Electronic Supplementary Material (ESI) for CrystEngComm.

Orientation-dependent conformational polymorphs in two similar pyridine/pyrazine phenolic esters

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Supporting Information

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Table S1. Neutron normalized C–H···N interaction geometrical parameters

	H···A/Å	D···A/Å	∠D–H···A/°	Symmetry Operation	
Ia					
C_{10}–H_{10}···N_1	2.67	3.57(1)	139	1-x, 1-y, 2-z	Py···Py
C_6–H_6···N_1	2.53	3.53(1)	153	1.5-x, -0.5+y, z	Py···Ph
Ib					
C_9–H_9···N_1	2.676	3.70(1)	157	1-x, -y, 2-z	Py···Py
IIa					
C_{11}–H_{11}···N_1	2.65	3.46(1)	130	-1+x, y, z	Pz···Pz
C_9–H_9···N_2	2.68	3.46(1)	128	1+x, y, z	Pz···Pz
IIb					
C_{11}–H_{11}···N_2	2.57	3.36(1)	128	-x, 1-y, 1-z	Pz···Pz
C_6–H_6···N_1	2.75	3.78(1)	157	x, -0.5-y, 0.5+z	Pz···Ph
C_{10}–H_{10}···N_1	2.47	3.36(1)	138	-x, 0.5+y, 0.5-z	Pz···Pz

Table S2. Neutron normalized C–H···O interaction geometrical parameters

Interaction	H···A/Å	D···A/Å	∠D–H···A/°	Symmetry Operation
Ia				
C_3–H_3···O_1	2.42	3.48(1)	164	2-x, 0.5+y, 1.5-z
C_4–H_4···O_1	2.40	3.47(1)	166	0.5+x, y, 1.5-z
Ib				
C_{11}–H_{11}···O_1	2.60	3.34(1)	125	1+x, y, z
C_2–H_2···O_1	2.44	3.31(1)	136	X, 1+y, z
IIa				
C_2–H_2···O_1	2.30	3.35(1)	162	1+x, y, z
C_{10}–H_{10}···O_1	2.46	3.35(1)	162	0.5-x, -y, -0.5+z
IIb				

C_2–H_2···O_1	2.47	3.52(1)	160	X, 1+y, z

Figure S1. FT-IR transmittance plots for I, II

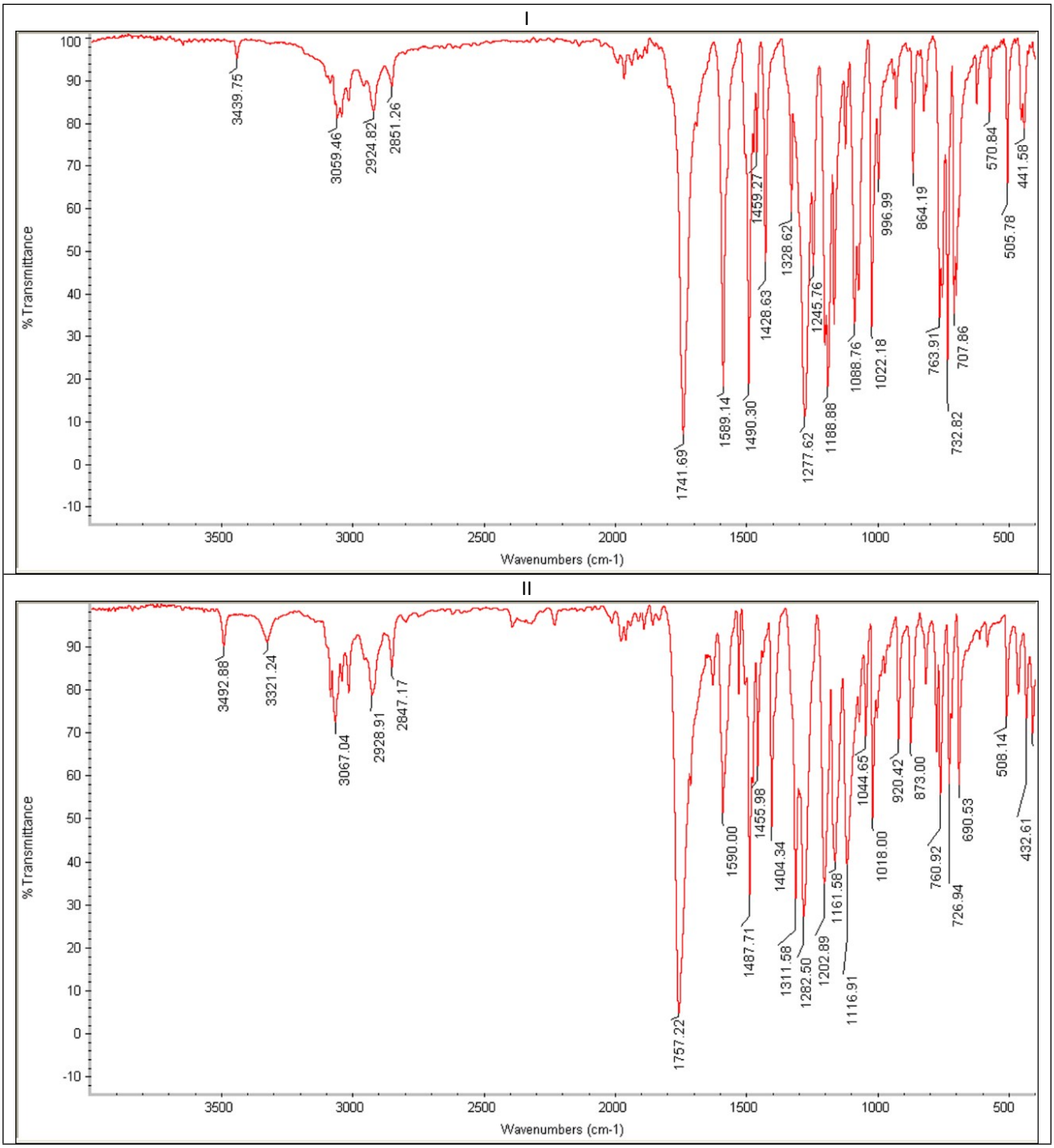
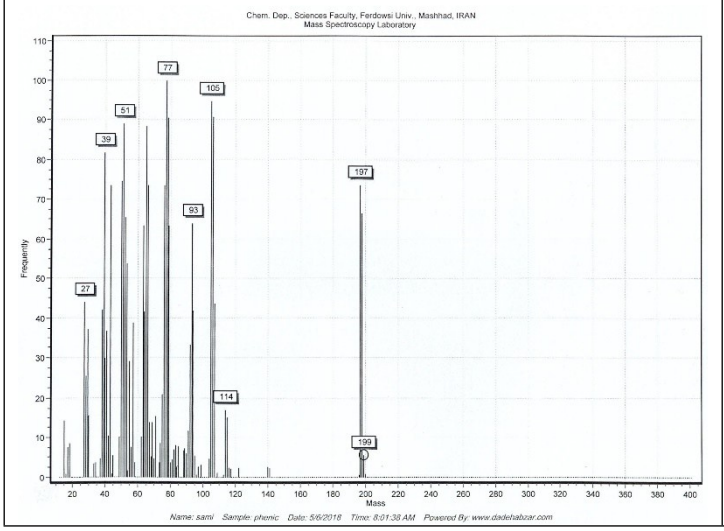


