Claudio Luchinat

List of Publications by Citations

623 papers	21,388 citations	73 h-index	107 g-index
651 ext. papers	23,562 ext. citations	6.7 avg, IF	6.7 L-index

#	Paper	IF	Citations
623	Magnetic susceptibility in paramagnetic NMR. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2002**, 40, 249-273	10.4	389
622	Perspectives on NMR in drug discovery: a technique comes of age. *Nature Reviews Drug Discovery*, **2008**, 7, 738-45	64.1	318
621	Solution structure of oxidized horse heart cytochrome c. *Biochemistry*, **1997**, 36, 9867-77	3.2	282
620	A new structural model of A40 fibrils. *Journal of the American Chemical Society*, **2011**, 133, 16013-22	16.4	265
619	NMR spectroscopy of paramagnetic metalloproteins. *ChemBioChem*, **2005**, 6, 1536-49	3.8	260
618	Standard operating procedures for pre-analytical handling of blood and urine for metabolomic studies and biobanks. *Journal of Biomolecular NMR*, **2011**, 49, 231-43	3	236
617	Facing and Overcoming Sensitivity Challenges in Biomolecular NMR Spectroscopy. *Angewandte Chemie - International Edition*, **2015**, 54, 9162-85	16.4	208
616	Evidence of different metabolic phenotypes in humans. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 1420-4	11.5	206
615	Lanthanide-Induced Pseudocontact Shifts for Solution Structure Refinements of Macromolecules in Shells up to 40 Å from the Metal Ion. *Journal of the American Chemical Society*, **2000**, 122, 4154-4161	16.4	198
614	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, 6841-6	11.5	197
613	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	4.7	171
612	Magnetic susceptibility tensor anisotropies for a lanthanide ion series in a fixed protein matrix. *Journal of the American Chemical Society*, **2001**, 123, 4181-8	16.4	170
611	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, 13881-6	11.5	155
610	Protonless NMR experiments for sequence-specific assignment of backbone nuclei in unfolded proteins. *Journal of the American Chemical Society*, **2006**, 128, 3918-9	16.4	155
609	Metabolomic NMR fingerprinting to identify and predict survival of patients with metastatic colorectal cancer. *Cancer Research*, **2012**, 72, 356-64	10.1	152
608	Accurate, fully-automated NMR spectral profiling for metabolomics. *PLoS ONE*, **2015**, 10, e0124219	3.7	149
607	Mechanistic studies of a calcium-dependent MRI contrast agent. *Inorganic Chemistry*, **2002**, 41, 4018-24	5.1	147

606	High-Throughput Metabolomics by 1D NMR. *Angewandte Chemie - International Edition*, **2019**, 58, 968-994	16.4	146
605	Solid-state NMR of proteins sedimented by ultracentrifugation. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 10396-9	11.5	141
604	Dynamic nuclear polarization at high magnetic fields in liquids. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2012**, 64, 4-28	10.4	140
603	The metabonomic signature of celiac disease. *Journal of Proteome Research*, **2009**, 8, 170-7	5.6	138
602	Conformational space of flexible biological macromolecules from average data. *Journal of the American Chemical Society*, **2010**, 132, 13553-8	16.4	135
601	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, 5334-9	11.5	134
600	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	16.4	134
599	Proton NOE studies on dicopper(II) dicobalt(II) superoxide dismutase. *Inorganic Chemistry*, **1989**, 28, 4650-4656	5.1	133
598	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, 51-6	11.5	129
597	Individual human phenotypes in metabolic space and time. *Journal of Proteome Research*, **2009**, 8, 4264-74	5.6	128
596	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, 6632-9	5.1	128
595	Cobalt(II) as a probe of the structure and function of carbonic anhydrase. *Accounts of Chemical Research*, **1983**, 16, 272-279	24.3	124
594	A modular system for the synthesis of multiplexed magnetic resonance probes. *Journal of the American Chemical Society*, **2011**, 133, 5329-37	16.4	114
593	Carbonic anhydrase: An insight into the zinc binding site and into the active cavity through metal substitution **1982**, 45-92		114
592	The G-triplex DNA. *Angewandte Chemie - International Edition*, **2013**, 52, 2269-73	16.4	113
591	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, 12786-94	16.4	112
590	High-resolution solid-state NMR structure of a 17.6 kDa protein. *Journal of the American Chemical Society*, **2010**, 132, 1032-40	16.4	110
589	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. *Metabolomics*, **2015**, 11, 1587-1597	4.7	109

588	High-field dynamic nuclear polarization with high-spin transition metal ions. *Journal of the American Chemical Society*, **2011**, 133, 5648-51	16.4	108
587	Paramagnetism-based restraints for Xplor-NIH. *Journal of Biomolecular NMR*, **2004**, 28, 249-61	3	107
586	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		107
585	Field dependent dynamic nuclear polarization with radicals in aqueous solution. *Journal of the American Chemical Society*, **2008**, 130, 3254-5	16.4	105
584	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	5.1	104
583	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	16.4	104
582	Ultrafast MAS solid-state NMR permits extensive 13C and 1H detection in paramagnetic metalloproteins. *Journal of the American Chemical Society*, **2010**, 132, 5558-9	16.4	103
581	Partial Orientation of Oxidized and Reduced Cytochrome b5 at High Magnetic Fields: Magnetic Susceptibility Anisotropy Contributions and Consequences for Protein Solution Structure Determination. *Journal of the American Chemical Society*, **1998**, 120, 12903-12909	16.4	102
580	Spectroscopic studies on Cu2Zn2SOD: a continuous advancement of investigation tools. *Coordination Chemistry Reviews*, **1990**, 100, 67-103	23.2	102
579	Paramagnetic constraints: An aid for quick solution structure determination of paramagnetic metalloproteins. *Concepts in Magnetic Resonance*, **2002**, 14, 259-286		101
578	Perspectives in paramagnetic NMR of metalloproteins. *Dalton Transactions*, **2008**, 3782-90	4.3	100
577	High-Field NMR Studies of Oxidized Blue Copper Proteins: The Case of Spinach Plastocyanin. *Journal of the American Chemical Society*, **1999**, 121, 2037-2046	16.4	99
576	Paramagnetism-based versus classical constraints: an analysis of the solution structure of Ca Ln calbindin D9k. *Journal of Biomolecular NMR*, **2001**, 21, 85-98	3	95
575	Recommendations and Standardization of Biomarker Quantification Using NMR-Based Metabolomics with Particular Focus on Urinary Analysis. *Journal of Proteome Research*, **2016**, 15, 360-73	5.6	94
574	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	4.2	94
573	High relaxivity Gd(III)-DNA gold nanostars: investigation of shape effects on proton relaxation. *ACS Nano*, **2015**, 9, 3385-96	16.7	92
572	Accurate solution structures of proteins from X-ray data and a minimal set of NMR data: calmodulin-peptide complexes as examples. *Journal of the American Chemical Society*, **2009**, 131, 5134-44	16.4	92
571	A strategy for the NMR characterization of type II copper(II) proteins: the case of the copper trafficking protein CopC from Pseudomonas Syringae. *Journal of the American Chemical Society*, **2003**, 125, 7200-8	16.4	92

570	NMR and Electronic Relaxation in Paramagnetic Dicopper(II) Compounds. *Journal of the American Chemical Society*, **1997**, 119, 2156-2162	16.4	91
569	Heme methyl 1H chemical shifts as structural parameters in some low-spin ferriheme proteins. *Journal of Biological Inorganic Chemistry*, **1999**, 4, 515-9	3.7	90
568	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	16.4	89
567	Structural basis for matrix metalloproteinase 1-catalyzed collagenolysis. *Journal of the American Chemical Society*, **2012**, 134, 2100-10	16.4	88
566	Snapshots of the reaction mechanism of matrix metalloproteinases. *Angewandte Chemie - International Edition*, **2006**, 45, 7952-5	16.4	88
565	Structural Information through NMR Hyperfine Shifts in Blue Copper Proteins. *Journal of the American Chemical Society*, **2000**, 122, 3701-3707	16.4	87
564	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, 715-25		87
563	Metabolomic fingerprint of severe obesity is dynamically affected by bariatric surgery in a procedure-dependent manner. *American Journal of Clinical Nutrition*, **2015**, 102, 1313-22	7	86
562	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, 17284-9	11.5	86
561	Tuning the affinity for lanthanides of calcium binding proteins. *Biochemistry*, **2003**, 42, 8011-21	3.2	83
560	Nuclear spin relaxation in paramagnetic complexes of S=1: Electron spin relaxation effects. *Journal of Chemical Physics*, **1999**, 111, 5795-5807	3.9	83
559	Solution structure of the paramagnetic complex of the N-terminal domain of calmodulin with two Ce3+ ions by 1H NMR. *Biochemistry*, **1997**, 36, 11605-18	3.2	82
558	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	0.9	79
557	The electronic structure of [Fe4S4]3+ clusters in proteins. An investigation of the oxidized high-potential iron-sulfur protein II from Ectothiorhodospira vacuolata. *Biochemistry*, **1993**, 32, 9387-97	3.2	79
556	Are true scalar proton□proton connectivities ever measured in COSY spectra of paramagnetic macromolecules?. *Chemical Physics Letters*, **1993**, 203, 445-449	2.5	79
555	Evidence of reciprocal reorientation of the catalytic and hemopexin-like domains of full-length MMP-12. *Journal of the American Chemical Society*, **2008**, 130, 7011-21	16.4	78
554	Paramagnetically induced residual dipolar couplings for solution structure determination of lanthanide binding proteins. *Journal of the American Chemical Society*, **2002**, 124, 5581-7	16.4	77
553	The 1H NMR parameters of magnetically coupled dimers□he Fe2S2 proteins as an example **1990**, 113-136		77

552	Paramagnetic ions provide structural restraints in solid-state NMR of proteins. *Journal of the American Chemical Society*, **2007**, 129, 2218-9	16.4	75
551	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	10.3	73
550	Solution structure of the oxidized 2[4Fe-4S] ferredoxin from Clostridium pasteurianum. *FEBS Journal*, **1995**, 232, 192-205		73
549	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, 128-39	7.9	72
548	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, 5902-10	3.6	72
547	The three-dimensional solution structure of the reduced high-potential iron-sulfur protein from Chromatium vinosum through NMR. *Biochemistry*, **1995**, 34, 206-19	3.2	72
546	Uncovering the metabolomic fingerprint of breast cancer. *International Journal of Biochemistry and Cell Biology*, **2011**, 43, 1010-20	5.6	71
545	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	16.4	71
544	Acyl positional distribution of glycerol tri-esters in vegetable oils: a 13C NMR study. *Chemistry and Physics of Lipids*, **1999**, 103, 47-55	3.7	68
543	Exploration of serum metabolomic profiles and outcomes in women with metastatic breast cancer: a pilot study. *Molecular Oncology*, **2012**, 6, 437-44	7.9	66
542	Entropic contribution to the linking coefficient in fragment based drug design: a case study. *Journal of Medicinal Chemistry*, **2010**, 53, 4285-9	8.3	66
541	Exploring the subtleties of drug-receptor interactions: the case of matrix metalloproteinases. *Journal of the American Chemical Society*, **2007**, 129, 2466-75	16.4	66
540	Metabolomics in breast cancer: A decade in review. *Cancer Treatment Reviews*, **2018**, 67, 88-96	14.4	65
539	Long-range correlated dynamics in intrinsically disordered proteins. *Journal of the American Chemical Society*, **2014**, 136, 16201-9	16.4	65
538	Interdomain flexibility in full-length matrix metalloproteinase-1 (MMP-1). *Journal of Biological Chemistry*, **2009**, 284, 12821-8	5.4	65
537	Mechanistic investigation of beta-galactosidase-activated MR contrast agents. *Inorganic Chemistry*, **2008**, 47, 56-68	5.1	65
536	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	16.4	65
535	Uniqueness of the NMR approach to metabolomics. *TrAC - Trends in Analytical Chemistry*, **2019**, 120, 115300	14.6	65

