Electronic Supplementary Material (ESI) for Analyst.

Supplementary Information

Confocal Raman micro-spectral evidence and physicochemical evaluation of triamterene salts

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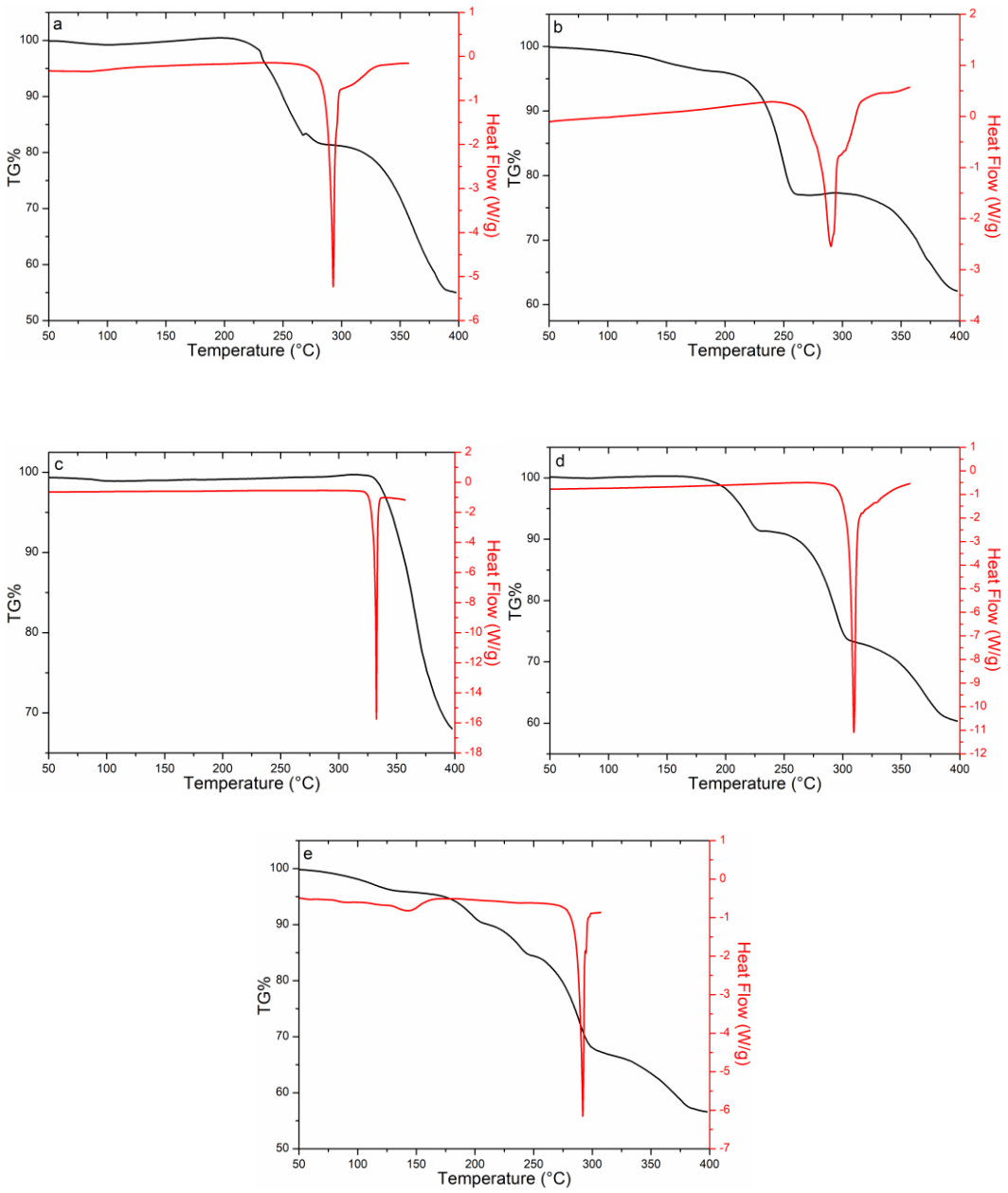


Fig. S1. TG and DSC curves of (a) Tri-NA, (b) Tri-BA, (c) Tri-TA, (d) Tri-INA and (e) Tri-NA·H_2O salts.

