

# Patrick McArdle

## List of Publications by Year in descending order

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96  
papers

1,789  
citations

304743

22  
h-index

330143

37  
g-index

107  
all docs

107  
docs citations

107  
times ranked

2201  
citing authors

#	ARTICLE	IF	CITATIONS
1	A method for the prediction of the crystal structure of ionic organic compounds—the crystal structures of o-toluidinium chloride and bromide and polymorphism of bicifadine hydrochloride. <i>CrystEngComm</i> , 2004, 6, 303-309.	2.6	131
2	Design of Lead(II) Metal-Organic Frameworks Based on Covalent and Tetrel Bonding. <i>Chemistry - A European Journal</i> , 2015, 21, 17951-17958.	3.3	93
3	Toward a comprehensive definition of oxidation state (IUPAC Technical Report). <i>Pure and Applied Chemistry</i> , 2014, 86, 1017-1081.	1.9	80
4	Comprehensive definition of oxidation state (IUPAC Recommendations 2016). <i>Pure and Applied Chemistry</i> , 2016, 88, 831-839.	1.9	80
5	Amorphous Solid Dispersions of Sulfonamide/Soluplus® and Sulfonamide/PVP Prepared by Ball Milling. <i>AAPS PharmSciTech</i> , 2013, 14, 464-474.	3.3	69
6	Mechanochemical Reaction of Sulfathiazole with Carboxylic Acids: Formation of a Cocrystal, a Salt, and Coamorphous Solids. <i>Crystal Growth and Design</i> , 2014, 14, 803-813.	3.0	69
7	Oscail, a program package for small-molecule single-crystal crystallography with crystal morphology prediction and molecular modelling. <i>Journal of Applied Crystallography</i> , 2017, 50, 320-326.	4.5	53
8	Nickel(II) and cobalt(II) complexes of lidocaine: Synthesis, structure and comparative in vitro evaluations of biological perspectives. <i>European Journal of Medicinal Chemistry</i> , 2015, 103, 516-529.	5.5	49
9	Predicting and understanding crystal morphology: the morphology of benzoic acid and the polymorphs of sulfathiazole. <i>CrystEngComm</i> , 2010, 12, 3119.	2.6	48
10	Solid-State Transformations of Sulfathiazole Polymorphs: The Effects of Milling and Humidity. <i>Crystal Growth and Design</i> , 2013, 13, 3404-3413.	3.0	45
11	The natural bile acid surfactant sodium taurocholate (NaTC) as a coformer in coamorphous systems: Enhanced physical stability and dissolution behavior of coamorphous drug-NaTC systems. <i>International Journal of Pharmaceutics</i> , 2018, 535, 132-139.	5.2	44
12	Planar [Ni7] discs as double-bowl, pseudometallacalix[6]arene host cavities. <i>CrystEngComm</i> , 2010, 12, 59-63.	2.6	36
13	Investigation of the formation of drug-drug cocrystals and coamorphous systems of the antidiabetic drug gliclazide. <i>International Journal of Pharmaceutics</i> , 2019, 561, 35-42.	5.2	29
14	Effects of Ball-Milling and Cryomilling on Sulfamerazine Polymorphs: A Quantitative Study. <i>Journal of Pharmaceutical Sciences</i> , 2014, 103, 1766-1778.	3.3	28
15	Regioselectivity and endo/exo selectivity in the cycloadditions of the phthalazinium dicyanomethanide 1,3-dipole with unsymmetrical alkene and alkyne dipolarophiles. Unexpected reversals of regiochemistry: a combined experimental and DFT theoretical study. <i>Journal of the Chemical Society, Perkin Transactions 1</i> , 2001, 1391-1397.	1.3	27
16	17 $\beta$ -Hydroxy-17 $\alpha$ -methylandrostan[3,2-c]pyrazole, Stanozolol: The Crystal Structures of Polymorphs 1 and 2 and 10 Solvates. <i>Crystal Growth and Design</i> , 2011, 11, 2829-2838.	3.0	26
17	Formation, Physical Stability, and Quantification of Process-Induced Disorder in Cryomilled Samples of a Model Polymorphic Drug. <i>Journal of Pharmaceutical Sciences</i> , 2013, 102, 93-103.	3.3	25
18	Sonochemical synthesis of a new cobalt(II) complex: Crystal structure, thermal behavior, Hirshfeld surface analysis and its usage as precursor for preparation of CoO/Co <sub>3</sub> O <sub>4</sub> nanoparticles. <i>Ultrasonics Sonochemistry</i> , 2017, 38, 134-144.	8.2	25