534	Bimodal Fluorescence-Magnetic Resonance Contrast Agent for Apoptosis Imaging. *Journal of the American Chemical Society*, **2019**, 141, 6224-6233	16.4	64
533	Characterization of a partially unfolded high potential iron protein. *Biochemistry*, **1997**, 36, 9332-9	3.2	64
532	A Serine -iCysteine Ligand Mutation in the High Potential Iron Sulfur Protein from Chromatium vinosum Provides Insight into the Electronic Structure of the [4Fe4S] Cluster. *Journal of the American Chemical Society*, **1996**, 118, 75-80	16.4	64
531	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, 440-52		64
530	Paramagnetic NMR spectroscopy and coordination structure of cobalt(II) Cys112Asp azurin. *Inorganic Chemistry*, **1995**, 34, 737-742	5.1	63
529	PSEUDYANA for NMR structure calculation of paramagnetic metalloproteins using torsion angle molecular dynamics. *Journal of Biomolecular NMR*, **1998**, 12, 553-7	3	62
528	The iron-sulfur cluster in the oxidized high-potential iron protein from Ectothiorhodospira halophila. *Journal of the American Chemical Society*, **1993**, 115, 3431-3440	16.4	62
527	Solid-state NMR crystallography through paramagnetic restraints. *Journal of the American Chemical Society*, **2012**, 134, 5006-9	16.4	61
526	The cardiovascular risk of healthy individuals studied by NMR metabonomics of plasma samples. *Journal of Proteome Research*, **2011**, 10, 4983-92	5.6	61
525	1H NMRD PROFILES OF PARAMAGNETIC COMPLEXES AND METALLOPROTEINS. *Advances in Inorganic Chemistry*, **2005**, 57, 105-172	2.1	61
524	Sulfonamide-Functionalized Gadolinium DTPA Complexes as Possible Contrast Agents for MRI: A Relaxometric Investigation **2000**, 2000, 625-630		61
523	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	5.1	61
522	Examination of matrix metalloproteinase-1 in solution: a preference for the pre-collagenolysis state. *Journal of Biological Chemistry*, **2013**, 288, 30659-30671	5.4	60
521	Locating the metal ion in calcium-binding proteins by using cerium(III) as a probe. *ChemBioChem*, **2001**, 2, 550-8	3.8	60
520	Bond-Mediated Electron Tunneling in Ruthenium-Modified High-Potential Iron Sulfur Protein. *Journal of the American Chemical Society*, **2000**, 122, 4532-4533	16.4	60
519	Paramagnetic probes in metalloproteins. *Methods in Enzymology*, **2001**, 339, 314-40	1.7	60
518	The solution structure of paramagnetic metalloproteins. *Progress in Biophysics and Molecular Biology*, **1996**, 66, 43-80	4.7	60
517	Liquid state DNP of water at 9.2 T: an experimental access to saturation. *Physical Chemistry Chemical Physics*, **2013**, 15, 6049-56	3.6	58

516	Analysis of the Temperature Dependence of the 1H and 13C Isotropic Shifts of Horse Heart Ferricytochrome c: 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	16.4	58
515	One-thousand-fold enhancement of high field liquid nuclear magnetic resonance signals at room temperature. *Nature Chemistry*, **2017**, 9, 676-680	17.6	57
514	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, 9851-8	3.2	57
513	Structural basis of serine/threonine phosphatase inhibition by the archetypal small molecules cantharidin and norcantharidin. *Journal of Medicinal Chemistry*, **2009**, 52, 4838-43	8.3	56
512	A critical assessment of methods to recover information from averaged data. *Physical Chemistry Chemical Physics*, **2016**, 18, 5686-701	3.6	55
511	Paramagnetic relaxation as a tool for solution structure determination: Clostridium pasteurianum ferredoxin as an example **1997**, 29, 348-358		55
510	The first solution structure of a paramagnetic copper(II) protein: the case of oxidized plastocyanin from the cyanobacterium Synechocystis PCC6803. *Journal of the American Chemical Society*, **2001**, 123, 2405-13	16.4	55
509	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	16.4	55
508	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	12.9	54
507	Thermotoga maritima IscU. Structural characterization and dynamics of a new class of metallochaperone. *Journal of Molecular Biology*, **2003**, 331, 907-24	6.5	54
506	1H NMRD profiles of diamagnetic proteins: a model-free analysis. *Magnetic Resonance in Chemistry*, **2000**, 38, 543-550	2.1	54
505	Dynamic nuclear polarization of (1)H, (13)C, and (59)Co in a tris(ethylenediamine)cobalt(III) crystalline lattice doped with Cr(III). *Journal of the American Chemical Society*, **2014**, 136, 11716-27	16.4	53
504	Dynamic nuclear polarization of sedimented solutes. *Journal of the American Chemical Society*, **2013** , 135, 1641-4	16.4	53
503	(1)H and (13)C 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, 15086-7	16.4	53
502	13C direct detected NMR increases the detectability of residual dipolar couplings. *Journal of the American Chemical Society*, **2006**, 128, 15042-3	16.4	52
501	G-triplex structure and formation propensity. *Nucleic Acids Research*, **2014**, 42, 13393-404	20.1	51
500	Are patients with potential celiac disease really potential? The answer of metabonomics. *Journal of Proteome Research*, **2011**, 10, 714-21	5.6	51
499	SedNMR: on the edge between solution and solid-state NMR. *Accounts of Chemical Research*, **2013**, 46, 2059-69	24.3	50

498	Metabolomic fingerprint of heart failure in humans: a nuclear magnetic resonance spectroscopy analysis. *International Journal of Cardiology*, **2013**, 168, e113-5	3.2	50
497	Paramagnetic metal ions in ligand screening: the Co(II) matrix metalloproteinase 12. *Angewandte Chemie - International Edition*, **2004**, 43, 2254-6	16.4	50
496	A Heteronuclear Direct-Detection NMR Spectroscopy Experiment for Protein-Backbone Assignment. *Angewandte Chemie - International Edition*, **2004**, 43, 2257-2259	16.4	50
495	Persistent contrast enhancement by sterically stabilized paramagnetic liposomes in murine melanoma. *Magnetic Resonance in Medicine*, **2004**, 52, 669-72	4.4	50
494	Quality assurance multicenter comparison of different MR scanners for quantitative diffusion-weighted imaging. *Journal of Magnetic Resonance Imaging*, **2016**, 43, 213-9	5.6	49
493	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, 1342-52	5.9	48
492	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, 110-27	4.2	48
491	Recognition pliability is coupled to structural heterogeneity: a calmodulin intrinsically disordered binding region complex. *Structure*, **2012**, 20, 522-33	5.2	47
490	The epr spectra of the inhibitor derivatives of cobalt carbonic anhydrase. *Journal of Inorganic Biochemistry*, **1981**, 14, 81-93	4.2	47
489	Neue Ansätze zur Empfindlichkeitssteigerung in der biomolekularen NMR-Spektroskopie. *Angewandte Chemie*, **2015**, 127, 9292-9317	3.6	46
488	Phenotyping COPD by 1H NMR metabolomics of exhaled breath condensate. *Metabolomics*, **2014**, 10, 302-311	4.7	46
487	Water exchange at the active site of carbonic anhydrase. A synthesis of the OH- and H2O-models. *Biophysical Journal*, **1983**, 41, 179-87	2.9	46
486	Hydrogen-1 NMR spectra of the coordination sphere of cobalt-substituted carbonic anhydrase. *Journal of the American Chemical Society*, **1981**, 103, 7784-7788	16.4	46
485	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. *Angewandte Chemie - International Edition*, **2016**, 55, 14713-14717	16.4	45
484	Unraveling hidden regulatory sites in structurally homologous metalloproteases. *Journal of Molecular Biology*, **2013**, 425, 2330-46	6.5	45
483	Collective relaxation of protein protons at very low magnetic field: a new window on protein dynamics and aggregation. *Journal of the American Chemical Society*, **2007**, 129, 1055-64	16.4	45
482	EF-hand protein dynamics and evolution of calcium signal transduction: an NMR view. *Journal of Biological Inorganic Chemistry*, **2006**, 11, 949-62	3.7	45
481	Solution structure of the oxidized Fe7S8 ferredoxin from the thermophilic bacterium Bacillus schlegelii by 1H NMR spectroscopy. *Biochemistry*, **1998**, 37, 9812-26	3.2	45

480	1H-NMR studies on partially and fully reduced 2(4Fe-4S) ferredoxin from Clostridium pasteurianum. *FEBS Journal*, **1992**, 204, 831-9		45
479	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	11.5	44
478	Nanodiamond-Gadolinium(III) Aggregates for Tracking Cancer Growth In Vivo at High Field. *Nano Letters*, **2016**, 16, 7551-7564	11.5	44
477	NMR properties of sedimented solutes. *Physical Chemistry Chemical Physics*, **2012**, 14, 439-47	3.6	44
476	Combining in silico tools and NMR data to validate protein-ligand structural models: application to matrix metalloproteinases. *Journal of Medicinal Chemistry*, **2005**, 48, 7544-59	8.3	44
475	The magnetic properties of myoglobin as studied by NMR spectroscopy. *Chemistry - A European Journal*, **2003**, 9, 2316-22	4.8	44
474	Age and Sex Effects on Plasma Metabolite Association Networks in Healthy Subjects. *Journal of Proteome Research*, **2018**, 17, 97-107	5.6	43
473	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	3	43
472	Individual Reduction Potentials of the Iron Ions in Fe(2)S(2) and High-Potential Fe(4)S(4) Ferredoxins. *Inorganic Chemistry*, **1996**, 35, 4248-4253	5.1	43
471	Proton NMR studies of the cobalt(II)-metallothionein system. *Journal of the American Chemical Society*, **1989**, 111, 7296-7300	16.4	43
470	Allostasis and Resilience of the Human Individual Metabolic Phenotype. *Journal of Proteome Research*, **2015**, 14, 2951-62	5.6	42
469	The catalytic domain of MMP-1 studied through tagged lanthanides. *FEBS Letters*, **2012**, 586, 557-67	3.8	42
468	Backbone dynamics of plastocyanin in both oxidation states. Solution structure of the reduced form and comparison with the oxidized state. *Journal of Biological Chemistry*, **2001**, 276, 47217-26	5.4	42
467	High resolution solution structure of the protein part of Cu7 metallothionein. *FEBS Journal*, **2000**, 267, 1008-18		42
466	Non-ionic bulky Gd(III) DTPA-bisamide complexes as potential contrast agents for magnetic resonance imaging. *Magnetic Resonance in Medicine*, **1999**, 41, 767-73	4.4	42
465	X-ray, NMR and molecular dynamics studies on reduced bovine superoxide dismutase: implications for the mechanism. *Biochemical and Biophysical Research Communications*, **1994**, 202, 1088-95	3.4	42
464	Regulation of HuR structure and function by dihydrotanshinone-I. *Nucleic Acids Research*, **2017**, 45, 9514-9527	11.5	41
463	Plasma and urinary metabolomic profiles of Down syndrome correlate with alteration of mitochondrial metabolism. *Scientific Reports*, **2018**, 8, 2977	4.9	41

