Marco Fragai

List of Publications by Year
in descending order

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132 papers	3,673 citations	126907 33 h-index	182427 51 g-index
141 all docs	141 docs citations	141 times ranked	3996 citing authors

#	Article	IF	Citations
1	Mechanistic Studies of a Calcium-Dependent MRI Contrast Agent. Inorganic Chemistry, 2002, 41, 4018-4024.	4.0	166
2	Conformational variability of matrix metalloproteinases: Beyond a single 3D structure. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 5334-5339.	7.1	143
3	The Gâ€Triplex DNA. Angewandte Chemie - International Edition, 2013, 52, 2269-2273.	13.8	133
4	Structural Basis for Matrix Metalloproteinase 1-Catalyzed Collagenolysis. Journal of the American Chemical Society, 2012, 134, 2100-2110.	13.7	105
5	Snapshots of the Reaction Mechanism of Matrix Metalloproteinases. Angewandte Chemie - International Edition, 2006, 45, 7952-7955.	13.8	98
6	Evidence of Reciprocal Reorientation of the Catalytic and Hemopexin-Like Domains of Full-Length MMP-12. Journal of the American Chemical Society, 2008, 130, 7011-7021.	13.7	84
7	Interdomain Flexibility in Full-length Matrix Metalloproteinase-1 (MMP-1). Journal of Biological Chemistry, 2009, 284, 12821-12828.	3.4	73
8	Exploring the Subtleties of Drugâ'Receptor Interactions:Â The Case of Matrix Metalloproteinases. Journal of the American Chemical Society, 2007, 129, 2466-2475.	13.7	72
9	G-triplex structure and formation propensity. Nucleic Acids Research, 2014, 42, 13393-13404.	14.5	71
10	Entropic Contribution to the Linking Coefficient in Fragment Based Drug Design: A Case Study. Journal of Medicinal Chemistry, 2010, 53, 4285-4289.	6.4	70
11	NMR-based techniques in the hit identification and optimisation processes. Expert Opinion on Therapeutic Targets, 2004, 8, 597-611.	3.4	69
12	Examination of Matrix Metalloproteinase-1 in Solution. Journal of Biological Chemistry, 2013, 288, 30659-30671.	3.4	68
13	Sulfonamide-Functionalized Gadolinium DTPA Complexes as Possible Contrast Agents for MRI: A Relaxometric Investigation. , 2000, 2000, 625-630.		64
14	Regulation of HuR structure and function by dihydrotanshinone-I. Nucleic Acids Research, 2017, 45, 9514-9527.	14.5	64
15	Structural Basis of Serine/Threonine Phosphatase Inhibition by the Archetypal Small Molecules Cantharidin and Norcantharidin. Journal of Medicinal Chemistry, 2009, 52, 4838-4843.	6.4	62
16	1H NMRD profiles of diamagnetic proteins: a model-free analysis. Magnetic Resonance in Chemistry, 2000, 38, 543-550.	1.9	60
17	Paramagnetic Metal Ions in Ligand Screening: The CoII Matrix Metalloproteinase 12. Angewandte Chemie - International Edition, 2004, 43, 2254-2256.	13.8	54
18	Persistent contrast enhancement by sterically stabilized paramagnetic liposomes in murine melanoma. Magnetic Resonance in Medicine, 2004, 52, 669-672.	3.0	52

