Electronic Supplementary Information

A dual-functional luminescent Tb(III) metal-organic framework for selective sensing of acetone and TNP in water

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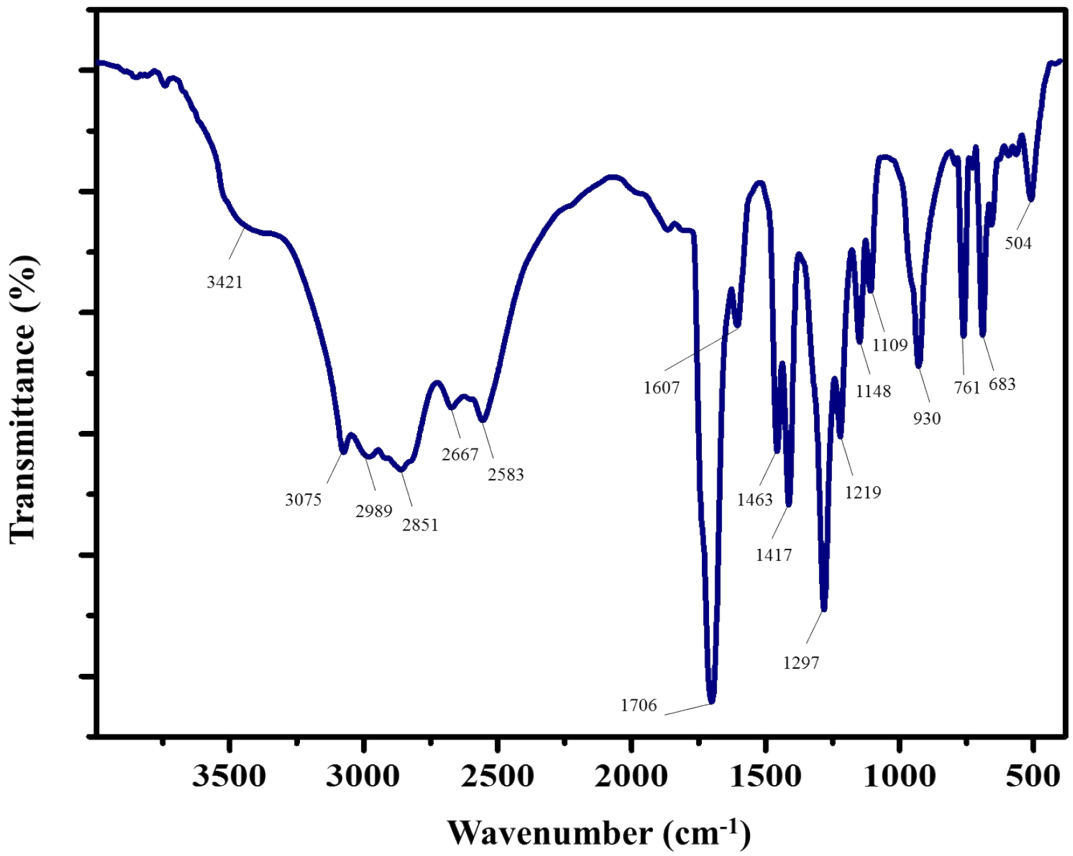

Figure S1. FT-IR spectrum of H_4abtc (L_2).

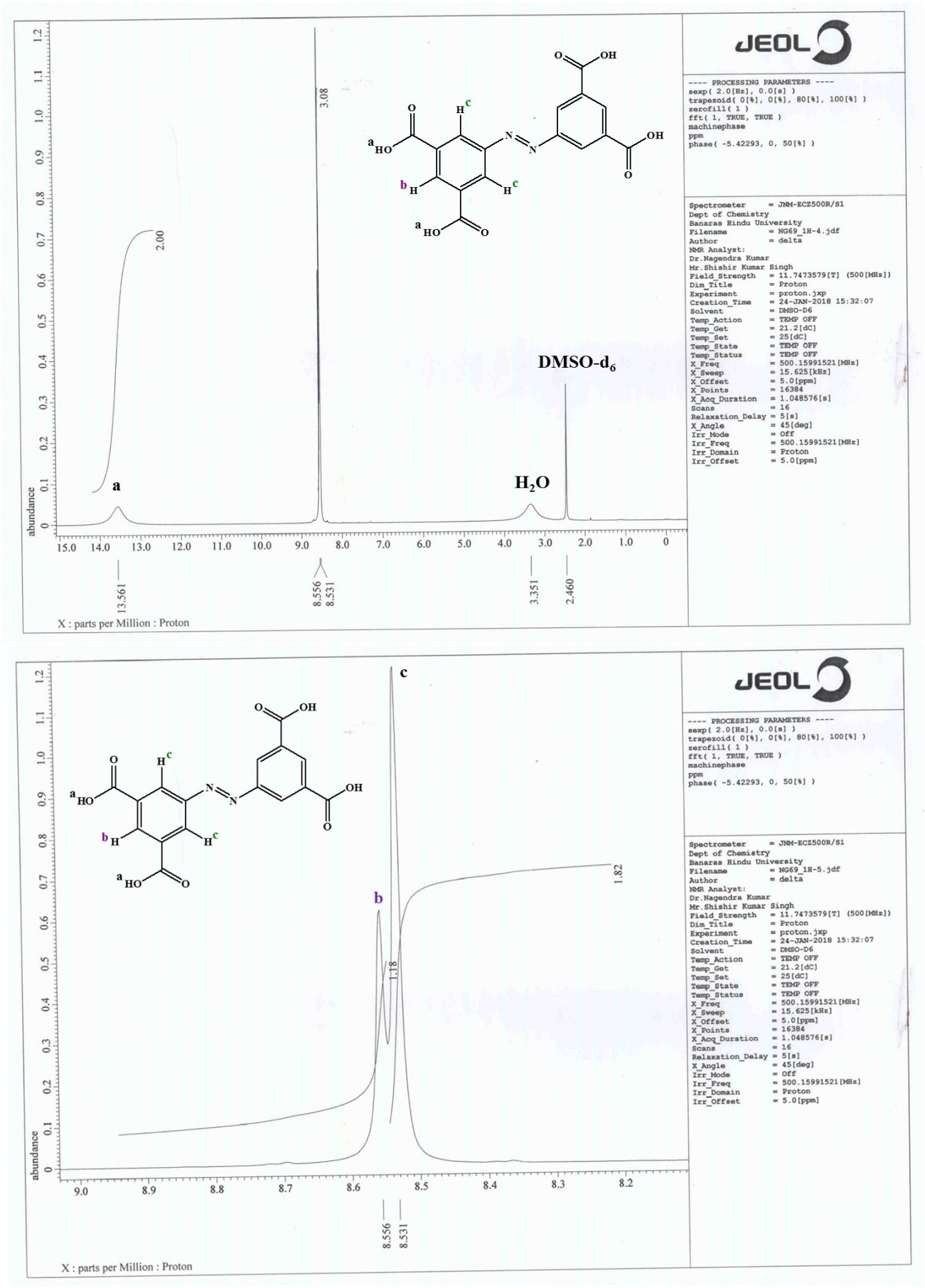

Figure S2. ^{1}H NMR spectra of L_2.

