224-230.	2.6	24
328	Atomic structural details of a protein grafted onto gold nanoparticles. Scientific Reports, 2017, 7, 17934.	3.3	24
329	13C NMR studies of d- and l-phenylalanine binding to cobalt(II) carboxypeptidase A. Journal of Inorganic Biochemistry, 1988, 32, 1-6.	3.5	23
330	Characterization of copper-nickel and silver-nickel bovine superoxide dismutases by proton NMR spectroscopy. Inorganic Chemistry, 1988, 27, 4458-4463.	4.0	23
331	The interaction of acetate and formate with cobalt carbonic anhydrase. An NMR study. FEBS Journal, 1992, 208, 607-615.	0.2	23
332	Rationalization of the reduction potentials within the series of the high potential iron-sulfur proteins. Inorganica Chimica Acta, 1995, 240, 251-256.	2.4	23
333	An exchange coupling model for the Fe4S43+ polymetallic center present in high potential iron-sulfur proteins. Inorganica Chimica Acta, 1996, 243, 91-99.	2.4	23
334	Characterization of the Unbound 2[Fe4S4]-Ferredoxin-Like Photosystem I Subunit PsaC from the Cyanobacterium Synechococcus elongatus. Biochemistry, 1997, 36, 13629-13637.	2.5	23
335	High Magnetic Field Consequences on the NMR Hyperfine Shifts in Solution. Journal of Magnetic Resonance, 1998, 134, 360-364.	2.1	23
336	Essential Dynamics of Helices Provide a Functional Classification of EF-Hand Proteins. Journal of Proteome Research, 2007, 6, 4245-4255.	3.7	23
337	Coordination of three and four Cu(I) to the Î±â˜’ and Î²-domain of vertebrate Zn-metallothionein-1, respectively, induces significant structural changes. FEBS Journal, 2007, 274, 2349-2362.	4.7	23
338	Entropy-Based Network Representation of the Individual Metabolic Phenotype. Journal of Proteome Research, 2016, 15, 3298-3307.	3.7	23
339	Biosilica and bioinspired silica studied by solid-state NMR. Coordination Chemistry Reviews, 2016, 327-328, 110-122.	18.8	23
340	Structural characterization of a protein adsorbed on aluminum hydroxide adjuvant in vaccine formulation. Npj Vaccines, 2019, 4, 20.	6.0	23
341	Plasma metabolome and cognitive skills in Down syndrome. Scientific Reports, 2020, 10, 10491.	3.3	23
342	Precision Oncology via NMR-Based Metabolomics: A Review on Breast Cancer. International Journal of Molecular Sciences, 2021, 22, 4687.	4.1	23

#	Article	IF	Citations
343	Spectroscopic investigation of copper(II) bovine carbonic anhydrase and its inhibitor derivatives. Journal of the Chemical Society Dalton Transactions, 1978, , 1269.	1.1	22
344	Preparation and characterization of the vanadium(III) derivative of transferrin. Inorganica Chimica Acta, 1982, 67, L21-L23.	2.4	22
345	A complete relaxation matrix refinement of the solution structure of a paramagnetic metalloprotein: Reduced HiPIP I fromEctothiorhodospira halophila. , 1996, 24, 158-164.		22
346	Nuclear and Electron Relaxation in Magnetic Exchange Coupled Dimers: Implications for NMR Spectroscopy. Journal of Magnetic Resonance, 1998, 130, 33-44.	2.1	22
347	A Refined Model for [Fe3S4]0 Clusters in Proteins. Angewandte Chemie - International Edition, 2000, 39, 3620-3622.	13.8	22
348	Of Monkeys and Men: A Metabolomic Analysis of Static and Dynamic Urinary Metabolic Phenotypes in Two Species. PLoS ONE, 2014, 9, e106077.	2.5	22
349	NMR of sedimented, fibrillized, silica-entrapped and microcrystalline (metallo)proteins. Journal of Magnetic Resonance, 2015, 253, 60-70.	2.1	22
350	1H-detected solid-state NMR of proteins entrapped in bioinspired silica: a new tool for biomaterials characterization. Scientific Reports, 2016, 6, 27851.	3.3	22
351	Improved Accuracy from Joint X-ray and NMR Refinement of a Proteinâ€“RNA Complex Structure. Journal of the American Chemical Society, 2016, 138, 1601-1610.	13.7	22
352	Long-range paramagnetic NMR data can provide a closer look on metal coordination in metalloproteins. Journal of Biological Inorganic Chemistry, 2018, 23, 71-80.	2.6	22
353	Simultaneous Targeting of RGD-Integrins and Dual Murine Double Minute Proteins in Glioblastoma Multiforme. Journal of Medicinal Chemistry, 2018, 61, 4791-4809.	6.4	22
354	Fast and Quantitative NMR Metabolite Analysis Afforded by a Paramagnetic Coâ€Solute. Angewandte Chemie - International Edition, 2019, 58, 15283-15286.	13.8	22
355	Effect of Estrogen Receptor Status on Circulatory Immune and Metabolomics Profiles of HER2-Positive Breast Cancer Patients Enrolled for Neoadjuvant Targeted Chemotherapy. Cancers, 2020, 12, 314.	3.7	22
356	A two-dimensional NMR study of Co(II)7 rabbit liver metallothionein. FEBS Journal, 1993, 211, 235-240.	0.2	21
357	Water-protein interaction in native and partially unfolded equine cytochrome c. Molecular Physics, 1998, 95, 797-808.	1.7	21
358	Waterâ€Based Ligand Screening for Paramagnetic Metalloproteins. Angewandte Chemie - International Edition, 2008, 47, 4533-4537.	13.8	21
359	Characterization of the Conjugation Pattern in Large Polysaccharideâ€“Protein Conjugates by NMR Spectroscopy. Angewandte Chemie - International Edition, 2017, 56, 14997-15001.	13.8	21
360	Perspectives on paramagnetic NMR from a life sciences infrastructure. Journal of Magnetic Resonance, 2017, 282, 154-169.	2.1	21

