Supporting information

Figure S1 Comparison of PXRD patterns collected at room temperature from bulk samples (black line) with that simulated from single crystal data (red dot).

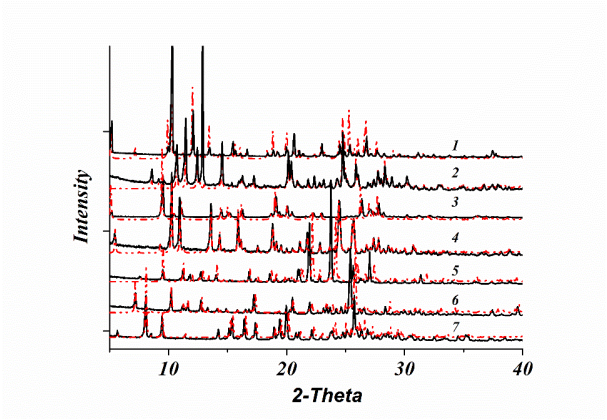


Figure S2 DSC and TGA diagrams of compound **1**

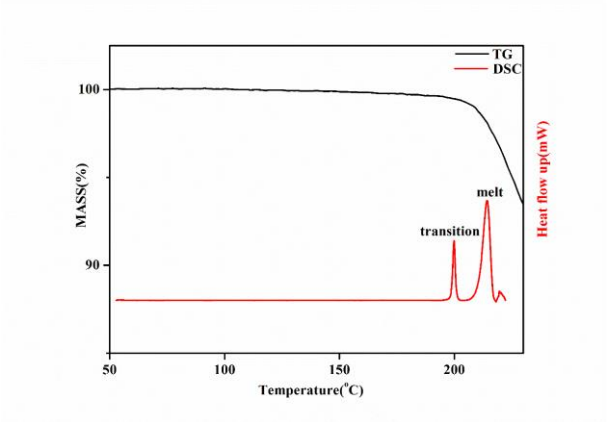


Figure S3 DSC and TGA diagrams of compound **2**

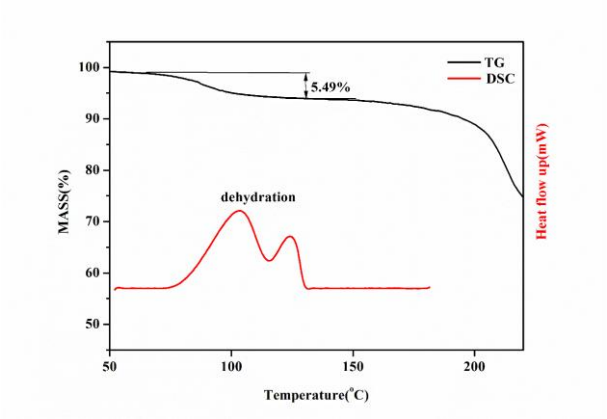


Figure S4 DSC and TGA diagrams of compound **3**

