Electronic Supplementary Material (ESI) for CrystEngComm.

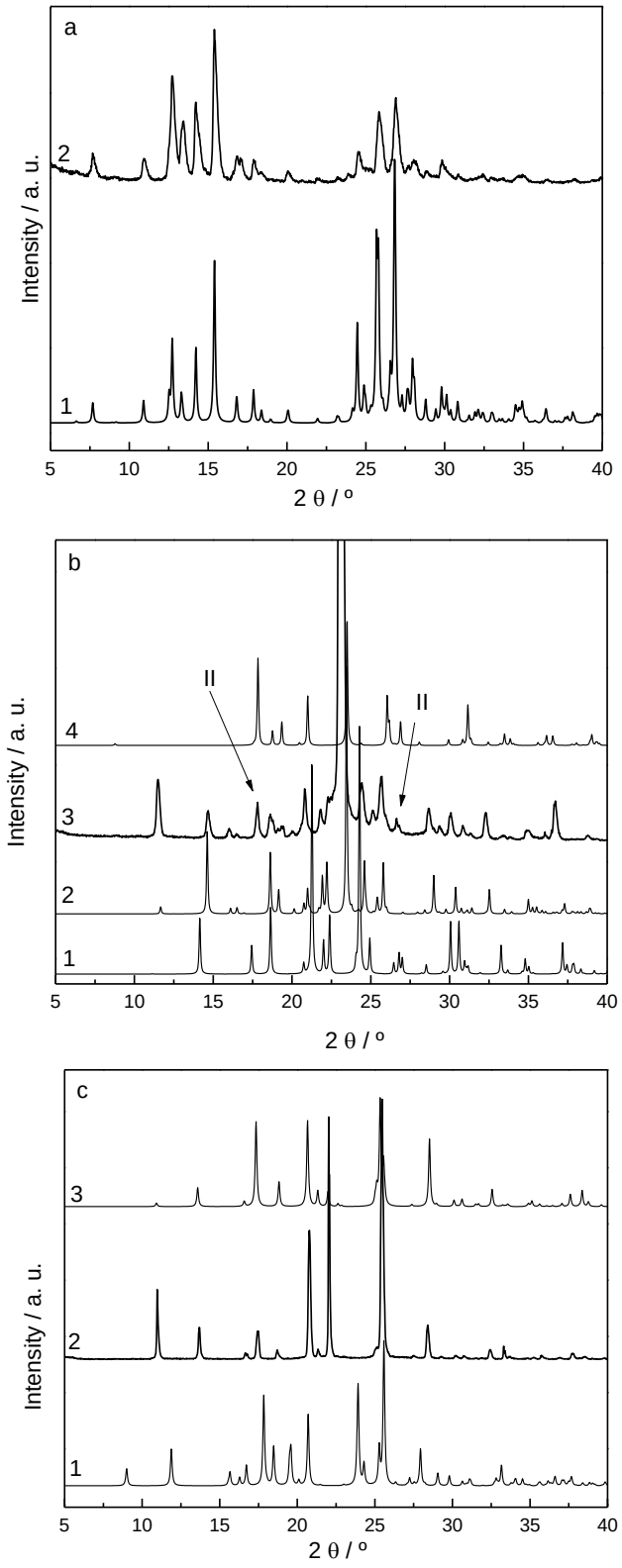

FIGURE S1. X-ray powder diffractograms **a.1.** Diflunisal, simulated for polymorph III [35]; **2.** Diflunisal crystallized from ethanol (Crystal16 experiments); **b.1.** Isonicotinamide, simulated for polymorph III [40]; **2.** Isonicotinamide, simulated for polymorph I [38]; **3.** Isonicotinamide, crystallized from ethanol (Crystal16 experiments); **4.** Isonicotinamide, simulated for polymorph II [38]; **c.1.** Picolinamide, simulated for polymorph I [36]; **2.** Picolinamide, crystallized from ethanol(Crystal16 experiments); **3.** Picolinamide, simulated for polymorph II [36, 37].