462	Simultaneous use of solution NMR and X-ray data in REFMAC5 for joint refinement/detection of structural differences. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 958-67		41
461	Gd(III)-labeled peptide nanofibers for reporting on biomaterial localization in vivo. *ACS Nano*, **2014**, 8, 7325-32	16.7	41
460	Narrowing the conformational space sampled by two-domain proteins with paramagnetic probes in both domains. *Journal of Biomolecular NMR*, **2011**, 51, 253-63	3	41
459	Crystal structure of the catalytic domain of human matrix metalloproteinase 10. *Journal of Molecular Biology*, **2004**, 336, 707-16	6.5	41
458	Coordination sphere versus protein environment as determinants of electronic and functional properties of iron-sulfur proteins. *Structure and Bonding*, **1998**, 127-160	0.9	41
457	2D 1H NMR studies of oxidized 2(Fe4S4) ferredoxin from Clostridium pasteurianum. *FEBS Letters*, **1991**, 289, 253-6	3.8	40
456	NMR crystallography on paramagnetic systems: solved and open issues. *CrystEngComm*, **2013**, 15, 8639	3.3	39
455	Probabilistic networks of blood metabolites in healthy subjects as indicators of latent cardiovascular risk. *Journal of Proteome Research*, **2015**, 14, 1101-11	5.6	39
454	On the use of ultracentrifugal devices for sedimented solute NMR. *Journal of Biomolecular NMR*, **2012**, 54, 123-7	3	39
453	Experimental determination of microsecond reorientation correlation times in protein solutions. *Journal of Physical Chemistry B*, **2013**, 117, 3548-53	3.4	39
452	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	16.4	39
451	Electron self-exchange in high-potential iron-sulfur proteins. Characterization of protein I from Ectothiorhodospira vacuolata. *Biochemistry*, **1993**, 32, 12887-93	3.2	39
450	Influence of surface charges on redox properties in high potential iron-sulfur proteins. *Biochemical and Biophysical Research Communications*, **1994**, 203, 436-42	3.4	39
449	Topical Developments in High-Field Dynamic Nuclear Polarization. *Israel Journal of Chemistry*, **2014**, 54, 207-221	3.4	38
448	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. *Analytical Chemistry*, **2018**, 90, 649-656	7.8	37
447	Paramagnetic relaxation enhancement for the characterization of the conformational heterogeneity in two-domain proteins. *Physical Chemistry Chemical Physics*, **2012**, 14, 9149-56	3.6	37
446	A Calix[4]arene Gd(III) Complex Endowed with High Stability, Relaxivity, and Binding Affinity to Serum Albumin This work was supported by CNR (Programma M.U.R.S.T. - Chimica Legge 95/95) "Agenti di contrasto, di shift e sonde luminescenti". We thank C.I.M. (Centro Interdipartimentale Misure) dell'Universit di Parma for the NMR and mass spectroscopy facilities.. *Angewandte Chemie*	16.4	37
445	Structural and dynamical properties of a partially unfolded Fe4S4 protein: role of the cofactor in protein folding. *Biochemistry*, **1999**, 38, 4669-80	3.2	37

444	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	11.4	37
443	NMR for sample quality assessment in metabolomics. *New Biotechnology*, **2019**, 52, 25-34	6.4	36
442	Conformational freedom of metalloproteins revealed by paramagnetism-assisted NMR. *Coordination Chemistry Reviews*, **2013**, 257, 2652-2667	23.2	36
441	Deconvoluting interrelationships between concentrations and chemical shifts in urine provides a powerful analysis tool. *Nature Communications*, **2017**, 8, 1662	17.4	36
440	Metabolomic profile of term infants of gestational diabetic mothers. *Journal of Maternal-Fetal and Neonatal Medicine*, **2014**, 27, 537-42	2	36
439	Solid-state NMR of matrix metalloproteinase 12: an approach complementary to solution NMR. *ChemBioChem*, **2007**, 8, 486-9	3.8	36
438	Solvent 1H NMRD study of biotinylated paramagnetic liposomes containing Gd-bis-SDA-DTPA or Gd-DMPE-DTPA. *Inorganica Chimica Acta*, **2002**, 331, 151-157	2.7	36
437	X-ray structures of binary and ternary enzyme-product-inhibitor complexes of matrix metalloproteinases. *Angewandte Chemie - International Edition*, **2003**, 42, 2673-6	16.4	36
436	Cross correlation between the dipole-dipole interaction and the Curie spin relaxation: the effect of anisotropic magnetic susceptibility. *Journal of Magnetic Resonance*, **2001**, 152, 103-8	3	36
435	Nuclear Spin Relaxation in Paramagnetic Systems:´Electron Spin Relaxation Effects under Near-Redfield Limit Conditions and Beyond. *Journal of Physical Chemistry A*, **2002**, 106, 7376-7382	2.8	36
434	New applications of paramagnetic NMR in chemical biology. *Current Opinion in Chemical Biology*, **1999**, 3, 145-51	9.7	36
433	Nuclear Magnetic Relaxation Dispersion Studies of Hexaaquo Mn(II) Ions in Water-Glycerol Mixtures. *Journal of Magnetic Resonance Series A*, **1993**, 101, 198-201		36
432	Proton NMR studies of the oxidized and partially reduced 2(4Fe-4S) ferredoxin from Clostridium pasteurianum. *Inorganic Chemistry*, **1990**, 29, 1874-1880	5.1	36
431	Basic facts and perspectives of Overhauser DNP NMR. *Journal of Magnetic Resonance*, **2016**, 264, 78-87	3	36
430	Metabolomic/lipidomic profiling of COVID-19 and individual response to tocilizumab. *PLoS Pathogens*, **2021**, 17, e1009243	7.6	36
429	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, 115-25	3	35
428	Sequence-Specific Assignment of Ligand Cysteine Protons of Oxidized, Recombinant HiPIP I from Ectothiorhodospira halophila. *Inorganic Chemistry*, **1995**, 34, 2516-2523	5.1	35
427	Nuclear and electron relaxation of hexaaquairon(3+). *The Journal of Physical Chemistry*, **1993**, 97, 1134-1137		35

426	COSY spectra of paramagnetic macromolecules: Observability, scalar effects, cross-correlation effects, relaxation-allowed coherence transfer. *Concepts in Magnetic Resonance*, **1994**, 6, 307-335		35
425	An investigation of a human erythrocyte SOD modified at position 137. *Journal of the American Chemical Society*, **1989**, 111, 714-719	16.4	35
424	Formation kinetics and structural features of Beta-amyloid aggregates by sedimented solute NMR. *ChemBioChem*, **2013**, 14, 1891-7	3.8	34
423	Are unit charges always negligible?. *Journal of Biological Inorganic Chemistry*, **1997**, 2, 114-118	3.7	34
422	Direct carbon detection in paramagnetic metalloproteins to further exploit pseudocontact shift restraints. *Journal of the American Chemical Society*, **2004**, 126, 10496-7	16.4	34
421	NMR and Spin Relaxation in Dimers. *Accounts of Chemical Research*, **1998**, 31, 351-361	24.3	34
420	Three-dimensional structure of the reduced C77S mutant of the Chromatium vinosum high-potential iron-sulfur protein through nuclear magnetic resonance: comparison with the solution structure of the wild-type protein. *Biochemistry*, **1996**, 35, 5928-36	3.2	34
419	A mössbauer investigation of oxidized Fe4S4 HiPIP II from Ectothiorhodospira halophila. *Journal of Inorganic Biochemistry*, **1993**, 52, 227-234	4.2	34
418	High-field liquid state NMR hyperpolarization: a combined DNP/NMRD approach. *Physical Chemistry Chemical Physics*, **2014**, 16, 18781-7	3.6	33
417	DNP-enhanced MAS NMR of bovine serum albumin sediments and solutions. *Journal of Physical Chemistry B*, **2014**, 118, 2957-65	3.4	33
416	Insights into domain-domain motions in proteins and RNA from solution NMR. *Accounts of Chemical Research*, **2014**, 47, 3118-26	24.3	33
415	An NMR study of the 7Fe-8S ferredoxin from Rhodopseudomonas palustris and reinterpretation of data on similar systems. *Biochemistry*, **1997**, 36, 3570-9	3.2	33
414	Efficient determination of the most favoured orientations of protein domains from paramagnetic NMR data. *Inverse Problems*, **2006**, 22, 1485-1502	2.3	33
413	1H NMRD studies of solutions of paramagnetic metal ions in ethyleneglycol. *Inorganica Chimica Acta*, **1985**, 100, 173-181	2.7	33
412	FANTEN: a new web-based interface for the analysis of magnetic anisotropy-induced NMR data. *Journal of Biomolecular NMR*, **2015**, 61, 21-34	3	32
411	Nuclear Relaxometry Helps Designing Systems for Solution DNP on Proteins. *Applied Magnetic Resonance*, **2008**, 34, 379-392	0.8	32
410	(13)C-(13)C NOESY: a constructive use of (13)C-(13)C spin-diffusion. *Journal of Biomolecular NMR*, **2004**, 30, 245-51	3	32
409	Concentration dependence of 13C NMR spectra of triglycerides: implications for the NMR analysis of olive oils. *Magnetic Resonance in Chemistry*, **2000**, 38, 886-890	2.1	32

408	Ab initio solution and refinement of two high-potential iron protein structures at atomic resolution. *Acta Crystallographica Section D: Biological Crystallography*, **1999**, 55, 1773-84		32
407	Probing Structural and Electronic Properties of the Oxidized [Fe4S4]3+ Cluster of Ectothiorhodospira halophila iso-II High-Potential Iron−Sulfur Protein by ENDOR Spectroscopy. *Journal of the American Chemical Society*, **1999**, 121, 1925-1935	16.4	32
406	Binding of gadobenate dimeglumine to proteins extravasated into interstitial space enhances conspicuity of reperfused infarcts. *Investigative Radiology*, **1994**, 29 Suppl 2, S50-3	10.1	32
405	Hydrogen-1 NOE and ligand field studies of copper-cobalt superoxide dismutase with anions. *Inorganic Chemistry*, **1990**, 29, 4867-4873	5.1	32
404	Interaction of anions with the active site of carboxypeptidase A. *Biochemistry*, **1988**, 27, 1050-7	3.2	32
403	Individual Human Metabolic Phenotype Analyzed by (1)H NMR of Saliva Samples. *Journal of Proteome Research*, **2016**, 15, 1787-93	5.6	32
402	Knowledge discovery by accuracy maximization. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 5117-22	11.5	31
401	SSNMR of biosilica-entrapped enzymes permits an easy assessment of preservation of native conformation in atomic detail. *Chemical Communications*, **2014**, 50, 421-3	5.8	31
400	MaxOcc: a web portal for maximum occurrence analysis. *Journal of Biomolecular NMR*, **2012**, 53, 271-80	3	31
399	Bioinformatic comparison of structures and homology-models of matrix metalloproteinases. *Journal of Proteome Research*, **2004**, 3, 21-31	5.6	31
398	NMR spectroscopic detection of protein protons and longitudinal relaxation rates between 0.01 and 50 MHz. *Angewandte Chemie - International Edition*, **2005**, 44, 2223-5	16.4	31
397	One- and two-dimensional NMR characterization of oxidized and reduced cytochrome c′ from Rhodocyclus gelatinosus. *Biochemistry*, **1993**, 32, 776-83	3.2	31
396	Electronic relaxation of a copper(II) dimer in a macromolecular complex as evaluated from solvent proton relaxation. *Inorganic Chemistry*, **1988**, 27, 951-953	5.1	31
395	Plasma and Serum Metabolite Association Networks: Comparability within and between Studies Using NMR and MS Profiling. *Journal of Proteome Research*, **2017**, 16, 2547-2559	5.6	30
394	Magnetic susceptibility and paramagnetism-based NMR. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2019**, 114-115, 211-236	10.4	30
393	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, 5723-9	5.6	30
392	Extreme Hypoxic Conditions Induce Selective Molecular Responses and Metabolic Reset in Detached Apple Fruit. *Frontiers in Plant Science*, **2016**, 7, 146	6.2	30
391	Molecular determinants of a selective matrix metalloprotease-12 inhibitor: insights from crystallography and thermodynamic studies. *Journal of Medicinal Chemistry*, **2013**, 56, 1149-59	8.3	29

