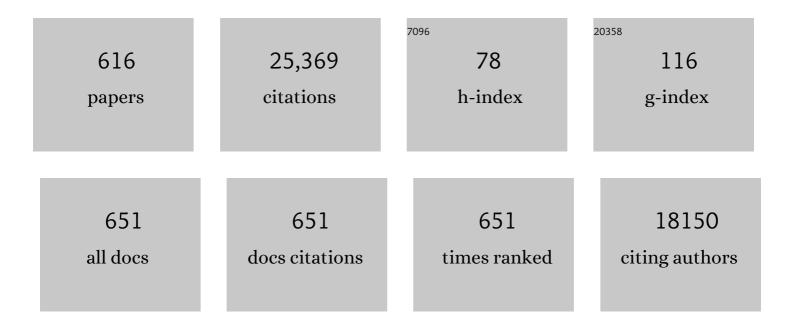
## **Claudio Luchinat**

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Using simple algebraic concepts to understand chemical composition problems. International Journal of Mathematical Education in Science and Technology, 2022, 53, 842-857.	1.4	1
2	Age- and Sex-Dependent Changes of Free Circulating Blood Metabolite and Lipid Abundances, Correlations, and Ratios. Journals of Gerontology - Series A Biological Sciences and Medical Sciences, 2022, 77, 918-926.	3.6	13
3	Impact of the pre-examination phase on multicenter metabolomic studies. New Biotechnology, 2022, 68, 37-47.	4.4	10
4	Metabolite and lipoprotein profiles reveal sex-related oxidative stress imbalance in de novo drug-naive Parkinson's disease patients. Npj Parkinson's Disease, 2022, 8, 14.	5.3	11
5	Serum or Plasma (and Which Plasma), That Is the Question. Journal of Proteome Research, 2022, 21, 1061-1072.	3.7	25
6	High Relaxivity with No Coordinated Waters: A Seemingly Paradoxical Behavior of [Gd(DOTP)] <sup>5–</sup> Embedded in Nanogels. Inorganic Chemistry, 2022, 61, 5380-5387.	4.0	7
7	Metabolomics Fingerprint Predicts Risk of Death in Dilated Cardiomyopathy and Heart Failure. Frontiers in Cardiovascular Medicine, 2022, 9, 851905.	2.4	3
8	Theoretical analysis of the long-distance limit of NMR chemical shieldings. Journal of Chemical Physics, 2022, 156, 154115.	3.0	5
9	Profiling metabolites and lipoproteins in COMETA, an Italian cohort of COVID-19 patients. PLoS Pathogens, 2022, 18, e1010443.	4.7	30
10	Paramagnetic effects in NMR for protein structures and ensembles: Studies of metalloproteins. Current Opinion in Structural Biology, 2022, 74, 102386.	5.7	9
11	Epitope Mapping and Binding Assessment by Solid-State NMR Provide a Way for the Development of Biologics under the Quality by Design Paradigm. Journal of the American Chemical Society, 2022, 144, 10006-10016.	13.7	9
12	Comparison of Different Reweighting Approaches for the Calculation of Conformational Variability of Macromolecules from Molecular Simulations. ChemPhysChem, 2021, 22, 127-138.	2.1	12
13	Differential Network Analysis Reveals Molecular Determinants Associated with Blood Pressure and Heart Rate in Healthy Subjects. Journal of Proteome Research, 2021, 20, 1040-1051.	3.7	3
14	A Quantum Chemistry View on Two Archetypical Paramagnetic Pentacoordinate Nickel(II) Complexes Offers a Fresh Look on Their NMR Spectra. Inorganic Chemistry, 2021, 60, 2068-2075.	4.0	18
15	Revisiting paramagnetic relaxation enhancements in slowly rotating systems: how long is the long range?. Magnetic Resonance, 2021, 2, 25-31.	1.9	2
16	Characterization of lanthanoid-binding proteins using NMR spectroscopy. Methods in Enzymology, 2021, 651, 103-137.	1.0	2
17	Metabolomic/lipidomic profiling of COVID-19 and individual response to tocilizumab. PLoS Pathogens, 2021, 17, e1009243.	4.7	76
18	A geroscience approach for Parkinson's disease: Conceptual framework and design of PROPAG-AGEING project. Mechanisms of Ageing and Development, 2021, 194, 111426.	4.6	14

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19	CXCR4 antagonism sensitizes cancer cells to novel indole-based MDM2/4 inhibitors in glioblastoma multiforme. European Journal of Pharmacology, 2021, 897, 173936.	3.5	11
