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Characterising the role of water in sildenafil citrate by NMR crystallography

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CrystEngComm, 2016, 18, 1054-1063.

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#	Paper	IF	Citations
24	Computational and experimental study of reversible hydration/dehydration processes in molecular crystals of natural products – the case of catechin. <i>CrystEngComm</i> , 2016 , 18, 5267-5277	3.3	14
23	Testing the limits of NMR crystallography: the case of caffeine–nitric acid hydrate. <i>CrystEngComm</i> , 2016 , 18, 6700-6707	3.3	21
22	Experimental tests for quality validation of computationally predicted crystal structures – the case of a conformationally flexible procyanidin A-2 dihydrate. <i>CrystEngComm</i> , 2017 , 19, 2903-2913	3.3	11
21	Invariom-based comparative electron density studies of iso-sildenafil and sildenafil. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2017 , 72, 1-10	1	0
20	Assessing the Detection Limit of a Minority Solid-State Form of a Pharmaceutical by H Double-Quantum Magic-Angle Spinning Nuclear Magnetic Resonance Spectroscopy. <i>Journal of Pharmaceutical Sciences</i> , 2017 , 106, 3372-3377	3.9	15
19	A combined NMR crystallographic and PXRD investigation of the structure-directing role of water molecules in orotic acid and its lithium and magnesium salts. <i>CrystEngComm</i> , 2017 , 19, 224-236	3.3	4
18	NMR crystallography: structure and properties of materials from solid-state nuclear magnetic resonance observables. <i>IUCrJ</i> , 2017 , 4, 350-359	4.7	86
17	Improving Confidence in Crystal Structure Solutions Using NMR Crystallography: The Case of Epiroxicam. <i>Crystal Growth and Design</i> , 2018 , 18, 3339-3351	3.5	20
16	DNP-enhanced solid-state NMR spectroscopy of active pharmaceutical ingredients. <i>Magnetic Resonance in Chemistry</i> , 2018 , 56, 583-609	2.1	48
15	Perspective: Current advances in solid-state NMR spectroscopy. <i>Journal of Chemical Physics</i> , 2018 , 149, 040901	3.9	21
14	Inversion dimers dominate the crystal packing in the structure of trimethyl citrate (trimethyl 2-hydroxy-propane-1,2,3-tri-carboxyl-ate). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018 , 74, 1362-1365	0.7	
13	The use of variable temperature C solid-state MAS NMR and GIPAW DFT calculations to explore the dynamics of diethylcarbamazine citrate. <i>Magnetic Resonance in Chemistry</i> , 2019 , 57, 200-210	2.1	5
12	Multiresolution 3D-DenseNet for Chemical Shift Prediction in NMR Crystallography. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 4558-4565	6.4	17
11	Successful Strategy for High Degree of Freedom Crystal Structure Determination from Powder X-Ray Diffraction Data: A Case Study for Selexipag Form I with 38 DOF. <i>Crystal Growth and Design</i> , 2019 , 19, 4625-4631	3.5	8
10	Understanding the formation of apremilast cocrystals. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019 , 75, 803-814	1.8	10
9	Pharmaceutical Hydrates Analysis-Overview of Methods and Recent Advances. <i>Pharmaceutics</i> , 2020 , 12,	6.4	15
8	NMR crystallography of molecular organics. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2020 , 118-119, 10-53	10.4	49

7	Sildenafil 4.0-Integrated Synthetic Chemistry, Formulation and Analytical Strategies Effecting Immense Therapeutic and Societal Impact in the Fourth Industrial Era. <i>Pharmaceuticals</i> , 2021 , 14,	5.2	5
6	The Solid State Landscape of the Sildenafil Drug. <i>Journal of Pharmaceutical Sciences</i> , 2021 ,	3.9	0
5	Resolving alternative structure determinations of indapamide using C solid-state NMR.. <i>Chemical Communications</i> , 2022 ,	5.8	
4	Chapter 6. Characterization of Pharmaceutical Solids Combining NMR, X-ray diffraction and Computer Modelling. <i>RSC Drug Discovery Series</i> , 120-169	0.6	
3	Combining X-ray and NMR Crystallography to Explore the Crystallographic Disorder in Salbutamol Oxalate. <i>Crystal Growth and Design</i> ,	3.5	
2	Hydrates of active pharmaceutical Ingredients:A ³⁵ Cl and ² H solid-state NMR and DFT study. 2022 , 101837		0
1	Solid state ¹³ C NMR spectroscopy as a tool for identification of counterfeit Viagra tablets and guide for develop new identification approach of falsified product. 2023 , 636, 122837		0