Doris Braun

List of Publications by Year
in descending order

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71	2,483	172386	206029
papers	citations	29	48
		h-index	g-index

74	74	74	2322
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Directing Crystallization Outcomes of Conformationally Flexible Molecules: Polymorphs, Solvates, and Desolvation Pathways of Fluconazole. Molecular Pharmaceutics, 2022, 19, 456-471.	2.3	13
2	Distinguishing liquid ammonia from sodium hydroxide mercerization in cotton textiles. Cellulose, 2022, 29, 4183-4202.	2.4	10
3	Efficient Screening of Coformers for Active Pharmaceutical Ingredient Cocrystallization. Crystal Growth and Design, 2022, 22, 4513-4527.	1.4	14
4	N , N â€Đimethoxyimidazolium Derivatives as Ion Pair Constituents of Energetic Redox Couples: Model Studies by Thermal Analysis and Crystallography. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2021, 647, 365-376.	0.6	2
5	Crystals and Crystallization in Drug Delivery Design. Crystal Growth and Design, 2021, 21, 1375-1377.	1.4	20
6	Crystals and Crystallization in Drug Delivery Design. Molecular Pharmaceutics, 2021, 18, 751-753.	2.3	9
7	In Vitro Investigation of Thiolated Chitosan Derivatives as Mucoadhesive Coating Materials for Solid Lipid Nanoparticles. Biomacromolecules, 2021, 22, 3980-3991.	2.6	24
8	The trimorphism of 3-hydroxybenzoic acid: an experimental and computational study. CrystEngComm, 2021, 23, 2513-2519.	1.3	3
9	Expanding the Solid Form Landscape of Bipyridines. Crystal Growth and Design, 2021, 21, 7201-7217.	1.4	5
10	The Eight Hydrates of Strychnine Sulfate. Crystal Growth and Design, 2020, 20, 6069-6083.	1.4	4
11	2-Mercaptoimidazolium halides: structural diversity, stability and spontaneous racemisation. CrystEngComm, 2020, 22, 6034-6046.	1.3	2
12	Supramolecular organisation of sulphate salt hydrates exemplified with brucine sulphate. CrystEngComm, 2020, 22, 7204-7216.	1.3	4
13	Experimental and computational approaches to produce and characterise isostructural solvates. CrystEngComm, 2019, 21, 5533-5545.	1.3	18
14	Experimental and computational approaches to rationalise multicomponent supramolecular assemblies: dapsone monosolvates. Physical Chemistry Chemical Physics, 2019, 21, 17288-17305.	1.3	13
15	Surface Induced Phenytoin Polymorph. 1. Full Structure Solution by Combining Grazing Incidence X-ray Diffraction and Crystal Structure Prediction. Crystal Growth and Design, 2019, 19, 6058-6066.	1.4	5
16	Surface Induced Phenytoin Polymorph. 2. Structure Validation by Comparing Experimental and Density Functional Theory Raman Spectra. Crystal Growth and Design, 2019, 19, 6067-6073.	1.4	1
17	Dapsone Form V: A Late Appearing Thermodynamic Polymorph of a Pharmaceutical. Molecular Pharmaceutics, 2019, 16, 3221-3236.	2.3	30
18	Inconvenient Truths about Solid Form Landscapes Revealed in the Polymorphs and Hydrates of Gandotinib. Crystal Growth and Design, 2019, 19, 2947-2962.	1.4	32

