

# Abigail G Doyle

## List of Publications by Year in descending order

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73  
papers

13,324  
citations

25034

57  
h-index

71685

76  
g-index

116  
all docs

116  
docs citations

116  
times ranked

9483  
citing authors

#	ARTICLE	IF	CITATIONS
1	A biohybrid strategy for enabling photoredox catalysis with low-energy light. <i>CheM</i> , 2022, 8, 174-185.	11.7	26
2	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.	13.7	74
3	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.	3.7	16
4	Oxidative Addition of Aryl Halides to a Ni(I)-Bipyridine Complex. <i>Journal of the American Chemical Society</i> , 2022, 144, 5575-5582.	13.7	60
5	Bioinspired Supercharging of Photoredox Catalysis for Applications in Energy and Chemical Manufacturing. <i>Accounts of Chemical Research</i> , 2022, 55, 1423-1434.	15.6	18
6	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.	15.6	144
7	Bayesian reaction optimization as a tool for chemical synthesis. <i>Nature</i> , 2021, 590, 89-96.	27.8	370
8	Predicting Reaction Yields via Supervised Learning. <i>Accounts of Chemical Research</i> , 2021, 54, 1856-1865.	15.6	72
9	Automation and computer-assisted planning for chemical synthesis. <i>Nature Reviews Methods Primers</i> , 2021, 1, .	21.2	83
10	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.	13.7	83
11	The Evolution of Data-Driven Modeling in Organic Chemistry. <i>ACS Central Science</i> , 2021, 7, 1622-1637.	11.3	58
12	Phosphine/Photoredox Catalyzed Anti-Markovnikov Hydroamination of Olefins with Primary Sulfonamides via $\beta$ -Scission from Phosphoranyl Radicals. <i>Journal of the American Chemical Society</i> , 2021, 143, 18331-18338.	13.7	47
13	Univariate classification of phosphine ligation state and reactivity in cross-coupling catalysis. <i>Science</i> , 2021, 374, 301-308.	12.6	97
14	The Open Reaction Database. <i>Journal of the American Chemical Society</i> , 2021, 143, 18820-18826.	13.7	112
15	A general strategy for C(sp <sup>3</sup> )-H functionalization with nucleophiles using methyl radical as a hydrogen atom abstractor. <i>Nature Communications</i> , 2021, 12, 6950.	12.8	54
16	Bioinspiration in light harvesting and catalysis. <i>Nature Reviews Materials</i> , 2020, 5, 828-846.	48.7	136
17	Regioselective Cross-Electrophile Coupling of Epoxides and (Hetero)aryl Iodides via Ni/Ti/Photoredox Catalysis. <i>ACS Catalysis</i> , 2020, 10, 5821-5827.	11.2	64
18	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.	13.7	110