Figure S2. mass spectroscopy analysis for I, II

I



II

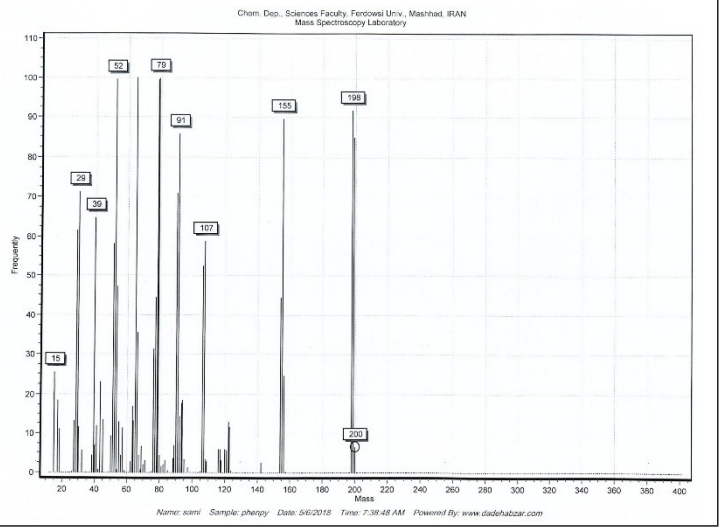


Figure S3. CHN elemental analysis for I, II

I

Eager 300 Summarize Results

Date : 06/05/2018 at 11:52:14
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
sami-55		

#	Group	Sample Name	Type	Weig.	Pro.F	---
55	1	phenic	UNK	0.652	6.25	---

Component name	Element %
Nitrogen%	6.053499222
Carbon%	72.08955383
Hydrogen%	4.733834267
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	6.053499222
Carbon%	72.08955383
Hydrogen%	4.733834267
Sulphur%	0

II

Eager 300 Summarize Results

Date : 06/05/2018 at 11:52:07
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
sami-54		

#	Group	Sample Name	Type	Weig.	Pro.F	---
54	1	phenpy	UNK	0.732	6.25	---

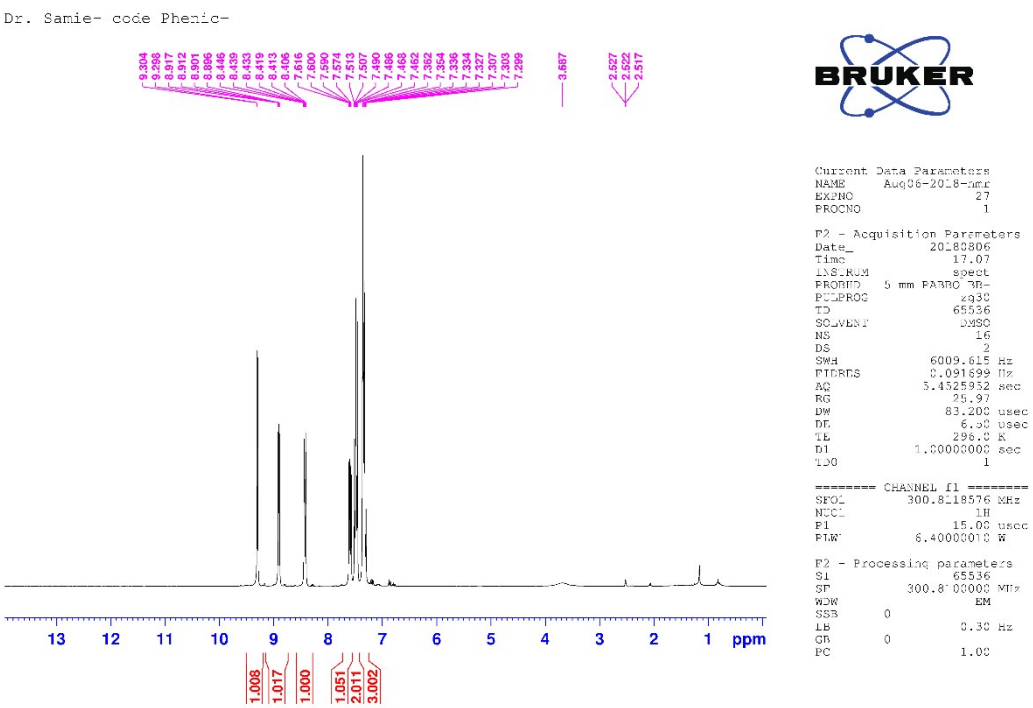
Component name	Element %
Nitrogen%	12.31163025
Carbon%	66.516922
Hydrogen%	4.478351593
Sulphur%	0

