Pharmaceutical Co-crystals with Isonicotinamide: Vitamin B3, Clofibric Acid and Diclofenac; and Two Isonicotinamide Hydrates.

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Table S1. Hydrogen bonds for 5 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(8W)	0.89(6)	2.12(6)	2.999(7)	167(5)
N(1)-H(1S)...O(2)	0.96(6)	1.92(6)	2.877(6)	173(4)
N(3)-H(3S)...O(1)	0.90(6)	2.05(6)	2.924(6)	166(5)
N(3)-H(3A)...O(1W)#1	1.04(4)	2.03(4)	3.062(6)	168(4)
N(5)-H(5A)...O(3W)	1.00(6)	2.04(6)	3.008(7)	162(4)
N(5)-H(5S)...O(4)	0.79(6)	2.08(6)	2.866(6)	173(6)
N(7)-H(7A)...O(7W)#2	0.81(5)	2.23(5)	3.005(6)	161(5)
N(7)-H(7S)...O(3)	0.94(5)	2.00(6)	2.927(7)	171(4)
N(9)-H(9A)...O(2W)#3	1.01(4)	2.03(5)	2.998(6)	160(4)
N(9)-H(9S)...O(6)	0.94(5)	2.01(5)	2.901(6)	158(4)
N(11)-H(11A)...O(6W)	0.87(5)	2.26(6)	3.121(7)	170(5)
N(11)-H(11S)...O(5)	0.95(5)	1.93(6)	2.868(7)	173(5)
N(13)-H(13A)...O(4W)	0.92(6)	2.22(6)	3.103(7)	159(5)
N(13)-H(13S)...O(8)	0.80(6)	2.08(6)	2.876(6)	173(6)
N(15)-H(15A)...O(5W)#2	0.80(5)	2.27(4)	3.046(6)	164(4)
N(15)-H(15S)...O(7)	0.92(5)	2.02(5)	2.924(6)	168(4)
O(1W)-H(1W)...N(14)	0.85	2.04	2.787(6)	146.9
O(1W)-H(2W)...O(2W)#4	0.85	1.92	2.760(5)	167.2
O(2W)-H(3W)...N(6)	0.85	2.01	2.799(6)	154.0
O(2W)-H(4W)...O(8W)#5	0.85	1.94	2.765(4)	162.1
O(3W)-H(5W)...N(10)	0.85	2.08	2.850(6)	150.8
O(3W)-H(6W)...O(4W)#6	0.85	1.99	2.809(5)	161.3

O(4W)-H(7W)...N(4)	0.85	2.07	2.799(6)	144.1
O(4W)-H(8W)...O(5W)#7	0.85	1.96	2.785(4)	162.2
O(5W)-H(9W)...N(12)	0.85	2.03	2.829(6)	156.7
O(5W)-H(10W)...O(7W)#6	0.85	1.96	2.779(5)	160.4
O(6W)-H(11W)...N(8)	0.85	2.04	2.810(6)	149.8
O(6W)-H(12W)...O(1W)#8	0.85	1.96	2.792(3)	165.2
O(7W)-H(13W)...N(2)	0.85	2.00	2.845(6)	169.6
O(7W)-H(14W)...O(3W)#9	0.85	1.96	2.755(4)	154.5
O(8W)-H(15W)...N(16)	0.85	1.99	2.832(6)	169.8
O(8W)-H(16W)...O(6W)#4	0.85	1.96	2.790(5)	163.9

Symmetry transformations used to generate equivalent atoms:

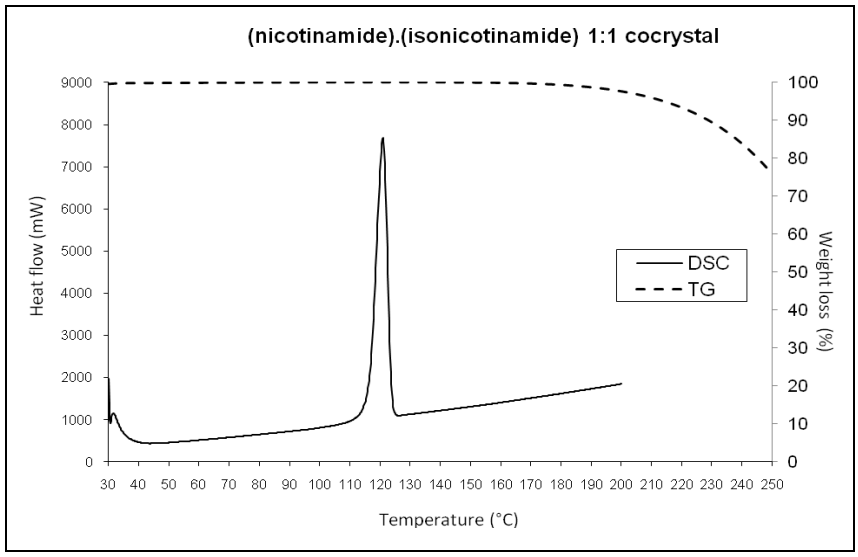
#1 x+1,-y+2,z+1/2 #2 x-1,-y+2,z-1/2 #3 x+1,-y+1,z+1/2