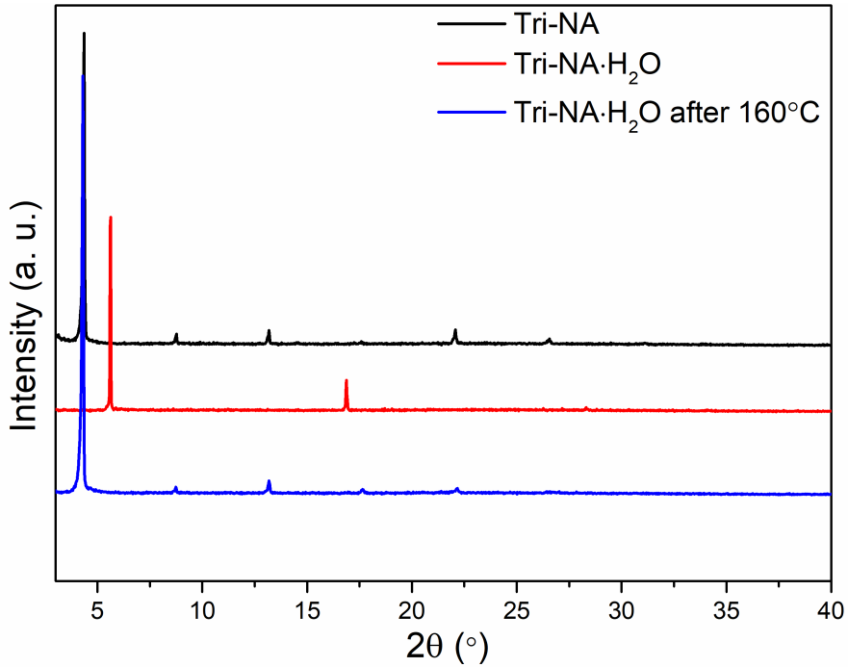


Fig. S2. The experimental PXRD of Tri-NA, Tri-NA·H_2O before and after heating.

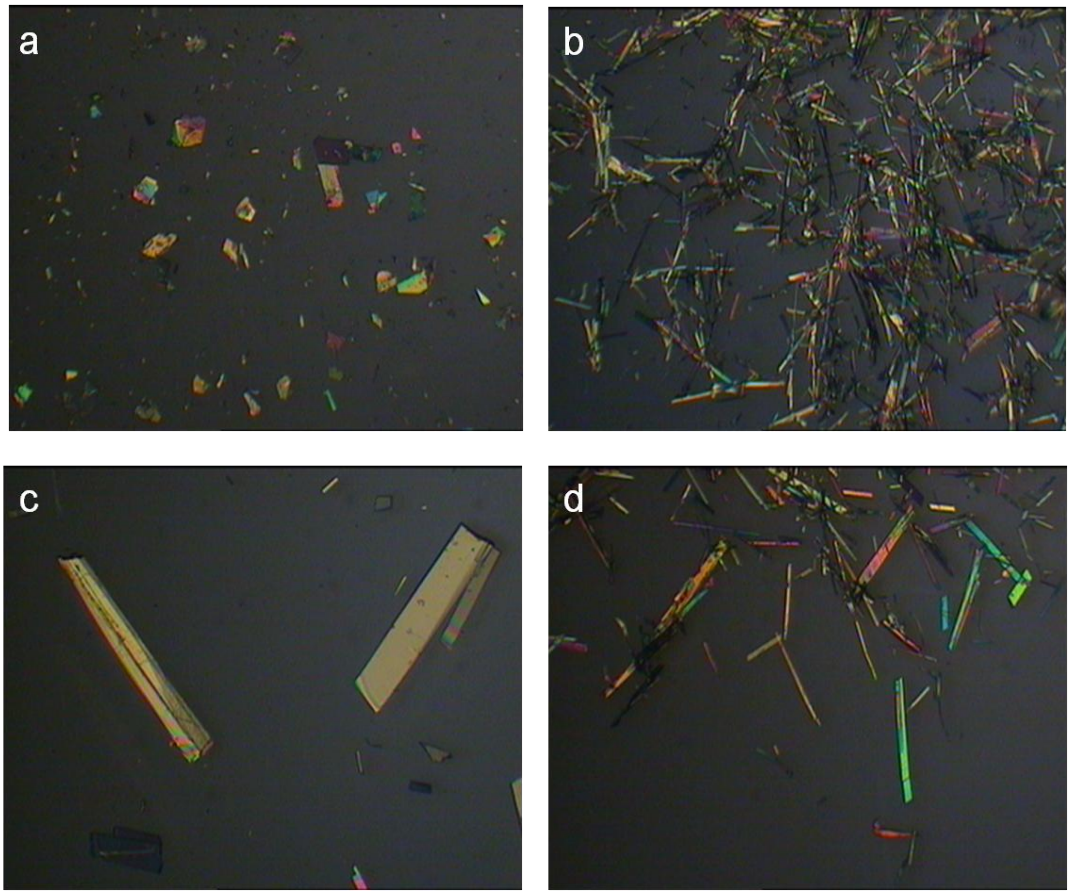


Fig. S3. Polarized light microscopies of (a) Tri-NA·H_2O, (b) Tri-BA, (c) Tri-TA, (d) Tri-INA salts.