1 Sample(s) in Group No : 1

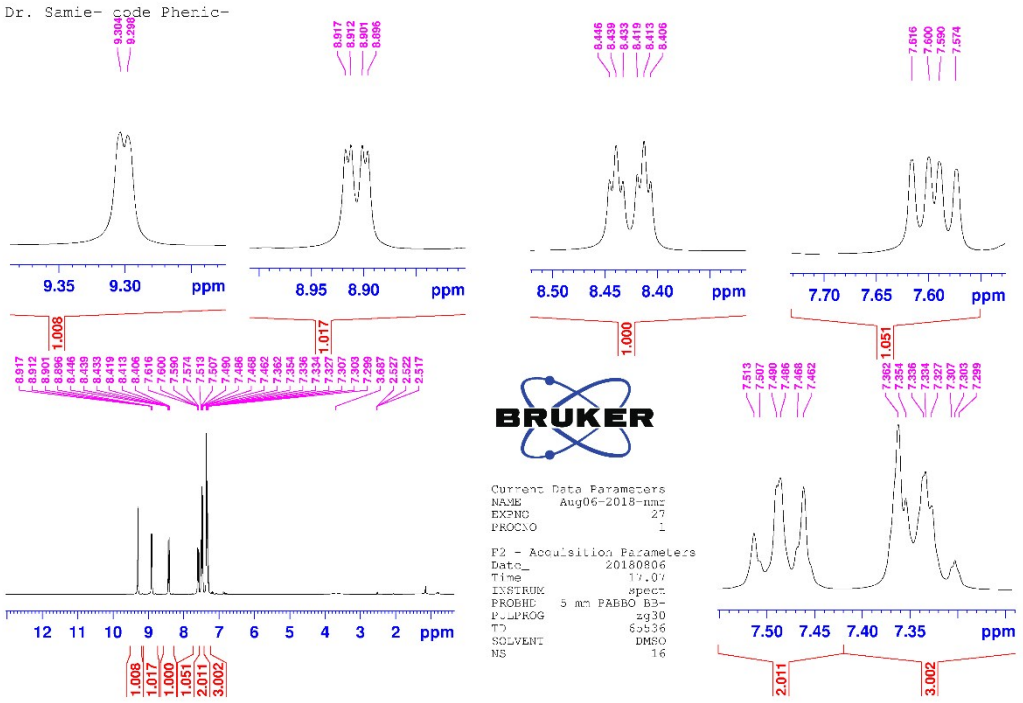
Component Name	Average
Nitrogen%	12.31163025
Carbon%	66.516922
Hydrogen%	4.478351593
Sulphur%	0

Figure S4. ^{1}H-NMR spectrums for I, II

I



I-expansion



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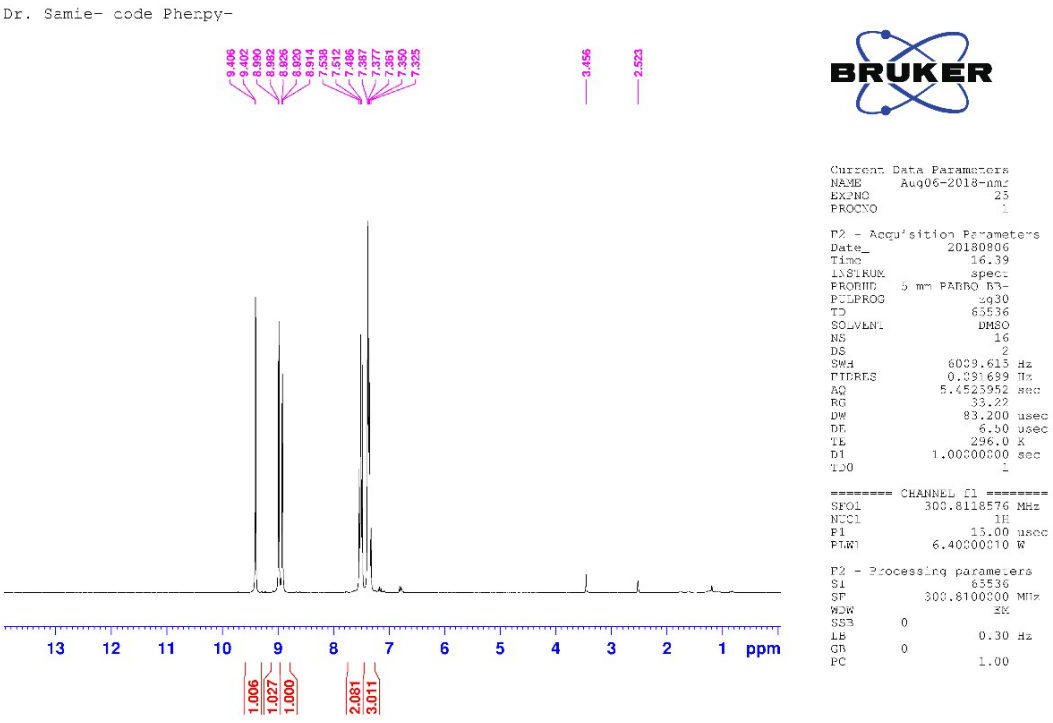