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19	Unraveling Hidden Regulatory Sites in Structurally Homologous Metalloproteases. Journal of Molecular Biology, 2013, 425, 2330-2346.	4.2	52
20	Crystal Structure of the Catalytic Domain of Human Matrix Metalloproteinase 10. Journal of Molecular Biology, 2004, 336, 707-716.	4.2	49
21	Combining in Silico Tools and NMR Data To Validate Proteinâ˜Ligand Structural Models:Â Application to Matrix Metalloproteinases. Journal of Medicinal Chemistry, 2005, 48, 7544-7559.	6.4	45
22	The catalytic domain of MMPâ€1 studied through tagged lanthanides. FEBS Letters, 2012, 586, 557-567.	2.8	45
23	A Calix[4]arene GdIII Complex Endowed with High Stability, Relaxivity, and Binding Affinity to Serum Albumin. Angewandte Chemie - International Edition, 2001, 40, 4737-4739.	13.8	41
24	X-ray Structures of Binary and Ternary Enzyme-Product-Inhibitor Complexes of Matrix Metalloproteinases. Angewandte Chemie - International Edition, 2003, 42, 2673-2676.	13.8	41
25	Conformational freedom of metalloproteins revealed by paramagnetism-assisted NMR. Coordination Chemistry Reviews, 2013, 257, 2652-2667.	18.8	41
26	Solidâ€State NMR of PEGylated Proteins. Angewandte Chemie - International Edition, 2016, 55, 2446-2449.	13.8	41
27	Solid-State NMR of Matrix Metalloproteinase 12: An Approach Complementary to Solution NMR. ChemBioChem, 2007, 8, 486-489.	2.6	40
28	SSNMR of biosilica-entrapped enzymes permits an easy assessment of preservation of native conformation in atomic detail. Chemical Communications, 2014, 50, 421-423.	4.1	40
29	Insights into Domainâ€“Domain Motions in Proteins and RNA from Solution NMR. Accounts of Chemical Research, 2014, 47, 3118-3126.	15.6	39
30	Interfering with HuRâ€“RNA Interaction: Design, Synthesis and Biological Characterization of Tanshinone Mimics as Novel, Effective HuR Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 1483-1498.	6.4	39
31	Mixing AÎ²(1â€“40) and AÎ²(1â€“42) peptides generates unique amyloid fibrils. Chemical Communications, 2020, 56, 8830-8833.	4.1	39
32	Solvent 1H NMRD study of biotinylated paramagnetic liposomes containing Gd-bis-SDA-DTPA or Gd-DMPE-DTPA. Inorganica Chimica Acta, 2002, 331, 151-157.	2.4	38
33	Molecular Determinants of a Selective Matrix Metalloprotease-12 Inhibitor: Insights from Crystallography and Thermodynamic Studies. Journal of Medicinal Chemistry, 2013, 56, 1149-1159.	6.4	37
34	Practical considerations over spectral quality in solid state NMR spectroscopy of soluble proteins. Journal of Biomolecular NMR, 2013, 57, 155-166.	2.8	36
35	Real-Time Insights into Biological Events: In-Cell Processes and Protein-Ligand Interactions. Biophysical Journal, 2019, 116, 239-247.	0.5	35
36	â€œFour-Dimensionalâ€•Protein Structures:â€‰ Examples from Metalloproteins. Accounts of Chemical Research, 2006, 39, 909-917.	15.6	33

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37	In Situ AP/MALDI-MS characterization of anchored matrix metalloproteinases. Journal of Mass Spectrometry, 2006, 41, 1561-1569.	1.6	32
38	Characterization of PEGylated Asparaginase: New Opportunities from NMR Analysis of Large PEGylated Therapeutics. Chemistry - A European Journal, 2019, 25, 1984-1991.	3.3	32
39	Activity of anchored human matrix metalloproteinase-1 catalytic domain on Au (111) surfaces monitored by ESI-MS. Journal of Mass Spectrometry, 2005, 40, 1565-1571.	1.6	31
40	Mechanism and Inhibition of Matrix Metalloproteinases. Current Medicinal Chemistry, 2019, 26, 2609-2633.	2.4	31
41	Structure-based approach to nanomolar, water soluble matrix metalloproteinases inhibitors (MMPIs). European Journal of Medicinal Chemistry, 2010, 45, 5919-5925.	5.5	30
42	Biosilicaâ€Entrapped Enzymes Studied by Using Dynamic Nuclearâ€Polarizationâ€Enhanced Highâ€Field NMR Spectroscopy. ChemPhysChem, 2015, 16, 2751-2754.	2.1	30
43	Aggregation kinetics of the AÎ²1â€“40 peptide monitored by NMR. Chemical Communications, 2018, 54, 7601-7604.	4.1	29
44	A High-Affinity Carbohydrate-Containing Inhibitor of Matrix Metalloproteinases. ChemMedChem, 2006, 1, 598-601.	3.2	28
45	A new methodology for monitoring the activity of cdMMP-12 anchored and freeze-dried on Au (111). Journal of the American Society for Mass Spectrometry, 2007, 18, 961-969.	2.8	27
46	Solvent 1H NMRD Study of Hexaaquochromium(III):â€‰ Inferences on Hydration and Electron Relaxation. Inorganic Chemistry, 2001, 40, 4030-4035.	4.0	25
47	Substrate Specificities of Matrix Metalloproteinase 1 in PAR-1 Exodomain Proteolysis. ChemBioChem, 2007, 8, 1367-1369.	2.6	25
48	Intra- and Interdomain Flexibility in Matrix Metalloproteinases: Functional Aspects and Drug Design. Current Pharmaceutical Design, 2009, 15, 3592-3605.	1.9	25
49	Atomicâ€Level Quality Assessment of Enzymes Encapsulated in Bioinspired Silica. Chemistry - A European Journal, 2016, 22, 425-432.	3.3	25
50	Dissecting the Interactions between Human Serum Albumin and Î±-Synuclein: New Insights on the Factors Influencing Î±-Synuclein Aggregation in Biological Fluids. Journal of Physical Chemistry B, 2019, 123, 4380-4386.	2.6	25
51	A paramagnetic probe to localize residues next to carboxylates on protein surfaces. Journal of Biological Inorganic Chemistry, 2002, 7, 617-622.	2.6	24
52	Atomic structural details of a protein grafted onto gold nanoparticles. Scientific Reports, 2017, 7, 17934.	3.3	24
53	Methyl group assignment using pseudocontact shifts with PARAssign. Journal of Biomolecular NMR, 2017, 69, 183-195.	2.8	24
54	Biosilica and bioinspired silica studied by solid-state NMR. Coordination Chemistry Reviews, 2016, 327-328, 110-122.	18.8	23

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55	Structural characterization of a protein adsorbed on aluminum hydroxide adjuvant in vaccine formulation. Npj Vaccines, 2019, 4, 20.	6.0	23
56	NMR quality control of fragment libraries for screening. Journal of Biomolecular NMR, 2020, 74, 555-563.	2.8	23
57	NMR of sedimented, fibrillized, silica-entrapped and microcrystalline (metallo)proteins. Journal of Magnetic Resonance, 2015, 253, 60-70.	2.1	22
58	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
59	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
60	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
61	Interhelical interactions within the STIM1 CC1 domain modulate CRAC channel activation. Nature Chemical Biology, 2021, 17, 196-204.	8.0	22
62	Synthesis of bicyclic molecular scaffolds (BTAa): An investigation towards new selective MMP-12 inhibitors. Bioorganic and Medicinal Chemistry, 2006, 14, 7392-7403.	3.0	21
63	Waterâ€Based Ligand Screening for Paramagnetic Metalloproteins. Angewandte Chemie - International Edition, 2008, 47, 4533-4537.	13.8	21
64	Characterization of the Conjugation Pattern in Large Polysaccharideâ€“Protein Conjugates by NMR Spectroscopy. Angewandte Chemie - International Edition, 2017, 56, 14997-15001.	13.8	21
65	Design In Silico, Synthesis and Binding Evaluation of a Carbohydrate-Based Scaffold for Structurally Novel Inhibitors of Matrix Metalloproteinases. ChemBioChem, 2005, 6, 1345-1349.	2.6	19
66	Targeting Matrix Metalloproteinases: Design of a Bifunctional Inhibitor for Presentation by Tumourâ€Associated Galectins. Chemistry - A European Journal, 2013, 19, 1896-1902.	3.3	19
67	Differences in Dynamics between Crosslinked and Nonâ€Crosslinked Hyaluronates Measured by using Fast Fieldâ€Cycling Relaxometry. ChemPhysChem, 2015, 16, 2803-2809.	2.1	19
68	Paramagnetic Properties of a Crystalline Ironâ€“Sulfur Protein by Magic-Angle Spinning NMR Spectroscopy. Inorganic Chemistry, 2017, 56, 6624-6629.	4.0	19
69	Computer-Aided Identification and Lead Optimization of Dual Murine Double Minute 2 and 4 Binders: Structureâ€“Activity Relationship Studies and Pharmacological Activity. Journal of Medicinal Chemistry, 2017, 60, 8115-8130.	6.4	19
70	Integrative Approaches in Structural Biology: A More Complete Picture from the Combination of Individual Techniques. Biomolecules, 2019, 9, 370.	4.0	19
71	Solution structure and dynamics of human S100A14. Journal of Biological Inorganic Chemistry, 2013, 18, 183-194.	2.6	18
72	Discovery of a New Class of Potent MMP Inhibitors by Structure-Based Optimization of the Arylsulfonamide Scaffold. ACS Medicinal Chemistry Letters, 2013, 4, 565-569.	2.8	18