#	Article	IF	Citations
361	NMR of Polymetallic Systems in Proteins. Biological Magnetic Resonance, 1993, , 357-420.	0.4	21
362	Nuclear magnetic resonance proton relaxation in bimetallic complexes containing cobalt(II). Journal of the American Chemical Society, 1987, 109, 5208-5212.	13.7	20
363	Proton NMR spectroscopy and the electronic structure of the high potential iron-sulfur protein from Chromatium vinosum [Erratum to document cited in CA114(9):77229m]. Journal of the American Chemical Society, 1991, 113, 7084-7084.	13.7	20
364	Simultaneous interpretation of MÃ¶ssbauer, EPR and 57Fe ENDOR spectra of the [Fe4S4] cluster in the high-potential iron protein I Ectothiorhodospira halophila. Journal of Biological Inorganic Chemistry, 1999, 4, 727-741.	2.6	20
365	NMR Characterization of Substrate Binding in the Phthalate Dioxygenase Systemâ€. Biochemistry, 1999, 38, 11051-11061.	2.5	20
366	Water and Protein Dynamics in Sedimented Systems: A Relaxometric Investigation. ChemPhysChem, 2013, 14, 3156-3161.	2.1	20
367	Global metabolomics characterization of bacteria: pre-analytical treatments and profiling. Metabolomics, 2014, 10, 241-249.	3.0	20
368	Assessing protein conformational landscapes: integration of DEER data in Maximum Occurrence analysis. Physical Chemistry Chemical Physics, 2018, 20, 27429-27438.	2.8	20
369	Maximizing Magnetic Resonance Contrast in Gd(III) Nanoconjugates: Investigation of Proton Relaxation in Zirconium Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2020, 12, 41157-41166.	8.0	20
370	Evidence of Histidine Coordination to the Catalytic Ferrous Ion in the Ring-Cleavlng 2,2â€²,3-Trihydroxybiphenyl Dioxygenase from the Dibenzofuran-Degrading Bacterium Sphingomonas sp Strain RW1. Biochemical and Biophysical Research Communications, 1995, 215, 855-860.	2.1	19
371	1H NMR Study of the Reduced Cytochromecâ€˜ fromRhodopseudomonaspalustrisContaining a High-Spin Iron(II) Heme Moiety. Inorganic Chemistry, 1998, 37, 4814-4821.	4.0	19
372	A15N NMR Mobility Study on the Dicalcium P43M Calbindin D9kand Its Mono-La3+-Substituted Formâ€. Biochemistry, 2002, 41, 5104-5111.	2.5	19
373	Energetics and Mechanism of Ca2+ Displacement by Lanthanides in a Calcium Binding Protein. Biochemistry, 2004, 43, 9320-9331.	2.5	19
374	EPR analysis of multiple forms of [4Feâ€“4S]3+ clusters in HiPIPs. Journal of Biological Inorganic Chemistry, 2005, 10, 417-424.	2.6	19
375	SPINE bioinformatics and data-management aspects of high-throughput structural biology. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 1184-1195.	2.5	19
376	Targeting Matrix Metalloproteinases: Design of a Bifunctional Inhibitor for Presentation by Tumourâ€Associated Galectins. Chemistry - A European Journal, 2013, 19, 1896-1902.	3.3	19
377	Differences in Dynamics between Crosslinked and Nonâ€Crosslinked Hyaluronates Measured by using Fast Fieldâ€Cycling Relaxometry. ChemPhysChem, 2015, 16, 2803-2809.	2.1	19
378	Information content of long-range NMR data for the characterization of conformational heterogeneity. Journal of Biomolecular NMR, 2015, 62, 353-371.	2.8	19

#	Article	IF	Citations
379	Paramagnetic Properties of a Crystalline Ironâ€“Sulfur Protein by Magic-Angle Spinning NMR Spectroscopy. Inorganic Chemistry, 2017, 56, 6624-6629.	4.0	19
380	Computer-Aided Identification and Lead Optimization of Dual Murine Double Minute 2 and 4 Binders: Structureâ€“Activity Relationship Studies and Pharmacological Activity. Journal of Medicinal Chemistry, 2017, 60, 8115-8130.	6.4	19
381	Pseudocontact shifts and paramagnetic susceptibility in semiempirical and quantum chemistry theories. Journal of Chemical Physics, 2019, 150, 144101.	3.0	19
382	Double exchange versus J inequality in Fe3S40 clusters. Inorganica Chimica Acta, 1990, 175, 9-10.	2.4	18
383	Off-resonance experiments and contrast agents to improve magnetic resonance imaging. Magnetic Resonance in Medicine, 1998, 39, 124-131.	3.0	18
384	A Structural and Dynamic Characterization of the EF-Hand Protein CLSP. Structure, 2006, 14, 1029-1038.	3.3	18
385	Structural characterization of human S100A16, a low-affinity calcium binder. Journal of Biological Inorganic Chemistry, 2011, 16, 243-256.	2.6	18
386	Solution structure and dynamics of human S100A14. Journal of Biological Inorganic Chemistry, 2013, 18, 183-194.	2.6	18
387	Discovery of a New Class of Potent MMP Inhibitors by Structure-Based Optimization of the Arylsulfonamide Scaffold. ACS Medicinal Chemistry Letters, 2013, 4, 565-569.	2.8	18
388	How Do Nuclei Couple to the Magnetic Moment of a Paramagnetic Center? A New Theory at the Gauntlet of the Experiments. Journal of Physical Chemistry Letters, 2019, 10, 3610-3614.	4.6	18
389	A Quantum Chemistry View on Two Archetypical Paramagnetic Pentacoordinate Nickel(II) Complexes Offers a Fresh Look on Their NMR Spectra. Inorganic Chemistry, 2021, 60, 2068-2075.	4.0	18
390	Unveiling protein dynamics in solution with field-cycling NMR relaxometry. Progress in Nuclear Magnetic Resonance Spectroscopy, 2021, 124-125, 85-98.	7.5	18
391	Detection of Metaboliteâ€“Protein Interactions in Complex Biological Samples by High-Resolution Relaxometry: Toward Interactomics by NMR. Journal of the American Chemical Society, 2021, 143, 9393-9404.	13.7	18
392	A water 17O NMR study of the pH dependent properties of superoxide dismutase. Biochemical and Biophysical Research Communications, 1981, 101, 577-583.	2.1	17
393	[12] Proton magnetic resonance of paramagnetic metalloproteins. Methods in Enzymology, 1989, 177, 246-263.	1.0	17
394	High-Resolution Solid-State NMR Characterization of Ligand Binding to a Protein Immobilized in a Silica Matrix. Journal of Physical Chemistry B, 2017, 121, 8094-8101.	2.6	17
395	Protein Glycosylation through Sulfur Fluoride Exchange (SuFEx) Chemistry: The Key Role of a Fluorosulfate Thiolactoside. Chemistry - A European Journal, 2018, 24, 18981-18987.	3.3	17
396	Electronic relaxation of the titanium(III) hexaaqua complex detected by solvent water proton-NMRD spectroscopy. Inorganic Chemistry, 1992, 31, 3152-3154.	4.0	16

