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How Good are the Crystallisation Methods for Co-Crystals - A Comparative Study of Piroxicam.

Katharina Fucke, Svetlana A. Myz, Tatyana P. Shakhtshneider, Elena V. Boldyreva, and Ulrich J. Griesser

Acid mixture	Melt		Evaporation					Fast cooling					Slow cooling					Precipitation					Solvent-drop grinding				
	1:1	98:50	EtOH	AcO	AcN	THF	$CHCl_3$	EtOH	AcO	AcN	THF	$CHCl_3$	EtOH	AcO	AcN	THF	$CHCl_3$	EtOH	AcO	AcN	THF	$CHCl_3$	EtOH	AcO	AcN	THF	$CHCl_3$
1 Oxalic acid	-	A	B	B	B	B	-	-	B	-	B	-	-	B	B	-	-	-	B Hy	-	B	-	B	B	B	B	B
2 Malonic acid	A	B	I	I Hy	I Hy	I	-	-	-	-	-	-	-	I	-	Hy	-	-	Hy	Hy I	-	-	C	C	C	Hy C	C
3 Succinic acid	A	B	C	A	A Hy	A	-	-	-	-	-	-	-	A	-	A	-	Hy	Hy	Hy	A	-	A	Hy	A	A	I
4 Maleic acid	A I	A	-	B	-	-	-	-	-	-	-	-	-	-	-	B	-	-	Hy	-	-	-	-	C	C	C	C
5 Fumaric acid	-	-	Hy	Hy I	A	A	-	-	Hy A	-	Hy	-	-	-	-	-	-	-	-	-	A	-	I	Hy	A	B	I
6 Glutaric acid	A B	C	-	I B	I Hy B	I B A	-	-	-	-	I	-	-	-	Hy	I A	-	-	Hy	Hy	I	B	B	B	B	B	B
7 Adipic acid	A	A	Hy	B I	B	B	-	-	-	-	A	-	-	B	-	A	-	-	Hy	Hy	B	C	B	B	B	B	B
8 Pimelic acid	A	B	-	C	C	I	D	-	-	-	-	-	-	-	-	I	-	-	-	-	-	-	I	D	D	I	D
9 Suberic acid	A B	B	Hy	A	I Hy A	A Hy	I	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	A	A	A	A	A
10 Azelaic acid	A I	A	Hy	I Hy	I	I	-	-	-	-	-	-	-	I	-	I	-	-	-	-	-	-	I	I	I	I	I
11 Sebacic acid	A	A	II Hy	Hy A	B Hy	I	II	-	-	-	-	-	-	-	-	I	-	-	-	-	-	-	I	Hy	I	I	Hy
12 Benzoic acid	I	A B	-	I	B	I	I B	-	-	-	-	B Hy	-	-	-	I Hy	B	-	Hy	Hy	C	B	B C	B	B	B	C
13 3-OH-benzoic acid	-	A B	D	C D	I D	I D	-	-	-	-	-	-	-	-	-	C I	-	-	Hy	Hy	-	-	D	B	D	D	D
14 4-OH-benzoic acid	-	A	-	B I	C I	-	-	-	I Hy C	-	Hy	-	-	C	-	-	-	-	Hy	Hy	I	-	C	C	C	C	C
15 3-(4-OH-phenyl)propionic acid	-	-	Hy	Hy	Hy	I	-	-	-	-	-	-	-	I	-	I	-	-	Hy	-	I	-	I	I	I	I	Hy
16 Hydrocaffeic acid	-	-	Hy	I	Hy	-	-	-	C Hy	C	-	-	-	-	-	I	-	-	Hy I	Hy	I	-	-	D	D	D	D
17 Phenylsuccinic acid	-	-	-	I B	I	I	-	-	II	B I	-	-	-	I	B	-	-	-	Hy	Hy	-	-	I	I	I	I	-
18 Isophthalic acid	A	-	A	A	A	A	B I	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	A	A	A	A	A
19 Terephthalic acid	I	-	I II Hy	I Hy	I	I	I	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	I	Hy	I	Hy	Hy
20 Trimesic acid	-	A	Hy	Hy B	Hy	B	I II	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	C	Hy B	C	Hy B	C

Table S 1 Crystallisation experiments and their results (A, B, C = co-crystal, I, II = anhydrous forms of PIR, Hy = hydrate of PIR)