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73	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
74	Therapeutic Targeting of MMP-12 for the Treatment of Chronic Obstructive Pulmonary Disease. Journal of Medicinal Chemistry, 2020, 63, 12911-12920.	6.4	18
75	Unveiling protein dynamics in solution with field-cycling NMR relaxometry. Progress in Nuclear Magnetic Resonance Spectroscopy, 2021, 124-125, 85-98.	7.5	18
76	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
77	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
78	Water Accessibility, Aggregation, and Motional Features of Polysaccharide-Protein Conjugate Vaccines. Biophysical Journal, 2004, 86, 3-9.	0.5	16
79	HTS by NMR for the Identification of Potent and Selective Inhibitors of Metalloenzymes. ACS Medicinal Chemistry Letters, 2018, 9, 137-142.	2.8	16
80	¹H NMR Relaxometric Study of Chitosan-Based Nanogels Containing Mono- and Bis-Hydrated Gd(III) Chelates: Clues for MRI Probes of Improved Sensitivity. ACS Applied Bio Materials, 2020, 3, 9065-9072.	4.6	16
81	Interfering with the Tumorâ€“Immune Interface: Making Way for Triazine-Based Small Molecules as Novel PD-L1 Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 16020-16045.	6.4	16
82	A Highly Soluble Matrix Metalloproteinaseâ€9 Inhibitor for Potential Treatment of Dry Eye Syndrome. Basic and Clinical Pharmacology and Toxicology, 2012, 111, 289-295.	2.5	14
83	Relaxivity of Gdâ€Based MRI Contrast Agents in Crosslinked Hyaluronic Acid as a Model for Tissues. ChemPhysChem, 2019, 20, 2204-2209.	2.1	14
84	A Structurally Simple Vaccine Candidate Reduces Progression and Dissemination of Triple-Negative Breast Cancer. IScience, 2020, 23, 101250.	4.1	14
85	Expression and high yield production of the catalytic domain of matrix metalloproteinase 12 and of an active mutant with increased solubility. Journal of Molecular Catalysis A, 2003, 204-205, 401-408.	4.8	13
86	Characterisation of the MMPâ€12â€“Elastin Adduct. Chemistry - A European Journal, 2009, 15, 7842-7845.	3.3	13
87	Bilayer Membrane Modulation of Membrane Type 1 Matrix Metalloproteinase (MT1-MMP) Structure and Proteolytic Activity. Scientific Reports, 2016, 6, 29511.	3.3	13
88	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
89	Solidâ€State NMR of PEGylated Proteins. Angewandte Chemie, 2016, 128, 2492-2495.	2.0	12
90	Lipoyl-Homotaurine Derivative (ADM_12) Reverts Oxaliplatin-Induced Neuropathy and Reduces Cancer Cells Malignancy by Inhibiting Carbonic Anhydrase IX (CAIX). Journal of Medicinal Chemistry, 2017, 60, 9003-9011.	6.4	12

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91	SARS-CoV-2 M^{pro}inhibition by a zinc ion: structural features and hints for drug design. Chemical Communications, 2021, 57, 7910-7913.	4.1	12
92	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
93	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
94	HuR-targeted agents: An insight into medicinal chemistry, biophysical, computational studies and pharmacological effects on cancer models. Advanced Drug Delivery Reviews, 2022, 181, 114088.	13.7	11
95	Biotin-Tagged Probes for MMP Expression and Activation: Design, Synthesis, and Binding Properties. Bioconjugate Chemistry, 2009, 20, 719-727.	3.6	10
96	Metal centers in biomolecular solid-state NMR. Journal of Structural Biology, 2019, 206, 99-109.	2.8	10
97	Title is missing!. Angewandte Chemie, 2003, 115, 2777-2780.	2.0	9
98	Algal autolysate medium to label proteins for NMR in mammalian cells. Journal of Biomolecular NMR, 2016, 64, 275-280.	2.8	9
99	Engineering <scp>l</scp>-asparaginase for spontaneous formation of calcium phosphate bioinspired microreactors. Physical Chemistry Chemical Physics, 2018, 20, 12719-12726.	2.8	9
100	NMR Spectroscopy and Metal Ions in Life Sciences. European Journal of Inorganic Chemistry, 2018, 2018, 4752-4770.	2.0	9
101	A small heterobifunctional ligand provides stable and water dispersible coreâ€“shell CdSe/ZnS quantum dots (QDs). Nanoscale, 2018, 10, 19720-19732.	5.6	9
102	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
103	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
104	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
105	Paramagnetic NMR as a new tool in structural biology. Emerging Topics in Life Sciences, 2018, 2, 19-28.	2.6	8
106	Fucosylated ubiquitin and orthogonally glycosylated mutant A28C: conceptually new ligands for Burkholderia ambifaria lectin (BambL). Chemical Science, 2020, 11, 12662-12670.	7.4	8
107	NMR characterization of the C-terminal tail of full-length RAGE in a membrane mimicking environment. Journal of Biomolecular NMR, 2012, 54, 285-290.	2.8	7
108	Quantum Dot-Based Probes for Labeling and Imaging of Cells that Express Matrix Metalloproteinases. ACS Omega, 2018, 3, 9822-9826.	3.5	7