#	Article	IF	Citations
397	Polymetallic macromolecules are potential contrast agents of improved efficiency. Magnetic Resonance in Medicine, 1994, 31, 58-60.	3.0	16
398	The Electronic Structure of the Fe₄S³⁺ ₄Cluster in Proteins: The Importance of Double Exchange Parameter. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1995, 50, 75-80.	1.5	16
399	From NOESY Cross Peaks to Structural Constraints in a Paramagnetic Metalloprotein. Magnetic Resonance in Chemistry, 1996, 34, 948-950.	1.9	16
400	Experimental evidence for the role of buried polar groups in determining the reduction potential of metalloproteins: the S79P variant of Chromatium vinosum HiPIP. Journal of Biological Inorganic Chemistry, 1999, 4, 692-700.	2.6	16
401	Water Accessibility, Aggregation, and Motional Features of Polysaccharide-Protein Conjugate Vaccines. Biophysical Journal, 2004, 86, 3-9.	0.5	16
402	HTS by NMR for the Identification of Potent and Selective Inhibitors of Metalloenzymes. ACS Medicinal Chemistry Letters, 2018, 9, 137-142.	2.8	16
403	What are the methodological and theoretical prospects for paramagnetic NMR in structural biology? A glimpse into the crystal ball. Journal of Magnetic Resonance, 2019, 306, 173-179.	2.1	16
404	Joint X-ray/NMR structure refinement of multidomain/multisubunit systems. Journal of Biomolecular NMR, 2019, 73, 265-278.	2.8	16
405	¹H 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
406	Nickel carbonic anhydrase: a re-examination of the electronic spectra with the help of CD spectra. Inorganica Chimica Acta, 1982, 67, 99-102.	2.4	15
407	Spectral characterization of vanadium-transferrin systems. Journal of Inorganic Biochemistry, 1985, 25, 57-60.	3.5	15
408	Determination of the [Fe4S4]Cys4cluster geometry ofDesulfovibrio africanusferredoxin I by1H NMR spectroscopy. FEBS Letters, 1995, 363, 199-204.	2.8	15
409	15N chemical shift changes in cytochromeÂb5: redox-dependent vs. guanidinium chloride-induced changes. Journal of Biological Inorganic Chemistry, 2000, 5, 761-764.	2.6	15
410	Global and Local Mobility of Apocalmodulin Monitored through Fast-Field Cycling Relaxometry. Biophysical Journal, 2009, 97, 1765-1771.	0.5	15
411	Maximum occurrence analysis of protein conformations for different distributions of paramagnetic metal ions within flexible two-domain proteins. Journal of Magnetic Resonance, 2012, 215, 85-93.	2.1	15
412	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
413	Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry. Molecular Physics, 2019, 117, 888-897.	1.7	15
414	Multivariate Curve Resolution for 2D Solid-State NMR spectra. Analytical Chemistry, 2020, 92, 4451-4458.	6.5	15

#	Article	IF	Citations
415	Carbon-13 longitudinal relaxation times of acetate ion in the presence of metal-substituted bovine carbonic anhydrases. Journal of the Chemical Society Dalton Transactions, 1977, , 1962.	1.1	14
416	Characterization of nickel(II) bovine carbonic anhydrase and its inhibitor derivatives. Bioinorganic Chemistry, 1978, 9, 495-504.	1.1	14
417	1H NMR detection of CoOH2 .dblharw. CoOH interconversions in high-spin cobalt(II) complexes. Inorganic Chemistry, 1982, 21, 3426-3429.	4.0	14
418	A theoretical investigation of the copper-super-oxide system. A model for the mechanism of copper-zinc superoxide dismutase. Inorganica Chimica Acta, 1985, 107, L21-L22.	2.4	14
419	Assignment of Pseudo-contact-shifted1H NMR resonances in the EF site of Yb3 +-substituted rabbit parvalbumin through a combination of 2D techniques and magnetic susceptibility tensor determination. Magnetic Resonance in Chemistry, 1993, 31, S118-S127.	1.9	14
420	NOE-NOESY, a Further Tool in NMR of Paramagnetic Metalloproteins. Journal of Magnetic Resonance Series B, 1994, 103, 278-283.	1.6	14
421	Paramagnetic Metal Centers in Proteins Investigated through Heterocorrelated NMR Spectroscopy. Journal of Magnetic Resonance Series B, 1994, 104, 95-98.	1.6	14
422	1H NMR of High-Potential Iron-Sulfur Protein from the Purple Non-Sulfur Bacterium Rhodoferax fermentans. FEBS Journal, 1996, 236, 405-411.	0.2	14
423	2H NMR Investigation of [Fe3S4]0Cluster in 7Fe8S Ferredoxin fromBacillus schlegelii. Inorganic Chemistry, 1998, 37, 969-972.	4.0	14
424	NMR Spectra of Iron-Sulfur Proteins. Advances in Inorganic Chemistry, 1999, 47, 251-282.	1.0	14
425	Structure-independent cross-validation between residual dipolar couplings originating from internal and external orienting media. Journal of Biomolecular NMR, 2002, 22, 365-368.	2.8	14
426	A simple protocol to study blue copper proteins by NMR. FEBS Journal, 2003, 270, 600-609.	0.2	14
427	An Italian contribution to structural genomics: Understanding metalloproteins. Coordination Chemistry Reviews, 2006, 250, 1419-1450.	18.8	14
428	Fragment Docking to S100 Proteins Reveals a Wide Diversity of Weak Interaction Sites. ChemMedChem, 2007, 2, 1648-1654.	3.2	14
429	A Highly Soluble Matrix Metalloproteinaseâ€9 Inhibitor for Potential Treatment of Dry Eye Syndrome. Basic and Clinical Pharmacology and Toxicology, 2012, 111, 289-295.	2.5	14
430	Pseudoâ€Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMPâ€12 from First Principles. Angewandte Chemie, 2016, 128, 14933-14937.	2.0	14
431	Relaxivity of Gdâ€Based MRI Contrast Agents in Crosslinked Hyaluronic Acid as a Model for Tissues. ChemPhysChem, 2019, 20, 2204-2209.	2.1	14
432	NMR-Based Metabolomics for the Assessment of Inhaled Pharmacotherapy in Chronic Obstructive Pulmonary Disease Patients. Journal of Proteome Research, 2020, 19, 64-74.	3.7	14