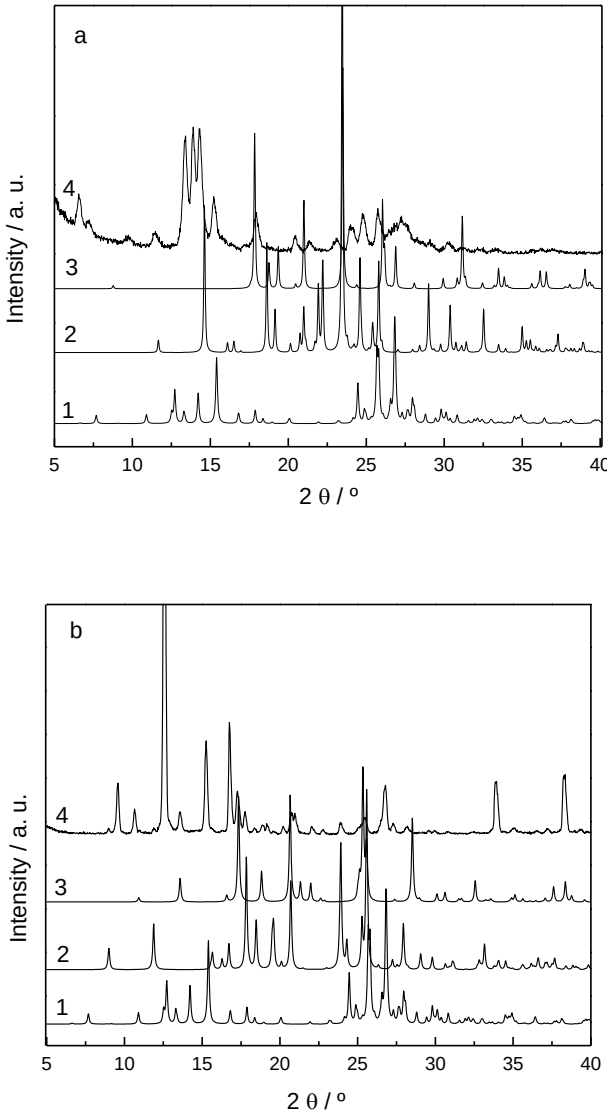

FIGURE S2. X-ray powder diffractograms **a.1.** Diflunisal, simulated for polymorph III [35]; **2.** Isonicotinamide, simulated for polymorph I [38]; **3.** Isonicotinamide, simulated for polymorph II [38]; **4.** Experimental obtained for diflunisal + isonicotinamide mixtures - crystallized from ethanol(Crystal16 experiments). **b.1.** Diflunisal, simulated for polymorph III [35]; **2.** Picolinamide, simulated for polymorph I [36]; **3.** Picolinamide, simulated for polymorph II [36, 37]; **4.** Experimental obtained for diflunisal + picolinamide mixtures - crystallized from ethanol(Crystal16 experiments).

