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	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
2	Can computed crystal energy landscapes help understand pharmaceutical solids?. Chemical Communications, 2016, 52, 7065-7077.	2.2	146
3	The impact of spray drying outlet temperature on the particle morphology of mannitol. Powder Technology, 2011, 213, 27-35.	2.1	125
4	Conformational polymorphism in aripiprazole: Preparation, stability and structure of five modifications. Journal of Pharmaceutical Sciences, 2009, 98, 2010-2026.	1.6	103
5	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
6	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
7	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
8	Which, if any, hydrates will crystallise? Predicting hydrate formation of two dihydroxybenzoic acids. Chemical Communications, 2011, 47, 5443-5445.	2.2	92
9	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
10	Navigating the Waters of Unconventional Crystalline Hydrates. Molecular Pharmaceutics, 2015, 12, 3069-3088.	2.3	62
11	The Complexity of Hydration of Phloroglucinol: A Comprehensive Structural and Thermodynamic Characterization. Journal of Physical Chemistry B, 2012, 116, 3961-3972.	1.2	60
12	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
13	Racemic Naproxen: A Multidisciplinary Structural and Thermodynamic Comparison with the Enantiopure Form. Crystal Growth and Design, 2011, 11, 5659-5669.	1.4	53
14	Packing polymorphism of a conformationally flexible molecule (aprepitant). New Journal of Chemistry, 2008, 32, 1677.	1.4	50
15	Expanding the crystal landscape of isonicotinamide: concomitant polymorphism and co-crystallisation. CrystEngComm, 2011, 13, 6923.	1.3	45
16	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
17	Screening for cocrystals of succinic acid and 4-aminobenzoic acid. CrystEngComm, 2012, 14, 2454.	1.3	41
18	Four Polymorphs of Methyl Paraben: Structural Relationships and Relative Energy Differences. Crystal Growth and Design, 2013, 13, 1206-1217.	1.4	41

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19	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
20	4-Aminoquinaldine monohydrate polymorphism: prediction and impurity aided discovery of a difficult to access stable form. CrystEngComm, 2016, 18, 4053-4067.	1.3	39
21	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
22	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
23	Stoichiometric and Nonstoichiometric Hydrates of Brucine. Crystal Growth and Design, 2016, 16, 6111-6121.	1.4	38
24	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
25	Creatine: Polymorphs Predicted and Found. Crystal Growth and Design, 2014, 14, 4895-4900.	1.4	33
26	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
27	Solid state characterisation of four solvates of R-cinacalcet hydrochloride. CrystEngComm, 2008, 10, 1617.	1.3	32
28	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
29	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
30	Structural Properties, Orderâ€“Disorder Phenomena, and Phase Stability of Orotic Acid Crystal Forms. Molecular Pharmaceutics, 2016, 13, 1012-1029.	2.3	31
31	Dapsone Form V: A Late Appearing Thermodynamic Polymorph of a Pharmaceutical. Molecular Pharmaceutics, 2019, 16, 3221-3236.	2.3	30
32	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
33	In Vitro Investigation of Thiolated Chitosan Derivatives as Mucoadhesive Coating Materials for Solid Lipid Nanoparticles. Biomacromolecules, 2021, 22, 3980-3991.	2.6	24
34	Supramolecular Organization of Nonstoichiometric Drug Hydrates: Dapsone. Frontiers in Chemistry, 2018, 6, 31.	1.8	23
35	Phase-out-compliant fluorosurfactants: unique methimazolium derivatives including room temperature ionic liquids. Green Chemistry, 2017, 19, 3225-3237.	4.6	22
36	Experimental and Computational Hydrate Screening: Cytosine, 5-Flucytosine, and Their Solid Solution. Crystal Growth and Design, 2017, 17, 4347-4364.	1.4	21

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37	Crystals and Crystallization in Drug Delivery Design. Crystal Growth and Design, 2021, 21, 1375-1377.	1.4	20
38	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
39	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
40	Experimental and computational approaches to produce and characterise isostructural solvates. CrystEngComm, 2019, 21, 5533-5545.	1.3	18
41	Structural and Thermodynamic Features of Crystal Polymorphs of R-Cinacalcet Hydrochloride. Crystal Growth and Design, 2008, 8, 4109-4119.	1.4	16
42	Efficient Screening of Coformers for Active Pharmaceutical Ingredient Cocrystallization. Crystal Growth and Design, 2022, 22, 4513-4527.	1.4	14
43	Experimental and computational approaches to rationalise multicomponent supramolecular assemblies: dapsone monosolvates. Physical Chemistry Chemical Physics, 2019, 21, 17288-17305.	1.3	13
44	Directing Crystallization Outcomes of Conformationally Flexible Molecules: Polymorphs, Solvates, and Desolvation Pathways of Fluconazole. Molecular Pharmaceutics, 2022, 19, 456-471.	2.3	13
45	Prediction and experimental validation of solid solutions and isopolymorphs of cytosine/5-flucytosine. CrystEngComm, 2017, 19, 3566-3572.	1.3	12
46	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
47	Specific energy contributions from competing hydrogen-bonded structures in six polymorphs of phenobarbital. Chemistry Central Journal, 2016, 10, 8.	2.6	11
48	Distinguishing liquid ammonia from sodium hydroxide mercerization in cotton textiles. Cellulose, 2022, 29, 4183-4202.	2.4	10
49	Crystals and Crystallization in Drug Delivery Design. Molecular Pharmaceutics, 2021, 18, 751-753.	2.3	9
50	Understanding the role of water in 1,10-phenanthroline monohydrate. CrystEngComm, 2017, 19, 6133-6145.	1.3	8
51	New Insights into Solid Form Stability and Hydrate Formation: o-Phenanthroline HCl and Neocuproine HCl. Molecules, 2017, 22, 2238.	1.7	8
52	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	1.6	8
53	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	1.6	7
54	Morphine hydrochloride anhydrate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3358-o3359.	0.2	6

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55	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
56	Structural and Ecotoxicological Profile of N-Alkoxymorpholinium-Based Ionic Liquids. Heterocycles, 2015, 90, 1018.	0.4	6
57	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
58	Stable polymorph of morphine. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o2-o2.	0.2	5
59	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
60	Expanding the Solid Form Landscape of Bipyridines. Crystal Growth and Design, 2021, 21, 7201-7217.	1.4	5
61	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
62	The Eight Hydrates of Strychnine Sulfate. Crystal Growth and Design, 2020, 20, 6069-6083.	1.4	4
63	Supramolecular organisation of sulphate salt hydrates exemplified with brucine sulphate. CrystEngComm, 2020, 22, 7204-7216.	1.3	4
64	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
65	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	1.6	3
66	The trimorphism of 3-hydroxybenzoic acid: an experimental and computational study. CrystEngComm, 2021, 23, 2513-2519.	1.3	3
67	2-Mercaptoimidazolium halides: structural diversity, stability and spontaneous racemisation. CrystEngComm, 2020, 22, 6034-6046.	1.3	2
68	N , N â€Ðimethoxyimidazolium 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
69	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
70	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
71	Crystal Structures of New Ammonium 5-Aminotetrazolates. Crystals, 2014, 4, 439-449.	1.0	0