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Theoretical and experimental study of pharmaceutical salts: A case of Trimethoprim

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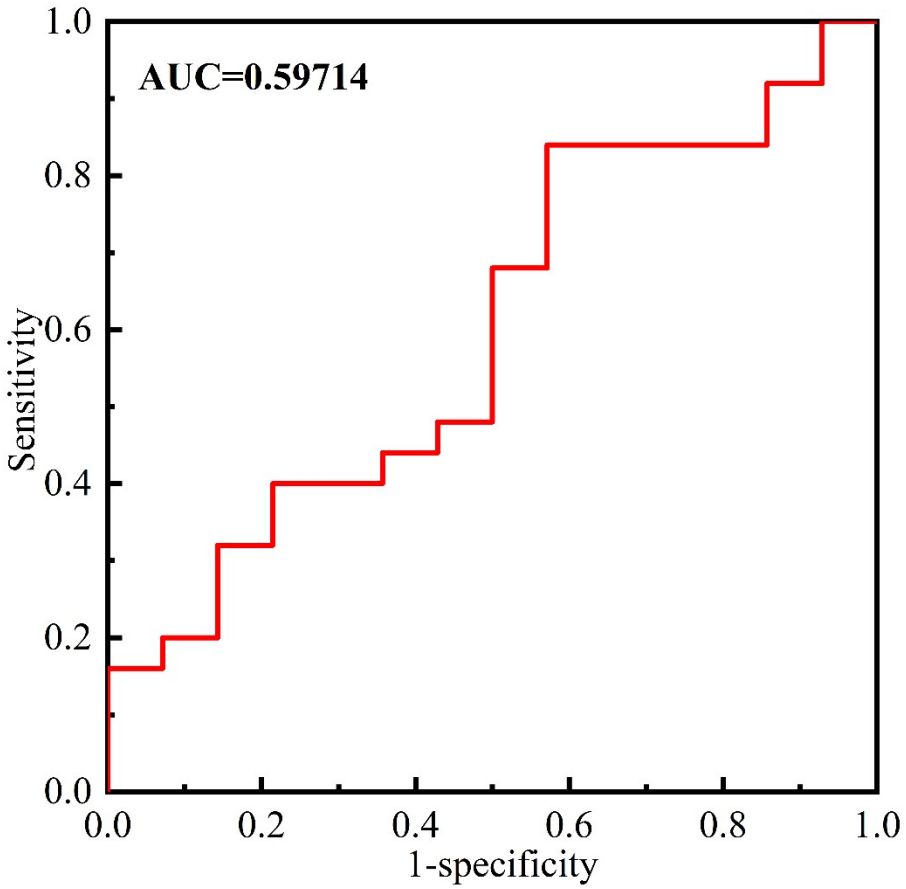


Fig. S1 ROC curve for COSMO-RS methodology.

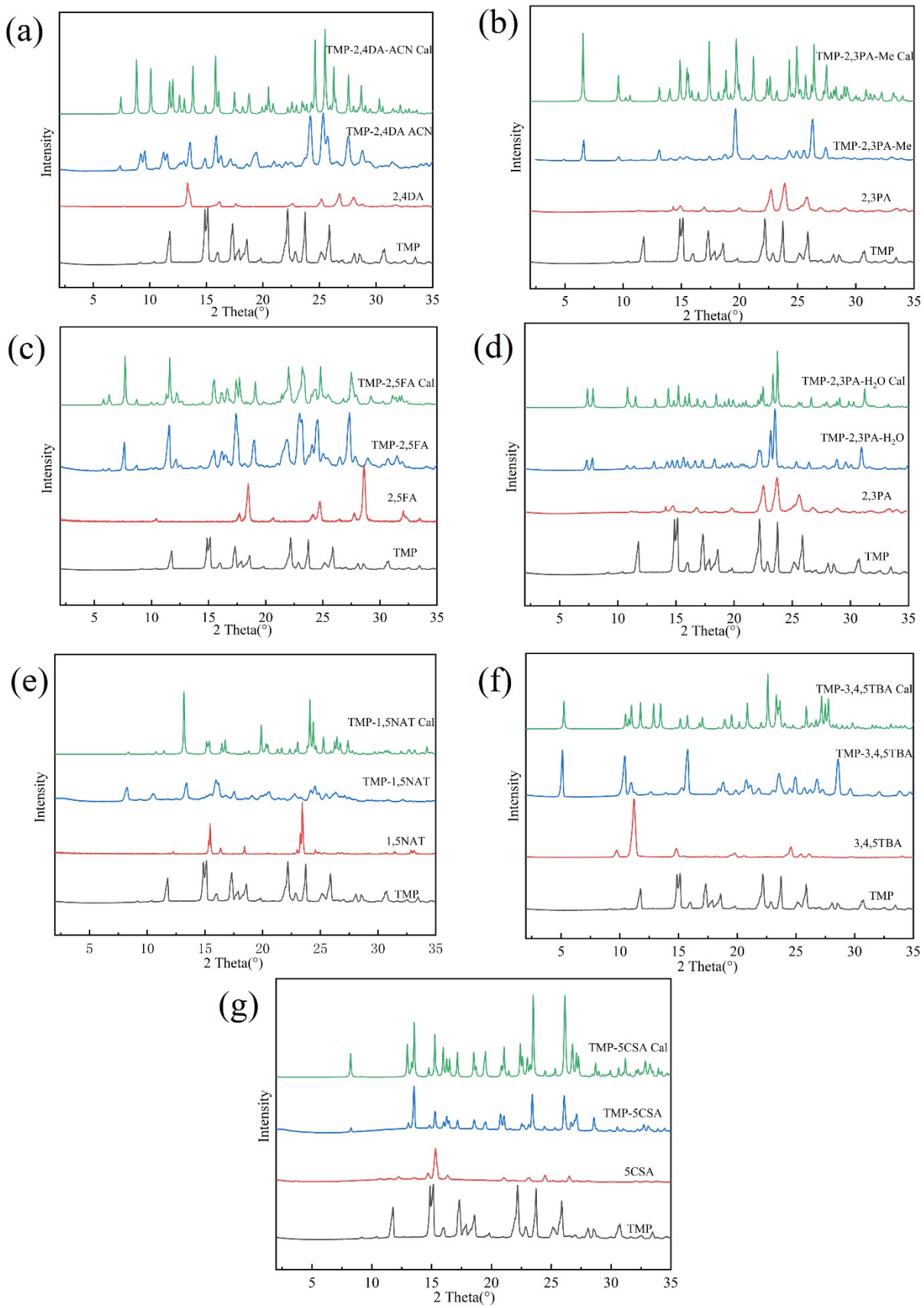


Fig. S2 PXRD patterns of TMP, coformers, salts and calculated from the single crystals. (Cal: Calculated from the crystal structure).