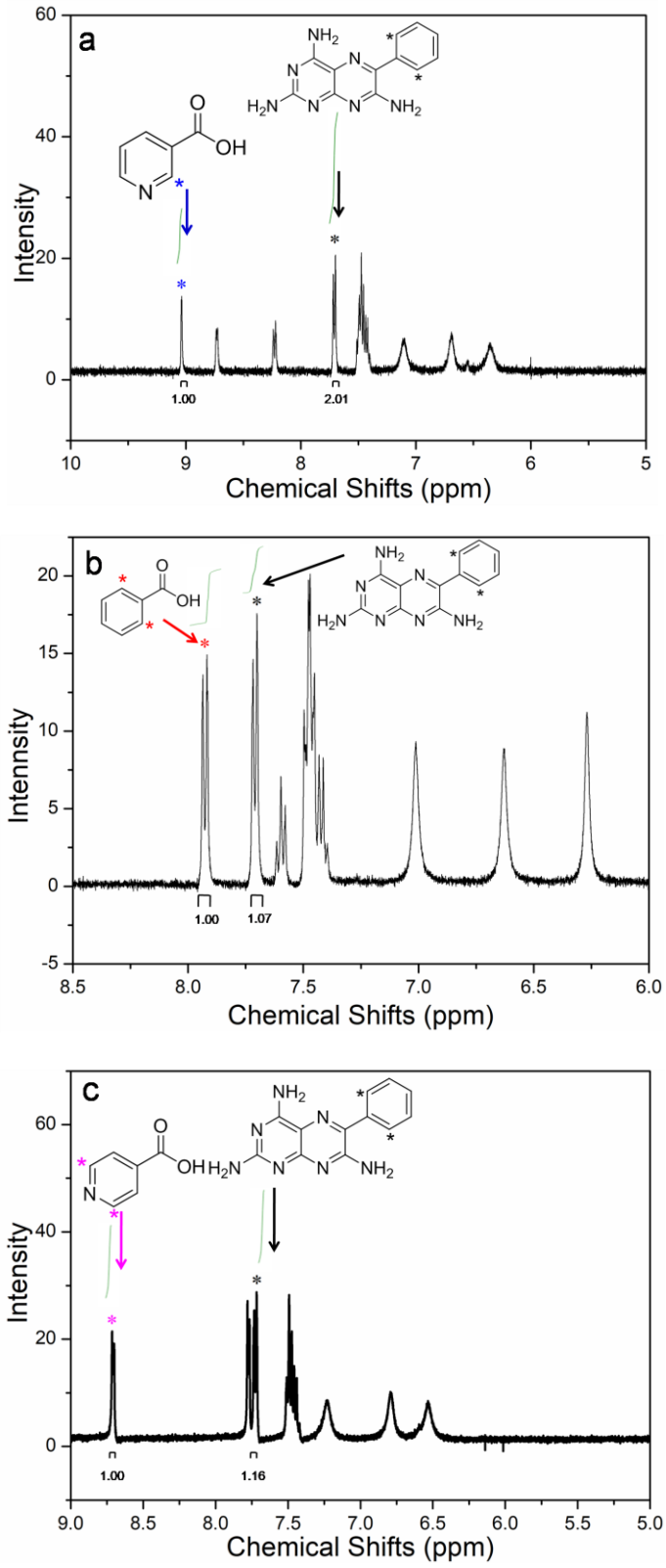


Fig. S4. ^{1}H-NMR (DMSO, 400 MHZ) of Tri-NA (a), Tri-BA (b). Tri-INA (c). The integration values suggested that the stoichiometry molar ratio of Tri : NA, Tri : BA, Tri : INA is 1:1, respectively.

