Electronic Supplementary Material (ESI) for CrystEngComm.

Preparation and solid-state characterization of dapsone pharmaceutical cocrystals through supramolecular synthon strategy

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Contents of Supporting Information

Table S1 Hydrogen-bond geometry of cocrystals

structure	X-H···A	(X-H)/Å	d (H···A)/ Å	D (X···A)/ Å	θ (X-H···A)/°
DAP-PYR（1:1）	N2-H2B···N3	0.906(19)	2.080(19)	2.9859(19)	179(2)
	N2-H2A···N5	0.87(2)	2.21(2)	3.0439(18)	162.3(17)
	N1-H1A···O2	0.87(2)	2.20(2)	3.0602(18)	176.6(17)
	N1-H1B···O1	0.851(19)	2.413(18)	3.1390(16)	143.5(17)
	N5 -H5A···O2	0.918(19)	2.204(19)	3.0972(16)	164.2(17)
DAP-PYR（2:1）	N2-H2A···N3	0.884(13)	2.130(16)	2.977(7)	160.3(15)
	N2-H2A···N5	0.884(13)	2.262(17)	3.111(9)	161.0(14)
	N5*-H5A···N2	0.88	2.30	3.111(9)	153
	N1-H1A···O1	0.887(16)	2.377(15)	3.223(2)	159.5(15)
	N1-H1B···O2	0.894(12)	2.558(15)	3.127(2)	122.1(12)
	N2-H2B···O2	0.883(16)	2.33(2)	3.081(2)	142.2(17)

There is disorder in the single crystal structure of DAP-PYR (2:1) cocrystal, and PYR molecules themselves turn over and overlap, so that the same repeating unit in a whole structure is located in different cells. This phenomenon is reflected in the same position in the structure of many identical structures, and have a certain atomic occupancy.

Table S2 Atomic occupancy for shelxl

atom	occupancy	atom	occupancy	atom	occupancy
N(3)	0.5	C(13)	0.5	H(13)	0.5
C(14)	0.5	H(14)	0.5	C(15)	0.5
C(16)	0.5	H(16)	0.5	C(17)	0.5
H(17)	0.5	N(4)	0.5	C(19)	0.5
H(19A)	0.5	H(19B)	0.5	C(18)	0.5
H(18A)	0.5	H(18b)	0.5	N(5)	0.5
H(5A)	0.5	C(21)	0.5	H(21A)	0.5
H(21B)	0.5	C(20)	0.5	H(20A)	0.5
H(20B)	0.5				

