Electronic Supplementary Material (ESI) for CrystEngComm

An insight into dapsone co-crystals: sulfones as participants in supramolecular interactions

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Electronic Supplementary Information

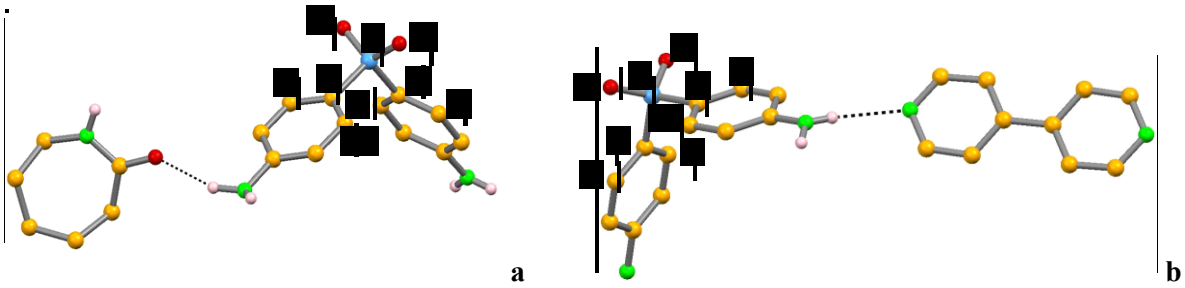

Figure S1. Crystallographic structures of co-crystals **1** (**a**) and **2** (**b**) with partial labeling atoms of DAP molecules

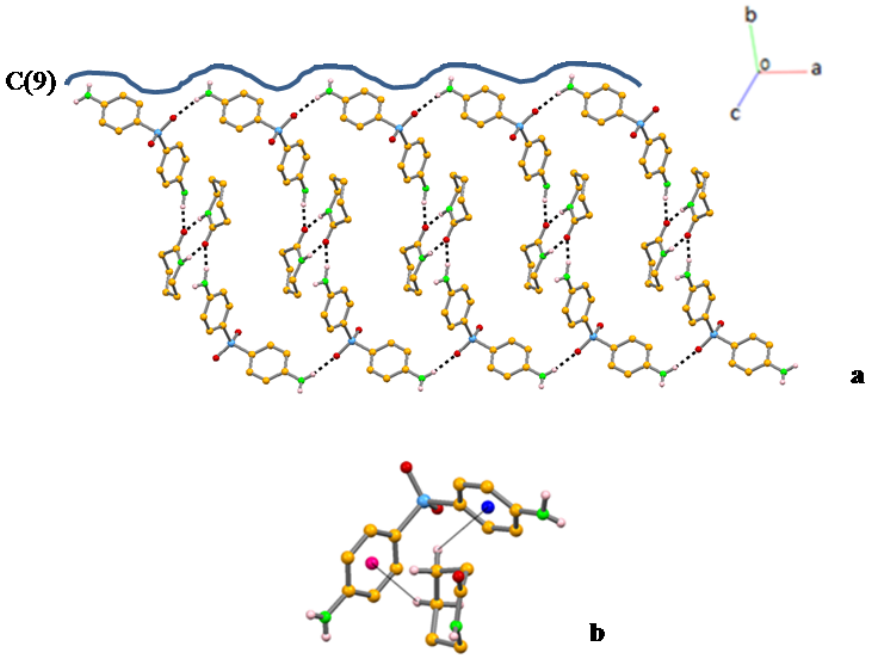

Figure S2. Packing diagrams for crystalline **1**: (**a**) detail of C(9) synthon responsible for DAP chain; (**b**) details of the different C-H···π interaction described above

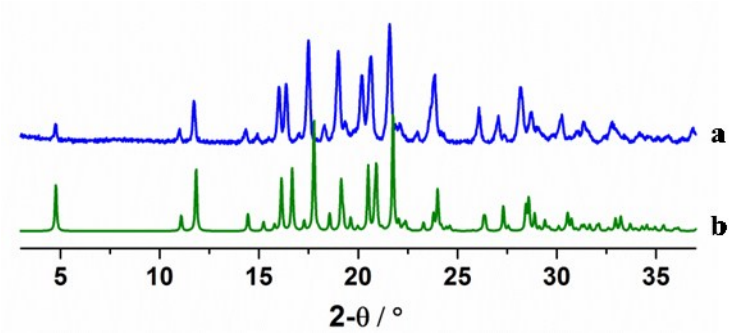

Figure S3. Experimental powder diffraction pattern of **1** as obtained (**a**) from solution, comparing with (**b**) the theoretical powder pattern calculated on the basis of single crystal data