#4 x,y+1,z #5 x-1,y-1,z-1 #6 x,y-1,z #7 x-1,y,z-1

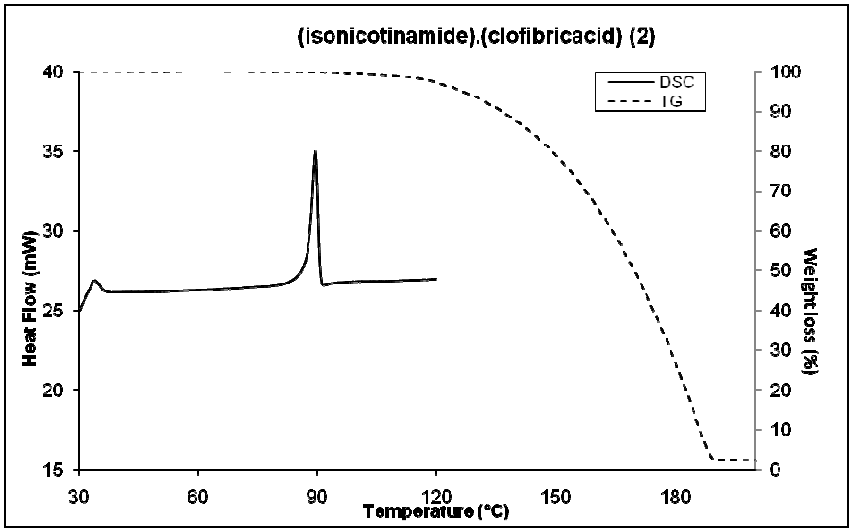
#8 x+1,y,z+1 #9 x+1,y+1,z+1

Figure S1. DSC and TG data for co-crystals **1** (a), **2** (b) and **3** (c). The diagrams show no presence of impurities or residual solvents.

(a)



(b)



(c)

