List of Publications by Year in descending order

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		145106	206121
132	3,673	33	51
papers	citations	h-index	g-index
141	141	141	4476
all docs	docs citations	times ranked	citing authors

#	Article	IF	CITATIONS
1	HuR-targeted agents: An insight into medicinal chemistry, biophysical, computational studies and pharmacological effects on cancer models. Advanced Drug Delivery Reviews, 2022, 181, 114088.	6.6	11
2	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.	6.6	9
3	Identification and Characterization of an RRM-Containing, RNA Binding Protein in Acinetobacter baumannii. Biomolecules, 2022, 12, 922.	1.8	0
4	Interhelical interactions within the STIM1 CC1 domain modulate CRAC channel activation. Nature Chemical Biology, 2021, 17, 196-204.	3.9	22
5	Revisiting paramagnetic relaxation enhancements in slowly rotating systems: how long is the long range?. Magnetic Resonance, 2021, 2, 25-31.	0.8	2
6	Characterization of lanthanoid-binding proteins using NMR spectroscopy. Methods in Enzymology, 2021, 651, 103-137.	0.4	2
7	CXCR4 antagonism sensitizes cancer cells to novel indole-based MDM2/4 inhibitors in glioblastoma multiforme. European Journal of Pharmacology, 2021, 897, 173936.	1.7	11
8	A Highâ€Resolution View of the Coordination Environment in a Paramagnetic Metalloprotein from its Magnetic Properties. Angewandte Chemie, 2021, 133, 15087-15093.	1.6	5
9	A Highâ€Resolution View of the Coordination Environment in a Paramagnetic Metalloprotein from its Magnetic Properties. Angewandte Chemie - International Edition, 2021, 60, 14960-14966.	7.2	13
10	Unveiling protein dynamics in solution with field-cycling NMR relaxometry. Progress in Nuclear Magnetic Resonance Spectroscopy, 2021, 124-125, 85-98.	3.9	18
11	Evaluation of the Higher Order Structure of Biotherapeutics Embedded in Hydrogels for Bioprinting and Drug Release. Analytical Chemistry, 2021, 93, 11208-11214.	3.2	6
12	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.	1.6	2
13	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.	5.1	4
14	SARS-CoV-2 M ^{pro} inhibition by a zinc ion: structural features and hints for drug design. Chemical Communications, 2021, 57, 7910-7913.	2.2	12
15	Origin of the MRI Contrast in Natural and Hydrogel Formulation of Pineapple Juice. Bioinorganic Chemistry and Applications, 2021, 2021, 1-12.	1.8	3
16	Molecular recognition of sialoglycans by streptococcal Siglec-like adhesins: toward the shape of specific inhibitors. RSC Chemical Biology, 2021, 2, 1618-1630.	2.0	6
17	Interfering with the Tumor–Immune Interface: Making Way for Triazine-Based Small Molecules as Novel PD-L1 Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 16020-16045.	2.9	16
18	Automated Determination of Nuclear Magnetic Resonance Chemical Shift Perturbations in Ligand Screening Experiments: The PICASSO Web Server. Journal of Chemical Information and Modeling, 2021, ,	2.5	4

