

# Leonard J Mueller

## List of Publications by Year in descending order

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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	pH-Responsive Nanogated Ensemble Based on Gold-Capped Mesoporous Silica through an Acid-Labile Acetal Linker. <i>Journal of the American Chemical Society</i> , 2010, 132, 1500-1501.	13.7	376
2	Crystallographic Evidence for a Free Silylium Ion. <i>Science</i> , 2002, 297, 825-827.	12.6	284
3	Taming Superacids: Stabilization of the Fullerene Cations HC <sub>60</sub> <sup>+</sup> and C <sub>60</sub> · <sup>+</sup> . <i>Science</i> , 2000, 289, 101-104.	12.6	233
4	Electronic Structures of Exciplexes and Excited Charge-Transfer Complexes. <i>Journal of the American Chemical Society</i> , 1994, 116, 8188-8199.	13.7	228
5	Mechanisms of Exciplex Formation. Roles of Superexchange, Solvent Polarity, and Driving Force for Electron Transfer. <i>Journal of the American Chemical Society</i> , 1994, 116, 8176-8187.	13.7	200
6	Mechanism of Photoinduced Bending and Twisting in Crystalline Microneedles and Microribbons Composed of 9-Methylanthracene. <i>Journal of the American Chemical Society</i> , 2014, 136, 6617-6625.	13.7	180
7	Isolating Benzenium Ion Salts. <i>Journal of the American Chemical Society</i> , 2003, 125, 1796-1804.	13.7	169
8	Efficient Multispin Homonuclear Double-Quantum Recoupling for Magic-Angle Spinning NMR: <sup>13</sup> C- <sup>13</sup> C Correlation Spectroscopy of U- <sup>13</sup> C-Erythromycin A. <i>Journal of the American Chemical Society</i> , 1998, 120, 10602-10612.	13.7	134
9	Determination of Multiple Torsion-Angle Constraints in U- <sup>13</sup> C, <sup>15</sup> N-Labeled Peptides: <sup>3</sup> D <sup>1</sup> H- <sup>15</sup> N- <sup>13</sup> C- <sup>1</sup> H Dipolar Chemical Shift NMR Spectroscopy in Rotating Solids. <i>Journal of the American Chemical Society</i> , 2002, 124, 11908-11922.	13.7	108
10	X-ray and NMR Crystallography in an Enzyme Active Site: The Indoline Quinonoid Intermediate in Tryptophan Synthase. <i>Journal of the American Chemical Society</i> , 2011, 133, 4-7.	13.7	101
11	Anion Stripping as a General Method to Create Cationic Porous Framework with Mobile Anions. <i>Journal of the American Chemical Society</i> , 2014, 136, 7579-7582.	13.7	97
12	Benchmark fragment-based <sup>1</sup> H, <sup>13</sup> C, <sup>15</sup> N and <sup>17</sup> O chemical shift predictions in molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21686-21709.	2.8	94
13	The Amide Rotational Barriers in Picolinamide and Nicotinamide: NMR and ab Initio Studies. <i>Journal of the American Chemical Society</i> , 2003, 125, 10125-10132.	13.7	81
14	Constant-Time Through-Bond <sup>13</sup> C Correlation Spectroscopy for Assigning Protein Resonances with Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2006, 128, 9992-9993.	13.7	80
15	State interrogation in nuclear magnetic resonance quantum-information processing. <i>Physical Review A</i> , 2004, 69, .	2.5	76
16	Solid-state photochemical and photomechanical properties of molecular crystal nanorods composed of anthracene ester derivatives. <i>Journal of Materials Chemistry</i> , 2011, 21, 6258.	6.7	76
17	Effect of Protonation on the Conformation of Cinchonidine. <i>Journal of the American Chemical Society</i> , 2006, 128, 15594-15595.	13.7	69
18	Through-Bond <sup>13</sup> C- <sup>13</sup> C Correlation at the Natural Abundance Level: Refining Dynamic Regions in the Crystal Structure of Vitamin-D3 with Solid-State NMR. <i>Journal of the American Chemical Society</i> , 2003, 125, 11784-11785.	13.7	67

