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Multicomponent solids of uracil derivatives, orotic and isoorotic acids

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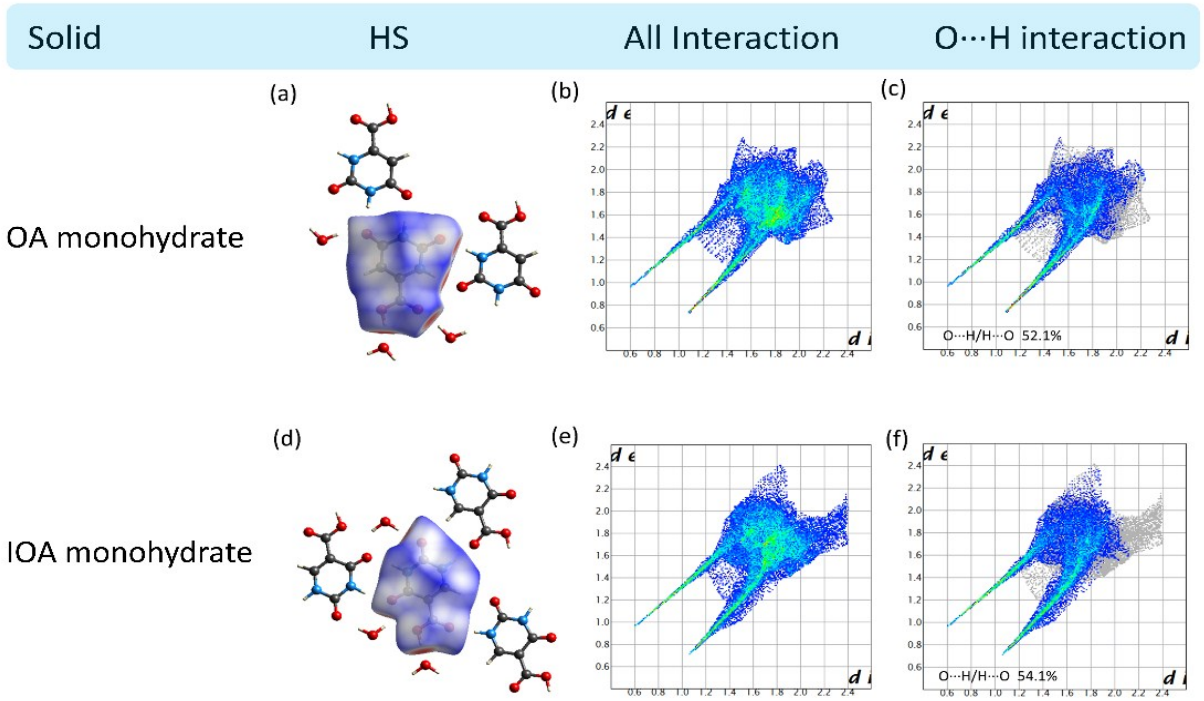


Fig. S1 (a and d) Structural environment of OA and IOA monohydrates have been shown through Hirshfeld surface. (b-f) Fingerprint plots of both the solids for all interaction, resolution of plot in O···H/H···O interactions. The presence of two spikes are characteristic of carboxylic acid.

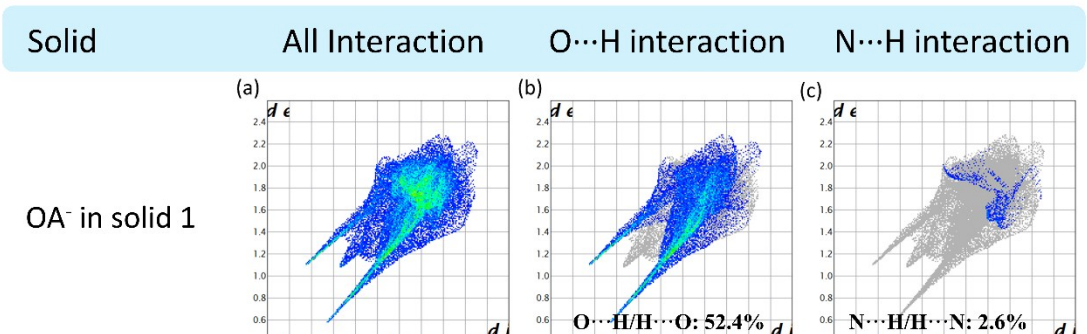


Fig. S2 (a-c) Fingerprint plot of OA^- in solid **1** $(OA)_2^-\cdot(bpeeH)^{+2}$, plot resolved in O···H/H···O and N···H/H···N interactions. (d-f) Fingerprint plot of IOA in solid **7** $(IOA)_2\cdot bpee$, resolved in O···H/ H···O and N···H/H···N interactions.

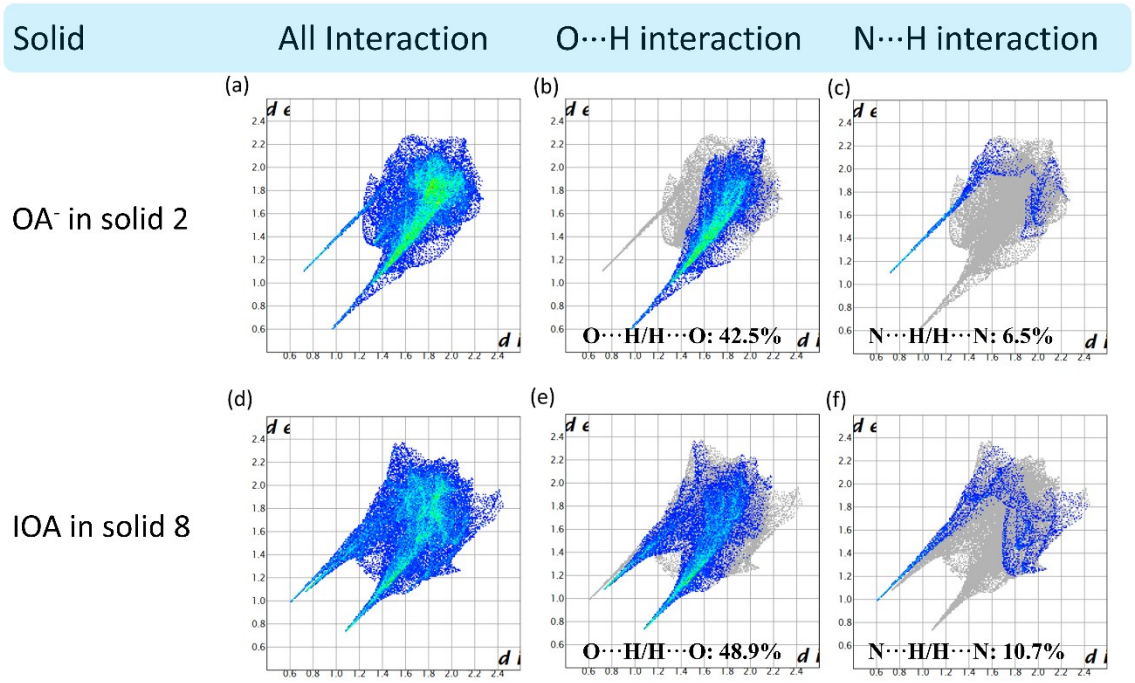


Fig. S3 (a-c) Fingerprint plot of OA^- in solid **2** $(OA)^{-}.(bpeH)^{+}$, plot resolved in O···H/ H···O and N···H/H···N interactions. (d) Fingerprint plot of solid **8** $(IOA)_2 \cdot (bpe)$ interaction resolved in O···H/ H···O and N···H/H···N interactions.

