Supplementary Data

This supplementary data is a part of paper entitled "Synthesis, Characterization and Morphological Study of Nicotinamide and *p*-Coumaric Acid Cocrystal".

In this supplementary material, the following experimental detail and data is provided comprising;

S1 Vibration bands observed in the NIC:COU cocrystals
S2 Bond lengths (Å) of NIC:COU (1:1) cocrystal
S3 Bond angles (°) of NIC:COU (1:1) cocrystal
S4 Torsion angles (°) of NIC:COU (1:1) cocrystal

Table S1 shows the differences in the interaction between NIC and COU molecules in the crystal lattice, based on the vibration band shifts from the parent compounds.

Table S1. Vibration bands observed in the NIC:COU cocrystals

	NIC:COU (1:1), cm^{-1}	NIC:COU (1:2), cm^{-1}	NIC:COU (2:1), cm^{-1}
C=O amide stretching	1667	1667	1667
Asymmetric $-NH_2$ stretching	3355	-	3356
Symmetric $-NH_2$ stretching	3181	3178	3177
-NH bending	1607	1627	-
N-pyridine stretching	1404	1404	1394
-OH carboxylic acid stretching	3425	3426	3426
-OH phenol stretching	1336	-	1340
O--H··N hydrogen bond	1900	1895	-

Table S2, S3, and S4 show the bond lengths, bond angles, and torsion angles of the NIC:COU (1:1) cocrystal, which are in expected values.

Table S2. Bond lengths (Å) of NIC:COU (1:1) cocrystal

O1-C9	1.331(3)	O4-C15	1.245(3)
O2-C9	1.215(3)	N1-C10	1.337(4)
O3-C3	1.353(3)	N1-C12	1.337(4)
C1-C2	1.373(3)	N2-C15	1.315(3)
C1-C6	1.396(4)	C10-C14	1.378(4)
C2-C3	1.384(4)	C11-C12	1.367(4)
C3-C4	1.397(4)	C11-C13	1.381(4)
C4-C5	1.382(4)	C13-C14	1.386(4)
C5-C6	1.397(4)	C14 > C15	1.486(3)
C6 > C7	1.463(3)	N2-H2A	0.86
C7-C8	1.331(4)	N2-H2B	0.86
C8 > C9	1.460(4)	C10-H10A	0.93
O1-H1	0.82(3)	C11-H11A	0.93
O3-H3A	0.82	C12-H12A	0.93
C1-H1A	0.93	C13-H13A	0.93
C2-H2C	0.93		
C4-H4A	0.93		
C5-H5A	0.93		
C7-H7A	0.93		
C8-H8A	0.93		

Table S3. Bond angles (°) of NIC:COU (1:1) cocrystal

C2-C1-C6	121.0(2)	C10-N1-C12	116.9(2)
C1-C2-C3	121.0(2)	N1-C10-C14	123.5(2)
O3-C3-C2	120.2(2)	C12-C11-C13	118.3(2)
O3-C3-C4	122.8(2)	N1-C12-C11	124.1(3)
C2-C3-C4	118.7(2)	C11-C13-C14	119.1(3)
C3-C4-C5	120.2(2)	C10-C14-C13	118.2(2)
C4-C5-C6	121.1(2)	C10-C14-C15	118.4(2)
C1-C6-C5	117.9(2)	C13-C14-C15	123.4(2)
C1-C6-C7	121.9(2)	O4-C15-N2	122.1(2)
C5-C6-C7	120.2(2)	O4-C15-C14	118.9(2)
C6-C7-C8	126.3(2)	N2-C15-C14	119.0(2)
C7-C8-C9	122.1(2)	C15-N2-H2A	120
O1-C9-O2	122.9(2)	C15-N2-H2B	120
O1-C9-C8	111.9(2)	H2A-N2-H2B	120
O2-C9-C8	125.2(2)	N1-C10-H10A	118
C9-O1-H1	104(2)	C14-C10-H10A	118
C3-O3-H3A	110	C12-C11-H11A	121
C2-C1-H1A	120	C13-C11-H11A	121
C6-C1-H1A	120	N1-C12-H12A	118
C1-C2-H2C	120	C11-C12-H12A	118
C3-C2-H2C	119	C11-C13-H13A	120
C3-C4-H4A	120	C14-C13-H13A	120
C5-C4-H4A	120		
C4-C5-H5A	119		
C6-C5-H5A	119		
C6-C7-H7A	117		
C8-C7-H7A	117		
C7-C8-H8A	119		
C9-C8-H8A	119		

Table S4. Torsion angles (°) of NIC:COU (1:1) cocrystal

C6-C1-C2-C3	-2.4(4)	C12-N1-C10-C14	1.6(4)
C2-C1-C6-C5	1.1(4)	C10-N1-C12-C11	-2.0(4)
C2-C1-C6-C7	-177.6(2)	N1-C10-C14-C13	-0.5(4)
C1-C2-C3-O3	-180.0(2)	N1-C10-C14-C15	-179.3(2)
C1-C2-C3-C4	1.7(4)	C13-C11-C12-N1	1.3(4)
O3-C3-C4-C5	-178.0(2)	C12-C11-C13-C14	0.0(4)
C2-C3-C4-C5	0.2(4)	C11-C13-C14-C10	-0.3(4)
C3-C4-C5-C6	-1.5(4)	C11-C13-C14-C15	178.4(2)
C4-C5-C6-C1	0.9(4)	C10-C14-C15-O4	20.0(3)
C4-C5-C6-C7	179.6(2)	C10-C14-C15-N2	-159.8(2)
C1-C6-C7-C8	-11.7(4)	C13-C14-C15-O4	-158.8(2)
C5-C6-C7-C8	169.7(2)	C13-C14-C15-N2	21.4(4)
C6-C7-C8-C9	179.5(2)	C12-N1-C10-H10A	-178
C7-C8-C9-O1	171.8(2)	C10-N1-C12-H12A	178
C7-C8-C9-O2	-6.8(4)	H2A-N2-C15-O4	0
H1-O1-C9-O2	-7(2)	H2A-N2-C15-C14	180
H1-O1-C9-C8	174(2)	H2B-N2-C15-O4	-180
H3A-O3-C3-C2	2	H2B-N2-C15-C14	0
H3A-O3-C3-C4	180	H10A-C10-C14-C13	179
C6-C1-C2-H2C	178	H10A-C10-C14-C15	1
H1A-C1-C2-C3	178	C13-C11-C12-H12A	-179
H1A-C1-C2-H2C	-2	H11A-C11-C12-N1	-179
H1A-C1-C6-C5	-179	H11A-C11-C12-H12A	1
H1A-C1-C6-C7	2	C12-C11-C13-H13A	180
H2C-C2-C3-O3	0	H11A-C11-C13-C14	180
H2C-C2-C3-C4	-178	H11A-C11-C13-H13A	0
O3-C3-C4-H4A	2	H13A-C13-C14-C10	180
C2-C3-C4-H4A	-180	H13A-C13-C14-C15	-2
C3-C4-C5-H5A	179		
H4A-C4-C5-C6	178		
H4A-C4-C5-H5A	-1		
H5A-C5-C6-C1	-179		
H5A-C5-C6-C7	0		
C1-C6-C7-H7A	168		
C5-C6-C7-H7A	-10		
C6-C7-C8-H8A	-1		
H7A-C7-C8-C9	-1		
H7A-C7-C8-H8A	179		
H8A-C8-C9-O1	-8		
H8A-C8-C9-O2	173		