390	NMR in structural proteomics and beyond. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2010**, 56, 247-66	10.4	29
389	Structure-based approach to nanomolar, water soluble matrix metalloproteinases inhibitors (MMPIs). *European Journal of Medicinal Chemistry*, **2010**, 45, 5919-25	6.8	29
388	Paramagnetism-based refinement strategy for the solution structure of human alpha-parvalbumin. *Biochemistry*, **2004**, 43, 5562-73	3.2	29
387	Solution structure of the unbound, oxidized Photosystem I subunit PsaC, containing [4Fe-4S] clusters F(A) and F(B): a conformational change occurs upon binding to photosystem I. *Journal of Biological Inorganic Chemistry*, **2002**, 7, 461-72	3.7	29
386	Structural and Dynamic Information on Double-Decker Yb3+ and Dy3+ Porphyrin Complexes in Solution through 1H NMR. *Inorganic Chemistry*, **1996**, 35, 6308-6315	5.1	29
385	A multinuclear ligand NMR investigation of cyanide, cyanate, and thiocyanate binding to zinc and cobalt carbonic anhydrase. *Inorganic Chemistry*, **1992**, 31, 3975-3979	5.1	29
384	Molecular dynamics simulations on HiPIP from Chromatium vinosum and comparison with NMR data. *Journal of the American Chemical Society*, **1992**, 114, 10683-10689	16.4	29
383	Water in the coordination sphere of metallocarbonic anhydrases: A solvent proton longitudinal relaxation study at several frequencies. *Inorganica Chimica Acta*, **1981**, 56, 99-107	2.7	29
382	Solid-State NMR of PEGylated Proteins. *Angewandte Chemie - International Edition*, **2016**, 55, 2446-9	16.4	29
381	Local and Global Dynamics in Intrinsically Disordered Synuclein. *Angewandte Chemie - International Edition*, **2018**, 57, 15262-15266	16.4	29
380	Practical considerations over spectral quality in solid state NMR spectroscopy of soluble proteins. *Journal of Biomolecular NMR*, **2013**, 57, 155-66	3	28
379	"Four-dimensional" protein structures: examples from metalloproteins. *Accounts of Chemical Research*, **2006**, 39, 909-17	24.3	28
378	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	3.2	28
377	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	10.4	28
376	Evidence of a DHA Signature in the Lipidome and Metabolome of Human Hepatocytes. *International Journal of Molecular Sciences*, **2017**, 18,	6.3	27
375	Paradoxically, Most Flexible Ligand Binds Most Entropy-Favored: Intriguing Impact of Ligand Flexibility and Solvation on Drug-Kinase Binding. *Journal of Medicinal Chemistry*, **2018**, 61, 5922-5933	8.3	27
374	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, 45-8	3.8	27
373	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	4.8	27

372	1H-NMR investigation of oxidized and reduced high-potential iron-sulfur protein from Rhodopseudomonas globiformis. *FEBS Journal*, **1993**, 212, 69-78		27
371	Magnetic relaxation of solvent protons by Cu2+- and VO2+-substituted transferrin: theoretical analysis and biochemical implications. *Biochemistry*, **1985**, 24, 6287-90	3.2	27
370	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, 158-60	3.4	27
369	Sarcolab pilot study into skeletal muscle adaptation to long-term spaceflight. *Npj Microgravity*, **2018**, 4, 18	5.3	27
368	NMR metabolomic fingerprinting distinguishes milk from different farms. *Food Research International*, **2018**, 113, 131-139	7	27
367	NMR-based metabolomic approach to study urine samples of chronic inflammatory rheumatic disease patients. *Analytical and Bioanalytical Chemistry*, **2017**, 409, 1405-1413	4.4	26
366	Moving the frontiers in solution and solid-state bioNMR. *Coordination Chemistry Reviews*, **2011**, 255, 649-663	23.2	26
365	Solution structure of human beta-parvalbumin and structural comparison with its paralog alpha-parvalbumin and with their rat orthologs. *Biochemistry*, **2004**, 43, 16076-85	3.2	26
364	Investigation of copper-zinc superoxide dismutase Ser-137 and Ala-137 mutants. *Inorganic Chemistry*, **1990**, 29, 2398-2403	5.1	26
363	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	5.1	26
362	The acid-base equilibria of carbonic anhydrase. *Inorganica Chimica Acta*, **1980**, 46, 85-89	2.7	26
361	pH-Dependent properties of a CoN4(OH2) chromophore: a spectroscopic model of cobalt carbonic anhydrase. *Inorganic Chemistry*, **1981**, 20, 1670-1673	5.1	26
360	Solution structure of reduced Clostridium pasteurianum rubredoxin. *Journal of Biological Inorganic Chemistry*, **1998**, 3, 401	3.7	26
359	The impact of free or standardized lifestyle and urine sampling protocol on metabolome recognition accuracy. *Genes and Nutrition*, **2015**, 10, 441	4.3	25
358	The effect of Gd on trityl-based dynamic nuclear polarisation in solids. *Physical Chemistry Chemical Physics*, **2015**, 17, 26969-78	3.6	25
357	A high-affinity carbohydrate-containing inhibitor of matrix metalloproteinases. *ChemMedChem*, **2006**, 1, 598-601	3.7	25
356	Principal component analysis of the conformational freedom within the EF-hand superfamily. *Journal of Proteome Research*, **2005**, 4, 1961-71	5.6	25
355	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, 416-26	3.7	25

354	Protein hydration and location of water molecules in oxidized horse heart cytochrome c by (1)H NMR. *Journal of Magnetic Resonance*, **2000**, 147, 1-8	3	25
353	Two-dimensional nuclear magnetic resonance spectra of paramagnetic systems. *Methods in Enzymology*, **1994**, 239, 485-514	1.7	25
352	1H NOE studies of oxidized high potential iron sulfur protein II from Ectothiorhodospira halophila. *Inorganica Chimica Acta*, **1991**, 180, 171-175	2.7	25
351	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	2.7	25
350	Water in the active cavity of copper/zinc superoxide dismutase. A water 1H-nuclear-magnetic-relaxation-dispersion study. *FEBS Journal*, **1989**, 184, 125-9		25
349	Investigation of the system copper(II) carbonic anhydrase and HCO3-/CO2. *Journal of Inorganic Biochemistry*, **1983**, 18, 221-9	4.2	25
348	Mechanisms of Gadographene-Mediated Proton Spin Relaxation. *Journal of Physical Chemistry C*, **2013**, 117,	3.8	24
347	Biosilica-Entrapped Enzymes Studied by Using Dynamic Nuclear-Polarization-Enhanced High-Field NMR Spectroscopy. *ChemPhysChem*, **2015**, 16, 2751-2754	3.2	24
346	Efficiency of paramagnetism-based constraints to determine the spatial arrangement of alpha-helical secondary structure elements. *Journal of Biomolecular NMR*, **2002**, 22, 123-36	3	24
345	Hyperfine Shifts in Low-Spin Iron(III) Hemes: A Ligand Field Analysis. *European Journal of Inorganic Chemistry*, **2000**, 2000, 2473-2480	2.3	24
344	Lanthanide induced residual dipolar couplings for the conformational investigation of peripheral 15NH2 moieties. *Journal of Biomolecular NMR*, **2000**, 18, 347-55	3	24
343	Chapter 8 considerations on high resolution solid state NMR in paramagnetic molecules. *Coordination Chemistry Reviews*, **1996**, 150, 221-242	23.2	24
342	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	16.4	24
341	Two-dimensional proton NMR studies of the paramagnetic metalloenzyme copper-nickel superoxide dismutase. *Inorganic Chemistry*, **1992**, 31, 4433-4435	5.1	24
340	The metabolic fingerprints of HCV and HBV infections studied by Nuclear Magnetic Resonance Spectroscopy. *Scientific Reports*, **2019**, 9, 4128	4.9	23
339	Overhauser DNP with 15N labelled Frhy© salt at 0.35 Tesla. *Physical Chemistry Chemical Physics*, **2012**, 14, 502-10	3.6	23
338	Intra- and interdomain flexibility in matrix metalloproteinases: functional aspects and drug design. *Current Pharmaceutical Design*, **2009**, 15, 3592-605	3.3	23
337	High magnetic field consequences on the NMR hyperfine shifts in solution. *Journal of Magnetic Resonance*, **1998**, 134, 360-4	3	23

336	Essential dynamics of helices provide a functional classification of EF-hand proteins. *Journal of Proteome Research*, **2007**, 6, 4245-55	5.6	23
335	Towards a protocol for solution structure determination of copper(II) proteins: the case of Cu(II)Zn(II) superoxide dismutase. *ChemBioChem*, **2007**, 8, 1422-9	3.8	23
334	Binding affinity of bicarboxylate ions for cobalt (II) bovine carbonic anhydrase. *Bioinorganic Chemistry*, **1978**, 9, 93-100		23
333	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	10.4	22
332	Breathomics for Assessing the Effects of Treatment and Withdrawal With Inhaled Beclomethasone/Formoterol in Patients With COPD. *Frontiers in Pharmacology*, **2018**, 9, 258	5.6	22
331	Exploring regions of conformational space occupied by two-domain proteins. *Journal of Physical Chemistry B*, **2014**, 118, 10576-87	3.4	22
330	1H and (13)C NMR Studies of an Oxidized HiPIP. *Inorganic Chemistry*, **1997**, 36, 4798-4803	5.1	22
329	The solution structure of parsley [2Fe-2S]ferredoxin. *FEBS Journal*, **1998**, 258, 465-77		22
328	A use of Ramachandran potentials in protein solution structure determinations. *Journal of Biomolecular NMR*, **2003**, 26, 355-66	3	22
327	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, 230-9		22
326	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, 703-14		22
325	Rationalization of the reduction potentials within the series of the high potential iron-sulfur proteins. *Inorganica Chimica Acta*, **1995**, 240, 251-256	2.7	22
324	Proton NMR spectra of the Co4S11 cluster in metallothioneins: a theoretical model. *Journal of the American Chemical Society*, **1989**, 111, 7300-7303	16.4	22
323	NMR proton relaxation in bimetallic complexes of zinc(II), nickel(II), and copper(II). *Journal of the American Chemical Society*, **1986**, 108, 3298-3303	16.4	22
322	Metabolomics in Breast Cancer: Current Status and Perspectives. *Advances in Experimental Medicine and Biology*, **2016**, 882, 217-34	3.6	21
321	Solution structure and dynamics of S100A5 in the apo and Ca2+-bound states. *Journal of Biological Inorganic Chemistry*, **2009**, 14, 1097-107	3.7	21
320	Coordination of three and four Cu(I) to the alpha- and beta-domain of vertebrate Zn-metallothionein-1, respectively, induces significant structural changes. *FEBS Journal*, **2007**, 274, 2349-62	5.7	21
319	NMR-validated structural model for oxidized Rhodopseudomonas palustris cytochrome c(556). *Journal of Biological Inorganic Chemistry*, **2004**, 9, 224-30	3.7	21