IR spectra of the co-crystals

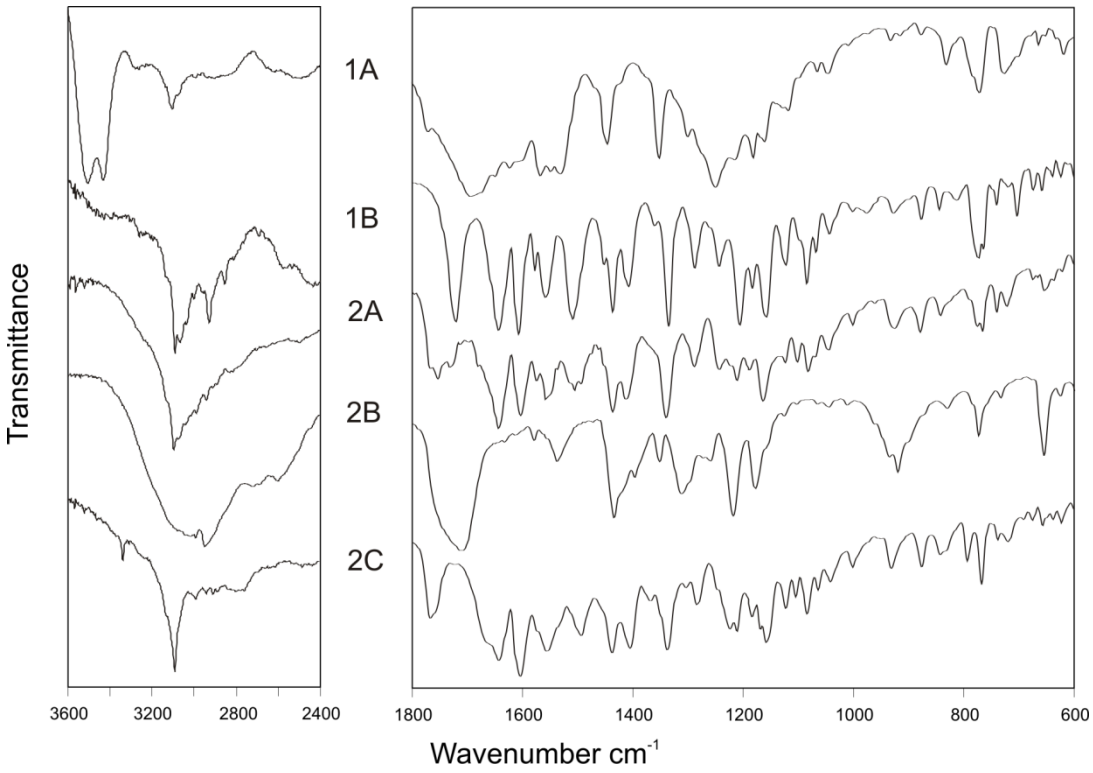

Fig. S 2 IR spectra of the co-crystals with oxalic acid and malonic acid as guest.