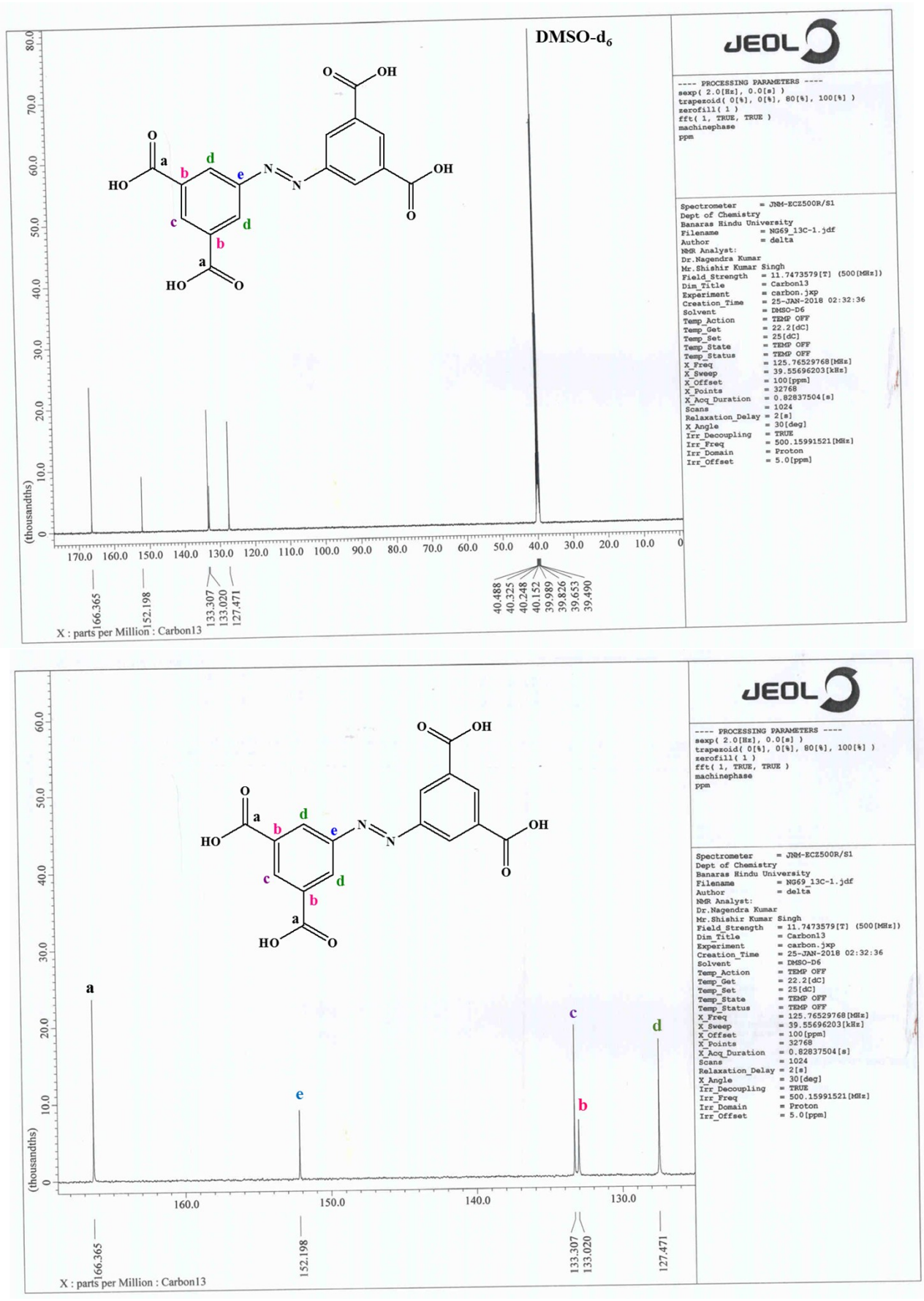

Figure S3. ^{13}C NMR spectra of L_2.

Display Report

Analysis Info

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Method	7. LC-MS tune_low meoh.m	Operator	Ghanashyam Bhavsar
Sample Name	h ak-nkg-001	Instrument	micrOTOF-Q II 10348
Comment			

Acquisition Parameter

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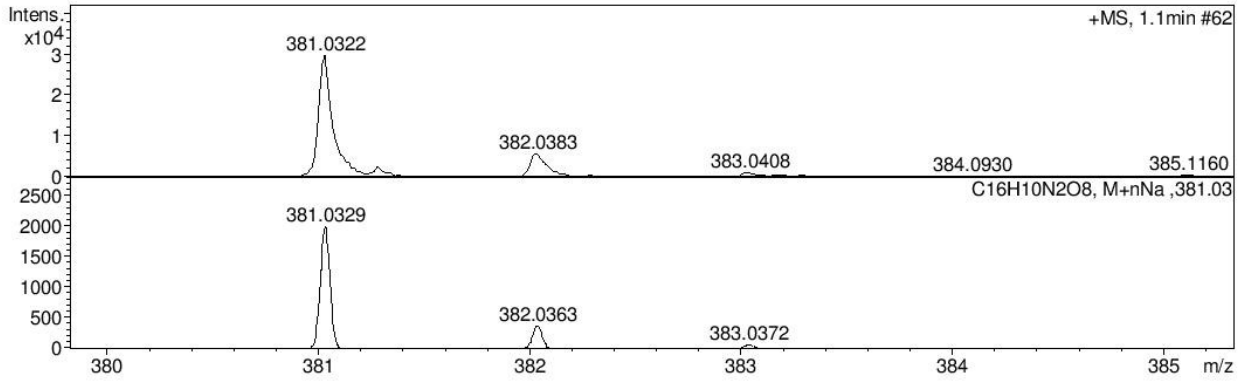
Scan End	2000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.0 printed: 1/19/2018 4:03:01 PM Page 1 of 1

Figure S4. HRMS spectra of L_2.