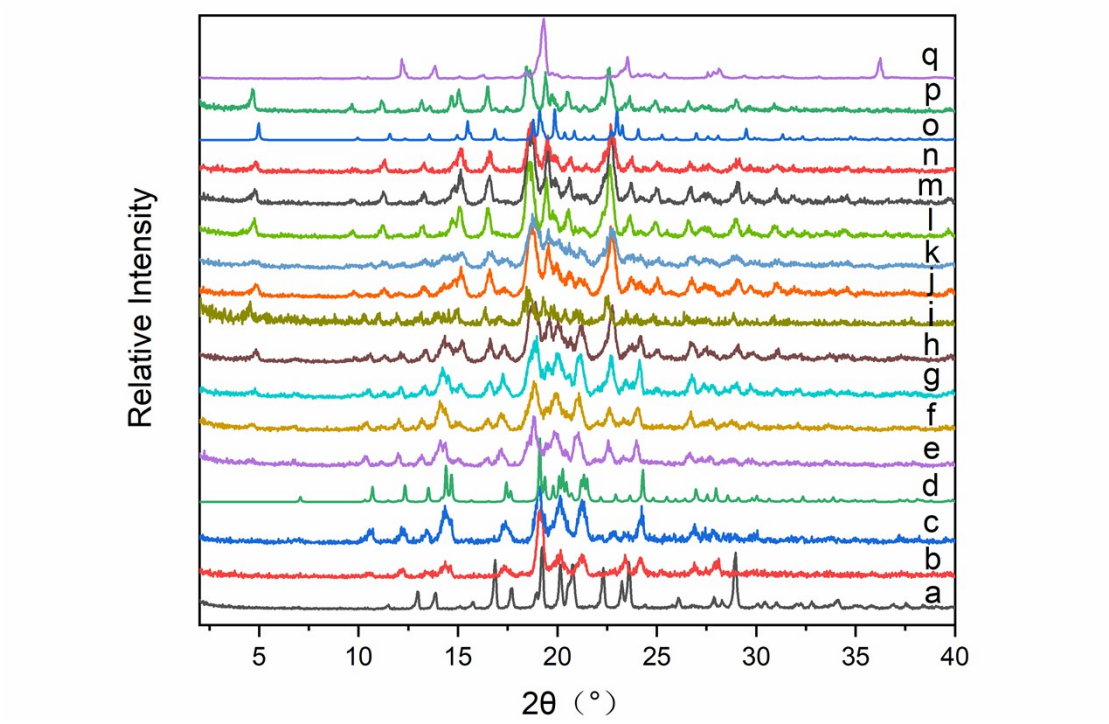

Fig. S1 PXRD pattern of (a) DAP; (b) 1:2; (c) 1:1; (d) simulated 1:1; (e) 1.1:1; (f) 1.2:1; (g) 1.3:1; (h) 1.4:1; (i) 1.5:1; (j) 1.6:1; (k) 1.7:1; (l) 1.8:1; (m) 1.9:1; (n) 2:1; (o) simulated 2:1; (p) 3:1; (q) PYR.

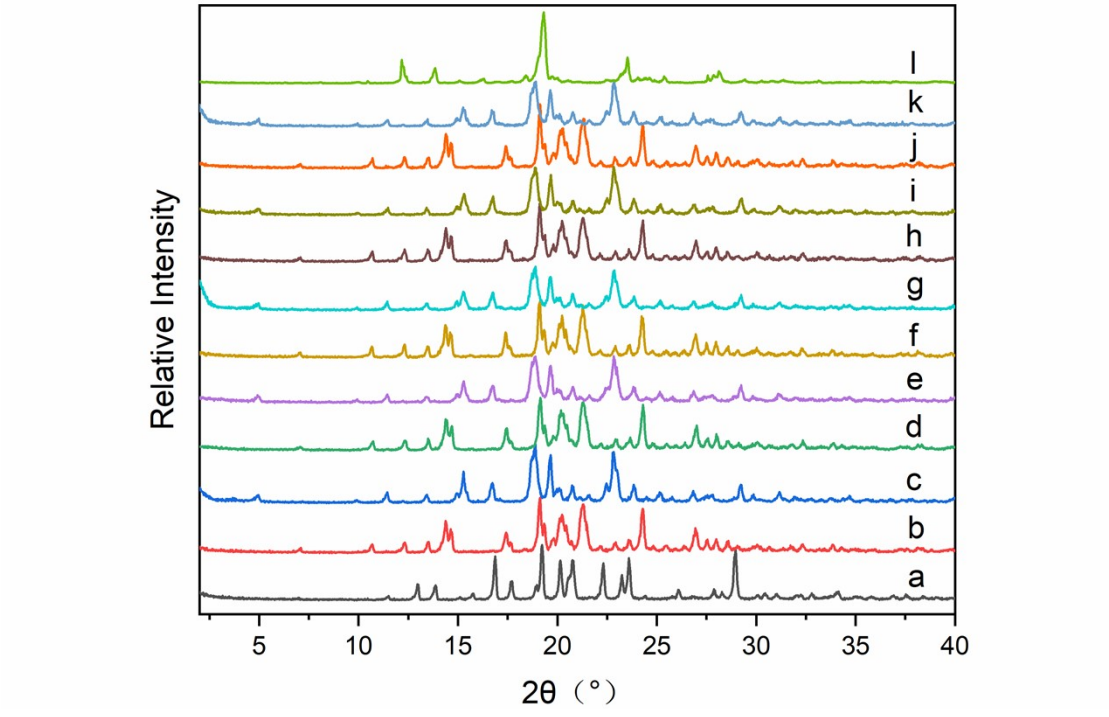

Fig. S2 PXRD pattern of (a) DAP; (b) dry grinding (1:1); (c) dry grinding (2:1); (d) LAG (1:1) in ethanol; (e) LAG (2:1) in ethanol; (f) LAG (1:1) in methanol; (g) LAG (2:1) in methanol; (h) LAG (1:1) in ethyl acetate; (i) LAG (2:1) in ethyl acetate; (j) LAG (1:1) in toluene; (k) LAG (2:1) in toluene; (l) PYR.