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19	Stereoselective Epimerizations of Glycosyl Thiols. <i>Organic Letters</i> , 2017, 19, 5802-5805.	4.6	25
20	Cocrystal Forms of the BCS Class IV Drug Sulfamethoxazole. <i>Crystal Growth and Design</i> , 2018, 18, 3902-3912.	3.0	25
21	Synthesis, crystal structure and spectroscopy of bioactive Cd(II) polymeric complex of the non-steroidal anti-inflammatory drug diclofenac sodium: Antiproliferative and biological activity. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 429-436.	3.9	24
22	Applications of Low Temperature Gradient Sublimation in Vacuo: Rapid Production of High Quality Crystals. The First Solvent-Free Crystals of Ethinyl Estradiol. <i>Crystal Growth and Design</i> , 2013, 13, 1122-1130.	3.0	23
23	Allylic Azide Rearrangement in Tandem with Huisgen Cycloaddition for Stereoselective Annulation: Synthesis of <i>C</i> -Glycosyl Iminosugars. <i>Organic Letters</i> , 2015, 17, 6226-6229.	4.6	23
24	Anisotropic Crystal Growth in Flat and Nonflat Systems: The Important Influence of van der Waals Contact Molecular Stacking on Crystal Growth and Dissolution. <i>Crystal Growth and Design</i> , 2015, 15, 3235-3248.	3.0	23
25	Tailoring Cocrystal and Salt Formation and Controlling the Crystal Habit of Diflunisal. <i>Crystal Growth and Design</i> , 2016, 16, 6468-6478.	3.0	22
26	Factors Controlling Persistent Needle Crystal Growth: The Importance of Dominant One-Dimensional Secondary Bonding, Stacked Structures, and van der Waals Contact. <i>Crystal Growth and Design</i> , 2021, 21, 3449-3460.	3.0	21
27	Use of Sublimation Catalysis and Polycrystalline Powder Templates for Polymorph Control of Gas Phase Crystallization. <i>Crystal Growth and Design</i> , 2018, 18, 3510-3516.	3.0	20
28	Determination of the Polymorphic Forms of Bicycladine Hydrochloride by Differential Scanning Calorimetry, Thermogravimetric Analysis, X-Ray Powder Diffraction, Attenuated Total Reflectance Infrared Spectroscopy, and Attenuated Total Reflectance Near-Infrared Spectroscopy. <i>Applied Spectroscopy</i> , 2005, 59, 1365-1371.	2.2	19
29	Unexpected Effects of Catalytic Amounts of Additives on Crystallization from the Gas Phase: Depression of the Sublimation Temperature and Polymorph Control. <i>Crystal Growth and Design</i> , 2016, 16, 2492-2495.	3.0	19
30	A Comprehensive Cocrystal Screening Study of Chlorothiazide. <i>Crystal Growth and Design</i> , 2017, 17, 5223-5232.	3.0	19
31	One-Pot Hydrogen Peroxide and Hydrohalic Acid Induced Ring Closure and Selective Aromatic Halogenation To Give New Ring-Fused Benzimidazoles. <i>Organic Letters</i> , 2015, 17, 2856-2859.	4.6	18
32	Influence of nitroxide structure on the 2,5- and 2,6-spirodicyclohexyl substituted cyclic nitroxide-mediated free-radical polymerization of styrene. <i>Journal of Polymer Science Part A</i> , 2003, 41, 3892-3900.	2.3	17
33	Hydrogen Bonding Networks and Solid-State Conversions in Benzamidinium Salts. <i>Crystal Growth and Design</i> , 2015, 15, 3905-3916.	3.0	17
34	Simultaneous double 1,3-dipolar cycloaddition reactions involving bisnitrones or bisdipolarophiles. 1H NMR investigation of the conformational preferences of N-methyl- and N-phenyl-isoxazolidines. <i>Perkin Transactions II</i> , 2001, , 373-378.	1.1	16
35	Synthesis and Toxicity of New Ring-Fused Imidazo[5,4-f]benzimidazolequinones and Mechanism Using Amine Oxide Cyclizations. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 1967-1975.	2.4	16
36	Investigation into solid and solution properties of quinizarin. <i>CrystEngComm</i> , 2015, 17, 3985-3997.	2.6	16

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37	One-Pot Synthesis of Dihalogenated Ring-Fused Benzimidazolequinones from 3,6-Dimethoxy-2-(cycloamino)anilines Using Hydrogen Peroxide and Hydrohalic Acid. <i>Organic Letters</i> , 2018, 20, 6970-6974.	4.6	15
38	Synthesis of pyrazolopyrimidinones using a "one-pot" approach under microwave irradiation. <i>Beilstein Journal of Organic Chemistry</i> , 2018, 14, 1222-1228.	2.2	15
39	Influence of Excipients on Cocrystal Stability and Formation. <i>Crystal Growth and Design</i> , 2020, 20, 4523-4532.	3.0	14
40	A comprehensive spectroscopic study of the polymorphs of diflunisal and their phase transformations. <i>International Journal of Pharmaceutics</i> , 2017, 528, 312-321.	5.2	13
41	Incorporating Morpholine and Oxetane into Benzimidazolequinone Antitumor Agents: The Discovery of 1,4,6,9-Tetramethoxyphenazine from Hydrogen Peroxide and Hydroiodic Acid-Mediated Oxidative Cyclizations. <i>Journal of Organic Chemistry</i> , 2019, 84, 9811-9818.	3.2	12
42	Unprecedented morphology control of gas phase cocrystal growth using multi zone heating and tailor made additives. <i>Chemical Communications</i> , 2020, 56, 5657-5660.	4.1	12
43	Pyrimidine annelated heterocycles - synthesis and cycloaddition of the first pyrimido[1,4]diazepine N-oxides. <i>Journal of the Chemical Society, Perkin Transactions 1</i> , 2001, , 622-632.	1.3	11
44	A new tricyclic ring and a nitrogen-sulfur analogue of the tri-pentagon bowl: cycloaddition reactions of the unstabilised 1,3,4-thiadiazolium-3-methanide 1,3-dipole: steric influences on the endo-effect: substituted pyrrolo[2,1-b]-1,3,4-thiadiazole systems: azolium 1,3-dipoles. <i>Journal of the Chemical Society, Perkin Transactions 1</i> , 2002, , 2851-2860.	1.3	11
45	A cobalt(II) complex with anionic and neutral N-donor ligands: synthesis, crystal structure, and application as a heterogeneous catalyst for olefin epoxidation with tert-BuOOH. <i>Journal of Coordination Chemistry</i> , 2015, 68, 980-992.	2.2	11
46	Synthesis and crystal structures of cobalt(II), cadmium(II), and zinc(II) complexes of 4-nitro phenylcyanamide: enhancing the biological properties through bound to human serum albumin. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 2055-2065.	3.5	11
47	Selective Methylmagnesium Chloride Mediated Acetylations of Isosorbide: A Route to Powerful Nitric Oxide Donor Furoxans. <i>Organic Letters</i> , 2018, 20, 3025-3029.	4.6	11
48	Application of Ball Milling for Highly Selective Mechanochemical Polymorph Transformations. <i>Organic Process Research and Development</i> , 2018, 22, 796-802.	2.7	11
49	Plastically bendable pregabalin multi-component systems with improved tabletability and compressibility. <i>CrystEngComm</i> , 2020, 22, 412-415.	2.6	11
50	ZnII and CuII-Based Coordination Polymers and Metal Organic Frameworks by the of Use of 2-Pyridyl Oximes and 1,3,5-Benzenetricarboxylic Acid. <i>Molecules</i> , 2021, 26, 491.	3.8	11
51	Expanding the NUIG MOF family: synthesis and characterization of new MOFs for selective CO <sub>2</sub> adsorption, metal ion removal from aqueous systems, and drug delivery applications. <i>Dalton Transactions</i> , 2021, 50, 6997-7006.	3.3	11
52	Formation of Salts and Molecular Ionic Cocrystals of Fluoroquinolones and $\pm$ -Dicarboxylic Acids. <i>Crystal Growth and Design</i> , 2022, 22, 3060-3071.	3.0	11
53	Solid Forms, Crystal Habits, and Solubility of Danthron. <i>Journal of Chemical &amp; Engineering Data</i> , 2015, 60, 2110-2118.	1.9	10
54	Sulfamerazine: Understanding the Influence of Slip Planes in the Polymorphic Phase Transformation through X-Ray Crystallographic Studies and <i>ab Initio</i> Lattice Dynamics. <i>Molecular Pharmaceutics</i> , 2015, 12, 3735-3748.	4.6	10