20	Precision Oncology via NMR-Based Metabolomics: A Review on Breast Cancer. International Journal of Molecular Sciences, 2021, 22, 4687.	4.1	23
21	A Highâ€Resolution View of the Coordination Environment in a Paramagnetic Metalloprotein from its Magnetic Properties. Angewandte Chemie, 2021, 133, 15087-15093.	2.0	5
22	A Highâ€Resolution View of the Coordination Environment in a Paramagnetic Metalloprotein from its Magnetic Properties. Angewandte Chemie - International Edition, 2021, 60, 14960-14966.	13.8	13
23	Exploration of Blood Lipoprotein and Lipid Fraction Profiles in Healthy Subjects through Integrated Univariate, Multivariate, and Network Analysis Reveals Association of Lipase Activity and Cholesterol Esterification with Sex and Age. Metabolites, 2021, 11, 326.	2.9	5
24	Unveiling protein dynamics in solution with field-cycling NMR relaxometry. Progress in Nuclear Magnetic Resonance Spectroscopy, 2021, 124-125, 85-98.	7.5	18
25	Prediagnostic circulating metabolites in female breast cancer cases with low and high mammographic breast density. Scientific Reports, 2021, 11, 13025.	3.3	10
26	A Serum Metabolomics Classifier Derived from Elderly Patients with Metastatic Colorectal Cancer Predicts Relapse in the Adjuvant Setting. Cancers, 2021, 13, 2762.	3.7	14
27	Detection of Metabolite–Protein Interactions in Complex Biological Samples by High-Resolution Relaxometry: Toward Interactomics by NMR. Journal of the American Chemical Society, 2021, 143, 9393-9404.	13.7	18
28	Lipid and metabolite correlation networks specific to clinical and biochemical covariate show differences associated with sexual dimorphism in a cohort of nonagenarians. GeroScience, 2021, , 1.	4.6	2
29	NMR for Single Ion Magnets. Magnetochemistry, 2021, 7, 96.	2.4	9
30	Structure and Dynamics Perturbations in Ubiquitin Adsorbed or Entrapped in Silica Materials Are Related to Disparate Surface Chemistries Resolved by Solid-State NMR Spectroscopy. Biomacromolecules, 2021, 22, 3718-3730.	5.4	4
31	Metabolomic Fingerprints in Large Population Cohorts: Impact of Preanalytical Heterogeneity. Clinical Chemistry, 2021, 67, 1153-1155.	3.2	10
32	Evaluation of the Higher Order Structure of Biotherapeutics Embedded in Hydrogels for Bioprinting and Drug Release. Analytical Chemistry, 2021, 93, 11208-11214.	6.5	6
33	Analysis of Metabolite and Lipid Association Networks Reveals Molecular Mechanisms Associated with 3-Month Mortality and Poor Functional Outcomes in Patients with Acute Ischemic Stroke after Thrombolytic Treatment with Recombinant Tissue Plasminogen Activator. Journal of Proteome Research. 2021. 20. 4758-4770.	3.7	8
34	Not only manganese, but fruit component effects dictate the efficiency of fruit juice as an oral magnetic resonance imaging contrast agent. NMR in Biomedicine, 2021, , e4623.	2.8	2
35	Origin of the MRI Contrast in Natural and Hydrogel Formulation of Pineapple Juice. Bioinorganic Chemistry and Applications, 2021, 2021, 1-12.	4.1	3
36	Fecal metabolomic profiles: A comparative study of patients with colorectal cancer <i>vs</i> adenomatous polyps. World Journal of Gastroenterology, 2021, 27, 6430-6441.	3.3	11

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37	On the Mechanism of Bioinspired Formation of Inorganic Oxides: Structural Evidence of the Electrostatic Nature of the Interaction between a Mononuclear Inorganic Precursor and Lysozyme. Biomolecules, 2021, 11, 43.	4.0	4