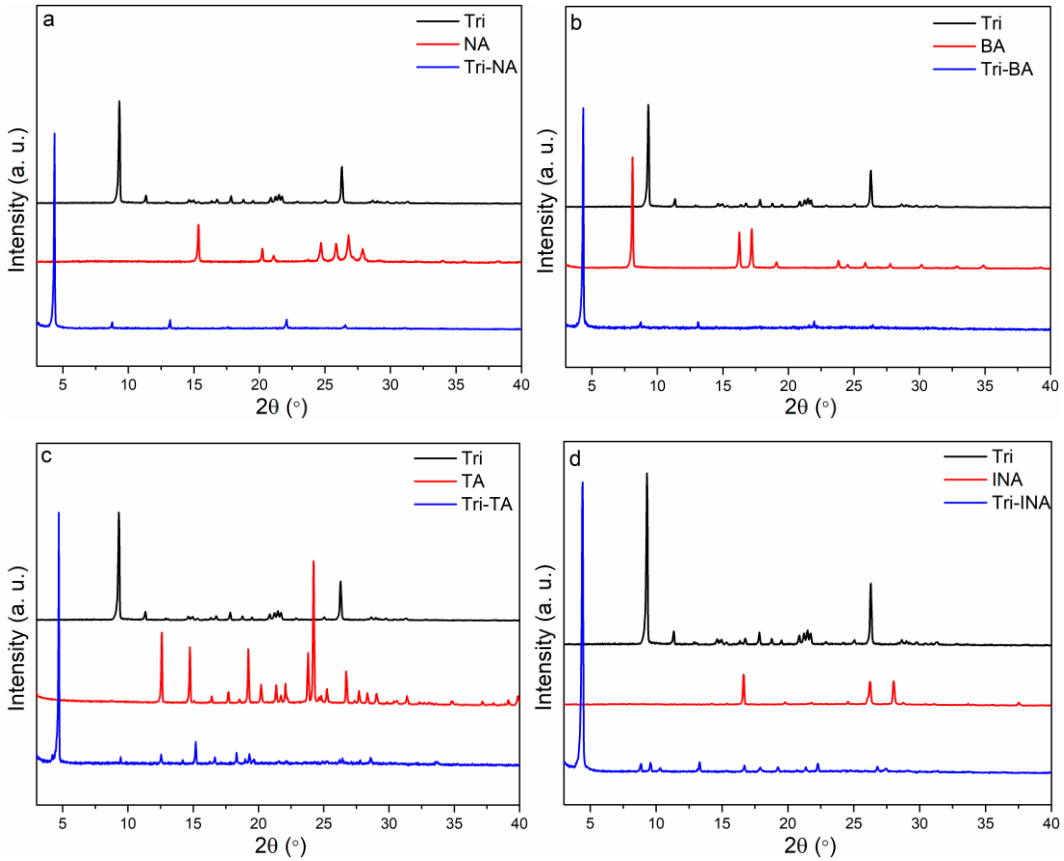


Fig. S5. The experimental PXRD of four salts and corresponding acids.

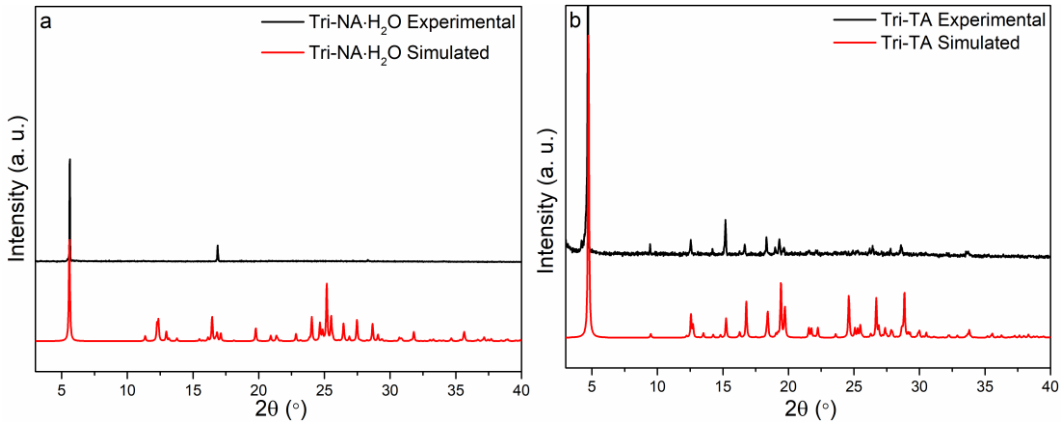


Fig. S6. Comparison between experimental and simulated PXRD of salts: (a) Tri-NA·H_2O, (b) Tri-TA.