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19	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.	1.9	3
20	A Structurally Simple Vaccine Candidate Reduces Progression and Dissemination of Triple-Negative Breast Cancer. IScience, 2020, 23, 101250.	1.9	14
21	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.	1.5	9
22	Therapeutic Targeting of MMP-12 for the Treatment of Chronic Obstructive Pulmonary Disease. Journal of Medicinal Chemistry, 2020, 63, 12911-12920.	2.9	18
23	Fucosylated ubiquitin and orthogonally glycosylated mutant A28C: conceptually new ligands for <i>Burkholderia ambifaria</i> lectin (BambL). Chemical Science, 2020, 11, 12662-12670.	3.7	8
24	Single Peptide Backbone Surrogate Mutations to Regulate Angiotensin GPCR Subtype Selectivity. Chemistry - A European Journal, 2020, 26, 10690-10694.	1.7	7
25	NMR quality control of fragment libraries for screening. Journal of Biomolecular NMR, 2020, 74, 555-563.	1.6	23
26	Mixing Aβ(1–40) and Aβ(1–42) peptides generates unique amyloid fibrils. Chemical Communications, 2020, 56, 8830-8833.	2.2	39
27	HOPPI-NMR: Hot-Peptide-Based Screening Assay for Inhibitors of Protein–Protein Interactions by NMR. ACS Medicinal Chemistry Letters, 2020, 11, 1047-1053.	1.3	5
28	The Photocatalyzed Thiolâ€ene reaction: A New Tag to Yield Fast, Selective and reversible Paramagnetic Tagging of Proteins. ChemPhysChem, 2020, 21, 863-869.	1.0	11
29	The NMR tube bioreactor. Methods in Enzymology, 2020, 633, 71-101.	0.4	3
30	¹ 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.	2.3	16
31	NMR of Immobilized Enzymes. Methods in Molecular Biology, 2020, 2100, 363-383.	0.4	1
32	Integrative Approaches in Structural Biology: A More Complete Picture from the Combination of Individual Techniques. Biomolecules, 2019, 9, 370.	1.8	19
33	Relaxivity of Gdâ€Based MRI Contrast Agents in Crosslinked Hyaluronic Acid as a Model for Tissues. ChemPhysChem, 2019, 20, 2204-2209.	1.0	14
34	Exploration of zinc-binding groups for the design of inhibitors for the oxytocinase subfamily of M1 aminopeptidases. Bioorganic and Medicinal Chemistry, 2019, 27, 115177.	1.4	4
35	Mechanism and Inhibition of Matrix Metalloproteinases. Current Medicinal Chemistry, 2019, 26, 2609-2633.	1.2	31
36	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.	2.1	18

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37	Structural characterization of a protein adsorbed on aluminum hydroxide adjuvant in vaccine formulation. Npj Vaccines, 2019, 4, 20.	2.9	23
38	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.	1.2	25
39	Real-Time Insights into Biological Events: In-Cell Processes and Protein-Ligand Interactions. Biophysical Journal, 2019, 116, 239-247.	0.2	35
40	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.	0.4	5
41	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.	0.9	3
42	Characterization of PEGylated Asparaginase: New Opportunities from NMR Analysis of Large PEGylated Therapeutics. Chemistry - A European Journal, 2019, 25, 1984-1991.	1.7	32
43	Metal centers in biomolecular solid-state NMR. Journal of Structural Biology, 2019, 206, 99-109.	1.3	10
44	Non-crystallographic symmetry in proteins: Jahn–Teller-like and Butterfly-like effects?. Journal of Biological Inorganic Chemistry, 2019, 24, 91-101.	1.1	2
45	HTS by NMR for the Identification of Potent and Selective Inhibitors of Metalloenzymes. ACS Medicinal Chemistry Letters, 2018, 9, 137-142.	1.3	16
46	Interfering with HuR–RNA Interaction: Design, Synthesis and Biological Characterization of Tanshinone Mimics as Novel, Effective HuR Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 1483-1498.	2.9	39
47	Engineering <scp>l</scp> -asparaginase for spontaneous formation of calcium phosphate bioinspired microreactors. Physical Chemistry Chemical Physics, 2018, 20, 12719-12726.	1.3	9
48	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.	1.1	8
49	Long-range paramagnetic NMR data can provide a closer look on metal coordination in metalloproteins. Journal of Biological Inorganic Chemistry, 2018, 23, 71-80.	1.1	22
50	Protein Glycosylation through Sulfur Fluoride Exchange (SuFEx) Chemistry: The Key Role of a Fluorosulfate Thiolactoside. Chemistry - A European Journal, 2018, 24, 18981-18987.	1.7	17
51	NMR Spectroscopy and Metal Ions in Life Sciences. European Journal of Inorganic Chemistry, 2018, 2018, 4752-4770.	1.0	9
52	A small heterobifunctional ligand provides stable and water dispersible core–shell CdSe/ZnS quantum dots (QDs). Nanoscale, 2018, 10, 19720-19732.	2.8	9
53	Simultaneous Targeting of RGD-Integrins and Dual Murine Double Minute Proteins in Glioblastoma Multiforme. Journal of Medicinal Chemistry, 2018, 61, 4791-4809.	2.9	22
54	Aggregation kinetics of the Al̂21–40 peptide monitored by NMR. Chemical Communications, 2018, 54, 7601-7604.	2.2	29

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55	Paramagnetic NMR as a new tool in structural biology. Emerging Topics in Life Sciences, 2018, 2, 19-28.	1.1	8
56	Quantum Dot-Based Probes for Labeling and Imaging of Cells that Express Matrix Metalloproteinases. ACS Omega, 2018, 3, 9822-9826.	1.6	7
57	Paramagnetic Properties of a Crystalline Iron–Sulfur Protein by Magic-Angle Spinning NMR Spectroscopy. Inorganic Chemistry, 2017, 56, 6624-6629.	1.9	19
58	Synthesis and binding monitoring of a new nanomolar PAMAM-based matrix metalloproteinases inhibitor (MMPIs). Bioorganic and Medicinal Chemistry, 2017, 25, 523-527.	1.4	6
59	Regulation of HuR structure and function by dihydrotanshinone-I. Nucleic Acids Research, 2017, 45, 9514-9527.	6.5	64
60	Characterization of the Conjugation Pattern in Large Polysaccharide–Protein Conjugates by NMR Spectroscopy. Angewandte Chemie - International Edition, 2017, 56, 14997-15001.	7.2	21
61	Characterization of the Conjugation Pattern in Large Polysaccharide–Protein Conjugates by NMR Spectroscopy. Angewandte Chemie, 2017, 129, 15193-15197.	1.6	3
62	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.	2.9	12
63	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.	2.9	19
64	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.	1.2	17
65	Atomic structural details of a protein grafted onto gold nanoparticles. Scientific Reports, 2017, 7, 17934.	1.6	24
66	Methyl group assignment using pseudocontact shifts with PARAssign. Journal of Biomolecular NMR, 2017, 69, 183-195.	1.6	24
67	Solidâ€&tate NMR of PEGylated Proteins. Angewandte Chemie - International Edition, 2016, 55, 2446-2449.	7.2	41
68	Solid‣tate NMR of PEGylated Proteins. Angewandte Chemie, 2016, 128, 2492-2495.	1.6	12
69	Atomicâ€Level Quality Assessment of Enzymes Encapsulated in Bioinspired Silica. Chemistry - A European Journal, 2016, 22, 425-432.	1.7	25
70	Algal autolysate medium to label proteins for NMR in mammalian cells. Journal of Biomolecular NMR, 2016, 64, 275-280.	1.6	9
71	Active‣ite Targeting Paramagnetic Probe for Matrix Metalloproteinases. ChemPlusChem, 2016, 81, 1333-1338.	1.3	2
72	1H-detected solid-state NMR of proteins entrapped in bioinspired silica: a new tool for biomaterials characterization. Scientific Reports, 2016, 6, 27851.	1.6	22