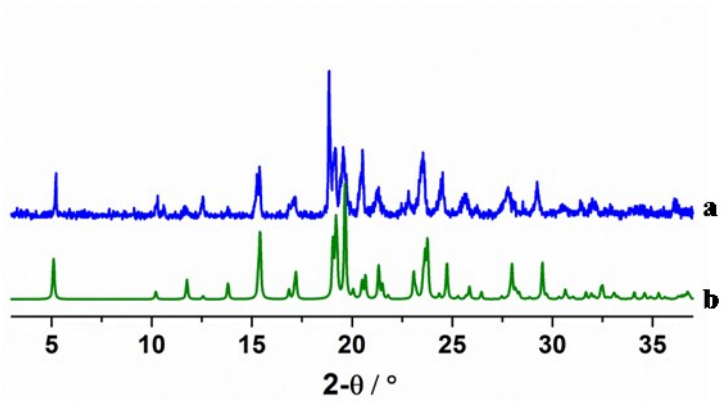

Figure S4. Experimental powder diffraction patterns of **2** as obtained (**a**) from solution, comparing with (**b**) the theoretical powder pattern calculated on the basis of single crystal data

Table S1. Unsuccessful experimental conditions tested

Coformer	Solvent	Volume of the solvent (mL)	Quantity and concentration of coformer (mg (mmol))	Quantity and concentration of dapsone(mg (mmol))	Time of stirring (min)	Heating (45ºC)
1,10 – Phenantroline	Ethanol+acetone	2+1	50.6 (0.278)	69.7 (0.281)	10	No
1,2-Bis(4-pyridil)ethane	Ethanol+acetone	2+1	51.6 (0.280)	69.4 (0.280)	10	Yes
Isonicotinic acid	Ethanol+acetone	3+2	39.8 (0.323)	81.1 (0.327)	10	Yes
Morpholine	Acetone	2	31.3 (0.359)	89.1 (0.359)	10	No
Nicotinamide	Ethanol+acetone	2+1	40.0 (0.327)	80.8 (0.325)	10	Yes
Isonicotinamide	Ethanol+acetone	2+1	39.6 (0.324)	80.4 (0.324)	10	Yes
DABCO	Ethanol+acetone	2+1	38.1 (0.340)	83.2 (0.335)	10	No
Piperazine	Ethanol+acetone	2+1	32.4 (0.376)	89.3 (0.360)	10	Yes
Paracetamol	Ethanol+acetone	3+1	45.4 (0.300)	74.6 (0.300)	10	No

Table S2. Torsion angles for dapsone and dapsone co-crystals

	Atoms label	**Torsion angle**
Dap	C2C1S1O1	37.4(3)º
	C6C1S1O2	-8.5(3)º
	C8C7S1O1	-31.0(3)º
	C12C7S1O2	21.0(3)º
1	C2C1S1O2	28.7(2)º
	C6C1S1O1	-20.0(2)º
	C8C7S1O2	-17.7(2)º
	C12C7S1O1	28.8(2)º
2	C2C1S1O2	17.8(1)º
	C6C1S1O1	-33.0(1)º
	C8C7S102	-24.6(1)º
	C12C7S1O1	28.1(1)º

Table S3. IR typical bands for co-crystals **1** and **2**

Compound	***IR (KBr, selected bands, cm^{-1})***
1	N-H from primary amine (3489.8 υ) N-H from amide (3380.0 υ) C-H from aliphatic chain (2928.3 υ) C-H from aromatic chain (3226.6 υ) C=O from amide (1671.9 υ) C=C (1608.0 υ) SO_2 (1301.2 υ, 1156.3 υ)
2	N-H from primary amine (3452.4 υ) C-H from aromatic chain (3208.7 υ) C=N (1653.2 υ) C=C (1599.4 υ) SO_2 (1283.3 υ, 1138.4 υ)