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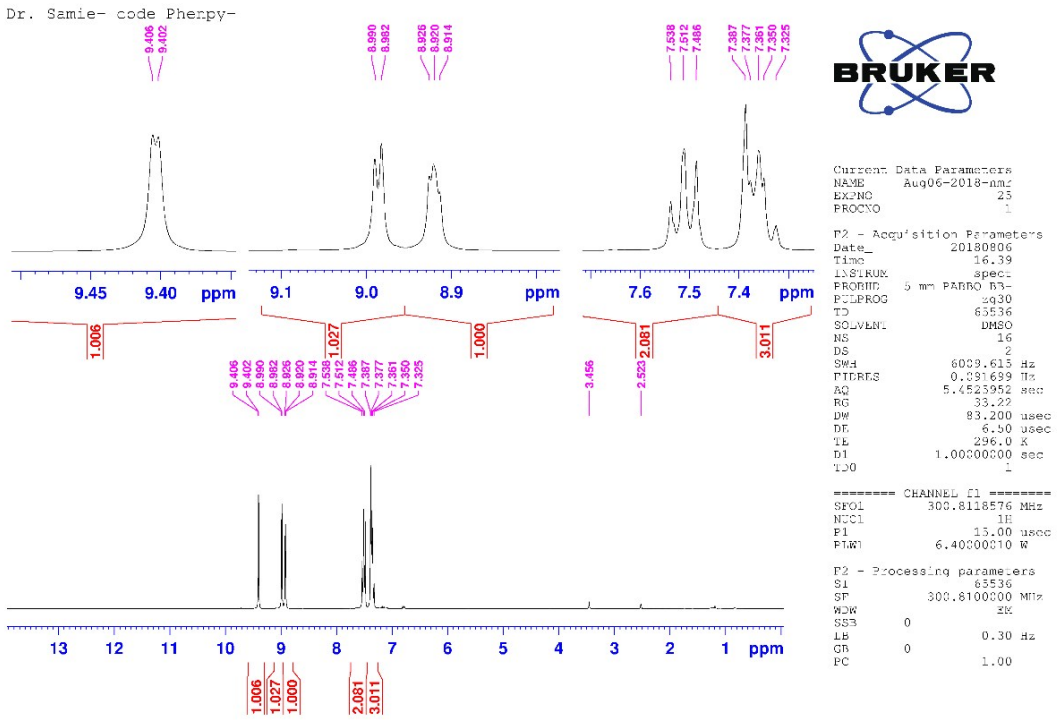
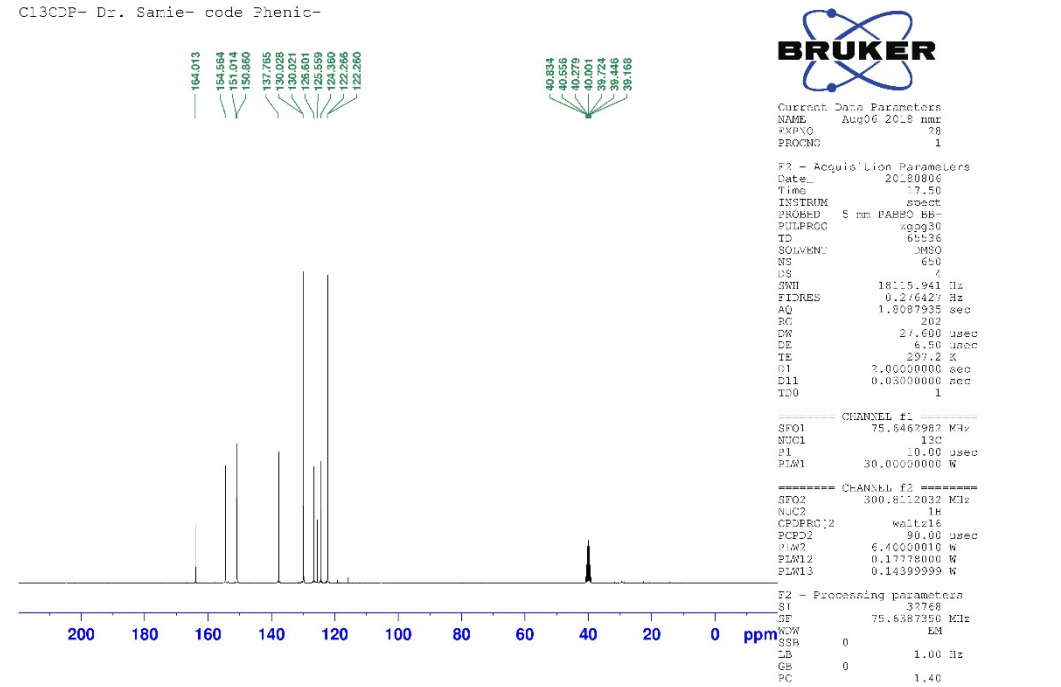