38	Exploring Serum NMR-Based Metabolomic Fingerprint of Colorectal Cancer Patients: Effects of Surgery and Possible Associations with Cancer Relapse. Applied Sciences (Switzerland), 2021, 11, 11120.	2.5	3
39	Phenotyping Green and Roasted Beans of Nicaraguan Coffea Arabica Varieties Processed with Different Post-Harvest Practices. Applied Sciences (Switzerland), 2021, 11, 11779.	2.5	2
40	NMR-Based Metabolomics for the Assessment of Inhaled Pharmacotherapy in Chronic Obstructive Pulmonary Disease Patients. Journal of Proteome Research, 2020, 19, 64-74.	3.7	14
41	On the complementarity of X-ray and NMR data. Journal of Structural Biology: X, 2020, 4, 100019.	1.3	7
42	DHA-Induced Perturbation of Human Serum Metabolome. Role of the Food Matrix and Co-Administration of Oat β-glucan and Anthocyanins. Nutrients, 2020, 12, 86.	4.1	7
43	A protocol to automatically calculate homo-oligomeric protein structures through the integration of evolutionary constraints and NMR ambiguous contacts. Computational and Structural Biotechnology Journal, 2020, 18, 114-124.	4.1	3
44	Differential Network Analysis Reveals Metabolic Determinants Associated with Mortality in Acute Myocardial Infarction Patients and Suggests Potential Mechanisms Underlying Different Clinical Scores Used To Predict Death. Journal of Proteome Research, 2020, 19, 949-961.	3.7	27
45	Different flavors of diffusion in paramagnetic systems: Unexpected NMR signal intensity and relaxation enhancements. Journal of Magnetic Resonance Open, 2020, 2-3, 100003.	1.1	3
46	Effects of Probiotics Administration on Human Metabolic Phenotype. Metabolites, 2020, 10, 396.	2.9	7
47	Metabolomics to Assess Response to Immune Checkpoint Inhibitors in Patients with Non-Small-Cell Lung Cancer. Cancers, 2020, 12, 3574.	3.7	42
48	Orientation of immobilized antigens on common surfaces by a simple computational model: Exposition of SARS-CoV-2 Spike protein RBD epitopes. Biophysical Chemistry, 2020, 265, 106441.	2.8	9
49	Solution of a Puzzle: High-Level Quantum-Chemical Treatment of Pseudocontact Chemical Shifts Confirms Classic Semiempirical Theory. Journal of Physical Chemistry Letters, 2020, 11, 8735-8744.	4.6	28
50	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.	8.0	20
51	Single Peptide Backbone Surrogate Mutations to Regulate Angiotensin GPCR Subtype Selectivity. Chemistry - A European Journal, 2020, 26, 10690-10694.	3.3	7
52	Nuclear Magnetic Resonance-Based Metabolomic Comparison of Breast Milk and Organic and Traditional Formula Milk Brands for Infants and Toddlers. OMICS A Journal of Integrative Biology, 2020, 24, 424-436.	2.0	5
53	Plasma metabolome and cognitive skills in Down syndrome. Scientific Reports, 2020, 10, 10491.	3.3	23
54	Mixing Aβ(1–40) and Aβ(1–42) peptides generates unique amyloid fibrils. Chemical Communications, 2020, 56, 8830-8833.	4.1	39

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55	Multivariate Curve Resolution for 2D Solid-State NMR spectra. Analytical Chemistry, 2020, 92, 4451-4458.	6.5	15
56	The Photocatalyzed Thiolâ€ene reaction: A New Tag to Yield Fast, Selective and reversible Paramagnetic Tagging of Proteins. ChemPhysChem, 2020, 21, 863-869.	2.1	11