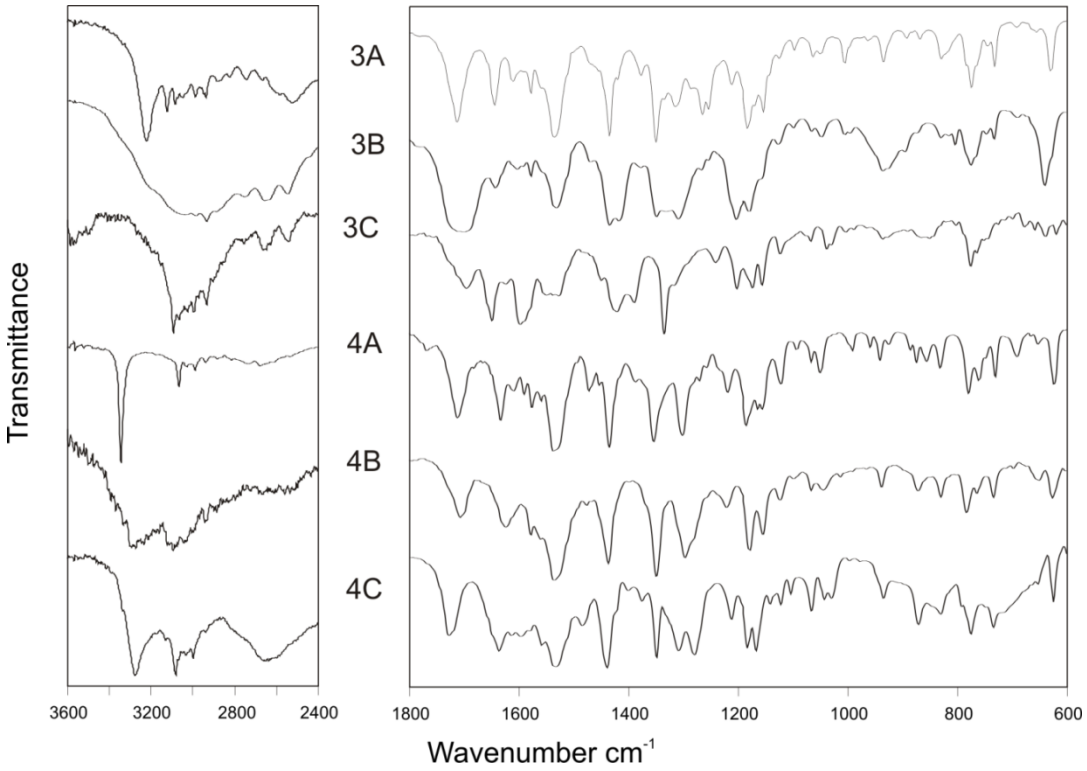

Fig. S 3 IR spectra of the co-crystals with succinic acid and maleic acid as guest.

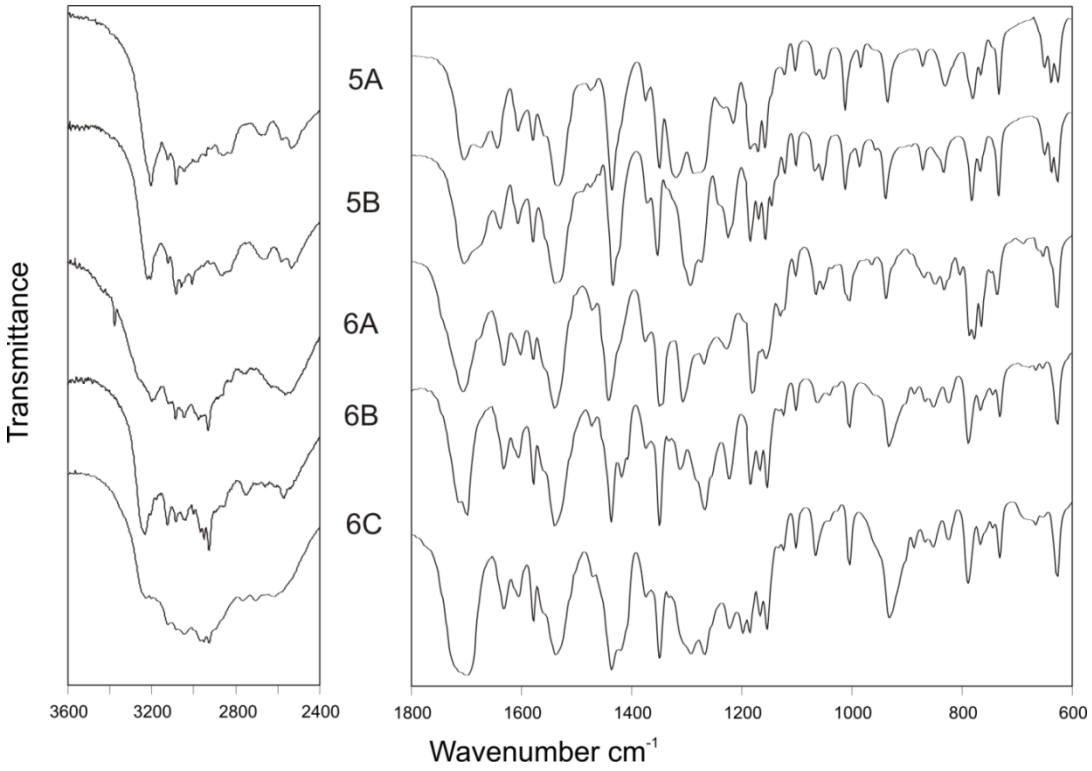

Fig. S 4 IR spectra of the co-crystals with fumaric acid and glutaric acid as guest.