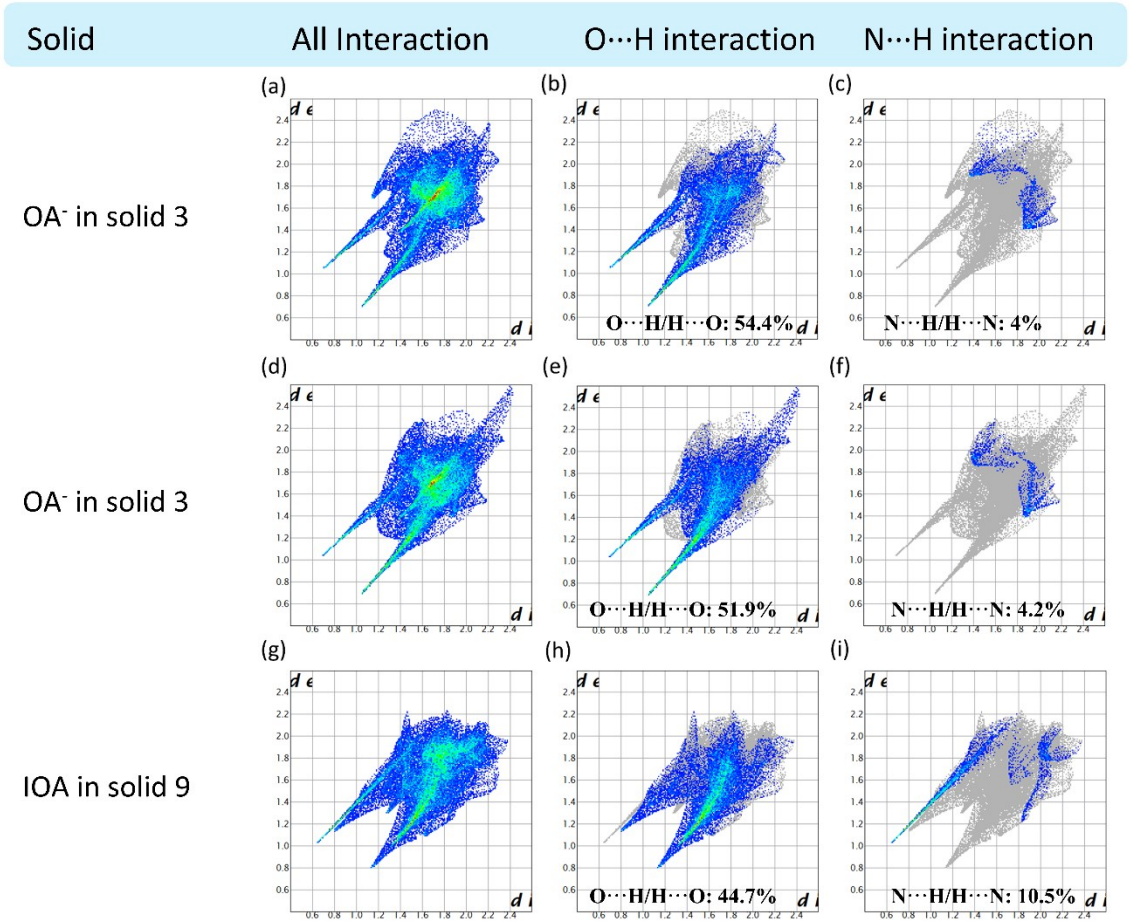


Fig. S4 (a- f) Fingerprint plot of both OA^- in solid **3** $(OA)^-_2.bppH_2^{2+}\cdot 2H_2O$, plot resolved in O···H/ H···O and N···H/H···N interactions. (g-h) Fingerprint plot of IOA in solid **9** (IOA)·(*bpp)* , interaction resolved in O···H/ H···O and N···H/H···N interactions.

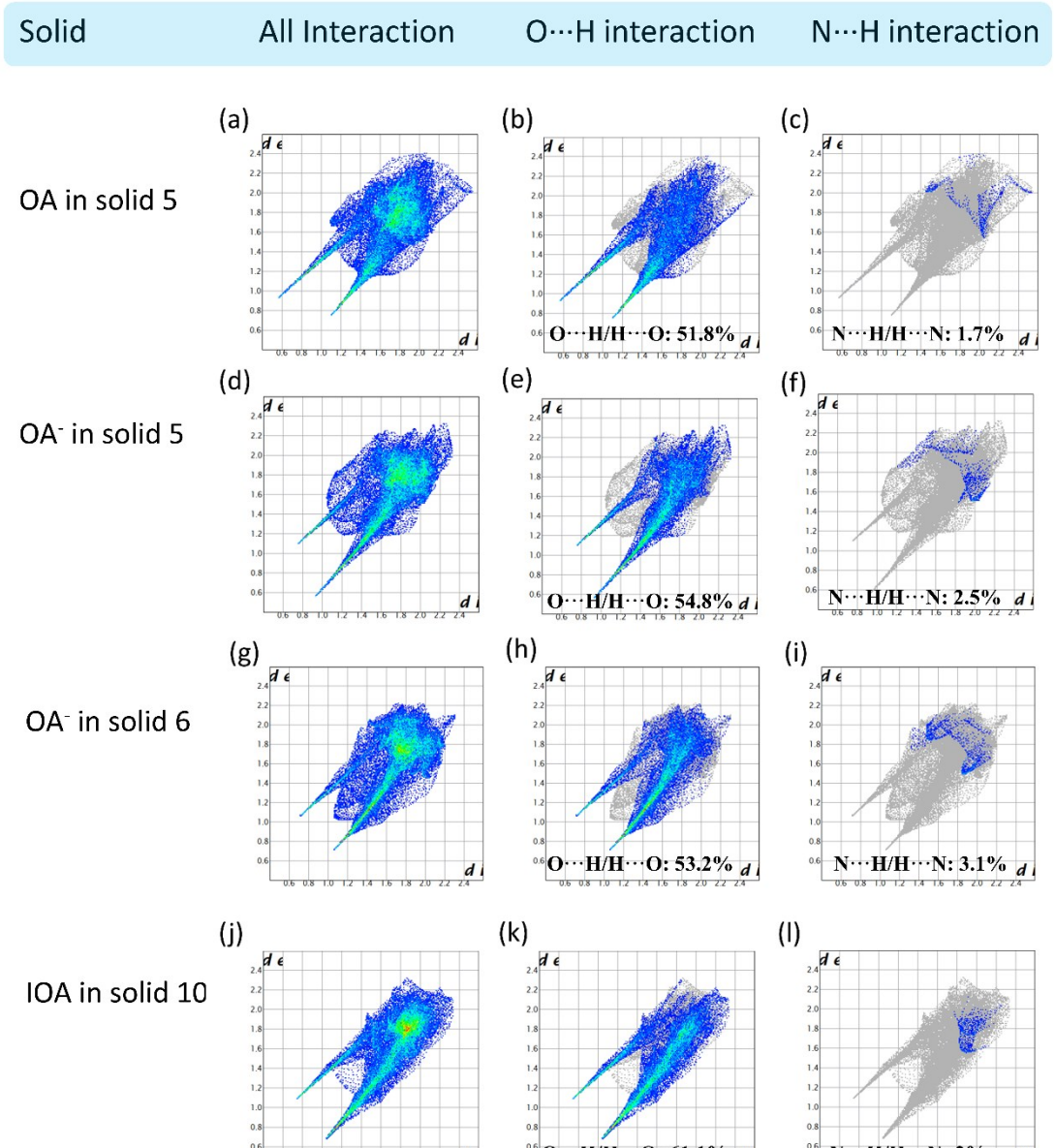
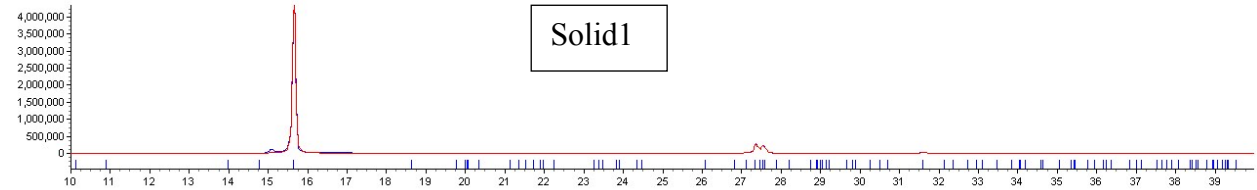
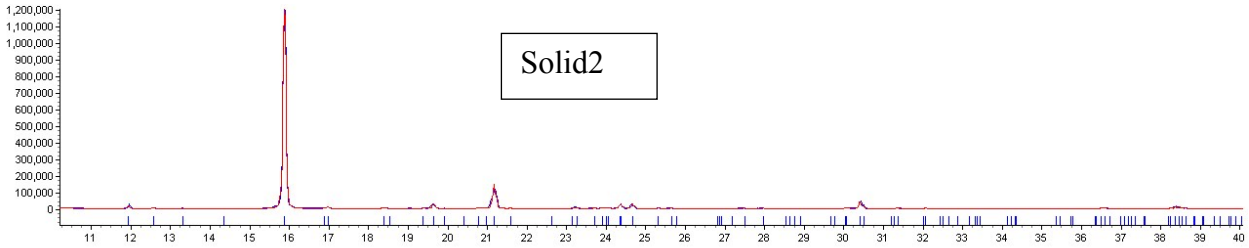
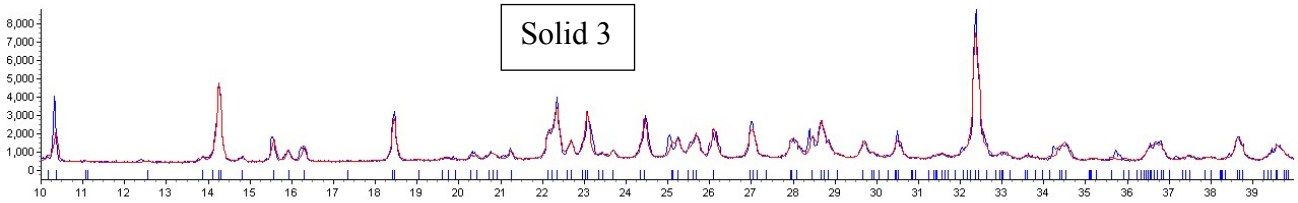
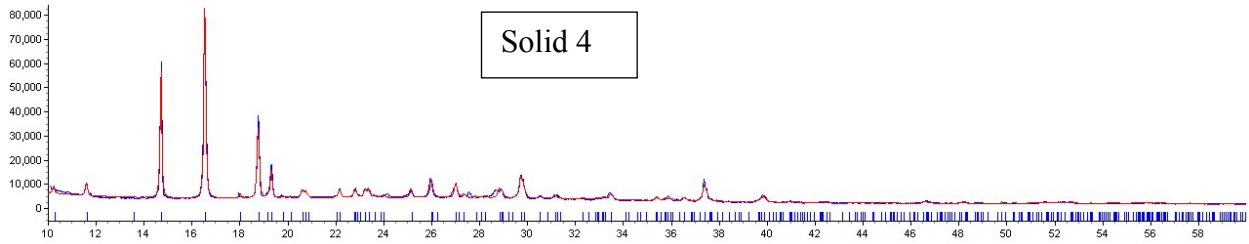