57	Fingerprinting Alzheimer's Disease by <sup>1</sup> H Nuclear Magnetic Resonance Spectroscopy of Cerebrospinal Fluid. Journal of Proteome Research, 2020, 19, 1696-1705.	3.7	32
58	Effect of Estrogen Receptor Status on Circulatory Immune and Metabolomics Profiles of HER2-Positive Breast Cancer Patients Enrolled for Neoadjuvant Targeted Chemotherapy. Cancers, 2020, 12, 314.	3.7	22
59	The NMR tube bioreactor. Methods in Enzymology, 2020, 633, 71-101.	1.0	3
60	<sup>1</sup> H NMR Relaxometric Study of Chitosan-Based Nanogels Containing Mono- and Bis-Hydrated Gd(III) Chelates: Clues for MRI Probes of Improved Sensitivity. ACS Applied Bio Materials, 2020, 3, 9065-9072.	4.6	16
61	NMR of Immobilized Enzymes. Methods in Molecular Biology, 2020, 2100, 363-383.	0.9	1
62	Highâ€Throughput Metabolomics by 1D NMR. Angewandte Chemie - International Edition, 2019, 58, 968-994.	13.8	254
63	Hochdurchsatzâ€Metabolomik mit 1Dâ€NMR. Angewandte Chemie, 2019, 131, 980-1007.	2.0	8
64	Investigation of Variations in the Human Urine Metabolome amongst European Populations: An Exploratory Search for Biomarkers of People at Riskâ€ofâ€Poverty. Molecular Nutrition and Food Research, 2019, 63, e1800216.	3.3	10
65	Fast and Quantitative NMR Metabolite Analysis Afforded by a Paramagnetic Coâ€Solute. Angewandte Chemie - International Edition, 2019, 58, 15283-15286.	13.8	22
66	Relaxivity of Gdâ€Based MRI Contrast Agents in Crosslinked Hyaluronic Acid as a Model for Tissues. ChemPhysChem, 2019, 20, 2204-2209.	2.1	14
67	What are the methodological and theoretical prospects for paramagnetic NMR in structural biology? A glimpse into the crystal ball. Journal of Magnetic Resonance, 2019, 306, 173-179.	2.1	16
68	Assessing Structural Preferences of Unstructured Protein Regions by NMR. Biophysical Journal, 2019, 117, 1948-1953.	0.5	4
69	Metabolomic analysis of serum may refine 21-gene expression assay risk recurrence stratification. Npj Breast Cancer, 2019, 5, 26.	5.2	12
70	Mechanism and Inhibition of Matrix Metalloproteinases. Current Medicinal Chemistry, 2019, 26, 2609-2633.	2.4	31
71	Magnetic susceptibility and paramagnetism-based NMR. Progress in Nuclear Magnetic Resonance Spectroscopy, 2019, 114-115, 211-236.	7.5	54
72	How Do Nuclei Couple to the Magnetic Moment of a Paramagnetic Center? A New Theory at the Gauntlet of the Experiments. Journal of Physical Chemistry Letters, 2019, 10, 3610-3614.	4.6	18

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73	Structural characterization of a protein adsorbed on aluminum hydroxide adjuvant in vaccine formulation. Npj Vaccines, 2019, 4, 20.	6.0	23
74	Pseudocontact shifts and paramagnetic susceptibility in semiempirical and quantum chemistry theories. Journal of Chemical Physics, 2019, 150, 144101.	3.0	19
75	Dissecting the Interactions between Human Serum Albumin and α-Synuclein: New Insights on the Factors Influencing α-Synuclein Aggregation in Biological Fluids. Journal of Physical Chemistry B, 2019, 123, 4380-4386.	2.6	25
76	NMR for sample quality assessment in metabolomics. New Biotechnology, 2019, 52, 25-34.	4.4	49
77	Bimodal Fluorescence-Magnetic Resonance Contrast Agent for Apoptosis Imaging. Journal of the American Chemical Society, 2019, 141, 6224-6233.	13.7	111
78	The metabolic fingerprints of HCV and HBV infections studied by Nuclear Magnetic Resonance Spectroscopy. Scientific Reports, 2019, 9, 4128.	3.3	36