#	Article	IF	Citations
433	A geroscience approach for Parkinsonâ€™s disease: Conceptual framework and design of PROPAG-AGEING project. Mechanisms of Ageing and Development, 2021, 194, 111426.	4.6	14
434	A Serum Metabolomics Classifier Derived from Elderly Patients with Metastatic Colorectal Cancer Predicts Relapse in the Adjuvant Setting. Cancers, 2021, 13, 2762.	3.7	14
435	The Structure of Cobalt(II)-substituted Carbonic Anhydrase and Its Implications for the Catalytic Mechanism of the Enzyme. Annals of the New York Academy of Sciences, 1984, 429, 89-98.	3.8	13
436	The electron-nucleus dipolar coupling in slow rotating systems. 4. The effect of zero-field splitting and hyperfine coupling when and. Journal of Magnetic Resonance, 1986, 66, 58-65.	0.5	13
437	Structural basis for sequential displacement of Ca2+ by Yb3+ in a protozoan EF-hand calcium binding protein. Protein Science, 2003, 12, 412-425.	7.6	13
438	The Cu(I)7 cluster in yeast copper thionein survives major shortening of the polypeptide backbone as deduced from electronic absorption, circular dichroism, luminescence and 1H NMR. Journal of Biological Inorganic Chemistry, 2003, 8, 353-359.	2.6	13
439	Characterisation of the MMPâ€12â€“Elastin Adduct. Chemistry - A European Journal, 2009, 15, 7842-7845.	3.3	13
440	SedNMR: a web tool for optimizing sedimentation of macromolecular solutes for SSNMR. Journal of Biomolecular NMR, 2013, 57, 319-326.	2.8	13
441	Metabolomic does not predict response to cardiac resynchronization therapy in patients with heart failure. Journal of Cardiovascular Medicine, 2014, 15, 295-300.	1.5	13
442	Can metal ion complexes be used as polarizing agents for solution DNP? A theoretical discussion. Journal of Biomolecular NMR, 2014, 58, 239-249.	2.8	13
443	Bilayer Membrane Modulation of Membrane Type 1 Matrix Metalloproteinase (MT1-MMP) Structure and Proteolytic Activity. Scientific Reports, 2016, 6, 29511.	3.3	13
444	A Highâ€Resolution View of the Coordination Environment in a Paramagnetic Metalloprotein from its Magnetic Properties. Angewandte Chemie - International Edition, 2021, 60, 14960-14966.	13.8	13
445	Age- and Sex-Dependent Changes of Free Circulating Blood Metabolite and Lipid Abundances, Correlations, and Ratios. Journals of Gerontology - Series A Biological Sciences and Medical Sciences, 2022, 77, 918-926.	3.6	13
446	A 31 P NMR study of phosphate in presence of cobalt(II)- and copper(II)-substituted bovine carbonic anhydrase B. FEBS Letters, 1978, 93, 251-254.	2.8	12
447	Characterization of oxovanadium(IV) substituted bovine carbonic anhydrase B. Inorganica Chimica Acta, 1979, 36, 9-12.	2.4	12
448	1H NMR relaxation rate and coordination number in high spin cobalt(II) complexes. Inorganica Chimica Acta, 1983, 80, 123-126.	2.4	12
449	The influence of anions and inhibitors on the catalytic metal ion in Co(II)-substituted horse liver alcohol dehydrogenase. European Biophysics Journal, 1987, 14, 431-9.	2.2	12
450	Copper(II) as a probe of the active centers of alkaline phosphatase. Inorganic Chemistry, 1989, 28, 352-358.	4.0	12

#	Article	IF	Citations
451	Oxidized and Reduced [Fe2Q2] (Q = S, Se) Cores of Spinach Ferredoxin: a Comparative Study Using 1H NMR Spectroscopy. Inorganic Chemistry, 1995, 34, 417-420.	4.0	12
452	Magnetic Resonance of Fe-S Clusters: Isolation and Characterization of a 7Fe Ferredoxin from Rhodopseudomonas palustris. Archives of Biochemistry and Biophysics, 1995, 320, 149-154.	3.0	12
453	The influence of a surface charge on the electronic and steric structure of a high potential iron-sulfur protein. Journal of Biological Inorganic Chemistry, 1996, 1, 257-263.	2.6	12
454	NMRD studies on phthalate dioxygenase: evidence for displacement of water on binding substrate. Journal of Biological Inorganic Chemistry, 1996, 1, 468-475.	2.6	12
455	Isolation and characterization of cytochrome c2 from Rhodopseudomonas palustris. Inorganica Chimica Acta, 1998, 269, 125-134.	2.4	12
456	Development of NMR Instrumentation to Achieve Excitation of Large Bandwidths in High-Resolution Spectra at High Field. Journal of Magnetic Resonance, 2001, 150, 161-166.	2.1	12
457	Lanthanide Modulation of the Orientation of Macromolecules Induced by Purple Membrane. Journal of the American Chemical Society, 2002, 124, 374-375.	13.7	12
458	NMR in the SPINE Structural Proteomics project. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 1150-1161.	2.5	12
459	NMR Characterization of a â€œFibril-Readyâ€•State of Demetalated Wild-Type Superoxide Dismutase. Journal of the American Chemical Society, 2011, 133, 345-349.	13.7	12
460	NMR fingerprinting as a tool to evaluate post-harvest time-related changes of peaches, tomatoes and plums. Food Research International, 2015, 75, 106-114.	6.2	12
461	Solidâ€State NMR of PEGylated Proteins. Angewandte Chemie, 2016, 128, 2492-2495.	2.0	12
462	Fingerprinting Acute Digestive Diseases by Untargeted NMR Based Metabolomics. International Journal of Molecular Sciences, 2018, 19, 3288.	4.1	12
463	Cancer cell death induced by ferritins and the peculiar role of their labile iron pool. Oncotarget, 2018, 9, 27974-27984.	1.8	12
464	Metabolomic analysis of serum may refine 21-gene expression assay risk recurrence stratification. Npj Breast Cancer, 2019, 5, 26.	5.2	12
465	Comparison of Different Reweighting Approaches for the Calculation of Conformational Variability of Macromolecules from Molecular Simulations. ChemPhysChem, 2021, 22, 127-138.	2.1	12
466	Interactions between Î±-amino acids and cobalt(II) bovine-carbonic anhydrase. Bioinorganic Chemistry, 1977, 7, 225-231.	1.1	11
467	Solution structure of an artificial Fe8S8 ferredoxin : the D13C variant of Bacillus schlegelii Fe7S8 ferredoxin. FEBS Journal, 1998, 258, 502-514.	0.2	11
468	Partial Orientation of Cytochrome c in a Lyotropic Liquid Crystal:â€‰ Residual Hâ^'H Dipolar Coupling. Journal of Physical Chemistry B, 2000, 104, 10653-10658.	2.6	11