Figure S5. ^{13}C-NMR spectrums for I, II

I



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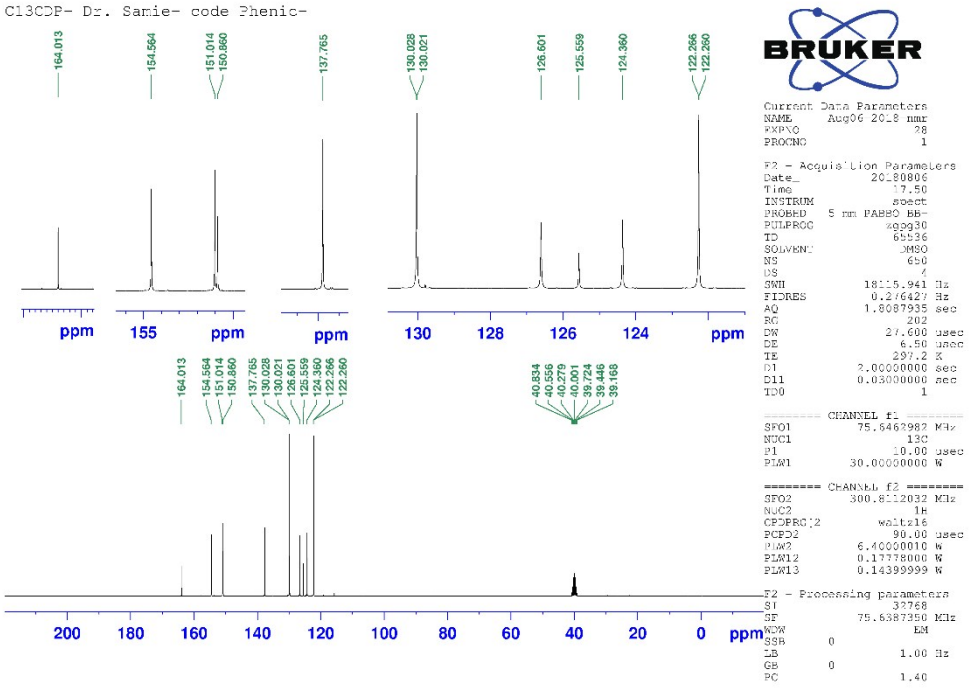

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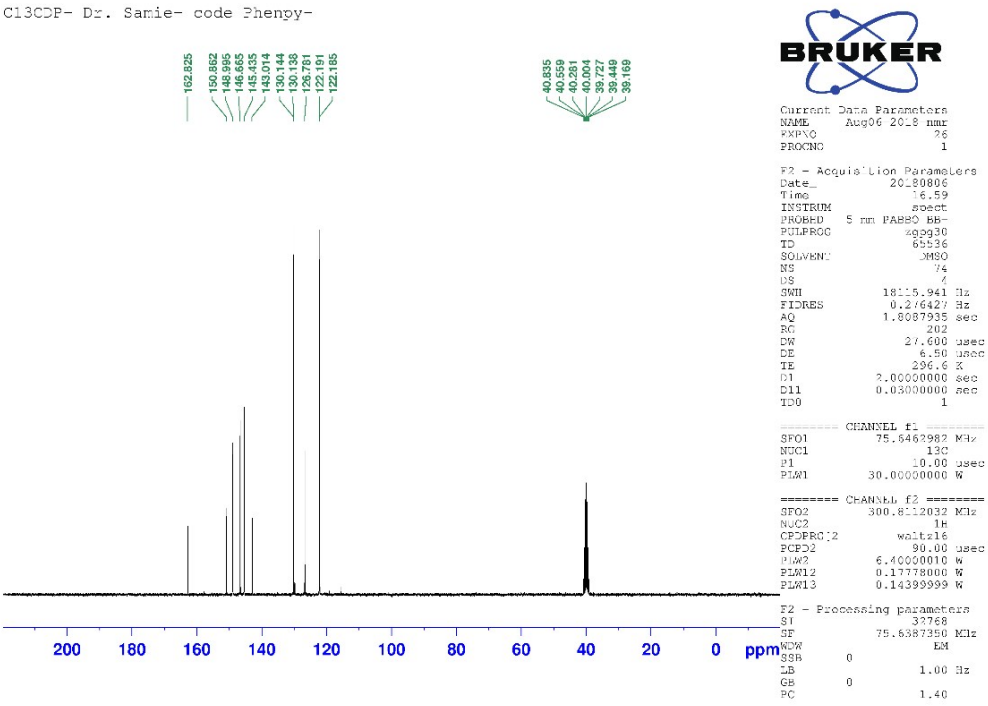