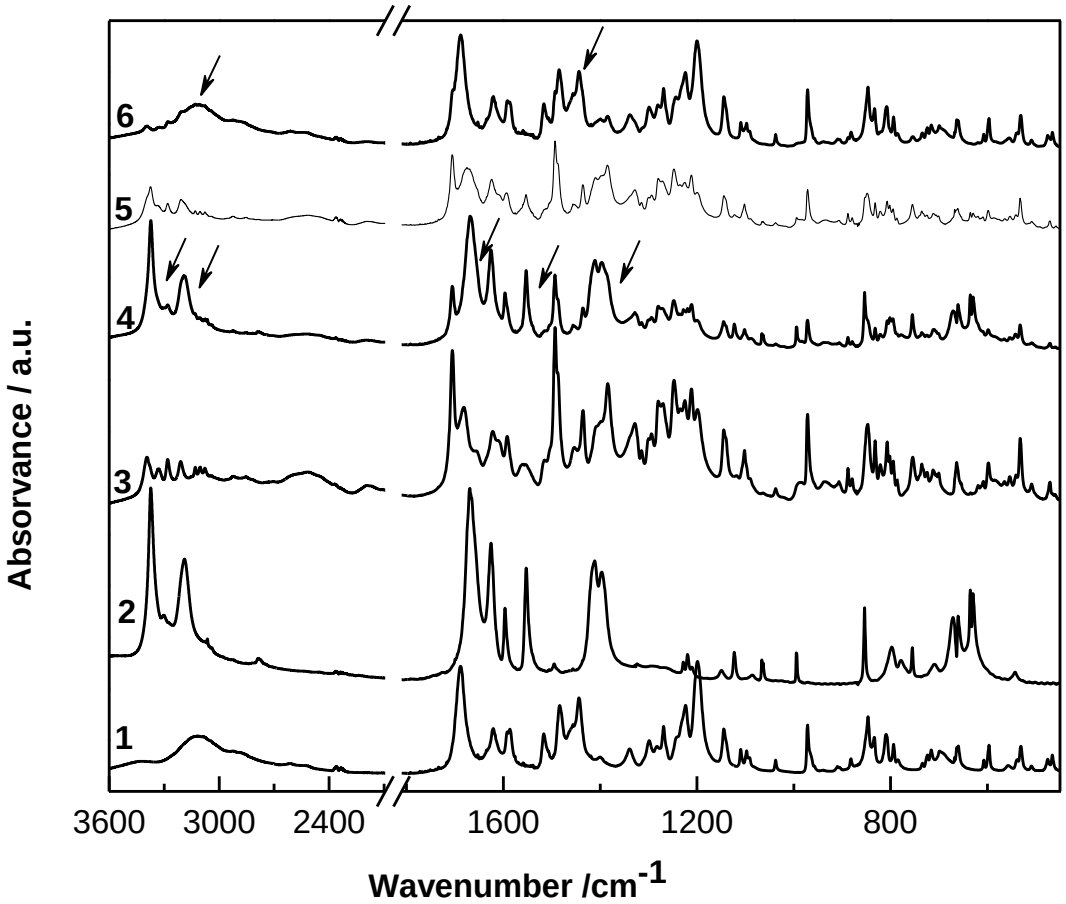

FIGURE S3. FTIR spectra, DIF +INA: **1.** DIF, polymorph I; **2.** INA, polymorph II; **3.** Co-crystal DIF + INA (2:1) x_{DIF} = 0.6667; **4.** x_{DIF} = 0.2501 (INA excess); **5.** x_{DIF} = 0.4999 (INA excess)**; 6.** x_{DIF} = 0.8954 (DIF excess).