#	Article	IF	Citations
469	Comparison and characterization of the [Fe4S4]2+/3+ centre in the wild-type and C77S mutated HiPIPs from Chromatium vinosum monitored by MÃ¶ssbauer, 57Fe ENDOR and EPR spectroscopies. Journal of Biological Inorganic Chemistry, 2001, 6, 232-246.	2.6	11
470	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
471	The Photocatalyzed Thiolâ€ene reaction: A New Tag to Yield Fast, Selective and reversible Paramagnetic Tagging of Proteins. ChemPhysChem, 2020, 21, 863-869.	2.1	11
472	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
473	Fecal metabolomic profiles: A comparative study of patients with colorectal cancer vs adenomatous polyps. World Journal of Gastroenterology, 2021, 27, 6430-6441.	3.3	11
474	Metabolite and lipoprotein profiles reveal sex-related oxidative stress imbalance in de novo drug-naive Parkinsonâ€™s disease patients. Npj Parkinson's Disease, 2022, 8, 14.	5.3	11
475	Different behavior of sulfonamides with respect to copper-substituted bovine and human carbonic anhydrases. Journal of Inorganic Biochemistry, 1982, 16, 155-160.	3.5	10
476	Nuclear spin relaxation in paramagnetic () systems. A comparison of two new theoretical approaches. Journal of Magnetic Resonance, 1985, 62, 235-241.	0.5	10
477	Applications of COSY to paramagnetic heme-containing systems. Journal of Magnetic Resonance, 1991, 95, 244-252.	0.5	10
478	The D13C variant ofBacillus schlegelii7Fe ferredoxin is an 8Fe ferredoxin as revealed by1H-NMR spectroscopy. FEBS Letters, 1997, 412, 501-505.	2.8	10
479	Model-free analysis of a thermophilic Fe7S8 protein compared with a mesophilic Fe4S4 protein. Proteins: Structure, Function and Bioinformatics, 2000, 41, 75-85.	2.6	10
480	Dynamics of wild-type HiPIPs: a Cys77Ser mutant and a partially unfolded HiPIP. Journal of Biological Inorganic Chemistry, 2002, 7, 691-703.	2.6	10
481	Monomorphism of human cytochrome c. Genomics, 2006, 88, 669-672.	2.9	10
482	Biotin-Tagged Probes for MMP Expression and Activation: Design, Synthesis, and Binding Properties. Bioconjugate Chemistry, 2009, 20, 719-727.	3.6	10
483	Acycloguanosyl 5â€²-thymidyltriphosphate, a Thymidine Analogue Prodrug Activated by Telomerase, Reduces Pancreatic Tumor Growth in Mice. Gastroenterology, 2011, 140, 709-720.e9.	1.3	10
484	Telomerase activated thymidine analogue pro-drug is a new molecule targeting hepatocellular carcinoma. Journal of Hepatology, 2014, 61, 1064-1072.	3.7	10
485	A protocol for the refinement of NMR structures using simultaneously pseudocontact shift restraints from multiple lanthanide ions. Journal of Biomolecular NMR, 2016, 66, 175-185.	2.8	10
486	Investigation of Variations in the Human Urine Metabolome amongst European Populations: An Exploratory Search for Biomarkers of People at Riskâ€ofâ€Poverty. Molecular Nutrition and Food Research, 2019, 63, e1800216.	3.3	10

#	Article	IF	Citations
487	Metal centers in biomolecular solid-state NMR. Journal of Structural Biology, 2019, 206, 99-109.	2.8	10
488	Prediagnostic circulating metabolites in female breast cancer cases with low and high mammographic breast density. Scientific Reports, 2021, 11, 13025.	3.3	10
489	Metabolomic Fingerprints in Large Population Cohorts: Impact of Preanalytical Heterogeneity. Clinical Chemistry, 2021, 67, 1153-1155.	3.2	10
490	Impact of the pre-examination phase on multicenter metabolomic studies. New Biotechnology, 2022, 68, 37-47.	4.4	10
491	Evidence of exchangeable protons in the acidic form of manganese(II) bovine carbonic anhydrase B. FEBS Letters, 1978, 87, 92-94.	2.8	9
492	metalloenzymes containing bipositive zinc(II) chromophores with a water molecule in the coordination sphere. Inorganica Chimica Acta, 1980, 46, L91-L92.	2.4	9
493	17O NMR investigation of copper(II) substituted carbonic anhydrases. Inorganica Chimica Acta, 1981, 56, 1-4.	2.4	9
494	Relaxometry and paramagnetic metal ions in biological systems. Magnetic Resonance in Chemistry, 1993, 31, S145-S153.	1.9	9
495	The structure of iron-sulfur clusters in proteins as monitored by NMR, mÃ¶ssbauer, EPR and molecular dynamics. Journal of Molecular Structure, 1993, 292, 207-219.	3.6	9
496	Carbonic Anhydrase: An Example of How the Cavity Governs the Reactivity at the Zinc Ion. Comments on Inorganic Chemistry, 1995, 17, 1-15.	5.2	9
497	Experimental data and calculated parameters in FeS polymetallic centers in proteins. Journal of Biological Inorganic Chemistry, 1996, 1, 183-185.	2.6	9
498	Title is missing!. Angewandte Chemie, 2003, 115, 2777-2780.	2.0	9
499	Application of NMRD to Hydration of Rubredoxin and a Variant Containing a (Cys-S)3FeIII(OH) Site. Biophysical Journal, 2003, 84, 545-551.	0.5	9
500	Backbone and Side-chains 1H, 13C and 15N NMR Assignment of Human Î²-parvalbumin. Journal of Biomolecular NMR, 2005, 33, 137-137.	2.8	9
501	The Da Vinci European BioBank: A Metabolomics-Driven Infrastructure. Journal of Personalized Medicine, 2015, 5, 107-119.	2.5	9
502	Mechanistic Insights into Polyion Complex Associations. Macromolecules, 2018, 51, 1427-1440.	4.8	9
503	Engineering <scp>l</scp>-asparaginase for spontaneous formation of calcium phosphate bioinspired microreactors. Physical Chemistry Chemical Physics, 2018, 20, 12719-12726.	2.8	9
504	1H 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