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19	Computational and analytical approaches for investigating hydrates: the neat and hydrated solid-state forms of 3-(3-methylimidazolium-1-yl)propanoate. CrystEngComm, 2018, 20, 7826-7837.	1.3	6
20	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	1.6	3
21	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	1.6	7
22	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	1.6	8
23	Supramolecular Organization of Nonstoichiometric Drug Hydrates: Dapsone. Frontiers in Chemistry, 2018, 6, 31.	1.8	23
24	Experimental and Computational Hydrate Screening: Cytosine, 5-Flucytosine, and Their Solid Solution. Crystal Growth and Design, 2017, 17, 4347-4364.	1.4	21
25	Prediction and experimental validation of solid solutions and isopolymorphs of cytosine/5-flucytosine. CrystEngComm, 2017, 19, 3566-3572.	1.3	12
26	Phase-out-compliant fluorosurfactants: unique methimazolium derivatives including room temperature ionic liquids. Green Chemistry, 2017, 19, 3225-3237.	4.6	22
27	Understanding the role of water in 1,10-phenanthroline monohydrate. CrystEngComm, 2017, 19, 6133-6145.	1.3	8
28	Molecular Level Understanding of the Reversible Phase Transformation between Forms III and II of Dapsone. Crystal Growth and Design, 2017, 17, 5054-5060.	1.4	19
29	Unraveling Complexity in the Solid Form Screening of a Pharmaceutical Salt: Why so Many Forms? Why so Few?. Crystal Growth and Design, 2017, 17, 5349-5365.	1.4	33
30	Temperature- and moisture-dependent studies on alunogen and the crystal structure of meta-alunogen determined from laboratory powder diffraction data. Physics and Chemistry of Minerals, 2017, 44, 95-107.	0.3	12
31	New Insights into Solid Form Stability and Hydrate Formation: o-Phenanthroline HCl and Neocuproine HCl. Molecules, 2017, 22, 2238.	1.7	8
32	The Hydrogen Bonded Structures of Two 5-Bromobarbituric Acids and Analysis of Unequal C5â€“X and C5â€“Xâ€² Bond Lengths (X = Xâ€² = F, Cl, Br or Me) in 5,5-Disubstituted Barbituric Acids. Crystals, 2016, 6, 47.	1.0	3
33	Can computed crystal energy landscapes help understand pharmaceutical solids?. Chemical Communications, 2016, 52, 7065-7077.	2.2	146
34	Computational and Experimental Characterization of Five Crystal Forms of Thymine: Packing Polymorphism, Polytypism/Disorder, and Stoichiometric 0.8-Hydrate. Crystal Growth and Design, 2016, 16, 3480-3496.	1.4	34
35	Why Do Hydrates (Solvates) Form in Small Neutral Organic Molecules? Exploring the Crystal Form Landscapes of the Alkaloids Brucine and Strychnine. Crystal Growth and Design, 2016, 16, 6405-6418.	1.4	32
36	Stoichiometric and Nonstoichiometric Hydrates of Brucine. Crystal Growth and Design, 2016, 16, 6111-6121.	1.4	38

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37	Specific energy contributions from competing hydrogen-bonded structures in six polymorphs of phenobarbital. Chemistry Central Journal, 2016, 10, 8.	2.6	11
38	Structural Properties, Orderâ€“Disorder Phenomena, and Phase Stability of Orotic Acid Crystal Forms. Molecular Pharmaceutics, 2016, 13, 1012-1029.	2.3	31
39	4-Aminoquinaldine monohydrate polymorphism: prediction and impurity aided discovery of a difficult to access stable form. CrystEngComm, 2016, 18, 4053-4067.	1.3	39
40	Investigations on alunogen under Mars-relevant temperature conditions: An example for a single-crystal-to-single-crystal phase transition. American Mineralogist, 2015, 100, 2548-2558.	0.9	6
41	New crystal structures in the realm of 5,5â€²-azotetrazolates. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2015, 70, 125-134.	0.3	4
42	Solid state forms of 4-aminoquinaldine â€“ from void structures with and without solvent inclusion to close packing. CrystEngComm, 2015, 17, 2504-2516.	1.3	18
43	Navigating the Waters of Unconventional Crystalline Hydrates. Molecular Pharmaceutics, 2015, 12, 3069-3088.	2.3	62
44	Building solids inside nano-space: from confined amorphous through confined solvate to confined â€˜metastableâ€™ polymorph. Physical Chemistry Chemical Physics, 2015, 17, 24761-24773.	1.3	26
45	Structural and Ecotoxicological Profile of N-Alkoxymorpholinium-Based Ionic Liquids. Heterocycles, 2015, 90, 1018.	0.4	6
46	Synthesis and Crystal Structures of 1,1â€²-Methylene-bis(imidazolidine-2,4-dione) and Alkali Metal Salts. Crystals, 2014, 4, 1-10.	1.0	0
47	Crystal Structures of New Ammonium 5-Aminotetrazolates. Crystals, 2014, 4, 439-449.	1.0	0
48	Contrasting Polymorphism of Related Small Molecule Drugs Correlated and Guided by the Computed Crystal Energy Landscape. Crystal Growth and Design, 2014, 14, 2056-2072.	1.4	72
49	Creatine: Polymorphs Predicted and Found. Crystal Growth and Design, 2014, 14, 4895-4900.	1.4	33
50	Insights into Hydrate Formation and Stability of Morphinanes from a Combination of Experimental and Computational Approaches. Molecular Pharmaceutics, 2014, 11, 3145-3163.	2.3	38
51	Absorbing a Little Water: The Structural, Thermodynamic, and Kinetic Relationship between Pyrogallol and Its Tetarto-Hydrate. Crystal Growth and Design, 2013, 13, 4071-4083.	1.4	39
52	Four Polymorphs of Methyl Paraben: Structural Relationships and Relative Energy Differences. Crystal Growth and Design, 2013, 13, 1206-1217.	1.4	41
53	Complex Polymorphic System of Gallic Acidâ€”Five Monohydrates, Three Anhydrates, and over 20 Solvates. Crystal Growth and Design, 2013, 13, 19-23.	1.4	97
54	Stable polymorph of morphine. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o2-o2.	0.2	5