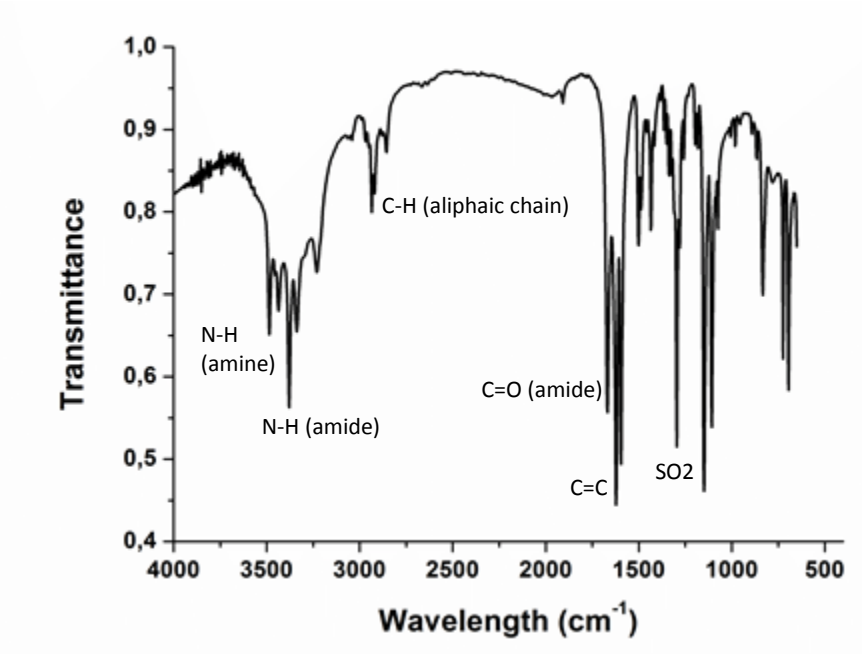

Figure S5. IR spectra of Co-crystal **1**

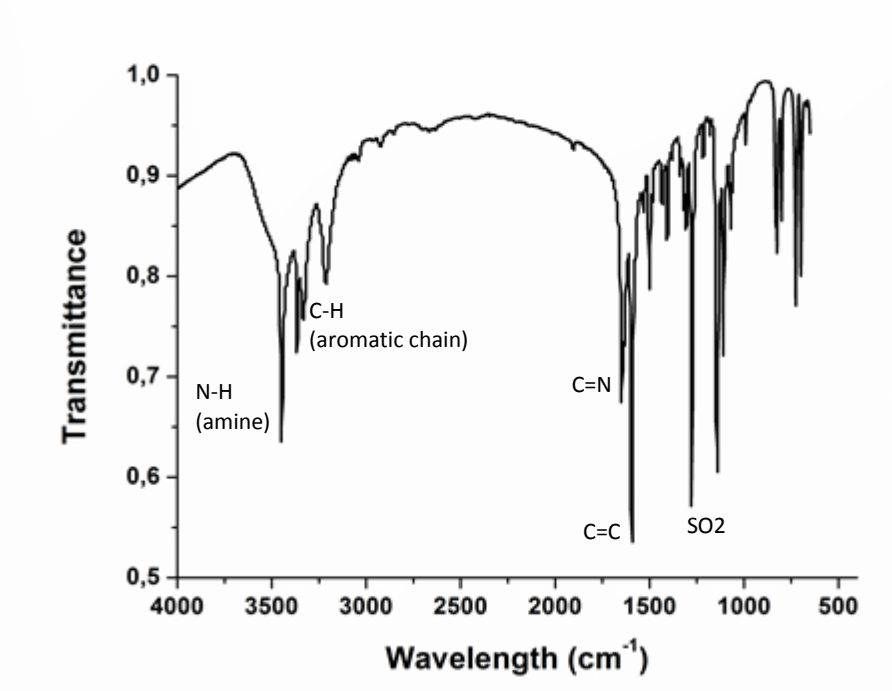

Figure S6. IR spectra of Co-crystal **2**