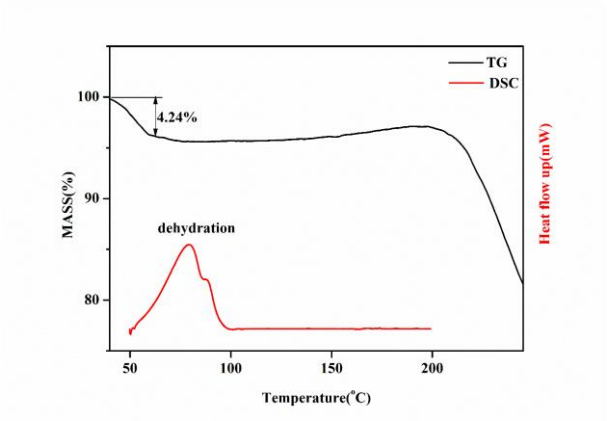


Figure S5 DSC and TGA diagrams of compound **4**

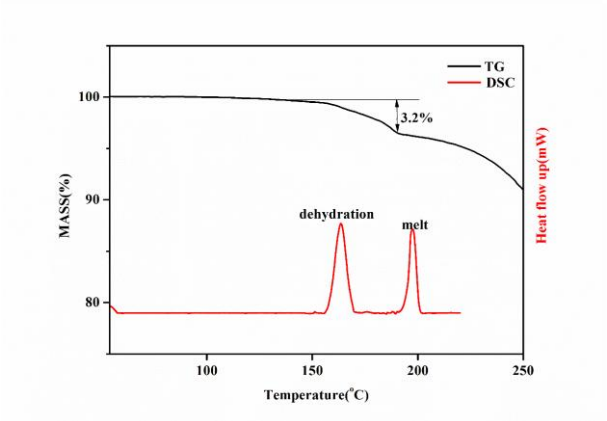


Figure S6 DSC and TGA diagrams of compound **5**

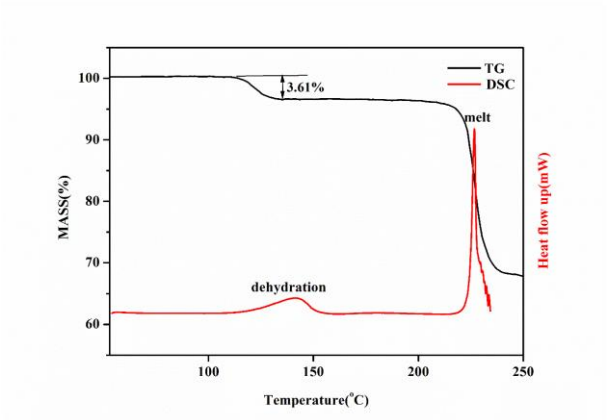


Figure S7 DSC and TGA diagrams of compound **6**

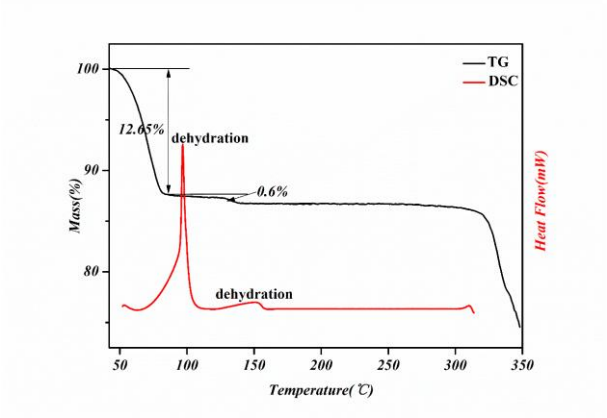


Figure S8 DSC and TGA diagrams of compound **7**

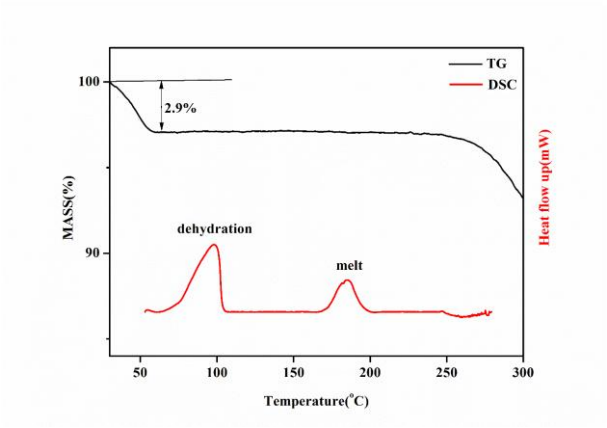
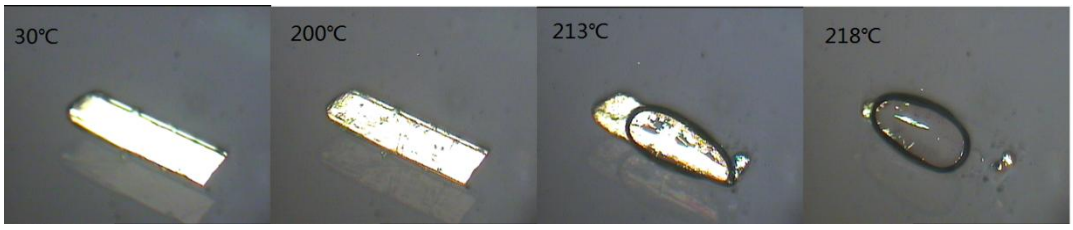
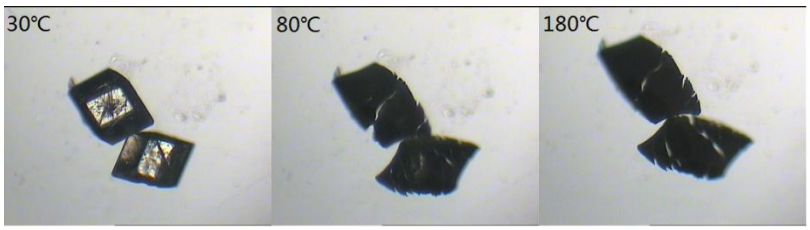