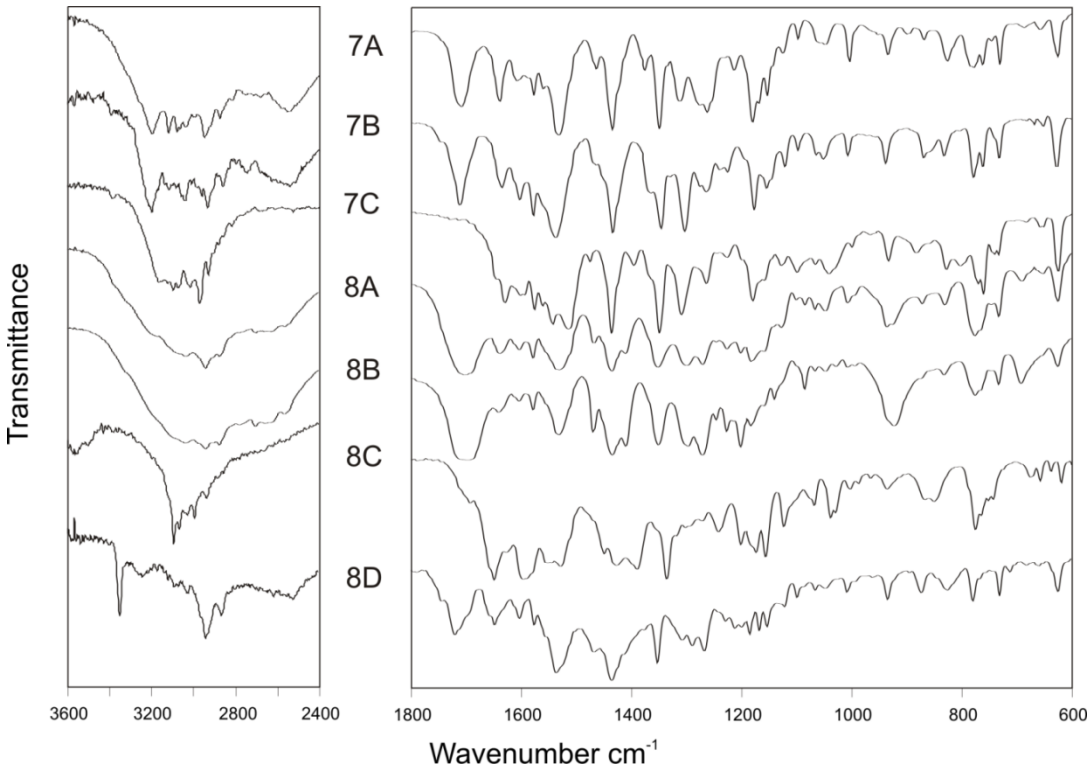

Fig. S 5 IR spectra of the co-crystals with adipic acid and pimelic acid as guest.