318	Solvent (1)H NMRD study of hexaaquochromium(III): inferences on hydration and electron relaxation. *Inorganic Chemistry*, **2001**, 40, 4030-5	5.1	21
317	Iron-sulfur interconversions in the anaerobic ribonucleotide reductase from Escherichia coli. *Journal of Biological Inorganic Chemistry*, **1999**, 4, 614-20	3.7	21
316	A theoretical analysis of the 1H nuclear magnetic relaxation dispersion profiles of diferric transferrin. *The Journal of Physical Chemistry*, **1995**, 99, 14217-14222		21
315	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	3.7	21
314	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, 92-9		21
313	Assignment of active-site protons in the 1H-NMR spectrum of reduced human Cu/Zn superoxide dismutase. *FEBS Journal*, **1991**, 197, 691-7		21
312	Relaxation of the electronic spin moment of copper(II)-macromolecular complexes in solution. *Journal of the American Chemical Society*, **1989**, 111, 3532-3536	16.4	21
311	Application of 2D NMR techniques to paramagnetic systems. *Inorganic Chemistry*, **1990**, 29, 4351-4353	5.1	21
310	Spectroscopic investigation of copper(II) bovine carbonic anhydrase and its inhibitor derivatives. *Journal of the Chemical Society Dalton Transactions*, **1978**, 1269		21
309	NMR of sedimented, fibrillized, silica-entrapped and microcrystalline (metallo)proteins. *Journal of Magnetic Resonance*, **2015**, 253, 60-70	3	20
308	Entropy-Based Network Representation of the Individual Metabolic Phenotype. *Journal of Proteome Research*, **2016**, 15, 3298-307	5.6	20
307	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- and FB-. *Journal of Biological Inorganic Chemistry*, **2000**, 5, 381-92	3.7	20
306	Water-protein interaction in native and partially unfolded equine cytochrome c. *Molecular Physics*, **1998**, 95, 797-808	1.7	20
305	An exchange coupling model for the Fe4S43+ polymetallic center present in high potential iron-sulfur proteins. *Inorganica Chimica Acta*, **1996**, 243, 91-99	2.7	20
304	The interaction of acetate and formate with cobalt carbonic anhydrase. An NMR study. *FEBS Journal*, **1992**, 208, 607-15		20
303	Transient versus steady state NOE in paramagnetic molecules Cu2Co2SOD as an example. *FEBS Letters*, **1990**, 272, 175-80	3.8	20
302	Atomic-Level Quality Assessment of Enzymes Encapsulated in Bioinspired Silica. *Chemistry - A European Journal*, **2016**, 22, 425-32	4.8	20
301	Mechanism and Inhibition of Matrix Metalloproteinases. *Current Medicinal Chemistry*, **2019**, 26, 2609-2632	4.3	19

300	Biosilica and bioinspired silica studied by solid-state NMR. *Coordination Chemistry Reviews*, **2016**, 327-328, 110-122	23.2	19
299	Of monkeys and men: a metabolomic analysis of static and dynamic urinary metabolic phenotypes in two species. *PLoS ONE*, **2014**, 9, e106077	3.7	19
298	A metabolomic perspective on coeliac disease. *Autoimmune Diseases*, **2014**, 2014, 756138	2.9	19
297	Water and protein dynamics in sedimented systems: a relaxometric investigation. *ChemPhysChem*, **2013**, 14, 3156-61	3.2	19
296	A paramagnetic probe to localize residues next to carboxylates on protein surfaces. *Journal of Biological Inorganic Chemistry*, **2002**, 7, 617-22	3.7	19
295	1H NMR Study of the Reduced Cytochrome cFrom Rhodopseudomonas palustris Containing a High-Spin Iron(II) Heme Moiety. *Inorganic Chemistry*, **1998**, 37, 4814-4821	5.1	19
294	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, 158-64	4.2	19
293	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	16.4	19
292	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	5.6	19
291	Aggregation kinetics of the Aβ1-40 peptide monitored by NMR. *Chemical Communications*, **2018**, 54, 7601-7604	5.8	19
290	Characterization of the Conjugation Pattern in Large Polysaccharide-Protein Conjugates by NMR Spectroscopy. *Angewandte Chemie - International Edition*, **2017**, 56, 14997-15001	16.4	18
289	(1)H-detected solid-state NMR of proteins entrapped in bioinspired silica: a new tool for biomaterials characterization. *Scientific Reports*, **2016**, 6, 27851	4.9	18
288	Improved Accuracy from Joint X-ray and NMR Refinement of a Protein-RNA Complex Structure. *Journal of the American Chemical Society*, **2016**, 138, 1601-10	16.4	18
287	Perspectives on paramagnetic NMR from a life sciences infrastructure. *Journal of Magnetic Resonance*, **2017**, 282, 154-169	3	18
286	Nuclear and Electron Relaxation in Magnetic Exchange Coupled Dimers: Implications for NMR Spectroscopy. *Journal of Magnetic Resonance*, **1998**, 130, 33-44	3	18
285	Water-based ligand screening for paramagnetic metalloproteins. *Angewandte Chemie - International Edition*, **2008**, 47, 4533-7	16.4	18
284	A 15N NMR mobility study on the dicalcium P43M calbindin D9k and its mono-La3+-substituted form. *Biochemistry*, **2002**, 41, 5104-11	3.2	18
283	Simultaneous interpretation of Mössbauer, EPR and 57Fe ENDOR spectra of the [Fe4S4] cluster in the high-potential iron protein I from Ectothiorhodospira halophila. *Journal of Biological Inorganic Chemistry*, **1999**, 4, 727-41	3.7	18

282	NMR characterization of substrate binding in the phthalate dioxygenase system. *Biochemistry*, **1999**, 38, 11051-61	3.2	18
281	Long-range paramagnetic NMR data can provide a closer look on metal coordination in metalloproteins. *Journal of Biological Inorganic Chemistry*, **2018**, 23, 71-80	3.7	18
280	NMR of Polymetallic Systems in Proteins. *Biological Magnetic Resonance*, **1993**, 357-420	0.5	18
279	Information content of long-range NMR data for the characterization of conformational heterogeneity. *Journal of Biomolecular NMR*, **2015**, 62, 353-71	3	17
278	Fingerprinting Alzheimer© Disease by H Nuclear Magnetic Resonance Spectroscopy of Cerebrospinal Fluid. *Journal of Proteome Research*, **2020**, 19, 1696-1705	5.6	17
277	Characterization of the unbound 2[Fe4S4]-ferredoxin-like photosystem I subunit PsaC from the Cyanobacterium synechococcus elongatus. *Biochemistry*, **1997**, 36, 13629-37	3.2	17
276	Off-resonance experiments and contrast agents to improve magnetic resonance imaging. *Magnetic Resonance in Medicine*, **1998**, 39, 124-31	4.4	17
275	Energetics and mechanism of Ca2+ displacement by lanthanides in a calcium binding protein. *Biochemistry*, **2004**, 43, 9320-31	3.2	17
274	Double exchange versus J inequality in Fe3S40 clusters. *Inorganica Chimica Acta*, **1990**, 175, 9-10	2.7	17
273	13C NMR studies of D- and L-phenylalanine binding to cobalt(II) carboxypeptidase A. *Journal of Inorganic Biochemistry*, **1988**, 32, 1-6	4.2	17
272	Characterization of PEGylated Asparaginase: New Opportunities from NMR Analysis of Large PEGylated Therapeutics. *Chemistry - A European Journal*, **2019**, 25, 1984-1991	4.8	17
271	Metabolic Signature of Primary Biliary Cholangitis and Its Comparison with Celiac Disease. *Journal of Proteome Research*, **2019**, 18, 1228-1236	5.6	17
270	Dependence of apparent diffusion coefficient measurement on diffusion gradient direction and spatial position - A quality assurance intercomparison study of forty-four scanners for quantitative diffusion-weighted imaging. *Physica Medica*, **2018**, 55, 135-141	2.7	17
269	Paramagnetic Properties of a Crystalline Iron-Sulfur Protein by Magic-Angle Spinning NMR Spectroscopy. *Inorganic Chemistry*, **2017**, 56, 6624-6629	5.1	16
268	Solution structure and dynamics of human S100A14. *Journal of Biological Inorganic Chemistry*, **2013**, 18, 183-94	3.7	16
267	Atomic structural details of a protein grafted onto gold nanoparticles. *Scientific Reports*, **2017**, 7, 17934	4.9	16
266	Differences in Dynamics between Crosslinked and Non-Crosslinked Hyaluronates Measured by using Fast Field-Cycling Relaxometry. *ChemPhysChem*, **2015**, 16, 2803-2809	3.2	16
265	A Refined Model for. *Angewandte Chemie - International Edition*, **2000**, 39, 3620-3622	16.4	16

264	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	3.7	16
263	Evidence of histidine coordination to the catalytic ferrous ion in the ring-cleaving 2,2Ø3-trihydroxybiphenyl dioxygenase from the dibenzofuran-degrading bacterium Sphingomonas sp. strain RW1. *Biochemical and Biophysical Research Communications*, **1995**, 215, 855-60	3.4	16
262	From NOESY Cross Peaks to Structural Constraints in a Paramagnetic Metalloprotein. *Magnetic Resonance in Chemistry*, **1996**, 34, 948-950	2.1	16
261	Proton magnetic resonance of paramagnetic metalloproteins. *Methods in Enzymology*, **1989**, 177, 246-63	1.7	16
260	Characterization of copper-nickel and silver-nickel bovine superoxide dismutases by proton NMR spectroscopy. *Inorganic Chemistry*, **1988**, 27, 4458-4463	5.1	16
259	A water 17O NMR study of the pH dependent properties of superoxide dismutase. *Biochemical and Biophysical Research Communications*, **1981**, 101, 577-83	3.4	16
258	Discovery of a New Class of Potent MMP Inhibitors by Structure-Based Optimization of the Arylsulfonamide Scaffold. *ACS Medicinal Chemistry Letters*, **2013**, 4, 565-9	4.3	15
257	Targeting matrix metalloproteinases: design of a bifunctional inhibitor for presentation by tumour-associated galectins. *Chemistry - A European Journal*, **2013**, 19, 1896-902	4.8	15
256	Structural characterization of human S100A16, a low-affinity calcium binder. *Journal of Biological Inorganic Chemistry*, **2011**, 16, 243-56	3.7	15
255	SPINE bioinformatics and data-management aspects of high-throughput structural biology. *Acta Crystallographica Section D: Biological Crystallography*, **2006**, 62, 1184-95		15
254	Paramagnetic Metal Ions in Ligand Screening: The CoII Matrix Metalloproteinase 12. *Angewandte Chemie*, **2004**, 116, 2304-2306	3.6	15
253	EPR analysis of multiple forms of [4Fe-4S](3+) clusters in HiPIPs. *Journal of Biological Inorganic Chemistry*, **2005**, 10, 417-24	3.7	15
252	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	1.4	15
251	Preparation and characterization of the vanadium(III) derivative of transferrin. *Inorganica Chimica Acta*, **1982**, 67, L21-L23	2.7	15
250	Structural characterization of a protein adsorbed on aluminum hydroxide adjuvant in vaccine formulation. *Npj Vaccines*, **2019**, 4, 20	9.5	14
249	Pseudocontact shifts and paramagnetic susceptibility in semiempirical and quantum chemistry theories. *Journal of Chemical Physics*, **2019**, 150, 144101	3.9	14
248	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,	6.6	14
247	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	3	14