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19	<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.	13.7	168
20	Synthesis of Î <sup>2</sup> -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.	13.7	71
21	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.	13.7	32
22	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.	13.7	95
23	Direct Use of Carboxylic Acids in the Photocatalytic Hydroacylation of Styrenes To Generate Dialkyl Ketones. <i>Organic Letters</i> , 2019, 21, 9940-9944.	4.6	59
24	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.	13.7	219
25	Predicting reaction performance in C-N cross-coupling using machine learning. <i>Science</i> , 2018, 360, 186-190.	12.6	613
26	Ni-Catalyzed Carbon-Carbon Bond-Forming Reductive Amination. <i>Journal of the American Chemical Society</i> , 2018, 140, 2292-2300.	13.7	81
27	Deoxyfluorination with Sulfonyl Fluorides: Navigating Reaction Space with Machine Learning. <i>Journal of the American Chemical Society</i> , 2018, 140, 5004-5008.	13.7	181
28	Response to Comment on "Predicting reaction performance in C-N cross-coupling using machine learning". <i>Science</i> , 2018, 362, .	12.6	49
29	Direct C-C Bond Formation from Alkanes Using Ni-Photoredox Catalysis. <i>Journal of the American Chemical Society</i> , 2018, 140, 14059-14063.	13.7	182
30	Generation of Phosphoranyl Radicals via Photoredox Catalysis Enables Voltage-Independent Activation of Strong C-O Bonds. <i>ACS Catalysis</i> , 2018, 8, 11134-11139.	11.2	211
31	Dual Nickel- and Photoredox-Catalyzed Enantioselective Desymmetrization of Cyclic meso-Anhydrides. <i>Angewandte Chemie</i> , 2017, 129, 3733-3737.	2.0	20
32	Dual Nickel- and Photoredox-Catalyzed Enantioselective Desymmetrization of Cyclic meso-Anhydrides. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 3679-3683.	13.8	99
33	Parameterization of phosphine ligands demonstrates enhancement of nickel catalysis via remote steric effects. <i>Nature Chemistry</i> , 2017, 9, 779-784.	13.6	183
34	Nickel-Catalyzed Enantioselective Reductive Cross-Coupling of Styrenyl Aziridines. <i>Journal of the American Chemical Society</i> , 2017, 139, 5688-5691.	13.7	214
35	Mild, Redox-Neutral Formylation of Aryl Chlorides through the Photocatalytic Generation of Chlorine Radicals. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 7191-7194.	13.8	165
36	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

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37	Direct Acylation of C(sp <sup>3</sup> )-H Bonds Enabled by Nickel and Photoredox Catalysis. <i>Angewandte Chemie</i> , 2016, 128, 4108-4111.	2.0	57
38	Direct Acylation of C(sp <sup>3</sup> )-H Bonds Enabled by Nickel and Photoredox Catalysis. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4040-4043.	13.8	204
39	Nucleophilic (Radio)Fluorination of $\alpha$ -Diazocarbonyl Compounds Enabled by Copper-Catalyzed H $\alpha$ -F Insertion. <i>Journal of the American Chemical Society</i> , 2016, 138, 10802-10805.	13.7	59
40	C $\alpha$ -H functionalization of amines with aryl halides by nickel-photoredox catalysis. <i>Chemical Science</i> , 2016, 7, 7002-7006.	7.4	141
41	Direct C(sp <sup>3</sup> )-H Cross Coupling Enabled by Catalytic Generation of Chlorine Radicals. <i>Journal of the American Chemical Society</i> , 2016, 138, 12719-12722.	13.7	505
42	Nickel-catalyzed enantioselective arylation of pyridine. <i>Chemical Science</i> , 2016, 7, 4105-4109.	7.4	72
43	Dialkyl Ether Formation by Nickel-Catalyzed Cross-Coupling of Acetals and Aryl Iodides. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9876-9880.	13.8	138
44	PyFluor: A Low-Cost, Stable, and Selective Deoxyfluorination Reagent. <i>Journal of the American Chemical Society</i> , 2015, 137, 9571-9574.	13.7	222
45	A Modular, Air-Stable Nickel Precatalyst. <i>Organic Letters</i> , 2015, 17, 2166-2169.	4.6	115
46	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.	13.7	110
47	The Chemistry of Transition Metals with Three-Membered Ring Heterocycles. <i>Chemical Reviews</i> , 2014, 114, 8153-8198.	47.7	416
48	Mechanistic Investigations of Palladium-Catalyzed Allylic Fluorination. <i>Organometallics</i> , 2014, 33, 2121-2133.	2.3	63
49	Enantioselective, Nickel-Catalyzed Suzuki Cross-Coupling of Quinolinium Ions. <i>Organic Letters</i> , 2014, 16, 142-145.	4.6	71
50	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.	13.7	85
51	Merging photoredox with nickel catalysis: Coupling of $\alpha$ -carboxyl sp <sup>3</sup> -carbons with aryl halides. <i>Science</i> , 2014, 345, 437-440.	12.6	1,309
52	Nickel-Catalyzed Enantioselective Arylation of Pyridinium Ions: Harnessing an Iminium Ion Activation Mode. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 9153-9156.	13.8	77
53	Directed Nickel-Catalyzed Negishi Cross Coupling of Alkyl Aziridines. <i>Journal of the American Chemical Society</i> , 2013, 135, 13605-13609.	13.7	95
54	Palladium-Catalyzed Allylic C $\alpha$ -H Fluorination. <i>Journal of the American Chemical Society</i> , 2013, 135, 12990-12993.	13.7	188