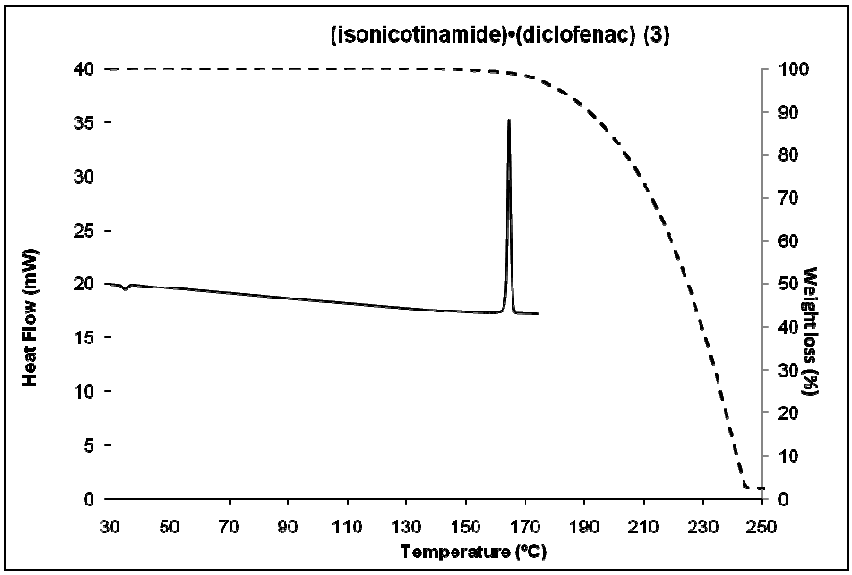
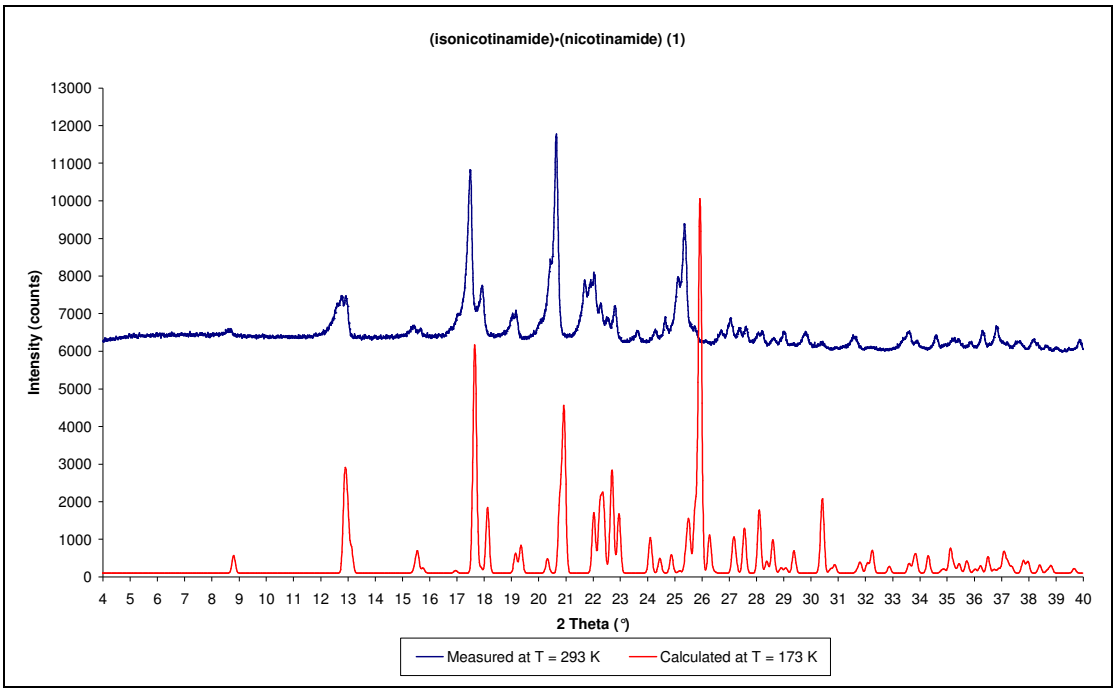
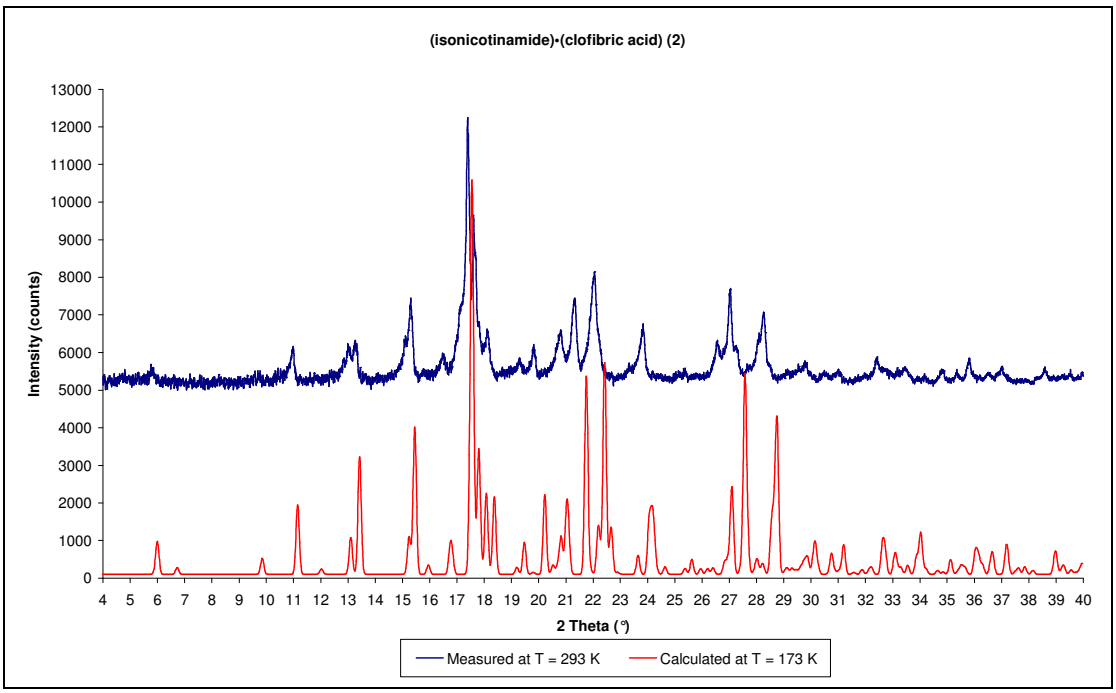


Figure S2. Comparative PXRDs of compounds **1-4**. In all cases, the calculated pattern of the single crystal structure shows good agreement with the measured pattern. Hence the single crystal structure is representative to the bulk material.