79	Reviewing the Crystal Structure of S100Z and Other Members of the S100 Family: Implications in Calcium-Regulated Quaternary Structure. Methods in Molecular Biology, 2019, 1929, 487-499.	0.9	5
80	Nanoparticles for the multivalent presentation of a TnThr mimetic and as tool for solid state NMR coating investigation. Pure and Applied Chemistry, 2019, 91, 1471-1478.	1.9	3
81	Fast and Quantitative NMR Metabolite Analysis Afforded by a Paramagnetic Coâ€Solute. Angewandte Chemie, 2019, 131, 15427-15430.	2.0	7
82	Uniqueness of the NMR approach to metabolomics. TrAC - Trends in Analytical Chemistry, 2019, 120, 115300.	11.4	103
83	Characterization of PEGylated Asparaginase: New Opportunities from NMR Analysis of Large PEGylated Therapeutics. Chemistry - A European Journal, 2019, 25, 1984-1991.	3.3	32
84	NMR-based metabolomics identifies patients at high risk of death within two years after acute myocardial infarction in the AMI-Florence II cohort. BMC Medicine, 2019, 17, 3.	5.5	66
85	Joint X-ray/NMR structure refinement of multidomain/multisubunit systems. Journal of Biomolecular NMR, 2019, 73, 265-278.	2.8	16
86	Metabolic Signature of Primary Biliary Cholangitis and Its Comparison with Celiac Disease. Journal of Proteome Research, 2019, 18, 1228-1236.	3.7	26
87	Metal centers in biomolecular solid-state NMR. Journal of Structural Biology, 2019, 206, 99-109.	2.8	10
88	Non-crystallographic symmetry in proteins: Jahn–Teller-like and Butterfly-like effects?. Journal of Biological Inorganic Chemistry, 2019, 24, 91-101.	2.6	2
89	Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry. Molecular Physics, 2019, 117, 888-897.	1.7	15
90	Plasma and urinary metabolomic profiles of Down syndrome correlate with alteration of mitochondrial metabolism. Scientific Reports, 2018, 8, 2977.	3.3	80

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91	HTS by NMR for the Identification of Potent and Selective Inhibitors of Metalloenzymes. ACS Medicinal Chemistry Letters, 2018, 9, 137-142.	2.8	16
92	Mechanistic Insights into Polyion Complex Associations. Macromolecules, 2018, 51, 1427-1440.	4.8	9
93	Metabolomics in breast cancer: A decade in review. Cancer Treatment Reviews, 2018, 67, 88-96.	7.7	87
94	Engineering <scp>l</scp> -asparaginase for spontaneous formation of calcium phosphate bioinspired microreactors. Physical Chemistry Chemical Physics, 2018, 20, 12719-12726.	2.8	9
95	Effect of Magnetic Coupling on Water Proton Relaxivity in a Series of Transition Metal Gd <sup>III</sup> Complexes. Inorganic Chemistry, 2018, 57, 5810-5819.	4.0	11
96	Age and Sex Effects on Plasma Metabolite Association Networks in Healthy Subjects. Journal of Proteome Research, 2018, 17, 97-107.	3.7	66
97	Enriching the biological space of natural products and charting drug metabolites, through real time biotransformation monitoring: The NMR tube bioreactor. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1-8.	2.4	8
98	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. Analytical Chemistry, 2018, 90, 649-656.	6.5	50
99	Long-range paramagnetic NMR data can provide a closer look on metal coordination in metalloproteins. Journal of Biological Inorganic Chemistry, 2018, 23, 71-80.	2.6	22
100	1H NMR Spectroscopy of [FeFe] Hydrogenase: Insight into the Electronic Structure of the Active Site. Journal of the American Chemical Society, 2018, 140, 131-134.	13.7	9