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55	Carbofluorination via a palladium-catalyzed cascade reaction. <i>Chemical Science</i> , 2013, 4, 1216.	7.4	83
56	Enantioselective fluoride ring opening of aziridines enabled by cooperative Lewis acid catalysis. <i>Tetrahedron</i> , 2013, 69, 5702-5709.	1.9	95
57	Synthesis of $\hat{1}^2$ -Fluoroamines by Lewis Base Catalyzed Hydrofluorination of Aziridines. <i>Journal of Organic Chemistry</i> , 2012, 77, 4177-4183.	3.2	94
58	Mechanistic Investigation of the Nickel-Catalyzed Suzuki Reaction of $\langle i \rangle N \langle /i \rangle, \langle i \rangle O \langle /i \rangle$ -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.	13.7	66
59	Nickel-Catalyzed Cross-Coupling of Chromene Acetals and Boronic Acids. <i>Organic Letters</i> , 2012, 14, 1616-1619.	4.6	79
60	Nickel-Catalyzed Negishi Alkylations of Styrenyl Aziridines. <i>Journal of the American Chemical Society</i> , 2012, 134, 9541-9544.	13.7	172
61	Transition metal-catalyzed cross coupling with N-acyliminium ions derived from quinolines and isoquinolines. <i>Chemical Science</i> , 2011, 2, 980-984.	7.4	61
62	Mechanistic Investigations of Cooperative Catalysis in the Enantioselective Fluorination of Epoxides. <i>Journal of the American Chemical Society</i> , 2011, 133, 16001-16012.	13.7	145
63	Palladium-Catalyzed Regio- and Enantioselective Fluorination of Acyclic Allylic Halides. <i>Journal of the American Chemical Society</i> , 2011, 133, 15902-15905.	13.7	174
64	Nickel-Catalyzed Cross-Coupling of Styrenyl Epoxides with Boronic Acids. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 6056-6059.	13.8	113
65	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.	13.7	255
66	Palladium-Catalyzed Asymmetric Synthesis of Allylic Fluorides. <i>Journal of the American Chemical Society</i> , 2010, 132, 17402-17404.	13.7	192
67	Enantioselective Thiourea-Catalyzed Additions to Oxocarbenium Ions. <i>Journal of the American Chemical Society</i> , 2008, 130, 7198-7199.	13.7	423
68	Small-Molecule H-Bond Donors in Asymmetric Catalysis. <i>Chemical Reviews</i> , 2007, 107, 5713-5743.	47.7	2,323
69	Enantioselective Alkylation of Acyclic $\hat{1}^{\pm}, \hat{1}^{\pm}$ -Disubstituted Tributyltin Enolates Catalyzed by a {Cr(salen)} Complex. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 3701-3705.	13.8	107
70	Enantioselective Alkylations of Tributyltin Enolates Catalyzed by Cr(salen)Cl: Access to Enantiomerically Enriched All-Carbon Quaternary Centers.. <i>ChemInform</i> , 2005, 36, no.	0.0	0
71	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.	13.7	129
72	C-Arylglycoside 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

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73	A Synthetically Useful, Self-Assembling MMO Mimic System for Catalytic Alkene Epoxidation with Aqueous H <sub>2</sub> O <sub>2</sub> . Journal of the American Chemical Society, 2001, 123, 7194-7195.	13.7	456