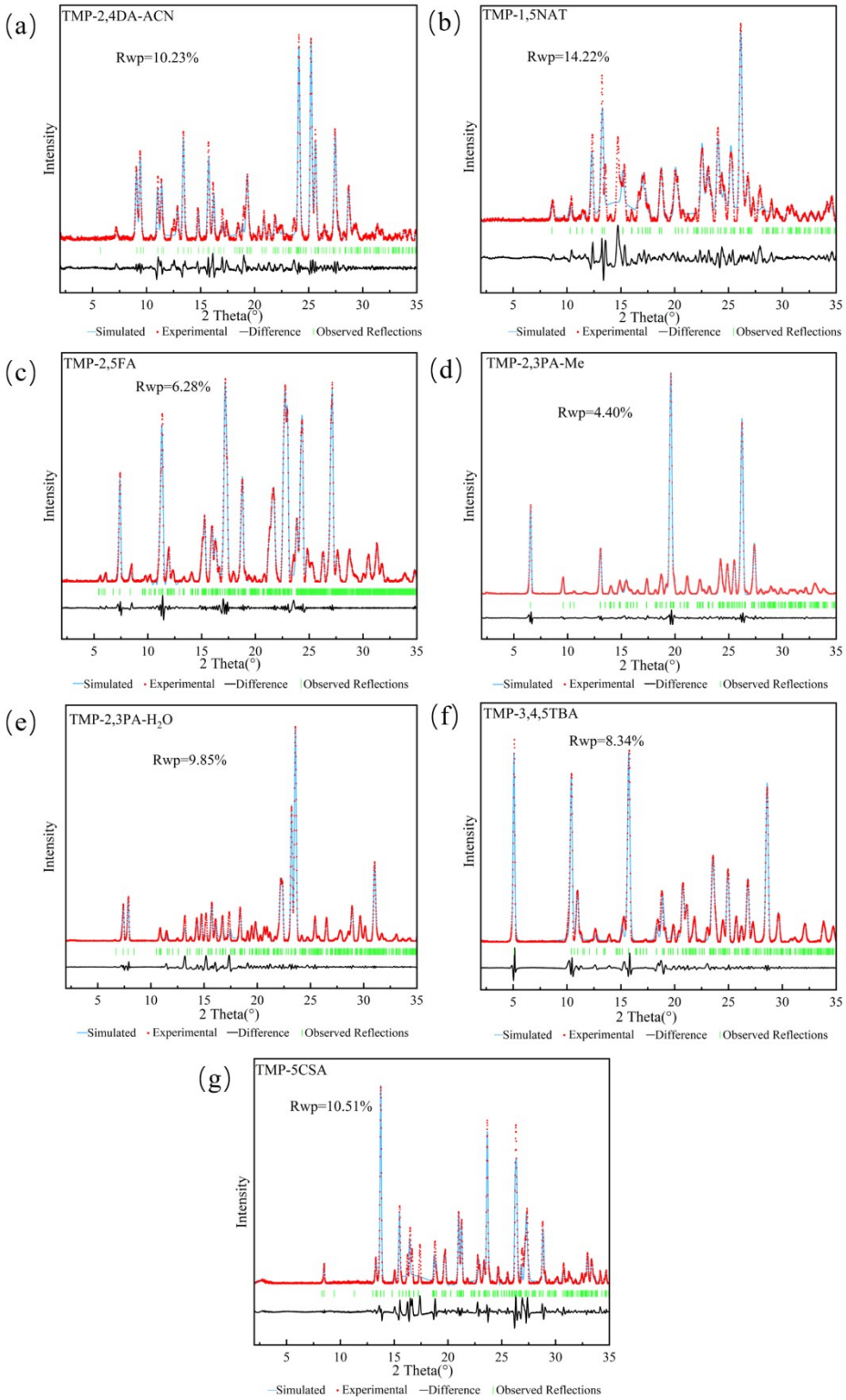
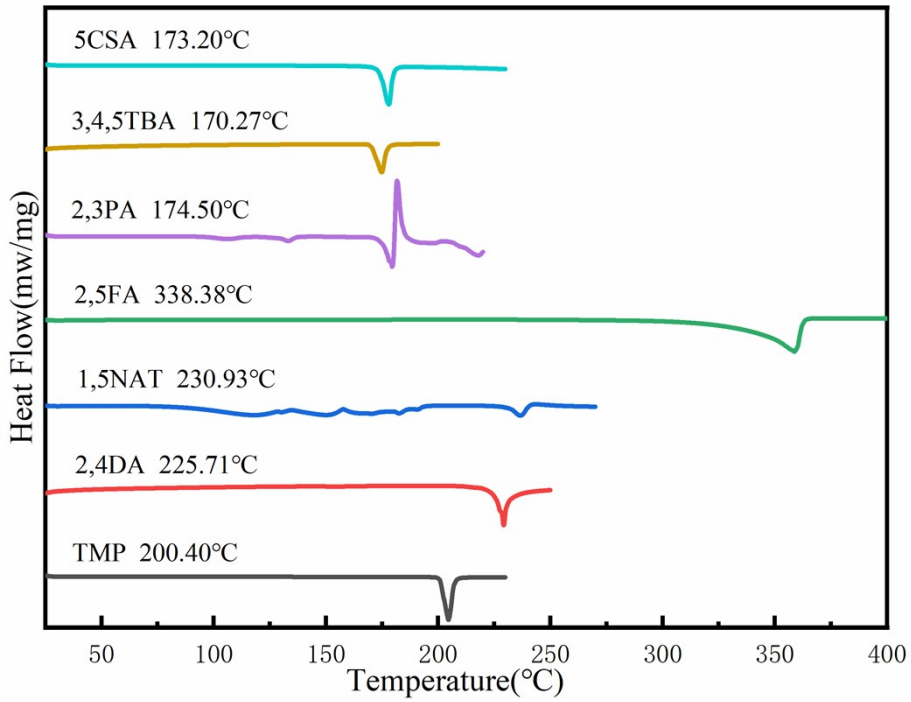


Fig. S3 Pawley fitting patterns of XRD of TMP salts.