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109	Single Peptide Backbone Surrogate Mutations to Regulate Angiotensin GPCR Subtype Selectivity. Chemistry - A European Journal, 2020, 26, 10690-10694.	3.3	7
110	Synthesis and binding monitoring of a new nanomolar PAMAM-based matrix metalloproteinases inhibitor (MMPIs). Bioorganic and Medicinal Chemistry, 2017, 25, 523-527.	3.0	6
111	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
112	Molecular recognition of sialoglycans by streptococcal Siglec-like adhesins: toward the shape of specific inhibitors. RSC Chemical Biology, 2021, 2, 1618-1630.	4.1	6
113	Probing the interaction of distamycin A with S100Î²: the â€œunexpectedâ€•ability of S100Î² to bind to DNAâ€binding ligands. Journal of Molecular Recognition, 2015, 28, 376-384.	2.1	5
114	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
115	HOPPI-NMR: Hot-Peptide-Based Screening Assay for Inhibitors of Proteinâ€“Protein Interactions by NMR. ACS Medicinal Chemistry Letters, 2020, 11, 1047-1053.	2.8	5
116	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
117	Exploration of zinc-binding groups for the design of inhibitors for the oxytocinase subfamily of M1 aminopeptidases. Bioorganic and Medicinal Chemistry, 2019, 27, 115177.	3.0	4
118	Sodium hyaluronate-g-2-((N-(6-aminohexyl)-4-methoxyphenyl)sulfonamido)-N-hydroxyacetamide with enhanced affinity towards MMP12 catalytic domain to be used as visco-supplement with increased degradation resistance. Carbohydrate Polymers, 2021, 271, 118452.	10.2	4
119	Automated Determination of Nuclear Magnetic Resonance Chemical Shift Perturbations in Ligand Screening Experiments: The PICASSO Web Server. Journal of Chemical Information and Modeling, 2021, , .	5.4	4
120	Characterization of the Conjugation Pattern in Large Polysaccharideâ€“Protein Conjugates by NMR Spectroscopy. Angewandte Chemie, 2017, 129, 15193-15197.	2.0	3
121	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
122	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
123	Origin of the MRI Contrast in Natural and Hydrogel Formulation of Pineapple Juice. Bioinorganic Chemistry and Applications, 2021, 2021, 1-12.	4.1	3
124	The NMR tube bioreactor. Methods in Enzymology, 2020, 633, 71-101.	1.0	3
125	Tuning Sensitivity in Paramagnetic NMR Detection of Ligandâ€“DNA Interactions. ChemMedChem, 2007, 2, 1153-1156.	3.2	2
126	Activeâ€Site Targeting Paramagnetic Probe for Matrix Metalloproteinases. ChemPlusChem, 2016, 81, 1333-1338.	2.8	2

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127	Non-crystallographic symmetry in proteins: Jahnâ€“Teller-like and Butterfly-like effects?. Journal of Biological Inorganic Chemistry, 2019, 24, 91-101.	2.6	2
128	Revisiting paramagnetic relaxation enhancements in slowly rotating systems: how long is the long range?. Magnetic Resonance, 2021, 2, 25-31.	1.9	2
129	Characterization of lanthanoid-binding proteins using NMR spectroscopy. Methods in Enzymology, 2021, 651, 103-137.	1.0	2
130	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
131	NMR of Immobilized Enzymes. Methods in Molecular Biology, 2020, 2100, 363-383.	0.9	1
132	Identification and Characterization of an RRM-Containing, RNA Binding Protein in Acinetobacter baumannii. Biomolecules, 2022, 12, 922.	4.0	0