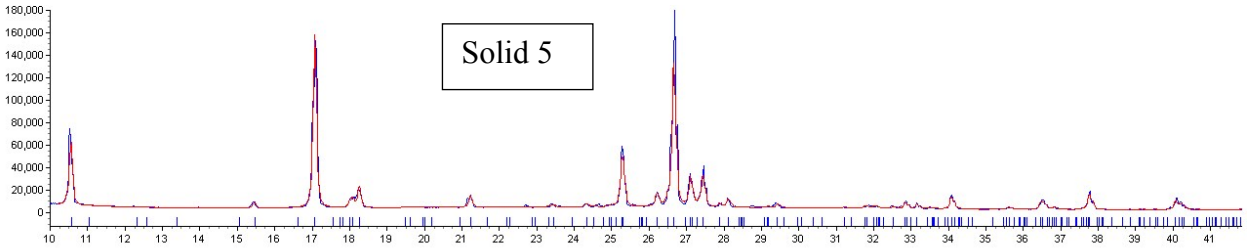
Fig. S5 (a-f) Fingerprint plot of both OA and OA^- in solid **5** $(OA)\cdot(OA)^{-}\cdot(4apH)^{+}$, interaction resolved in O···H/ H···O and N···H/H···N interactions. (g-i) Fingerprint plot of OA^- in solid **6** $(OA)^{-}.(4ap\mathrm{H})^{+}$, interaction resolved in O···H/ H···O and N···H/H···N interactions. (j-l) Fingerprint plot of IOA in solid **10** $(IOA)^{-}\cdot(4apH)^{+}\cdot 3H_2O$, plot is resolved in O···H/ H···O and N···H/H···N interactions.