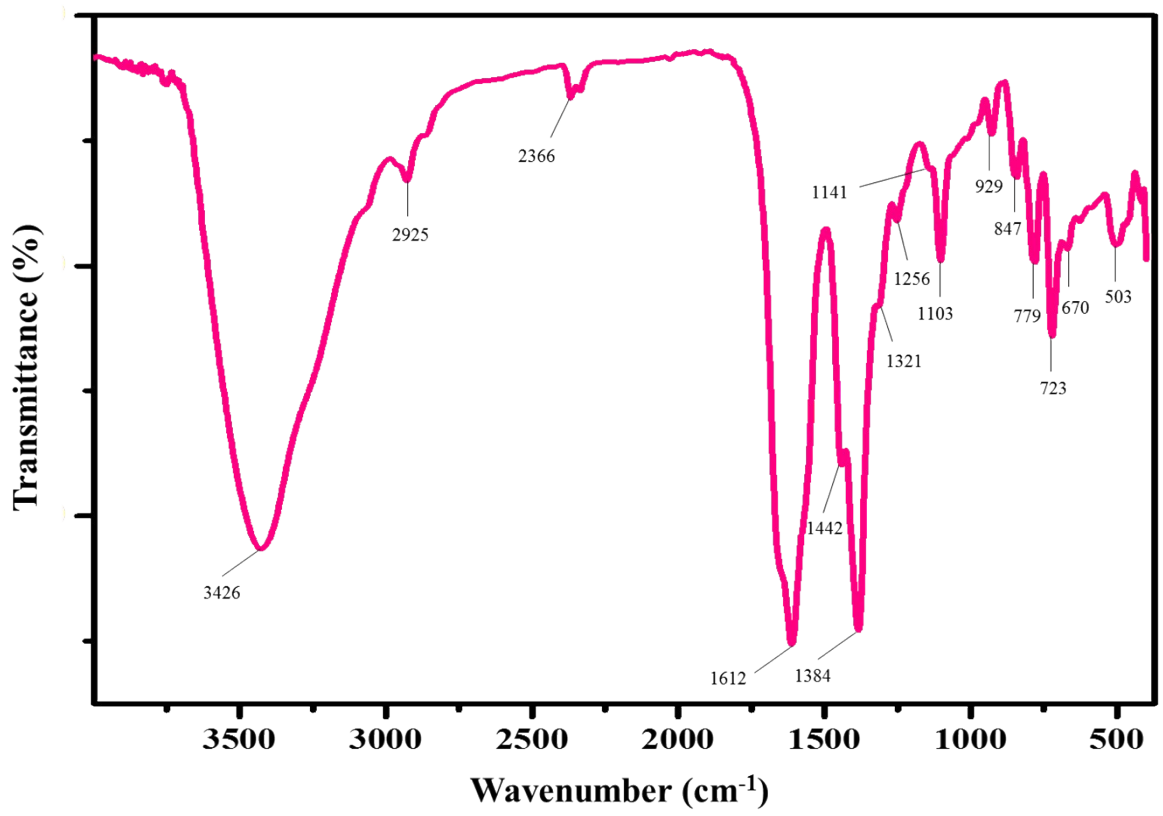
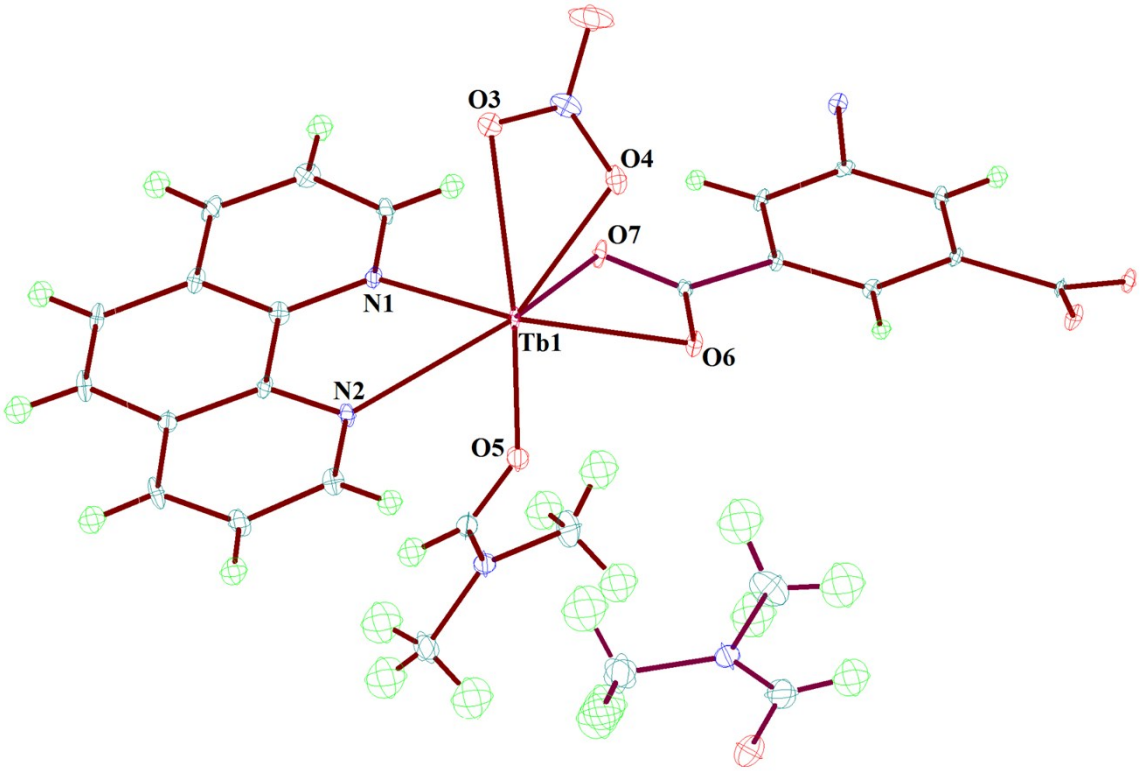
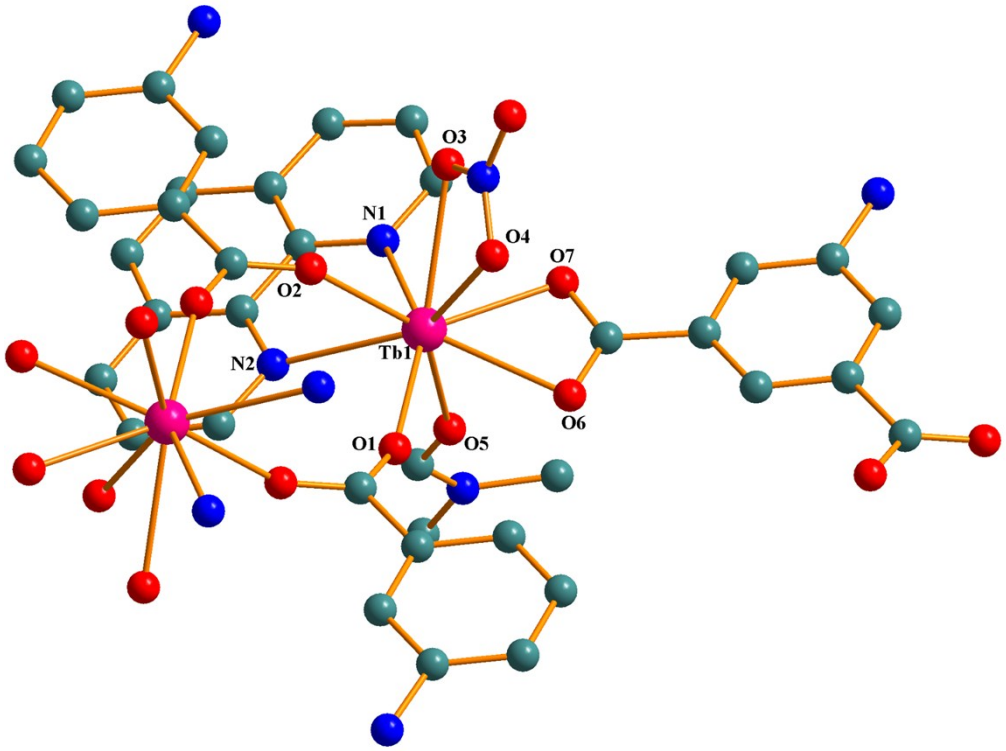


Figure S5. FT-IR spectrum of TPA-MOF.



(a)



(b)

Figure S6. (a) ORTEP representation of TPA-MOF in asymmetric unit. Thermal ellipsoids were drawn at the 30% probability level, **(b)** coordination behaviour around Tb metal centre (Hydrogens have been omitted for clarity). Color code: Tb; pink, O; red, N; blue, C; teal.

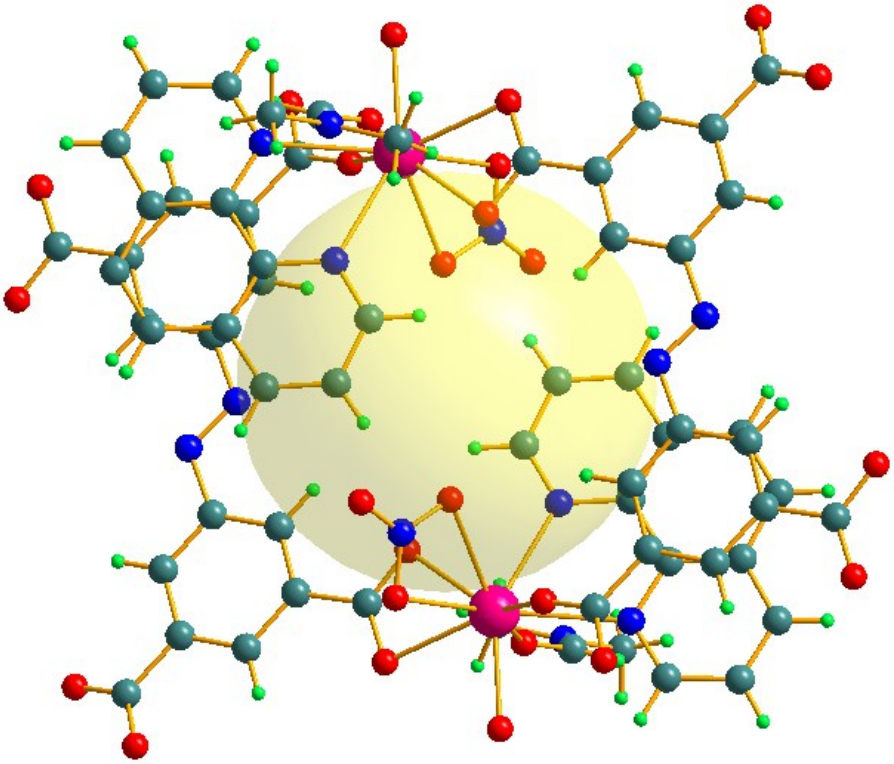


Figure S7. Micro-channel having 4Å Vander Wall radius. Color code: Tb; pink, O; red, N; blue, C; teal, and H; green.