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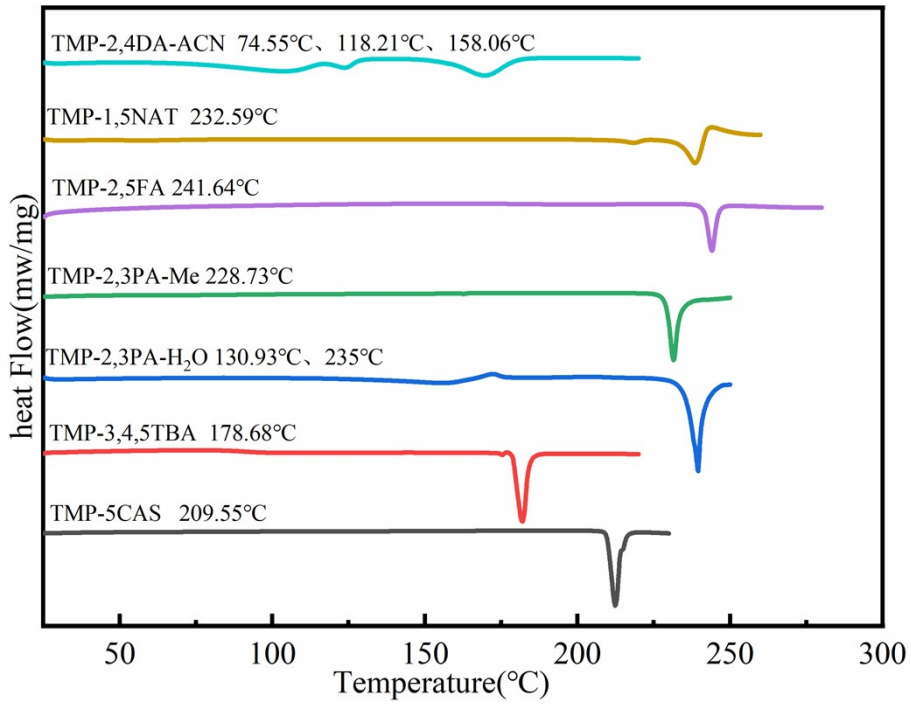
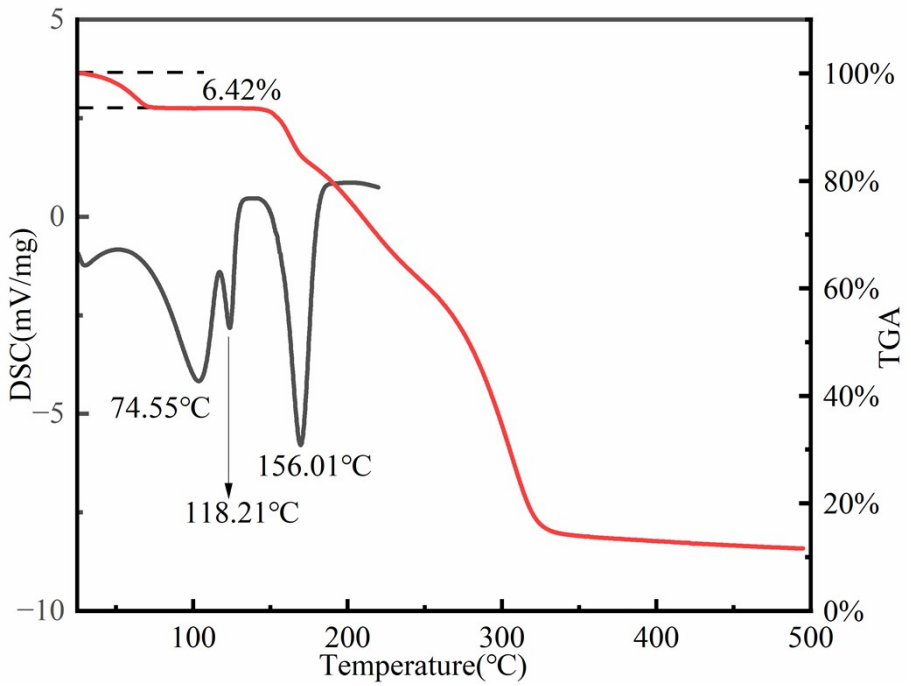


Fig. S5 DSC curves of salts.



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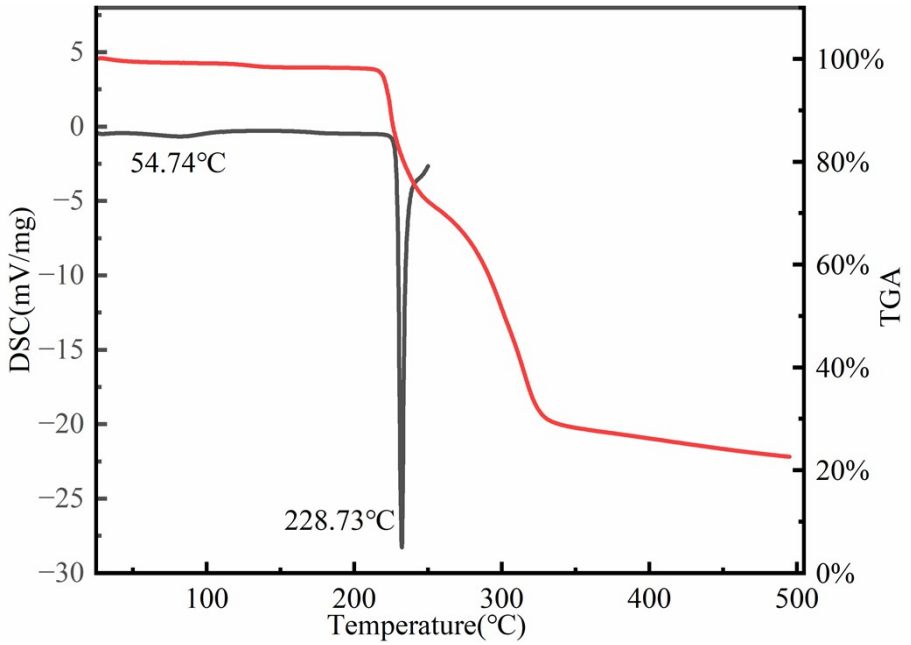
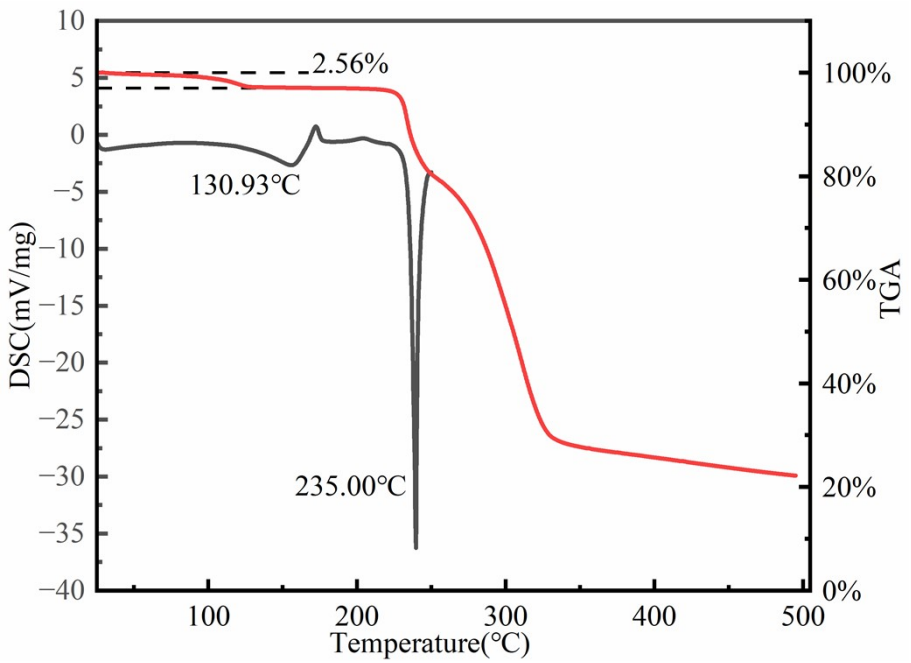


Fig. S7 DSC and TGA curves of TMP-2,3PA-Me.