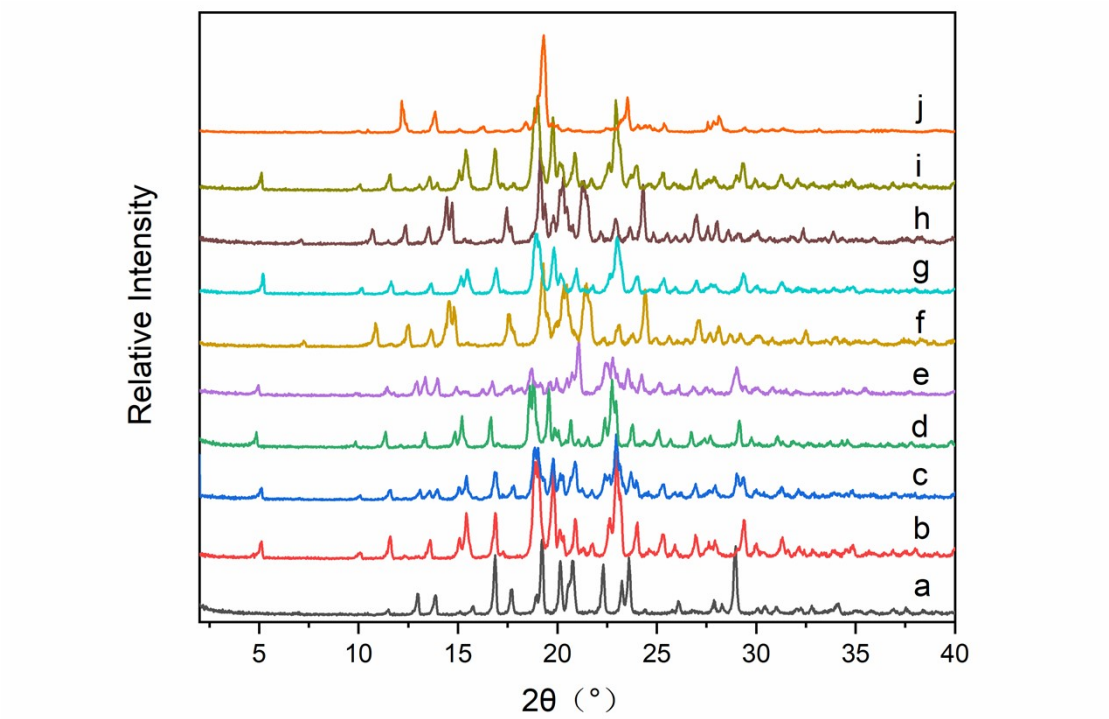

Fig. S3 PXRD pattern of (a) DAP; (b) suspension (1:1) in ethanol; (c) suspension (2:1) in ethanol; (d) suspension (1:1) in methanol; (e) suspension (2:1) in methanol; (f) suspension (1:1) in ethyl acetate; (g) suspension (2:1) in ethyl acetate; (h) suspension (1:1) in toluene; (i) suspension (2:1) in toluene; (j) PYR.

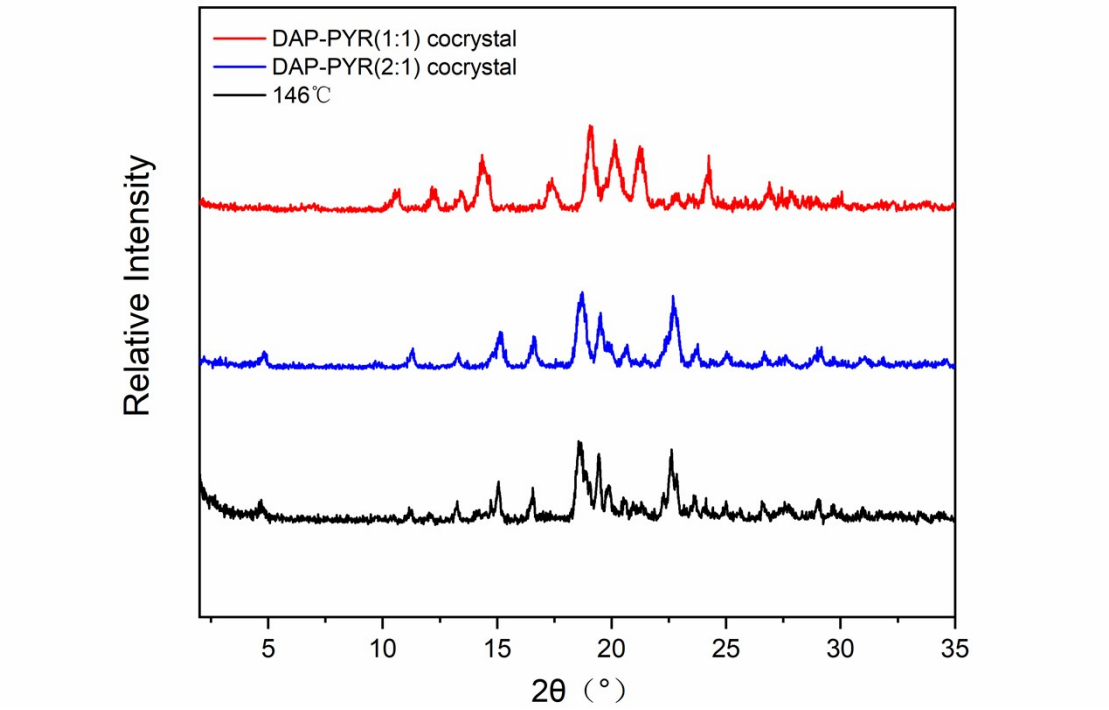

Fig. S4 PXRD pattern of DAP-PYR（1:1）after heating to 146 ℃.