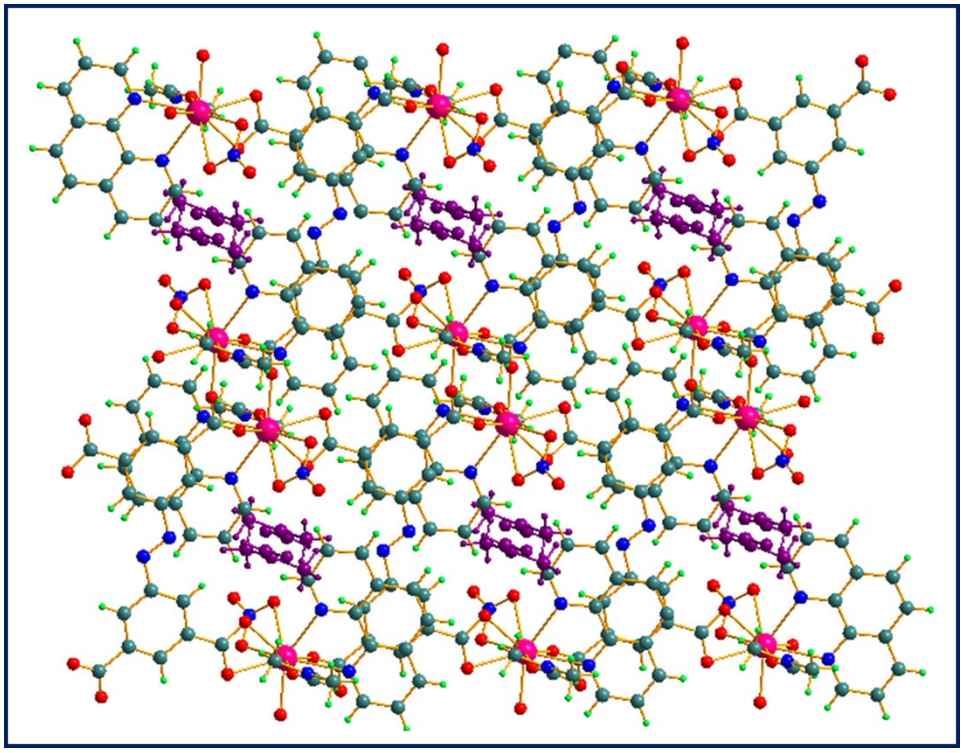
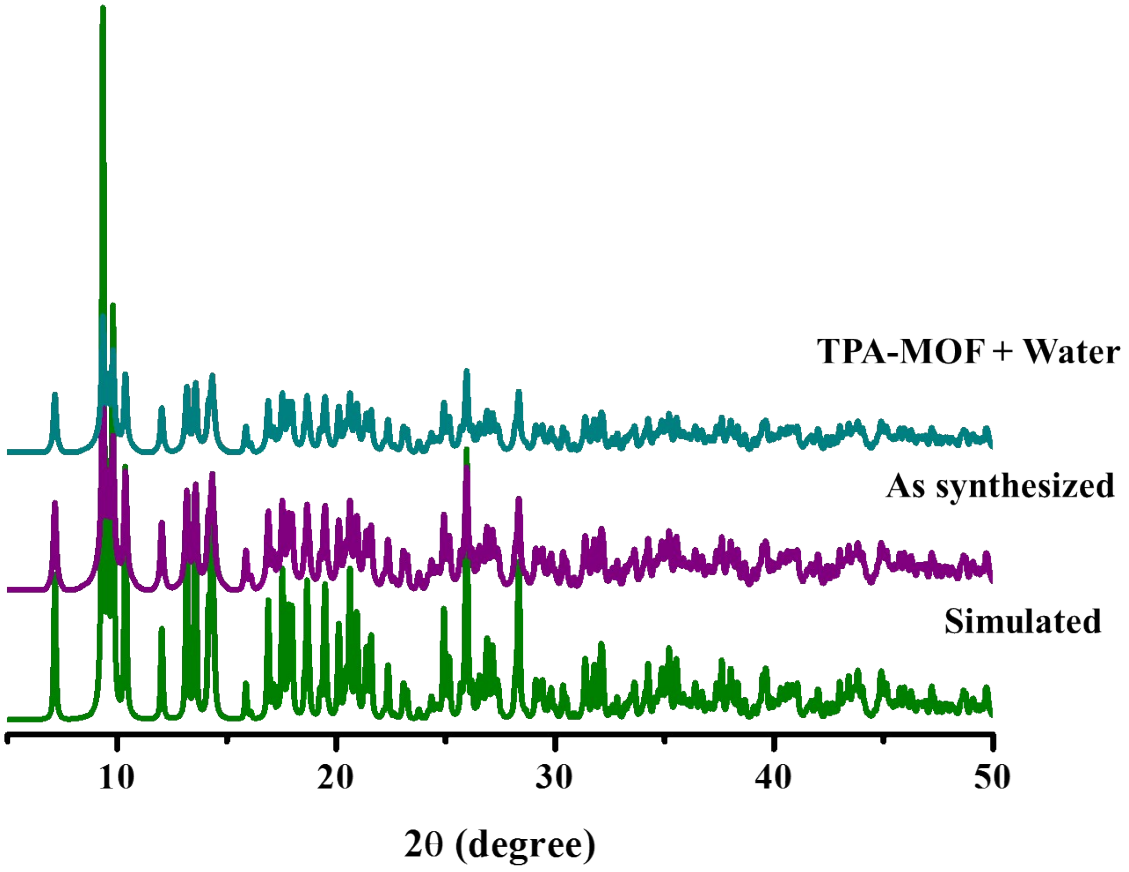
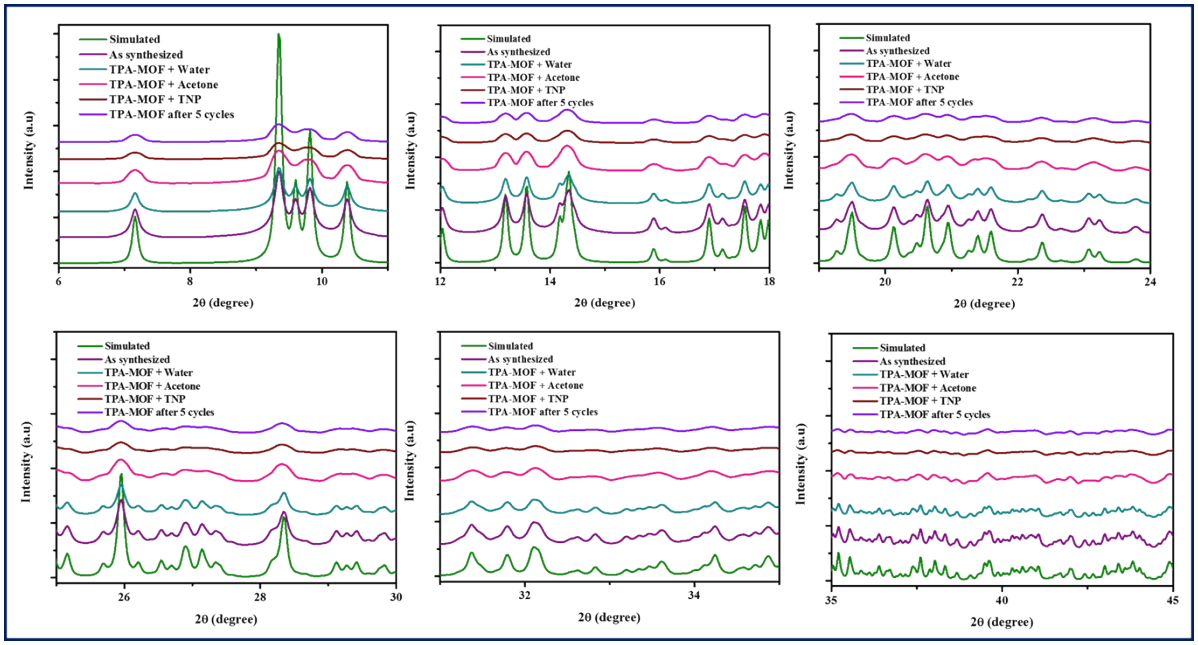


Figure S8. Perspective view of TPA-MOF. Color code: Tb; pink, O; red, N; blue, C; teal, H; green and DMF (guest), purple.



(a)



(b)

Figure S9. (a) Simulated and experimental powder X-ray diffraction pattern of TPA-MOF and TPA-MOF in water, **(b)** magnifying PXRD images in the scan range of 6-45° (2θ), obtained after immersing in H_2O (4 days), acetone, TNP for 72 h and recycled sample after five cycles.