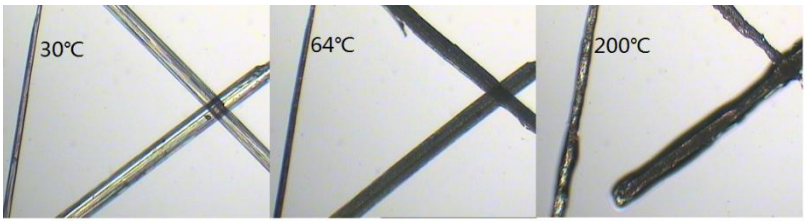
Figure S9 Hot stage microscopy pictures of compound **1**-**7**. (a) Adipate (b) Mucate (c) o-OH-benzoate (d) m-OH-benzoate (e) p-OH-benzoate(f) Naphthalene-1, 5-disulfonicate (g) Naphthalene-2-sulfonicate.



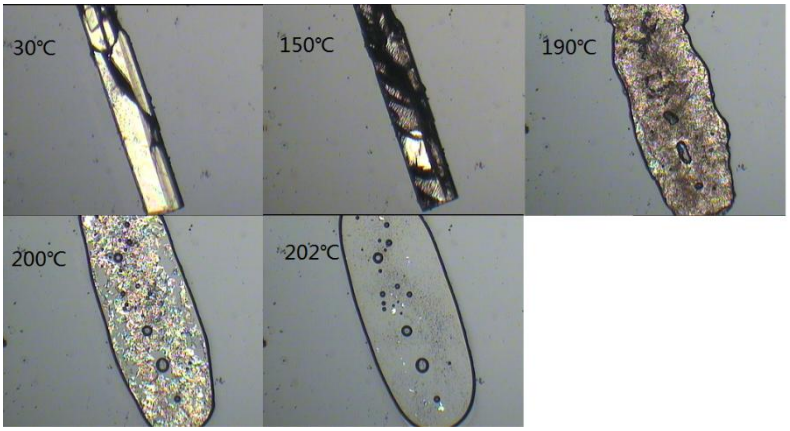
(a)



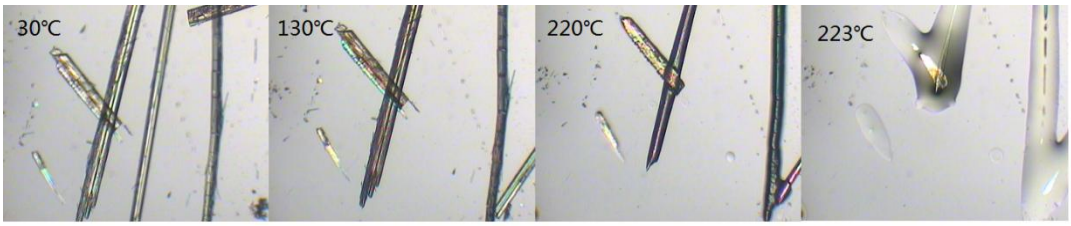
(b)