101	Assessing protein conformational landscapes: integration of DEER data in Maximum Occurrence analysis. Physical Chemistry Chemical Physics, 2018, 20, 27429-27438.	2.8	20
102	Fingerprinting Acute Digestive Diseases by Untargeted NMR Based Metabolomics. International Journal of Molecular Sciences, 2018, 19, 3288.	4.1	12
103	Protein Glycosylation through Sulfur Fluoride Exchange (SuFEx) Chemistry: The Key Role of a Fluorosulfate Thiolactoside. Chemistry - A European Journal, 2018, 24, 18981-18987.	3.3	17
104	Sarcolab pilot study into skeletal muscle's adaptation to long-term spaceflight. Npj Microgravity, 2018, 4, 18.	3.7	62
105	Cancer cell death induced by ferritins and the peculiar role of their labile iron pool. Oncotarget, 2018, 9, 27974-27984.	1.8	12
106	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.	0.7	30
107	Local and Global Dynamics in Intrinsically Disordered Synuclein. Angewandte Chemie - International Edition, 2018, 57, 15262-15266.	13.8	49
108	Lokale und globale Dynamik im ungeordneten Synukleinâ€Protein. Angewandte Chemie, 2018, 130, 15482-15486.	2.0	0

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109	NMR Spectroscopy and Metal Ions in Life Sciences. European Journal of Inorganic Chemistry, 2018, 2018, 4752-4770.	2.0	9
110	Simultaneous Targeting of RGD-Integrins and Dual Murine Double Minute Proteins in Glioblastoma Multiforme. Journal of Medicinal Chemistry, 2018, 61, 4791-4809.	6.4	22
111	Aggregation kinetics of the Aβ1–40 peptide monitored by NMR. Chemical Communications, 2018, 54, 7601-7604.	4.1	29
112	NMR metabolomic fingerprinting distinguishes milk from different farms. Food Research International, 2018, 113, 131-139.	6.2	39
113	Breathomics for Assessing the Effects of Treatment and Withdrawal With Inhaled Beclomethasone/Formoterol in Patients With COPD. Frontiers in Pharmacology, 2018, 9, 258.	3.5	25
114	Paramagnetic NMR as a new tool in structural biology. Emerging Topics in Life Sciences, 2018, 2, 19-28.	2.6	8
115	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.	6.4	36
116	NMR Consequences of the Nucleusâ $\in$ "Electron Spin Interactions. New Developments in NMR, 2018, , 1-41.	0.1	6
117	KODAMA: an R package for knowledge discovery and data mining. Bioinformatics, 2017, 33, 621-623.	4.1	33
118	Serum Metabolomic Profiles Identify ER-Positive Early Breast Cancer Patients at Increased Risk of Disease Recurrence in a Multicenter Population. Clinical Cancer Research, 2017, 23, 1422-1431.	7.0	65
119	Identification of productive and futile encounters in an electron transfer protein complex. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E1840-E1847.	7.1	51
120	One-thousand-fold enhancement of high field liquid nuclear magnetic resonance signals at room temperature. Nature Chemistry, 2017, 9, 676-680.	13.6	77
121	NMR-based metabolomic approach to study urine samples of chronic inflammatory rheumatic disease patients. Analytical and Bioanalytical Chemistry, 2017, 409, 1405-1413.	3.7	28
122	Plasma and Serum Metabolite Association Networks: Comparability within and between Studies Using NMR and MS Profiling. Journal of Proteome Research, 2017, 16, 2547-2559.	3.7	43
123	Paramagnetic Properties of a Crystalline Iron–Sulfur Protein by Magic-Angle Spinning NMR Spectroscopy. Inorganic Chemistry, 2017, 56, 6624-6629.	4.0	19
