

# Abigail G Doyle

## List of Publications by Year in descending order

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73  
papers

13,324  
citations

25185

57  
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71999

76  
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116  
all docs

116  
docs citations

116  
times ranked

9483  
citing authors

#	ARTICLE	IF	CITATIONS
1	Small-Molecule H-Bond Donors in Asymmetric Catalysis. <i>Chemical Reviews</i> , 2007, 107, 5713-5743.	49.1	2,323
2	Merging photoredox with nickel catalysis: Coupling of $\beta$ -carboxyl $\text{sp}^3$ -carbons with aryl halides. <i>Science</i> , 2014, 345, 437-440.	12.8	1,309
3	Predicting reaction performance in $\text{C}^{\text{N}}$ cross-coupling using machine learning. <i>Science</i> , 2018, 360, 186-190.	12.8	613
4	Direct $\text{C}(\text{sp}^3)\text{-H}$ Cross Coupling Enabled by Catalytic Generation of Chlorine Radicals. <i>Journal of the American Chemical Society</i> , 2016, 138, 12719-12722.	14.2	505
5	A Synthetically Useful, Self-Assembling MMO Mimic System for Catalytic Alkene Epoxidation with Aqueous $\text{H}_2\text{O}_2$ . <i>Journal of the American Chemical Society</i> , 2001, 123, 7194-7195.	14.2	456
6	Enantioselective Thiourea-Catalyzed Additions to Oxocarbenium Ions. <i>Journal of the American Chemical Society</i> , 2008, 130, 7198-7199.	14.2	423
7	The Chemistry of Transition Metals with Three-Membered Ring Heterocycles. <i>Chemical Reviews</i> , 2014, 114, 8153-8198.	49.1	416
8	Bayesian reaction optimization as a tool for chemical synthesis. <i>Nature</i> , 2021, 590, 89-96.	28.1	370
9	Enantioselective Ring Opening of Epoxides by Fluoride Anion Promoted by a Cooperative Dual-Catalyst System. <i>Journal of the American Chemical Society</i> , 2010, 132, 3268-3269.	14.2	255
10	PyFluor: A Low-Cost, Stable, and Selective Deoxyfluorination Reagent. <i>Journal of the American Chemical Society</i> , 2015, 137, 9571-9574.	14.2	222
11	Long-Lived Charge-Transfer States of Nickel(II) Aryl Halide Complexes Facilitate Bimolecular Photoinduced Electron Transfer. <i>Journal of the American Chemical Society</i> , 2018, 140, 3035-3039.	14.2	219
12	Nickel-Catalyzed Enantioselective Reductive Cross-Coupling of Styrenyl Aziridines. <i>Journal of the American Chemical Society</i> , 2017, 139, 5688-5691.	14.2	214
13	Generation of Phosphoranyl Radicals via Photoredox Catalysis Enables Voltage-Independent Activation of Strong $\text{C}^{\text{O}}$ Bonds. <i>ACS Catalysis</i> , 2018, 8, 11134-11139.	11.4	211
14	Direct Acylation of $\text{C}(\text{sp}^3)\text{-H}$ Bonds Enabled by Nickel and Photoredox Catalysis. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4040-4043.	14.2	204
15	Palladium-Catalyzed Asymmetric Synthesis of Allylic Fluorides. <i>Journal of the American Chemical Society</i> , 2010, 132, 17402-17404.	14.2	192
16	Palladium-Catalyzed Allylic $\text{C}^{\text{H}}$ Fluorination. <i>Journal of the American Chemical Society</i> , 2013, 135, 12990-12993.	14.2	188
17	Parameterization of phosphine ligands demonstrates enhancement of nickel catalysis via remote steric effects. <i>Nature Chemistry</i> , 2017, 9, 779-784.	14.2	183
18	Direct $\text{C}^{\text{C}}$ Bond Formation from Alkanes Using Ni-Photoredox Catalysis. <i>Journal of the American Chemical Society</i> , 2018, 140, 14059-14063.	14.2	182