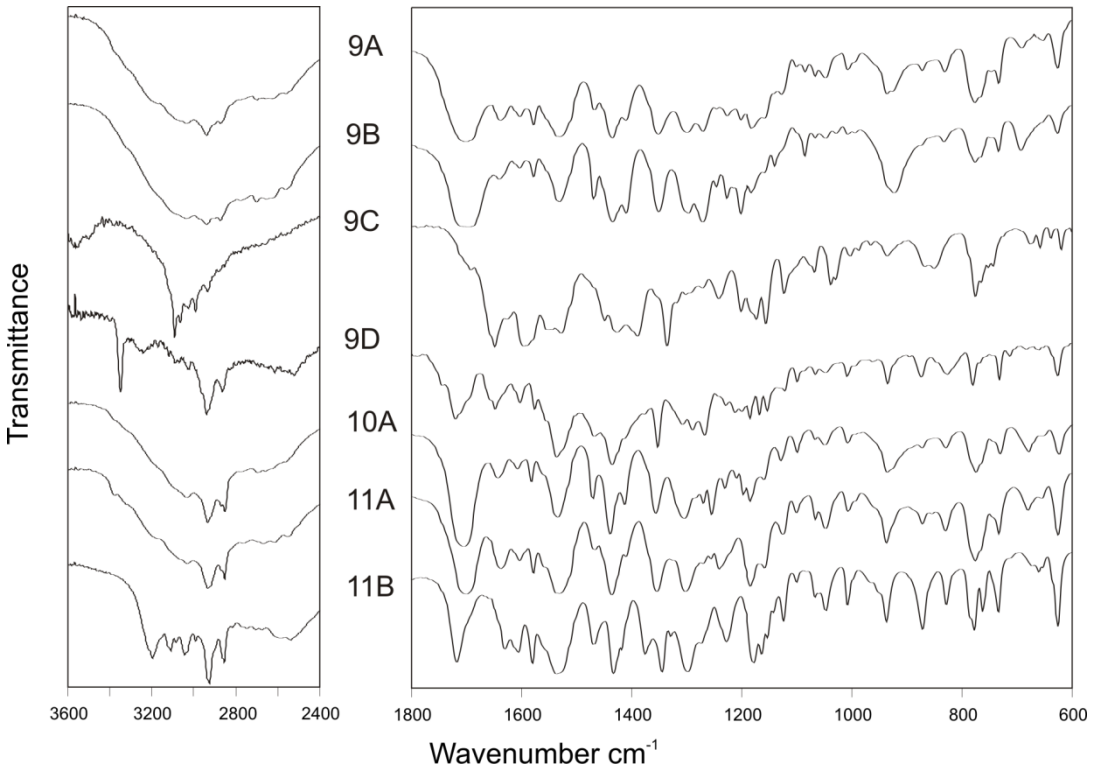

Fig. S 6 IR spectra of the co-crystals with suberic acid, azelaic acid and sebacic acid as guest.

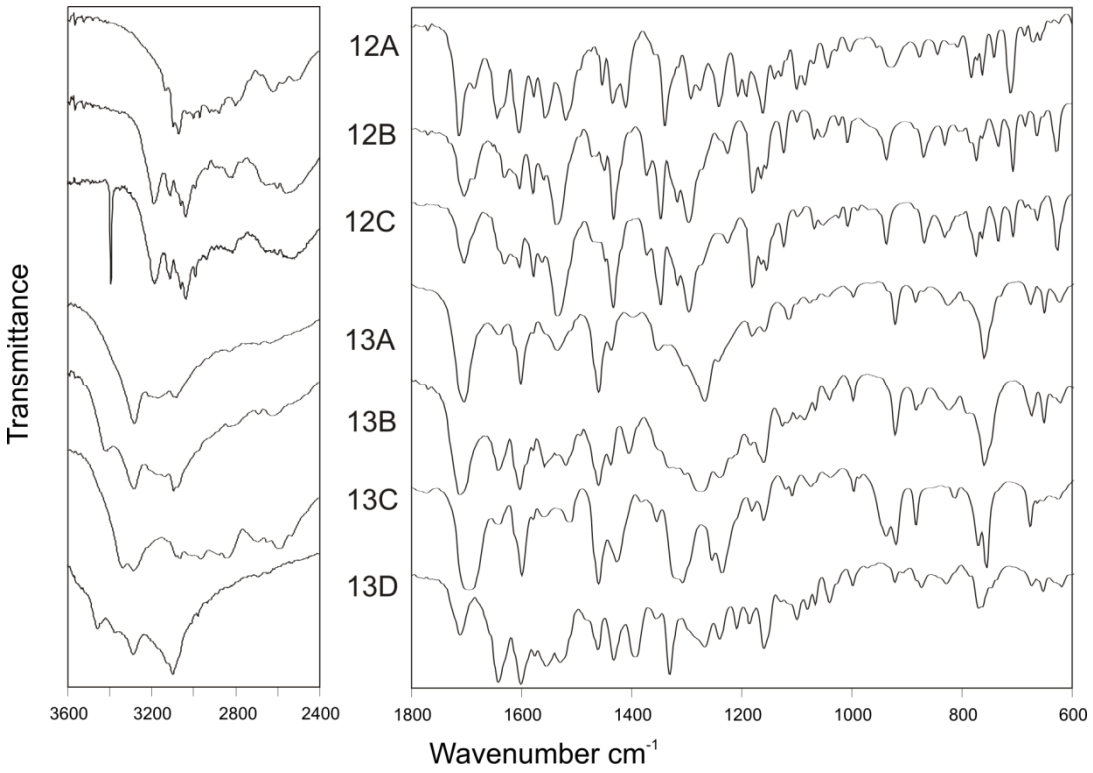

Fig. S 7 IR spectra of the co-crystals with benzoic acid and 3-OH-benzoic acid as guest.