246	Global metabolomics characterization of bacteria: pre-analytical treatments and profiling. *Metabolomics*, **2014**, 10, 241-249	4.7	14
245	Global and local mobility of apocalmodulin monitored through fast-field cycling relaxometry. *Biophysical Journal*, **2009**, 97, 1765-71	2.9	14
244	Fragment docking to S100 proteins reveals a wide diversity of weak interaction sites. *ChemMedChem*, **2007**, 2, 1648-54	3.7	14
243	Water accessibility, aggregation, and motional features of polysaccharide-protein conjugate vaccines. *Biophysical Journal*, **2004**, 86, 3-9	2.9	14
242	Determination of the [Fe4S4]Cys4 cluster geometry of Desulfovibrio africanus ferredoxin I by 1H NMR spectroscopy. *FEBS Letters*, **1995**, 363, 199-204	3.8	14
241	Assignment of Pseudo-contact-shifted 1H 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	2.1	14
240	A two-dimensional NMR study of Co(II)7 rabbit liver metallothionein. *FEBS Journal*, **1993**, 211, 235-40		14
239	Nuclear magnetic resonance proton relaxation in bimetallic complexes containing cobalt(II). *Journal of the American Chemical Society*, **1987**, 109, 5208-5212	16.4	14
238	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	2.7	14
237	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	6.4	13
236	Dissecting the Interactions between Human Serum Albumin and □Synuclein: New Insights on the Factors Influencing □Synuclein Aggregation in Biological Fluids. *Journal of Physical Chemistry B*, **2019**, 123, 4380-4386	3.4	13
235	Mixing A□(1-40) and A□(1-42) peptides generates unique amyloid fibrils. *Chemical Communications*, **2020**, 56, 8830-8833	5.8	13
234	A highly soluble matrix metalloproteinase-9 inhibitor for potential treatment of dry eye syndrome. *Basic and Clinical Pharmacology and Toxicology*, **2012**, 111, 289-95	3.1	13
233	Characterisation of the MMP-12-elastin adduct. *Chemistry - A European Journal*, **2009**, 15, 7842-5	4.8	13
232	A structural and dynamic characterization of the EF-hand protein CLSP. *Structure*, **2006**, 14, 1029-38	5.2	13
231	Structural basis for sequential displacement of Ca(2+) by Yb(3+) in a protozoan EF-hand calcium binding protein. *Protein Science*, **2003**, 12, 412-25	6.3	13
230	Polymetallic macromolecules are potential contrast agents of improved efficiency. *Magnetic Resonance in Medicine*, **1994**, 31, 58-60	4.4	13
229	Electronic relaxation of the titanium(III) hexaaqua complex detected by solvent water proton-NMRD spectroscopy. *Inorganic Chemistry*, **1992**, 31, 3152-3154	5.1	13

228	Spectral characterization of vanadium-transferrin systems. *Journal of Inorganic Biochemistry*, **1985**, 25, 57-60	4.2	13
227	Nickel carbonic anhydrase: a re-examination of the electronic spectra with the help of CD spectra. *Inorganica Chimica Acta*, **1982**, 67, 99-102	2.7	13
226	Characterization of nickel(II) bovine carbonic anhydrase and its inhibitor derivatives. *Bioinorganic Chemistry*, **1978**, 9, 495-504		13
225	Metabolomics to Assess Response to Immune Checkpoint Inhibitors in Patients with Non-Small-Cell Lung Cancer. *Cancers*, **2020**, 12,	6.6	13
224	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	6.4	13
223	KODAMA: an R package for knowledge discovery and data mining. *Bioinformatics*, **2017**, 33, 621-623	7.2	13
222	Assessing protein conformational landscapes: integration of DEER data in Maximum Occurrence analysis. *Physical Chemistry Chemical Physics*, **2018**, 20, 27429-27438	3.6	13
221	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, 5743-52	3.6	12
220	Plasma metabolome and cognitive skills in Down syndrome. *Scientific Reports*, **2020**, 10, 10491	4.9	12
219	HTS by NMR for the Identification of Potent and Selective Inhibitors of Metalloenzymes. *ACS Medicinal Chemistry Letters*, **2018**, 9, 137-142	4.3	12
218	Relaxivity of Gd-Based MRI Contrast Agents in Crosslinked Hyaluronic Acid as a Model for Tissues. *ChemPhysChem*, **2019**, 20, 2204-2209	3.2	12
217	SedNMR: a web tool for optimizing sedimentation of macromolecular solutes for SSNMR. *Journal of Biomolecular NMR*, **2013**, 57, 319-26	3	12
216	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	3.4	12
215	Isolation and characterization of cytochrome c2 from Rhodopseudomonas palustris. *Inorganica Chimica Acta*, **1998**, 269, 125-134	2.7	12
214	An Italian contribution to structural genomics: Understanding metalloproteins. *Coordination Chemistry Reviews*, **2006**, 250, 1419-1450	23.2	12
213	A Heteronuclear Direct-Detection NMR Spectroscopy Experiment for Protein-Backbone Assignment. *Angewandte Chemie*, **2004**, 116, 2307-2309	3.6	12
212	A simple protocol to study blue copper proteins by NMR. *FEBS Journal*, **2003**, 270, 600-9		12
211	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(1)H NMR. *Journal of Biological Inorganic Chemistry*, **2003**, 8, 353-9	3.7	12

210	15N chemical shift changes in cytochrome b5: redox-dependent vs. guanidinium chloride-induced changes. *Journal of Biological Inorganic Chemistry*, **2000**, 5, 761-4	3.7	12
209	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	3.7	12
208	1H NMR of high-potential iron-sulfur protein from the purple non-sulfurbacterium Rhodoferax fermentans. *FEBS Journal*, **1996**, 236, 405-11		12
207	NOE-NOESY, a Further Tool in NMR of Paramagnetic Metalloproteins. *Journal of Magnetic Resonance Series B*, **1994**, 103, 278-283		12
206	Paramagnetic Metal Centers in Proteins Investigated through Heterocorrelated NMR Spectroscopy. *Journal of Magnetic Resonance Series B*, **1994**, 104, 95-98		12
205	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. *Angewandte Chemie*, **2016**, 128, 14933-14937	3.6	11
204	Fast and Quantitative NMR Metabolite Analysis Afforded by a Paramagnetic Co-Solute. *Angewandte Chemie - International Edition*, **2019**, 58, 15283-15286	16.4	11
203	Computer-Aided Identification and Lead Optimization of Dual Murine Double Minute 2 and 4 Binders: Structure-Activity Relationship Studies and Pharmacological Activity. *Journal of Medicinal Chemistry*, **2017**, 60, 8115-8130	8.3	11
202	Metabolomic does not predict response to cardiac resynchronization therapy in patients with heart failure. *Journal of Cardiovascular Medicine*, **2014**, 15, 295-300	1.9	11
201	Can metal ion complexes be used as polarizing agents for solution DNP? A theoretical discussion. *Journal of Biomolecular NMR*, **2014**, 58, 239-49	3	11
200	NMR characterization of a "fibril-ready" state of demetalated wild-type superoxide dismutase. *Journal of the American Chemical Society*, **2011**, 133, 345-9	16.4	11
199	Structure-independent cross-validation between residual dipolar couplings originating from internal and external orienting media. *Journal of Biomolecular NMR*, **2002**, 22, 365-8	3	11
198	Partial Orientation of Cytochrome c in a Lyotropic Liquid Crystal: Residual HH Dipolar Coupling. *Journal of Physical Chemistry B*, **2000**, 104, 10653-10658	3.4	11
197	Oxidized and Reduced [Fe2Q2] (Q = S, Se) Cores of Spinach Ferredoxin: a Comparative Study Using 1H NMR Spectroscopy. *Inorganic Chemistry*, **1995**, 34, 417-420	5.1	11
196	NMRD studies on phthalate dioxygenase: evidence for displacement of water on binding substrate. *Journal of Biological Inorganic Chemistry*, **1996**, 1, 468-475	3.7	11
195	Copper(II) as a probe of the active centers of alkaline phosphatase. *Inorganic Chemistry*, **1989**, 28, 352-358	5.1	11
194	1H NMR relaxation rate and coordination number in high spin cobalt(II) complexes. *Inorganica Chimica Acta*, **1983**, 80, 123-126	2.7	11
193	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	6.5	11

192	Characterization of oxovanadium(IV) substituted bovine carbonic anhydrase B. *Inorganica Chimica Acta*, **1979**, 36, 9-12	2.7	11
191	1H NMR detection of CoOH2 .dblharw. CoOH interconversions in high-spin cobalt(II) complexes. *Inorganic Chemistry*, **1982**, 21, 3426-3429	5.1	11
190	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		11
189	The Photocatalyzed Thiol-ene reaction: A New Tag to Yield Fast, Selective and reversible Paramagnetic Tagging of Proteins. *ChemPhysChem*, **2020**, 21, 863-869	3.2	10
188	Bilayer Membrane Modulation of Membrane Type 1 Matrix Metalloproteinase (MT1-MMP) Structure and Proteolytic Activity. *Scientific Reports*, **2016**, 6, 29511	4.9	10
187	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	3	10
186	NMR in the SPINE Structural Proteomics project. *Acta Crystallographica Section D: Biological Crystallography*, **2006**, 62, 1150-61		10
185	Comparison and characterization of the [Fe4S4]2+/3+ centre in the wild-type and C77S mutated HiPIPs from Chromatium vinosum monitored by MÆsbauer, 57Fe ENDOR and EPR spectroscopies. *Journal of Biological Inorganic Chemistry*, **2001**, 6, 232-46	3.7	10
184	Development of NMR instrumentation to achieve excitation of large bandwidths in high-resolution spectra at high field. *Journal of Magnetic Resonance*, **2001**, 150, 161-6	3	10
183	Lanthanide modulation of the orientation of macromolecules induced by purple membrane. *Journal of the American Chemical Society*, **2002**, 124, 374-5	16.4	10
182	Model-free analysis of a thermophilic Fe(7)S(8) protein compared with a mesophilic Fe(4)S(4) protein. *Proteins: Structure, Function and Bioinformatics*, **2000**, 41, 75-85	4.2	10
181	2H NMR Investigation of [Fe3S4]0Cluster in 7Fe8S Ferredoxin fromBacillus schlegelii. *Inorganic Chemistry*, **1998**, 37, 969-972	5.1	10
180	NMR Spectra of Iron-Sulfur Proteins. *Advances in Inorganic Chemistry*, **1999**, 47, 251-282	2.1	10
179	Magnetic resonance of Fe-S clusters: isolation and characterization of a 7Fe ferredoxin from Rhodopseudomonas palustris. *Archives of Biochemistry and Biophysics*, **1995**, 320, 149-54	4.1	10
178	Maximizing Magnetic Resonance Contrast in Gd(III) Nanoconjugates: Investigation of Proton Relaxation in Zirconium Metal-Organic Frameworks. *ACS Applied Materials & Interfaces*, **2020**, 12, 41157-41166	9.5	10
177	Joint X-ray/NMR structure refinement of multidomain/multisubunit systems. *Journal of Biomolecular NMR*, **2019**, 73, 265-278	3	10
176	Mechanistic Insights into Polyion Complex Associations. *Macromolecules*, **2018**, 51, 1427-1440	5.5	9
175	Effect of Magnetic Coupling on Water Proton Relaxivity in a Series of Transition Metal Gd Complexes. *Inorganic Chemistry*, **2018**, 57, 5810-5819	5.1	9

174	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	3	9
173	Acycloguanosyl 5′-thymidyltriphosphate, a thymidine analogue prodrug activated by telomerase, reduces pancreatic tumor growth in mice. *Gastroenterology*, **2011**, 140, 709-720.e9	13.3	9
172	The D13C variant of Bacillus schlegelii 7Fe ferredoxin is an 8Fe ferredoxin as revealed by 1H-NMR spectroscopy. *FEBS Letters*, **1997**, 412, 501-5	3.8	9
171	Solution structure of an artificial Fe8S8 ferredoxin: the D13C variant of Bacillus schlegelii Fe7S8 ferredoxin. *FEBS Journal*, **1998**, 258, 502-14		9
170	Dynamics of wild-type HiPIPs: a Cys77Ser mutant and a partially unfolded HiPIP. *Journal of Biological Inorganic Chemistry*, **2002**, 7, 691-703	3.7	9
169	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		9
168	Interactions between alpha-amino acids and cobalt(II) bovine-carbonic anhydrase. *Bioinorganic Chemistry*, **1977**, 7, 225-31		9
167	A 31P NMR study of phosphate in presence of cobalt(II)- and copper(II)- substituted bovine carbonic anhydrase B. *FEBS Letters*, **1978**, 93, 251-4	3.8	9
166	Solid-State NMR of PEGylated Proteins. *Angewandte Chemie*, **2016**, 128, 2492-2495	3.6	9
165	Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry. *Molecular Physics*, **2019**, 117, 888-897	1.7	9
164	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	5.1	9
163	H NMR Spectroscopy of [FeFe] Hydrogenase: Insight into the Electronic Structure of the Active Site. *Journal of the American Chemical Society*, **2018**, 140, 131-134	16.4	9
162	Protein Glycosylation through Sulfur Fluoride Exchange (SuFEx) Chemistry: The Key Role of a Fluorosulfate Thiolactoside. *Chemistry - A European Journal*, **2018**, 24, 18981-18987	4.8	9
161	Simultaneous Targeting of RGD-Integrins and Dual Murine Double Minute Proteins in Glioblastoma Multiforme. *Journal of Medicinal Chemistry*, **2018**, 61, 4791-4809	8.3	9
160	Metabolomic analysis of serum may refine 21-gene expression assay risk recurrence stratification. *Npj Breast Cancer*, **2019**, 5, 26	7.8	8
159	Telomerase activated thymidine analogue pro-drug is a new molecule targeting hepatocellular carcinoma. *Journal of Hepatology*, **2014**, 61, 1064-72	13.4	8
158	The Da Vinci European BioBank: A Metabolomics-Driven Infrastructure. *Journal of Personalized Medicine*, **2015**, 5, 107-19	3.6	8
157	Biotin-tagged probes for MMP expression and activation: design, synthesis, and binding properties. *Bioconjugate Chemistry*, **2009**, 20, 719-27	6.3	8