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19	Deoxyfluorination with Sulfonyl Fluorides: Navigating Reaction Space with Machine Learning. <i>Journal of the American Chemical Society</i> , 2018, 140, 5004-5008.	14.2	181
20	Palladium-Catalyzed Regio- and Enantioselective Fluorination of Acyclic Allylic Halides. <i>Journal of the American Chemical Society</i> , 2011, 133, 15902-15905.	14.2	174
21	Nickel-Catalyzed Negishi Alkylations of Styrenyl Aziridines. <i>Journal of the American Chemical Society</i> , 2012, 134, 9541-9544.	14.2	172
22	<sup>3</sup> d-d Excited States of Ni(II) Complexes Relevant to Photoredox Catalysis: Spectroscopic Identification and Mechanistic Implications. <i>Journal of the American Chemical Society</i> , 2020, 142, 5800-5810.	14.2	168
23	Mild, Redox-Neutral Formylation of Aryl Chlorides through the Photocatalytic Generation of Chlorine Radicals. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 7191-7194.	14.2	165
24	Mechanistic Investigations of Cooperative Catalysis in the Enantioselective Fluorination of Epoxides. <i>Journal of the American Chemical Society</i> , 2011, 133, 16001-16012.	14.2	145
25	Synthetic and Mechanistic Implications of Chlorine Photoelimination in Nickel/Photoredox C(sp <sup>3</sup> )-H Cross-Coupling. <i>Accounts of Chemical Research</i> , 2021, 54, 988-1000.	16.1	144
26	C-H functionalization of amines with aryl halides by nickel-photoredox catalysis. <i>Chemical Science</i> , 2016, 7, 7002-7006.	7.6	141
27	Dialkyl Ether Formation by Nickel-Catalyzed Cross-Coupling of Acetals and Aryl Iodides. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9876-9880.	14.2	138
28	Bioinspiration in light harvesting and catalysis. <i>Nature Reviews Materials</i> , 2020, 5, 828-846.	49.6	136
29	Enantioselective Alkylations of Tributyltin Enolates Catalyzed by Cr(salen)Cl: Access to Enantiomerically Enriched All-Carbon Quaternary Centers. <i>Journal of the American Chemical Society</i> , 2005, 127, 62-63.	14.2	129
30	A Modular, Air-Stable Nickel Precatalyst. <i>Organic Letters</i> , 2015, 17, 2166-2169.	4.8	115
31	Nickel-Catalyzed Cross-Coupling of Styrenyl Epoxides with Boronic Acids. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 6056-6059.	14.2	113
32	The Open Reaction Database. <i>Journal of the American Chemical Society</i> , 2021, 143, 18820-18826.	14.2	112
33	Electron-Deficient Olefin Ligands Enable Generation of Quaternary Carbons by Ni-Catalyzed Cross-Coupling. <i>Journal of the American Chemical Society</i> , 2015, 137, 5638-5641.	14.2	110
34	Nucleophilic (Radio)Fluorination of Redox-Active Esters via Radical-Polar Crossover Enabled by Photoredox Catalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 9493-9500.	14.2	110
35	Enantioselective Alkylation of Acyclic $\hat{1},\hat{1}$ -Disubstituted Tributyltin Enolates Catalyzed by a {Cr(salen)} Complex. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 3701-3705.	14.2	107
36	Dual Nickel- and Photoredox-Catalyzed Enantioselective Desymmetrization of Cyclic <i>meso</i> -Anhydrides. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 3679-3683.	14.2	99