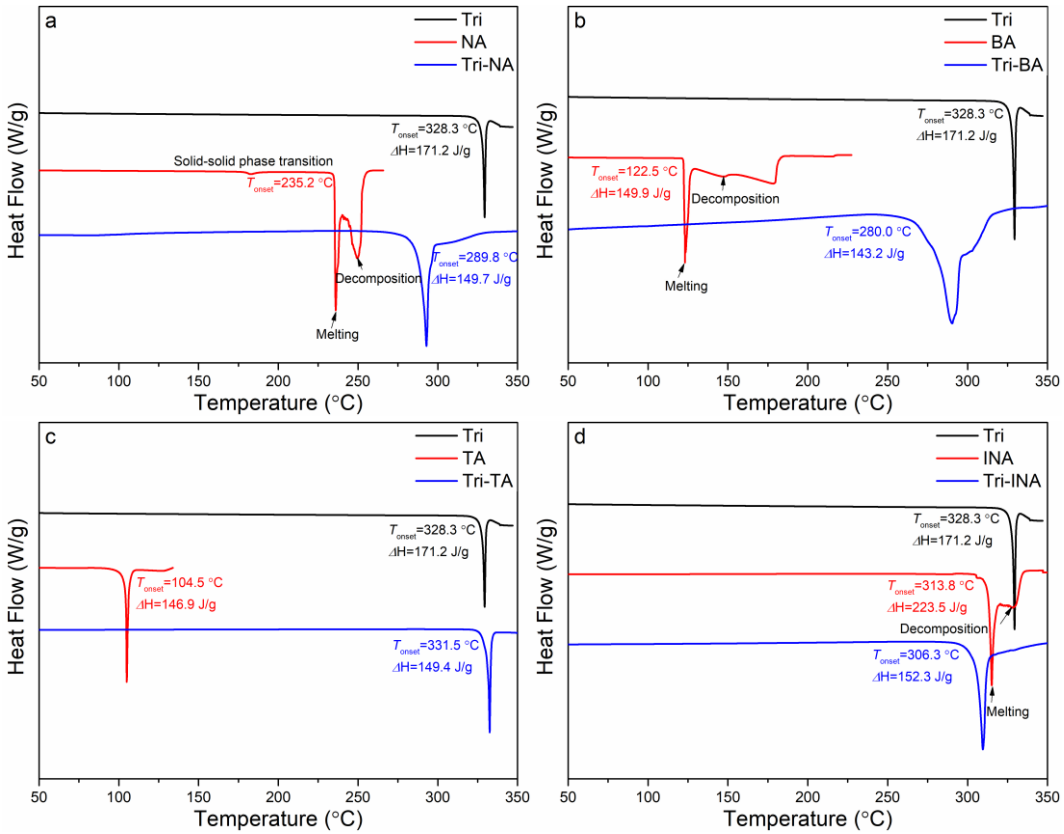
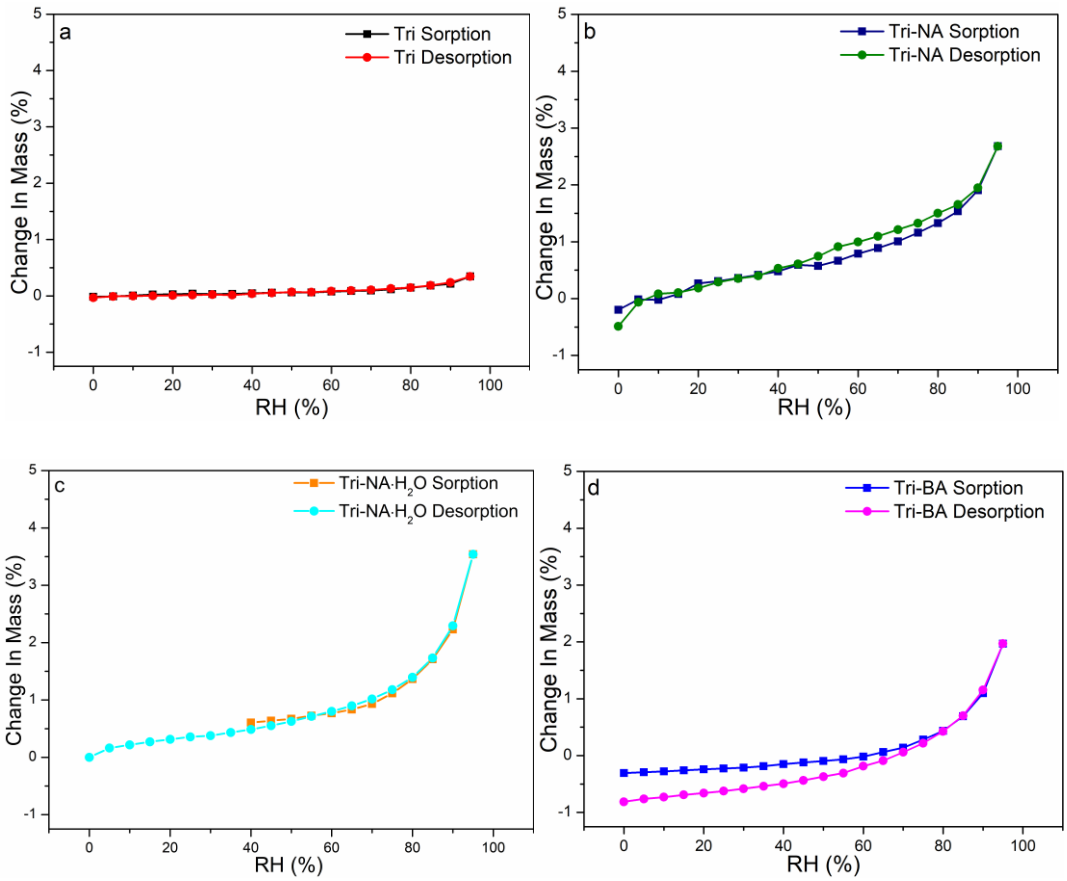


Fig. S7. Comparison of DSC curves among (a) Tri, NA and Tri-NA, (b) Tri, BA and Tri-BA, (c) Tri, TA and Tri-TA, (d) Tri, INA and Tri-INA.



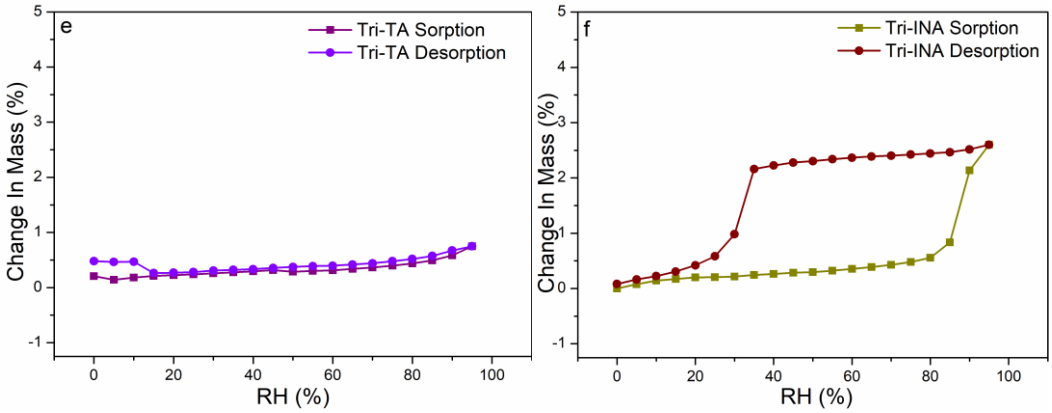


Fig. S8. Water vapour sorption and desorption isotherm curves of (a) Tri, (b) Tri-NA, (c) Tri-NA·H_2O, (d) Tri-BA, (e) Tri-TA, (f) Tri-INA salts.