II-expansion

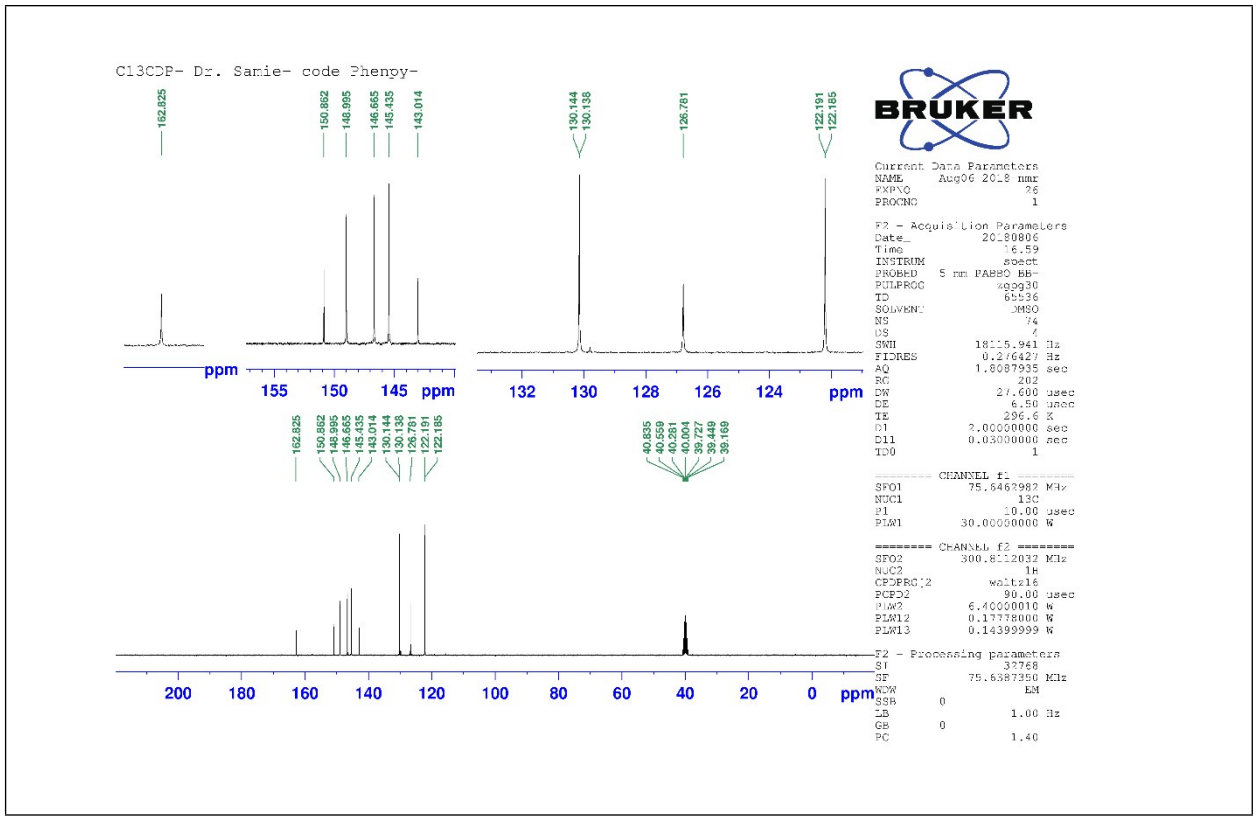


Figure S6. CSD-search for distances and angles