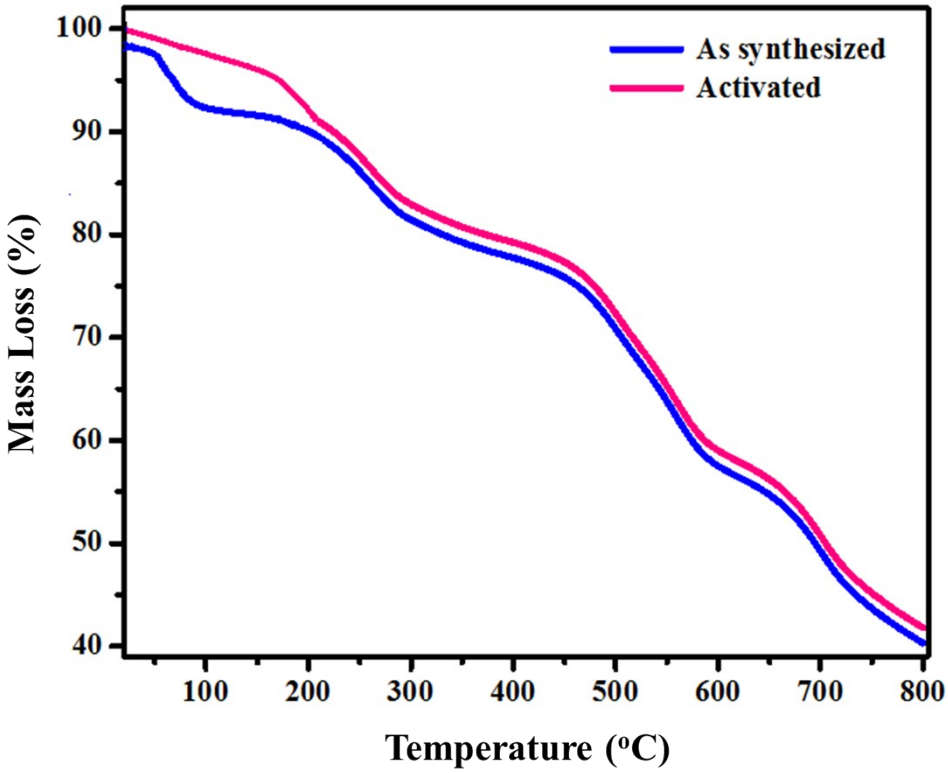


Figure S10. As synthesized and activated TG of TPA-MOF.

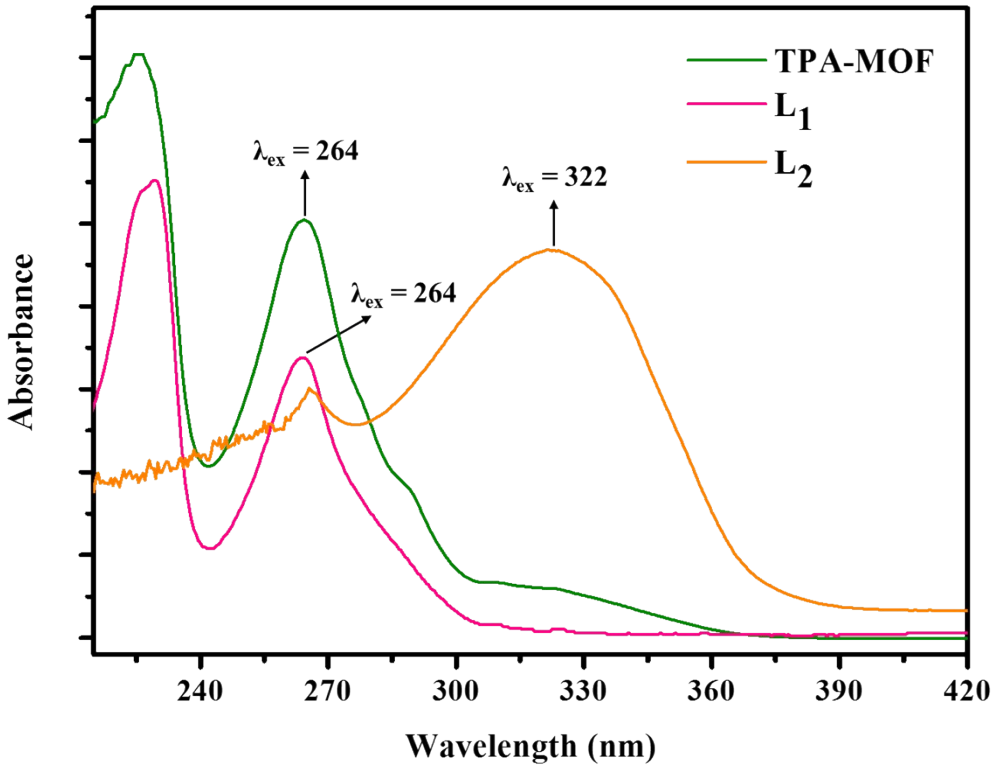


Figure S11. Comparative absorption spectra of ligands (L_1 and L_2) and TPA-MOF.

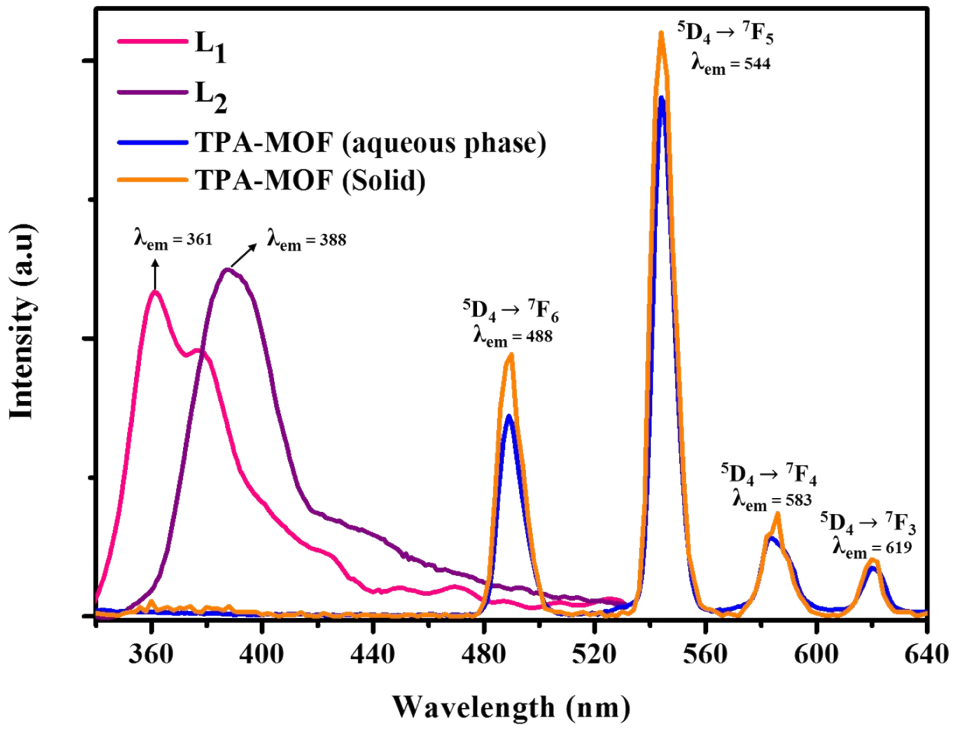


Figure S12. Comparative emission spectra of ligands (L_1 and L_2) and TPA-MOF.

The relative fluorescence intensity is linear with TNP concentration in the range of (0-400 ppm).
F_0/F = 15.971[TNP(ppm)] + 1, (R^2 = 0.99025)
K_{sv} = 15.971 ppm^{-1}
1M = 35,500 ppm
1/35,500 ppm^{-1} = $1M^{-1}$
15.971 ppm^{-1} = 5.67 × 10^5 M^{-1}

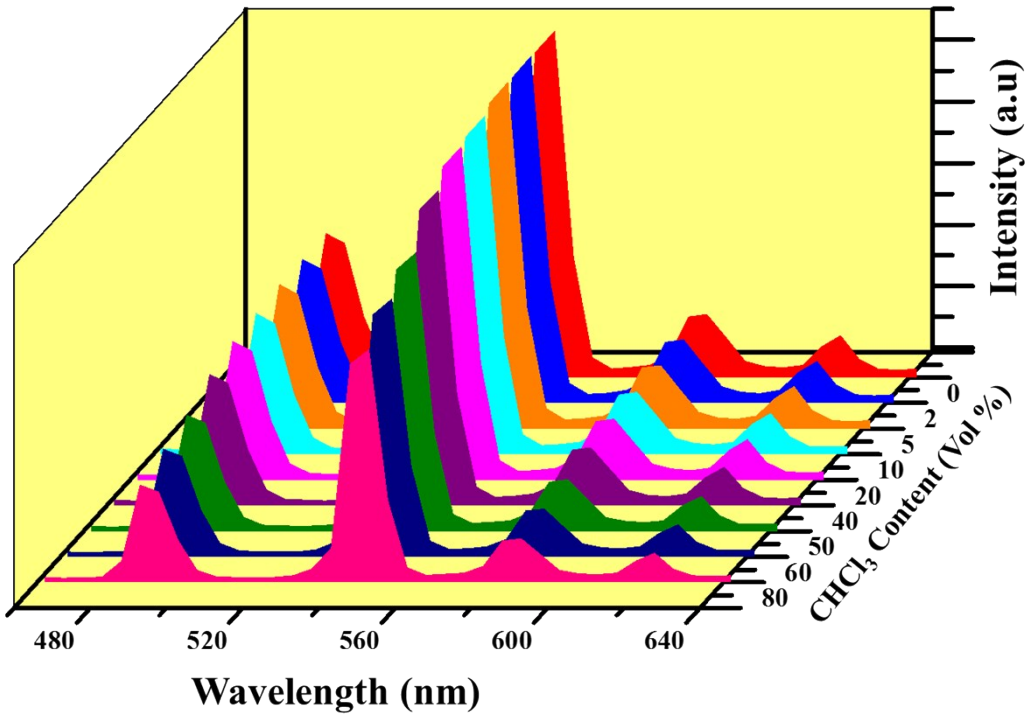


Figure S13. Spectra of TPA-MOF in presence of variable amounts of chloroform.

Table S1. Bond lengths (Å) for TPA-MOF.

Tb1—O1	2.283(3)	C4—C11	1.403(5)
Tb1—O2^{i}	2.346(4)	C4—C5	1.437(6)
Tb1—O5	2.360(4)	C5—C6	1.349(7)
Tb1—O7^{ii}	2.402(4)	C5—H5	0.950(4)
Tb1—O4	2.474(5)	C6—C7	1.431(6)
Tb1—O6^{ii}	2.486(4)	C6—H6	0.950(4)
Tb1—N1	2.538(6)	C7—C12	1.403(6)
Tb1—O3	2.595(4)	C7—C8	1.404(7)
Tb1—N2	2.599(5)	C8—C9	1.365(5)
Tb1—C20^{ii}	2.800(5)	C8—H8	0.950(4)
Tb1—N3	2.953(5)	C9—C10	1.395(6)
O1—C13	1.261(5)	C9—H9	0.950(5)
O2—C13	1.252(6)	C10—H10	0.950(4)
O2—Tb1^{i}	2.346(4)	C11—C12	1.443(7)
O3—N3	1.267(5)	C13—C14	1.503(6)
O4—N3	1.265(5)	C14—C19	1.392(6)
O5—C21	1.240(5)	C14—C15	1.407(7)
O6—C20	1.256(5)	C15—C16	1.395(6)
O6—Tb1^{ii}	2.486(4)	C15—H15	0.950(4)
O7—C20	1.268(5)	C16—C17	1.397(6)
O7—Tb1^{ii}	2.402(4)	C16—C20	1.500(7)
O8—N3	1.228(6)	C17—C18	1.390(7)
O9—C24	1.275(9)	C17—H17	0.950(4)
N1—C1	1.326(6)	C18—C19	1.390(6)
N1—C11	1.363(5)	C19—H19	0.950(5)
N2—C10	1.326(6)	C20—Tb1^{ii}	2.800(5)
N2—C12	1.359(5)	C21—H21	0.951(5)
N4—N4^{iii}	1.245(4)	C22—H22A	0.979(7)
N4—C18	1.442(5)	C22—H22B	0.980(6)
N5—C21	1.311(7)	C22—H22C	0.980(6)
N5—C23	1.455(8)	C23—H23A	0.980(6)
N5—C22	1.459(6)	C23—H23B	0.980(5)
N6—C24	1.302(7)	C23—H23C	0.979(6)
N6—C26	1.443(7)	C24—H24	0.950(6)
N6—C25	1.458(9)	C25—H25A	0.980(6)
C1—C2	1.399(6)	C25—H25B	0.979(7)
C1—H1	0.950(4)	C25—H25C	0.980(6)
C2—C3	1.365(7)	C26—H26A	0.981(8)
C2—H2	0.950(5)	C26—H26B	0.980(7)
C3—C4	1.412(7)	C26—H26C	0.980(8)
C3—H3	0.950(4)		

Table S2. Bond angles (°) for TPA-MOF.

O1—Tb1—O2^{i}	82.13(10)	C2—C3—C4	118.65(44)
O1—Tb1—O5	86.76(10)	C2—C3—H3	120.67(44)
O2^{i}—Tb1—O5	141.45(11)	C4—C3—H3	120.68(37)
O1—Tb1—O7^{ii}	128.54(9)	C11—C4—C3	118.53(34)
O2^{i}—Tb1—O7^{ii}	137.02(10)	C11—C4—C5	119.94(37)
O5—Tb1—O7^{ii}	76.94(10)	C3—C4—C5	121.51(40)
O1—Tb1—O4	90.08(10)	C6—C5—C4	120.32(39)
O2^{i}—Tb1—O4	72.91(11)	C6—C5—H5	119.86(37)
O5—Tb1—O4	144.15(11)	C4—C5—H5	119.81(39)
O7^{ii}—Tb1—O4	77.36(10)	C5—C6—C7	121.30(35)
O1—Tb1—O6^{ii}	75.26(10)	C5—C6—H6	119.36(43)
O2^{i}—Tb1—O6^{ii}	136.16(11)	C7—C6—H6	119.34(39)
O5—Tb1—O6^{ii}	74.57(11)	C12—C7—C8	117.53(39)
O7^{ii}—Tb1—O6^{ii}	53.44(11)	C12—C7—C6	119.73(37)
O4—Tb1—O6^{ii}	70.12(10)	C8—C7—C6	122.73(34)
O1—Tb1—N1	147.03(10)	C9—C8—C7	119.12(35)
O2^{i}—Tb1—N1	92.21(10)	C9—C8—H8	120.43(41)
O5—Tb1—N1	77.59(10)	C7—C8—H8	120.45(42)
O7^{ii}—Tb1—N1	76.1(1)	C8—C9—C10	119.48(38)
O4—Tb1—N1	119.37(10)	C8—C9—H9	120.25(37)
O6^{ii}—Tb1—N1	126.31(10)	C10—C9—H9	120.27(41)
O1—Tb1—O3	135.14(9)	N2—C10—C9	123.38(39)
O2^{i}—Tb1—O3	67.87(11)	N2—C10—H10	118.30(37)
O5—Tb1—O3	137.13(11)	C9—C10—H10	118.32(40)
O7^{ii}—Tb1—O3	69.31(10)	N1—C11—C4	122.05(37)
O4—Tb1—O3	50.35(11)	N1—C11—C12	118.56(38)
O6^{ii}—Tb1—O3	103.73(10)	C4—C11—C12	119.38(34)
N1—Tb1—O3	69.38(10)	N2—C12—C7	123.13(37)
O1—Tb1—N2	83.80(11)	N2—C12—C11	117.54(34)
O2^{i}—Tb1—N2	69.05(11)	C7—C12—C11	119.30(38)
O5—Tb1—N2	73.13(11)	O2—C13—O1	124.06(37)
O7^{ii}—Tb1—N2	134.02(11)	O2—C13—C14	118.27(38)
O4—Tb1—N2	141.94(11)	O1—C13—C14	117.65(32)
O6^{ii}—Tb1—N2	142.20(11)	C19—C14—C15	119.57(37)
N1—Tb1—N2	64.01(11)	C19—C14—C13	119.96(33)
O3—Tb1—N2	113.22(10)	C15—C14—C13	120.47(38)
O1—Tb1—C20^{ii}	101.91(11)	C16—C15—C14	119.35(39)
O2^{i}—Tb1—C20^{ii}	143.18(12)	C16—C15—H15	120.37(37)
O5—Tb1—C20^{ii}	75.25(12)	C14—C15—H15	120.27(39)
O7^{ii}—Tb1—C20^{ii}	26.84(11)	C15—C16—C17	120.78(35)
O4—Tb1—C20^{ii}	70.52(12)	C15—C16—C20	121.15(38)
O6^{ii}—Tb1—C20^{ii}	26.66(12)	C17—C16—C20	118.00(36)
N1—Tb1—C20^{ii}	101.85(11)	C18—C17—C16	119.43(37)
O3—Tb1—C20^{ii}	85.41(11)	C18—C17—H17	120.25(42)
N2—Tb1—C20^{ii}	147.47(12)	C16—C17—H17	120.31(37)
O1—Tb1—N3	112.82(11)	C17—C18—C19	120.26(40)
O2^{i}—Tb1—N3	67.98(12)	C17—C18—N4	123.78(36)