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37	Univariate classification of phosphine ligation state and reactivity in cross-coupling catalysis. <i>Science</i> , 2021, 374, 301-308.	12.8	97
38	Directed Nickel-Catalyzed Negishi Cross Coupling of Alkyl Aziridines. <i>Journal of the American Chemical Society</i> , 2013, 135, 13605-13609.	14.2	95
39	Enantioselective fluoride ring opening of aziridines enabled by cooperative Lewis acid catalysis. <i>Tetrahedron</i> , 2013, 69, 5702-5709.	2.0	95
40	Nickel/Photoredox-Catalyzed Methylation of (Hetero)aryl Chlorides Using Trimethyl Orthoformate as a Methyl Radical Source. <i>Journal of the American Chemical Society</i> , 2020, 142, 7683-7689.	14.2	95
41	Synthesis of $\hat{I}^2$ -Fluoroamines by Lewis Base Catalyzed Hydrofluorination of Aziridines. <i>Journal of Organic Chemistry</i> , 2012, 77, 4177-4183.	3.3	94
42	Enantioselective Radiosynthesis of Positron Emission Tomography (PET) Tracers Containing [ <sup>18</sup> F]Fluorohydrins. <i>Journal of the American Chemical Society</i> , 2014, 136, 5291-5294.	14.2	85
43	Carbofluorination via a palladium-catalyzed cascade reaction. <i>Chemical Science</i> , 2013, 4, 1216.	7.6	83
44	Automation and computer-assisted planning for chemical synthesis. <i>Nature Reviews Methods Primers</i> , 2021, 1, .	21.7	83
45	Ni/Photoredox-Catalyzed Enantioselective Cross-Electrophile Coupling of Styrene Oxides with Aryl Iodides. <i>Journal of the American Chemical Society</i> , 2021, 143, 15873-15881.	14.2	83
46	Ni-Catalyzed Carbon-Carbon Bond-Forming Reductive Amination. <i>Journal of the American Chemical Society</i> , 2018, 140, 2292-2300.	14.2	81
47	Nickel-Catalyzed Cross-Coupling of Chromene Acetals and Boronic Acids. <i>Organic Letters</i> , 2012, 14, 1616-1619.	4.8	79
48	Nickel-Catalyzed Enantioselective Arylation of Pyridinium Ions: Harnessing an Iminium Ion Activation Mode. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 9153-9156.	14.2	77
49	Using Data Science To Guide Aryl Bromide Substrate Scope Analysis in a Ni/Photoredox-Catalyzed Cross-Coupling with Acetals as Alcohol-Derived Radical Sources. <i>Journal of the American Chemical Society</i> , 2022, 144, 1045-1055.	14.2	74
50	Nickel-catalyzed enantioselective arylation of pyridine. <i>Chemical Science</i> , 2016, 7, 4105-4109.	7.6	72
51	Predicting Reaction Yields via Supervised Learning. <i>Accounts of Chemical Research</i> , 2021, 54, 1856-1865.	16.1	72
52	Enantioselective, Nickel-Catalyzed Suzuki Cross-Coupling of Quinolinium Ions. <i>Organic Letters</i> , 2014, 16, 142-145.	4.8	71
53	Synthesis of $\hat{I}^2$ -Phenethylamines via Ni/Photoredox Cross-Electrophile Coupling of Aliphatic Aziridines and Aryl Iodides. <i>Journal of the American Chemical Society</i> , 2020, 142, 7598-7605.	14.2	71
54	Mechanistic Investigation of the Nickel-Catalyzed Suzuki Reaction of <i>N</i> -Acetals: Evidence for Boronic Acid Assisted Oxidative Addition and an Iminium Activation Pathway. <i>Journal of the American Chemical Society</i> , 2012, 134, 16967-16970.	14.2	66