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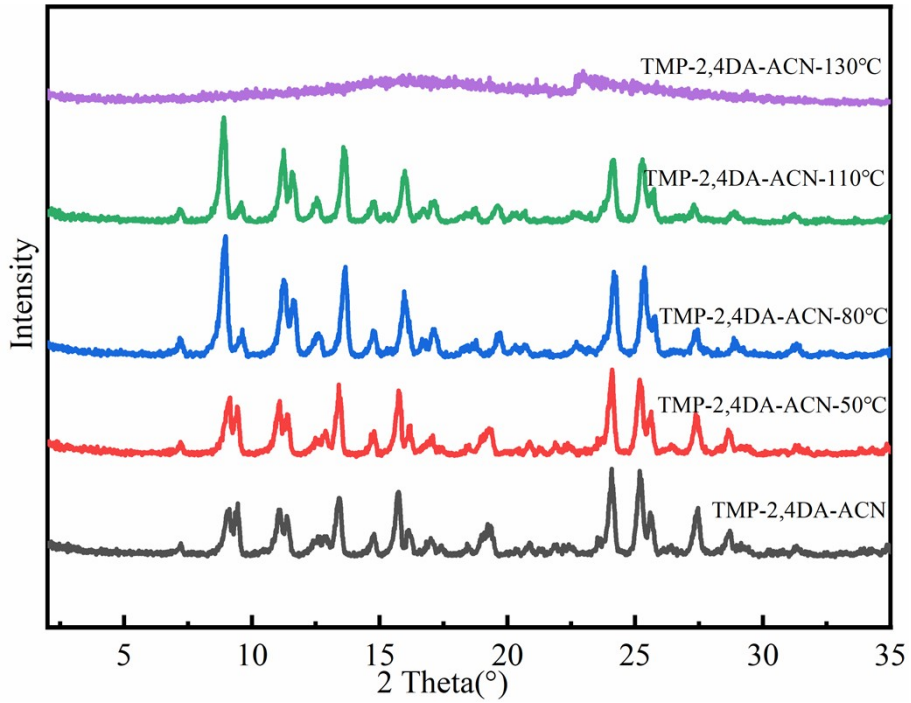

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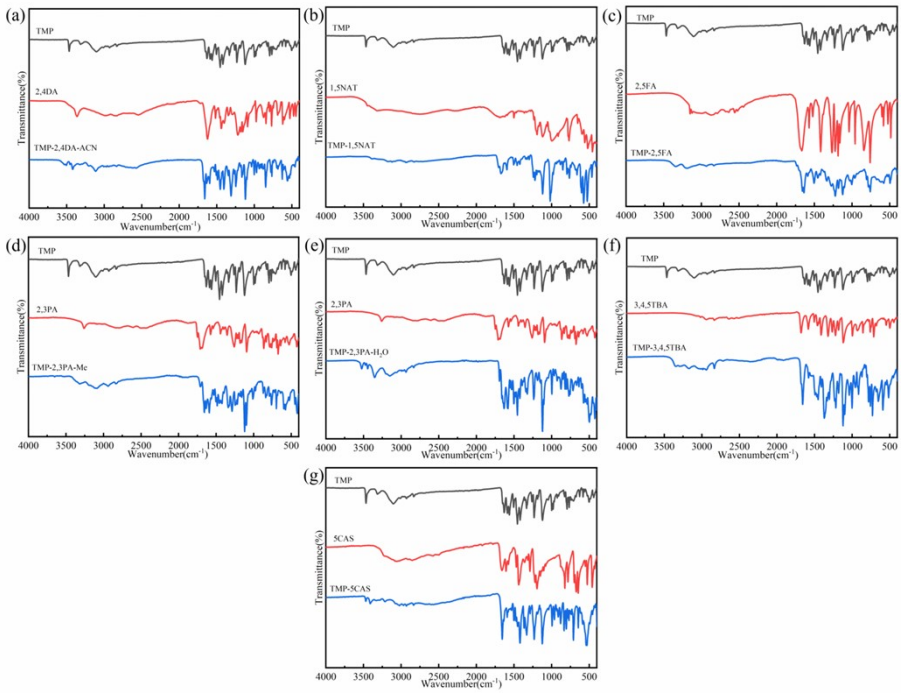

Fig. S10 FTIR spectrogram of TMP, coformers and salts. (a) TMP-2,4DA-ACN, (b) TMP-1,5NAT, (c) TMP-2,5FA, (d) TMP-2,3PA-Me, (e) TMP-2,3PA-H_2O, (f) TMP-3,4,5TBA, (g) TMP-5CSA.

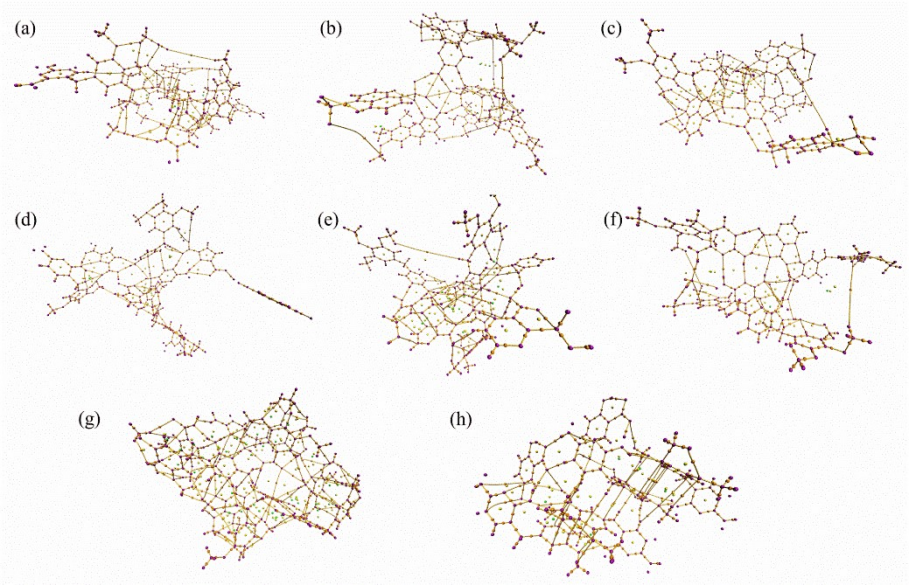

Fig. S11 Topological geometry of eight salts of TMP. The purple, orange, yellow and green spheres correspond to the (3, -3), (3, -1), (3, +1), (3, +3) critical points of electron density (nuclear critical point, bond critical point, ring critical point, cage critical point), respectively. The orange curve corresponds to the bond diameter. (a) TMP-2,4DA-ACN, (b) TMP-1,5NAT, (c) TMP-1,5NAT-Me, (d) TMP-2,5FA, (e) TMP-2,3PA-Me, (f) TMP-2,3PA-H_2O, (g) TMP-3,4,5TBA, (h) TMP-5CSA.

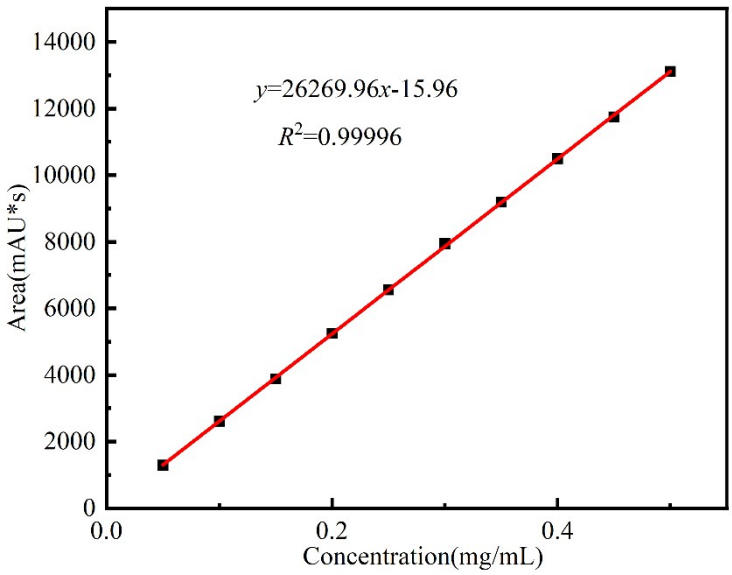

Fig. S12 HPLC standard curve of TMP.