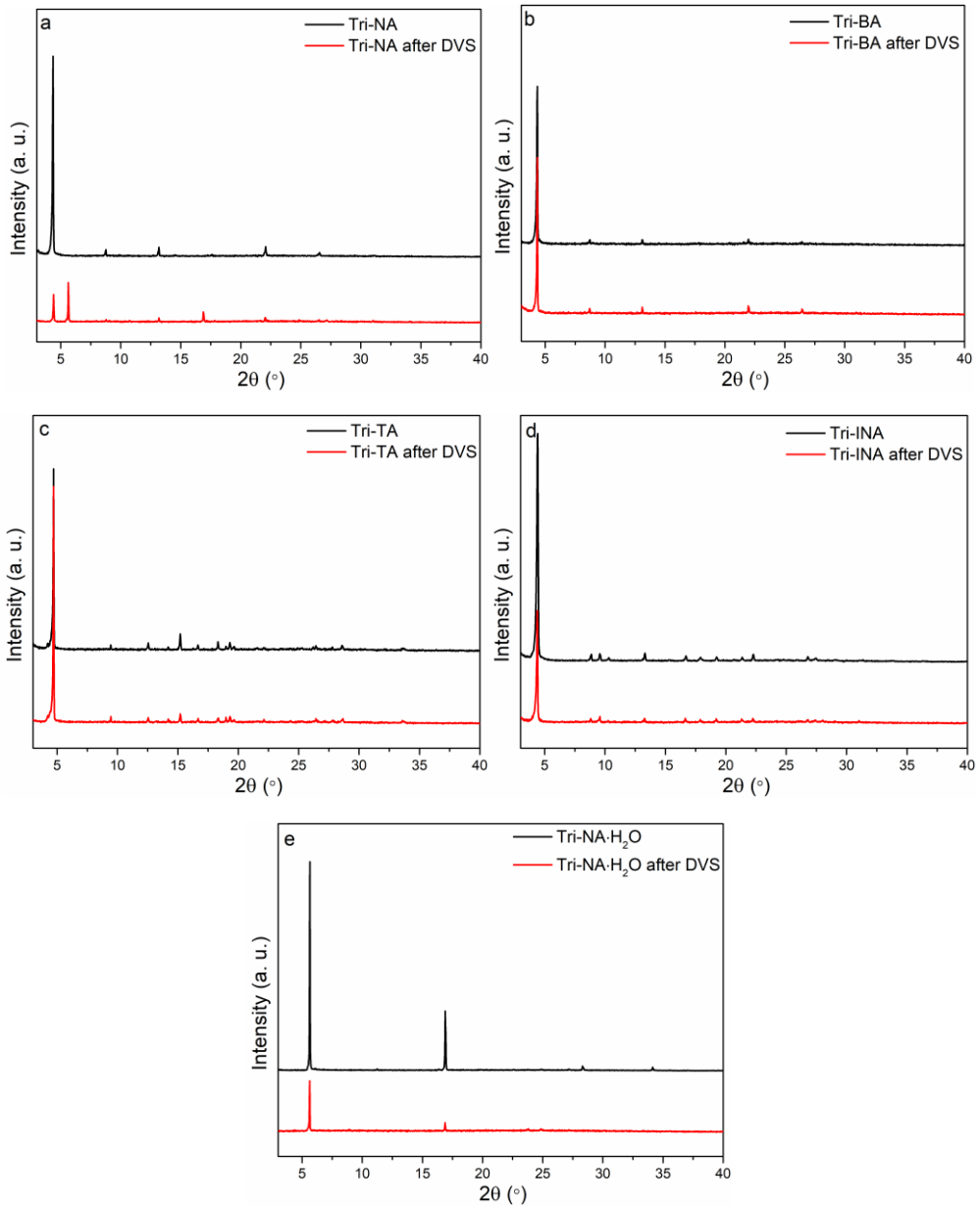


Fig. S9. PXRD patterns of Tri salts after DVS experiments (a) Tri-NA, (b) Tri-BA, (c)

Tri-TA, (d) Tri-INA and (e) Tri-NA·H_2O.