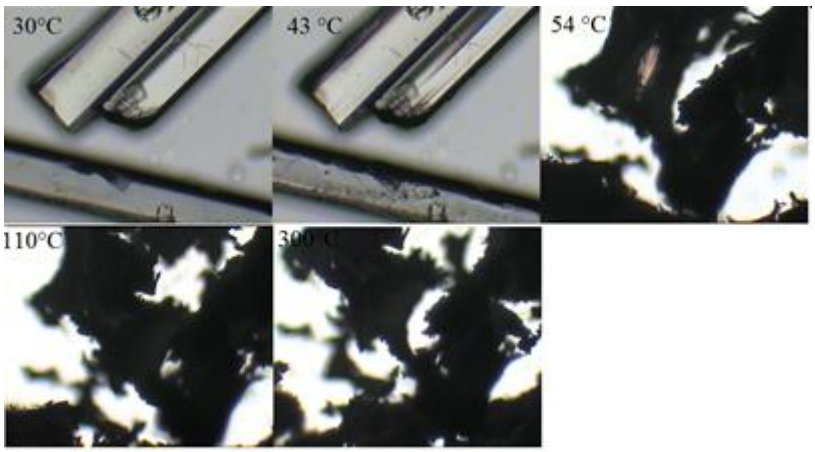
(c)



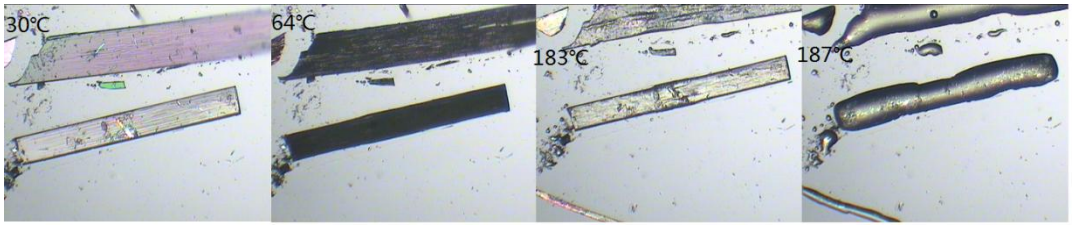
(d)



(e)



(f)



(g)

Figure S10 Solubility data of compound **1-7** and **NF** in aqueous solution.

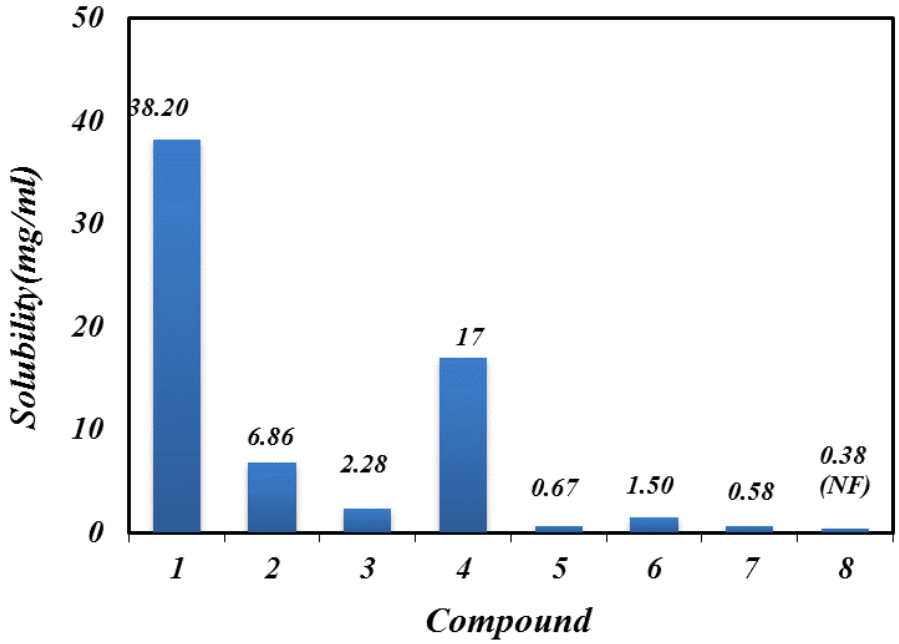


Figure S11IDR data of compound **1-7** and **NF** under aqueous solution.