156	Folding properties of iron–sulfur proteins. *Inorganica Chimica Acta*, **1998**, 283, 12-16	2.7	8
155	Monomorphism of human cytochrome c. *Genomics*, **2006**, 88, 669-72	4.3	8
154	Carbonic Anhydrase: An Example of How the Cavity Governs the Reactivity at the Zinc Ion. *Comments on Inorganic Chemistry*, **1995**, 17, 1-15	3.9	8
153	The structure of iron-sulfur clusters in proteins as monitored by NMR, mössbauer, EPR and molecular dynamics. *Journal of Molecular Structure*, **1993**, 292, 207-219	3.4	8
152	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	1.9	8
151	17O NMR investigation of copper(II) substituted carbonic anhydrases. *Inorganica Chimica Acta*, **1981**, 56, 1-4	2.7	8
150	Different behavior of sulfonamides with respect to copper-substituted bovine and human carbonic anhydrases. *Journal of Inorganic Biochemistry*, **1982**, 16, 155-60	4.2	8
149	Evidence of exchangeable protons in the acidic form of manganese(II) bovine carbonic anhydrase B. *FEBS Letters*, **1978**, 87, 92-4	3.8	8
148	Precision Oncology via NMR-Based Metabolomics: A Review on Breast Cancer. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	8
147	A High-Resolution View of the Coordination Environment in a Paramagnetic Metalloprotein from its Magnetic Properties. *Angewandte Chemie - International Edition*, **2021**, 60, 14960-14966	16.4	8
146	Metal centers in biomolecular solid-state NMR. *Journal of Structural Biology*, **2019**, 206, 99-109	3.4	8
145	NMR-Based Metabolomics for the Assessment of Inhaled Pharmacotherapy in Chronic Obstructive Pulmonary Disease Patients. *Journal of Proteome Research*, **2020**, 19, 64-74	5.6	8
144	Cancer cell death induced by ferritins and the peculiar role of their labile iron pool. *Oncotarget*, **2018**, 9, 27974-27984	3.3	8
143	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	4	7
142	Paramagnetic NMR as a new tool in structural biology. *Emerging Topics in Life Sciences*, **2018**, 2, 19-28	3.5	7
141	Investigation of Variations in the Human Urine Metabolome amongst European Populations: An Exploratory Search for Biomarkers of People at Risk-of-Poverty. *Molecular Nutrition and Food Research*, **2019**, 63, e1800216	5.9	7
140	NMR characterization of the C-terminal tail of full-length RAGE in a membrane mimicking environment. *Journal of Biomolecular NMR*, **2012**, 54, 285-90	3	7
139	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, 1712-22	8.3	7

138	Snapshots of the Reaction Mechanism of Matrix Metalloproteinases. *Angewandte Chemie*, **2006**, 118, 8120-8123	3.6	7
137	Direct measurement of dynamic frequency shift induced by cross-correlations in 15N-enriched proteins. *ChemPhysChem*, **2004**, 5, 959-65	3.2	7
136	X-ray Structures of Binary and Ternary Enzyme-Product-Inhibitor Complexes of Matrix Metalloproteinases. *Angewandte Chemie*, **2003**, 115, 2777-2780	3.6	7
135	Application of NMRD to hydration of rubredoxin and a variant containing a (Cys-S)3FeIII(OH) site. *Biophysical Journal*, **2003**, 84, 545-51	2.9	7
134	Redox-related chemical shift perturbations on backbone nuclei of high-potential iron-sulfur proteins. *Inorganic Chemistry*, **2002**, 41, 1679-83	5.1	7
133	A Refined Model for [Fe3S4]0 Clusters in Proteins. *Angewandte Chemie*, **2000**, 112, 3766-3768	3.6	7
132	Redox-dependent hydration of cytochrome c and cytochrome b(5) studied through (17)O NMRD. *Journal of the American Chemical Society*, **2001**, 123, 12925-6	16.4	7
131	Experimental data and calculated parameters in FeS polymetallic centers in proteins. *Journal of Biological Inorganic Chemistry*, **1996**, 1, 183-185	3.7	7
130	Applications of COSY to paramagnetic heme-containing systems. *Journal of Magnetic Resonance*, **1991**, 95, 244-252		7
129	Paramagnetism and dynamic properties of electrons and nuclei. *Coordination Chemistry Reviews*, **1992**, 120, 281-307	23.2	7
128	Relaxometry and paramagnetic metal ions in biological systems. *Magnetic Resonance in Chemistry*, **1993**, 31, S145-S153	2.1	7
127	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	2.7	7
126	Solvent 1H NMRD of copper(II) complexes. *Chemical Physics Letters*, **1985**, 118, 345-347	2.5	7
125	The complex cation [Co{tris(3,5-dimethyl-1-parazolylmethyl)amine)amine}H2O]2+: a model for metalloenzymes containing bipositive zinc(II) chromophores with a water molecule in the coordination sphere. *Inorganica Chimica Acta*, **1980**, 46, L91-L92	2.7	7
124	H NMR Relaxometric Study of Chitosan-Based Nanogels Containing Mono- and Bis-Hydrated Gd(III) Chelates: Clues for MRI Probes of Improved Sensitivity.. *ACS Applied Bio Materials*, **2020**, 3, 9065-9072	4.1	7
123	NMR fingerprinting as a tool to evaluate post-harvest time-related changes of peaches, tomatoes and plums. *Food Research International*, **2015**, 75, 106-114	7	6
122	Hochdurchsatz-Metabolomik mit 1D-NMR. *Angewandte Chemie*, **2019**, 131, 980-1007	3.6	6
121	De-escalating and escalating treatment beyond endocrine therapy in patients with luminal breast cancer. *Breast*, **2017**, 34 Suppl 1, S13-S18	3.6	6

120	Transition metal ions: shift and relaxation **2017**, 175-253		6
119	Backbone and side-chains 1H, 13C and 15N NMR assignment of human beta-parvalbumin. *Journal of Biomolecular NMR*, **2005**, 33, 137	3	6
118	Frontiers in 2D NMR of paramagnetic metalloproteins. *Applied Magnetic Resonance*, **1993**, 4, 461-476	0.8	6
117	Azide and chloride binding to carboxypeptidase A in the presence of L-phenylalanine. *Journal of Inorganic Biochemistry*, **1990**, 39, 9-16	4.2	6
116	DHA-Induced Perturbation of Human Serum Metabolome. Role of the Food Matrix and Co-Administration of Oat β-glucan and Anthocyanins. *Nutrients*, **2019**, 12,	6.7	6
115	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	3.5	6
114	A geroscience approach for Parkinson's disease: Conceptual framework and design of PROPAG-AGEING project. *Mechanisms of Ageing and Development*, **2021**, 194, 111426	5.6	6
113	Detection of Metabolite-Protein Interactions in Complex Biological Samples by High-Resolution Relaxometry: Toward Interactomics by NMR. *Journal of the American Chemical Society*, **2021**,	16.4	6
112	Fingerprinting Acute Digestive Diseases by Untargeted NMR Based Metabolomics. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	6
111	NMR Spectroscopy and Metal Ions in Life Sciences. *European Journal of Inorganic Chemistry*, **2018**, 2018, 4752-4770	2.3	6
110	Multivariate Curve Resolution for 2D Solid-State NMR spectra. *Analytical Chemistry*, **2020**, 92, 4451-4458	7.8	5
109	Engineering l-asparaginase for spontaneous formation of calcium phosphate bioinspired microreactors. *Physical Chemistry Chemical Physics*, **2018**, 20, 12719-12726	3.6	5
108	The hyperfine shift **2017**, 25-60		5
107	Detecting Small Structural Changes in Metalloproteins by the Use of NMR Pseudocontact Shifts. *European Journal of Inorganic Chemistry*, **2002**, 2002, 2121-2127	2.3	5
106	An NMR method for studying the kinetics of metal exchange in biomolecular systems. *Journal of Biomolecular NMR*, **2002**, 23, 303-9	3	5
105	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	2.1	5
104	Active-site modification of superoxide dismutase by H2O2 studied through 1H NMR of the cobalt derivatives. *Archives of Biochemistry and Biophysics*, **1989**, 269, 586-94	4.1	5
103	NMR of Paramagnetic Systems. *ACS Symposium Series*, **1988**, 70-84	0.4	5

102	Are there other acidic groups capable of affecting the electronic spectra of cobalt(II) substituted carbonic anhydrase?. *Inorganica Chimica Acta*, **1984**, 91, 173-177	2.7	5
101	Investigation of zinc-deprived bovine superoxide dismutase. *Inorganica Chimica Acta*, **1984**, 91, 109-111	2.7	5
100	Investigation of cobalt(II) substituted carboxypeptidase a interacting with azide and cyanate ions. *Inorganica Chimica Acta*, **1985**, 107, 153-157	2.7	5
99	Nuclear spin relaxation in paramagnetic () systems. A comparison of two new theoretical approaches. *Journal of Magnetic Resonance*, **1985**, 62, 235-241		5
98	Chapter 1:NMR Consequences of the Nucleus□Electron Spin Interactions. *New Developments in NMR*, **2018**, 1-41	0.9	5
97	CXCR4 antagonism sensitizes cancer cells to novel indole-based MDM2/4 inhibitors in glioblastoma multiforme. *European Journal of Pharmacology*, **2021**, 897, 173936	5.3	5
96	A Serum Metabolomics Classifier Derived from Elderly Patients with Metastatic Colorectal Cancer Predicts Relapse in the Adjuvant Setting. *Cancers*, **2021**, 13,	6.6	5
95	Gelified Biofluids for High-Resolution Magic Angle Spinning H NMR Analysis: The Case of Urine. *Analytical Chemistry*, **2017**, 89, 1054-1058	7.8	4
94	Solid-state NMR studies of metal-free SOD1 fibrillar structures. *Journal of Biological Inorganic Chemistry*, **2014**, 19, 659-66	3.7	4
93	High resolution solid-state NMR in paramagnetic molecules **2017**, 127-150		4
92	Lanthanoids and actinoids: shift and relaxation **2017**, 255-276		4
91	Targeting Metabolomics in Breast Cancer. *Current Breast Cancer Reports*, **2012**, 4, 249-256	0.8	4
90	Metabolomics for the future of personalized medicine through information and communication technologies. *Personalized Medicine*, **2012**, 9, 133-136	2.2	4
89	Paramagnetic Systems in Biochemistry: Solution NMR Studies **2010**,		4
88	Selective versus non-selective T1 experiments to determine metal-nucleus distances in paramagnetic metalloproteins. *Inorganica Chimica Acta*, **1998**, 275-276, 373-379	2.7	4
87	Water-Based Ligand Screening for Paramagnetic Metalloproteins. *Angewandte Chemie*, **2008**, 120, 4609-4613	3.6	4
86	Electronic Isomerism in Oxidized High-Potential Iron-Sulfur Proteins Revisited. *ACS Symposium Series*, **2003**, 272-286	0.4	4
85	NMR Spectroscopic Detection of Protein Protons and Longitudinal Relaxation Rates between 0.01 and 50 MHz. *Angewandte Chemie*, **2005**, 117, 2263-2265	3.6	4