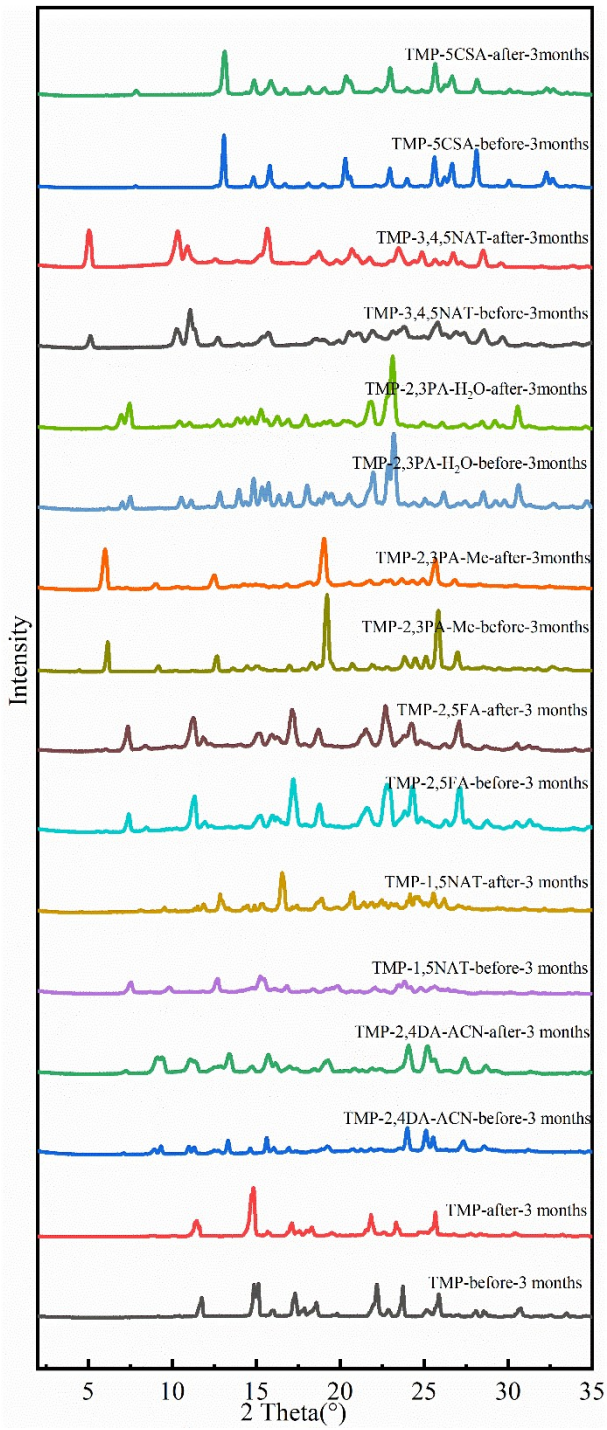

Fig. S13 PXRD comparison of samples before and after storage (40°C, RH=75%) for 3 months.

Table S1. The preparation conditions for multicomponent crystals.

Compound	Detail
	Slow solvent evaporation method
TMP-2,4DA-ACN	TMP (29 mg, 0.1mmol), 2,4DA (15.4 mg, 0.1mmol), acetonitrile (4 ml)
TMP-1,5NAT	TMP (58 mg, 0.1mmol), 1,5NAT (36 mg, 0.1mmol), methanol (4ml)

TMP-2,5FA	TMP (29 mg, 0.1mmol), 2,5FA (15.6 mg, 0.1mmol), methanol (4ml)
TMP-2,3PA-Me	TMP (29 mg, 0.1mmol), 2,3PA (16.8 mg, 0.1mmol), methanol (4ml)
TMP-2,3PA-H_2O	TMP (58 mg, 0.2mmol), 2,3PA (16.8 mg, 0.1mmol), ethanol (4ml)
TMP-3,4,5TBA	TMP (29 mg, 0.1mmol), 3,4,5TBA (21.2 mg, 0.1mmol) methanol (4ml)
TMP-5CSA	TMP (29 mg, 0.1mmol), 5CSA (17.3 mg, 0.1mmol) methanol (4ml)
	Cooling crystallization method
TMP-1,5NAT-Me	TMP (1.45 g, 0.1mmol), 1,5NAT (36 mg, 0.1mmol), methanol (4ml)
	Slurry suspension method
TMP-2,4DA-ACN	TMP (1.45 g, 5 mol), 2,4DA (0.77 g, 5 mol), acetonitrile (20 ml)
TMP-1,5NAT	TMP (1.45 g, 5 mol), 1,5NAT (0.9 g, 2.5 mol), methanol (20 ml)
TMP-2,5FA	TMP (1.45 g, 5 mol), 2,5FA (0.78 g, 5 mol), ethyl acetate (20 ml)
TMP-2,3PA-Me	TMP (1.45 g, 5 mol), 2,3PA (0.84 g, 5 mol), methanol (20 ml)
TMP-2,3PA-H_2O	TMP (1.45 g, 5 mol), 2,3PA (0.42 g, 2.5 mol), ethanol (20 ml)
TMP-3,4,5TBA	TMP (1.45 g, 5 mol), 3,4,5TBA (1.06 g, 5 mol), ethanol (20ml)
TMP-5CSA	TMP (1.45 g, 5 mol), 5CSA (0.865 g, 5 mol), methanol (20ml)

Table S2. The excess enthalpy (ΔH_{ex}) and ΔpK_a values of the reported TMP salts[a].

API/Coformer	ΔH_{ex}(kcal/mol)	pK_a	ΔpK_a
TMP		7.12	
Oxalic acid	-5.357665	1.23	5.89
Sulfosalicylic acid	-5.326675	2.48	4.64
2,5-Dihydroxybenzoic acid	-4.247795	2.75	4.37
Gallic acid	-4.065365	4.24	2.88
Phthalic acid	-3.979215	2.89	4.23
Benzenesulfonic acid	-3.934695	0.70	6.42
Sulfanilic acid	-3.92702	3.24	3.88
p-Toluenesulfonic acid	-3.88384	-0.51	7.63
2-Ketoglutaric acid	-3.774315	2.47	4.65
Fumaric acid	-3.76432	3.02	4.10
3-Nitrobenzoic acid	-3.720265	3.47	3.65
3,5-Dinitrosalicylic acid	-3.701945	0.3	6.82
DL-Malic acid	-3.4344	3.46	3.66
Terephthalic acid	-3.36769	3.51	3.61
Pyridine-2,6-dicarboxylic acid	-3.343745	2.16	4.96

p-Nitrobenzoic acid	-2.97194	3.41	3.71
Succinic acid	-2.919295	4.16	2.96
Salicylic acid	-2.87963	2.98	4.14
2,6-Dihydroxybenzoic acid	-2.63133	1.30	5.82
2-Picolinic acid	-2.5365	1.07	6.05
Malonic acid	-2.51721	2.83	4.29
Glutaric acid	-2.409645	4.31	2.81
5-Methyl-2-thiophenecarboxylic acid	-2.337725	3.75	3.37
Adipic acid	-2.28998	4.43	2.69
Sebacic acid	-2.10115	4359	2.53
Flufenamic acid	-2.09056	3.90	3.22
Tolfenamic acid	-2.050175	3.66	3.46
3-Chlorobenzoic acid	-2.02994	3.82	3.30
Mefenamic acid	-2.01616	4.20	2.92
Syringic acid	-2.013465	4.20	2.92
2-Nitrobenzoic acid	-1.61943	2.16	4.96
trans-Cinnamic acid	-1.497265	4.44	2.68
Trifluoroacetic acid	-1.425355	0.30	6.82
Sorbic acid	-1.34473	4.76	2.36
Nicotinic acid	-1.167365	4.85	2.27

[a]All the reported TMP salt were obtained from the CCDC database; all the pK_a values were obtained from CAS SciFinder.