124	Gelified Biofluids for High-Resolution Magic Angle Spinning <sup>1</sup> H NMR Analysis: The Case of Urine. Analytical Chemistry, 2017, 89, 1054-1058.	6.5	5
125	Regulation of HuR structure and function by dihydrotanshinone-I. Nucleic Acids Research, 2017, 45, 9514-9527.	14.5	64
126	Characterization of the Conjugation Pattern in Large Polysaccharide–Protein Conjugates by NMR Spectroscopy. Angewandte Chemie - International Edition, 2017, 56, 14997-15001.	13.8	21

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127	Characterization of the Conjugation Pattern in Large Polysaccharide–Protein Conjugates by NMR Spectroscopy. Angewandte Chemie, 2017, 129, 15193-15197.	2.0	3
128	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.	6.4	19
129	High-Resolution Solid-State NMR Characterization of Ligand Binding to a Protein Immobilized in a Silica Matrix. Journal of Physical Chemistry B, 2017, 121, 8094-8101.	2.6	17
130	De-escalating and escalating treatment beyond endocrine therapy in patients with luminal breast cancer. Breast, 2017, 34, S13-S18.	2.2	6
131	The hyperfine shift. , 2017, , 25-60.		7
132	The effect of partial orientation: residual dipolar couplings. , 2017, , 61-76.		0
133	High resolution solid-state NMR in paramagnetic molecules. , 2017, , 127-150.		4
134	Chemical exchange, chemical equilibria, andÂdynamics. , 2017, , 151-173.		1
135	Paramagnetic restraints for structure and dynamics of biomolecules. , 2017, , 277-312.		0
136	Transition metal ions: shift and relaxation. , 2017, , 175-253.		7
137	Magnetic coupled systems. , 2017, , 347-381.		3
138	Hints on experimental techniques. , 2017, , 383-456.		2
139	Lanthanoids and actinoids: shift and relaxation. , 2017, , 255-276.		4
140	Relaxometry and contrast agents for MRI. , 2017, , 313-345.		2
141	Deconvoluting interrelationships between concentrations and chemical shifts in urine provides a powerful analysis tool. Nature Communications, 2017, 8, 1662.	12.8	48
142	Atomic structural details of a protein grafted onto gold nanoparticles. Scientific Reports, 2017, 7, 17934.	3.3	24
143	Perspectives on paramagnetic NMR from a life sciences infrastructure. Journal of Magnetic Resonance, 2017, 282, 154-169.	2.1	21
144	Evidence of a DHA Signature in the Lipidome and Metabolome of Human Hepatocytes. International Journal of Molecular Sciences, 2017, 18, 359.	4.1	66

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145	Extreme Hypoxic Conditions Induce Selective Molecular Responses and Metabolic Reset in Detached Apple Fruit. Frontiers in Plant Science, 2016, 7, 146.	3.6	48
146	Solid‣tate NMR of PEGylated Proteins. Angewandte Chemie - International Edition, 2016, 55, 2446-2449.	13.8	41
147	Solidâ€State NMR of PEGylated Proteins. Angewandte Chemie, 2016, 128, 2492-2495.	2.0	12
148	Quality assurance multicenter comparison of different MR scanners for quantitative diffusion-weighted imaging. Journal of Magnetic Resonance Imaging, 2016, 43, 213-219.	3.4	67
149	Basic facts and perspectives of Overhauser DNP NMR. Journal of Magnetic Resonance, 2016, 264, 78-87.	2.1	50
150	Atomic‣evel Quality Assessment of Enzymes Encapsulated in Bioinspired Silica. Chemistry - A European Journal, 2016, 22, 425-432.	3.3	25