#	Article	IF	Citations
505	NMR Spectroscopy and Metal Ions in Life Sciences. European Journal of Inorganic Chemistry, 2018, 2018, 4752-4770.	2.0	9
506	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
507	NMR for Single Ion Magnets. Magnetochemistry, 2021, 7, 96.	2.4	9
508	Paramagnetic effects in NMR for protein structures and ensembles: Studies of metalloproteins. Current Opinion in Structural Biology, 2022, 74, 102386.	5.7	9
509	Epitope Mapping and Binding Assessment by Solid-State NMR Provide a Way for the Development of Biologics under the Quality by Design Paradigm. Journal of the American Chemical Society, 2022, 144, 10006-10016.	13.7	9
510	Investigation of cobalt(II) substituted carboxypeptidase a interacting with azide and cyanate ions. Inorganica Chimica Acta, 1985, 107, 153-157.	2.4	8
511	Solvent 1H NMRD of copper(II) complexes. Chemical Physics Letters, 1985, 118, 345-347.	2.6	8
512	Active-site modification of superoxide dismutase by H2O2 studied through 1H NMR of the cobalt derivatives. Archives of Biochemistry and Biophysics, 1989, 269, 586-594.	3.0	8
513	Azide and chloride binding to carboxypeptidase A in the presence of L-phenylalanine. Journal of Inorganic Biochemistry, 1990, 39, 9-16.	3.5	8
514	Folding properties of ironâ€"sulfur proteins. Inorganica Chimica Acta, 1998, 283, 12-16.	2.4	8
515	Redox-Dependent Hydration of Cytochromecand Cytochromeb5Studied through17O NMRD. Journal of the American Chemical Society, 2001, 123, 12925-12926.	13.7	8
516	Redox-Related Chemical Shift Perturbations on Backbone Nuclei of High-Potential Ironâ^'Sulfur Proteins. Inorganic Chemistry, 2002, 41, 1679-1683.	4.0	8
517	Direct Measurement of Dynamic Frequency Shift Induced by Cross-Correlations in15N-Enriched Proteins. ChemPhysChem, 2004, 5, 959-965.	2.1	8
518	Enriching the biological space of natural products and charting drug metabolites, through real time biotransformation monitoring: The NMR tube bioreactor. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1-8.	2.4	8
519	Paramagnetic NMR as a new tool in structural biology. Emerging Topics in Life Sciences, 2018, 2, 19-28.	2.6	8
520	Hochdurchsatzâ€Metabolomik mit 1Dâ€NMR. Angewandte Chemie, 2019, 131, 980-1007.	2.0	8
521	Analysis of Metabolite and Lipid Association Networks Reveals Molecular Mechanisms Associated with 3-Month Mortality and Poor Functional Outcomes in Patients with Acute Ischemic Stroke after Thrombolytic Treatment with Recombinant Tissue Plasminogen Activator. Journal of Proteome Research, 2021, 20, 4758-4770.	3.7	8
522	13C and 1H NMR studies of imidazole binding to native and Co(II)-substituted human carbonic anhydrase I. Inorganica Chimica Acta, 1990, 177, 133-139.	2.4	7

#	Article	IF	Citations
523	Paramagnetism and dynamic properties of electrons and nuclei. Coordination Chemistry Reviews, 1992, 120, 281-307.	18.8	7
524	An NMR method for studying the kinetics of metal exchange in biomolecular systems. Journal of Biomolecular NMR, 2002, 23, 303-309.	2.8	7
525	Does a Fast Nuclear Magnetic Resonance Spectroscopy- and X-Ray Crystallography Hybrid Approach Provide Reliable Structural Information of Ligand-Protein Complexes? A Case Study of Metalloproteinases. Journal of Medicinal Chemistry, 2009, 52, 1712-1722.	6.4	7
526	NMR characterization of the C-terminal tail of full-length RAGE in a membrane mimicking environment. Journal of Biomolecular NMR, 2012, 54, 285-290.	2.8	7
527	The hyperfine shift. , 2017, , 25-60.		7
528	Transition metal ions: shift and relaxation. , 2017, , 175-253.		7
529	Fast and Quantitative NMR Metabolite Analysis Afforded by a Paramagnetic Coâ€Solute. Angewandte Chemie, 2019, 131, 15427-15430.	2.0	7
530	On the complementarity of X-ray and NMR data. Journal of Structural Biology: X, 2020, 4, 100019.	1.3	7
531	DHA-Induced Perturbation of Human Serum Metabolome. Role of the Food Matrix and Co-Administration of Oat Î²-glucan and Anthocyanins. Nutrients, 2020, 12, 86.	4.1	7
532	Effects of Probiotics Administration on Human Metabolic Phenotype. Metabolites, 2020, 10, 396.	2.9	7
533	Single Peptide Backbone Surrogate Mutations to Regulate Angiotensin GPCR Subtype Selectivity. Chemistry - A European Journal, 2020, 26, 10690-10694.	3.3	7
534	High Relaxivity with No Coordinated Waters: A Seemingly Paradoxical Behavior of [Gd(DOTP)]^{5â€“} Embedded in Nanogels. Inorganic Chemistry, 2022, 61, 5380-5387.	4.0	7
535	Investigation of the system cobalt(II) bovine carbonic anhydrase b-trichloroacetaldehyde. Journal of Inorganic Biochemistry, 1979, 11, 49-56.	3.5	6
536	Are there other acidic groups capable of affecting the electronic spectra of cobalt(II) substituted carbonic anhydrase?. Inorganica Chimica Acta, 1984, 91, 173-177.	2.4	6
537	Frontiers in 2D NMR of paramagnetic metalloproteins. Applied Magnetic Resonance, 1993, 4, 461-476.	1.2	6
538	Detecting Small Structural Changes in Metalloproteins by the Use of NMR Pseudocontact Shifts. European Journal of Inorganic Chemistry, 2002, 2002, 2121-2127.	2.0	6
539	Electronic Isomerism in Oxidized High-Potential Iron-Sulfur Proteins Revisited. ACS Symposium Series, 2003, , 272-286.	0.5	6
540	De-escalating and escalating treatment beyond endocrine therapy in patients with luminal breast cancer. Breast, 2017, 34, S13-S18.	2.2	6