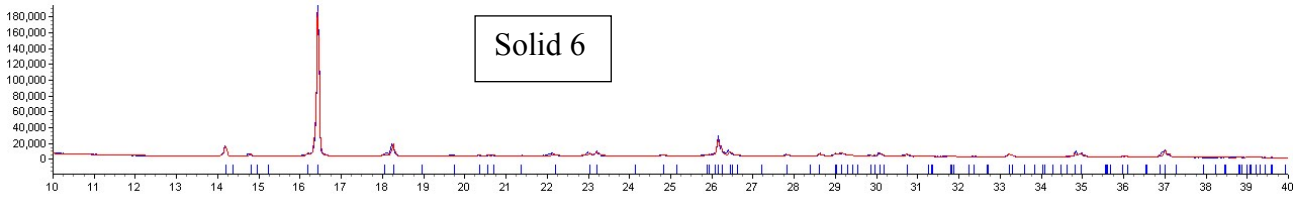


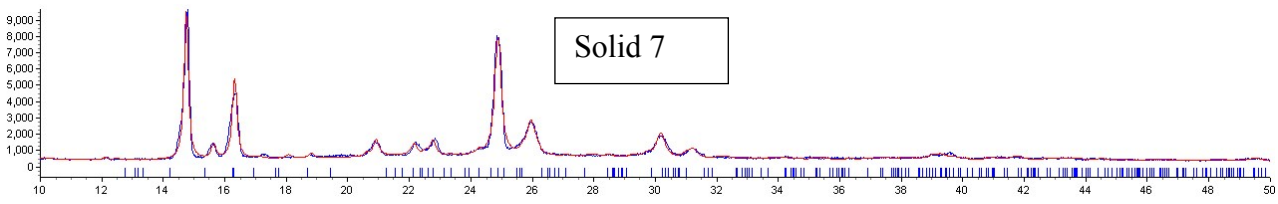





Solid 4


Solid 5


Solid 6


Solid 7

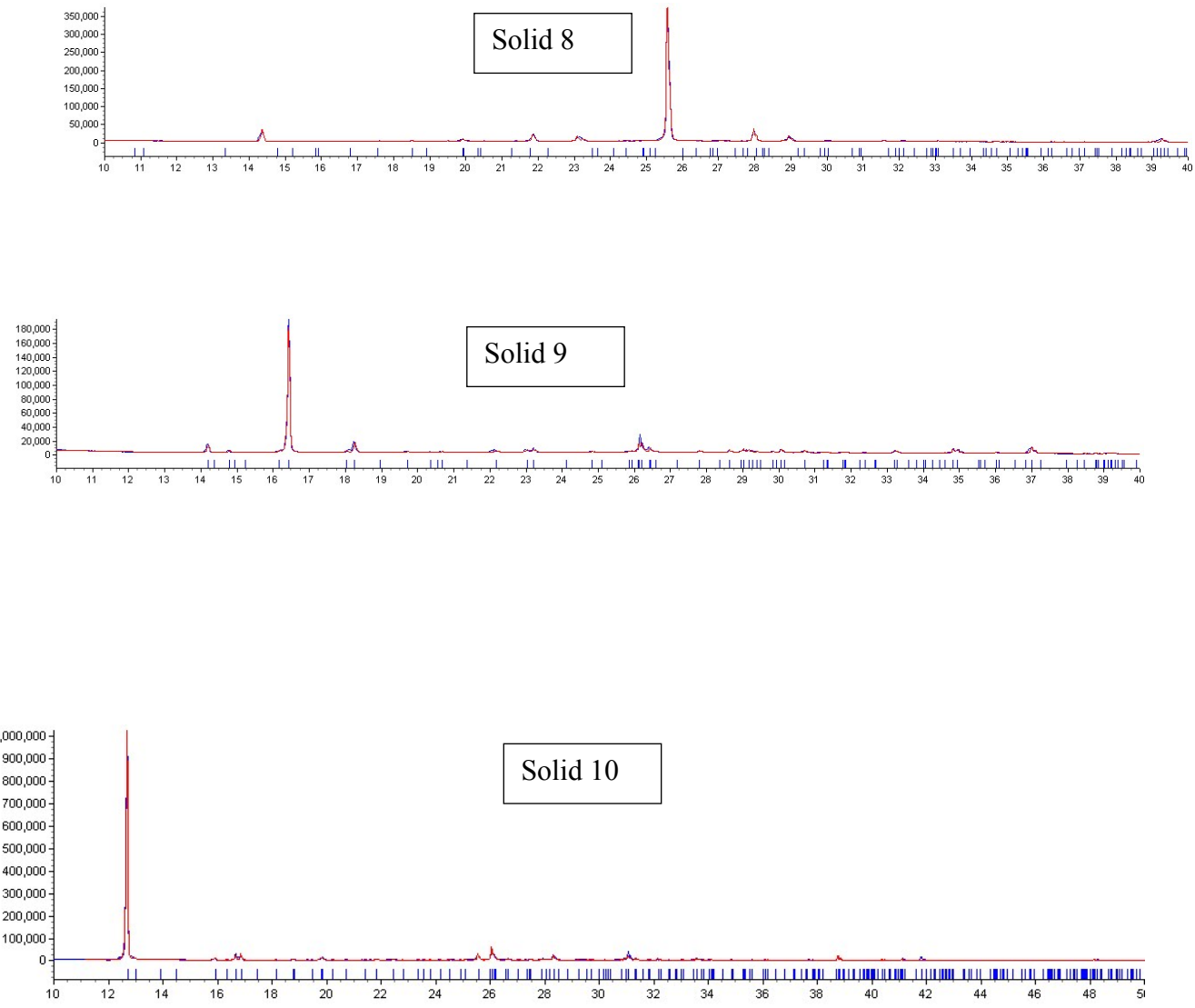
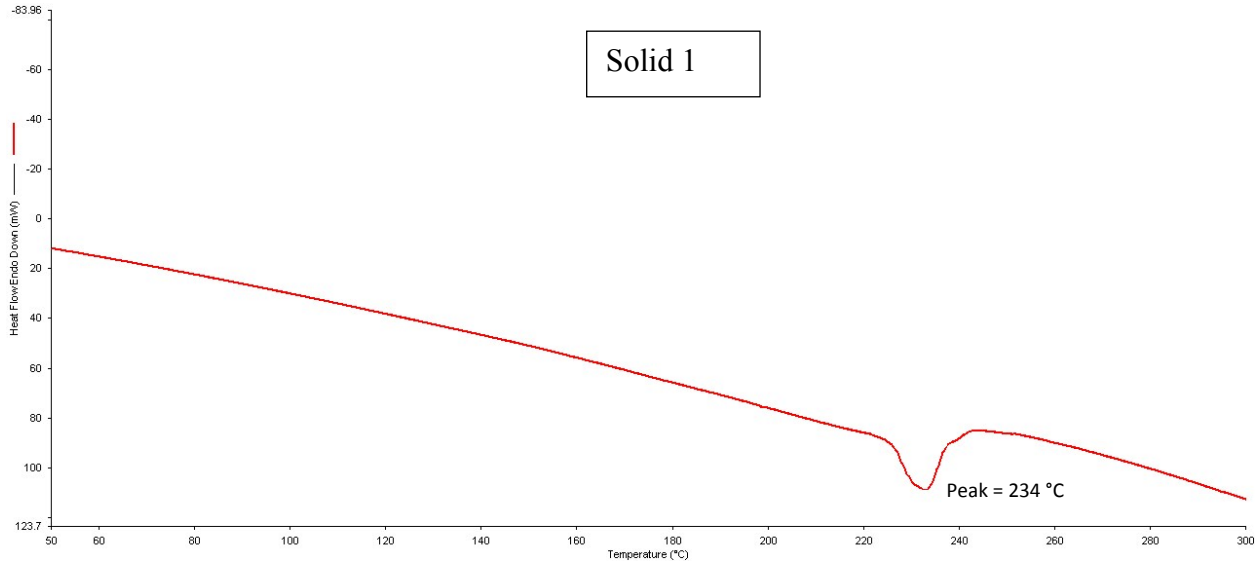
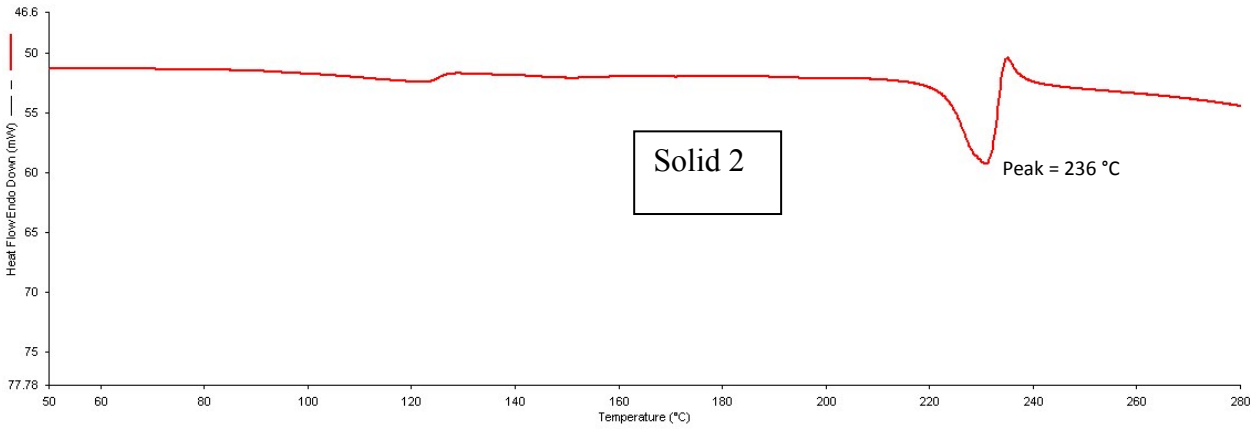
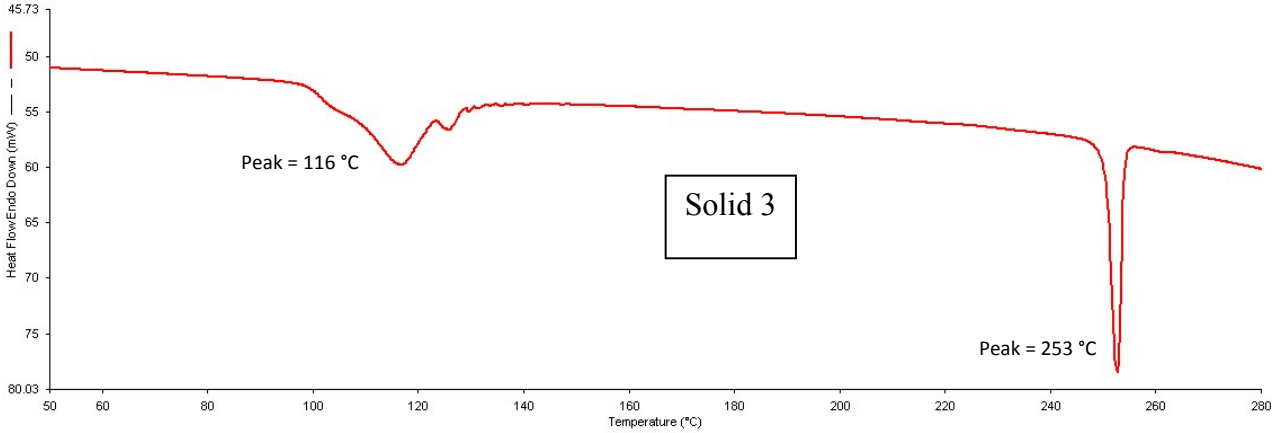
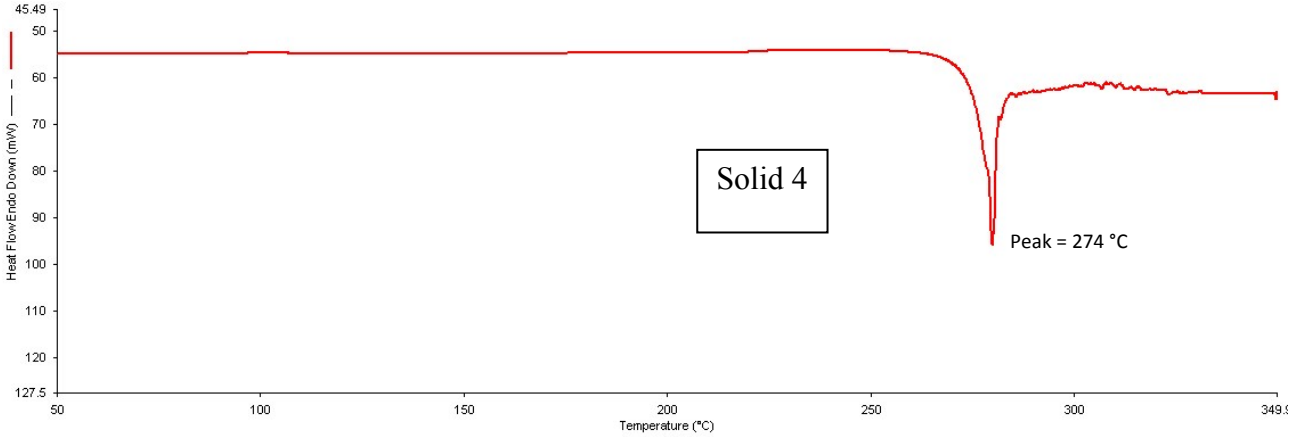


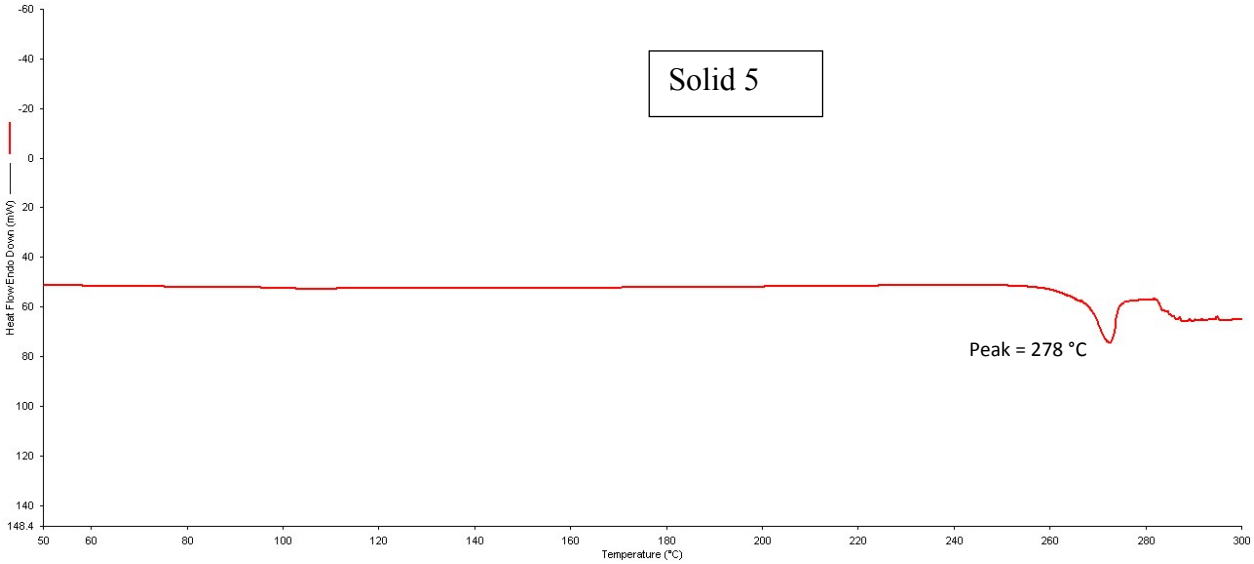
Fig. S6 Rietveld refinement plots for **1–10**, indicating the homogeneity of the bulk samples. The plot shows the experimental powder XRD profile (blue line), the calculated (red line), and blue tick lines shows Bragg positions in the bottom.