Table S3 Crystal structure parameters and fitting parameters of TMP salts.

Compounds		a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Rwp(%)
TMP-2,4DA-ACN	Single crystal	12.0964	9.7449	20.4019	90	101.150	90	
	Pawley fit	11.9428	9.7353	20.2245	90	101.290	90	10.23
TMP-1,5NAT	Single crystal	12.2812	11.5143	14.0953	90	107.887	90	
	Pawley fit	12.2238	11.6123	14.0885	90	107.726	90	14.22
TMP-2,5FA	Single crystal	16.9699	17.1267	17.9029	63.782	64.481	84.746	
	Pawley fit	16.8877	17.1563	17.9839	64.028	64.797	84.718	6.28
TMP-2,3PA-Me	Single crystal	14.4664	12.6295	12.7478	90	111.155	90	
	Pawley fit	14.2329	12.3525	12.4719	90	111.202	90	4.40
TMP-2,3PA-H_2O	Single crystal	10.6038	12.9331	14.4781	67.818	84.598	84.690	
	Pawley fit	10.2182	12.5668	13.8210	67.208	85.659	84.740	9.85

TMP-3,4,5TBA	Single crystal	17.5775	8.5067	16.7661	90	106.408	90	
	Pawley fit	17.1566	8.3423	16.2581	90	107.076	90	8.34
TMP-5CSA	Single crystal	11.7204	8.4362	21.7076	90	98.393	90	
	Pawley fit	11.9513	8.7628	22.0095	90	98.906	90	10.51

Table S4. Crystallographic parameters of salts.

compound	TMP-5CSA	TMP-3,4,5TBA	TMP-1,5NAT	TMP-2,4DA-ACN
Empirical formula	$C_{21}H_{23}ClN_4O_6$	$C_{24}H_{30}N_4O_8$	$C_{38}H_{44}N_8O_{12}S_2$	$C_{23}H_{27}N_5O_7$
Formula weight	462.88	502.52	868.93	485.49
Temperature (K)	113.15	293	113.15	293
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/n$	$P2_1/c$
a (Å)	11.7204(2)	17.5775(9)	12.2812(2)	12.0964(3)
b (Å)	8.4362(2)	8.5067(4)	11.5143(2)	9.7449(2)
c (Å)	21.7076 (5)	16.7661(9)	14.0952(2)	20.4019(6)
α (°)	90	90	90	90
β (°)	98.393(2)	106.408(6)	107.887(2)	101.150(2)
γ (°)	90	90	90	90
Z	4	4	2	4
Volume(Å^3)	2123.37(8)	2404.9(2)	1896.85(6)	2359.54(10)
ρ_{calc} (g/cm^3)	1.448	1.388	1.521	1.367
μ(mm^{-1})	0.227	0.105	0.219	0.103
F(000)	968.0	1064.0	912.0	1024.0
Reflections collected	29871	19423	26794	50758
R_{int}	0.0484	0.0993	0.0334	0.0862
Goodness-of-fit on F^2	1.036	1.144	1.009	1.062
R_1 indexes [I > 2σ (I)]	0.0441	0.0918	0.0365	0.0944

wR_2 indexes (all data)	0.1178	0.2000	0.0984	0.2138
CCDC	2283871	2283924	2283930	2283958

compound	TMP-1,5NAT-2Me	2TMP-2,3PA-H_2O	TMP-2,3PA-Me	TMP-2,5FA
Empirical formula	$C_{26}H_{34}N_4O_{11}S_2$	$C_{34}H_{42}N_{10}O_{11}$	$C_{20.37}H_{23.49}N_6O_{7.37}$	$C_{20}H_{22}N_4O_8$
Formula weight	642.69	766.77	470.37	446.41
Temperature (K)	293(2)	293(2)	113.15	113.15
Crystal system	triclinic	triclinic	monoclinic	triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P\bar{1}$
a (Å)	11.43180(10)	10.6038(7)	14.4664(4)	16.9699(4)
b (Å)	11.93110(10)	12.9331(11)	12.6295(2)	17.1267(5)
c (Å)	12.8427(2)	14.4781(8)	12.7478(4)	17.9029(3)
α (°)	83.4930(10)	67.818(6)	90	63.782(3)
β (°)	68.6770(10)	84.598(5)	111.155(3)	64.481(2)
γ (°)	61.8010(10)	84.690(6)	90	84.746(2)
Z	2	2	4	8
Volume($Å^3$)	1434.43(3)	1826.9(2)	2172.10(11)	4181.1(2)
ρ_{calc} (g/cm^3)	1.488	1.394	1.438	1.418
$\mu(mm^{-1})$	0.254	0.893	0.112	0.111
F(000)	676.0	808.0	987.0	1872.0
Reflections collected	37718	24796	30763	17016
R_{int}	0.0416	0.0774	0.0854	
Goodness-of-fit on F^2	1.037	1.026	1.020	1.030
R_1 indexes [$I > 2\sigma(I)$]	0.0464	0.0600	0.0512	0.0595
wR_2 indexes (all data)	0.1201	0.1786	0.1395	0.1662
CCDC	2288509	2288508	2283935	2286188

Table S5. Hydrogen bond geometrical parameters of salts.