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19	Evidence for the Coexistence of Two Bond-Stretch Isomers in Solution. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 4880-4883.	13.8	67
20	Dependence of the solid-state photomechanical response of 4-chlorocinnamic acid on crystal shape and size. <i>CrystEngComm</i> , 2012, 14, 7792.	2.6	67
21	Backbone Assignments in Solid-State Proteins Using J-Based 3D Heteronuclear Correlation Spectroscopy. <i>Journal of the American Chemical Society</i> , 2007, 129, 10650-10651.	13.7	59
22	NMR Crystallography of a Carbanionic Intermediate in Tryptophan Synthase: Chemical Structure, Tautomerization, and Reaction Specificity. <i>Journal of the American Chemical Society</i> , 2016, 138, 15214-15226.	13.7	59
23	Protein Refolding Assisted by Periodic Mesoporous Organosilicas. <i>Langmuir</i> , 2007, 23, 5735-5739.	3.5	55
24	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-5P-Phosphate. <i>Journal of the American Chemical Society</i> , 2014, 136, 12824-12827.	13.7	52
25	Allostery and Substrate Channeling in the Tryptophan Synthase Bienenzyme Complex: Evidence for Two Subunit Conformations and Four Quaternary States. <i>Biochemistry</i> , 2013, 52, 6396-6411.	2.5	49
26	Establishing Through-Bond Connectivity in Solids with NMR: Structure and Dynamics in HC60+. <i>Journal of the American Chemical Society</i> , 2002, 124, 9360-9361.	13.7	48
27	Electronic Coupling Matrix Elements in Acceptor-Donor Excited States and the Effect of Charge-Transfer Character on Their Radiative Rate Constants. <i>Journal of the American Chemical Society</i> , 1994, 116, 3147-3148.	13.7	47
28	<sup>31</sup> P NMR Investigation of Backbone Dynamics in DNA Binding Sites. <i>Journal of Physical Chemistry B</i> , 2009, 113, 2596-2603.	2.6	47
29	Converging nuclear magnetic shielding calculations with respect to basis and system size in protein systems. <i>Journal of Biomolecular NMR</i> , 2015, 62, 327-340.	2.8	47
30	The Physico-chemical Properties of Cinchona Alkaloids Responsible for their Unique Performance in Chiral Catalysis. <i>Topics in Catalysis</i> , 2008, 48, 120-127.	2.8	46
31	Sulfamate proton solvent exchange in heparin oligosaccharides: Evidence for a persistent hydrogen bond in the antithrombin-binding pentasaccharide Arixtra. <i>Glycobiology</i> , 2012, 22, 1173-1182.	2.5	46
32	Influence of Peripheral Groups on the Physical and Chemical Behavior of Cinchona Alkaloids. <i>Journal of Physical Chemistry B</i> , 2009, 113, 11696-11701.	2.6	42
33	Uniform-sign cross-peak double-quantum-filtered correlation spectroscopy. <i>Journal of Magnetic Resonance</i> , 2004, 168, 327-335.	2.1	40
34	Photopolymerization of Organic Molecular Crystal Nanorods. <i>Macromolecules</i> , 2007, 40, 9040-9044.	4.8	39
35	NMR Crystallography of Enzyme Active Sites: Probing Chemically Detailed, Three-Dimensional Structure in Tryptophan Synthase. <i>Accounts of Chemical Research</i> , 2013, 46, 2008-2017.	15.6	36
36	J-based 2D homonuclear and heteronuclear correlation in solid-state proteins. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, S84-S92.	1.9	33

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37	Tensors and rotations in NMR. Concepts in Magnetic Resonance Part A: Bridging Education and Research, 2011, 38A, 221-235.	0.5	33
38	Solution <sup>17</sup> O <sup>15</sup> N Quadrupole Central Transition NMR Spectroscopy in the Active Site of Tryptophan Synthase. Angewandte Chemie - International Edition, 2016, 55, 1350-1354.	13.8	31
39	Atomic-resolution chemical characterization of (2x)72-kDa tryptophan synthase via four- and five-dimensional <sup>1</sup> H-detected solid-state NMR. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	31
40	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
41	TensorView: A software tool for displaying NMR tensors. Magnetic Resonance in Chemistry, 2019, 57, 211-223.	1.9	27
42	Synthesis and NMR Studies of <sup>13</sup> C-Labeled Vitamin D Metabolites 1. Journal of Organic Chemistry, 2002, 67, 1637-1650.	3.2	26
43	Three-qubit nuclear magnetic resonance quantum information processing with a single-crystal solid. Journal of Chemical Physics, 2003, 119, 1643-1649.	3.0	26
44	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
45	J-Based 3D sidechain correlation in solid-state proteins. Physical Chemistry Chemical Physics, 2009, 11, 7078.	2.8	25
46	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
47	The Amide Rotational Barrier in Isonicotinamide: A Dynamic NMR and Ab Initio Studies. Journal of Physical Chemistry A, 2005, 109, 1152-1158.	2.5	23
48	Sensitive absorptive refocused scalar correlation NMR spectroscopy in solids. Physical Chemistry Chemical Physics, 2009, 11, 3547.	2.8	23
49	Hydroxyl-Proton Hydrogen Bonding in the Heparin Oligosaccharide Arixtra in Aqueous Solution. Journal of Physical Chemistry B, 2014, 118, 482-491.	2.6	23
50	Protonation states and catalysis: Molecular dynamics studies of intermediates in tryptophan synthase. Protein Science, 2016, 25, 166-183.	7.6	23
51	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
52	Chelation of a Proton by an Aliphatic Tertiary Diamine. Journal of the American Chemical Society, 2008, 130, 7836-7838.	13.7	22
53	High resolution <sup>13</sup> C-detected solid-state NMR spectroscopy of a deuterated protein. Journal of Biomolecular NMR, 2010, 48, 103-111.	2.8	22
54	Correlating Reaction Dynamics and Size Change during the Photomechanical Transformation of 9-Methylanthracene Single Crystals. Angewandte Chemie - International Edition, 2022, 61, .	13.8	21

