Daniel J O'leary

List of Publications by Year
in descending order

61 papers	3,337 citations	257101 24 h-index	161609 54 g-index
109 all docs	109 docs citations	109 times ranked	3462 citing authors

#	Article	IF	Citations
1	Macromolecular stereochemistry: the out-of-proportion influence of optically active comonomers on the conformational characteristics of polyisocyanates. The sergeants and soldiers experiment. Journal of the American Chemical Society, 1989, 111, 6452-6454.	6.6	623
2	Recent advances in ruthenium-based olefin metathesis. Chemical Society Reviews, 2018, 47, 4510-4544.	18.7	501
3	New Approaches to Olefin Cross-Metathesis. Journal of the American Chemical Society, 2000, 122, 58-71.	6.6	363
4	Ring-Closing Metathesis of Olefinic Peptides:Â Design, Synthesis, and Structural Characterization of Macrocyclic Helical Peptides. Journal of Organic Chemistry, 2001, 66, 5291-5302.	1.7	216
5	Synthesis and Reactivity of Olefin Metathesis Catalysts Bearing Cyclic (Alkyl)(Amino)Carbenes. Angewandte Chemie - International Edition, 2007, 46, 7262-7265.	7.2	153
6	Conformations of N-Heterocyclic Carbene Ligands in Ruthenium Complexes Relevant to Olefin Metathesis. Journal of the American Chemical Society, 2009, 131, 1931-1938.	6.6	106
7	Z-Selective Olefin Metathesis on Peptides: Investigation of Side-Chain Influence, Preorganization, and Guidelines in Substrate Selection. Journal of the American Chemical Society, 2014, 136, 12469-12478.	6.6	78
8	Facile and E-Selective Intramolecular Ring-Closing Metathesis Reactions in 310-Helical Peptides:â€‰ A 3D Structural Study. Journal of the American Chemical Society, 2007, 129, 6986-6987.	6.6	73
9	The shielding tensor. Part I: Understanding its symmetry properties. Concepts in Magnetic Resonance, 1991, 3, 193-214.	1.3	72
10	Model Compounds of Rutheniumâ”Alkene Intermediates in Olefin Metathesis Reactions. Journal of the American Chemical Society, 2006, 128, 8386-8387.	6.6	69
11	Carboxylate-Assisted C(sp³)â€“H Activation in Olefin Metathesis-Relevant Ruthenium Complexes. Journal of the American Chemical Society, 2014, 136, 6733-6743.	6.6	61
12	A new method for cross-metathesis of terminal olefins. Tetrahedron Letters, 1998, 39, 7427-7430.	0.7	49
13	The shielding tensor part II: Understanding its strange effects on relaxation. Concepts in Magnetic Resonance, 1992, 4, 35-52.	1.3	47
14	Isotopic Perturbation of Intramolecular Hydrogen Bonds in Rigid 1,3-Diols:Â NMR Studies Reveal Unusually Large Equilibrium Isotope Effects. Journal of Organic Chemistry, 1996, 61, 9610-9613.	1.7	43
15	Scalar Coupling Across the Hydrogen Bond in 1,3- and 1,4-Diols. Organic Letters, 2000, 2, 2077-2080.	2.4	41
16	Rutheniumâ€“Olefin Complexes: Effect of Ligand Variation upon Geometry. Chemistry - A European Journal, 2008, 14, 7536-7544.	1.7	41
17	Using Equilibrium Isotope Effects To Detect Intramolecular OH/OH Hydrogen Bonds:Â Structural and Solvent Effects. Journal of the American Chemical Society, 2002, 124, 2931-2938.	6.6	40
18	NMR relaxation by the antisymmetric component of the shielding tensor: a longer transverse than longitudinal relaxation time. Chemical Physics Letters, 1990, 171, 401-405.	1.2	36

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19	Solvent dependence of the chain dimensions of poly(n-hexyl isocyanate). Macromolecules, 1990, 23, 3454-3458.	2.2	36
20	Terminal olefin cross-metathesis with acrolein acetals. Tetrahedron Letters, 1999, 40, 1091-1094.	0.7	34
21	H-D coupling constants and deuterium isotope effects on the proton chemical shifts in partially deuteriated methanes. Tetrahedron Letters, 1989, 30, 2755-2758.	0.7	33
22	Preferred conformation of C-glycosides. 11. C-Sucrose: new practical synthesis, structural reassignment, and solid-state and solution conformation of its octaacetate. Journal of Organic Chemistry, 1993, 58, 304-306.	1.7	29
23	Theoretical and NMR Studies of Deuterium Isotopic Perturbation of Hydrogen Bonding in Symmetrical Dihydroxy Compounds. Journal of Organic Chemistry, 2010, 75, 1331-1342.	1.7	26
24	Structureâ€“Activity Relationship-based Optimization of Small Temporin-SHf Analogs with Potent Antibacterial Activity. ACS Chemical Biology, 2015, 10, 2257-2266.	1.6	26
25	An Isosparteine Derivative for Stereochemical Assignment of Stereogenic (Chiral) Methyl Groups Using Tritium NMR:Â Theory and Experiment. Journal of the American Chemical Society, 2005, 127, 412-420.	6.6	25
26	Stereogenic (chiral) methyl groups: determination of configuration by direct tritium NMR spectroscopy. Journal of the American Chemical Society, 1989, 111, 8935-8936.	6.6	22
27	Qualitative and Quantitative Measurements of Hydrogen Bond Mediated Scalar Couplings in Acyclic 1,3-Diols. Organic Letters, 2006, 8, 5321-5323.	2.4	22
28	¹H and ¹³C NMR Assignments for the Cyanine Dyes SYBR Safe and Thiazole Orange. Journal of Organic Chemistry, 2012, 77, 10967-10971.	1.7	22
29	The conformational preference (a value) of deuterium in monodeuteriocyclohexane from deuteron integration at low temperatures. Tetrahedron Letters, 1989, 30, 1059-1062.	0.7	17
30	Direct Assignment of the Relative Configuration in Acyclic 1,3-Diols by1H NMR Spectroscopy. Organic Letters, 2005, 7, 5721-5723.	2.4	17
31	Nuclear singlet relaxation by scalar relaxation of the second kind in the slow-fluctuation regime. Journal of Chemical Physics, 2019, 150, 064315.	1.2	16
32	Density functional theory studies of transannular1H?1HJ-coupling in half-cage alcohols and rigid 1,3- and 1,4-diols: conformational dependencies and implications for intramolecular hydrogen bond detection in carbohydrates. Magnetic Resonance in Chemistry, 2001, 39, S115-S125.	1.1	15
33	On the Origin of Conformational Kinetic Isotope Effects. Angewandte Chemie - International Edition, 2011, 50, 2564-2567.	7.2	14
34	NMR Detection of Intramolecular OH/OH Hydrogen Bond Networks: An Approach Using Isotopic Perturbation and Hydrogen Bond Mediated OHÂ·Â·Â·OH J-Coupling. Heterocycles, 2007, 72, 469.	0.4	14
35	Fomenting Proton Anisochronicity in the CH2D Group. Journal of the American Chemical Society, 2003, 125, 9018-9019.	6.6	13
36	Following Molecular Mobility during Chemical Reactions: No Evidence for Active Propulsion. Journal of the American Chemical Society, 2021, 143, 20884-20890.	6.6	13