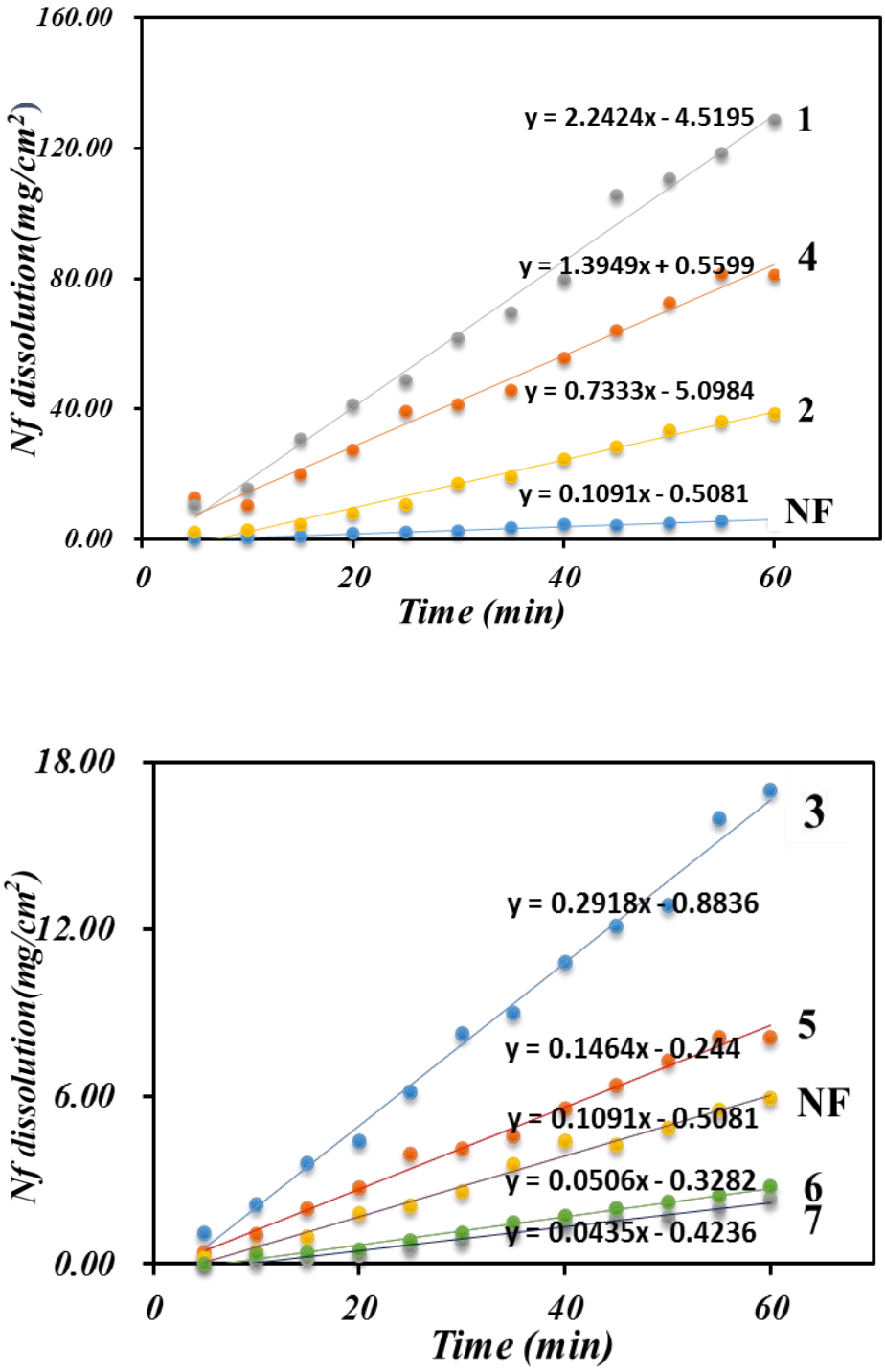


Table S1 Geometrical parameters of hydrogen bonds in compounds **1-6.**

D-H···A	D···A(Å)	H···A(Å)	D-H···A(deg)
	Compound 1		
O2X-H1'···O3Y	2.59	1.637	171.87
O4X-H10'···O1Y	2.522	1.582	172.96
intra O2B-H28···O3B	2.526	1.758	155.19
N3A-H14···O2Y	2.67	1.72	166.45
N3A-H15···O3Y	2.792	1.873	161.52
intra O2A-H9···O3A	2.536	1.656	160.67
N3B-H34···O4Y	2.674	1.698	169.04
N3B-H33···O1Y	2.774	1.862	169.23
	Compound 2		
O2S-H2B···O2A	2.983	2.094	153.32
O2S-H2B···O1A	3.262	2.417	146.73
O2S-H2A···O1Y	2.771	1.955	168.63
O3Y-H1'···O2Y	2.599	2.131	116.15
intra O3X-H6'···O2X	2.575	2.072	119.42
O3X-H6'···O3Z	2.929	2.239	142.04
O4X-H8'···O1X	2.7	1.897	166.01
intra O2A-H1···O3A	2.492	1.733	153.16
O4Z-H12'···O4X	2.743	1.927	166.53
N3B-H34···O2S	3.069	2.221	157.03
N3B-H33···O1Y	2.735	1.889	155.74
N3A-H15···O2X	2.682	1.695	178.73
N3A-H14···O3X	2.75	1.903	162.61
O3S-H3A···O4Z	3.181	2.333	175.43
O3S-H3B···O3B	2.837	2.026	159.37
O1S-H1B···O2Y	2.722	1.802	170.62
O1S-H1A···O2S	2.918	2.008	174.1
O1Z-H9'···O1X	2.583	1.675	169.84
intra O2B-H20···O3B	2.532	1.621	151.61
	Compound 3		
N3-H14···O1S	2.756	1.864	170.97
N3-H15···O1'	2.729	1.845	167.18
intra O2-H2···O3	2.570	1.658	154.34
O1S-H1A···O1'	2.811	1.929	168.83
O1S-H1B···O2'	2.770	1.899	171.48
