Claudio Luchinat

List of Publications by Year in Descending Order

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

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	Impact of the pre-examination phase on multicenter metabolomic studies.. *New Biotechnology*, **2022**, 68, 37-37	6.4	2
622	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
621	Serum or Plasma (and Which Plasma), That Is the Question.. *Journal of Proteome Research*, **2022**,	5.6	4
620	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
619	Metabolomics Fingerprint Predicts Risk of Death in Dilated Cardiomyopathy and Heart Failure.. *Frontiers in Cardiovascular Medicine*, **2022**, 9, 851905	5.4	0
618	Theoretical analysis of the long-distance limit of NMR chemical shieldings.. *Journal of Chemical Physics*, **2022**, 156, 154115	3.9	0
617	Profiling metabolites and lipoproteins in COMETA, an Italian cohort of COVID-19 patients.. *PLoS Pathogens*, **2022**, 18, e1010443	7.6	3
616	Paramagnetic effects in NMR for protein structures and ensembles: Studies of metalloproteins.. *Current Opinion in Structural Biology*, **2022**, 74, 102386	8.1	2
615	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
614	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
613	Fecal metabolomic profiles: A comparative study of patients with colorectal cancer adenomatous polyps. *World Journal of Gastroenterology*, **2021**, 27, 6430-6441	5.6	1
612	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
611	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
610	Precision Oncology via NMR-Based Metabolomics: A Review on Breast Cancer. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	8
609	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
608	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
607	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

606	Unveiling protein dynamics in solution with field-cycling NMR relaxometry. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2021**, 124-125, 85-98	10.4	3
605	Prediagnostic circulating metabolites in female breast cancer cases with low and high mammographic breast density. *Scientific Reports*, **2021**, 11, 13025	4.9	2
604	A Serum Metabolomics Classifier Derived from Elderly Patients with Metastatic Colorectal Cancer Predicts Relapse in the Adjuvant Setting. *Cancers*, **2021**, 13,	6.6	5
603	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
602	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
601	NMR for Single Ion Magnets. *Magnetochemistry*, **2021**, 7, 96	3.1	3
600	Comparison of Different Reweighting Approaches for the Calculation of Conformational Variability of Macromolecules from Molecular Simulations. *ChemPhysChem*, **2021**, 22, 127-138	3.2	3
599	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
598	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
597	Revisiting paramagnetic relaxation enhancements in slowly rotating systems: how long is the long range?. *Magnetic Resonance*, **2021**, 2, 25-31	2.9	2
596	Characterization of lanthanoid-binding proteins using NMR spectroscopy. *Methods in Enzymology*, **2021**, 651, 103-137	1.7	1
595	Metabolomic/lipidomic profiling of COVID-19 and individual response to tocilizumab. *PLoS Pathogens*, **2021**, 17, e1009243	7.6	36
594	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
593	Metabolomic Fingerprints in Large Population Cohorts: Impact of Preanalytical Heterogeneity. *Clinical Chemistry*, **2021**, 67, 1153-1155	5.5	3
592	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
591	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
590	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
589	Origin of the MRI Contrast in Natural and Hydrogel Formulation of Pineapple Juice. *Bioinorganic Chemistry and Applications*, **2021**, 2021, 6666018	4.2	3

588	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
587	Single Peptide Backbone Surrogate Mutations to Regulate Angiotensin GPCR Subtype Selectivity. *Chemistry - A European Journal*, **2020**, 26, 10690-10694	4.8	3
586	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
585	Plasma metabolome and cognitive skills in Down syndrome. *Scientific Reports*, **2020**, 10, 10491	4.9	12
584	Mixing A[1-40) and A[1-42) peptides generates unique amyloid fibrils. *Chemical Communications*, **2020**, 56, 8830-8833	5.8	13
583	Using simple algebraic concepts to understand chemical composition problems. *International Journal of Mathematical Education in Science and Technology*, **2020**, 1-16	0.5	1
582	Multivariate Curve Resolution for 2D Solid-State NMR spectra. *Analytical Chemistry*, **2020**, 92, 4451-4458	7.8	5
581	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
580	Fingerprinting Alzheimer's Disease by H Nuclear Magnetic Resonance Spectroscopy of Cerebrospinal Fluid. *Journal of Proteome Research*, **2020**, 19, 1696-1705	5.6	17
579	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
578	NMR of Immobilized Enzymes. *Methods in Molecular Biology*, **2020**, 2100, 363-383	1.4	1
577	The NMR tube bioreactor. *Methods in Enzymology*, **2020**, 633, 71-101	1.7	2
576	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
575	On the complementarity of X-ray and NMR data. *Journal of Structural Biology: X*, **2020**, 4, 100019	2.9	2
574	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
573	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
572	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
571	Effects of Probiotics Administration on Human Metabolic Phenotype. *Metabolites*, **2020**, 10,	5.6	3

570	Metabolomics to Assess Response to Immune Checkpoint Inhibitors in Patients with Non-Small-Cell Lung Cancer. *Cancers*, **2020**, 12,	6.6	13
569	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
568	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
567	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
566	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
565	Metabolomic analysis of serum may refine 21-gene expression assay risk recurrence stratification. *Npj Breast Cancer*, **2019**, 5, 26	7.8	8
564	Mechanism and Inhibition of Matrix Metalloproteinases. *Current Medicinal Chemistry*, **2019**, 26, 2609-2632	4.3	19
563	Magnetic susceptibility and paramagnetism-based NMR. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2019**, 114-115, 211-236	10.4	30
562	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
561	Structural characterization of a protein adsorbed on aluminum hydroxide adjuvant in vaccine formulation. *Npj Vaccines*, **2019**, 4, 20	9.5	14
560	Pseudocontact shifts and paramagnetic susceptibility in semiempirical and quantum chemistry theories. *Journal of Chemical Physics*, **2019**, 150, 144101	3.9	14
559	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
558	NMR for sample quality assessment in metabolomics. *New Biotechnology*, **2019**, 52, 25-34	6.4	36
557	Bimodal Fluorescence-Magnetic Resonance Contrast Agent for Apoptosis Imaging. *Journal of the American Chemical Society*, **2019**, 141, 6224-6233	16.4	64
556	The metabolic fingerprints of HCV and HBV infections studied by Nuclear Magnetic Resonance Spectroscopy. *Scientific Reports*, **2019**, 9, 4128	4.9	23
555	Reviewing the Crystal Structure of S100Z and Other Members of the S100 Family: Implications in Calcium-Regulated Quaternary Structure. *Methods in Molecular Biology*, **2019**, 1929, 487-499	1.4	2
554	High-Throughput Metabolomics by 1D NMR. *Angewandte Chemie - International Edition*, **2019**, 58, 968-994	16.4	146
553	Hochdurchsatz-Metabolomik mit 1D-NMR. *Angewandte Chemie*, **2019**, 131, 980-1007	3.6	6

552	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
551	Fast and Quantitative NMR Metabolite Analysis Afforded by a Paramagnetic Co-Solute. *Angewandte Chemie - International Edition*, **2019**, 58, 15283-15286	16.4	11
550	Relaxivity of Gd-Based MRI Contrast Agents in Crosslinked Hyaluronic Acid as a Model for Tissues. *ChemPhysChem*, **2019**, 20, 2204-2209	3.2	12
549	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
548	Assessing Structural Preferences of Unstructured Protein Regions by NMR. *Biophysical Journal*, **2019**, 117, 1948-1953	2.9	3
547	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
546	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
545	Fast and Quantitative NMR Metabolite Analysis Afforded by a Paramagnetic Co-Solute. *Angewandte Chemie*, **2019**, 131, 15427-15430	3.6	3
544	Uniqueness of the NMR approach to metabolomics. *TrAC - Trends in Analytical Chemistry*, **2019**, 120, 115300	14.6	65
543	Characterization of PEGylated Asparaginase: New Opportunities from NMR Analysis of Large PEGylated Therapeutics. *Chemistry - A European Journal*, **2019**, 25, 1984-1991	4.8	17
542	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
541	Joint X-ray/NMR structure refinement of multidomain/multisubunit systems. *Journal of Biomolecular NMR*, **2019**, 73, 265-278	3	10
540	Metabolic Signature of Primary Biliary Cholangitis and Its Comparison with Celiac Disease. *Journal of Proteome Research*, **2019**, 18, 1228-1236	5.6	17
539	Metal centers in biomolecular solid-state NMR. *Journal of Structural Biology*, **2019**, 206, 99-109	3.4	8
538	Non-crystallographic symmetry in proteins: Jahn-Teller-like and Butterfly-like effects?. *Journal of Biological Inorganic Chemistry*, **2019**, 24, 91-101	3.7	0
537	Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry. *Molecular Physics*, **2019**, 117, 888-897	1.7	9
536	Plasma and urinary metabolomic profiles of Down syndrome correlate with alteration of mitochondrial metabolism. *Scientific Reports*, **2018**, 8, 2977	4.9	41
535	HTS by NMR for the Identification of Potent and Selective Inhibitors of Metalloenzymes. *ACS Medicinal Chemistry Letters*, **2018**, 9, 137-142	4.3	12

534	Mechanistic Insights into Polyion Complex Associations. *Macromolecules*, **2018**, 51, 1427-1440	5.5	9
533	Metabolomics in breast cancer: A decade in review. *Cancer Treatment Reviews*, **2018**, 67, 88-96	14.4	65
532	Engineering l-asparaginase for spontaneous formation of calcium phosphate bioinspired microreactors. *Physical Chemistry Chemical Physics*, **2018**, 20, 12719-12726	3.6	5
531	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
530	Age and Sex Effects on Plasma Metabolite Association Networks in Healthy Subjects. *Journal of Proteome Research*, **2018**, 17, 97-107	5.6	43
529	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
528	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
527	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
526	Paramagnetic NMR as a new tool in structural biology. *Emerging Topics in Life Sciences*, **2018**, 2, 19-28	3.5	7
525	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
524	Chapter 1:NMR Consequences of the Nucleus□Electron Spin Interactions. *New Developments in NMR*, **2018**, 1-41	0.9	5
523	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
522	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
521	Assessing protein conformational landscapes: integration of DEER data in Maximum Occurrence analysis. *Physical Chemistry Chemical Physics*, **2018**, 20, 27429-27438	3.6	13
520	Fingerprinting Acute Digestive Diseases by Untargeted NMR Based Metabolomics. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	6
519	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
518	Sarcolab pilot study into skeletal muscle□ adaptation to long-term spaceflight. *Npj Microgravity*, **2018**, 4, 18	5.3	27
517	Cancer cell death induced by ferritins and the peculiar role of their labile iron pool. *Oncotarget*, **2018**, 9, 27974-27984	3.3	8

516	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
515	Local and Global Dynamics in Intrinsically Disordered Synuclein. *Angewandte Chemie - International Edition*, **2018**, 57, 15262-15266	16.4	29
514	Lokale und globale Dynamik im ungeordneten Synuklein-Protein. *Angewandte Chemie*, **2018**, 130, 15482-15486	3	16
513	NMR Spectroscopy and Metal Ions in Life Sciences. *European Journal of Inorganic Chemistry*, **2018**, 2018, 4752-4770	2.3	6
512	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
511	Aggregation kinetics of the A□1-40 peptide monitored by NMR. *Chemical Communications*, **2018**, 54, 7601-7604	5.8	19
510	NMR metabolomic fingerprinting distinguishes milk from different farms. *Food Research International*, **2018**, 113, 131-139	7	27
509	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
508	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
507	One-thousand-fold enhancement of high field liquid nuclear magnetic resonance signals at room temperature. *Nature Chemistry*, **2017**, 9, 676-680	17.6	57
506	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
505	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
504	Paramagnetic Properties of a Crystalline Iron-Sulfur Protein by Magic-Angle Spinning NMR Spectroscopy. *Inorganic Chemistry*, **2017**, 56, 6624-6629	5.1	16
503	Gelified Biofluids for High-Resolution Magic Angle Spinning H NMR Analysis: The Case of Urine. *Analytical Chemistry*, **2017**, 89, 1054-1058	7.8	4
502	Regulation of HuR structure and function by dihydrotanshinone-I. *Nucleic Acids Research*, **2017**, 45, 9514-9527	2	41
501	Characterization of the Conjugation Pattern in Large Polysaccharide-Protein Conjugates by NMR Spectroscopy. *Angewandte Chemie - International Edition*, **2017**, 56, 14997-15001	16.4	18
500	Characterization of the Conjugation Pattern in Large Polysaccharide-Protein Conjugates by NMR Spectroscopy. *Angewandte Chemie*, **2017**, 129, 15193-15197	3.6	3
499	Evidence of a DHA Signature in the Lipidome and Metabolome of Human Hepatocytes. *International Journal of Molecular Sciences*, **2017**, 18,	6.3	27

