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Supporting information for article:

Temperature-induced polymorphism of salt cocrystal solvates of a pyridyl bis-urea macrocycle and naphthalene-1,5-disulfonic acid

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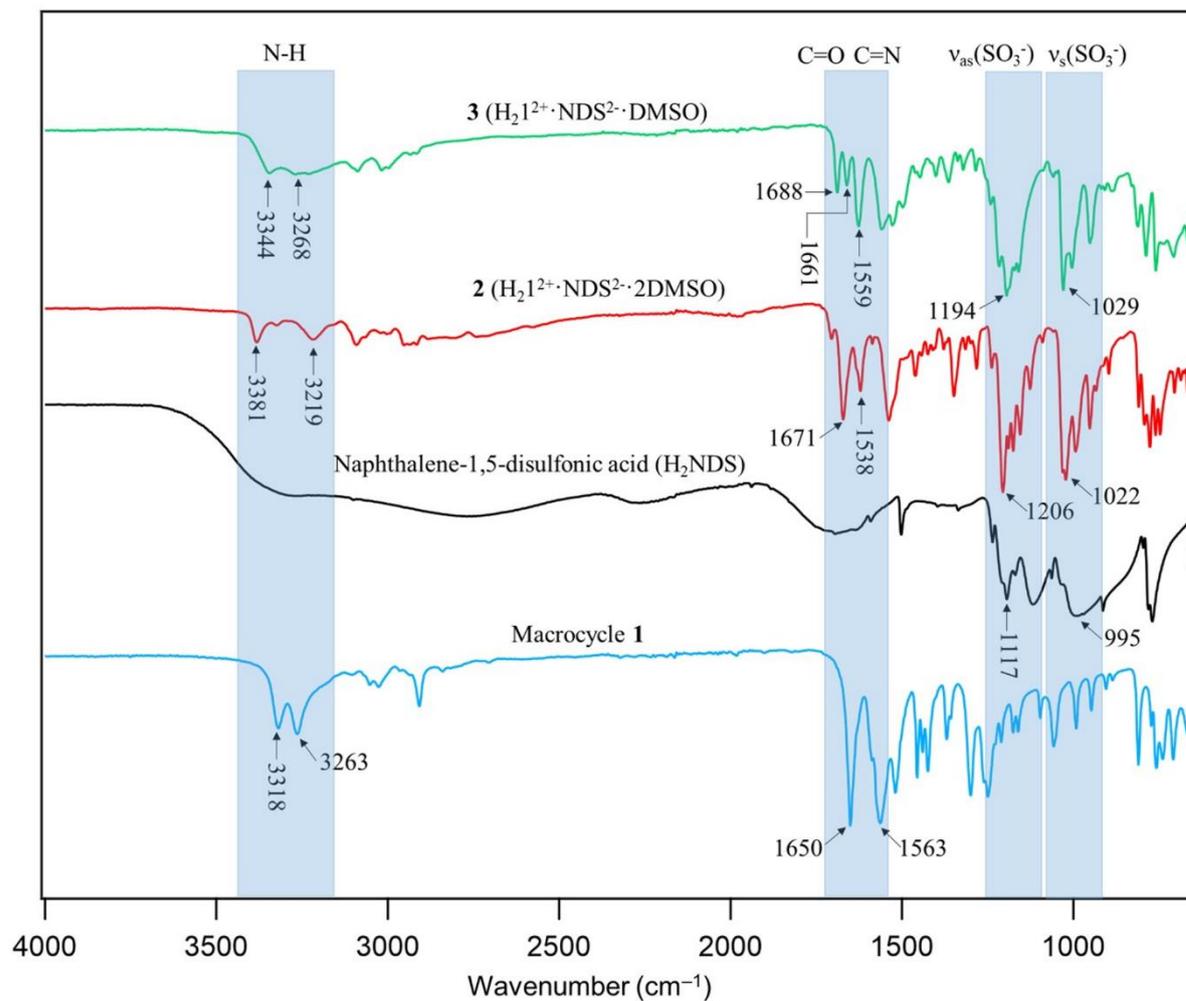
S1. FT-IR Spectroscopy**S1.**

Figure S1. FT-IR profiles of co-formers (**1** & H_2NDS) DMSO-solvated salts (**2** & **3**) in the range 4000–650 cm^{-1} .

Table S1 Comparison of key FT-IR peaks of cofomers (**1** and H₂NDS) and the DMSO-solvated salts.

	IR bands (cm ⁻¹)				
	$\nu(\text{N-H})$	$\nu(\text{C=O})$	$\nu(\text{C=N})$	$\nu_{\text{as}}(\text{SO}_3^-)$	$\nu_{\text{s}}(\text{SO}_3^-)$
1	3318, 3263	1650	1563		
H ₂ NDS				1117	995
2 (H ₂ 1 ²⁺)·(NDS ²⁻)·(DMSO) ₂	3381, 3219	1671	1538	1206	1022
3 (H ₂ 1 ²⁺)·(NDS ²⁻)·(DMSO)	3344, 3268	1661, 1688	1559	1194	1029