

# Daniel J O'leary

## List of Publications by Year in descending order

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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	An Examination of Factors Influencing Small Proton Chemical Shift Differences in Nitrogen-Substituted Monodeuterated Methyl Groups. <i>Symmetry</i> , 2021, 13, 1610.	1.1	1
2	<sup>1</sup> H NMR Studies of Intramolecular OH/OH Hydrogen Bonds via Titratable Isotope Shifts. <i>Journal of Organic Chemistry</i> , 2021, , .	1.7	1
3	Following Molecular Mobility during Chemical Reactions: No Evidence for Active Propulsion. <i>Journal of the American Chemical Society</i> , 2021, 143, 20884-20890.	6.6	13
4	Comment on "An equilibrium isotope effect due to a strong hydrogen bond". <i>Chemical Physics Letters</i> , 2019, 730, 302-305.	1.2	2
5	Nuclear singlet relaxation by scalar relaxation of the second kind in the slow-fluctuation regime. <i>Journal of Chemical Physics</i> , 2019, 150, 064315.	1.2	16
6	<sup>1</sup> H and <sup>13</sup> C NMR assignments for (N-methyl)lacosparteinium iodide and (N-methyl)sparteinium iodide. <i>Magnetic Resonance in Chemistry</i> , 2019, 57, 55-64.	1.1	1
7	Field-cycling long-lived-state NMR of <sup>15</sup> N <sub>2</sub> spin pairs. <i>Molecular Physics</i> , 2019, 117, 861-867.	0.8	11
8	Vibrational analysis of a rate-slowing conformational kinetic isotope effect. <i>Tetrahedron</i> , 2019, 75, 545-550.	1.0	1
9	Spreadsheet-Based Computational Predictions of Isotope Effects. , 2018, , 403-450.		0
10	Recent advances in ruthenium-based olefin metathesis. <i>Chemical Society Reviews</i> , 2018, 47, 4510-4544.	18.7	501
11	Origins of Small Proton Chemical Shift Differences in Monodeuterated Methyl Groups. <i>Journal of Organic Chemistry</i> , 2017, 82, 8943-8949.	1.7	4
12	Index, Volume 3: Polymer Synthesis. , 2015, , 391-403.		0
13	Index, Volume 2: Applications in Organic Synthesis. , 2015, , 727-743.		0
14	Structure-Activity Relationship-based Optimization of Small Temporin-SHf Analogs with Potent Antibacterial Activity. <i>ACS Chemical Biology</i> , 2015, 10, 2257-2266.	1.6	26
15	Front Matter, Volume 1: Catalyst Development and Mechanism. , 2015, , I-XVII.		0
16	Front Matter, Volume 2: Applications in Organic Synthesis. , 2015, , I-XXVI.		0
17	Front Matter, Volume 3: Polymer Synthesis. , 2015, , I-XVII.		0
18	Index, Volume 1: Catalyst Development and Mechanism. , 2015, , 417-423.		0