of similar C–H···N

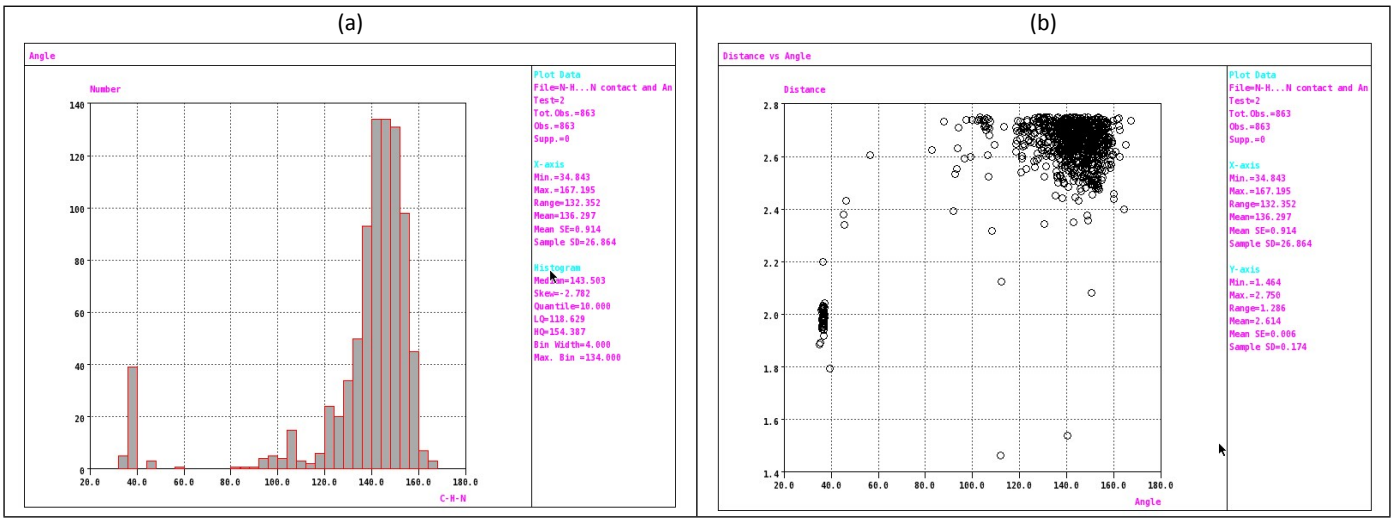
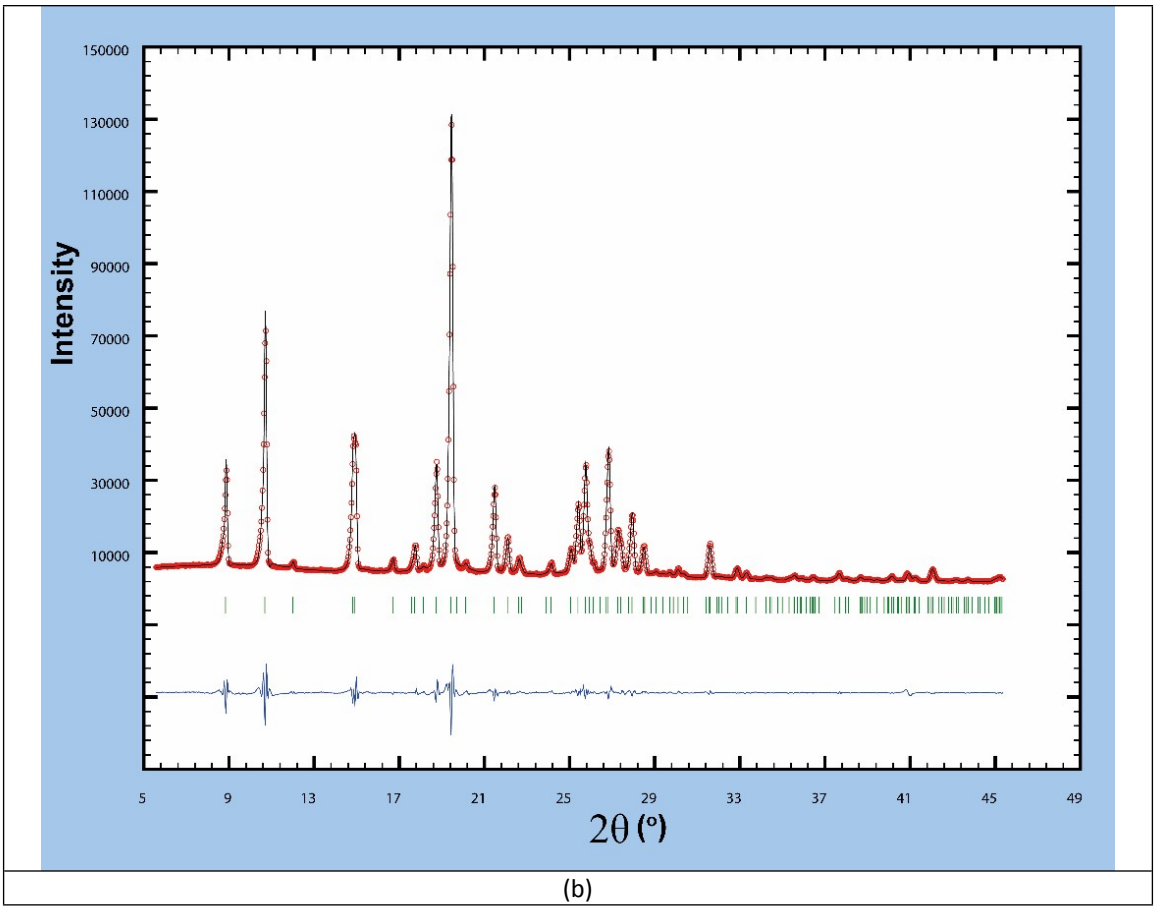