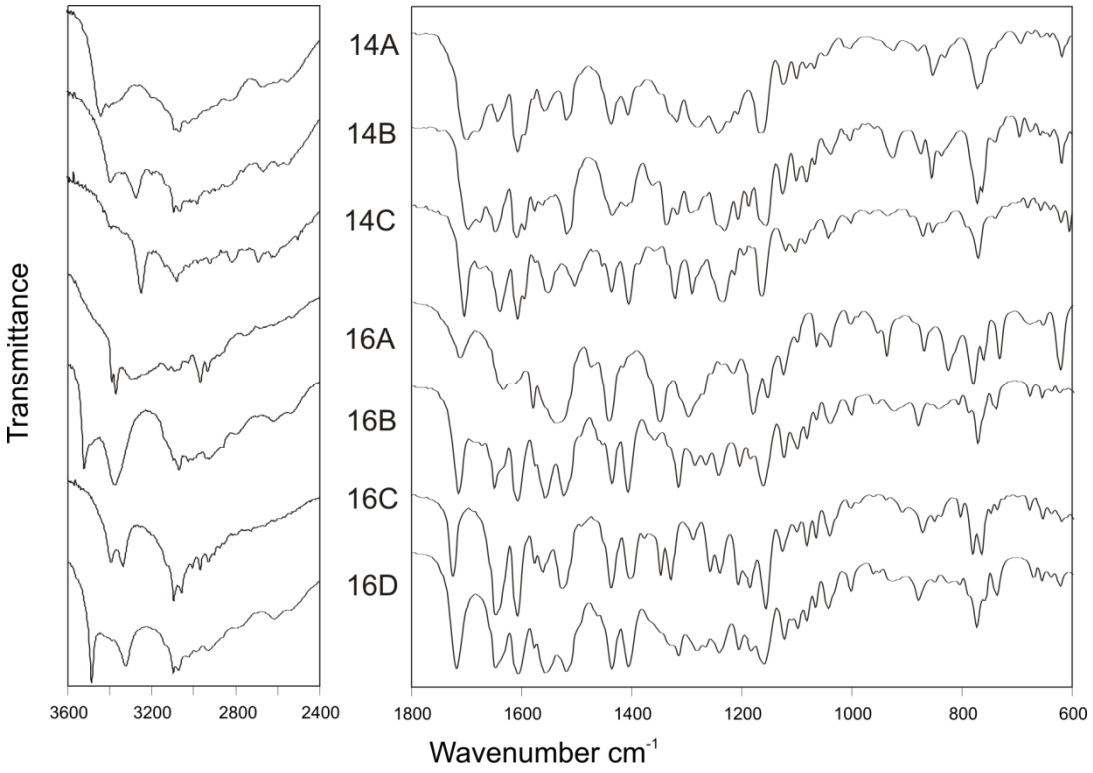

Fig. S 8 IR spectra of the co-crystals with 4-OH-benzoic acid and hydrocaffeic acid as guest.