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73	Visible-light unmasking of heterocyclic quinone methide radicals from alkoxyamines. <i>Chemical Communications</i> , 2019, 55, 14665-14668.	4.1	6
74	A new tricyclic ring and a nitrogen-sulfur analogue of the tri-pentagon bowl. Substituted 5,6,7,7a-tetrahydropyrrolo[2,1-b]-1,3,4-thiadiazole-endo-6,7-dicarboxyimides. <i>Chemical Communications</i> , 2001, , 1950-1951.	4.1	5
75	Synthesis, characterization, and molecular structures of Ni(II) and Cd(II) complexes derived from dithiophosphate. <i>Heteroatom Chemistry</i> , 2016, 27, 353-360.	0.7	5
76	Dinuclear cadmium indomethacin and Lawsone complexes: synthesis, crystal structures, antiproliferative and biological evaluations. <i>Journal of Coordination Chemistry</i> , 2016, 69, 3021-3034.	2.2	5
77	Quantitative assessment of copper proteinates used as animal feed additives using ATR-FTIR spectroscopy and powder X-ray diffraction (PXRD) analysis. <i>Food Additives and Contaminants - Part A Chemistry, Analysis, Control, Exposure and Risk Assessment</i> , 2017, 34, 1344-1352.	2.3	5
78	Conversion of Gel-Forming Crystal Needles To Easily Processable More Equant Crystals Using High-Shear Ultralow Attrition Agitation: Accelerated Ostwald Ripening without Crystal Attrition. <i>Crystal Growth and Design</i> , 2019, 19, 1502-1504.	3.0	5
79	Shining Light on Growth-Dependent Surface Chemistry of Organic Crystals: A Polarized Raman Spectroscopic and Computational Study of Aspirin. <i>Crystal Growth and Design</i> , 2019, 19, 1288-1298.	3.0	5
80	Synthesis of a Spirocyclic Oxetane-Fused Benzimidazole. <i>Molecules</i> , 2015, 20, 13864-13874.	3.8	4
81	Crystallization of Organic Salts from the Gas Phase: When Does Proton Transfer Take Place?. <i>Crystal Growth and Design</i> , 2021, 21, 23-27.	3.0	4
82	Pixel calculations using Orca or GAUSSIAN for electron density automated within the Oscail package. <i>Journal of Applied Crystallography</i> , 2021, 54, 1535-1541.	4.5	4
83	Differences in Coformer Interactions of the 2,4-Diaminopyrimidines Pyrimethamine and Trimethoprim. <i>Crystal Growth and Design</i> , 2022, 22, 3163-3173.	3.0	4
84	The first organo-tungsten pyrylium salt and structural characterization of its pseudobase. <i>Chemical Communications</i> , 2001, , 1504-1505.	4.1	3
85	Preparation and Structure of Novel Chiral 4,6-Disubstituted Tetrahydropyrimidinones. <i>Organic Chemistry International</i> , 2012, 2012, 1-5.	1.0	3
86	Photochemical Aryl Radical Cyclizations to Give (E)-3-Ylideneoxindoles. <i>Molecules</i> , 2014, 19, 15891-15899.	3.8	3
87	Synthesis, characterization, crystal structure, and antibacterial evaluation of Ni (II) complex with new dithiophosphorus compound. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2016, 191, 1313-1317.	1.6	3
88	Synthesis and characterization of new coordination compounds by the use of 2-pyridinemethanol and di- or tricarboxylic acids. <i>CrystEngComm</i> , 2021, 23, 5489-5497.	2.6	3
89	Ring-fused dimethoxybenzimidazole-benzimidazolequinone (DMBBQ): tunable halogenation and quinone formation using NaX/Oxone. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 2716-2724.	2.8	3
90	Spectral, Structural, and Antibacterial Study of Copper(II) Complex with N2O2 Donor Schiff Base Ligand and Its Usage in Preparation of CuO Nanoparticles. <i>Journal of Chemistry</i> , 2022, 2022, 1-13.	1.9	3

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91	Nitrogen-containing heterocycles: 1,3-dipolar cycloaddition of stabilized nitrones with alkynes; primary cycloadducts, first and second generation rearrangement processes. <i>Journal of the Chemical Society, Perkin Transactions 1</i> , 2001, , 3382-3392.	1.3	2
92	Dual-drug amorphous formulation of gliclazide. <i>Drug Development and Industrial Pharmacy</i> , 2021, 47, 302-307.	2.0	2
93	The Very Different Effect of Water on Nucleation, Crystallization, and Hydrate Stability of Zingerone and Vanillate Esters. <i>Crystal Growth and Design</i> , 2020, 20, 627-635.	3.0	1
94	Synthesis, characterization, and molecular structures of Ni(II) and Cd(II) complexes derived from dithiophosphonate. <i>Heteroatom Chemistry</i> , 2017, 28, e21367.	0.7	0
95	1-Fluoro-2,5-dimethoxy-4-nitrobenzene. <i>MolBank</i> , 2018, 2018, M984.	0.5	0
96	Crystallization from the Gas Phase: Morphology Control, Co-Crystal and Salt Formation. <i>Proceedings (mdpi)</i> , 2021, 78, 1.	0.2	0