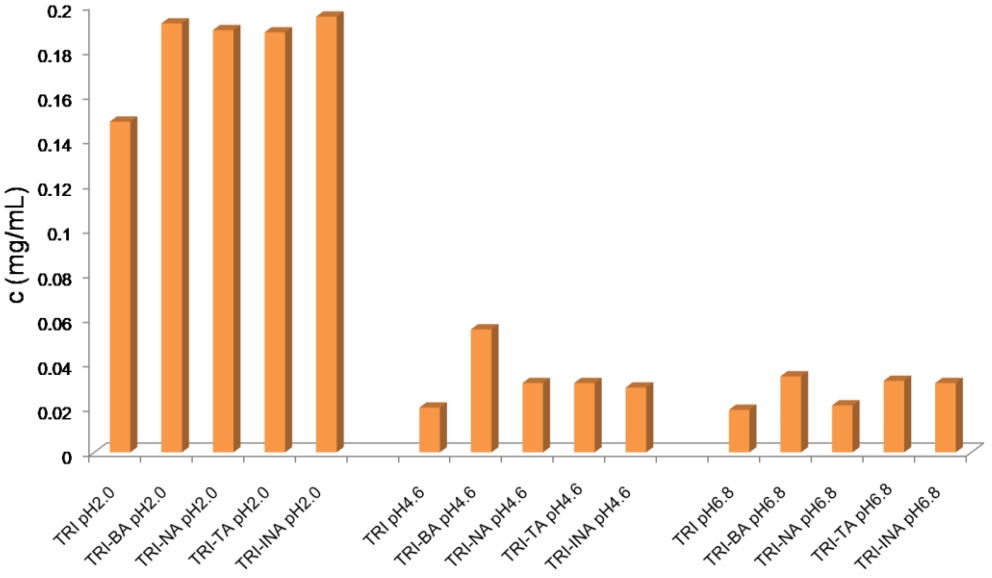


Fig. S10. Apparent equilibrium solubility of Tri and its four salts in pH 2.0, 4.6 and 6.8 buffer solution.

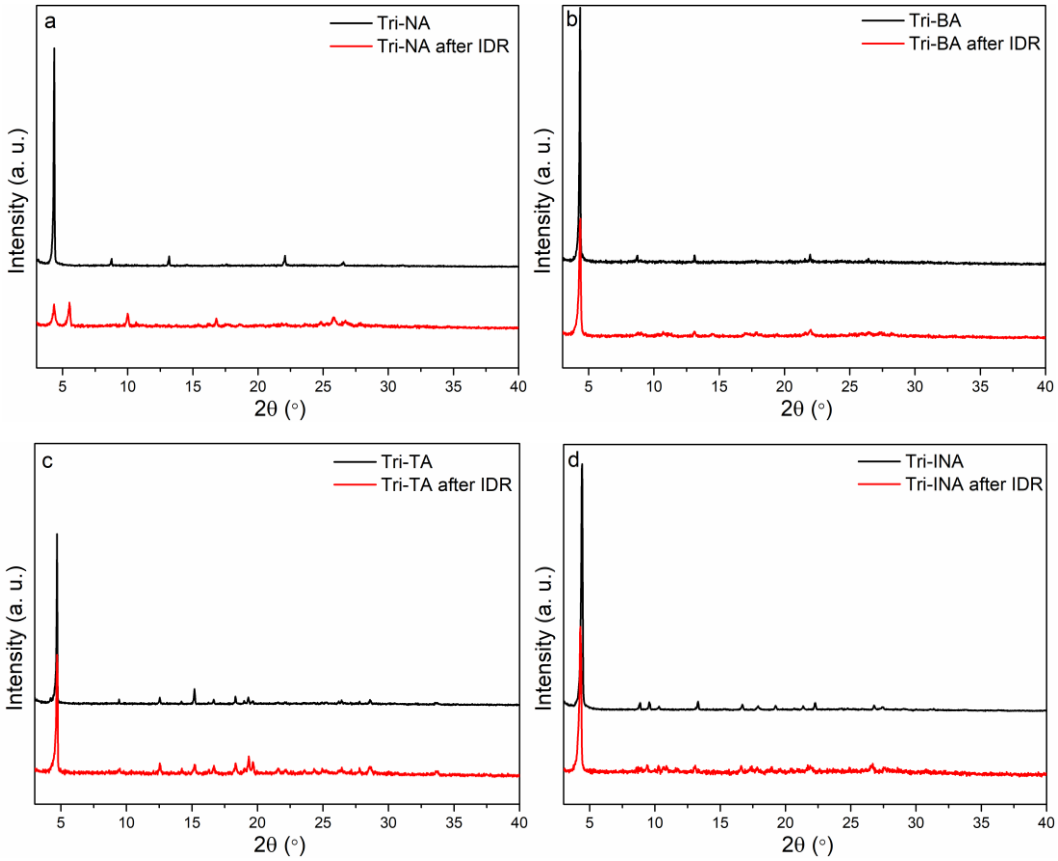


Fig. S11. PXRD patterns of Tri salts after IDR tests (a) Tri-NA, (b) Tri-BA, (c) Tri-TA, (d) Tri-INA.

Table S1. Crystallographic Data for two salts of Tri.