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37	Vicinal Deuterium Perturbations on Hydrogen NMR Chemical Shifts in Cyclohexanes. Journal of the American Chemical Society, 2008, 130, 13659-13663.	6.6	12
38	Field-cycling long-lived-state NMR of ¹⁵N₂ spin pairs. Molecular Physics, 2019, 117, 861-867.	0.8	11
39	Tritium NMR in conformational analysis: isotopic perturbation of the ring inversion equilibrium in [3H]cyclohexane. Journal of the Chemical Society Chemical Communications, 1990, , 1427.	2.0	10
40	On the1H NMR chemical shift assignments for ampicillin. Magnetic Resonance in Chemistry, 2000, 38, 126-128.	1.1	10
41	Visual Isotope Effects: Demonstrating the Primary Kinetic Isotope Effect in the Chromium(VI) Oxidation of 2-Propanol-d₈ and Methanol-d₄. Journal of Chemical Education, 2013, 90, 1044-1047.	1.1	9
42	C-sucrose vs. O-sucrose: Different conformational behavior in methanol solutions containing Ca2+. Tetrahedron Letters, 1994, 35, 5591-5594.	0.7	8
43	Enthalpy/Entropy Contributions to Conformational KIEs: Theoretical Predictions and Comparison with Experiment. Molecules, 2013, 18, 2281-2296.	1.7	7
44	Conformational Analysis of Alkylated Biuret and Triuret:â€‰ Evidence for Helicity and Helical Inversion in Oligoisocyanates. Organic Letters, 2000, 2, 3063-3066.	2.4	6
45	Origins of Small Proton Chemical Shift Differences in Monodeuterated Methyl Groups. Journal of Organic Chemistry, 2017, 82, 8943-8949.	1.7	4
46	A hydrazino nicotinamide derivative of cholesterol for radiolabelling liposomes with99mTc. Journal of Labelled Compounds and Radiopharmaceuticals, 1999, 42, 23-28.	0.5	3
47	From the teaching laboratory: A half-cage isodrin derivative for demonstrating the nuclear Overhauser effect. Concepts in Magnetic Resonance, 2000, 12, 1-5.	1.3	2
48	Comment on â€œAn equilibrium isotope effect due to a strong hydrogen bondâ€. Chemical Physics Letters, 2019, 730, 302-305.	1.2	2
49	Elective and Capstone Undergraduate Experiences in NMR Spectroscopy. ACS Symposium Series, 2007, , 36-47.	0.5	1
50	¹H and ¹³C NMR assignments for (Nâ€Methyl)â€(â^')â€(Î±)â€isosparteinium iodide and (Nâ€Methyl)â€(â^')â€sparteinium iodide. Magnetic Resonance in Chemistry, 2019, 57, 55-64.	1.1	1
51	Vibrational analysis of a rate-slowing conformational kinetic isotope effect. Tetrahedron, 2019, 75, 545-550.	1.0	1
52	An Examination of Factors Influencing Small Proton Chemical Shift Differences in Nitrogen-Substituted Monodeuterated Methyl Groups. Symmetry, 2021, 13, 1610.	1.1	1
53	1H NMR Studies of Intramolecular OH/OH Hydrogen Bonds via Titratable Isotope Shifts. Journal of Organic Chemistry, 2021, , .	1.7	1
54	Letter to the Editor-in-Chief. Concepts in Magnetic Resonance, 2000, 12, i-i.	1.3	0

#	Article	IF	Citations
55	Index, Volume 3: Polymer Synthesis. , 2015, , 391-403.		0
56	Index, Volume 2: Applications in Organic Synthesis. , 2015, , 727-743.		0
57	Front Matter, Volume 1: Catalyst Development and Mechanism. , 2015, , I-XVII.		0
58	Front Matter, Volume 2: Applications in Organic Synthesis. , 2015, , I-XXVI.		0
59	Front Matter, Volume 3: Polymer Synthesis. , 2015, , I-XVII.		0
60	Index, Volume 1: Catalyst Development and Mechanism. , 2015, , 417-423.		0
61	Spreadsheet-Based Computational Predictions of Isotope Effects. , 2018, , 403-450.		0