Figure S7. Rietveld refinement for PXRD profiles of **(a)** Ia and **(b)** IIa; experimental (up), calculated (down) and difference (middle).

(a)


Intensity
150000
130000
110000
90000
70000
50000
30000
10000
5
9
13
17
21
25
29
33
37
41
45
49
2θ (°)

(b)

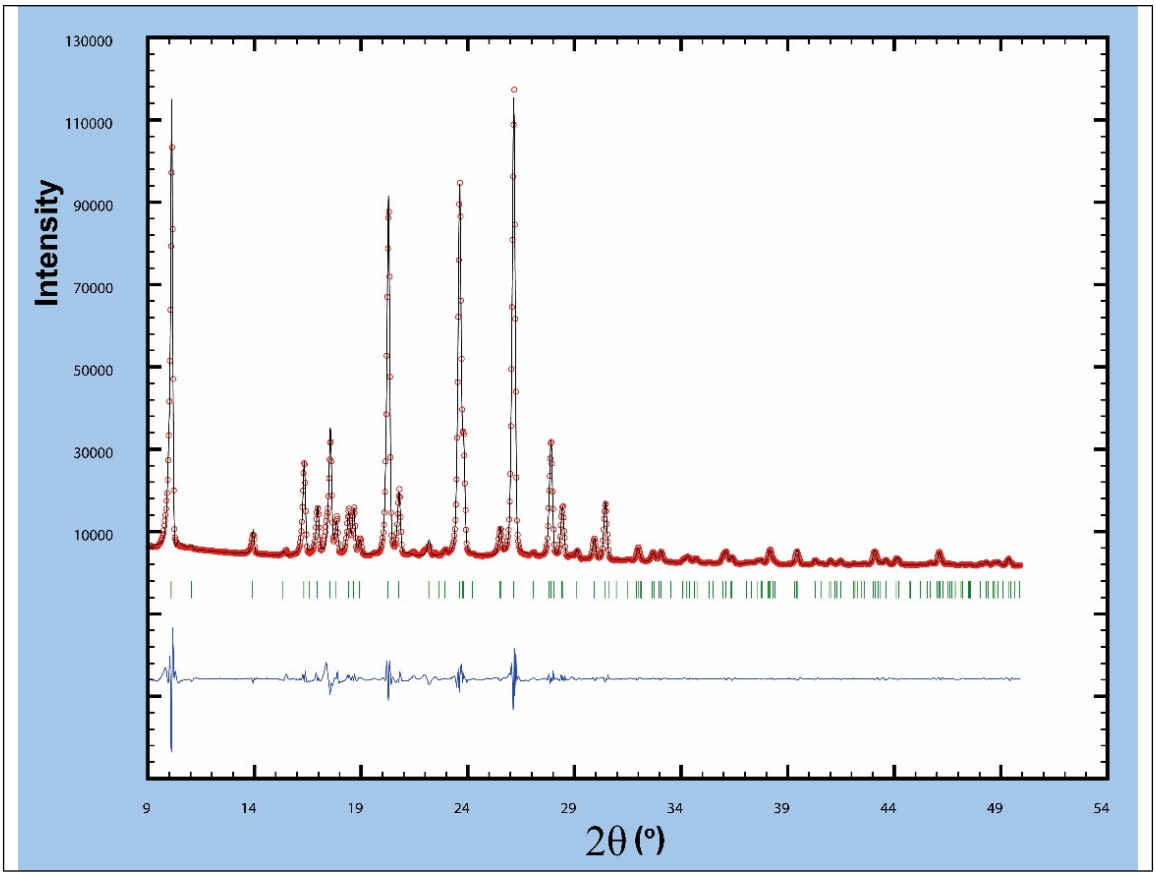
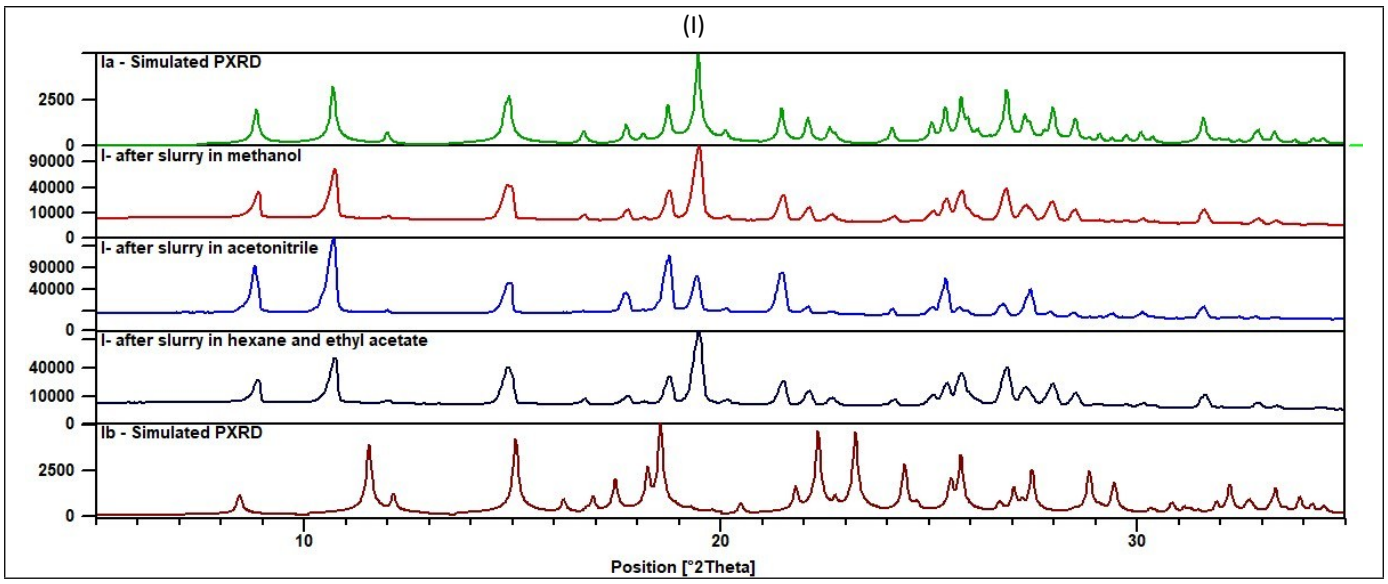
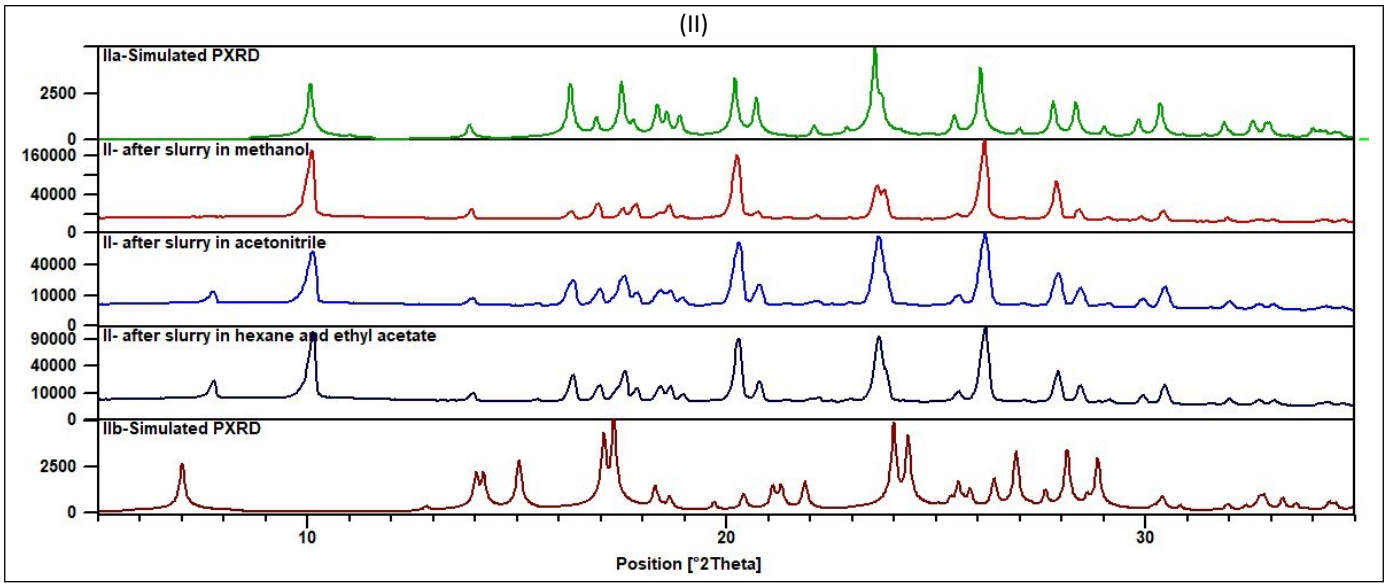


Figure S8. PXRD after slurry experiment




(II)
IIa-Simulated PXRD
2500
0
II- after slurry in methanol
160000
40000
0
II- after slurry in acetonitrile
40000
10000
0
II- after slurry in hexane and ethyl acetate
90000
40000
10000
0
IIb-Simulated PXRD
2500
0
10
20
30
Position [°2Theta]