498	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
497	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
496	De-escalating and escalating treatment beyond endocrine therapy in patients with luminal breast cancer. *Breast*, **2017**, 34 Suppl 1, S13-S18	3.6	6
495	The hyperfine shift **2017**, 25-60		5
494	The effect of partial orientation: residual dipolar couplings **2017**, 61-76		
493	High resolution solid-state NMR in paramagnetic molecules **2017**, 127-150		4
492	Chemical exchange, chemical equilibria, and dynamics **2017**, 151-173		1
491	Paramagnetic restraints for structure and dynamics of biomolecules **2017**, 277-312		
490	Transition metal ions: shift and relaxation **2017**, 175-253		6
489	Magnetic coupled systems **2017**, 347-381		3
488	Hints on experimental techniques **2017**, 383-456		2
487	Lanthanoids and actinoids: shift and relaxation **2017**, 255-276		4
486	Relaxometry and contrast agents for MRI **2017**, 313-345		0
485	Deconvoluting interrelationships between concentrations and chemical shifts in urine provides a powerful analysis tool. *Nature Communications*, **2017**, 8, 1662	17.4	36
484	Atomic structural details of a protein grafted onto gold nanoparticles. *Scientific Reports*, **2017**, 7, 17934	4.9	16
483	Perspectives on paramagnetic NMR from a life sciences infrastructure. *Journal of Magnetic Resonance*, **2017**, 282, 154-169	3	18
482	KODAMA: an R package for knowledge discovery and data mining. *Bioinformatics*, **2017**, 33, 621-623	7.2	13
481	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

480	Nanodiamond-Gadolinium(III) Aggregates for Tracking Cancer Growth In Vivo at High Field. *Nano Letters*, **2016**, 16, 7551-7564	11.5	44
479	Entropy-Based Network Representation of the Individual Metabolic Phenotype. *Journal of Proteome Research*, **2016**, 15, 3298-307	5.6	20
478	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
477	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. *Angewandte Chemie - International Edition*, **2016**, 55, 14713-14717	16.4	45
476	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. *Angewandte Chemie*, **2016**, 128, 14933-14937	3.6	11
475	(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
474	Bilayer Membrane Modulation of Membrane Type 1 Matrix Metalloproteinase (MT1-MMP) Structure and Proteolytic Activity. *Scientific Reports*, **2016**, 6, 29511	4.9	10
473	Biosilica and bioinspired silica studied by solid-state NMR. *Coordination Chemistry Reviews*, **2016**, 327-328, 110-122	23.2	19
472	Metabolomics in Breast Cancer: Current Status and Perspectives. *Advances in Experimental Medicine and Biology*, **2016**, 882, 217-34	3.6	21
471	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
470	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
469	A critical assessment of methods to recover information from averaged data. *Physical Chemistry Chemical Physics*, **2016**, 18, 5686-701	3.6	55
468	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
467	Extreme Hypoxic Conditions Induce Selective Molecular Responses and Metabolic Reset in Detached Apple Fruit. *Frontiers in Plant Science*, **2016**, 7, 146	6.2	30
466	Solid-State NMR of PEGylated Proteins. *Angewandte Chemie - International Edition*, **2016**, 55, 2446-9	16.4	29
465	Solid-State NMR of PEGylated Proteins. *Angewandte Chemie*, **2016**, 128, 2492-2495	3.6	9
464	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
463	Basic facts and perspectives of Overhauser DNP NMR. *Journal of Magnetic Resonance*, **2016**, 264, 78-87	3	36

462	Atomic-Level Quality Assessment of Enzymes Encapsulated in Bioinspired Silica. *Chemistry - A European Journal*, **2016**, 22, 425-32	4.8	20
461	Individual Human Metabolic Phenotype Analyzed by (1)H NMR of Saliva Samples. *Journal of Proteome Research*, **2016**, 15, 1787-93	5.6	32
460	Active-Site Targeting Paramagnetic Probe for Matrix Metalloproteinases. *ChemPlusChem*, **2016**, 81, 1333-1338	2.8	2
459	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
458	NMR of sedimented, fibrillized, silica-entrapped and microcrystalline (metallo)proteins. *Journal of Magnetic Resonance*, **2015**, 253, 60-70	3	20
457	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
456	Allostasis and Resilience of the Human Individual Metabolic Phenotype. *Journal of Proteome Research*, **2015**, 14, 2951-62	5.6	42
455	The impact of free or standardized lifestyle and urine sampling protocol on metabolome recognition accuracy. *Genes and Nutrition*, **2015**, 10, 441	4.3	25
454	High relaxivity Gd(III)-DNA gold nanostars: investigation of shape effects on proton relaxation. *ACS Nano*, **2015**, 9, 3385-96	16.7	92
453	The effect of Gd on trityl-based dynamic nuclear polarisation in solids. *Physical Chemistry Chemical Physics*, **2015**, 17, 26969-78	3.6	25
452	Information content of long-range NMR data for the characterization of conformational heterogeneity. *Journal of Biomolecular NMR*, **2015**, 62, 353-71	3	17
451	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
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