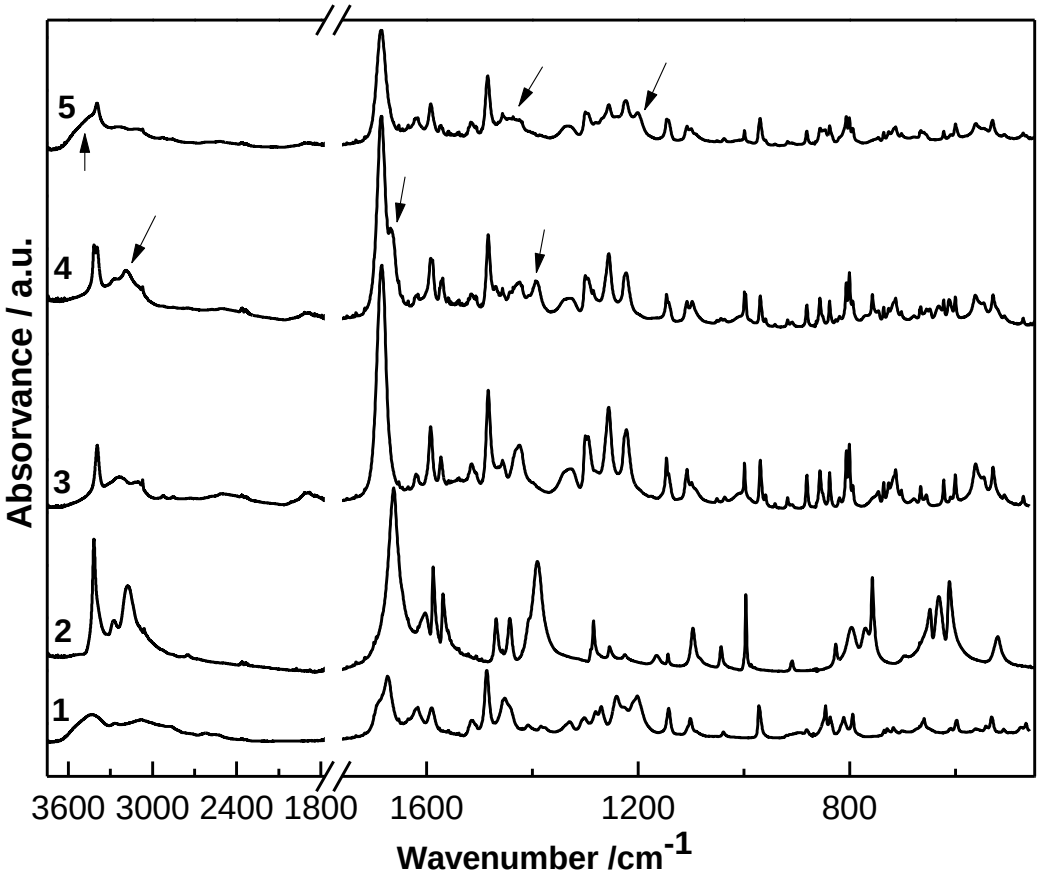

FIGURE S4. FTIR spectra, DIF + PA: **1.** DIF, polymorph III; **2.** PA, polymorph II; **3.** Co-crystal DIF + PA (1:1) x_{DIF} = 0.5000; **4.** x_{DIF} = 0.3334 (PA II excess); **5.** x_{DIF} = 0.6654 EAG (DIF III excess).

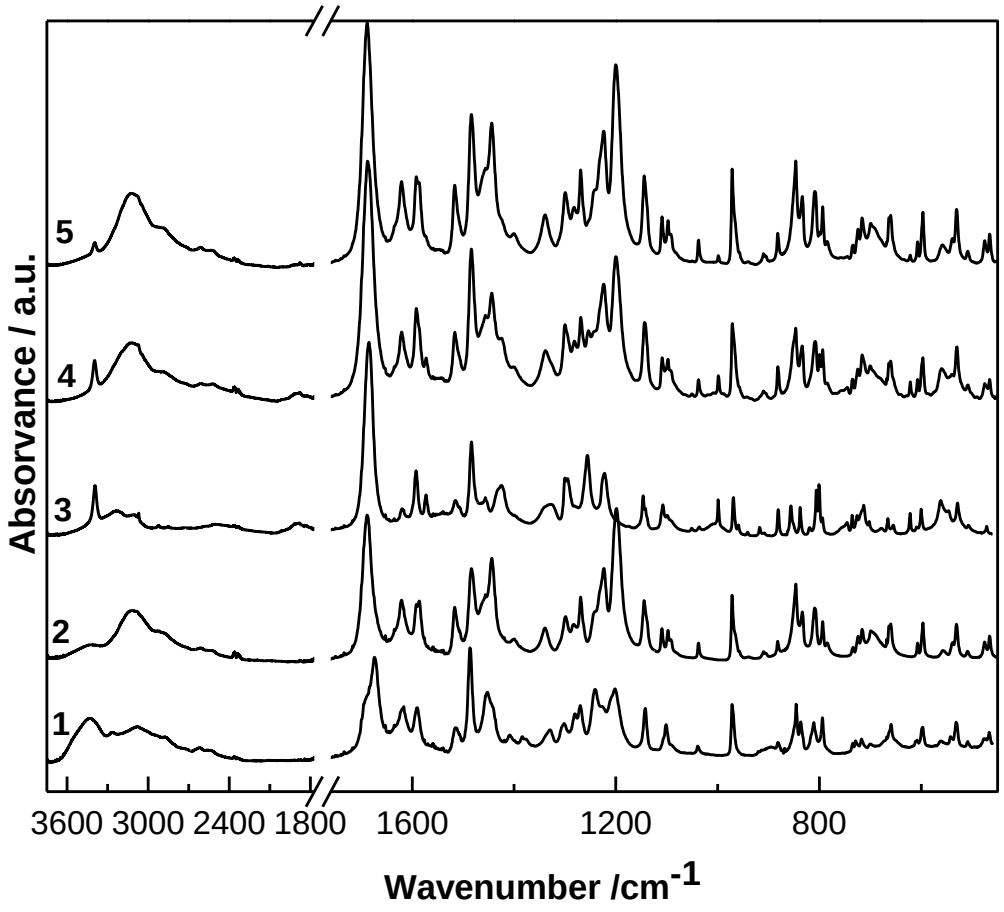

FIGURE S5. FTIR spectra, DIF + PA: **1.** DIF, III; **2.** DIF, I; **3.** Co-crystal DIF + PA (1:1) x_{DIF} = 0.5000; **4.** x_{DIF} = 0.7492 neat grinding (DIF I excess); **5.** x_{DIF} = 0.8990 neat grinding (DIF I excess).