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19	Carboxylate-Assisted C(sp <sup>3</sup> )â€“H Activation in Olefin Metathesis-Relevant Ruthenium Complexes. <i>Journal of the American Chemical Society</i> , 2014, 136, 6733-6743.	6.6	61
20	Z-Selective Olefin Metathesis on Peptides: Investigation of Side-Chain Influence, Preorganization, and Guidelines in Substrate Selection. <i>Journal of the American Chemical Society</i> , 2014, 136, 12469-12478.	6.6	78
21	Visual Isotope Effects: Demonstrating the Primary Kinetic Isotope Effect in the Chromium(VI) Oxidation of 2-Propanol- <i>d</i> <sub>8</sub> and Methanol- <i>d</i> <sub>4</sub> . <i>Journal of Chemical Education</i> , 2013, 90, 1044-1047.	1.1	9
22	Enthalpy/Entropy Contributions to Conformational KIEs: Theoretical Predictions and Comparison with Experiment. <i>Molecules</i> , 2013, 18, 2281-2296.	1.7	7
23	<sup>1</sup> H and <sup>13</sup> C NMR Assignments for the Cyanine Dyes SYBR Safe and Thiazole Orange. <i>Journal of Organic Chemistry</i> , 2012, 77, 10967-10971.	1.7	22
24	On the Origin of Conformational Kinetic Isotope Effects. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 2564-2567.	7.2	14
25	Theoretical and NMR Studies of Deuterium Isotopic Perturbation of Hydrogen Bonding in Symmetrical Dihydroxy Compounds. <i>Journal of Organic Chemistry</i> , 2010, 75, 1331-1342.	1.7	26
26	Conformations of N-Heterocyclic Carbene Ligands in Ruthenium Complexes Relevant to Olefin Metathesis. <i>Journal of the American Chemical Society</i> , 2009, 131, 1931-1938.	6.6	106
27	Rutheniumâ€“Olefin Complexes: Effect of Ligand Variation upon Geometry. <i>Chemistry - A European Journal</i> , 2008, 14, 7536-7544.	1.7	41
28	Vicinal Deuterium Perturbations on Hydrogen NMR Chemical Shifts in Cyclohexanes. <i>Journal of the American Chemical Society</i> , 2008, 130, 13659-13663.	6.6	12
29	Elective and Capstone Undergraduate Experiences in NMR Spectroscopy. <i>ACS Symposium Series</i> , 2007, , 36-47.	0.5	1
30	Synthesis and Reactivity of Olefin Metathesis Catalysts Bearing Cyclic (Alkyl)(Amino)Carbenes. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 7262-7265.	7.2	153
31	Facile and E-Selective Intramolecular Ring-Closing Metathesis Reactions in 310-Helical Peptides:â€“ A 3D Structural Study. <i>Journal of the American Chemical Society</i> , 2007, 129, 6986-6987.	6.6	73
32	NMR Detection of Intramolecular OH/OH Hydrogen Bond Networks: An Approach Using Isotopic Perturbation and Hydrogen Bond Mediated OHAâ€“OH J-Coupling. <i>Heterocycles</i> , 2007, 72, 469.	0.4	14
33	Qualitative and Quantitative Measurements of Hydrogen Bond Mediated Scalar Couplings in Acyclic 1,3-Diols. <i>Organic Letters</i> , 2006, 8, 5321-5323.	2.4	22
34	Model Compounds of Rutheniumâ€“Alkene Intermediates in Olefin Metathesis Reactions. <i>Journal of the American Chemical Society</i> , 2006, 128, 8386-8387.	6.6	69
35	An Isosparteine Derivative for Stereochemical Assignment of Stereogenic (Chiral) Methyl Groups Using Tritium NMR:â€“ Theory and Experiment. <i>Journal of the American Chemical Society</i> , 2005, 127, 412-420.	6.6	25
36	Direct Assignment of the Relative Configuration in Acyclic 1,3-Diols by <sup>1</sup> H NMR Spectroscopy. <i>Organic Letters</i> , 2005, 7, 5721-5723.	2.4	17