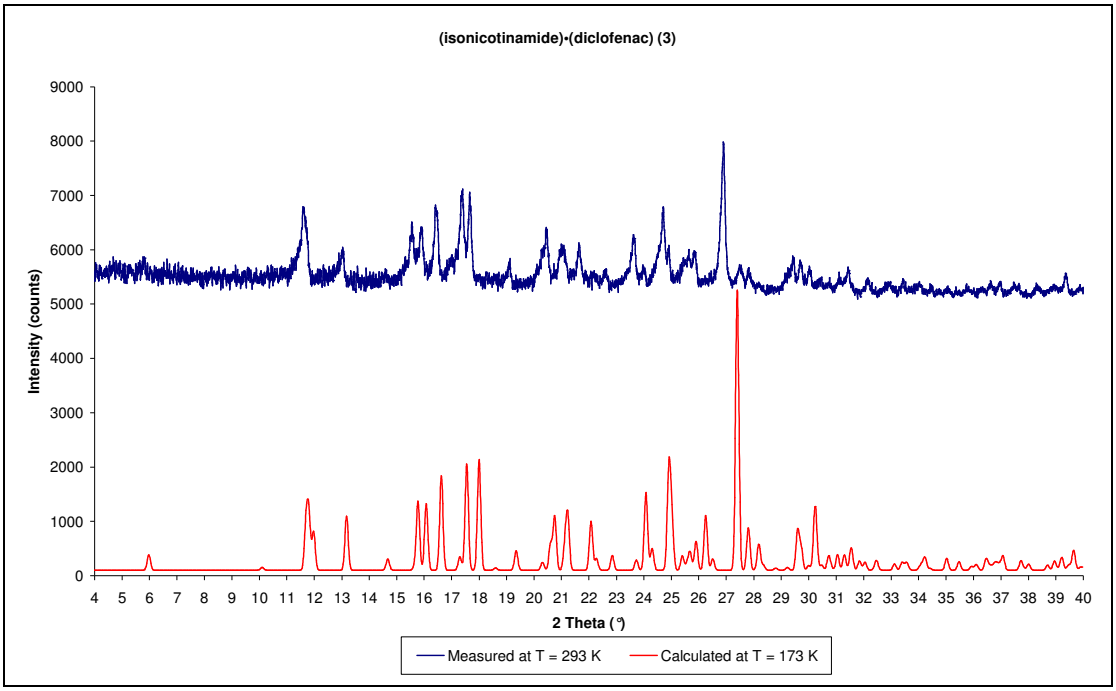
(a)



(b)



(c)


(isonicotinamide)·(diclofenac) (3)
Intensity (counts)
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40
2 Theta (°)
Measured at T = 293 K
Calculated at T = 173 K

(d)