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55	Regioselective Cross-Electrophile Coupling of Epoxides and (Hetero)aryl Iodides via Ni/Ti/Photoredox Catalysis. <i>ACS Catalysis</i> , 2020, 10, 5821-5827.	11.4	64
56	Mechanistic Investigations of Palladium-Catalyzed Allylic Fluorination. <i>Organometallics</i> , 2014, 33, 2121-2133.	2.5	63
57	Transition metal-catalyzed cross coupling with N-acyliminium ions derived from quinolines and isoquinolines. <i>Chemical Science</i> , 2011, 2, 980-984.	7.6	61
58	Oxidative Addition of Aryl Halides to a Ni(I)-Bipyridine Complex. <i>Journal of the American Chemical Society</i> , 2022, 144, 5575-5582.	14.2	60
59	Nucleophilic (Radio)Fluorination of $\hat{\text{I}}\pm$ -Diazocarbonyl Compounds Enabled by Copper-Catalyzed $\text{H}\hat{\text{A}}\text{F}$ Insertion. <i>Journal of the American Chemical Society</i> , 2016, 138, 10802-10805.	14.2	59
60	Direct Use of Carboxylic Acids in the Photocatalytic Hydroacylation of Styrenes To Generate Dialkyl Ketones. <i>Organic Letters</i> , 2019, 21, 9940-9944.	4.8	59
61	The Evolution of Data-Driven Modeling in Organic Chemistry. <i>ACS Central Science</i> , 2021, 7, 1622-1637.	11.6	58
62	Direct Acylation of $\text{C}(\text{sp}^3)\hat{\text{A}}\text{H}$ Bonds Enabled by Nickel and Photoredox Catalysis. <i>Angewandte Chemie</i> , 2016, 128, 4108-4111.	2.0	57
63	A general strategy for $\text{C}(\text{sp}^3)\hat{\text{A}}\text{H}$ functionalization with nucleophiles using methyl radical as a hydrogen atom abstractor. <i>Nature Communications</i> , 2021, 12, 6950.	13.0	54
64	Response to Comment on $\hat{\text{A}}\text{Predicting reaction performance in C}\hat{\text{A}}\text{N cross-coupling using machine learning}\hat{\text{A}}$ . <i>Science</i> , 2018, 362, .	12.8	49
65	Phosphine/Photoredox Catalyzed Anti-Markovnikov Hydroamination of Olefins with Primary Sulfonamides via $\hat{\text{I}}\pm$ Scission from Phosphoranyl Radicals. <i>Journal of the American Chemical Society</i> , 2021, 143, 18331-18338.	14.2	47
66	Mild, Redox-Neutral Formylation of Aryl Chlorides through the Photocatalytic Generation of Chlorine Radicals. <i>Angewandte Chemie</i> , 2017, 129, 7297-7300.	2.0	46
67	C-Arylglucoside synthesis: triisopropylsilane as a selective reagent for the reduction of an anomeric C-phenyl ketal. <i>Tetrahedron: Asymmetry</i> , 2003, 14, 3243-3247.	1.8	42
68	Role of Electron-Deficient Olefin Ligands in a Ni-Catalyzed Aziridine Cross-Coupling To Generate Quaternary Carbons. <i>Journal of the American Chemical Society</i> , 2020, 142, 8928-8937.	14.2	32
69	A biohybrid strategy for enabling photoredox catalysis with low-energy light. <i>CheM</i> , 2022, 8, 174-185.	12.0	26
70	Dual Nickel- and Photoredox-Catalyzed Enantioselective Desymmetrization of Cyclic meso -Anhydrides. <i>Angewandte Chemie</i> , 2017, 129, 3733-3737.	2.0	20
71	Bioinspired Supercharging of Photoredox Catalysis for Applications in Energy and Chemical Manufacturing. <i>Accounts of Chemical Research</i> , 2022, 55, 1423-1434.	16.1	18
72	Auto-QChem: an automated workflow for the generation and storage of DFT calculations for organic molecules. <i>Reaction Chemistry and Engineering</i> , 2022, 7, 1276-1284.	3.5	16

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73	Enantioselective Alkylations of Tributyltin Enolates Catalyzed by Cr(salen)Cl: Access to Enantiomerically Enriched All-Carbon Quaternary Centers.. ChemInform, 2005, 36, no.	0.0	0