#	Article	IF	Citations
541	Evaluation of the Higher Order Structure of Biotherapeutics Embedded in Hydrogels for Bioprinting and Drug Release. Analytical Chemistry, 2021, 93, 11208-11214.	6.5	6
542	NMR Consequences of the Nucleusâ€“Electron Spin Interactions. New Developments in NMR, 2018, , 1-41.	0.1	6
543	13C Nmr spectra of hexakis pyridine-N-oxide cobalt(II) and nickel(II) complexes. Inorganica Chimica Acta, 1976, 19, 201-202.	2.4	5
544	31P NMR spectra of paramagnetic MBr2 (OPPh3)2 complexes. A breakdown in the validity of the Solomon-Bloembergen equations. Inorganic and Nuclear Chemistry Letters, 1979, 15, 89-91.	0.7	5
545	Cyanometallates and cobalt(II) bovine carbonic anhydrase B. Five coordination with dicyanoaurate(I). Inorganica Chimica Acta, 1980, 46, 211-214.	2.4	5
546	Investigation of the copperî—¸magnesiumî—¸alkaline phosphatase system. Inorganica Chimica Acta, 1983, 78, 19-22.	2.4	5
547	Investigation of zinc-deprived bovine superoxide dismutase. Inorganica Chimica Acta, 1984, 91, 109-111.	2.4	5
548	NMR of Paramagnetic Systems. ACS Symposium Series, 1988, , 70-84.	0.5	5
549	The effect of magnetic anisotropy on the longitudinal nuclear relaxation time in paramagnetic systems. Journal of Magnetic Resonance, 1990, 89, 243-254.	0.5	5
550	1H 3D NOE-NOE spectrum of met-cyanomyoglobin: The first 3D NMR spectrum of a paramagnetic protein. Magnetic Resonance in Chemistry, 1993, 31, S3-S7.	1.9	5
551	Selective versus non-selective T1 experiments to determine metal-nucleus distances in paramagnetic metalloproteins. Inorganica Chimica Acta, 1998, 275-276, 373-379.	2.4	5
552	Targeting Metabolomics in Breast Cancer. Current Breast Cancer Reports, 2012, 4, 249-256.	1.0	5
553	Solid-state NMR studies of metal-free SOD1 fibrillar structures. Journal of Biological Inorganic Chemistry, 2014, 19, 659-666.	2.6	5
554	Gelified Biofluids for High-Resolution Magic Angle Spinning ¹H NMR Analysis: The Case of Urine. Analytical Chemistry, 2017, 89, 1054-1058.	6.5	5
555	Reviewing the Crystal Structure of S100Z and Other Members of the S100 Family: Implications in Calcium-Regulated Quaternary Structure. Methods in Molecular Biology, 2019, 1929, 487-499.	0.9	5
556	Nuclear Magnetic Resonance-Based Metabolomic Comparison of Breast Milk and Organic and Traditional Formula Milk Brands for Infants and Toddlers. OMICS A Journal of Integrative Biology, 2020, 24, 424-436.	2.0	5
557	A Highâ€Resolution View of the Coordination Environment in a Paramagnetic Metalloprotein from its Magnetic Properties. Angewandte Chemie, 2021, 133, 15087-15093.	2.0	5
558	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. Metabolites, 2021, 11, 326.	2.9	5

#	Article	IF	Citations
559	New Approaches to NMR of Paramagnetic Molecules. , 1995, , 1-28.		5
560	Theoretical analysis of the long-distance limit of NMR chemical shieldings. Journal of Chemical Physics, 2022, 156, 154115.	3.0	5
561	A water 1H and 17O N.M.R. study on PHG-modified SOD. Inorganica Chimica Acta, 1984, 93, 51-53.	2.4	4
562	A spectroscopic investigation of cobalt(II) substituted alkaline phosphatase. Journal of Inorganic Biochemistry, 1987, 30, 77-85.	3.5	4
563	Evaluation of paramagnetic relaxation rates in a J-coupled two-spin system. Chemical Physics Letters, 1996, 250, 495-504.	2.6	4
564	The use of propionate Î±-proton contact shifts as structural constraints. Inorganica Chimica Acta, 2000, 297, 199-205.	2.4	4
565	The CrIIL Reduction of [2Fe-2S] Ferredoxins and Site of Attachment of CrIIIUsing1H NMR and Site-Directed Mutagenesis. Inorganic Chemistry, 2000, 39, 1755-1764.	4.0	4
566	NMR Spectroscopic Detection of Protein Protons and Longitudinal Relaxation Rates between 0.01 and 50 MHz. Angewandte Chemie, 2005, 117, 2263-2265.	2.0	4
567	Metabolomics for the future of personalized medicine through information and communication technologies. Personalized Medicine, 2012, 9, 133-136.	1.5	4
568	High resolution solid-state NMR in paramagnetic molecules. , 2017, , 127-150.		4
569	Lanthanoids and actinoids: shift and relaxation. , 2017, , 255-276.		4
570	Assessing Structural Preferences of Unstructured Protein Regions by NMR. Biophysical Journal, 2019, 117, 1948-1953.	0.5	4
571	Structure and Dynamics Perturbations in Ubiquitin Adsorbed or Entrapped in Silica Materials Are Related to Disparate Surface Chemistries Resolved by Solid-State NMR Spectroscopy. Biomacromolecules, 2021, 22, 3718-3730.	5.4	4
572	On the Mechanism of Bioinspired Formation of Inorganic Oxides: Structural Evidence of the Electrostatic Nature of the Interaction between a Mononuclear Inorganic Precursor and Lysozyme. Biomolecules, 2021, 11, 43.	4.0	4
573	Multinuclear NMR investigation of the metal binding sites of transferrins. Journal of Molecular Structure, 1984, 113, 191-200.	3.6	3
574	Water proton relaxation rate enhancements as a function of magnetic field strength and nature and size of paramagnetic solutes. Magnetic Resonance Imaging, 1991, 9, 849-853.	1.8	3
575	Solvent water1H NMRD study of oxovanadium(IV) aquo ion. Journal of Magnetic Resonance, 1992, 99, 235-246.	0.5	3
576	Polymetallic hydrolytic zinc enzymes. Probing the site of nuclease P1 through cobalt(II) substitution. Inorganica Chimica Acta, 1995, 234, 9-11.	2.4	3