TABLE S1. Transition temperatures T_{E1}, T_{E2}, T_{E3} and T_{liq} obtained for the various phase transitions observed in DSC heating runs of mixtures of (diflunisal +isonicotinamide) of different diflunisal mole fraction, x_{DIF}.

x_{DIF}	T_{E1} / K	T_{E2} / K	T_{E3} / K	T_{liq} / K	x_{DIF}	T_{E1} / K	T_{E2} / K	T_{E3} / K	T_{liq} / K
β = 2 K /min					β = 10 K /min				
0.0000				428.9	0.0000				428.9
0.0502	409.3	411.8		425.1	0.0502		412.2		425.2
0.1008	408.8	412.2		421.5	0.3001	405.3			425.6
0.1667	408.5	412.0		415.2	0.3323	404.2			426.2
0.1999	408.8	411.8			0.4002	405.1			434.4
0.2501	409.3	413.6		416.7	0.4169	405.1			437.2
0.3323	407.0	412.5		428.0	0.4999	403.1			444.2
0.4004	407.5	412.4		435.2	0.6667				452.1
0.4169	406.9	411.9		436.3	0.7142			450.8	454.6
0.4999	404.2			445.2	0.8572			447.2	469.9
0.5556	404.9			447.7	0.8988			451.5	476.0
0.6003	403.8			449.5	1.0000				486.0
0.6254	403.8			449.5					
0.6667				452.6					
0.6916			449.9						
0.7141			450.1						
0.7484			450.8	457.5					
0.7996			451.0	466.0					
0.8572			451.0	469.2					
0.8988			451.1	475.1					
1.000				486.0					

TABLE S2. Transition temperatures T_{E1}, T_{E2}, T_{E3} and T_{liq} obtained for the various phase transitions observed in DSC heating runs of mixtures of (diflunisal + picolinamide) of different diflunisal mole fraction, x_{DIF}.

x_{DIF}	T_{E1} / K	T_{E2} / K	T_{E3} / K	T_{liq} / K	x_{DIF}	T_{E1} / K	T_{E2} / K	T_{E3} / K	T_{liq} /K
β = 2 K /min					β = 10 K /min				
0.0000				375.2	0.0000				375.2
0.0000				379.5	0.000				379.5
0.0259	373.3			393.5	0.0259		378.7		392.3
0.0501	373.7			398.6	0.0501	372.2	377.2		404.2
0.1080	373.7	378.0		421.5	0.1080	373.2	377.4		418.2
0.1636	374.0	377.2		434.0	0.1636	367.2	371.3		433.2
0.2001	372.9	377.7		438.6	0.2509	368.3	376.3		445.4
0.2509	373.6	377.9		445.6	0.3334	373.7	378.6		453.5
0.3334	373.6	377.9		452.6	0.3996	373.2	378.2		457.2
0.3996		377.2		456.2	0.4502	363.9	372.0		459.6
0.5000				459.8	0.5000				460.2
0.5569[(a)]			453.2	458.2	0.5991			451.2	458.1
0.5991			453.2	457.2	0.6497			453.4	
0.6061[(a)]			452.9	457.0	0.6654			455.1	
0.6557[(a)]			452.9		0.7492[(a)]			453.2	466.2
0.6654			454.0		0.9357			453.4	478.4
0.7482			454.0	463.5	0.9499			451.4	484.2
0.7492[(a)]			454.2	463.0	1.000				485.9
0.8547			453.4	472.1					
0.8954			451.4	476.6					
0.8990[(a)]			454.0	478.2					
0.9357			448.8	480.4					
1.0000				485.0					

(a) These mixtures were obtained by neat grinding.