Supplementary Files

Solid-State Dehydration Mechanism of Diclofenac Sodium Salt Hydrates

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The Supplementary File contains a table (**Table S1**) and a figure (**Figure S1**).

Table S1. Crystal structures of diclofenac sodium (DIC-Na) hydrates published thus far.

	pentahydrate	4.75-hydrate	tetrahydrate (3.94-hydrate)	3.5-hydrate
Publication year	2002	2007	1988	2020
Author(s)	Muangsin et al.	Llinàs et al.	Reck et al.	Nieto et al.
Space group	$P2_1/m$	$P2_1$	$P2_1/m$	$P\bar{1}$
a / Å	9.508(4)	9.554(1)	9.464(2)	9.4370(4)
b / Å	39.591(1)	39.491(1)	39.405(7)	9.5675(5)
c / Å	9.997(4)	9.841(1)	9.972(3)	19.1526(10)
α / °	90	90	90	90.331(4)
β / °	90.69(1)	90.73(1)	90.74(2)	99.828(4)
γ / °	90	90	90	90.436(4)
Z, Z'	8, 2	8, 4	8, 2	4, 2
R-factor	0.0706	0.0323	-	0.0414
CSD identifier	AKOTAV 1102110	LIQFUN 630862	-	LAHBAB 2044232
Reference	[33]	[34]	[35]	[37]

Figure S1. DSC diagram of DIC-Na 4.75H, collected at +10°C min^{-1} up to 300°C in a sealed Al pan with flowing N_2 gas (100 mL min^{-1}), using Thermo plus EVO (Rigaku, Japan). The sample weight was 6.5 mg.