D-H···A	d(D-H)/ Å	d(H···A)/ Å	d(D···A)/ Å	θ(D-H···A)/°	Symmetry code
TMP-2,4DA-ACN					
N_1–H_1···O_7	0.86	1.84	2.696(2)	172	
N_3–H_{3A}···O_1	0.86	2.18	3.005(2)	160	1+x,y,z
N_3–H_{3B}···O_6	0.86	2.00	2.855(2)	174	
N_4–H_{4B}···N_{22}	0.86	2.31	3.100(3)	154	
O_4–H_{4C}···O_7	0.82	1.81	2.623(2)	148	1-x,-1/2+y,3/2-z
O_5–H_5···O_6	0.82	1.77	2.500(2)	148	
C_5–H_{5A}···O_5	0.96	2.35	3.219(3)	150	-1+x,3/2-y,-1/2+z
C_5–H_{5B}···O_5	0.96	2.42	3.210(3)	139	-x,2-y,1-z
C_5–H_{5B}···O_3	0.96	2.31	3.122(3)	142	-x,2-y,1-z
C_7–H_7···N_2	0.93	2.57	3.471(2)	162	1-x,2-y,1-z
TMP-1,5NAT					
N_1–H_{1A}···O_6	0.879(19)	2.200(19)	2.9944(15)	150.2(16)	2-x,-y,1-z
N_1–H_{1B}···O_5	0.875(19)	2.08(2)	2.9258(15)	162.5(18)	
N_2–H_{2A}···O_6	0.864(19)	2.081(18)	2.8405(14)	146.3(17)	1/2+x,1/2-y,1/2+z
N_2–H_{2B}···O_3	0.89(2)	2.47(2)	3.3210(15)	159.2(17)	1/2+x,3/2-y,1/2+z
N_4–H_4···O_4	0.888(17)	1.863(17)	2.7503(13)	177.2(14)	
C_4–H_{4A}···O_1	0.95	2.28	3.1515(14)	152	1-x,1-y,1-z
C_{16}–H_{16}···O_5	0.95	2.41	2.8328(14)	107	
C_{18}–H_{18}···O_4	0.95	2.49	3.0552(15)	118	1-x,-y,1-z
TMP-1,5NAT-Me					
N_1–H_{1A}···O_{10}	0.86	2.14	2.8648(15)	141	
N_1–H_{1B}···O_9	0.86	2.05	2.8490(19)	154	1-x,1-y,-z
N_2–H_2···O_7	0.86	1.82	2.6731(15)	175	
N_3–H_{3A}···O_5	0.86	1.95	2.8021(17)	170	
N_3–H_{3B}···O_8	0.86	2.08	2.8895(15)	158	
N_4–H_4···O_6	0.86	1.84	2.6777(16)	164	
O_{10}–H_{10}···O_{11}	0.82	1.94	2.753(2)	170	
O_{11}–H_{11}···O_8	0.86	2.06	2.8897(15)	161	1-x,1-y,-z
C_1–H_{1D}···N_3	0.96	2.57	3.5088(17)	167	x,-1+y,z
C_3–H_{3C}···O_4	0.96	2.56	3.412(2)	148	-1+x,y,z
C_{10}–H_{10A}···O_9	0.97	2.59	3.3171(17)	132	1-x,1-y,-z
C_{12}–H_{12}···O_1	0.93	2.30	3.1033(15)	144	1-x,-y,1-z
C_{15}–H_{15}···O_4	0.93	2.60	3.1861(16)	122	2-x,-y,1-z
TMP-2,5FA					
N_1–H_1···O_{21}	0.88	1.94	2.752(3)	153	1+x,1+y,-2+z
N_1–H_{2A}···N_7	0.88	2.23	3.082(4)	162	1-x,-y,-z

N_2–H_{2B}···O_{22}	0.88	2.37	3.247(3)	178	1+x,1+y,-2+z
N_2–H_{2B}···O_{23}	0.88	2.52	2.985(3)	114	1+x,1+y,-2+z
N_4–H_{4A}···O_5	0.88	2.18	3.049(3)	171	
N_4–H_{4A}···O_6	0.88	2.56	2.895(3)	104	
N_4–H_{4B}···O_7	0.88	2.35	3.130(3)	148	
O_4–H_{4C}···O_{12}	0.860(13)	1.627(14)	2.485(2)	175(4)	x,y,-1+z
N_5–H_{5A}···O_{18}	0.88	2.02	2.898(3)	178	-x,-y,1-z
N_5–H_{5B}···O_8	0.88	2.11	2.971(3)	167	
N_6–H_6···O_{12}	0.88	1.90	2.729(3)	155	1-x,-y,1-z
N_8–H_{8A}···O_{23}	0.88	1.93	2.805(3)	175	x,y,-1+z
N_8–H_{8B}···O_{20}	0.88	2.37	3.030(3)	132	x,y,-1+z
O_9–H_{9A}···O_8	0.85(7)	1.61(7)	2.447(3)	169(8)	
C_4–H_4···O_7	0.95	2.46	3.343(4)	154	
C_{10}–H_{10D}···O_7	0.99	2.49	3.417(4)	155	
C_{17}–H_{17}···N_5	0.95	2.54	3.400(3)	150	
TMP-2,3PA-Me					
N_1–H_{1A}···O_5	0.87(2)	1.95(2)	2.8117(17)	170(2)	-x,-1/2+y,1/2-z
N_1–H_{1B}···N_5	0.85(2)	2.20(2)	3.0151(16)	162.8(19)	
N_1–H_2···O_4	0.89(2)	1.91(2)	2.7689(15)	161.3(19)	
N_4–H_{4A}···O_4	0.897(19)	2.364(19)	3.1907(17)	153.3(15)	-x,1-y,-z
N_4–H_{4B}···N_6	0.90(2)	2.126(19)	2.9761(16)	158.0(18)	x,y,-1+z
O_7–H_{7B}···O_4	0.92(2)	1.66(2)	2.5729(13)	171(2)	x,3/2-y,1/2+z
C_2–H_{2A}···O_6	0.95	2.46	3.1713(15)	131	x,3/2-y,-1/2+z
TMP-2,3PA-H_2O					
N_1–H_{1A}···O_{11}	0.88(3)	2.41(3)	3.039(3)	129(2)	-1+x,y,z
N_1–H_{1B}···O_9	0.87(4)	2.28(4)	3.145(3)	172(4)	1-x,1-y,1-z
N_3–H_{3A}···O_5	0.84(3)	2.09(3)	2.916(3)	167(3)	1-x,1-y,1-z
N_3–H_{3B}···O_4	0.90(4)	1.99(4)	2.799(3)	148(4)	
N_4–H_4···O_4	0.92(4)	1.97(4)	2.792(3)	148(4)	
N_4–H_4···N_5	0.92(4)	2.33(4)	3.047(3)	135(3)	
N_7–H_{7A}···O_5	0.93(3)	2.05(3)	2.801(4)	138(3)	
N_7–H_{7B}···N_2	0.90(4)	2.05(4)	2.938(3)	166(4)	1-x,1-y,1-z
N_8–H_8···O_7	1.04(3)	1.55(4)	2.592(3)	176(4)	
N_{10}–H_{10A}···O_{11}	0.91(4)	1.95(4)	2.842(3)	165(3)	2-x,1-y,1-z
O_{11}–H_{11A}···O_8	0.80(4)	2.19(4)	2.922(4)	152(4)	-1+x,-1+y,z
O_{11}–H_{11B}···O_4	1.00(5)	1.79(5)	2.779(3)	171(4)	
C_1–H_{1D}···N_6	0.96	2.61	3.570(4)	177	1-x,1-y,-z
C_2–H_{2A}···O_3	0.96	2.46	2.817(5)	102	

C_{10}–H_{10D}···O_5	0.97	2.47	3.433(4)	172	-1+x,-1+y,z
C_{17}–H_{17}···O_2	0.93	2.37	3.275(4)	164	-x,1-y,-z
C_{25}–H_{25A}···N_6	0.97	2.55	3.434(3)	152	2-x,2-y,-z
C_{27}–H_{27}···O_6	0.93	2.42	3.308(4)	160	1+x,y,z
TMP-3,4,5TBA					
N_1–H_1···O_5	0.86	1.79	2.641(4)	168	
N_3–H_{3A}···O_4	0.88(4)	2.08(4)	2.949(4)	166(4)	1-x,-1/2+y,3/2-z
N_3–H_{3B}···O_4	1.02(5)	1.09(5)	2.914(4)	171(4)	
N_4–H_{4A}···N_2	0.86	2.29	3.131(4)	164	1-x,-y,1-z
N_4–H_{4B}···O_4	0.86	2.20	2.865(4)	134	x,1/2-y,-1/2+z
C_2–H_{2B}···O_3	0.96	2.49	2.874(4)	104	
C_3–H_{3D}···O_2	0.96	2.41	2.924(4)	113	
C_3–H_{3E}···O_5	0.96	2.58	3.376(4)	141	x,1/2-y,-1/2+z
TMP-5CSA					
N_1–H_{1A}···O_5	0.88(2)	1.91(2)	2.7860(17)	173.8(19)	
N_1–H_{1B}···O_4	0.866(18)	2.42(2)	2.9868(18)	123.9(15)	-1/2-x,1/2+y,1/2-z
N_2–H_{2A}···O_6	0.902(18)	2.198(18)	3.0455(17)	156.4(18)	x,1+y,z
N_2–H_{2B}···O_2	0.89(2)	2.445(19)	3.2278(17)	147.2(16)	1-x,3-y,1-z
N_2–H_{2B}···O_3	0.89(2)	2.535(19)	3.0538(16)	118.0(14)	1-x,3-y,1-z
N_4–H_4···O_6	0.902(17)	1.840(17)	2.7350(16)	171.7(18)	
O_4–H_{4B}···O_5	0.97(3)	1.60(3)	2.5201(17)	157(2)	
C_4–H_{4A}···O_3	0.95	2.47	3.3174(17)	148	1-x,2-y,1-z
C_{13}–H_{13A}···O_1	0.98	2.36	2.9535(19)	118	
C_{14}–H_{14C}···O_6	0.98	2.59	3.2719(19)	127	1-x,2-y,1-z
C_{19}–H_{19}···O_1	0.95	2.50	3.4300(19)	168	1/2-x,-3/2+y,1/2-z