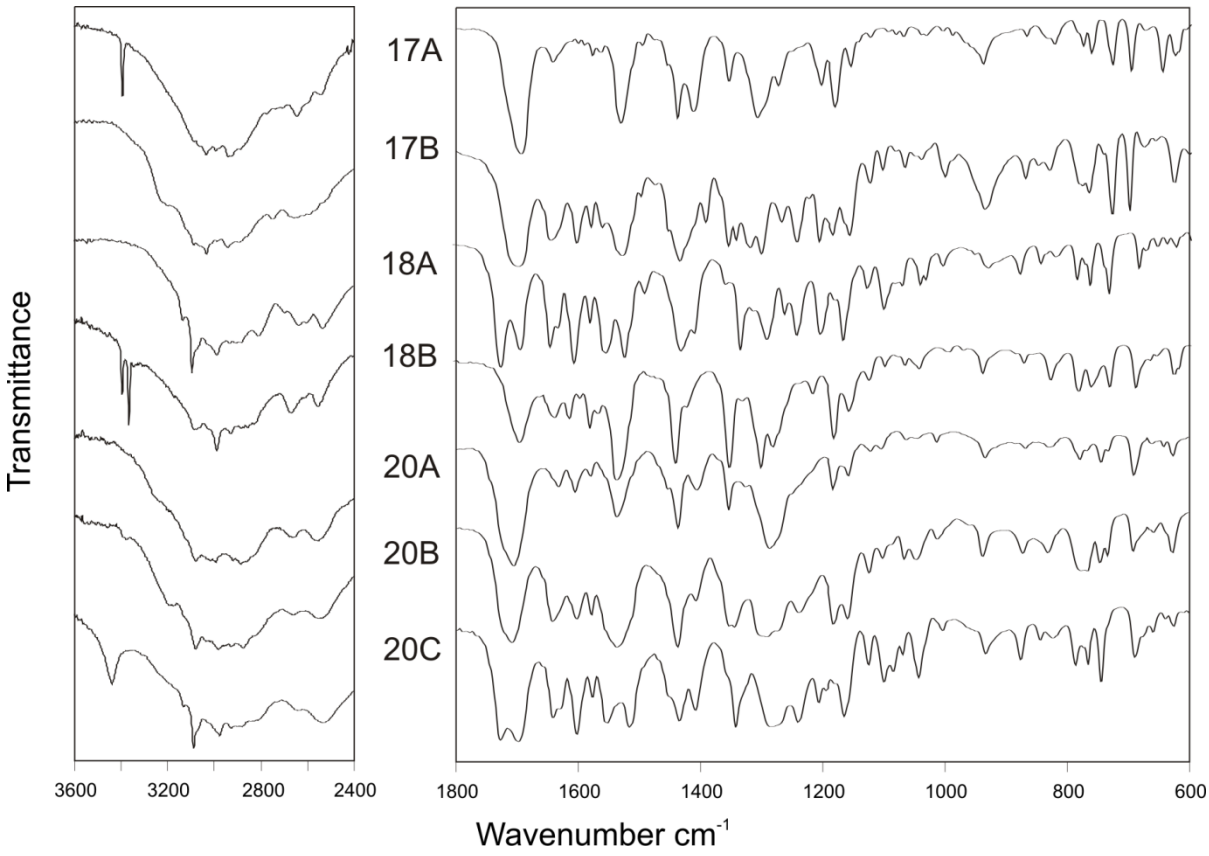

Fig. S 9 IR spectra of the co-crystals with phenylsuccinic acid, isophthalic acid and trimesic acid as guest.

