Electronic Supplementary Material (ESI) for CrystEngComm

Synthon identification in co-crystals and polymorphs with IR spectroscopy. Primary amides as a case study.

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S1. IR spectrum of ground mixture of 5-hydroxyquinoline and trimesic acid taken in 9:1 ratio

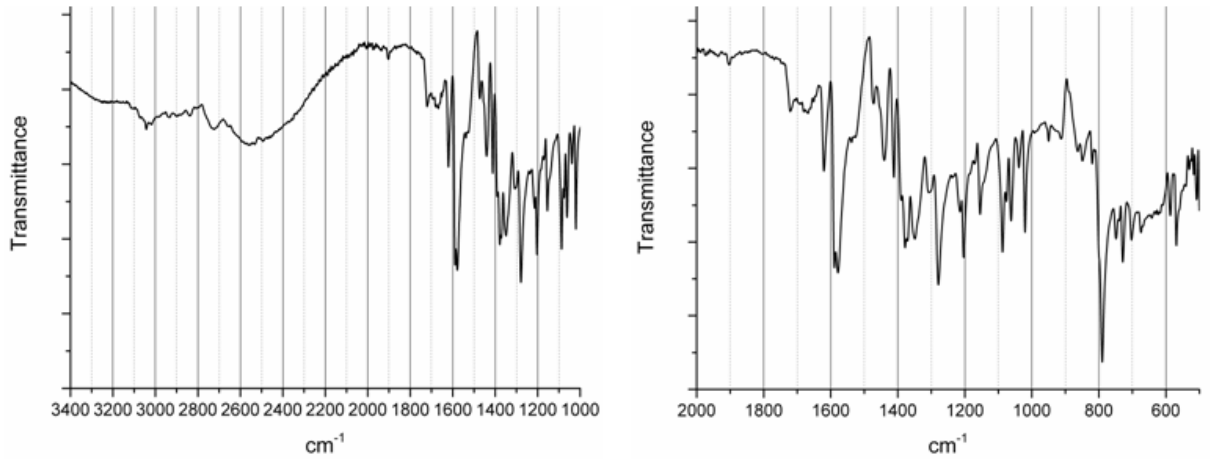


Fig. S1 IR spectrum of 9:1 mixture of 5-hydroxyquinoline and trimesic acid

5-Hydroxyquinoline and trimesic acid were taken in a mortar in 9: 1 molar ratio and ground with a pestle after the addition of a few drops of MeOH (solvent drop grinding). The ground mixture was taken for IR study. A clear 2500-2600 cm^{-1} band is seen which is representative of synthon **B**. A weak shoulder at 2400 cm^{-1} and the 1900 cm^{-1} band (though weak) shows the presence of synthon **D**. A split peak at 1600 cm^{-1} indicates the presence of both synthons **B** and **D** (excess 5-hydroxyquinoline). A strong split band at 1440-1430 cm^{-1} of the dimeric O–H in plane bending can be seen (synthon **A**). A weak but clear 920 cm^{-1} (O–H out of plane wag of dimer) is seen which confirms the presence of synthon **A**.

S2. Crystallographic information table

	5-Hydroxyquinoline	1,2-Di(4-pyridyl)ethylene: 4-hydroxybenzoic acid (1:2)	Quinoxaline: 4-hydroxybenzoic acid (1:2)	2,6-Difluorobenzamide	Adamantanecarboxamide
Formula	$C_9 H_7 N O$	$2(C_7 H_6 O_3), C_{12} H_{10} N_2$	$2(C_7 H_6 O_3), C_8 H_6 N_2$	$C_7H_5F_2NO$	$C_{11}H_{17}NO$
Molecular weight	145.16	458.46	406.38	157.08	179.26
Crystal system	Orthorhombic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	$P2_12_12_1$	$P2_1/c$	$P1$	$P2_1/c$	$C2/c$
a (Å)	3.8348(9)	3.9080(6)	6.9109(14)	5.1396(15)	23.283(19)
b (Å)	12.718(3)	23.780(4)	12.289(3)	12.118(4)	7.758(6)
c (Å)	14.067(3)	11.839(2)	12.647(3)	11.792(3)	10.744(8)
α (°)	90	90	112.713(8)	90	90
β (°)	90	100.833(9)	93.424(7)	112.482(11)	96.435(9)
γ (°)	90	90	103.103(7)	90	90
Volume ($Å^3$)	686.1(3)	1080.6(3)	951.9(4)	678.6(3)	1929(3)
Z	4	2	2	4	8
ρ_{calc} (g/cm^3)	1.405	1.409	1.418	1.537	1.235
F(000)	304	480	424	320	836
μ (MoK_α) (mm^{-1})	0.093	0.101	0.105	0.141	0.078
Temp. (K)	150	150	150	150	150