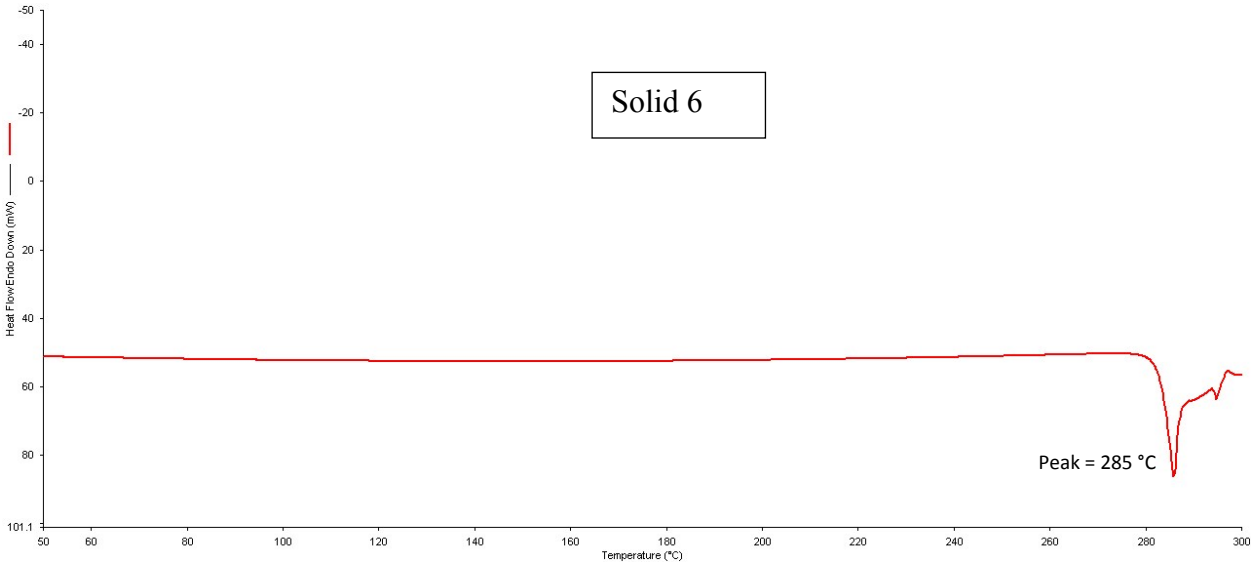

Solid 1
Peak = 234 °C
Heat Flow Endo Down (mW)
Temperature (°C)
-83.96
-60
-40
-20
0
20
40
60
80
100
123.7
50
60
80
100
120
140
160
180
200
220
240
260
280
300

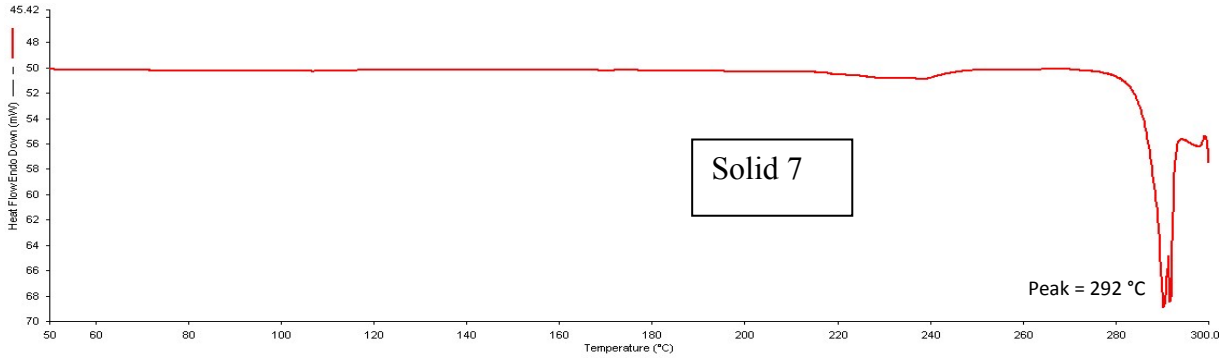

Solid 2
Peak = 236 °C
Heat Flow Endo Down (mW)
Temperature (°C)
46.6
50
55
60
65
70
75
77.78
50
60
80
100
120
140
160
180
200
220
240
260
280

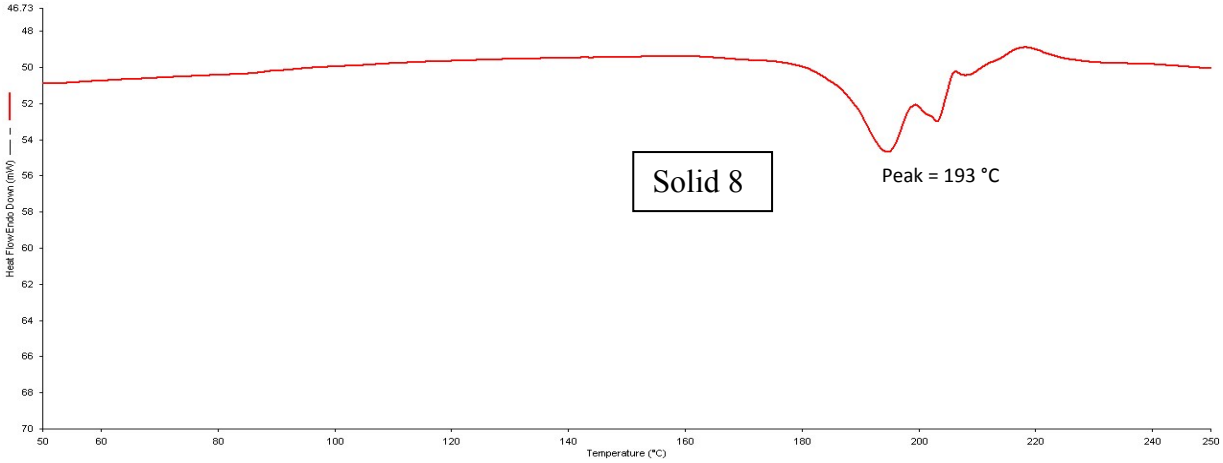

45.73
50
55
60
65
70
75
80.03
Heat Flow Endo Down (mW)
50
60
80
100
120
140
160
180
200
220
240
260
280
Temperature (°C)
Peak = 116 °C
Solid 3
Peak = 253 °C

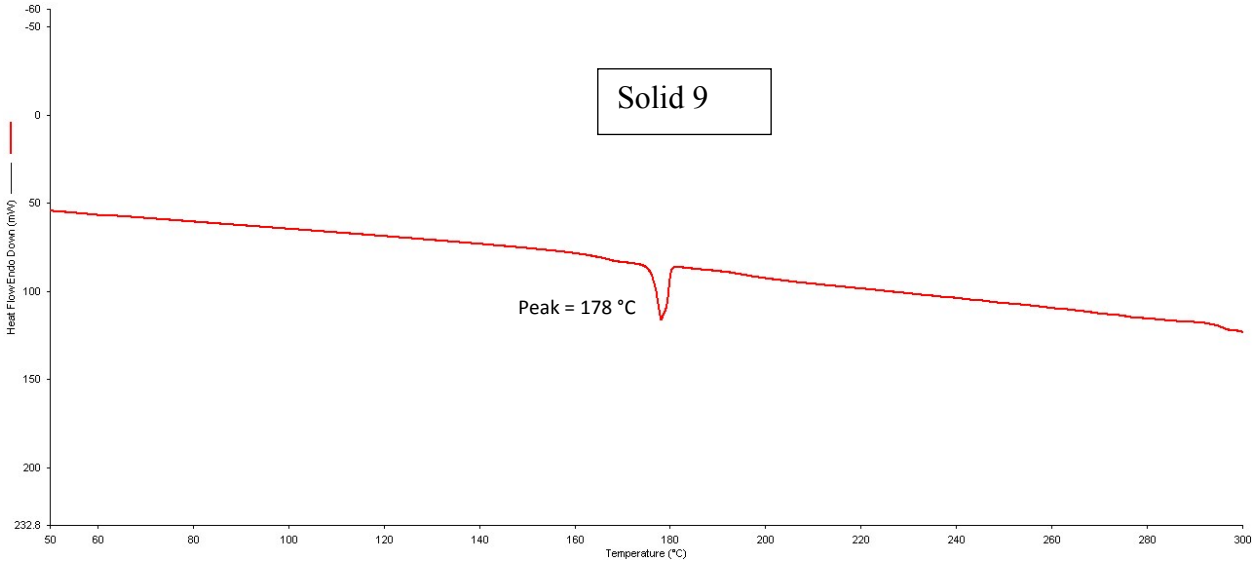

45.49
50
60
70
80
90
100
110
120
127.5
Heat Flow Endo Down (mW)
50
100
150
200
250
300
Temperature (°C)
Solid 4
Peak = 274 °C