Powder X-ray diffraction patterns of the co-crystal forms

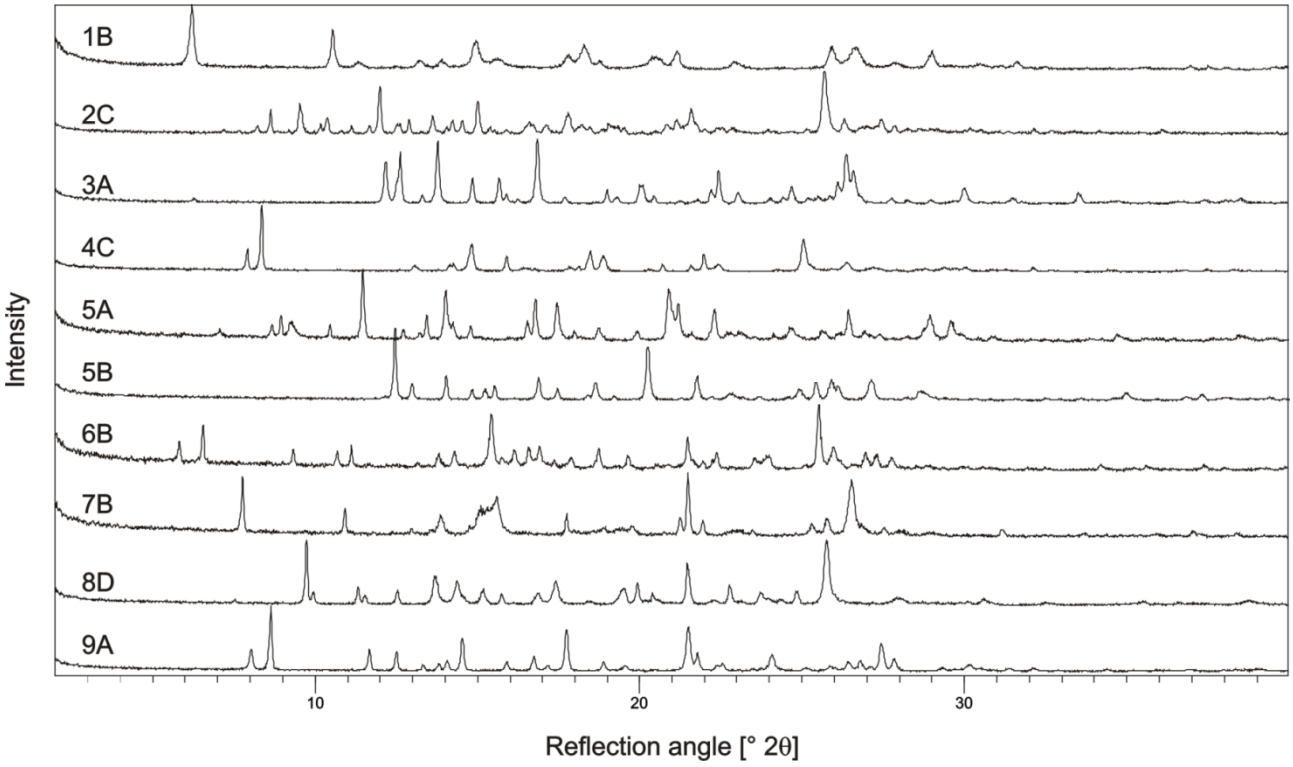

Fig. S 10 PXRD patterns of the co-crystals with oxalic acid, malonic acid, succinic acid, maleic acid, fumaric acid, glutaric acid, adipic acid, pimelic acid and suberic acid as guest.

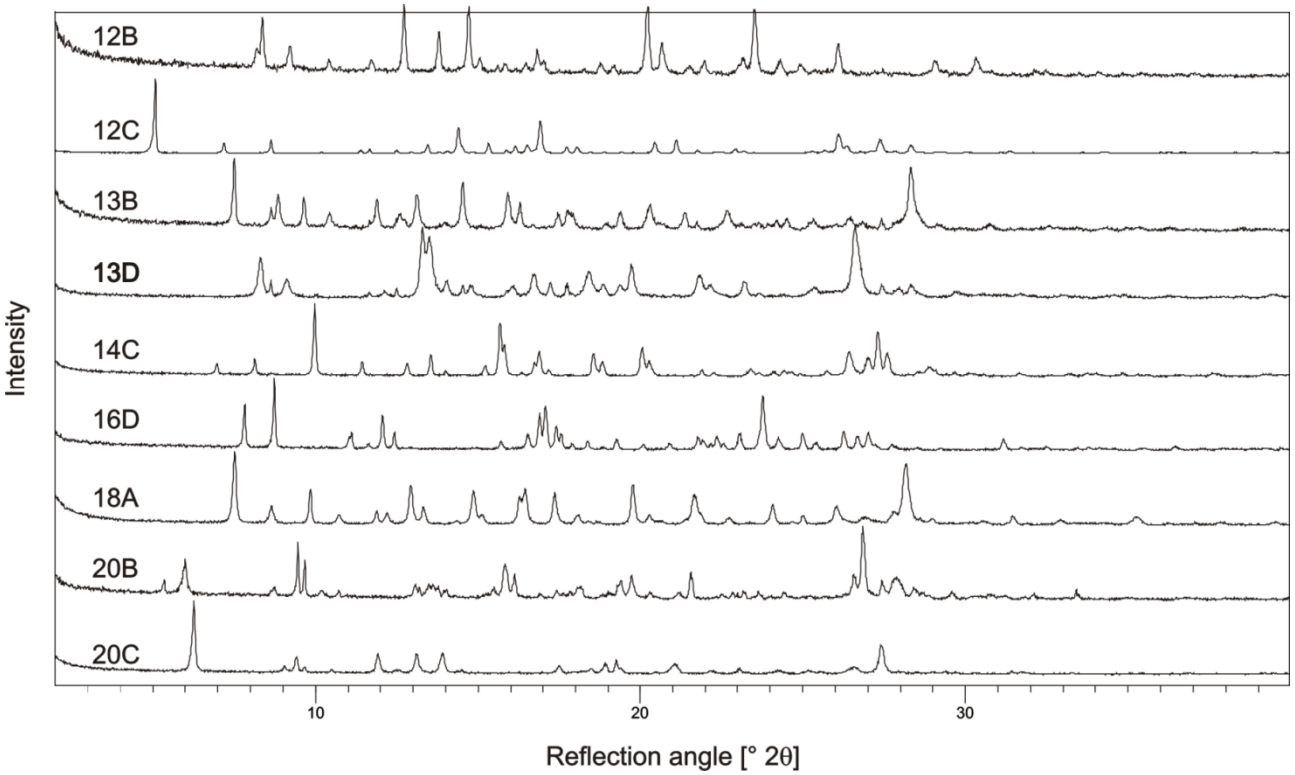

Fig. S 11 PXRD patterns of the co-crystals with benzoic acid, 3-OH-benzoic acid, 4-OH-benzoic acid, hydrocaffeic acid, isophthalic acid and trimesic acid as guest.