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73	Bilayer Membrane Modulation of Membrane Type 1 Matrix Metalloproteinase (MT1-MMP) Structure and Proteolytic Activity. Scientific Reports, 2016, 6, 29511.	1.6	13
74	Biosilica and bioinspired silica studied by solid-state NMR. Coordination Chemistry Reviews, 2016, 327-328, 110-122.	9.5	23
75	Probing the interaction of distamycin A with S100β: the "unexpected―ability of S100β to bind to DNAâ€binding ligands. Journal of Molecular Recognition, 2015, 28, 376-384.	1.1	5
76	Biosilicaâ€Entrapped Enzymes Studied by Using Dynamic Nuclearâ€Polarizationâ€Enhanced Highâ€Field NMR Spectroscopy. ChemPhysChem, 2015, 16, 2751-2754.	1.0	30
77	Differences in Dynamics between Crosslinked and Nonâ€Crosslinked Hyaluronates Measured by using Fast Fieldâ€Cycling Relaxometry. ChemPhysChem, 2015, 16, 2803-2809.	1.0	19
78	NMR of sedimented, fibrillized, silica-entrapped and microcrystalline (metallo)proteins. Journal of Magnetic Resonance, 2015, 253, 60-70.	1.2	22
79	G-triplex structure and formation propensity. Nucleic Acids Research, 2014, 42, 13393-13404.	6.5	71
80	SSNMR of biosilica-entrapped enzymes permits an easy assessment of preservation of native conformation in atomic detail. Chemical Communications, 2014, 50, 421-423.	2.2	40
81	Insights into Domain–Domain Motions in Proteins and RNA from Solution NMR. Accounts of Chemical Research, 2014, 47, 3118-3126.	7.6	39
82	Solution structure and dynamics of human S100A14. Journal of Biological Inorganic Chemistry, 2013, 18, 183-194.	1.1	18
83	Conformational freedom of metalloproteins revealed by paramagnetism-assisted NMR. Coordination Chemistry Reviews, 2013, 257, 2652-2667.	9.5	41
84	Practical considerations over spectral quality in solid state NMR spectroscopy of soluble proteins. Journal of Biomolecular NMR, 2013, 57, 155-166.	1.6	36
85	The Gâ€Triplex DNA. Angewandte Chemie - International Edition, 2013, 52, 2269-2273.	7.2	133
86	Molecular Determinants of a Selective Matrix Metalloprotease-12 Inhibitor: Insights from Crystallography and Thermodynamic Studies. Journal of Medicinal Chemistry, 2013, 56, 1149-1159.	2.9	37
87	Unraveling Hidden Regulatory Sites in Structurally Homologous Metalloproteases. Journal of Molecular Biology, 2013, 425, 2330-2346.	2.0	52
88	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.	1.3	18
89	Examination of Matrix Metalloproteinase-1 in Solution. Journal of Biological Chemistry, 2013, 288, 30659-30671.	1.6	68
90	Targeting Matrix Metalloproteinases: Design of a Bifunctional Inhibitor for Presentation by Tumourâ€Associated Galectins. Chemistry - A European Journal, 2013, 19, 1896-1902.	1.7	19

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91	NMR characterization of the C-terminal tail of full-length RAGE in a membrane mimicking environment. Journal of Biomolecular NMR, 2012, 54, 285-290.	1.6	7
92	Structural Basis for Matrix Metalloproteinase 1-Catalyzed Collagenolysis. Journal of the American Chemical Society, 2012, 134, 2100-2110.	6.6	105
93	The catalytic domain of MMPâ€1 studied through tagged lanthanides. FEBS Letters, 2012, 586, 557-567.	1.3	45
94	A Highly Soluble Matrix Metalloproteinaseâ€9 Inhibitor for Potential Treatment of Dry Eye Syndrome. Basic and Clinical Pharmacology and Toxicology, 2012, 111, 289-295.	1.2	14
95	Structure-based approach to nanomolar, water soluble matrix metalloproteinases inhibitors (MMPIs). European Journal of Medicinal Chemistry, 2010, 45, 5919-5925.	2.6	30
96	Entropic Contribution to the Linking Coefficient in Fragment Based Drug Design: A Case Study. Journal of Medicinal Chemistry, 2010, 53, 4285-4289.	2.9	70
97	Interdomain Flexibility in Full-length Matrix Metalloproteinase-1 (MMP-1). Journal of Biological Chemistry, 2009, 284, 12821-12828.	1.6	73
98	Characterisation of the MMPâ€12–Elastin Adduct. Chemistry - A European Journal, 2009, 15, 7842-7845.	1.7	13
99	Biotin-Tagged Probes for MMP Expression and Activation: Design, Synthesis, and Binding Properties. Bioconjugate Chemistry, 2009, 20, 719-727.	1.8	10
100	Structural Basis of Serine/Threonine Phosphatase Inhibition by the Archetypal Small Molecules Cantharidin and Norcantharidin. Journal of Medicinal Chemistry, 2009, 52, 4838-4843.	2.9	62
101	Intra- and Interdomain Flexibility in Matrix Metalloproteinases: Functional Aspects and Drug Design. Current Pharmaceutical Design, 2009, 15, 3592-3605.	0.9	25
102	Waterâ€Based Ligand Screening for Paramagnetic Metalloproteins. Angewandte Chemie - International Edition, 2008, 47, 4533-4537.	7.2	21
103	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.	6.6	84
104	Exploring the Subtleties of Drugâ^'Receptor Interactions:Â The Case of Matrix Metalloproteinases. Journal of the American Chemical Society, 2007, 129, 2466-2475.	6.6	72
105	Solid-State NMR of Matrix Metalloproteinase 12: An Approach Complementary to Solution NMR. ChemBioChem, 2007, 8, 486-489.	1.3	40
106	Substrate Specificities of Matrix Metalloproteinase 1 in PAR-1 Exodomain Proteolysis. ChemBioChem, 2007, 8, 1367-1369.	1.3	25
107	Tuning Sensitivity in Paramagnetic NMR Detection of Ligand–DNA Interactions. ChemMedChem, 2007, 2, 1153-1156	1.6	2
108	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.	1.2	27

