Leonard J Mueller

List of Publications by Year
in descending order

82 papers	4,227 citations	117625 34 h-index	110387 64 g-index
87 all docs	87 docs citations	87 times ranked	4606 citing authors

#	Article	IF	Citations
1	Correlating Reaction Dynamics and Size Change during the Photomechanical Transformation of 9â€Methylanthracene Single Crystals. Angewandte Chemie - International Edition, 2022, 61, .	13.8	21
2	Correlating Reaction Dynamics and Size Change during the Photomechanical Transformation of 9â€Methylanthracene Single Crystals. Angewandte Chemie, 2022, 134, e202114089.	2.0	6
3	Discovery of antimicrobial agent targeting tryptophan synthase. Protein Science, 2022, 31, 432-442.	7.6	10
4	Imaging active site chemistry and protonation states: NMR crystallography of the tryptophan synthase Î±-aminoacrylate intermediate. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	18
5	Atomic-resolution chemical characterization of (2x)72-kDa tryptophan synthase via four- and five-dimensional ¹ H-detected solid-state NMR. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	31
6	Moderated Basicity of Endohedral Amine Groups in an Octaâ€Cationic Selfâ€Assembled Cage. Angewandte Chemie - International Edition, 2022, 61, .	13.8	14
7	InnenrÃ¼cktitelbild: Correlating Reaction Dynamics and Size Change during the Photomechanical Transformation of 9â€Methylanthracene Single Crystals (Angew. Chem. 2/2022). Angewandte Chemie, 2022, 134, .	2.0	0
8	Bridging photochemistry and photomechanics with NMR crystallography: the molecular basis for the macroscopic expansion of an anthracene ester nanorod. Chemical Science, 2021, 12, 453-463.	7.4	23
9	Toho-1 Î²-lactamase: backbone chemical shift assignments and changes in dynamics upon binding with avibactam. Journal of Biomolecular NMR, 2021, 75, 303-318.	2.8	2
10	Mutation of Î²Gln114 to Ala Alters the Stabilities of Allosteric States in Tryptophan Synthase Catalysis. Biochemistry, 2021, 60, 3173-3186.	2.5	8
11	Selective, cofactor-mediated catalytic oxidation of alkanethiols in a self-assembled cage host. Chemical Communications, 2020, 56, 14263-14266.	4.1	2
12	Backbone assignments and conformational dynamics in the S. typhimurium tryptophan synthase Î±-subunit from solution-state NMR. Journal of Biomolecular NMR, 2020, 74, 341-354.	2.8	6
13	Non-Uniform Sampling in NMR Spectroscopy and the Preservation of Spectral Knowledge in the Time and Frequency Domains. Journal of Physical Chemistry A, 2020, 124, 5474-5486.	2.5	11
14	PCR Mutagenesis, Cloning, Expression, Fast Protein Purification Protocols and Crystallization of the Wild Type and Mutant Forms of Tryptophan Synthase. Journal of Visualized Experiments, 2020, , .	0.3	1
15	Cofactor-Mediated Nucleophilic Substitution Catalyzed by a Self-Assembled Holoenzyme Mimic. Journal of Organic Chemistry, 2019, 84, 12000-12008.	3.2	9
16	Investigation of the Amide Proton Solvent Exchange Properties of Glycosaminoglycan Oligosaccharides. Journal of Physical Chemistry B, 2019, 123, 4653-4662.	2.6	2
17	Direct dynamic nuclear polarization of 15N and 13C spins at 14.1 T using a trityl radical and magic angle spinning. Solid State Nuclear Magnetic Resonance, 2019, 100, 85-91.	2.3	9
18	TensorView: A software tool for displaying NMR tensors. Magnetic Resonance in Chemistry, 2019, 57, 211-223.	1.9	27