151	Individual Human Metabolic Phenotype Analyzed by <sup>1</sup> H NMR of Saliva Samples. Journal of Proteome Research, 2016, 15, 1787-1793.	3.7	38
152	Activeâ€5ite Targeting Paramagnetic Probe for Matrix Metalloproteinases. ChemPlusChem, 2016, 81, 1333-1338.	2.8	2
153	Nanodiamond–Gadolinium(III) Aggregates for Tracking Cancer Growth In Vivo at High Field. Nano Letters, 2016, 16, 7551-7564.	9.1	60
154	Entropy-Based Network Representation of the Individual Metabolic Phenotype. Journal of Proteome Research, 2016, 15, 3298-3307.	3.7	23
155	A protocol for the refinement of NMR structures using simultaneously pseudocontact shift restraints from multiple lanthanide ions. Journal of Biomolecular NMR, 2016, 66, 175-185.	2.8	10
156	Pseudoâ€Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMPâ€12 from First Principles. Angewandte Chemie - International Edition, 2016, 55, 14713-14717.	13.8	51
157	Pseudoâ€Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMPâ€12 from First Principles. Angewandte Chemie, 2016, 128, 14933-14937.	2.0	14
158	1H-detected solid-state NMR of proteins entrapped in bioinspired silica: a new tool for biomaterials characterization. Scientific Reports, 2016, 6, 27851.	3.3	22
159	Bilayer Membrane Modulation of Membrane Type 1 Matrix Metalloproteinase (MT1-MMP) Structure and Proteolytic Activity. Scientific Reports, 2016, 6, 29511.	3.3	13
160	Biosilica and bioinspired silica studied by solid-state NMR. Coordination Chemistry Reviews, 2016, 327-328, 110-122.	18.8	23
161	Metabolomics in Breast Cancer: Current Status and Perspectives. Advances in Experimental Medicine and Biology, 2016, 882, 217-234.	1.6	28
162	How to tackle protein structural data from solution and solid state: An integrated approach. Progress in Nuclear Magnetic Resonance Spectroscopy, 2016, 92-93, 54-70.	7.5	27

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163	Improved Accuracy from Joint X-ray and NMR Refinement of a Protein–RNA Complex Structure. Journal of the American Chemical Society, 2016, 138, 1601-1610.	13.7	22
164	A critical assessment of methods to recover information from averaged data. Physical Chemistry Chemical Physics, 2016, 18, 5686-5701.	2.8	70
165	Recommendations and Standardization of Biomarker Quantification Using NMR-Based Metabolomics with Particular Focus on Urinary Analysis. Journal of Proteome Research, 2016, 15, 360-373.	3.7	122
166	Inter-helical conformational preferences of HIV-1 TAR-RNA from maximum occurrence analysis of NMR data and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2016, 18, 5743-5752.	2.8	15
167	Biosilicaâ€Entrapped Enzymes Studied by Using Dynamic Nuclearâ€Polarizationâ€Enhanced Highâ€Field NMR Spectroscopy. ChemPhysChem, 2015, 16, 2751-2754.	2.1	30
168	Differences in Dynamics between Crosslinked and Nonâ€Crosslinked Hyaluronates Measured by using Fast Fieldâ€Cycling Relaxometry. ChemPhysChem, 2015, 16, 2803-2809.	2.1	19
169	Facing and Overcoming Sensitivity Challenges in Biomolecular NMR Spectroscopy. Angewandte Chemie - International Edition, 2015, 54, 9162-9185.	13.8	258
170	The Da Vinci European BioBank: A Metabolomics-Driven Infrastructure. Journal of Personalized Medicine, 2015, 5, 107-119.	2.5	9
171	Accurate, Fully-Automated NMR Spectral Profiling for Metabolomics. PLoS ONE, 2015, 10, e0124219.	2.5	206
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