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55	Predicting anisotropic thermal displacements for hydrogens from solid-state NMR: a study on hydrogen bonding in polymorphs of palmitic acid. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8475-8487.	2.8	18
56	Imaging active site chemistry and protonation states: NMR crystallography of the tryptophan synthase $\hat{\text{L}}\pm$ -aminoacrylate intermediate. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	7.1	18
57	Long-observation-window band-selective homonuclear decoupling: Increased sensitivity and resolution in solid-state NMR spectroscopy of proteins. <i>Journal of Magnetic Resonance</i> , 2013, 236, 89-94.	2.1	16
58	Measuring and Modeling Highly Accurate $^{15}\text{N}$ Chemical Shift Tensors in a Peptide.. <i>ChemPhysChem</i> , 2017, 18, 2225-2232.	2.1	16
59	Vibrations of a chelated proton in a protonated tertiary diamine. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20380.	2.8	15
60	Proton-bound dimers of 1-methylcytosine and its derivatives: vibrational and NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19001.	2.8	14
61	Moderated Basicity of Endohedral Amine Groups in an Octa $\hat{\text{C}}$ ationic Self $\hat{\text{A}}$ ssembled Cage. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	14
62	Catalytic roles of $\hat{\text{L}}^2\text{Lys87}$ in tryptophan synthase: $^{15}\text{N}$ solid state NMR studies. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2015, 1854, 1194-1199.	2.3	13
63	Investigation of Structural Dynamics of Enzymes and Protonation States of Substrates Using Computational Tools. <i>Catalysts</i> , 2016, 6, 82.	3.5	12
64	Lipid bilayer environments control exchange kinetics of deep cavitand hosts and enhance disfavored guest conformations. <i>Chemical Science</i> , 2018, 9, 1836-1845.	7.4	11
65	Non-Uniform Sampling in NMR Spectroscopy and the Preservation of Spectral Knowledge in the Time and Frequency Domains. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5474-5486.	2.5	11
66	Discovery of antimicrobial agent targeting tryptophan synthase. <i>Protein Science</i> , 2022, 31, 432-442.	7.6	10
67	Cofactor-Mediated Nucleophilic Substitution Catalyzed by a Self-Assembled Holoenzyme Mimic. <i>Journal of Organic Chemistry</i> , 2019, 84, 12000-12008.	3.2	9
68	Direct dynamic nuclear polarization of $^{15}\text{N}$ and $^{13}\text{C}$ spins at 14.1 T using a trityl radical and magic angle spinning. <i>Solid State Nuclear Magnetic Resonance</i> , 2019, 100, 85-91.	2.3	9
69	Moderated Basicity of Endohedral Amine Groups in an Octa $\hat{\text{C}}$ ationic Self $\hat{\text{A}}$ ssembled Cage. <i>Angewandte Chemie</i> , 0, , .	2.0	9
70	Mutation of $\hat{\text{L}}^2\text{Gln114}$ to Ala Alters the Stabilities of Allosteric States in Tryptophan Synthase Catalysis. <i>Biochemistry</i> , 2021, 60, 3173-3186.	2.5	8
71	Backbone assignments and conformational dynamics in the <i>S. typhimurium</i> tryptophan synthase $\hat{\text{L}}\pm$ -subunit from solution-state NMR. <i>Journal of Biomolecular NMR</i> , 2020, 74, 341-354.	2.8	6
72	Correlating Reaction Dynamics and Size Change during the Photomechanical Transformation of $9\hat{\text{A}}$ -Methylantracene Single Crystals. <i>Angewandte Chemie</i> , 2022, 134, e202114089.	2.0	6