	Tri-NA·H_2O	**Tri-TA**
Formula	$C_{18}H_{18}N_8O_3$	$C_{19}H_{19}N_7O_3S$
Crystal system	triclinic	triclinic
Space group	*P*-1	*P*-1
Temperature (*K*)	205	205
a (Å)	7.3398(4)	7.0799(10)
b (Å)	7.9181(5)	7.2853(10)
c (Å)	15.8561(9)	18.725(3)
α (°)	85.936(2)	94.786(7)
β (°)	85.998(2)	93.483(7)
γ (°)	79.919(2)	94.630(7)
V ($Å^3$)	903.46(9)	957.1(2)
D_{Cal}(g/cm^3)	1.450	1.476
Z	2	2
λ	1.54178 (Cu-Kα)	0.71073(Mo-Kα)
Independent reflns.	2789	3525
S	0.941	0.928
R_{int}	0	0.0736
R_1	0.0734	0.0599
wR_2	0.2111	0.1383

Table S2. Gradient HPLC system for the determination of Tri content.

Time (min)	KH_2PO_4 %	MeOH %	Flow rate (mL/min)
0	70	30	1.0
6	40	60	1.0

8	40	60	1.0
8.01	70	30	1.0
10	70	30	1.0

Table S3. List of intermolecular and intramolecular hydrogen bond lengths and angles for two Tri salts.

Crystal form	Interactions	H…A (Å)	D…A (Å)	<D-H…A (°)	Symmetry code
Tri-NA·H_2O	N1-H1…O1 (Inter)	1.91	2.769 (4)	171	x, y, z
	N2-H2A…O2 (Inter)	2.00	2.804 (5)	163	x, y, z
	N2-H2B…O3 (Inter)	2.02 (5)	2.909 (5)	167 (5)	-1+x,1+y,z
	O3-H3A…O1 (Inter)	2.12	2.971 (4)	170	x,-1+y,z
	O3-H3B…N8 (Inter)	1.95	2.755 (5)	156	x, y, z
	N4-H4A…N3 (Inter)	2.12	2.988 (4)	175	-x,2-y,1-z
	N4-H4B…N5 (Intra)	2.47	2.790 (4)	102	x, y, z
	N4-H4B…O3 (Inter)	2.22	2.888 (4)	134	1-x,1-y,1-z
	N7-H7A…N6 (Inter)	2.19	3.043 (5)	168	2-x,1-y,1-z
	N7-H7B…O1 (Inter)	2.17	2.830 (4)	132	2-x,1-y,1-z
	C6-H6…N7 (Intra)	2.62	3.058 (6)	109	x, y, z
	C18-H18…O1 (Intra)	2.50	2.817 (6)	100	x, y, z
Tri-TA	N1-H1…O2 (Inter)	1.90	2.746 (4)	162	x, y, z
	N2-H2A…O3 (Inter)	2.17	2.835 (4)	133	-1+x,y,z
	N2-H2B…O2 (Inter)	2.42	3.136 (4)	139	x, y, z
	N4-H4A…N3 (Inter)	2.20	3.061 (4)	170	-x,1-y,1-z
	N4-H4B…N5	2.42	2.757 (4)	104	x, y, z

	(Intra)				
	N4-H4B…O1 (Inter)	2.03	2.871 (4)	161	1-x,1-y,1-z
	N7-H7A…N6 (Inter)	2.19	3.056 (4)	177	2-x,2-y,1-z
	N7-H7B…O2 (Inter)	2.36	2.989 (4)	129	2-x,2-y,1-z

For Tri-NA·H_2O, the N_1-H_1···O_1, N_2-H_{2A}···O_2, N_2-H_{2B}···O_3, O_3-H_{3A}···O_1, O_3-H_{3B}···N_8, N_4-H_{4A}···N_3, N_4-H_{4B}···O_3, N_7-H_{7A}···N_6, N_7-H_{7B}···O_1 intermolecular H-bonding interaction are existed in Tri-NA·H_2O. In addition, the N_4-H_{4B}···N_5, C_6-H_6···N_7 and C_{18}-H_{18}···O_1 intramolecular H-bonding interaction are also existed in Tri-NA·H_2O. For Tri-TA, the N_1-H_1···O_2, N_2-H_{2A}···O_3, N_2-H_{2B}···O_2, N_4-H_{4A}···N_3, N_4-H_{4B}···O_1, N_7-H_{7A}···N_6, N_7-H_{7B}···O_2 intermolecular H-bonding interaction are existed in Tri-TA, and only the N_4-H_{4B}···N_5 intramolecular H-bonding interaction is existed in Tri-TA. Thus, the remaining five H-bond donors are involved in intermolecular H-bonding interactions in Tri-NA·H_2O, while for Tri-TA, four H-bond donors are involved in intermolecular H-bonding interactions.

The Alert level B of Tri-NA·H_2O single crystal structure occurring “The value of sine (theta_max)/wavelength is less than 0.575 Calculated sin (theta_max)/wavelength = 0.5750” error is mainly due to lacking of diffraction point in high angle region.