Solid 5
Peak = 278 °C
Heat Flow Endo Down (mW)
Temperature (°C)
-60
-40
-20
0
20
40
60
80
100
120
140
148.4
50
60
80
100
120
140
160
180
200
220
240
260
280
300


Solid 6
Peak = 285 °C
Heat Flow Endo Down (mW)
Temperature (°C)
-50
-40
-20
0
20
40
60
80
101.1
50
60
80
100
120
140
160
180
200
220
240
260
280
300


45.42
48
50
52
54
56
58
60
62
64
66
68
70
Heat Flow Endo Down (mW)
50
60
80
100
120
140
160
180
200
220
240
260
280
300.0
Temperature (°C)
Solid 7
Peak = 292 °C


46.73
48
50
52
54
56
58
60
62
64
66
68
70
Heat Flow Endo Down (mW)
50
60
80
100
120
140
160
180
200
220
240
250
Temperature (°C)
Solid 8
Peak = 193 °C


Solid 9
Peak = 178 °C
Heat Flow Endo Down (mW)
Temperature (°C)
-60
-50
0
50
100
150
200
232.8
50
60
80
100
120
140
160
180
200
220
240
260
280
300

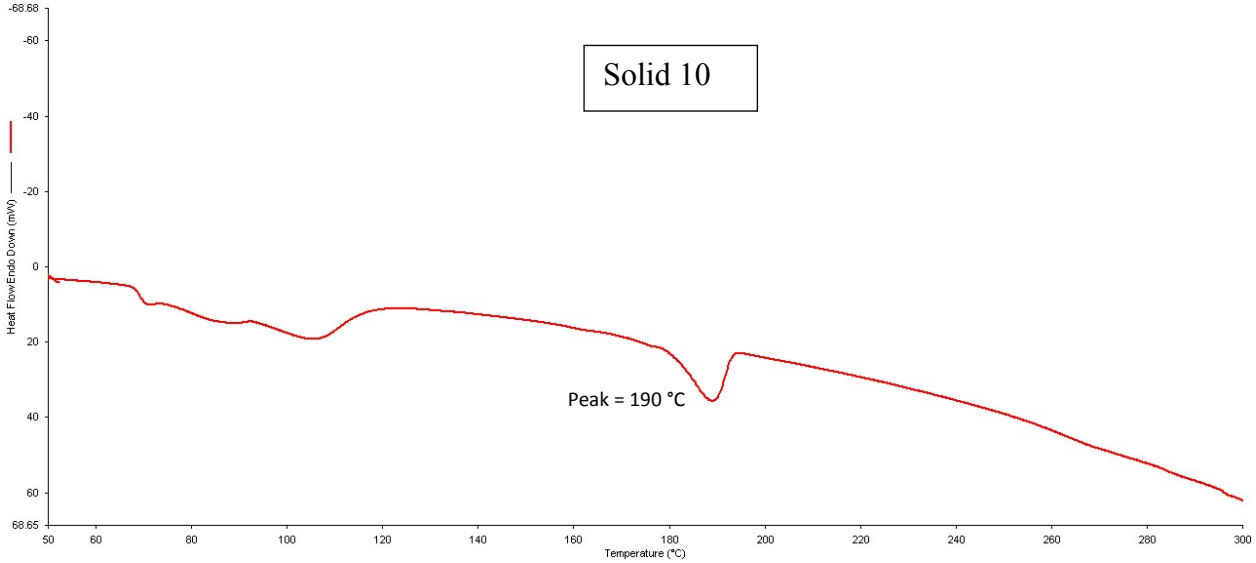

Solid 10
Peak = 190 °C
Heat Flow Endo Down (mW)
Temperature (°C)
-68.68
-60
-40
-20
0
20
40
60
68.65
50
60
80
100
120
140
160
180
200
220
240
260
280
300

Fig. S7 DSC thermograms of solids **1** to **10** showing endothermic peak corresponding to its melting point except solids **3**, **10** where first peak correspond to removal of water.

Orotic Acid solubility calculation

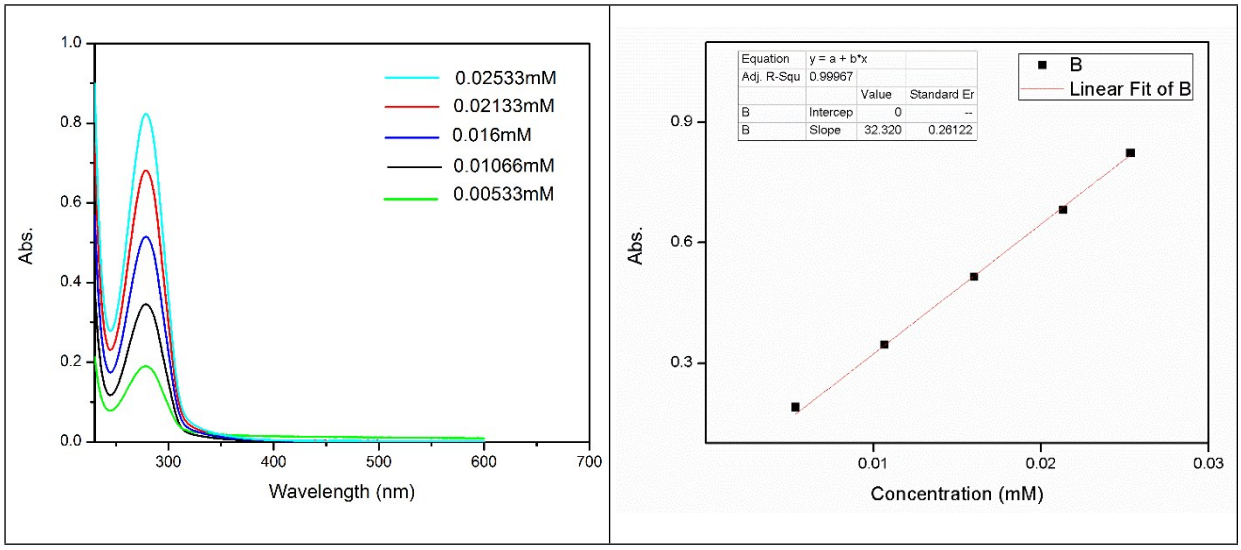


Fig. S8 Absorbance vs. wavelength and absorbance vs. concentration curves for the standard solutions of Orotic Acid in distilled water

Standard solutions of Orotic Acid in distilled water:

A suspension of OA in distilled water was stirred at room temperature for 24 hours. The excess solids were filtered and the solution was diluted to get the absorbance value within 1 in the UV-Vis spectrum. The PXRD of the residual solids was analyzed to assess it solid form nature.

Calculation:

Beer Lambert's law: $A=\varepsilon cl$

Where A is the absorbance, ε ix coefficient of absorbance, c is the concentration and *l* is the path length of the sample.

$\varepsilon = 32.32\ mmol^{-1}cm^{-1}$

Orotic Acid in distilled water:

For the saturated solution, A = 0.6965 (300 times dilution) at λ = 279 nm, ε = 32.32 $mmol^{-1}cm^{-1}$, *l* = 1 cm

A × dilution = ε × c × *l*

0.6965× 300 = 32.32 × c × 1

c = 6.465 mM

c = (6.465×156)/1000 mg/ml (Mol. wt. of OA= 156.1)

Hence concentration of saturated solution is c = 1.00 mg/ml

Solubility of all solids was calculated in the same way. Absorbance vs. concentration curves for the standard solutions of all solids is given below.

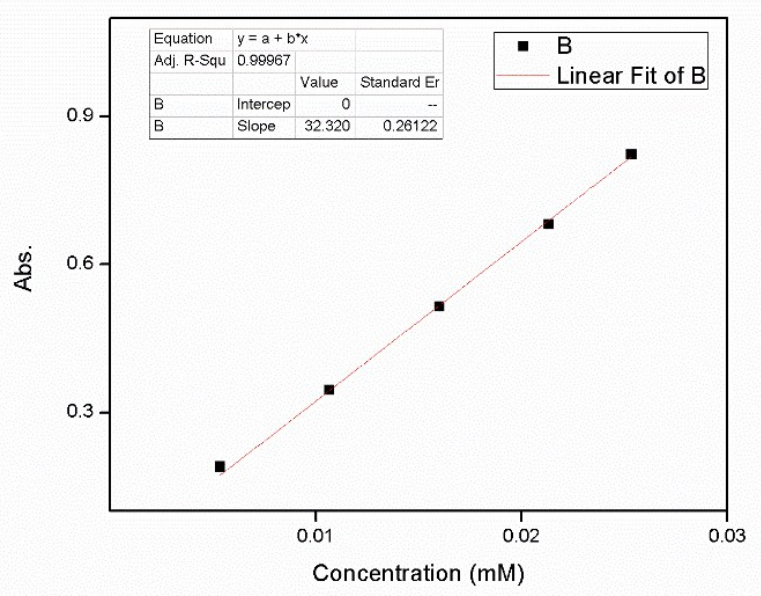


Fig. S9 Calibration curve of Orotic Acid in distilled water at 279 nm wavelength.

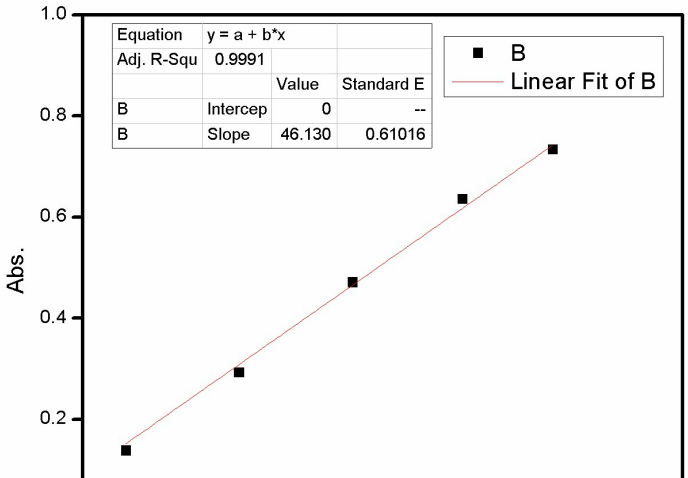


Fig. S10 Calibration curve of solid **1** in distilled water at 279 nm wavelength.

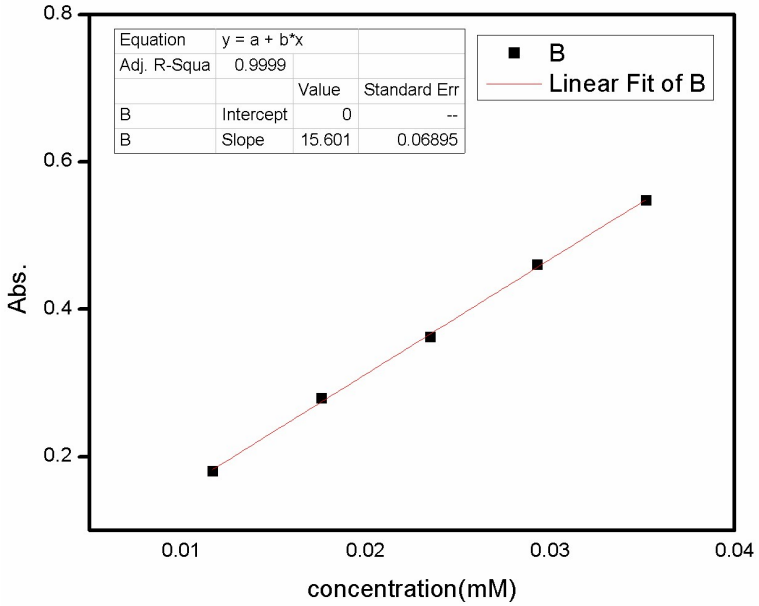


Fig. S11 Calibration curve of solid **2** in distilled water at 279 nm wavelength.

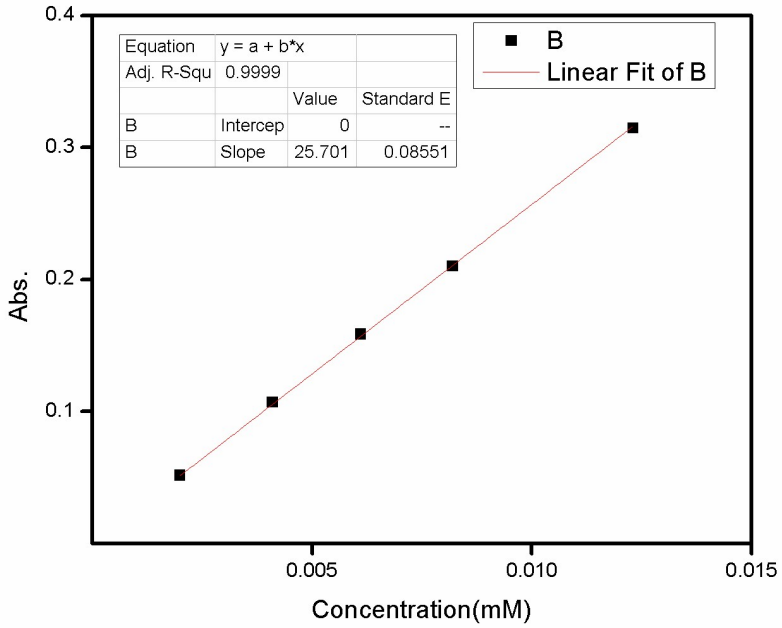


Fig. S12 Calibration curve of solid **3** in distilled water at 279 nm wavelength.

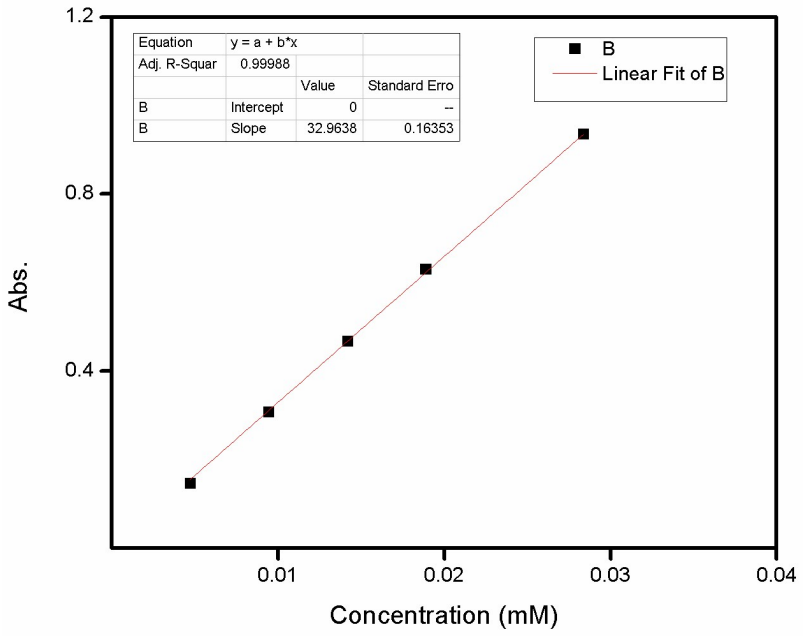


Fig. S13 Calibration curve of solid **4** in distilled water at 279 nm wavelength.

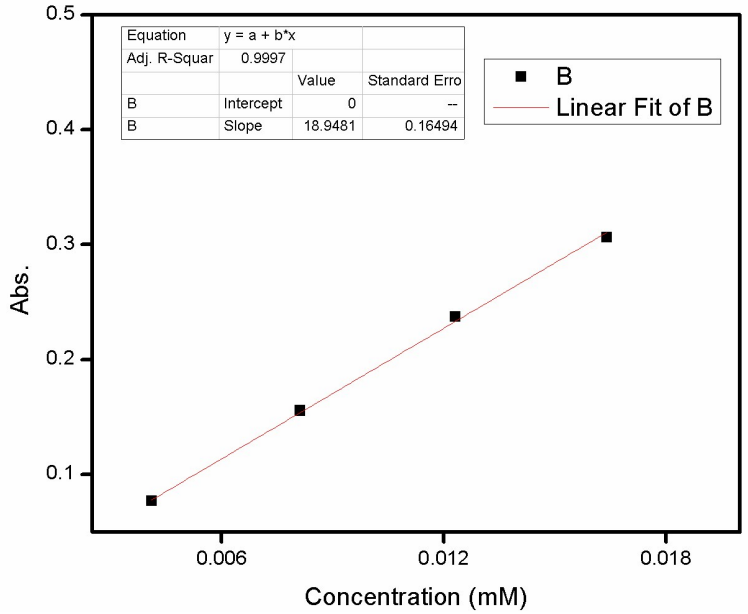


Fig. S14 Calibration curve of solid **5** in distilled water at 279 nm wavelength.

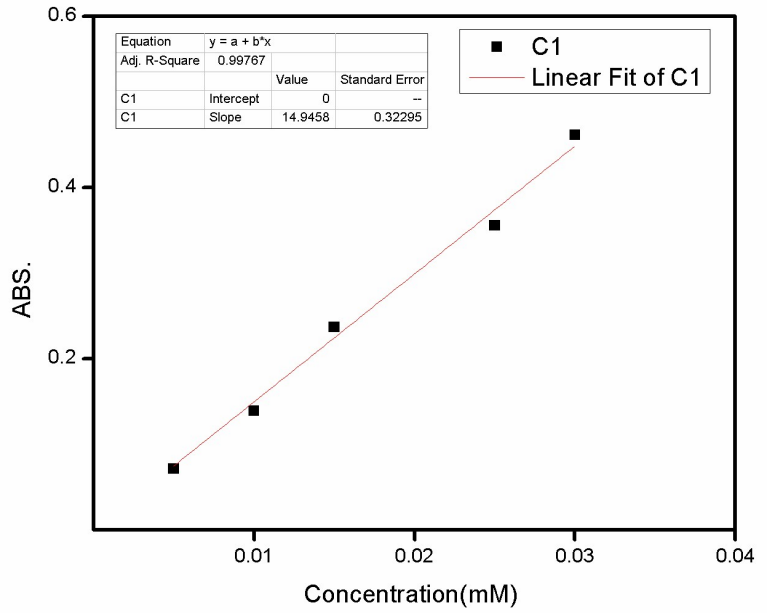


Fig. S15 Calibration curve of solid **6** in distilled water at 279 nm wavelength.

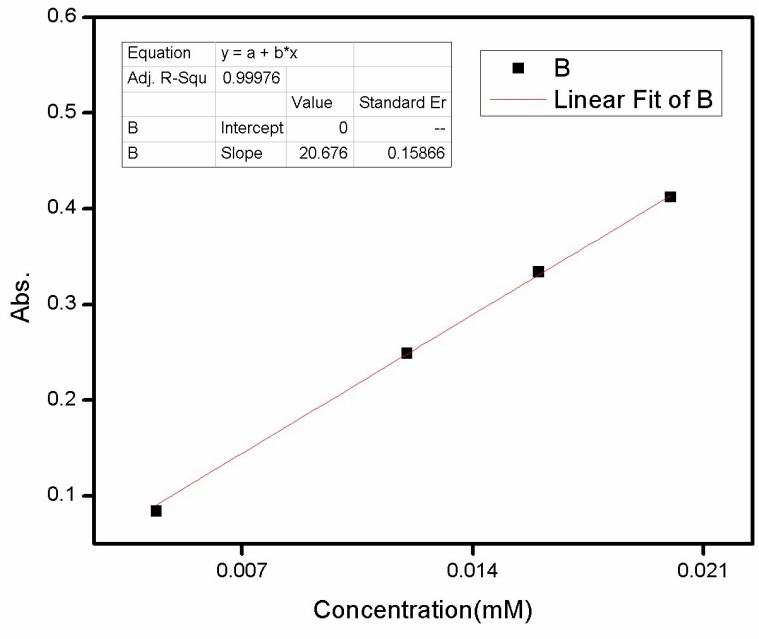


Fig. S16 Calibration curve of solid **7** in distilled water at 271 nm wavelength.

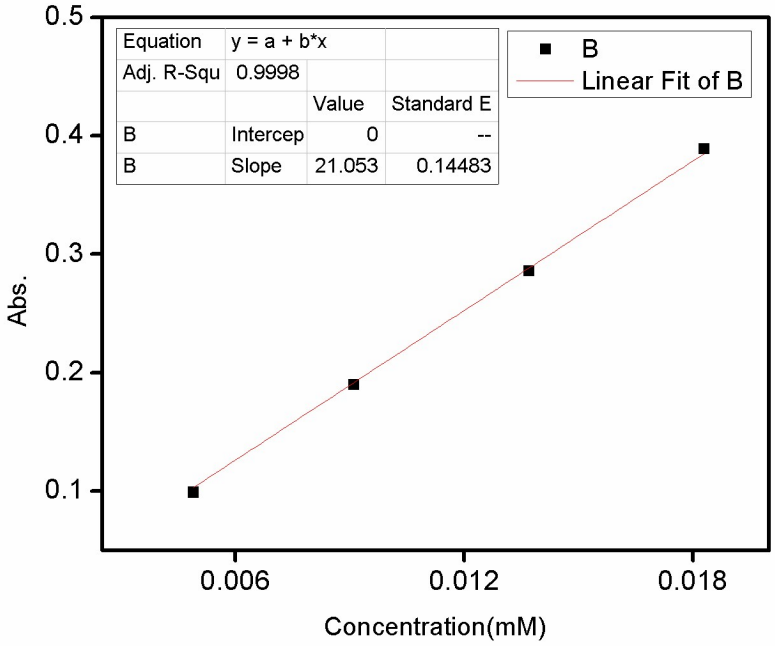


Fig. S17 Calibration curve of solid **8** in distilled water at 271 nm wavelength.

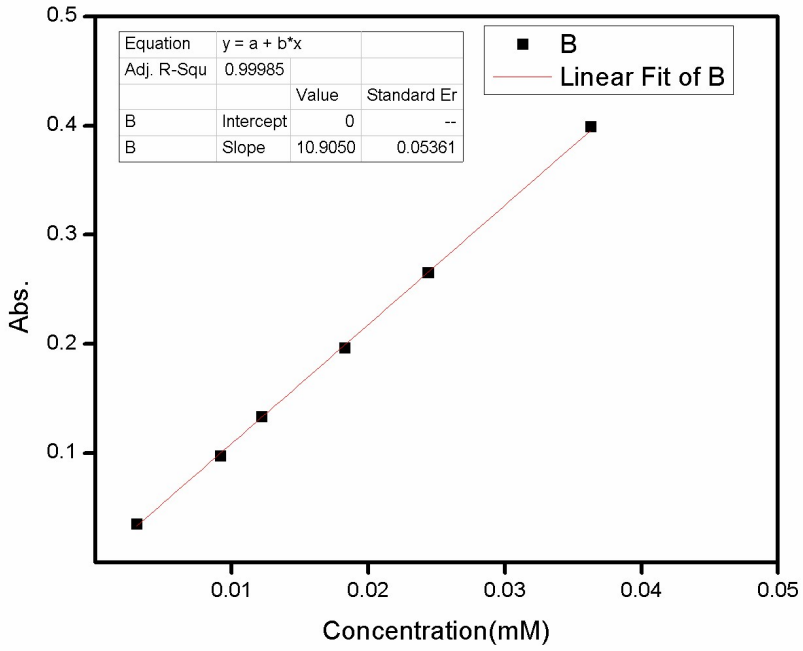


Fig. S18 Calibration curve of solid **9** in distilled water at 271 nm wavelength.

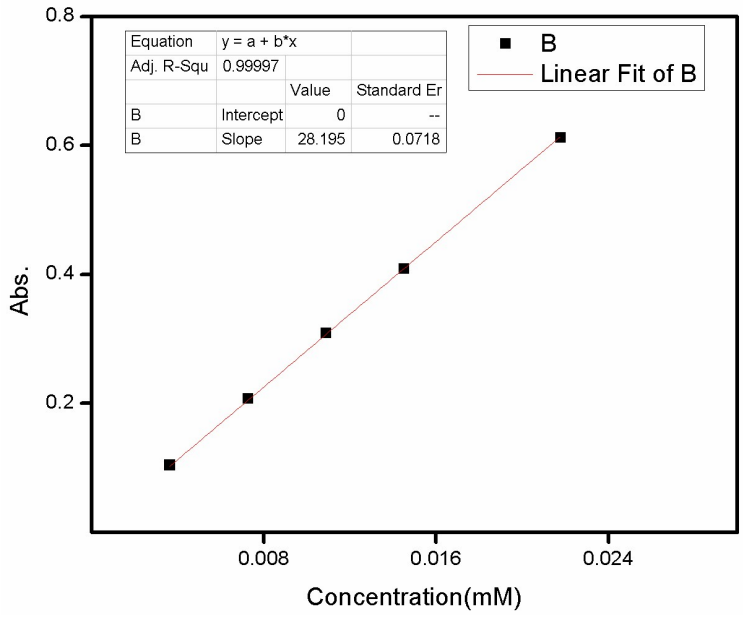


Fig. S18 Calibration curve of solid **10** in distilled water at 271 nm wavelength.