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19	Predicting anisotropic thermal displacements for hydrogens from solid-state NMR: a study on hydrogen bonding in polymorphs of palmitic acid. Physical Chemistry Chemical Physics, 2018, 20, 8475-8487.	2.8	18
20	Lipid bilayer environments control exchange kinetics of deep cavitand hosts and enhance disfavored guest conformations. Chemical Science, 2018, 9, 1836-1845.	7.4	11
21	Measuring and Modeling Highly Accurate 15 N Chemical Shift Tensors in a Peptide.. ChemPhysChem, 2017, 18, 2225-2232.	2.1	16
22	Investigation of Structural Dynamics of Enzymes and Protonation States of Substrates Using Computational Tools. Catalysts, 2016, 6, 82.	3.5	12
23	Solutionâ€State ¹⁷Oâ€…Quadrupole Centralâ€Transition NMR Spectroscopy in the Active Site of Tryptophan Synthase. Angewandte Chemie - International Edition, 2016, 55, 1350-1354.	13.8	31
24	Solutionâ€State 17 Oâ€…Quadrupole Centralâ€Transition NMR Spectroscopy in the Active Site of Tryptophan Synthase. Angewandte Chemie, 2016, 128, 1372-1376.	2.0	4
25	Protonation states and catalysis: Molecular dynamics studies of intermediates in tryptophan synthase. Protein Science, 2016, 25, 166-183.	7.6	23
26	Benchmark fragment-based¹H,¹³C,¹⁵N and¹⁷O chemical shift predictions in molecular crystals. Physical Chemistry Chemical Physics, 2016, 18, 21686-21709.	2.8	94
27	NMR Crystallography of a Carbanionic Intermediate in Tryptophan Synthase: Chemical Structure, Tautomerization, and Reaction Specificity. Journal of the American Chemical Society, 2016, 138, 15214-15226.	13.7	59
28	Crystal structure of the meta-stable intermediate in the photomechanical, crystal-to-crystal reaction of 9-tert-butyl anthracene ester. CrystEngComm, 2016, 18, 7319-7329.	2.6	29
29	Visualizing the tunnel in tryptophan synthase with crystallography: Insights into a selective filter for accommodating indole and rejecting water. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2016, 1864, 268-279.	2.3	26
30	Converging nuclear magnetic shielding calculations with respect to basis and system size in protein systems. Journal of Biomolecular NMR, 2015, 62, 327-340.	2.8	47
31	Catalytic roles of Î²Lys87 in tryptophan synthase: 15N solid state NMR studies. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1194-1199.	2.3	13
32	Anion Stripping as a General Method to Create Cationic Porous Framework with Mobile Anions. Journal of the American Chemical Society, 2014, 136, 7579-7582.	13.7	97
33	Protonation States of the Tryptophan Synthase Internal Aldimine Active Site from Solid-State NMR Spectroscopy: Direct Observation of the Protonated Schiff Base Linkage to Pyridoxal-5â€²-Phosphate. Journal of the American Chemical Society, 2014, 136, 12824-12827.	13.7	52
34	Hydroxyl-Proton Hydrogen Bonding in the Heparin Oligosaccharide Arixtra in Aqueous Solution. Journal of Physical Chemistry B, 2014, 118, 482-491.	2.6	23
35	Mechanism of Photoinduced Bending and Twisting in Crystalline Microneedles and Microribbons Composed of 9-Methylanthracene. Journal of the American Chemical Society, 2014, 136, 6617-6625.	13.7	180
36	NMR Crystallography of Enzyme Active Sites: Probing Chemically Detailed, Three-Dimensional Structure in Tryptophan Synthase. Accounts of Chemical Research, 2013, 46, 2008-2017.	15.6	36

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37	Resolution and measurement of heteronuclear dipolar couplings of a noncrystalline protein immobilized in a biological supramolecular assembly by proton-detected MAS solid-state NMR spectroscopy. Journal of Magnetic Resonance, 2013, 237, 164-168.	2.1	25
38	Proton-bound dimers of 1-methylcytosine and its derivatives: vibrational and NMR spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 19001.	2.8	14
39	Long-observation-window band-selective homonuclear decoupling: Increased sensitivity and resolution in solid-state NMR spectroscopy of proteins. Journal of Magnetic Resonance, 2013, 236, 89-94.	2.1	16
40	J-Based NMR Correlation Spectroscopy of Biological Solids. , 2013, , 1168-1173.		0
41	Allostery and Substrate Channeling in the Tryptophan Synthase Bienzyme Complex: Evidence for Two Subunit Conformations and Four Quaternary States. Biochemistry, 2013, 52, 6396-6411.	2.5	49
42	Sulfamate proton solvent exchange in heparin oligosaccharides: Evidence for a persistent hydrogen bond in the antithrombin-binding pentasaccharide Arixtra. Glycobiology, 2012, 22, 1173-1182.	2.5	46
43	Dependence of the solid-state photomechanical response of 4-chlorocinnamic acid on crystal shape and size. CrystEngComm, 2012, 14, 7792.	2.6	67
44	Vibrations of a chelated proton in a protonated tertiary diamine. Physical Chemistry Chemical Physics, 2011, 13, 20380.	2.8	15
45	Solid-state photochemical and photomechanical properties of molecular crystal nanorods composed of anthracene ester derivatives. Journal of Materials Chemistry, 2011, 21, 6258.	6.7	76
46	X-ray and NMR Crystallography in an Enzyme Active Site: The Indoline Quinonoid Intermediate in Tryptophan Synthase. Journal of the American Chemical Society, 2011, 133, 4-7.	13.7	101
47	Tensors and rotations in NMR. Concepts in Magnetic Resonance Part A: Bridging Education and Research, 2011, 38A, 221-235.	0.5	33
48	High resolution 13C-detected solid-state NMR spectroscopy of a deuterated protein. Journal of Biomolecular NMR, 2010, 48, 103-111.	2.8	22
49	pH-Responsive Nanogated Ensemble Based on Gold-Capped Mesoporous Silica through an Acid-Labile Acetal Linker. Journal of the American Chemical Society, 2010, 132, 1500-1501.	13.7	376
50	³¹P NMR Investigation of Backbone Dynamics in DNA Binding Sites. Journal of Physical Chemistry B, 2009, 113, 2596-2603.	2.6	47
51	Influence of Peripheral Groups on the Physical and Chemical Behavior of Cinchona Alkaloids. Journal of Physical Chemistry B, 2009, 113, 11696-11701.	2.6	42
52	Sensitive absorptive refocused scalar correlation NMR spectroscopy in solids. Physical Chemistry Chemical Physics, 2009, 11, 3547.	2.8	23
53	J-Based 3D sidechain correlation in solid-state proteins. Physical Chemistry Chemical Physics, 2009, 11, 7078.	2.8	25
54	The Physico-chemical Properties of Cinchona Alkaloids Responsible for their Unique Performance in Chiral Catalysis. Topics in Catalysis, 2008, 48, 120-127.	2.8	46