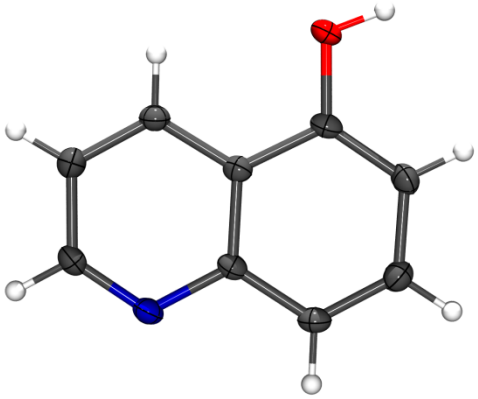
θ Range for data collection (°)	3.2, 27.5	1.7, 27.5	3.1, 25.2	3.36, 27.48	2.8, 27.5
R_1	0.0354	0.0482	0.0603	0.393	0.0561
wR_2	0.0908	0.1360	0.1647	0.0934	0.1957
Goodness-of fit	1.04	1.07	1.21	1.055	0.923
Reflns collected	7008	11126	8123	6733	9834
Unique reflns	1559	2461	3426	1555	2200
Observed reflns	1444	2239	3002	1401	1865
CCDC No.	908102	908104	908103	919101	931820

S3. Hydrogen bonding table

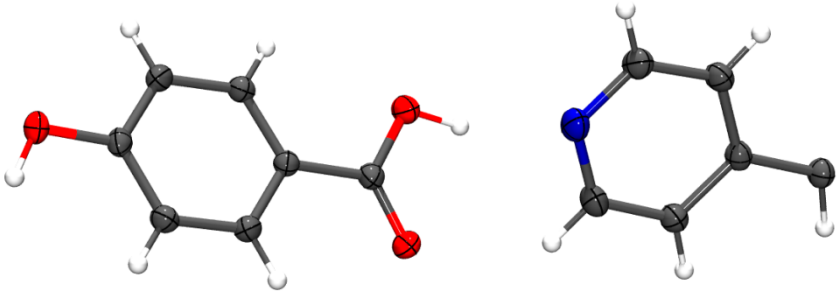
	D–H···A	Symmetry code	D–H	H···A	D–H···A
5-Hydroxyquinoline	O1–H1O···N1	1/2-x,1-y,1/2+z	0.98	1.75	166
1,2-Di(4-pyridyl)ethylene: 4-hydroxybenzoic acid (1:2)	O1–H1O···O2	1+x,-1/2-y,1/2+z	0.98	1.73	168
	O3–H3O···N1	-1+x,y,z	0.98	1.65	172
	C9–H9···O1	x,-1/2-y,-1/2+z	1.08	2.46	142
	C10–H10···O2	1+x,-1/2-y,1/2+z	1.08	2.44	127
Quinoxaline: 4-hydroxybenzoic acid and (1:2)	O1–H1O···N1		0.87	1.85	176
	O3–H3O···N2	x,1+y,1+z	0.89	1.95	145
	O4–H4O···O5	2-x,2-y,2-z	0.90	1.75	175
	O6–H6O···O2	-x,1-y,1-z	0.87	1.84	169
	C1–H1···O2		0.93	2.51	130
	C1–H1···O5	1-x,1-y,1-z	0.93	2.56	134
	C7–H7···O6	-x,1-y,-z	0.93	2.45	153
2,6-Difluorobenzamide	N1–H4···F1	-1+x,y,z	0.90	2.53	142
	N1–H4···O1	-1+x,y,z	0.90	2.17	140
	N1–H5···O1	2-x,-y,1-z	0.96	1.99	175
	C1–H2···F2	1-x,1/2+y,1/2-z	0.93	2.52	148
Adamantanecarboxamide	N1–H2···O1	x, -y, z-1/2	0.86	2.61	163
	N1–H1···O1	-x+1/2, -y+1/2, -z	0.91	2.06	174