#	Article	IF	Citations
577	Characterization of the Conjugation Pattern in Large Polysaccharideâ€“Protein Conjugates by NMR Spectroscopy. Angewandte Chemie, 2017, 129, 15193-15197.	2.0	3
578	Magnetic coupled systems. , 2017, , 347-381.		3
579	Nanoparticles for the multivalent presentation of a TnThr mimetic and as tool for solid state NMR coating investigation. Pure and Applied Chemistry, 2019, 91, 1471-1478.	1.9	3
580	A protocol to automatically calculate homo-oligomeric protein structures through the integration of evolutionary constraints and NMR ambiguous contacts. Computational and Structural Biotechnology Journal, 2020, 18, 114-124.	4.1	3
581	Different flavors of diffusion in paramagnetic systems: Unexpected NMR signal intensity and relaxation enhancements. Journal of Magnetic Resonance Open, 2020, 2-3, 100003.	1.1	3
582	Differential Network Analysis Reveals Molecular Determinants Associated with Blood Pressure and Heart Rate in Healthy Subjects. Journal of Proteome Research, 2021, 20, 1040-1051.	3.7	3
583	Origin of the MRI Contrast in Natural and Hydrogel Formulation of Pineapple Juice. Bioinorganic Chemistry and Applications, 2021, 2021, 1-12.	4.1	3
584	Iron-Sulfur Proteins: An Insight into their Electronic Structure Through 1H NMR Spectroscopy. Topics in Molecular Organization and Engineering, 1991, , 73-90.	0.1	3
585	The NMR tube bioreactor. Methods in Enzymology, 2020, 633, 71-101.	1.0	3
586	Exploring Serum NMR-Based Metabolomic Fingerprint of Colorectal Cancer Patients: Effects of Surgery and Possible Associations with Cancer Relapse. Applied Sciences (Switzerland), 2021, 11, 11120.	2.5	3
587	Metabolomics Fingerprint Predicts Risk of Death in Dilated Cardiomyopathy and Heart Failure. Frontiers in Cardiovascular Medicine, 2022, 9, 851905.	2.4	3
588	1H-NMR and relaxometry of copper-containing dimers in proteins. Biology of Metals, 1990, 3, 146-150.	1.1	2
589	A new lipid component identified in avocado pear by GC-MS and NMR spectroscopy. Chemistry and Physics of Lipids, 1991, 60, 133-142.	3.2	2
590	Unexpected interactions. Nature, 2011, 470, 469-470.	27.8	2
591	Activeâ€Site Targeting Paramagnetic Probe for Matrix Metalloproteinases. ChemPlusChem, 2016, 81, 1333-1338.	2.8	2
592	Hints on experimental techniques. , 2017, , 383-456.		2
593	Relaxometry and contrast agents for MRI. , 2017, , 313-345.		2
594	Non-crystallographic symmetry in proteins: Jahnâ€“Teller-like and Butterfly-like effects?. Journal of Biological Inorganic Chemistry, 2019, 24, 91-101.	2.6	2

#	Article	IF	Citations
595	Revisiting paramagnetic relaxation enhancements in slowly rotating systems: how long is the long range?. Magnetic Resonance, 2021, 2, 25-31.	1.9	2
596	Characterization of lanthanoid-binding proteins using NMR spectroscopy. Methods in Enzymology, 2021, 651, 103-137.	1.0	2
597	Lipid and metabolite correlation networks specific to clinical and biochemical covariate show differences associated with sexual dimorphism in a cohort of nonagenarians. GeroScience, 2021, , 1.	4.6	2
598	Not only manganese, but fruit component effects dictate the efficiency of fruit juice as an oral magnetic resonance imaging contrast agent. NMR in Biomedicine, 2021, , e4623.	2.8	2
599	A complete relaxation matrix refinement of the solution structure of a paramagnetic metalloprotein: Reduced HiPIP I from Ectothiorhodospira halophila. Proteins: Structure, Function and Bioinformatics, 1996, 24, 158-164.	2.6	2
600	Solvent Proton Nuclear Magnetic Relaxation Dispersion (NMRD) in Solutions of Paramagnetic Macromolecules. , 1986, , 165-195.		2
601	Phenotyping Green and Roasted Beans of Nicaraguan Coffea Arabica Varieties Processed with Different Post-Harvest Practices. Applied Sciences (Switzerland), 2021, 11, 11779.	2.5	2
602	The electron-nucleus coupling: A breakthrough in the investigation of paramagnetic metalloproteins. International Journal of Quantum Chemistry, 1992, 42, 1383-1396.	2.0	1
603	The competitive world of RAS biology. Nature Chemical Biology, 2014, 10, 173-174.	8.0	1
604	Chemical exchange, chemical equilibria, andÂdynamics. , 2017, , 151-173.		1
605	Using simple algebraic concepts to understand chemical composition problems. International Journal of Mathematical Education in Science and Technology, 2022, 53, 842-857.	1.4	1
606	Pseudocontact shifts as constraints for energy minimization and molecular dynamics calculations on solution structures of paramagnetic metalloproteins. , 1997, 29, 68.		1
607	NMR of Immobilized Enzymes. Methods in Molecular Biology, 2020, 2100, 363-383.	0.9	1
608	Differences between high activity bovine carbonic anhydrase B and low activity human carbonic anhydrase B monitored through metal substitution. Journal of Molecular Catalysis, 1984, 23, 133-144.	1.2	0
609	Evaluation of systematic exploitation of tolerance with respect to a declared nutrient content in the production of fertilizers. Fertilizer Research, 1992, 32, 45-53.	0.5	0
610	NMR of FeS Proteins. ACS Symposium Series, 1998, , 302-313.	0.5	0
611	Biological inorganic chemists pay tribute to Ivano Bertini. Journal of Biological Inorganic Chemistry, 2014, 19, 487-489.	2.6	0
612	The effect of partial orientation: residual dipolar couplings. , 2017, , 61-76.		0

#	Article	IF	Citations
613	Paramagnetic restraints for structure and dynamics of biomolecules. , 2017, , 277-312.		0
614	Lokale und globale Dynamik im ungeordneten Synukleinâ€Protein. Angewandte Chemie, 2018, 130, 15482-15486.	2.0	0
615	The use of the Electron-Nucleus Hyperfine Interaction for Solution Structure Determination. , 2000, , 1-17.		0
616	NMR and Unpaired Electrons in Biomolecules. , 1994, , 199-216.		0