Table S6. Parameters of the hydrogen bonds for eight salts in AIM analysis.

Bond type	ρ (a.u.)	$\nabla^2\rho$ (a.u.)	G (a.u.)	V (a.u.)	H (a.u.)	E (kcal/mol)
TMP-2,4DA-ACN						
N_1–H_1···O_7	0.03350	0.13192	0.03113	-0.02927	0.00185	-12.19949
N_3–H_{3B}···O_6	0.02309	0.09353	0.02038	-0.01738	0.00300	-8.73983
N_3–H_{3A}···O_1	0.01416	0.06047	0.01238	-0.00965	0.00273	-5.77203
TMP-1,5NAT						
N_4–H_4···O_4	0.03017	0.12467	0.02867	-0.02616	0.00250	-11.09280
N_2–H_{2B}···O_6	0.01879	0.07936	0.01672	-0.01360	0.00312	-7.31077
N_1–H_{1B}···O_5	0.01837	0.07624	0.01613	-0.01320	0.00293	-7.17119
N_1–H_{1A}···O_6	0.01437	0.05696	0.01189	-0.00954	0.00235	-5.84183
TMP-1,5NAT-Me						

N_2–H_2···O_7	0.03298	0.15890	0.03599	-0.03225	0.00374	-12.02667
N_4–H_4···O_6	0.03151	0.15024	0.03375	-0.02994	0.00381	-11.53813
O_{10}–H_{10}···O_{11}	0.02545	0.10823	0.02435	-0.02165	0.00271	-9.52415
N_3–H_{3A}···O_5	0.02429	0.11048	0.02378	-0.01995	0.00384	-9.13864
N_1–H_{1B}···O_9	0.01982	0.08624	0.01818	-0.01480	0.00338	-7.65308
O_{11}–H_{11}···O_8	0.01917	0.07656	0.01682	-0.01449	0.00233	-7.43706
N_3–H_{3B}···O_8	0.01915	0.08193	0.01733	-0.01419	0.00315	-7.43041
N_1–H_{1A}···O_{10}	0.01857	0.07295	0.01573	-0.01322	0.00251	-7.23765
TMP-2,5FA						
N_9–H_9···O_{28}	0.02583	0.12160	0.02623	-0.02206	0.00417	-9.65044
N_5–H_{5B}···O_8	0.01784	0.06840	0.01455	-0.01199	0.00255	-6.99505
N_4–H_{4A}···O_5	0.01430	0.05735	0.01178	-0.00921	0.00256	-5.81856
N_{12}–H_{12A}···O_{13}	0.01323	0.04584	0.00959	-0.00773	0.00186	-5.46296
N_{12}–H_{12B}···O_{10}	0.01137	0.04181	0.00879	-0.00712	0.00167	-4.84481
N_4–H_{4B}···O_7	0.01120	0.03979	0.00838	-0.00681	0.00157	-4.78831
N_{10}–H_{10B}···O_{27}	0.00970	0.03874	0.00776	-0.00584	0.00192	-4.28980
TMP-2,3-Me						
N_2–H_2···O_4	0.02622	0.11627	0.02551	-0.02196	0.00356	-9.78005
N_4–H_{4A}···O_4	0.02593	0.08290	0.01997	-0.01921	0.00076	-9.68368
N_1–H_{1A}···O_5	0.02369	0.10464	0.02237	-0.01858	0.00379	-8.93923
N_1–H_{1B}···N_5	0.01827	0.06392	0.01347	-0.01097	0.00251	-7.13795
C_2–H_{2A}···O_6	0.00908	0.03365	0.00695	-0.00550	0.00146	-4.08375
TMP-2,3PA-H_2O						
N_8–H_8···O_7	0.07027	0.14088	0.05427	-0.07332	-0.01905	-24.41963
N_4–H_4···O_4	0.02605	0.09347	0.02151	-0.01965	0.00186	-9.72356
N_{10}–H_{10A}···O_{11}	0.02513	0.10461	0.02307	-0.01998	0.00308	-9.41780
N_7–H_{7B}···N_2	0.02358	0.08510	0.01870	-0.01613	0.00258	-8.90268
N_3–H_{3B}···O_4	0.02253	0.09867	0.02064	-0.01737	0.00327	-8.55372
N_7–H_{7A}···O_5	0.01891	0.08582	0.01778	-0.01410	0.00368	-7.35065
N_3–H_{3A}···O_5	0.01888	0.07470	0.01590	-0.01312	0.00278	-7.34068
N_1–H_{1B}···N_9	0.01503	0.05126	0.01054	-0.00826	0.00228	-6.06117
N_4–H_4···N_5	0.01427	0.05027	0.01046	-0.00835	0.00211	-5.80860
N_1–H_{1A}···O_{11}	0.00955	0.03875	0.00799	-0.00630	0.00169	-4.23995
TMP-3,4,5TBA						
N_1–H_1···O_5	0.03713	0.15322	0.03670	-0.03509	0.00161	-13.40588
N_3–H_{3B}···O_4	0.02804	0.10040	0.02337	-0.02165	0.00173	-10.38491
N_3–H_{3A}···O_4	0.02288	0.09496	0.02084	-0.01795	0.00290	-8.67004
N_4–H_{4B}···O_4	0.01483	0.06626	0.01359	-0.01061	0.00298	-5.99470

N_4–H_{4A}···N_2	0.01443	0.05137	0.01053	-0.00821	0.00232	-5.86177
C_{17}–H_{17}···N_4	0.00802	0.02230	0.00493	-0.00410	0.00082	-3.73147
			TMP-5CSA			
N_4–H_4···O_6	0.03351	0.12525	0.03007	-0.02883	0.00124	-12.20281
N_1–H_{1A}···O_5	0.02742	0.11411	0.02548	-0.02243	0.00304	-10.17886
N_2–H_{2A}···O_6	0.01429	0.05328	0.01115	-0.00898	0.00217	-5.81524
N_2–H_{2B}···O_2	0.00856	0.03238	0.00667	-0.00525	0.00142	-3.91093
N_2–H_{2B}···O_3	0.00833	0.03331	0.00690	-0.00547	0.00143	-3.83450