84	The use of propionate proton contact shifts as structural constraints. *Inorganica Chimica Acta*, **2000**, 297, 199-205	2.7	4
83	Evaluation of paramagnetic relaxation rates in a J-coupled two-spin system. *Chemical Physics Letters*, **1996**, 250, 495-504	2.5	4
82	A spectroscopic investigation of cobalt(II) substituted alkaline phosphatase. *Journal of Inorganic Biochemistry*, **1987**, 30, 77-85	4.2	4
81	Investigation of the copper?magnesium?alkaline phosphatase system. *Inorganica Chimica Acta*, **1983**, 78, 19-22	2.7	4
80	Investigation of the system cobalt(II) bovine carbonic anhydrase B-trichloroacetaldehyde. *Journal of Inorganic Biochemistry*, **1979**, 11, 49-56	4.2	4
79	13C Nmr spectra of hexakis pyridine-N-oxide cobalt(II) and nickel(II) complexes. *Inorganica Chimica Acta*, **1976**, 19, 201-202	2.7	4
78	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		4
77	New Approaches to NMR of Paramagnetic Molecules **1995**, 1-28		4
76	Creation and multi-omics characterization of a genomically hybrid strain in the nitrogen-fixing symbiotic bacteriumSinorhizobium meliloti		4
75	Serum or Plasma (and Which Plasma), That Is the Question.. *Journal of Proteome Research*, **2022**,	5.6	4
74	Characterization of the Conjugation Pattern in Large Polysaccharide Protein Conjugates by NMR Spectroscopy. *Angewandte Chemie*, **2017**, 129, 15193-15197	3.6	3
73	Single Peptide Backbone Surrogate Mutations to Regulate Angiotensin GPCR Subtype Selectivity. *Chemistry - A European Journal*, **2020**, 26, 10690-10694	4.8	3
72	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	3.8	3
71	Assessing Structural Preferences of Unstructured Protein Regions by NMR. *Biophysical Journal*, **2019**, 117, 1948-1953	2.9	3
70	Magnetic coupled systems **2017**, 347-381		3
69	Paramagnetic Molecules **2012**, 154-171		3
68	The CrIIL reduction of [2Fe-2S] ferredoxins and site of attachment of CrIII using 1H NMR and site-directed mutagenesis. *Inorganic Chemistry*, **2000**, 39, 1755-64	5.1	3
67	Polymetallic hydrolytic zinc enzymes. Probing the site of nuclease P1 through cobalt(II) substitution. *Inorganica Chimica Acta*, **1995**, 234, 9-11	2.7	3

66	Cyanometallates and cobalt(II) bovine carbonic anhydrase B. Five coordination with dicyanoaurate(I). *Inorganica Chimica Acta*, **1980**, 46, 211-214	2.7	3
65	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*, **2021**,	6.4	3
64	Iron-Sulfur Proteins: An Insight into their Electronic Structure Through 1H NMR Spectroscopy. *Topics in Molecular Organization and Engineering*, **1991**, 73-90		3
63	Different flavors of diffusion in paramagnetic systems: Unexpected NMR signal intensity and relaxation enhancements. *Journal of Magnetic Resonance Open*, **2020**, 2-3, 100003	0.4	3
62	Effects of Probiotics Administration on Human Metabolic Phenotype. *Metabolites*, **2020**, 10,	5.6	3
61	Unveiling protein dynamics in solution with field-cycling NMR relaxometry. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2021**, 124-125, 85-98	10.4	3
60	NMR for Single Ion Magnets. *Magnetochemistry*, **2021**, 7, 96	3.1	3
59	Fast and Quantitative NMR Metabolite Analysis Afforded by a Paramagnetic Co-Solute. *Angewandte Chemie*, **2019**, 131, 15427-15430	3.6	3
58	Comparison of Different Reweighting Approaches for the Calculation of Conformational Variability of Macromolecules from Molecular Simulations. *ChemPhysChem*, **2021**, 22, 127-138	3.2	3
57	Metabolomic Fingerprints in Large Population Cohorts: Impact of Preanalytical Heterogeneity. *Clinical Chemistry*, **2021**, 67, 1153-1155	5.5	3
56	Origin of the MRI Contrast in Natural and Hydrogel Formulation of Pineapple Juice. *Bioinorganic Chemistry and Applications*, **2021**, 2021, 6666018	4.2	3
55	Profiling metabolites and lipoproteins in COMETA, an Italian cohort of COVID-19 patients.. *PLoS Pathogens*, **2022**, 18, e1010443	7.6	3
54	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	1.4	2
53	Hints on experimental techniques **2017**, 383-456		2
52	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	3.3	2
51	1H-NMR and relaxometry of copper-containing dimers in proteins. *Biology of Metals*, **1990**, 3, 146-150		2
50	The effect of magnetic anisotropy on the longitudinal nuclear relaxation time in paramagnetic systems. *Journal of Magnetic Resonance*, **1990**, 89, 243-254		2
49	A water 1H and 17O N.M.R. study on PHG-modified SOD. *Inorganica Chimica Acta*, **1984**, 93, 51-53	2.7	2

48	Multinuclear NMR investigation of the metal binding sites of transferrins. *Journal of Molecular Structure*, **1984**, 113, 191-200	3.4	2
47	Impact of the pre-examination phase on multicenter metabolomic studies.. *New Biotechnology*, **2022**, 68, 37-37	6.4	2
46	The NMR tube bioreactor. *Methods in Enzymology*, **2020**, 633, 71-101	1.7	2
45	On the complementarity of X-ray and NMR data. *Journal of Structural Biology: X*, **2020**, 4, 100019	2.9	2
44	A High-Resolution View of the Coordination Environment in a Paramagnetic Metalloprotein from its Magnetic Properties. *Angewandte Chemie*, **2021**, 133, 15087-15093	3.6	2
43	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,	5.6	2
42	Prediagnostic circulating metabolites in female breast cancer cases with low and high mammographic breast density. *Scientific Reports*, **2021**, 11, 13025	4.9	2
41	Active-Site Targeting Paramagnetic Probe for Matrix Metalloproteinases. *ChemPlusChem*, **2016**, 81, 1333-1338	2.8	2
40	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	2.1	2
39	Differential Network Analysis Reveals Molecular Determinants Associated with Blood Pressure and Heart Rate in Healthy Subjects. *Journal of Proteome Research*, **2021**, 20, 1040-1051	5.6	2
38	Revisiting paramagnetic relaxation enhancements in slowly rotating systems: how long is the long range?. *Magnetic Resonance*, **2021**, 2, 25-31	2.9	2
37	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	5.6	2
36	A complete relaxation matrix refinement of the solution structure of a paramagnetic metalloprotein: Reduced HiPIP I from Ectothiorhodospira halophila **1996**, 24, 158		2
35	Solvent Proton Nuclear Magnetic Relaxation Dispersion (NMRD) in Solutions of Paramagnetic Macromolecules **1986**, 165-195		2
34	Paramagnetic effects in NMR for protein structures and ensembles: Studies of metalloproteins.. *Current Opinion in Structural Biology*, **2022**, 74, 102386	8.1	2
33	Using simple algebraic concepts to understand chemical composition problems. *International Journal of Mathematical Education in Science and Technology*, **2020**, 1-16	0.5	1
32	Chemical exchange, chemical equilibria, and dynamics **2017**, 151-173		1
31	Matrix Metalloproteinases: From Structure to Function **2015**, 41-60		1

30	Microcrystalline Proteins □An Ideal Benchmark for Methodology Development **2012**, 376-392		1
29	Solvent water1H NMRD study of oxovanadium(IV) aquo ion. *Journal of Magnetic Resonance*, **1992**, 99, 235-246		1
28	Metabolite and lipoprotein profiles reveal sex-related oxidative stress imbalance in de novo drug-naive Parkinson□s disease patients.. *Npj Parkinson□s Disease*, **2022**, 8, 14	9.7	1
27	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	2.6	1
26	Fecal metabolomic profiles: A comparative study of patients with colorectal cancer adenomatous polyps. *World Journal of Gastroenterology*, **2021**, 27, 6430-6441	5.6	1
25	NMR of Immobilized Enzymes. *Methods in Molecular Biology*, **2020**, 2100, 363-383	1.4	1
24	Characterization of lanthanoid-binding proteins using NMR spectroscopy. *Methods in Enzymology*, **2021**, 651, 103-137	1.7	1
23	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	4.4	1
22	Pseudocontact shifts as constraints for energy minimization and molecular dynamics calculations on solution structures of paramagnetic metalloproteins **1997**, 29, 68		1
21	Relaxometry and contrast agents for MRI **2017**, 313-345		0
20	A new lipid component identified in avocado pear by GC-MS and NMR spectroscopy. *Chemistry and Physics of Lipids*, **1991**, 60, 133-142	3.7	0
19	The electron□nucleus coupling: A breakthrough in the investigation of paramagnetic metalloproteins. *International Journal of Quantum Chemistry*, **1992**, 42, 1383-1396	2.1	0
18	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	6.8	0
17	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	8.9	0
16	Non-crystallographic symmetry in proteins: Jahn-Teller-like and Butterfly-like effects?. *Journal of Biological Inorganic Chemistry*, **2019**, 24, 91-101	3.7	0
15	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	6.9	0
14	Evaluation of the Higher Order Structure of Biotherapeutics Embedded in Hydrogels for Bioprinting and Drug Release. *Analytical Chemistry*, **2021**, 93, 11208-11214	7.8	0
13	High Relaxivity with No Coordinated Waters: A Seemingly Paradoxical Behavior of [Gd(DOTP)] Embedded in Nanogels.. *Inorganic Chemistry*, **2022**, 61, 5380-5387	5.1	0

12	Metabolomics Fingerprint Predicts Risk of Death in Dilated Cardiomyopathy and Heart Failure.. *Frontiers in Cardiovascular Medicine*, **2022**, 9, 851905	5.4	0
11	Phenotyping Green and Roasted Beans of Nicaraguan Coffea Arabica Varieties Processed with Different Post-Harvest Practices. *Applied Sciences (Switzerland)*, **2021**, 11, 11779	2.6	0
10	Theoretical analysis of the long-distance limit of NMR chemical shieldings.. *Journal of Chemical Physics*, **2022**, 156, 154115	3.9	0
9	Biological inorganic chemists pay tribute to Ivano Bertini. *Journal of Biological Inorganic Chemistry*, **2014**, 19, 487-9	3.7	
8	The effect of partial orientation: residual dipolar couplings **2017**, 61-76		
7	Paramagnetic restraints for structure and dynamics of biomolecules **2017**, 277-312		
6	NMR of FeS Proteins. *ACS Symposium Series*, **1998**, 302-313	0.4	
5	Evaluation of systematic exploitation of tolerance with respect to a declared nutrient content in the production of fertilizers. *Fertilizer Research*, **1992**, 32, 45-53		
4	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		
3	The use of the Electron-Nucleus Hyperfine Interaction for Solution Structure Determination **2000**, 1-17		
2	NMR and Unpaired Electrons in Biomolecules **1994**, 199-216		
1	Lokale und globale Dynamik im ungeordneten Synuklein-Protein. *Angewandte Chemie*, **2018**, 130, 15482–15486		