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37	Fomenting Proton Anisochronicity in the CH <sub>2</sub> D Group. <i>Journal of the American Chemical Society</i> , 2003, 125, 9018-9019.	6.6	13
38	Using Equilibrium Isotope Effects To Detect Intramolecular OH/OH Hydrogen Bonds: A Structural and Solvent Effects. <i>Journal of the American Chemical Society</i> , 2002, 124, 2931-2938.	6.6	40
39	Ring-Closing Metathesis of Olefinic Peptides: A Design, Synthesis, and Structural Characterization of Macrocyclic Helical Peptides. <i>Journal of Organic Chemistry</i> , 2001, 66, 5291-5302.	1.7	216
40	Density functional theory studies of transannular <sup>1</sup> H- <sup>1</sup> HJ-coupling in half-cage alcohols and rigid 1,3- and 1,4-diols: conformational dependencies and implications for intramolecular hydrogen bond detection in carbohydrates. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, S115-S125.	1.1	15
41	On the <sup>1</sup> H NMR chemical shift assignments for ampicillin. <i>Magnetic Resonance in Chemistry</i> , 2000, 38, 126-128.	1.1	10
42	From the teaching laboratory: A half-cage isodrin derivative for demonstrating the nuclear Overhauser effect. <i>Concepts in Magnetic Resonance</i> , 2000, 12, 1-5.	1.3	2
43	Letter to the Editor-in-Chief. <i>Concepts in Magnetic Resonance</i> , 2000, 12, i-i.	1.3	0
44	New Approaches to Olefin Cross-Metathesis. <i>Journal of the American Chemical Society</i> , 2000, 122, 58-71.	6.6	363
45	Conformational Analysis of Alkylated Biuret and Triuret: Evidence for Helicity and Helical Inversion in Oligoisocyanates. <i>Organic Letters</i> , 2000, 2, 3063-3066.	2.4	6
46	Scalar Coupling Across the Hydrogen Bond in 1,3- and 1,4-Diols. <i>Organic Letters</i> , 2000, 2, 2077-2080.	2.4	41
47	Terminal olefin cross-metathesis with acrolein acetals. <i>Tetrahedron Letters</i> , 1999, 40, 1091-1094.	0.7	34
48	A hydrazino nicotinamide derivative of cholesterol for radiolabelling liposomes with <sup>99m</sup> Tc. <i>Journal of Labelled Compounds and Radiopharmaceuticals</i> , 1999, 42, 23-28.	0.5	3
49	A new method for cross-metathesis of terminal olefins. <i>Tetrahedron Letters</i> , 1998, 39, 7427-7430.	0.7	49
50	Isotopic Perturbation of Intramolecular Hydrogen Bonds in Rigid 1,3-Diols: NMR Studies Reveal Unusually Large Equilibrium Isotope Effects. <i>Journal of Organic Chemistry</i> , 1996, 61, 9610-9613.	1.7	43
51	C-sucrose vs. O-sucrose: Different conformational behavior in methanol solutions containing Ca <sup>2+</sup> . <i>Tetrahedron Letters</i> , 1994, 35, 5591-5594.	0.7	8
52	Preferred conformation of C-glycosides. 11. C-Sucrose: new practical synthesis, structural reassignment, and solid-state and solution conformation of its octaacetate. <i>Journal of Organic Chemistry</i> , 1993, 58, 304-306.	1.7	29
53	The shielding tensor part II: Understanding its strange effects on relaxation. <i>Concepts in Magnetic Resonance</i> , 1992, 4, 35-52.	1.3	47
54	The shielding tensor. Part I: Understanding its symmetry properties. <i>Concepts in Magnetic Resonance</i> , 1991, 3, 193-214.	1.3	72

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55	NMR relaxation by the antisymmetric component of the shielding tensor: a longer transverse than longitudinal relaxation time. <i>Chemical Physics Letters</i> , 1990, 171, 401-405.	1.2	36
56	Tritium NMR in conformational analysis: isotopic perturbation of the ring inversion equilibrium in [3H]cyclohexane. <i>Journal of the Chemical Society Chemical Communications</i> , 1990, , 1427.	2.0	10
57	Solvent dependence of the chain dimensions of poly(n-hexyl isocyanate). <i>Macromolecules</i> , 1990, 23, 3454-3458.	2.2	36
58	Stereogenic (chiral) methyl groups: determination of configuration by direct tritium NMR spectroscopy. <i>Journal of the American Chemical Society</i> , 1989, 111, 8935-8936.	6.6	22
59	The conformational preference (a value) of deuterium in monodeuteriocyclohexane from deuterium integration at low temperatures. <i>Tetrahedron Letters</i> , 1989, 30, 1059-1062.	0.7	17
60	H-D coupling constants and deuterium isotope effects on the proton chemical shifts in partially deuteriated methanes. <i>Tetrahedron Letters</i> , 1989, 30, 2755-2758.	0.7	33
61	Macromolecular stereochemistry: the out-of-proportion influence of optically active comonomers on the conformational characteristics of polyisocyanates. The sergeants and soldiers experiment. <i>Journal of the American Chemical Society</i> , 1989, 111, 6452-6454.	6.6	623