intra O3'-H1'···O2'	2.533	1.645	150.11
	Compound 4		

intra O2-H1···O3	2.545	1.694	155.98
O3'-H3'···O1'	2.581	1.654	174.03
O1S-H1B···O2'	2.865	2.029	163.68
O1S-H1A···O1'	2.905	2.034	171.21
N3-H14···O2'	2.704	1.734	172.22
N3-H15···O3	2.962	2.071	157.74
Compound 5			
O2A-H2···O3A	2.540	1.666	156.04
O3X-H37···O3S	2.629	1.820	172.54
O2C-H42···O3C	2.495	1.604	153.81
O3Y-H61···O1S	2.630	1.714	176.26
O3Z-H66···O2S	2.635	1.804	176.25
N3A-H14A···O1Y	2.693	1.808	167.14
N3A-H15A···O2Z	2.798	1.902	173.53
O2B-H20···O3B	2.504	1.691	151.34
N3C-H14C···O2Y	2.702	1.845	158.35
N3C-H15C···O1Z	2.712	1.813	176.85
N3B-H14B···O1X	2.805	1.861	175.85
N3B-H15B···O2X	2.711	1.819	164.73
O2S-H2B···O2X	2.737	1.895	175.94
O2S-H2A···O1X	2.755	1.875	170.12
O3S-H3A···O2Y	2.745	1.891	171.15
O3S-H3B···O1Z	2.749	1.878	174.55
O1S-H1A···O2Z	2.758	1.895	174.17
O1S-H1B···O1Y	2.762	1.858	166.86
Compound 6			
N3-H14···O4S	2.826	1.903	161.16
N3-H15···O1S	2.894	2.024	145.15
N3-H15···O3'	2.786	2.224	114.55
O1S-H1A···O2'	2.885	2.161	149.64
O1S-H1A···O3	2.96	2.541	113.86
O3S-H3B···O2S	2.759	1.958	171.05
O1S-H1B···O1	2.769	1.942	164.38
O4S-H4B···O3S	2.88	2.008	160.56
O4S-H4A···O3S	2.842	2.022	168
O3S-H3A···O1'	2.802	1.895	178.49
O2S-H2A···O2	2.891	1.965	174.1
O2S-H2B···O1S	2.832	1.999	172.08
intra O2-H1···O3	2.446	1.303	153.1