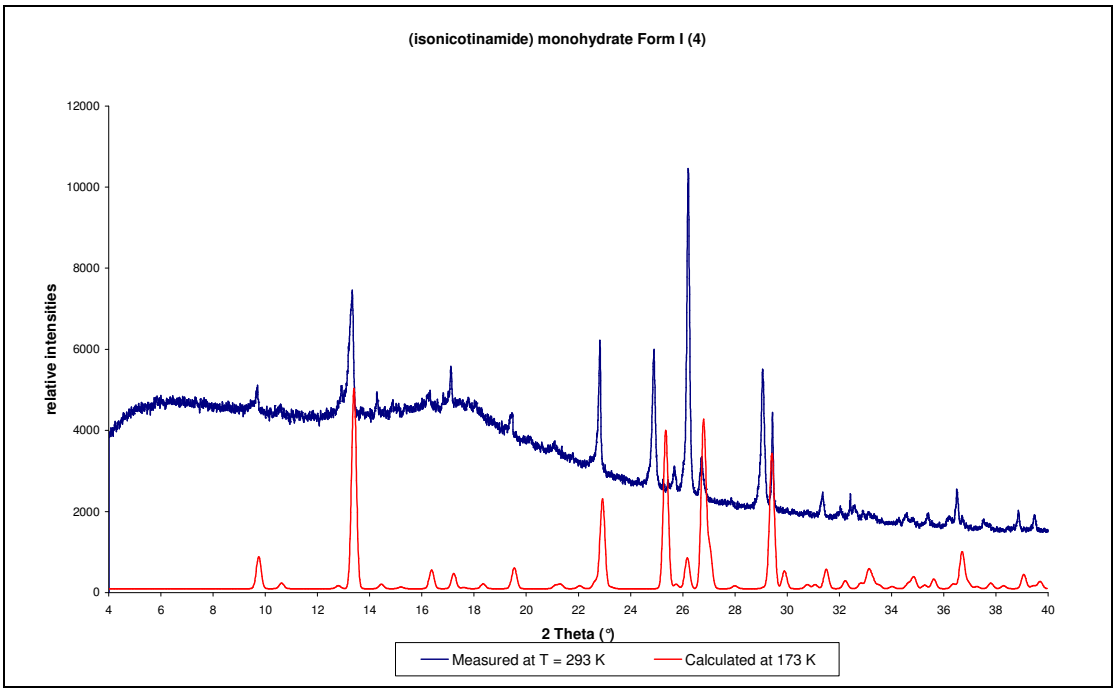
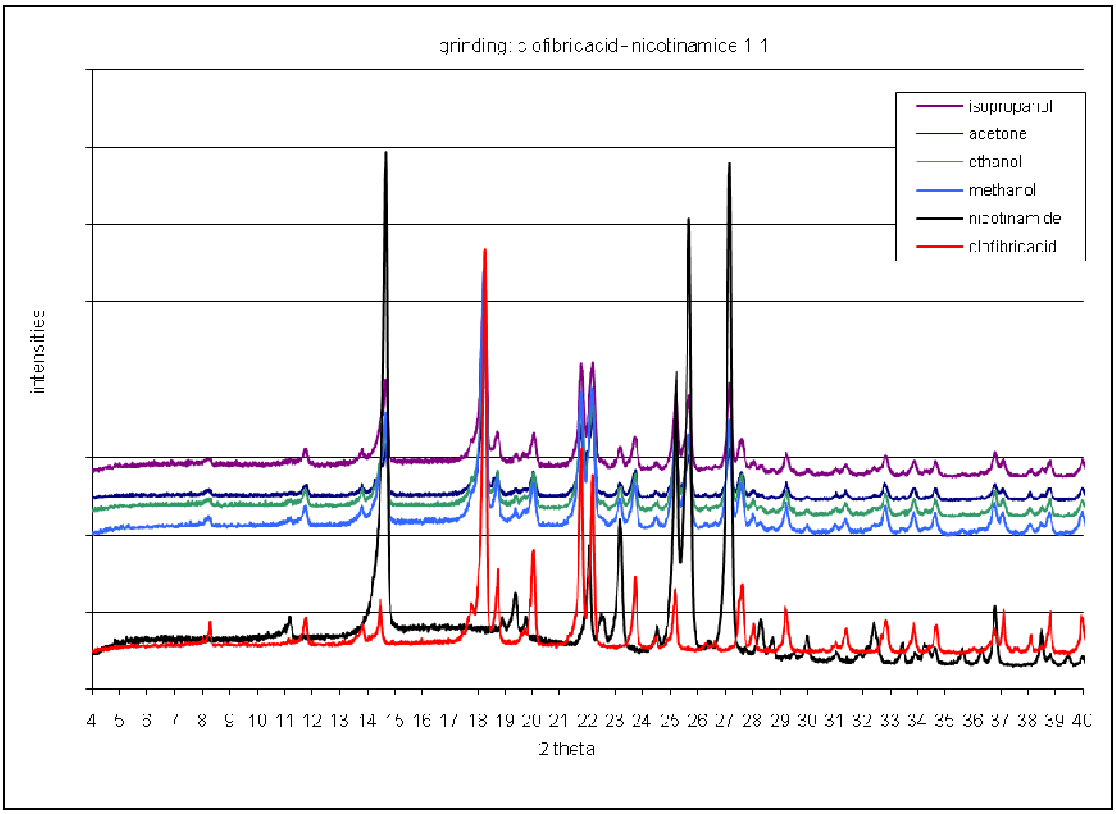

(isonicotinamide) monohydrate Form I (4)
relative intensities
12000
10000
8000
6000
4000
2000
0
4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36 38 40
2 Theta (°)
Measured at T = 293 K
Calculated at 173 K

Figure S3. PXRDs of failed co-grinding experiments between nicotinamide and clofibric acid (a) and diclofenac (b). In both cases, such attempts were unsuccessful, the PXRD traces agree well with the physical mixtures of the starting materials.

(a)



(b)