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55	Chelation of a Proton by an Aliphatic Tertiary Diamine. Journal of the American Chemical Society, 2008, 130, 7836-7838.	13.7	22
56	Photopolymerization of Organic Molecular Crystal Nanorods. Macromolecules, 2007, 40, 9040-9044.	4.8	39
57	Backbone Assignments in Solid-State Proteins UsingJ-Based 3D Heteronuclear Correlation Spectroscopy. Journal of the American Chemical Society, 2007, 129, 10650-10651.	13.7	59
58	Protein Refolding Assisted by Periodic Mesoporous Organosilicas. Langmuir, 2007, 23, 5735-5739.	3.5	55
59	J-based 2D homonuclear and heteronuclear correlation in solid-state proteins. Magnetic Resonance in Chemistry, 2007, 45, S84-S92.	1.9	33
60	Editorial. Magnetic Resonance in Chemistry, 2007, 45, S1-S1.	1.9	0
61	Effect of Protonation on the Conformation of Cinchonidine. Journal of the American Chemical Society, 2006, 128, 15594-15595.	13.7	69
62	Constant-Time Through-Bond13C Correlation Spectroscopy for Assigning Protein Resonances with Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2006, 128, 9992-9993.	13.7	80
63	The Amide Rotational Barrier in Isonicotinamide:â€‰ Dynamic NMR and Ab Initio Studies. Journal of Physical Chemistry A, 2005, 109, 1152-1158.	2.5	23
64	State interrogation in nuclear magnetic resonance quantum-information processing. Physical Review A, 2004, 69, .	2.5	76
65	Evidence for the Coexistence of Two Bond-Stretch Isomers in Solution. Angewandte Chemie - International Edition, 2004, 43, 4880-4883.	13.8	67
66	Uniform-sign cross-peak double-quantum-filtered correlation spectroscopy. Journal of Magnetic Resonance, 2004, 168, 327-335.	2.1	40
67	The Amide Rotational Barriers in Picolinamide and Nicotinamide:Â NMR and ab Initio Studies. Journal of the American Chemical Society, 2003, 125, 10125-10132.	13.7	81
68	Through-Bond 13Câ^'13C Correlation at the Natural Abundance Level:â€‰ Refining Dynamic Regions in the Crystal Structure of Vitamin-D3 with Solid-State NMR. Journal of the American Chemical Society, 2003, 125, 11784-11785.	13.7	67
69	Isolating Benzenium Ion Salts. Journal of the American Chemical Society, 2003, 125, 1796-1804.	13.7	169
70	Three-qubit nuclear magnetic resonance quantum information processing with a single-crystal solid. Journal of Chemical Physics, 2003, 119, 1643-1649.	3.0	26
71	Correlated tensor interactions and rotational-echo double resonance of spin clusters. Journal of Chemical Physics, 2003, 118, 8873-8881.	3.0	4
72	Crystallographic Evidence for a Free Silylium Ion. Science, 2002, 297, 825-827.	12.6	284

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73	Determination of Multiple Torsion-Angle Constraints in Uâ^'13C,15N-Labeled Peptides:Â 3D1Hâ^'15Nâ^'13Câ^'1H Dipolar Chemical Shift NMR Spectroscopy in Rotating Solids. Journal of the American Chemical Society, 2002, 124, 11908-11922.	13.7	108
74	Establishing Through-Bond Connectivity in Solids with NMR:Â Structure and Dynamics in HC60+. Journal of the American Chemical Society, 2002, 124, 9360-9361.	13.7	48
75	Synthesis and NMR Studies of13C-Labeled Vitamin D Metabolites1. Journal of Organic Chemistry, 2002, 67, 1637-1650.	3.2	26
76	Taming Superacids: Stabilization of the Fullerene Cations HC60+ and C60middle dot+. Science, 2000, 289, 101-104.	12.6	233
77	Quantum Statistical Corrections to Dynamic Nuclear Magnetic Resonance. Science, 1999, 283, 61-65.	12.6	5
78	Efficient Multispin Homonuclear Double-Quantum Recoupling for Magic-Angle Spinning NMR:â€‰ 13Câ^'13C Correlation Spectroscopy of U-13C-Erythromycin A. Journal of the American Chemical Society, 1998, 120, 10602-10612.	13.7	134
79	Mechanisms of Exciplex Formation. Roles of Superexchange, Solvent Polarity, and Driving Force for Electron Transfer. Journal of the American Chemical Society, 1994, 116, 8176-8187.	13.7	200
80	Electronic Coupling Matrix Elements in Acceptor-Donor Excited States and the Effect of Charge-Transfer Character on Their Radiative Rate Constants. Journal of the American Chemical Society, 1994, 116, 3147-3148.	13.7	47
81	Electronic Structures of Exciplexes and Excited Charge-Transfer Complexes. Journal of the American Chemical Society, 1994, 116, 8188-8199.	13.7	228
82	Moderated Basicity of Endohedral Amine Groups in an Octaâ€Cationic Selfâ€Assembled Cage. Angewandte Chemie, 0, , .	2.0	9