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55	Morphine hydrochloride anhydrate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3358-o3359.	0.2	6
56	Screening for cocrystals of succinic acid and 4-aminobenzoic acid. CrystEngComm, 2012, 14, 2454.	1.3	41
57	The Complexity of Hydration of Phloroglucinol: A Comprehensive Structural and Thermodynamic Characterization. Journal of Physical Chemistry B, 2012, 116, 3961-3972.	1.2	60
58	Which, if any, hydrates will crystallise? Predicting hydrate formation of two dihydroxybenzoic acids. Chemical Communications, 2011, 47, 5443-5445.	2.2	92
59	Solid-State Forms of Î²-Resorcylic Acid: How Exhaustive Should a Polymorph Screen Be?. Crystal Growth and Design, 2011, 11, 210-220.	1.4	55
60	Racemic Naproxen: A Multidisciplinary Structural and Thermodynamic Comparison with the Enantiopure Form. Crystal Growth and Design, 2011, 11, 5659-5669.	1.4	53
61	The impact of spray drying outlet temperature on the particle morphology of mannitol. Powder Technology, 2011, 213, 27-35.	2.1	125
62	Expanding the crystal landscape of isonicotinamide: concomitant polymorphism and co-crystallisation. CrystEngComm, 2011, 13, 6923.	1.3	45
63	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
64	Simultaneous quantitative analysis of ternary mixtures of d-mannitol polymorphs by FT-Raman spectroscopy and multivariate calibration models. International Journal of Pharmaceutics, 2010, 385, 29-36.	2.6	42
65	Conformational polymorphism in aripiprazole: Preparation, stability and structure of five modifications. Journal of Pharmaceutical Sciences, 2009, 98, 2010-2026.	1.6	103
66	Stability of Solvates and Packing Systematics of Nine Crystal Forms of the Antipsychotic Drug Aripiprazole. Crystal Growth and Design, 2009, 9, 1054-1065.	1.4	98
67	Solid state characterisation of four solvates of R-cinacalcet hydrochloride. CrystEngComm, 2008, 10, 1617.	1.3	32
68	Structural and Thermodynamic Features of Crystal Polymorphs of R-Cinacalcet Hydrochloride. Crystal Growth and Design, 2008, 8, 4109-4119.	1.4	16
69	Colored Polymorphs: Thermochemical and Structural Features of N-Picryl- p-toluidine Polymorphs and Solvates. Crystal Growth and Design, 2008, 8, 1977-1989.	1.4	38
70	Packing polymorphism of a conformationally flexible molecule (aprepitant). New Journal of Chemistry, 2008, 32, 1677.	1.4	50
71	Quantitative analysis of paracetamol polymorphs in powder mixtures by FT-Raman spectroscopy and PLS regression. Journal of Pharmaceutical and Biomedical Analysis, 2007, 43, 407-412.	1.4	93