S4. ORTEP Diagrams:

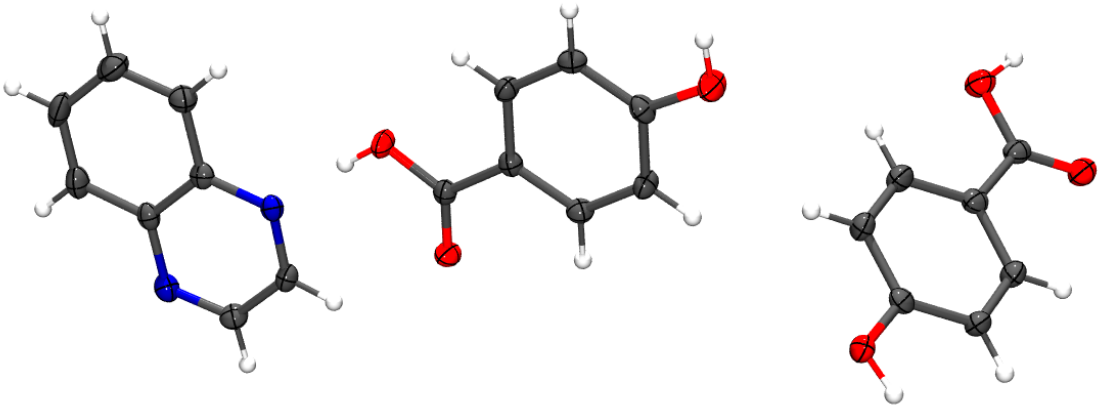
5-Hydroxyquinoline



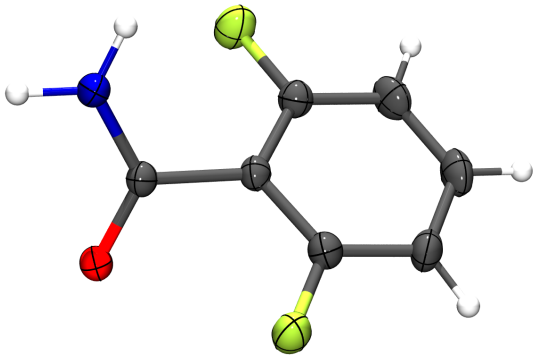
1,2-Di(4-pyridyl)ethylene: 4-hydroxybenzoic acid (1:2)



Quinoxaline: 4-hydroxybenzoic acid (1:2)



2,6-Difluorobenzamide



S5. Packing Diagram of 5-hydroxyquinoline:

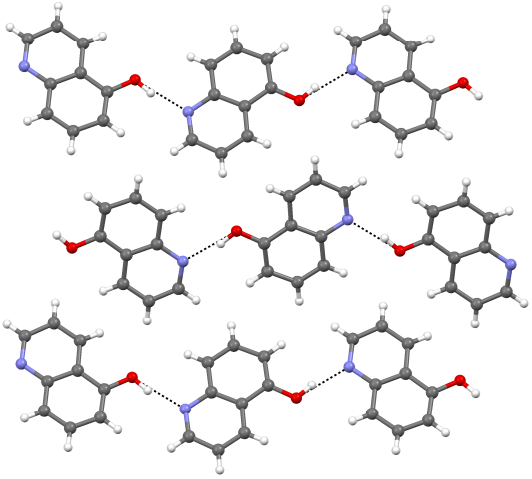


Fig. S5. Packing diagram of 5-hydroxyquinoline

S6. IR spectrum and packing diagram of adamantanecarboxamide: