Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information

Crystal Structure and Physical Stability of Ginsenoside Compound-K Solvates

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1. **Tables**
2. **Figures**

Table S1. Hydrogen bonds between solvent and GCK molecule in solvates

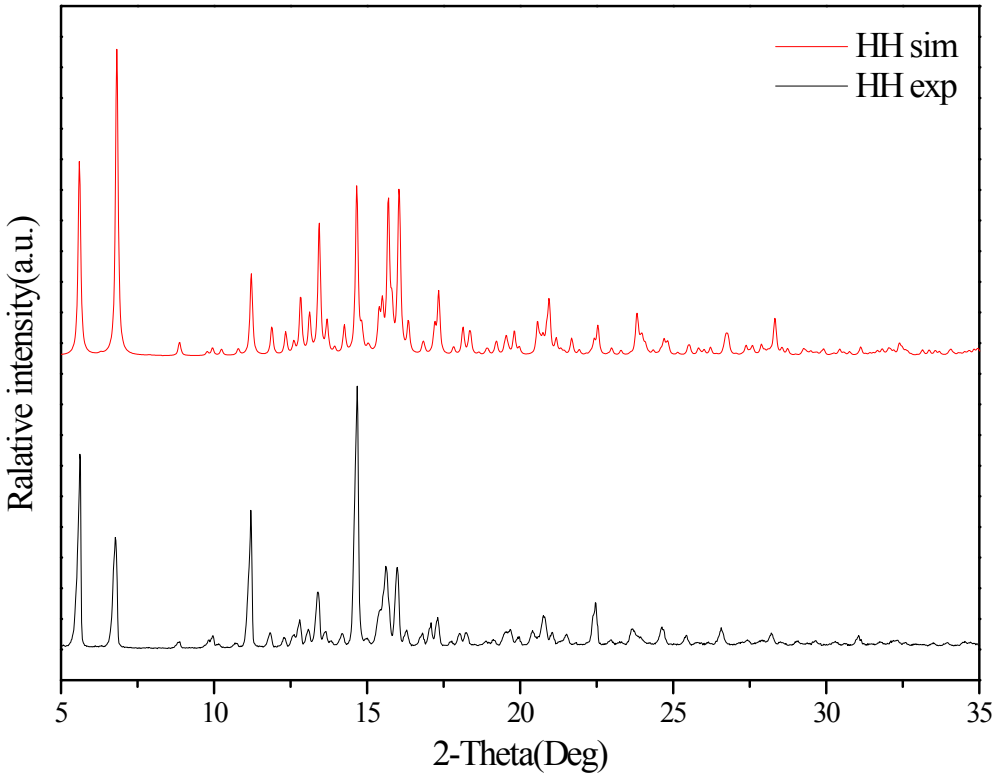
Donor-H…Acceptor	D-H (Å)	H…A (Å)	D…A (Å)	∠D-H…A (°)	Symmetry codes
HH					
O_{8A}-H_{8A}…O_9	0.94(4)	1.98(5)	2.859(4)	157(4)	1-x, 1/2+y, 1-z
O_9-H_{9C}…O_{5A}	0.73(8)	2.06(8)	2.781(4)	172(6)	x, y, z
O_9-H_{9B}…O_{2A}	0.95(9)	2.25(9)	3.186(4)	171(7)	1-x, -1/2+y, 1-z
MH					
O_4-H_4…O_9	0.84	2.06	2.868(3)	162	x, y, z
O_8-H_8…O_9	0.79(5)	2.14(5)	2.895(4)	161(4)	x, 1+y, z
O_9-H_{9A}…O_2	0.87	1.93	2.763(3)	160	2-x, -1/2+y, 2-z
S_{Et}					
O_4-H_4…O_{10}	0.82(8)	2.08(8)	2.870(7)	162(6)	x, y, z
O_5-H_5…O_9	0.84	2.08	2.880(7)	159	x, y, z
O_{10}-H_{10}…O_1	0.84	2.00	2.824(7)	167	1-x, 1/2+y, 1-z
O_9-H_{9B}…O_{8A}	0.84	2.39	2.899 (7)	119	1-x, 1/2+y, 2-z
S_{MeW}					
O_4-H_4…O_{11}	0.83(3)	1.98(3)	2.802(3)	174(3)	x, y, z
O_6-H_6…O_{10}	0.84	1.94	2.746(3)	159	-x, -1/2+y, -1-z
O_{11}-H_{11C}…O_1	0.90(5)	1.98(5)	2.849(3)	163(4)	x, -1+y, z
O_8-H_8…O_{10}	0.84	2.02	2.807(3)	155	x, y, z
O_9-H_{9A}…O_4	0.84	2.00	2.829(3)	169	x, y, z
O_{10}-H_{10A}…O_2	0.84	1.82	2.659(3)	177	x, y, z
O_{11}-H_{11D}…O_9	0.81(5)	2.08(5)	2.868(3)	166(5)	-1-x, 1/2+y, -1-z
S_{EtW}					
O_4-H_4…O_{11}	0.84	1.98	2.815(3)	170	-1+x, y, z
O_6-H_6…O_9	0.84	2.01	2.819(3)	160	1-x, -1/2+y, -z
O_8-H_8…O_9	0.84	2.05	2.819(3)	153	x, y, z
O_9-H_{9A}…O_2	0.84	1.88	2.706(3)	169	x, y, z
O_{10}-H_{10}…O_4	0.78(7)	2.12(7)	2.885(3)	167(6)	1-x, 1/2+y, 1-z
O_{11}-H_{11C}…O_1	0.85	2.07	2.911 (3)	171	1+x, -1+y, z
O_{11}-H_{11D}⋯O_{10}	0.80(5)	2.08(5)	2.869(4)	168(5)	x, y, -1+z
S_{iPrW}					
O_4-H_4…O_{10}	0.76(6)	2.05(6)	2.795(4)	170(5)	x, y, z
O_6-H_6…O_9	0.71(4)	2.05(4)	2.746(4)	166(4)	2-x, -1/2+y, 1-z
O_8-H_8…O_9	0.80(5)	2.04(5)	2.817(4)	163(4)	x, y, z
O_9-H_{9A}…O_2	0.84(6)	1.86(6)	2.687(4)	170(6)	x, y, z
O_{10}-H_{10B}…O_{11}	0.86(6)	2.06(5)	2.894(5)	163(5)	1-x, 1/2+y, 1-z
O_{10}-H_{10A}…O_1	0.86(6)	1.97(6)	2.818(5)	171(5)	x, -1+y, z
O_{11}-H_{11D}⋯O_8	0.90(19)	2.56(18)	3.319(5)	142(14)	2-x, -1/2+y, 1-z
O_{11}-H_{11C}⋯O_4	0.81(10)	2.05(10)	2.849(5)	172(5)	x, y, z

Table S2. Relative proportion of the close contact for water molecule in hydrates and

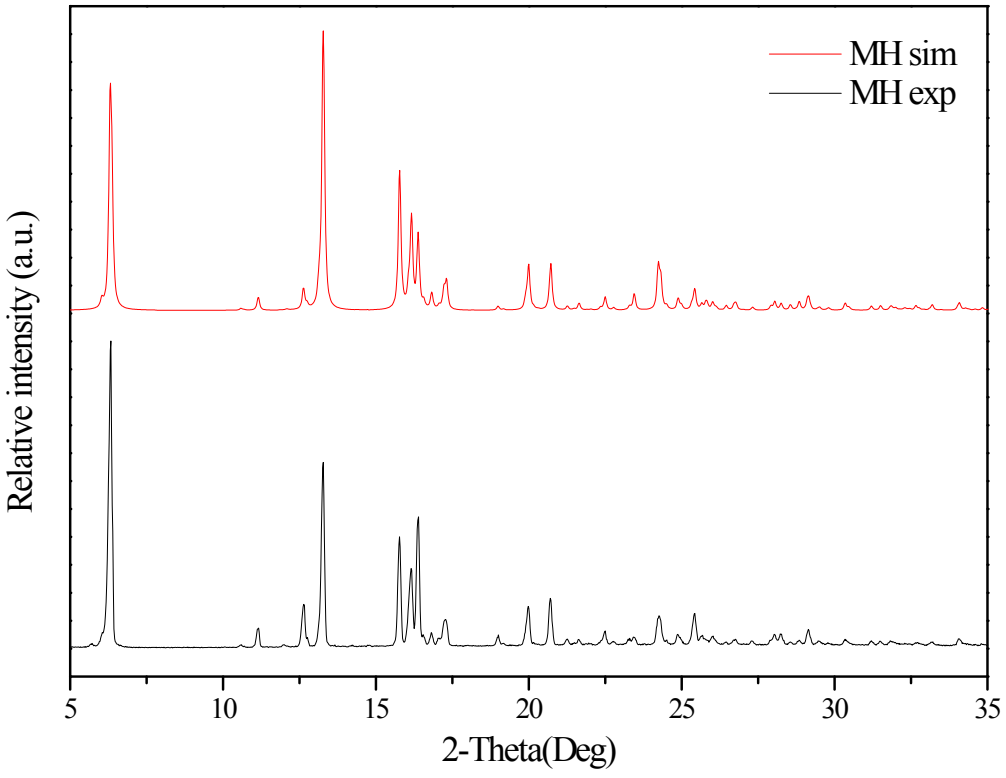
mixed solvates.

Form / contact	H-O	O-H	H-H
HH	23.9	29.3	46.8
MH	23.2	30.3	46.6
S_{MeW}	20.8	30.5	48.7
S_{EtW}	21.5	30.1	48.4
S_{iPrW}-1	22.1	28	50.1
S_{iPrW}-2	17.5	27.2	55.3

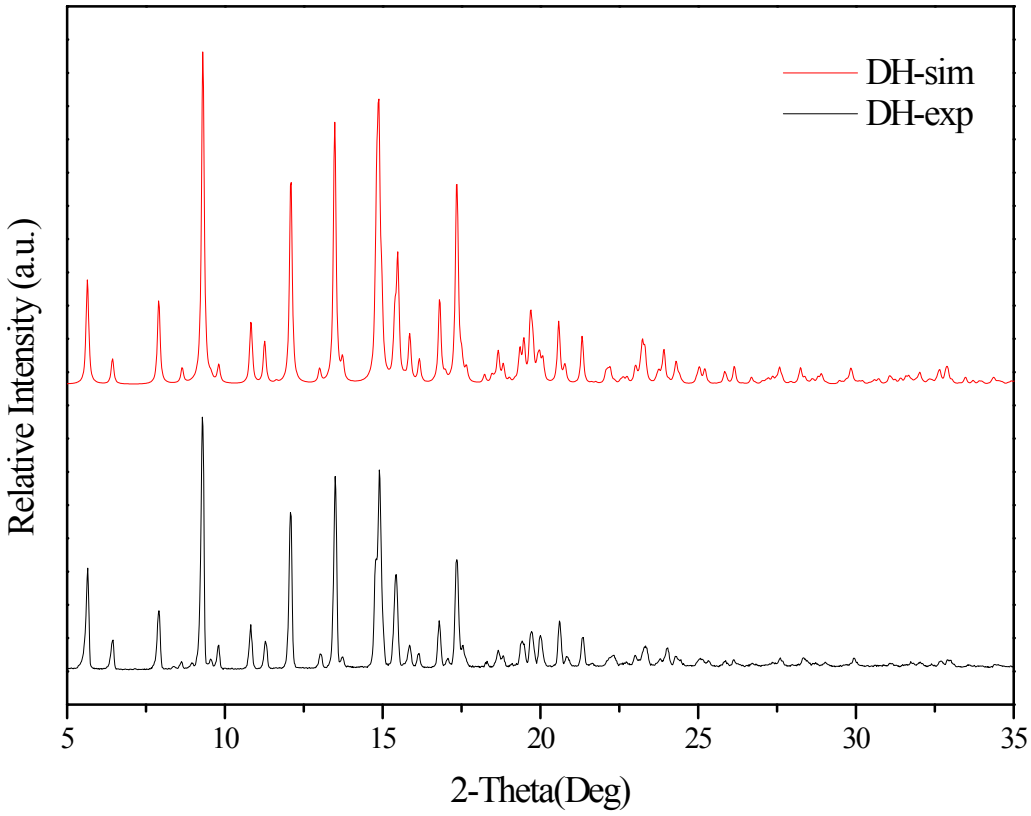
2. Figures.


HH sim
HH exp
Ralative intensity(a.u.)
5
10
15
20
25
30
35
2-Theta(Deg)

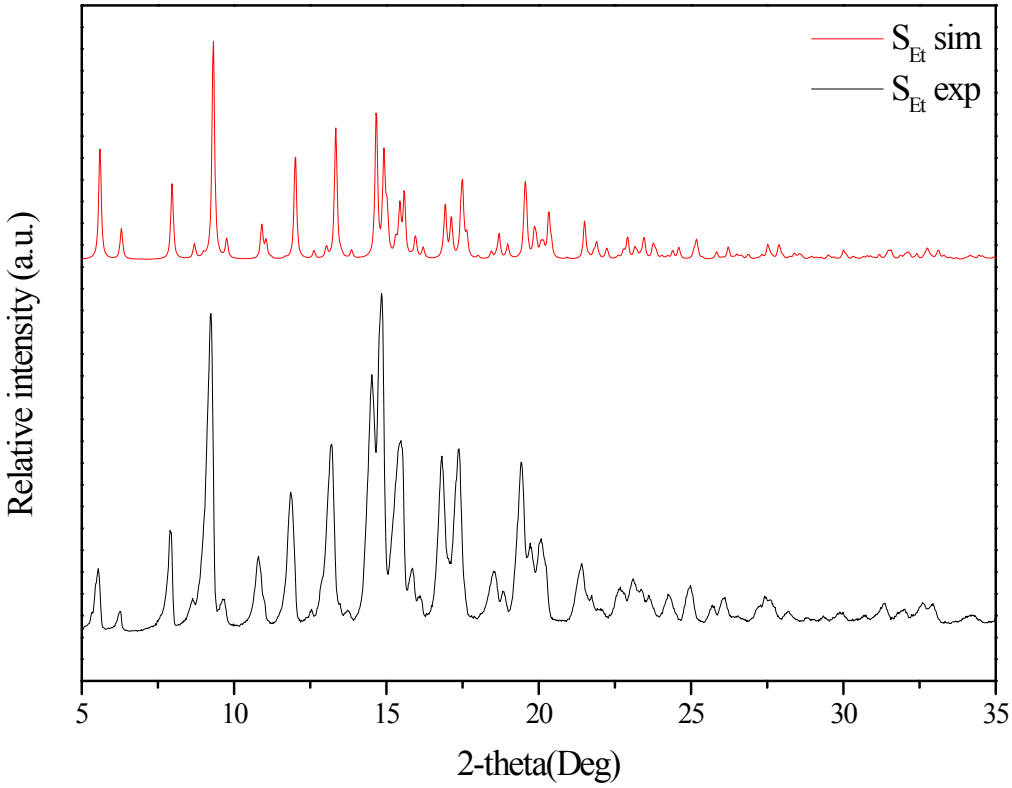
(a)


MH sim
MH exp
Relative intensity (a.u.)
5
10
15
20
25
30
35
2-Theta(Deg)

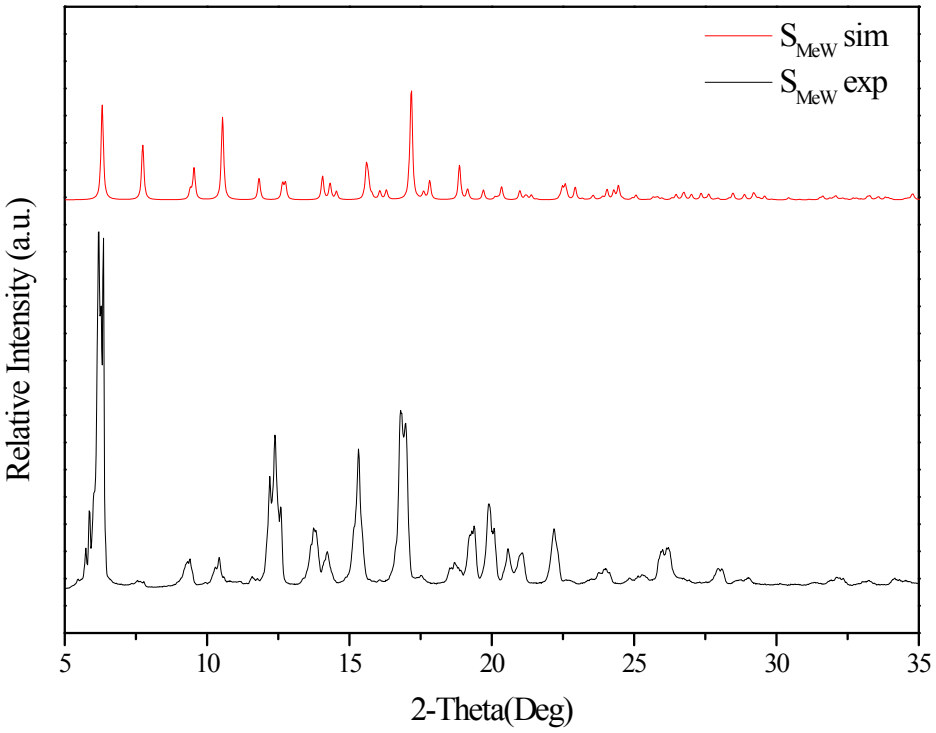
(b)


DH-sim
DH-exp
Relative Intensity (a.u.)
5
10
15
20
25
30
35
2-Theta(Deg)

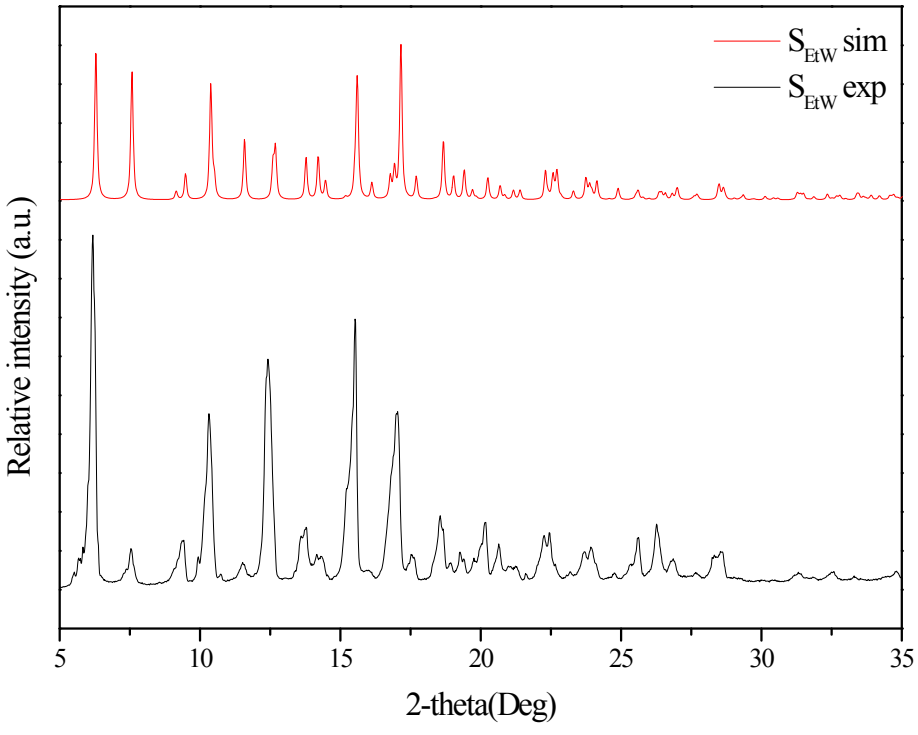
(c)


S_Et sim
S_Et exp
Relative intensity (a.u.)
5
10
15
20
25
30
35
2-theta(Deg)

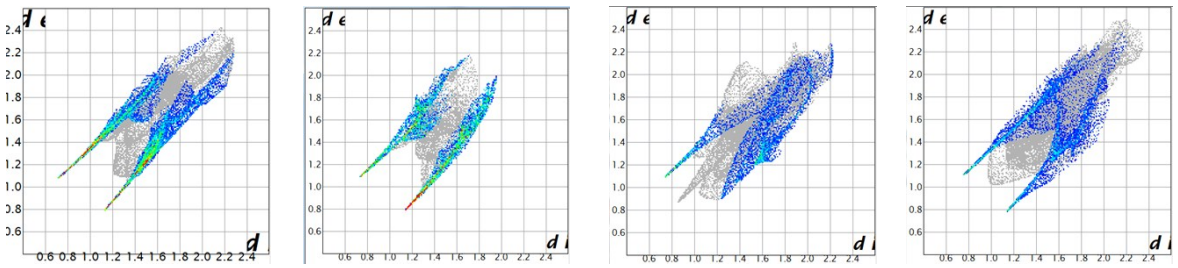
(d)


S_MeW sim
S_MeW exp
Relative Intensity (a.u.)
5
10
15
20
25
30
35
2-Theta(Deg)

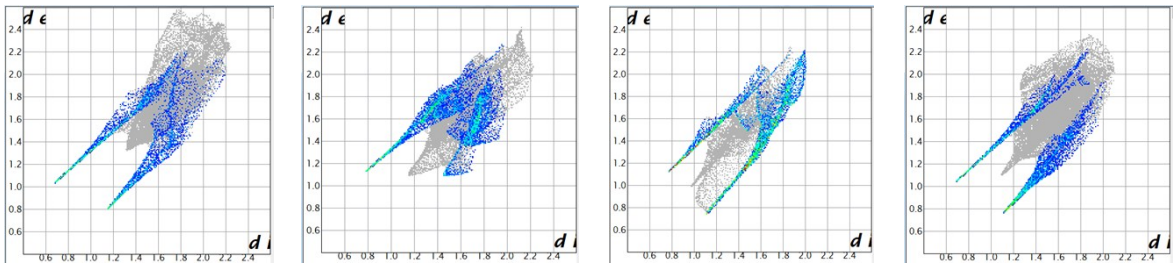
(e)


S_EtW sim
S_EtW exp
Relative intensity (a.u.)
5
10
15
20
25
30
35
2-theta(Deg)

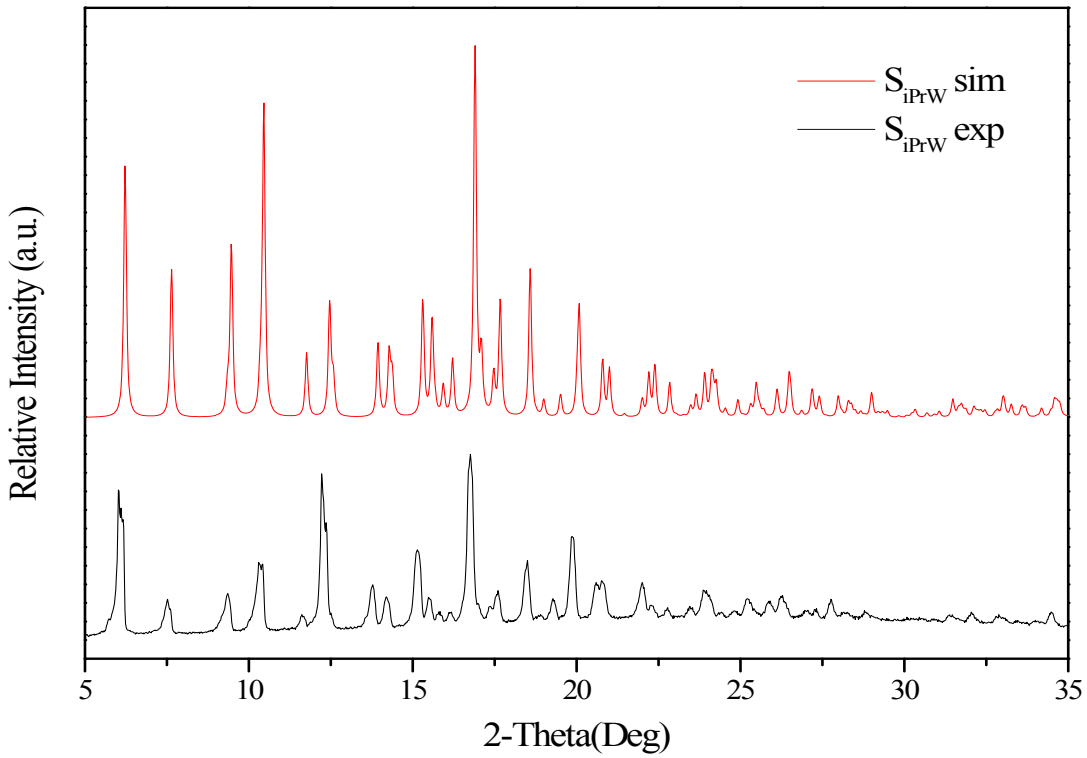
(f)



(a) HH-water (b) MH-water (c) S_{Et}-EtOH-O9 (d) S_{Et}-EtOH-O10

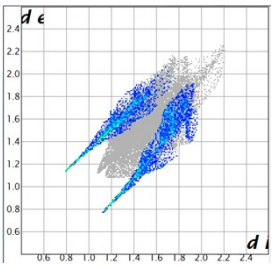


(e) S_{MeW}-MeOH-O9 (f) S_{MeW}-MeOH-O10 (g) S_{MeW}-water (h) S_{EtW}-EtOH-O9

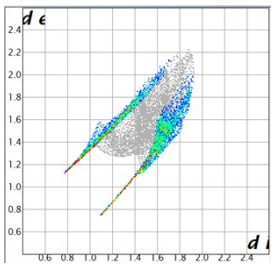


(g)

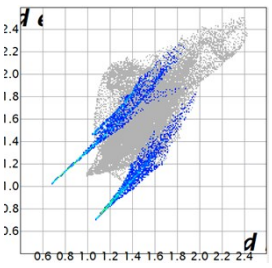
Figure S1. The comparison between the powder patterns obtained experimentally and simulated patterns generated from the single-crystal diffraction data.



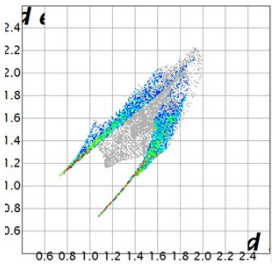
(i) S_{EtW}-EtOH-O10



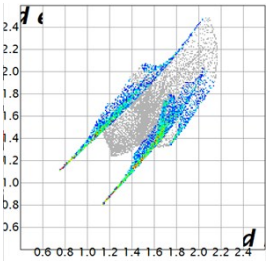
(j) S_{EtW}-water



(k) S_{iPrW}-iPrOH

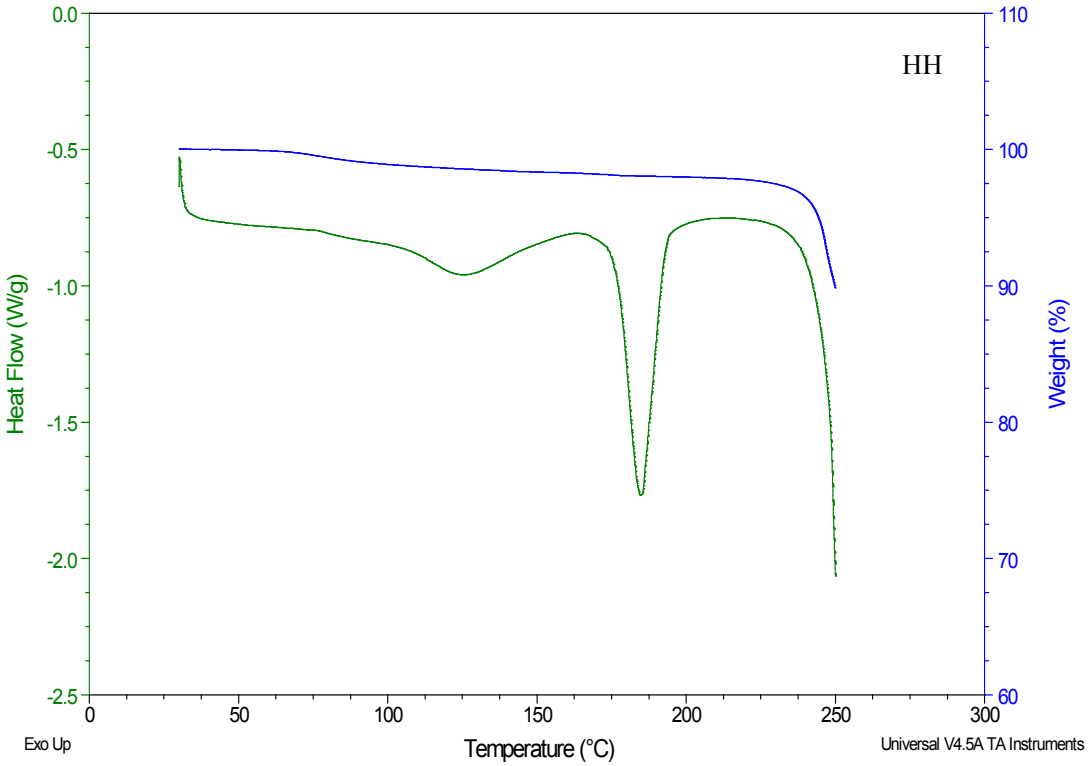


(l) S_{iPrW}-water-O10

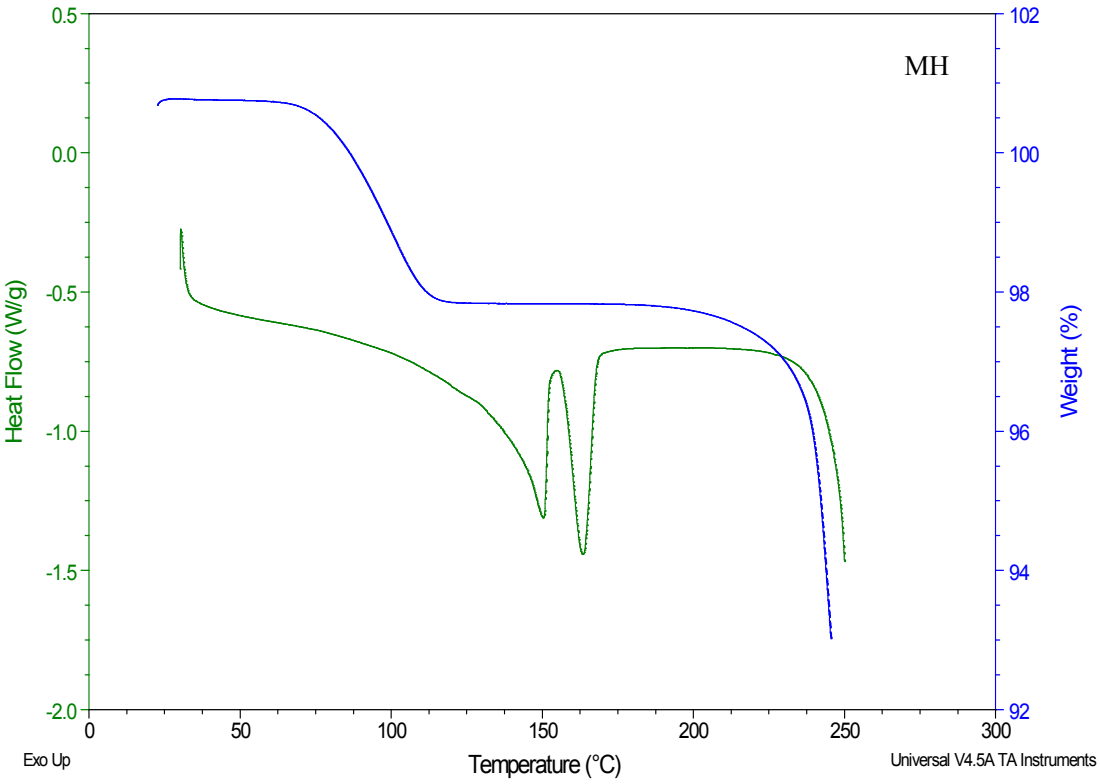


(m) S_{iPrW}-water-O11

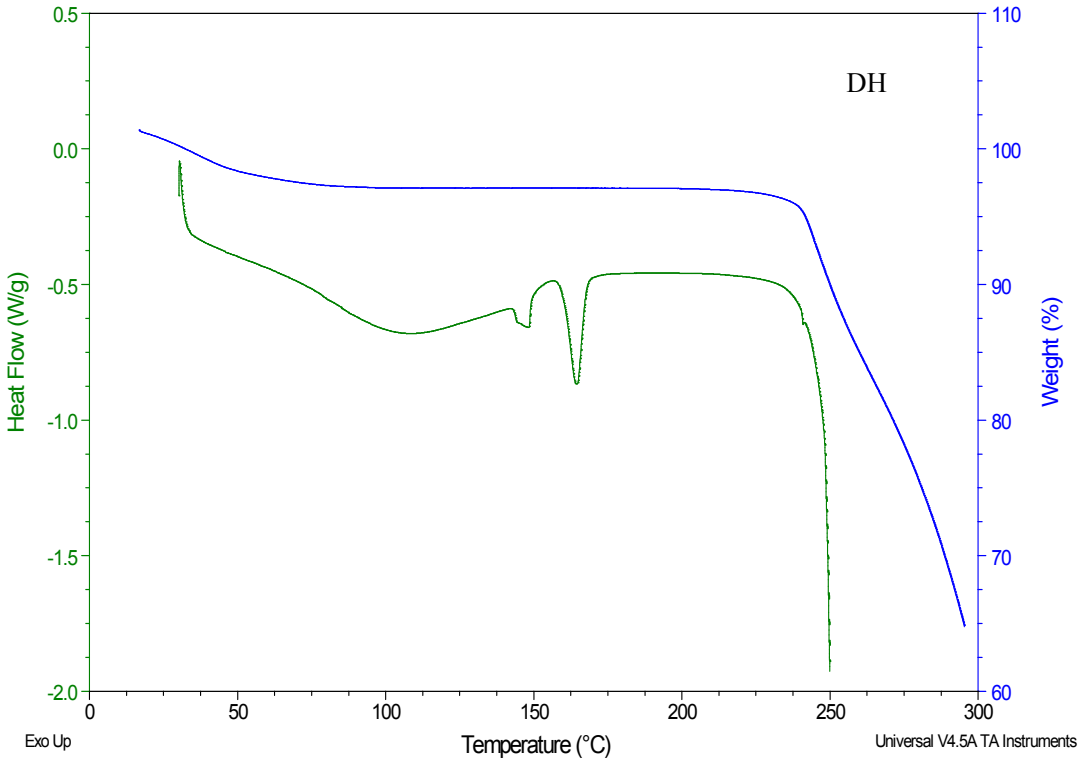
Figure S2. The O···H intermolecular contacts of 2D fingerprint plots from Hirshfeld surface analyses of solvent molecules.


HH
Heat Flow (W/g)
Weight (%)
Temperature (°C)
Exo Up
Universal V4.5A TA Instruments
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
110
100
90
80
70
60
0
50
100
150
200
250
300

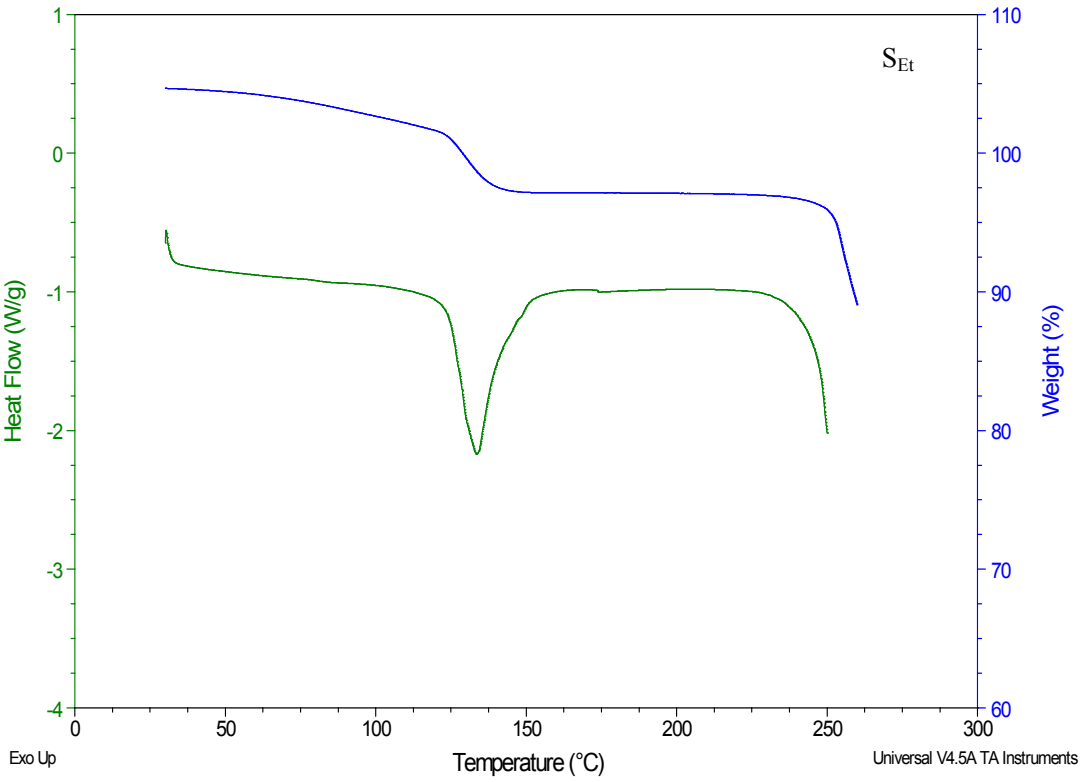
(a)


MH
Heat Flow (W/g)
Weight (%)
Temperature (°C)
Exo Up
Universal V4.5A TA Instruments
0.5
0.0
-0.5
-1.0
-1.5
-2.0
102
100
98
96
94
92
0
50
100
150
200
250
300

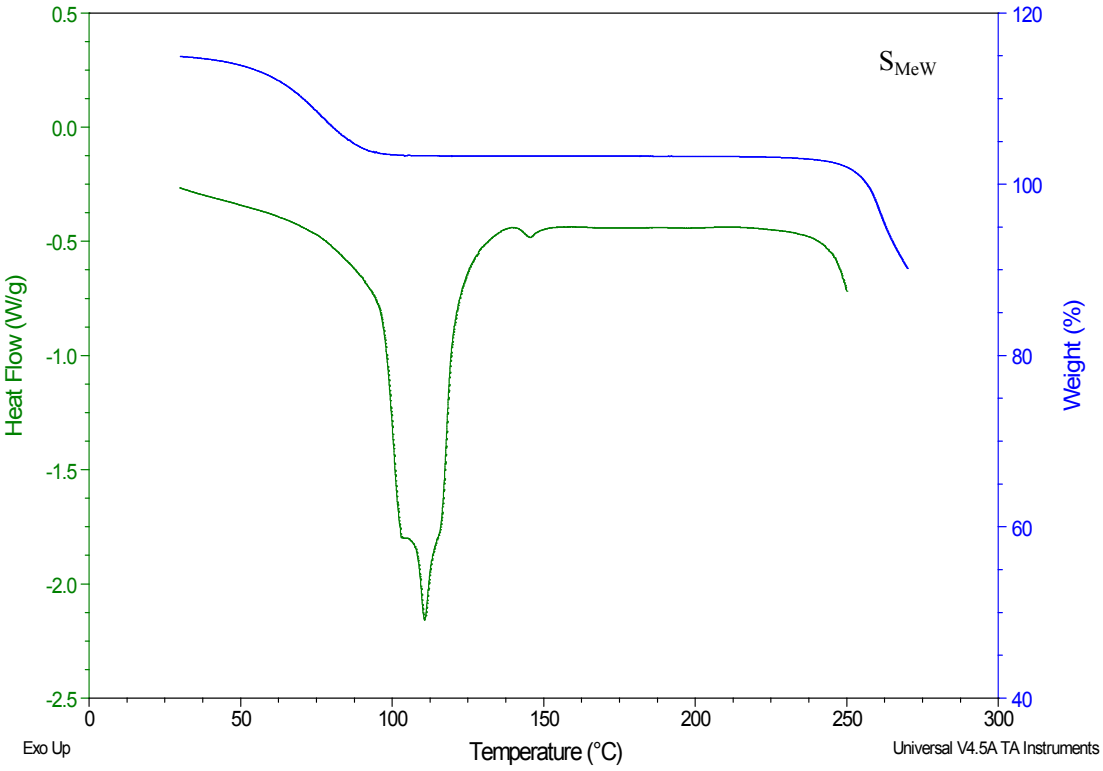
(b)


DH
Heat Flow (W/g)
Weight (%)
Temperature (°C)
Exo Up
Universal V4.5A TA Instruments

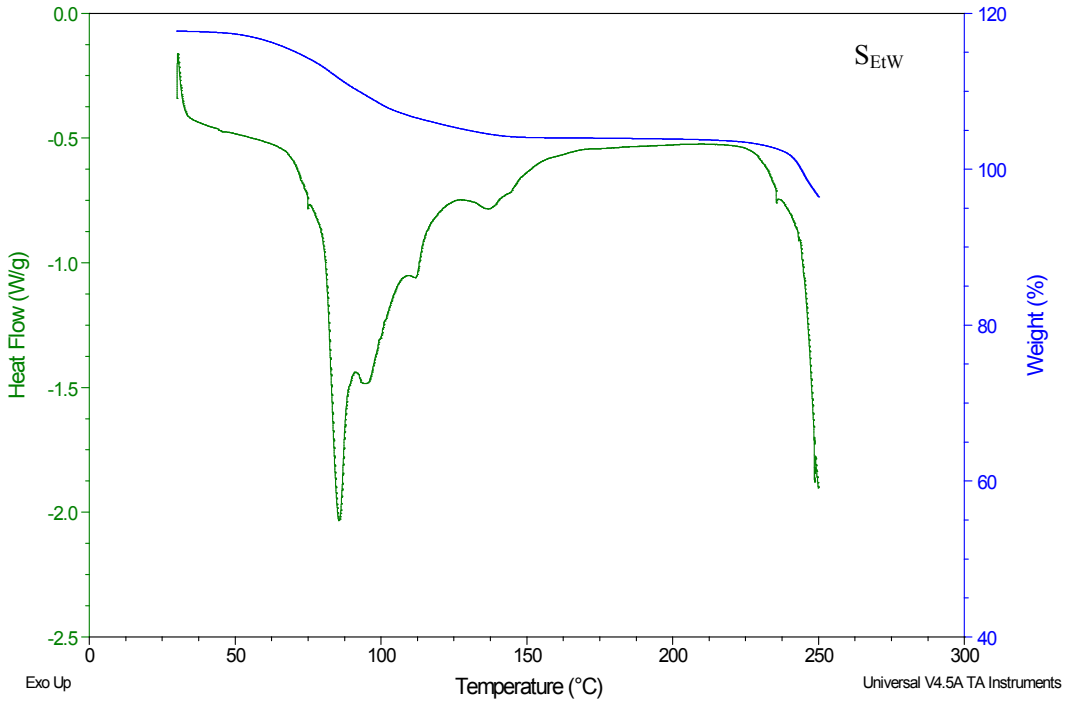
(c)


S$_{Et}$
Heat Flow (W/g)
Weight (%)
Temperature (°C)
Exo Up
Universal V4.5A TA Instruments

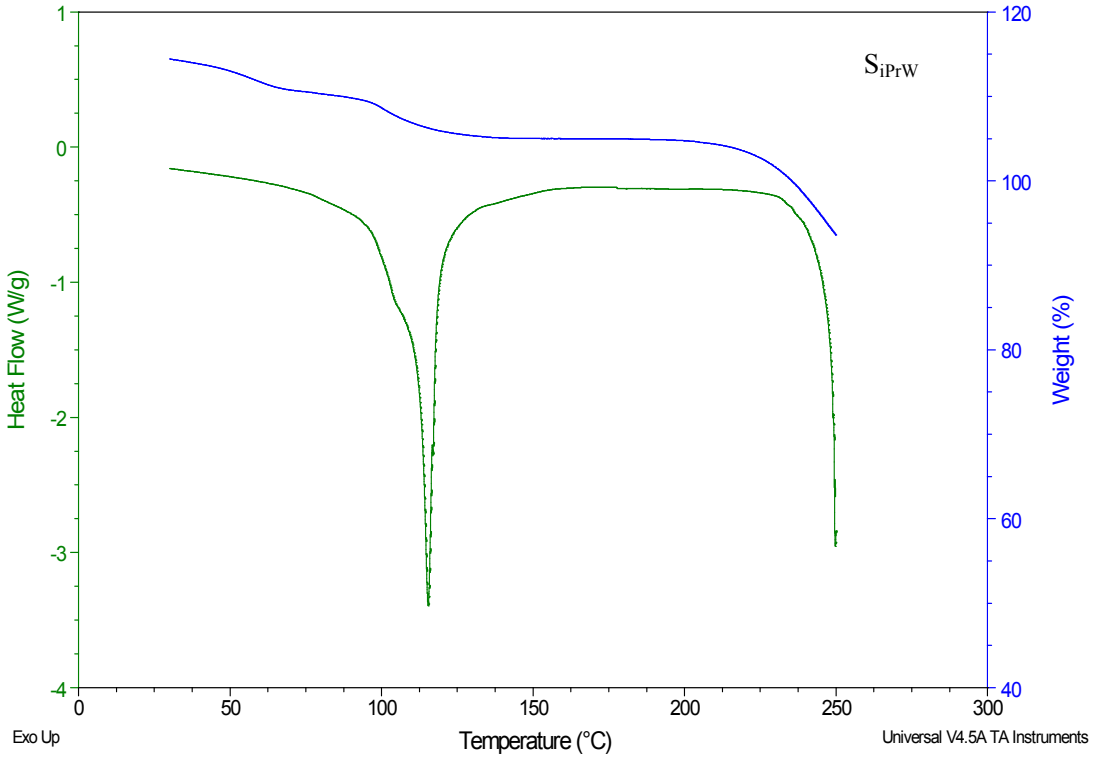
(d)


S_{MeW}
Heat Flow (W/g)
Weight (%)
Temperature (°C)
Exo Up
Universal V4.5A TA Instruments

(e)

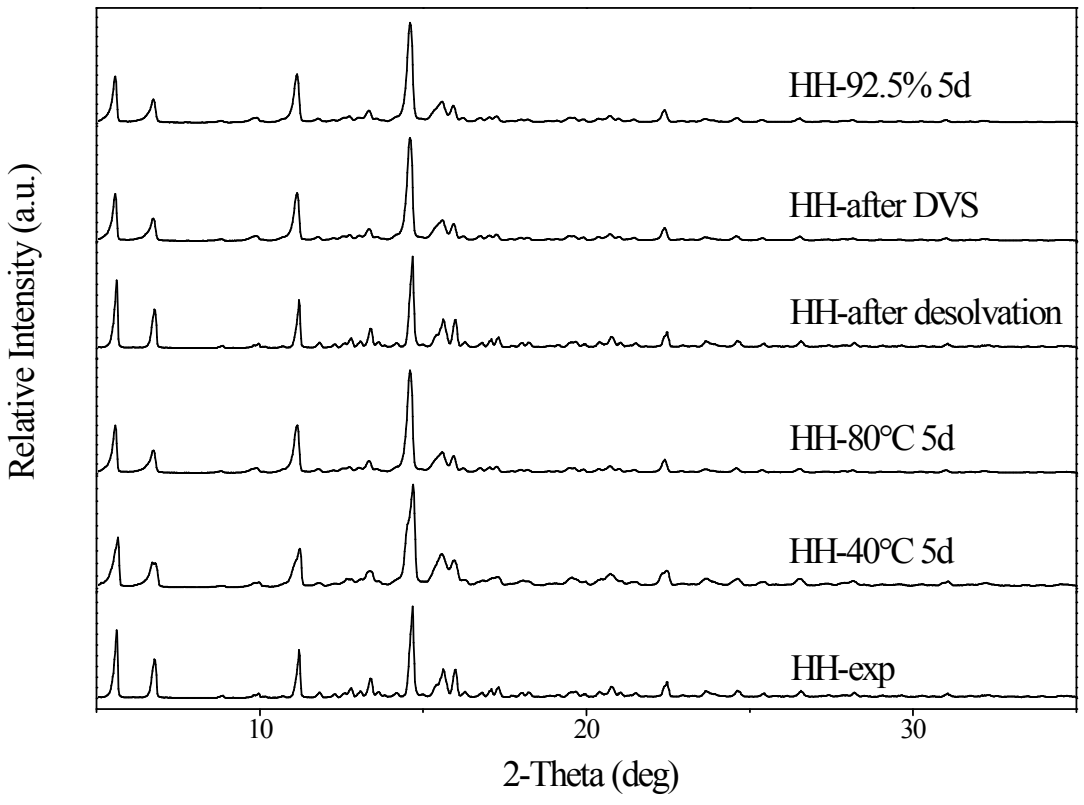

S_{EtW}
Heat Flow (W/g)
Weight (%)
Temperature (°C)
Exo Up
Universal V4.5A TA Instruments

(f)

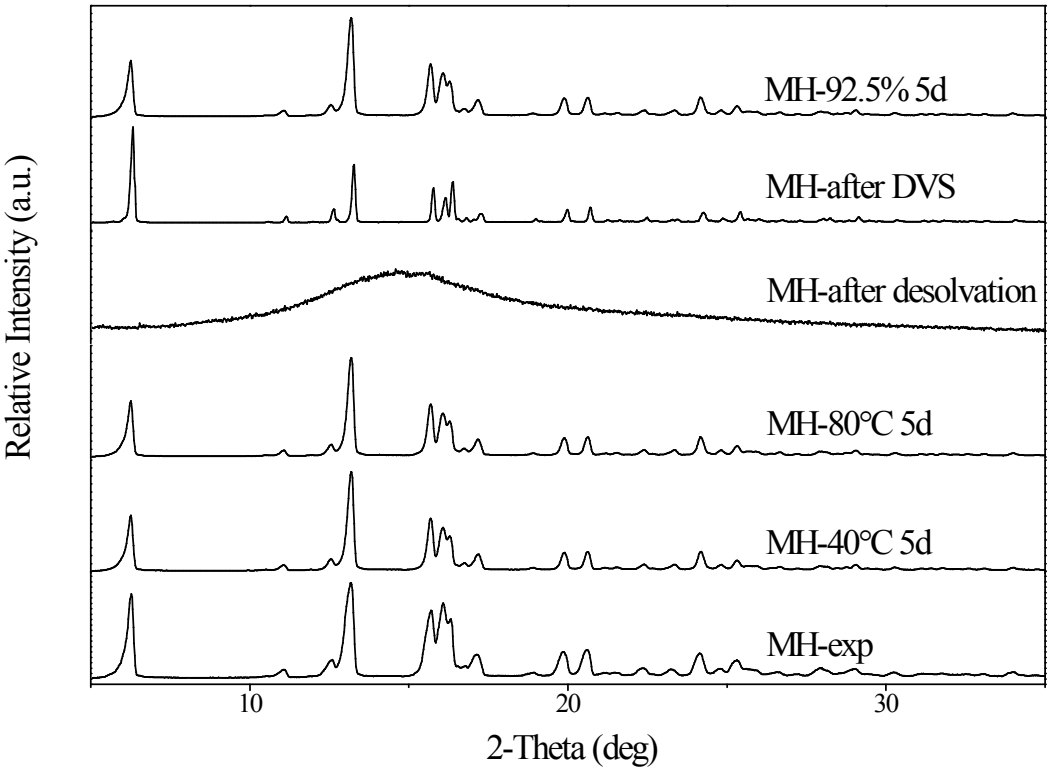


(g)

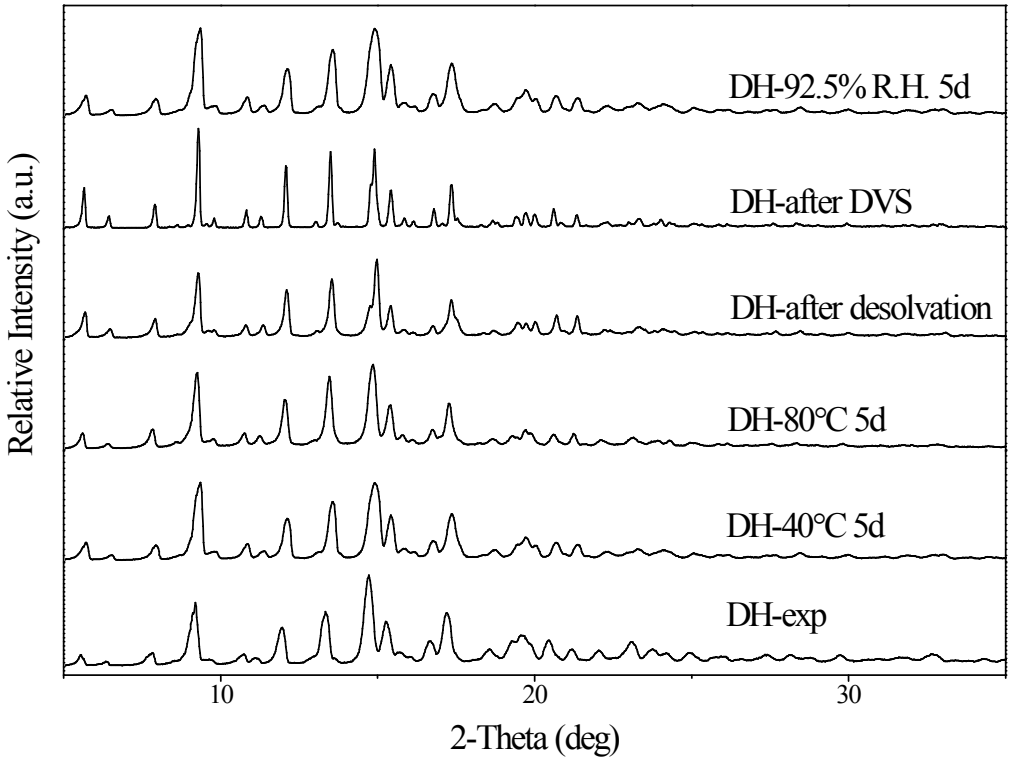
Figure S3. DSC diagrams of all GCK solvates.



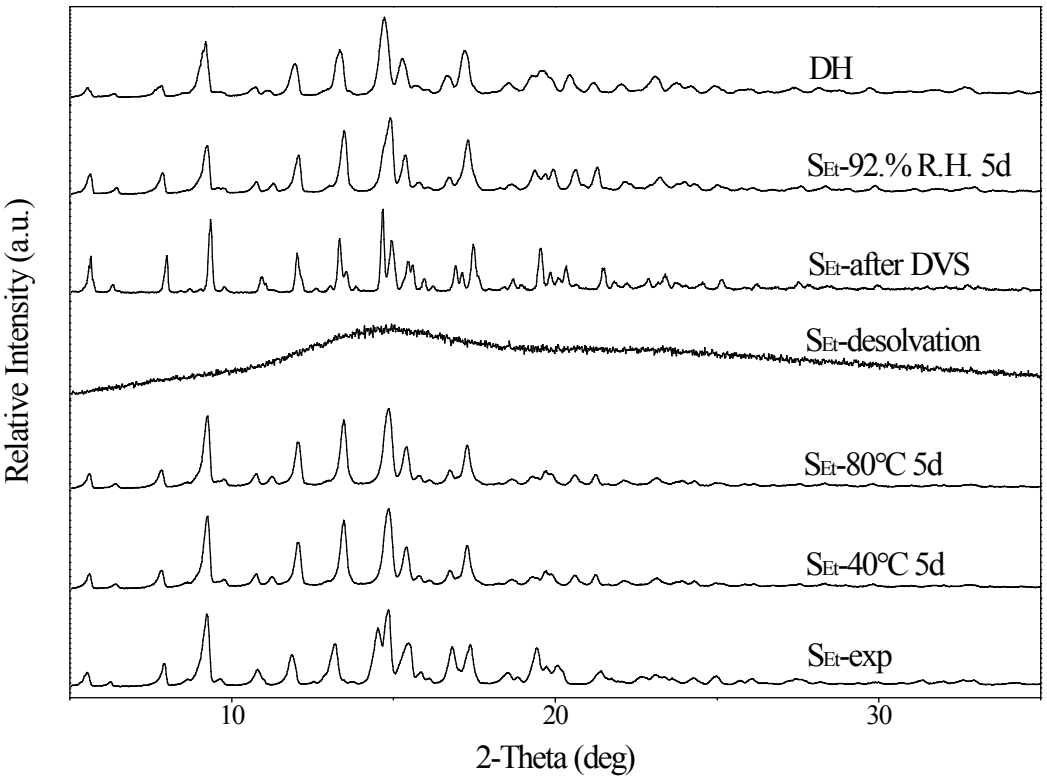
(a)


MH-92.5% 5d
MH-after DVS
MH-after desolvation
MH-80℃ 5d
MH-40℃ 5d
MH-exp
Relative Intensity (a.u.)
10
20
30
2-Theta (deg)

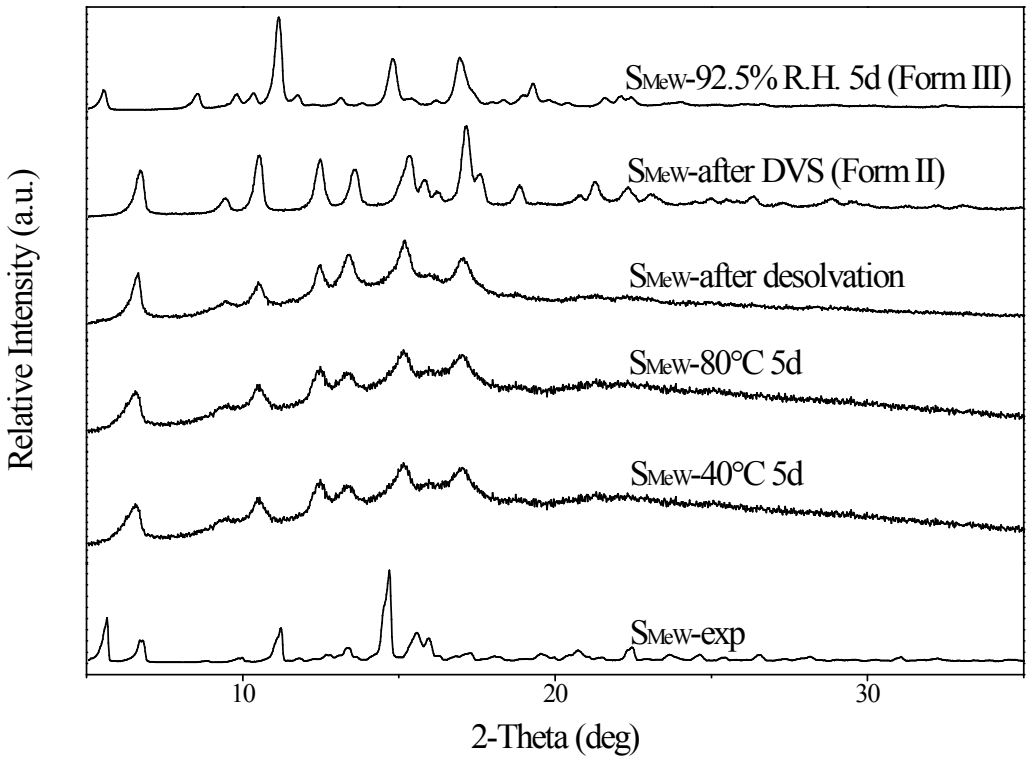
(b)


DH-92.5% R.H. 5d
DH-after DVS
DH-after desolvation
DH-80℃ 5d
DH-40℃ 5d
DH-exp
Relative Intensity (a.u.)
10
20
30
2-Theta (deg)

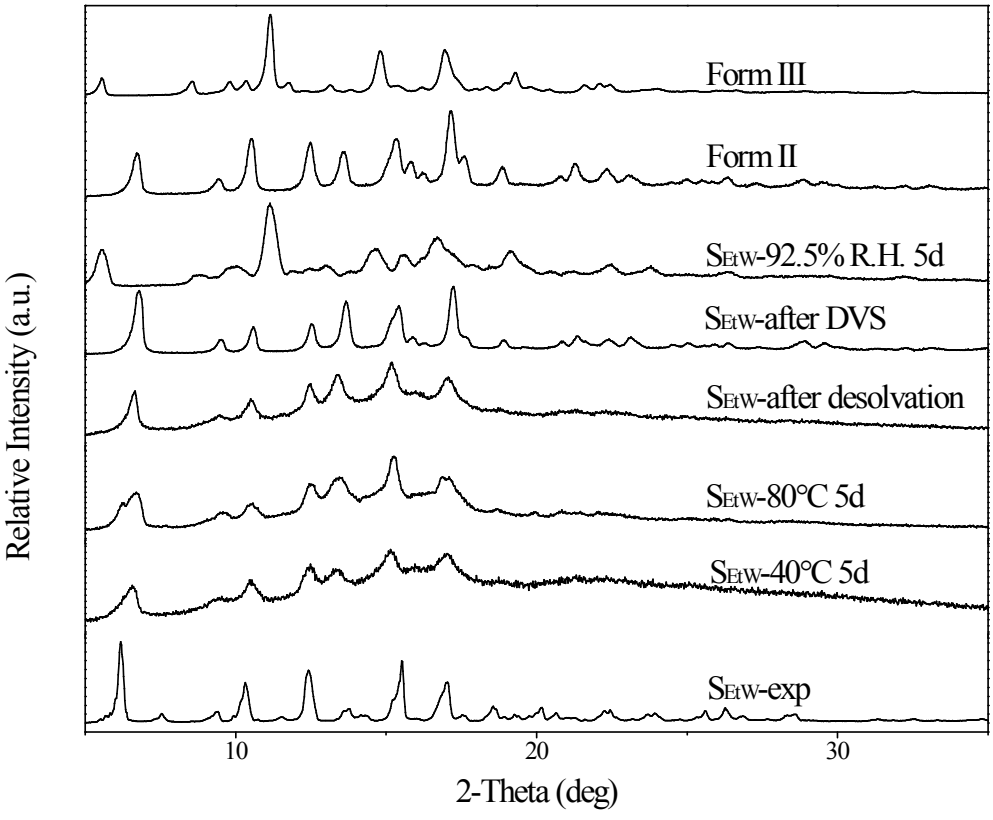
(c)


DH
SEt-92.% R.H. 5d
SEt-after DVS
SEt-desolvation
SEt-80℃ 5d
SEt-40℃ 5d
SEt-exp
Relative Intensity (a.u.)
10
20
30
2-Theta (deg)

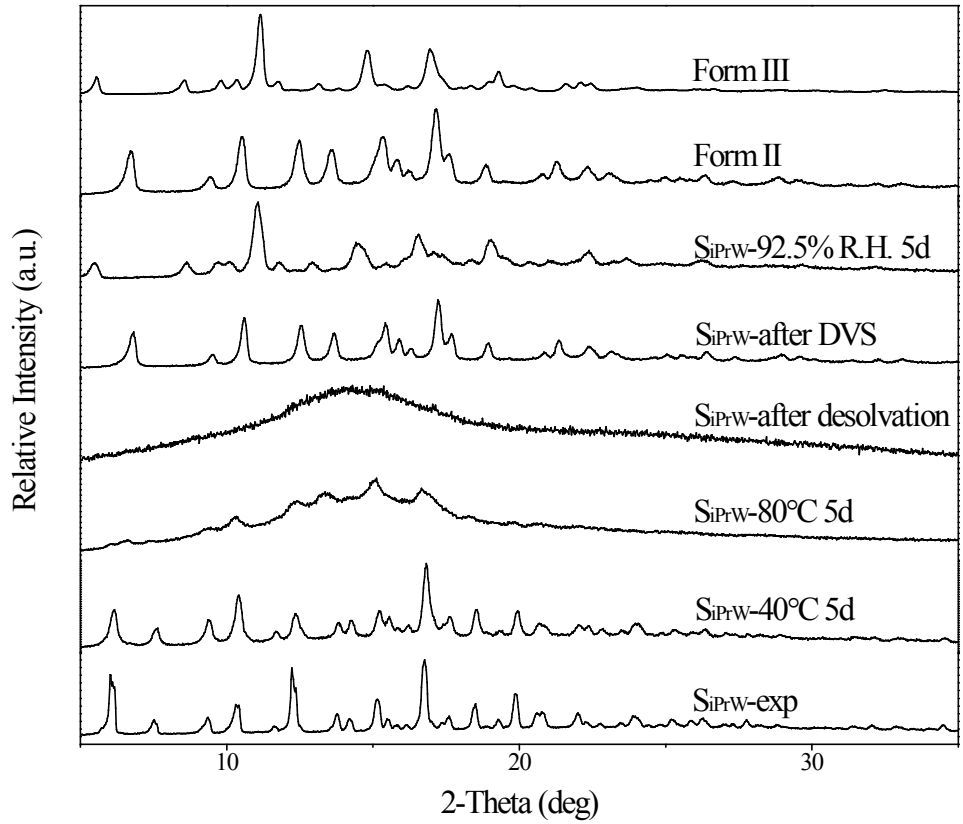
(d)


SMeW-92.5% R.H. 5d (Form III)
SMeW-after DVS (Form II)
SMeW-after desolvation
SMeW-80℃ 5d
SMeW-40℃ 5d
SMeW-exp
Relative Intensity (a.u.)
10
20
30
2-Theta (deg)

(e)



(f)



(g)

Figure S4. PXRD patterns of the resulting solid after desolvation and DVS experiments for GCK solvates.

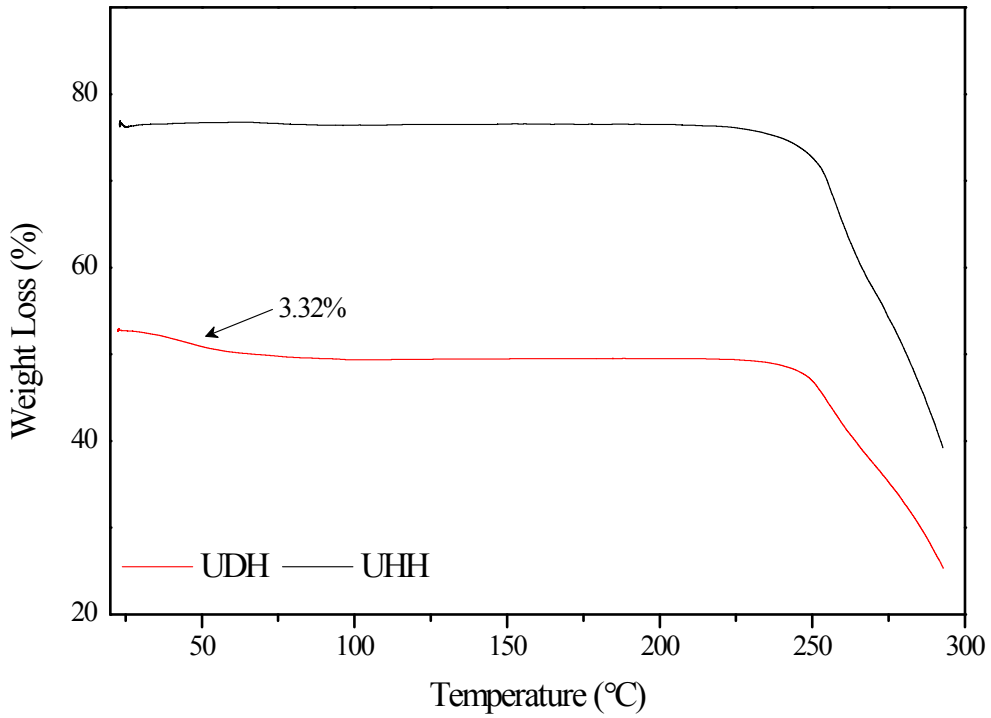


Figure S5. TGA cycle curves of UHH and UDH after PXRD performance.

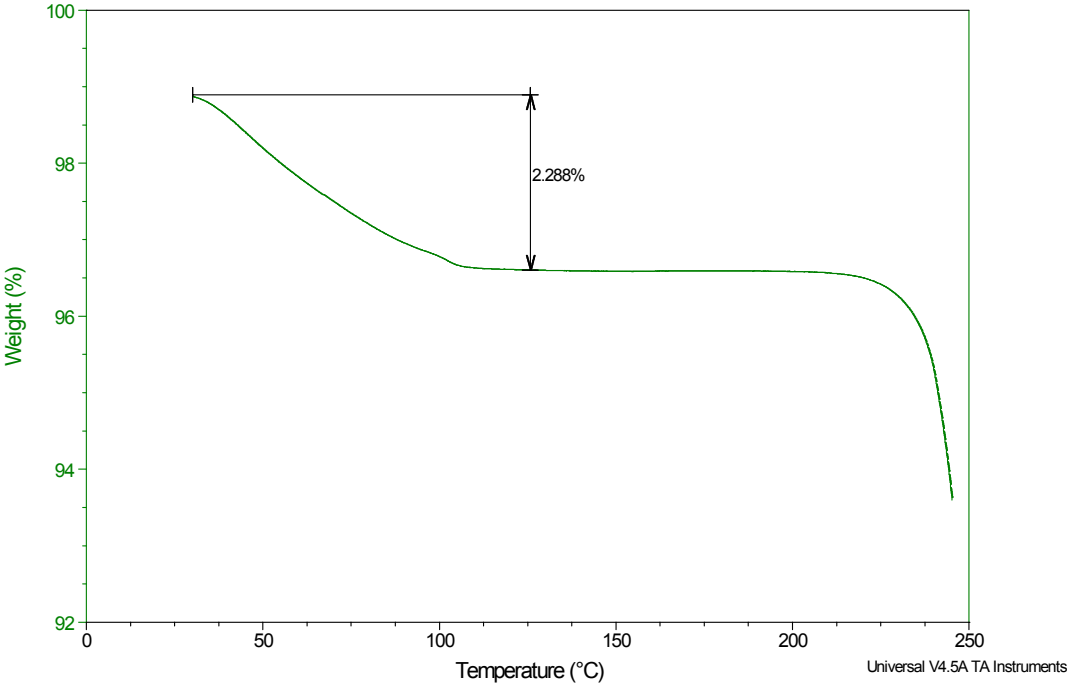
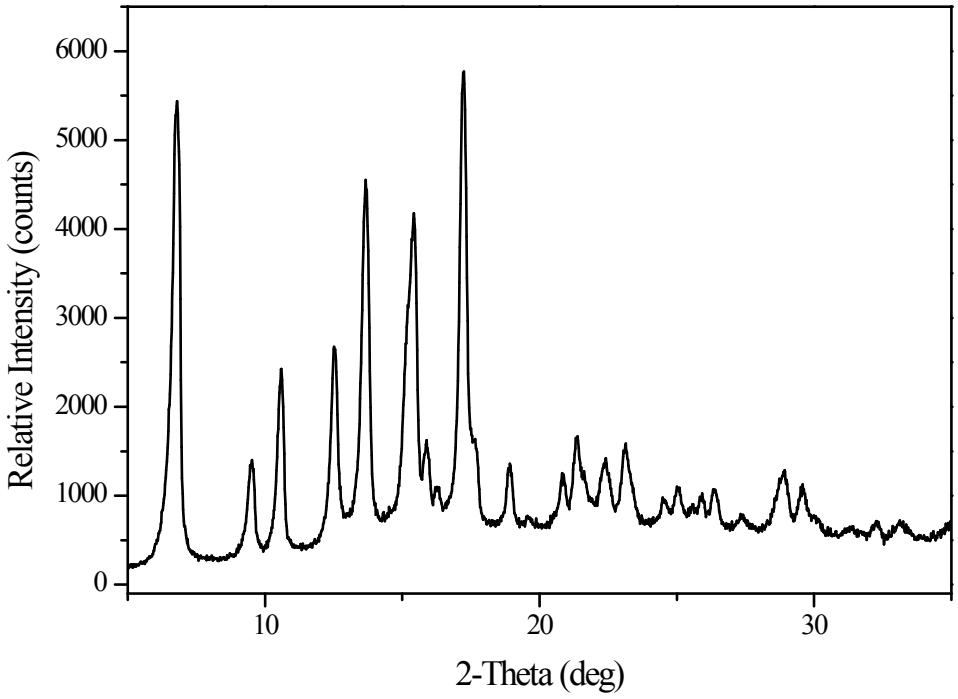
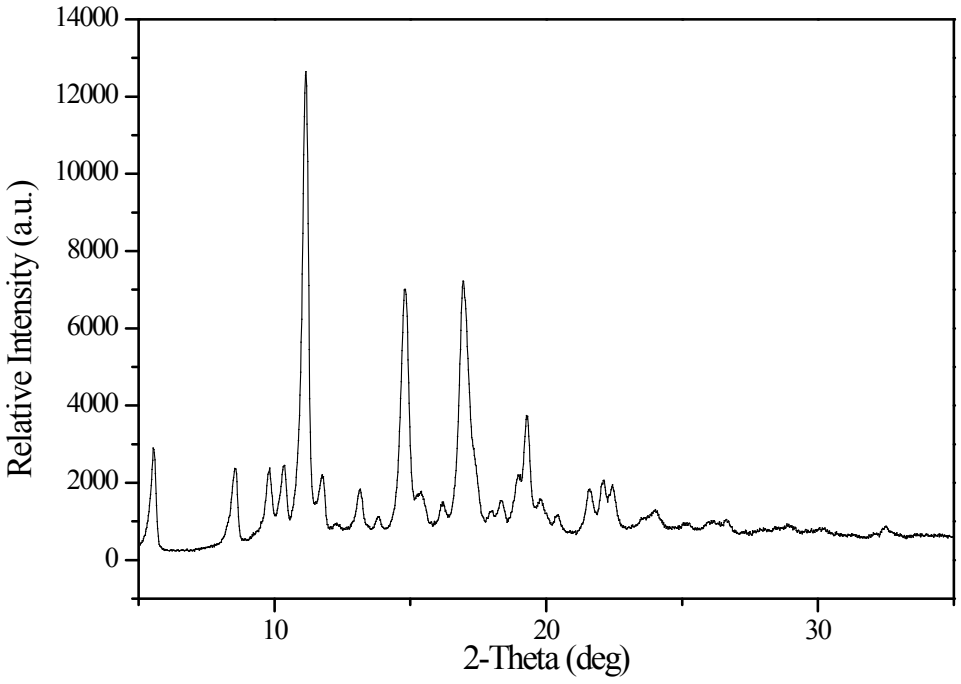


Figure S6. TGA curve of the resulting solid after DVS experiments for DH.

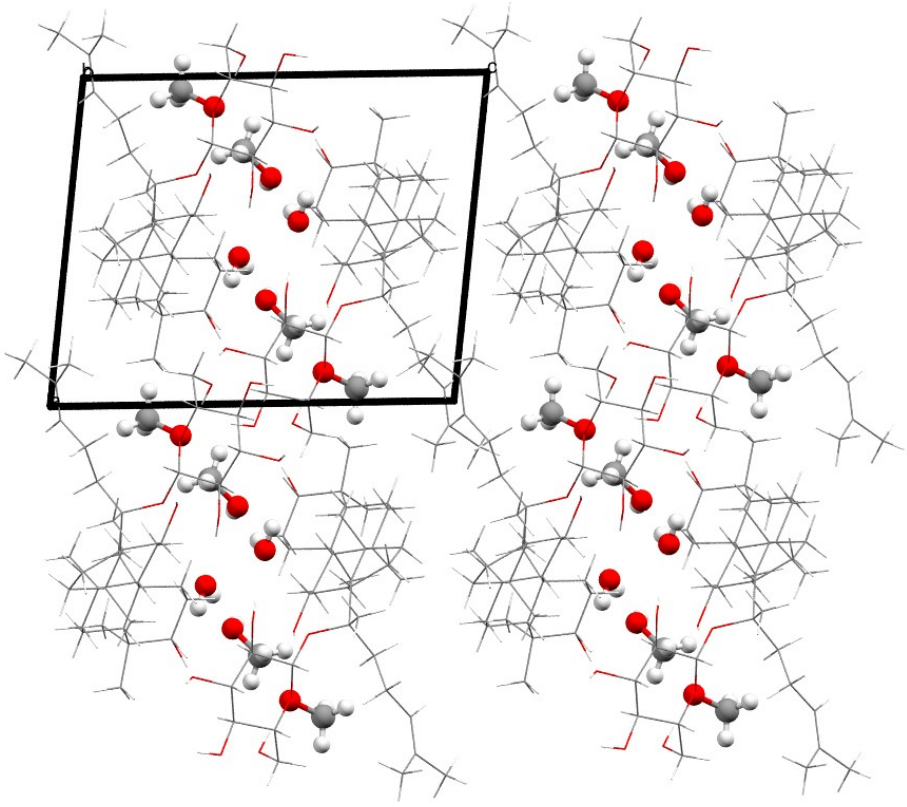


(a)

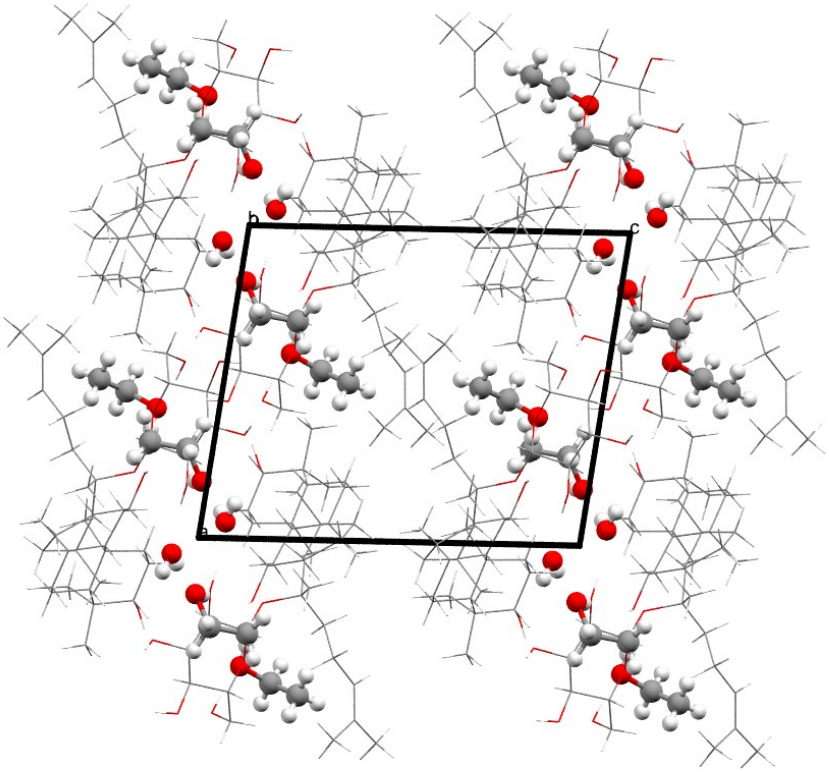


(b)

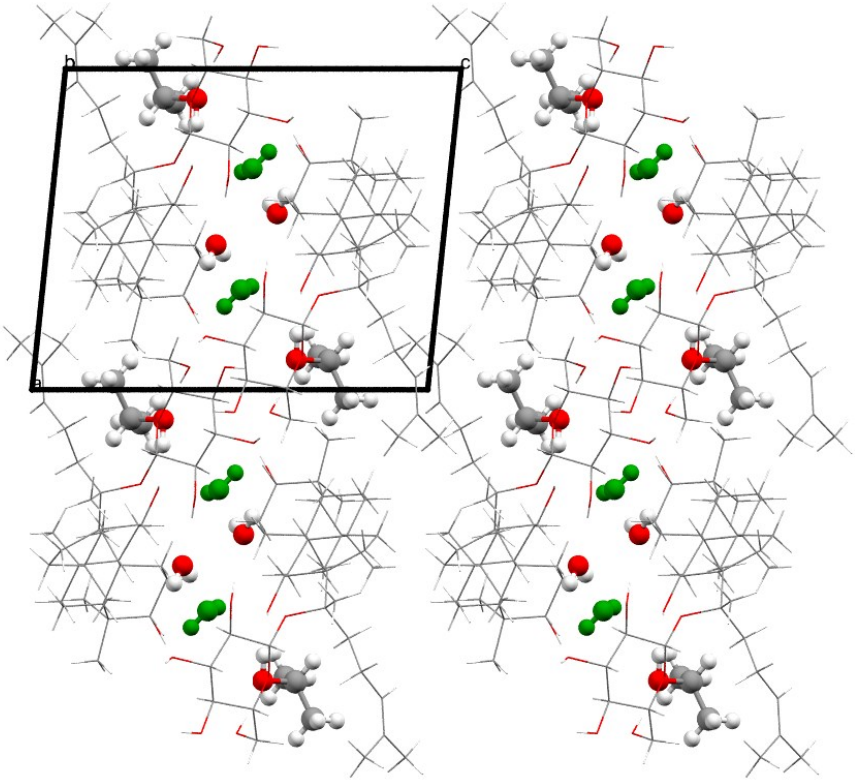
Figure S7. PXRD patterns of form II (a) and form III (b) for GCK compound.



(a)



(b)



(c)

Fig. S8 crystal packing of type 2 solvates: (a) S_{MeW}, (b) S_{EtW} and (c) S_{iPrW}, some of water molecule (green) occupied the channel of S_{iPrW} structure.