O5—Tb1—N3	148.83(12)	C19—C18—N4	115.94(32)
O7^{ii}—Tb1—N3	71.89(11)	C18—C19—C14	120.60(35)
O4—Tb1—N3	25.00(11)	C18—C19—H19	119.71(42)
O6^{ii}—Tb1—N3	86.84(11)	C14—C19—H19	119.68(40)
N1—Tb1—N3	94.58(11)	O6—C20—O7	121.17(34)
O3—Tb1—N3	25.35(11)	O6—C20—C16	120.13(36)
N2—Tb1—N3	130.63(11)	O7—C20—C16	118.67(38)
C20^{ii}—Tb1—N3	77.02(12)	O6—C20—Tb1^{ii}	62.58(22)
C13—O1—Tb1	154.63(24)	O7—C20—Tb1^{ii}	58.78(22)
C13—O2—Tb1^{i}	150.65(29)	C16—C20—Tb1^{ii}	173.45(30)
N3—O3—Tb1	93.33(26)	O5—C21—N5	124.10(44)
N3—O4—Tb1	99.22(27)	O5—C21—H21	117.95(51)
C21—O5—Tb1	145.17(32)	N5—C21—H21	117.96(47)
C20—O6—Tb1^{ii}	90.76(26)	N5—C22—H22A	109.52(49)
C20—O7—Tb1^{ii}	94.38(25)	N5—C22—H22B	109.43(49)
C1—N1—C11	117.82(36)	H22A—C22—H22B	109.52(55)
C1—N1—Tb1	121.59(27)	N5—C22—H22C	109.49(50)
C11—N1—Tb1	120.02(26)	H22A—C22—H22C	109.49(58)
C10—N2—C12	117.34(35)	H22B—C22—H22C	109.38(56)
C10—N2—Tb1	123.36(28)	N5—C23—H23A	109.41(49)
C12—N2—Tb1	118.58(27)	N5—C23—H23B	109.49(45)
O8—N3—O4	121.79(42)	H23A—C23—H23B	109.50(51)
O8—N3—O3	121.09(42)	N5—C23—H23C	109.41(49)
O4—N3—O3	117.09(34)	H23A—C23—H23C	109.49(63)
O8—N3—Tb1	177.45(37)	H23B—C23—H23C	109.53(49)
O4—N3—Tb1	55.78(22)	O9—C24—N6	125.59(55)
O3—N3—Tb1	61.32(23)	O9—C24—H24	117.22(63)
N4^{iii}—N4—C18	113.74(26)	N6—C24—H24	117.19(59)
C21—N5—C23	121.20(43)	N6—C25—H25A	109.43(63)
C21—N5—C22	122.27(44)	N6—C25—H25B	109.45(56)
C23—N5—C22	116.40(44)	H25A—C25—H25B	109.44(66)
C24—N6—C26	121.53(47)	N6—C25—H25C	109.47(55)
C24—N6—C25	122.30(46)	H25A—C25—H25C	109.51(62)
C26—N6—C25	116.03(49)	H25B—C25—H25C	109.51(65)
N1—C1—C2	123.64(36)	N6—C26—H26A	109.49(57)
N1—C1—H1	118.23(41)	N6—C26—H26B	109.48(55)
C2—C1—H1	118.14(40)	H26A—C26—H26B	109.42(61)
C3—C2—C1	119.29(40)	N6—C26—H26C	109.49(57)
C3—C2—H2	120.34(49)	H26A—C26—H26C	109.49(65)
C1—C2—H2	120.36(37)	H26B—C26—H26C	109.45(73)

Table S3. Coordinates for L_1, L_2 and selected NAC explosives.

Phen (L_1)					
Centre Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms)**		
			X	**Y**	**Z**
1	6	C	3.469208	-0.362207	0.000469
2	6	C	2.815625	0.844984	0.001390
3	6	C	1.409083	0.862424	0.000325
4	6	C	0.719870	-0.379404	-0.000261
5	6	C	2.708066	-1.545443	-0.000923
6	6	C	0.677902	2.098675	0.000011
7	6	C	-0.719867	-0.379408	-0.000218
8	6	C	-1.409072	0.862402	-0.000598
9	6	C	-0.677920	2.098662	-0.000817
10	6	C	-2.815634	0.845000	-0.000339
11	1	H	-3.363771	1.783984	-0.000609
12	6	C	-3.469197	-0.362196	0.000433
13	6	C	-2.708047	-1.545448	0.000844
14	1	H	1.238186	3.031105	0.000227
15	1	H	4.555802	-0.409375	0.000741
16	1	H	3.363702	1.784007	0.002544
17	1	H	3.204108	-2.511981	-0.001944
18	1	H	-1.238089	3.031159	-0.001364
19	1	H	-4.555792	-0.409381	0.000745
20	1	H	-3.204201	-2.511932	0.001515
21	7	N	1.380688	-1.572547	-0.000978
22	7	N	-1.380694	-1.572572	0.000442

H_4abtc (L_2)					
Centre Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms)**		
			X	**Y**	**Z**
1	6	C	-1.762238	-0.181573	-0.005030
2	6	C	-2.292627	1.110762	0.021986
3	6	C	-2.618328	-1.286227	-0.027001
4	6	C	4.161500	-2.726844	0.031232
5	6	C	-4.002892	-1.112272	-0.020543
6	6	C	-4.528215	0.182039	-0.016461
7	6	C	-3.674130	1.287889	0.015234
8	6	C	-4.192934	2.688766	0.035583
9	6	C	1.770723	0.193509	0.003969
10	6	C	2.630484	1.294809	-0.003602
11	6	C	2.292120	-1.103420	0.016747
12	6	C	4.010775	1.097714	-0.001454
13	6	C	4.527940	-0.199214	0.002101
14	6	C	3.671557	-1.303318	0.000776
15	6	C	-4.978850	-2.255926	-0.069081
16	6	C	4.981562	2.229156	0.005240
17	1	H	-2.153136	-2.264932	-0.078246
18	1	H	-5.601474	0.311152	-0.039348

19	1	H	-1.635764	1.969333	0.041695
20	1	H	2.209272	2.290964	-0.006554
21	1	H	1.628465	-1.956387	0.041478
22	1	H	5.607469	-0.298753	0.035532
23	1	H	5.847969	-2.137530	-0.685031
24	1	H	-5.784481	3.680147	0.041624
25	1	H	-3.629187	-3.409529	0.673822
26	1	H	5.080109	4.101516	0.014118
27	7	N	0.384759	0.503299	0.010150
28	7	N	-0.377221	-0.488637	-0.019272
29	8	O	-5.542441	2.742477	0.030943
30	8	O	-6.122661	-2.120129	-0.404295
31	8	O	-4.509123	-3.477473	0.285979
32	8	O	6.181157	2.096070	0.004135
33	8	O	-3.497063	3.673426	0.054271
34	8	O	5.451949	-2.938823	-0.323596
35	8	O	3.461572	-3.646899	0.352506
36	8	O	4.376525	3.435887	0.010880