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109	"Four-Dimensional―Protein Structures:  Examples from Metalloproteins. Accounts of Chemical Research, 2006, 39, 909-917.	7.6	33
110	Synthesis of bicyclic molecular scaffolds (BTAa): An investigation towards new selective MMP-12 inhibitors. Bioorganic and Medicinal Chemistry, 2006, 14, 7392-7403.	1.4	21
111	Snapshots of the Reaction Mechanism of Matrix Metalloproteinases. Angewandte Chemie - International Edition, 2006, 45, 7952-7955.	7.2	98
112	A High-Affinity Carbohydrate-Containing Inhibitor of Matrix Metalloproteinases. ChemMedChem, 2006, 1, 598-601.	1.6	28
113	In Situ AP/MALDI-MS characterization of anchored matrix metalloproteinases. Journal of Mass Spectrometry, 2006, 41, 1561-1569.	0.7	32
114	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.	0.7	31
115	Design In Silico, Synthesis and Binding Evaluation of a Carbohydrate-Based Scaffold for Structurally Novel Inhibitors of Matrix Metalloproteinases. ChemBioChem, 2005, 6, 1345-1349.	1.3	19
116	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.	3.3	143
117	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.	2.9	45
118	Paramagnetic Metal Ions in Ligand Screening: The Coll Matrix Metalloproteinase 12. Angewandte Chemie - International Edition, 2004, 43, 2254-2256.	7.2	54
119	Persistent contrast enhancement by sterically stabilized paramagnetic liposomes in murine melanoma. Magnetic Resonance in Medicine, 2004, 52, 669-672.	1.9	52
120	NMR-based techniques in the hit identification and optimisation processes. Expert Opinion on Therapeutic Targets, 2004, 8, 597-611.	1.5	69
121	Crystal Structure of the Catalytic Domain of Human Matrix Metalloproteinase 10. Journal of Molecular Biology, 2004, 336, 707-716.	2.0	49
122	Water Accessibility, Aggregation, and Motional Features of Polysaccharide-Protein Conjugate Vaccines. Biophysical Journal, 2004, 86, 3-9.	0.2	16
123	Title is missing!. Angewandte Chemie, 2003, 115, 2777-2780.	1.6	9
124	X-ray Structures of Binary and Ternary Enzyme-Product-Inhibitor Complexes of Matrix Metalloproteinases. Angewandte Chemie - International Edition, 2003, 42, 2673-2676.	7.2	41
125	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
126	Mechanistic Studies of a Calcium-Dependent MRI Contrast Agent. Inorganic Chemistry, 2002, 41, 4018-4024.	1.9	166

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127	Solvent 1H NMRD study of biotinylated paramagnetic liposomes containing Gd-bis-SDA-DTPA or Gd-DMPE-DTPA. Inorganica Chimica Acta, 2002, 331, 151-157.	1.2	38
128	A paramagnetic probe to localize residues next to carboxylates on protein surfaces. Journal of Biological Inorganic Chemistry, 2002, 7, 617-622.	1.1	24
129	Solvent 1H NMRD Study of Hexaaquochromium(III):  Inferences on Hydration and Electron Relaxation. Inorganic Chemistry, 2001, 40, 4030-4035.	1.9	25
130	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.	7.2	41
131	Sulfonamide-Functionalized Gadolinium DTPA Complexes as Possible Contrast Agents for MRI: A Relaxometric Investigation. , 2000, 2000, 625-630.		64
132	1H NMRD profiles of diamagnetic proteins: a model-free analysis. Magnetic Resonance in Chemistry, 2000, 38, 543-550.	1.1	60