NB					
Centre Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms)**		
			X	**Y**	**Z**
1	6	C	-0.432283	1.216904	0.000440
2	6	C	0.240633	-0.000015	0.000542
3	6	C	-0.432255	-1.216858	0.000202
4	6	C	-1.822620	-1.209207	-0.000271
5	6	C	-2.517471	-0.000035	-0.000364
6	6	C	-1.822583	1.209228	0.000026
7	1	H	0.132736	2.136105	0.000705
8	1	H	0.132649	-2.136120	0.000319
9	1	H	-2.361108	-2.147204	-0.000565
10	1	H	-3.599743	0.000016	-0.000705
11	1	H	-2.361211	2.147156	-0.000049
12	7	N	1.724881	-0.000003	0.001048
13	8	O	2.293882	-1.083401	-0.000320
14	8	O	2.293866	1.083398	-0.000991

1,3-DNB					
Centre Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms)**		
			X	**Y**	**Z**
1	6	C	1.198840	1.557649	-0.000230
2	6	C	-0.100360	2.042293	0.000042
3	6	C	-1.225145	1.201843	-0.000020
4	6	C	-0.962443	-0.183144	-0.000378
5	6	C	0.329016	-0.698692	-0.000651
6	6	C	1.394481	0.182320	-0.000593
7	1	H	2.053675	2.219547	-0.000183
8	1	H	-0.260666	3.113683	0.000315

9	1	H	0.490970	-1.765766	-0.000918
10	7	N	2.772913	-0.357687	-0.000906
11	8	O	2.903080	-1.572068	0.001395
12	8	O	3.689264	0.451992	0.001727
13	7	N	-2.053160	-1.196623	-0.000486
14	8	O	-1.727623	-2.373904	-0.000658
15	8	O	-3.209576	-0.797314	-0.000141
16	1	H	-2.194715	1.654430	0.000206

4-NT					
Centre Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms)**		
			X	**Y**	**Z**
1	6	C	-0.003372	-1.209901	0.000306
2	6	C	1.383628	-1.201558	0.000299
3	6	C	2.076616	0.015200	-0.000004
4	6	C	1.372752	1.226090	-0.000282
5	6	C	-0.011282	1.219253	-0.000274
6	6	C	-0.688486	0.000622	0.000008
7	1	H	-0.562488	-2.135012	0.000494
8	1	H	1.930584	-2.139067	0.000480
9	1	H	1.929928	2.154175	-0.000519
10	1	H	-0.579306	2.138964	-0.000471
11	7	N	-2.158243	-0.006856	0.000008
12	8	O	-2.732887	1.075226	0.000720
13	8	O	-2.722394	-1.094902	-0.000747
14	6	C	3.614503	0.095837	-0.000027
15	1	H	3.944266	0.618026	-0.873797
16	1	H	3.944272	0.618421	0.873506
17	1	H	4.023504	-0.892909	0.000196

2,4-DNT					
Centre Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms)**		
			X	**Y**	**Z**
1	6	C	1.198844	1.557965	0.000353
2	6	C	-0.100721	2.042311	0.000329
3	6	C	-1.225385	1.201998	0.000114
4	6	C	-0.962043	-0.182770	-0.000076
5	6	C	0.328884	-0.698346	-0.000051
6	6	C	1.394562	0.182721	0.000164
7	1	H	2.053433	2.220161	0.000514
8	1	H	-0.261137	3.113682	0.000480
9	1	H	0.491224	-1.765495	-0.000194
10	7	N	2.772845	-0.357500	0.000192
11	8	O	2.902924	-1.571945	-0.000077
12	8	O	3.689377	0.451976	0.000175
13	6	C	-2.590942	1.837854	0.000107
14	1	H	-3.172201	1.533877	-0.871596
15	1	H	-3.172339	1.533597	0.871620

16	1	H	-2.488703	2.923796	0.000289
17	7	N	-2.052817	-1.196439	-0.000318
18	8	O	-1.726421	-2.373708	-0.000467
19	8	O	-3.209586	-0.797877	-0.000366

TNT					
Centre Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms)**		
			X	**Y**	**Z**
1	6	C	0.84356	-1.23139	0.00529
2	6	C	1.55185	-0.04249	0.00582
3	6	C	0.9074	1.18209	-0.00982
4	6	C	-0.47916	1.18913	-0.04283
5	6	C	-1.27769	0.03185	-0.09211
6	6	C	-0.54142	-1.16537	-0.02853
7	1	H	1.34803	-2.18712	0.02407
8	1	H	1.46178	2.10993	-0.00275
9	7	N	-1.10171	2.54526	0.00205
10	8	O	-2.17797	2.64913	0.5687
11	8	O	-0.44823	3.46714	-0.45659
12	7	N	3.03407	-0.0815	0.03489
13	8	O	3.61309	0.99016	0.10654
14	8	O	3.55562	-1.18126	0.12072
15	7	N	-1.23486	-2.48597	0.0329
16	8	O	-2.34323	-2.51444	0.54376
17	8	O	-0.65844	-3.43619	-0.46919
18	6	C	-2.76555	0.06946	-0.3036
19	1	H	-3.29303	0.0846	0.6531
20	1	H	-3.05745	0.96694	-0.84215
21	1	H	-3.1024	-0.81485	-0.83798

4-NP					
Centre Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms)**		
			X	**Y**	**Z**
1	6	C	0.363080	-1.556813	0.000682
2	6	C	1.758240	-1.556813	0.000682
3	6	C	2.455778	-0.349062	0.000682
4	6	C	1.758124	0.859447	-0.000517
5	6	C	0.363299	0.859369	-0.000996
6	6	C	-0.334302	-0.348837	0.000000
7	1	H	-0.186679	-2.509130	0.001132
8	1	H	2.307748	-2.509326	0.001997
9	1	H	2.308324	1.811590	-0.000576
10	1	H	-0.186823	1.811650	-0.001949
11	7	N	-1.804302	-0.348593	-0.000241
12	8	O	-2.374441	0.706566	-0.000830
13	8	O	-2.374777	-1.403565	0.000161
14	8	O	3.885777	-0.348958	0.001506
15	1	H	4.206754	-0.350230	-0.903244

2,6-DNP					
Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	C	1.207504	1.542137	0.000222
2	6	C	0.000462	2.235170	0.000136
3	6	C	-1.207115	1.542031	-0.000065
4	6	C	-1.183179	0.151545	-0.000177
5	6	C	0.000168	-0.572733	-0.000090
6	6	C	1.183096	0.150954	0.000121
7	1	H	2.160116	2.053113	0.000397
8	1	H	-0.000011	3.317768	0.000237
9	1	H	-0.000345	-1.652510	-0.000156
10	7	N	2.468965	-0.590427	0.000235
11	8	O	2.413454	-1.809944	0.000279
12	8	O	3.495766	0.072260	0.000513
13	7	N	-2.469490	-0.590280	-0.000369
14	8	O	-2.413150	-1.809592	-0.000430
15	8	O	-3.496342	0.072052	-0.000397
16	1	H	-2.159523	2.053757	-0.000140

TNP					
Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	C	0.75179	-1.28867	-0.0274
2	6	C	1.54418	-0.14728	-0.06905
3	6	C	0.99525	1.12222	-0.03557
4	6	C	-0.38332	1.23846	0.02249
5	6	C	-1.24837	0.11188	0.01733
6	6	C	-0.62204	-1.15007	-0.00739
7	1	H	1.2105	-2.26817	-0.02676
8	7	N	-1.42767	-2.39996	-0.02459
9	8	O	-2.41505	-2.42257	-0.72917
10	8	O	-1.13044	-3.22789	0.82212
11	7	N	-0.95324	2.58883	0.08881
12	8	O	-2.1414	2.72357	-0.23756
13	8	O	-0.2132	3.51619	0.33088
14	1	H	1.62834	1.99875	-0.03066
15	8	O	-2.56828	0.17068	0.08474
16	1	H	-2.82225	1.11621	0.05867
17	7	N	3.0139	-0.29178	-0.13743
18	8	O	3.67326	0.73456	-0.07467
19	8	O	3.46107	-1.42525	-0.05775

Table S4. A comparative study of the K_{sv}, and medium used for TNP detection of some recent representative reports.

Tb-MOFs	K_{sv}	Medium used	Publications
$[Tb(1,3,5\text{-}BTC)]_n$ BTC = 1,3,5-benzenetricarboxylate	34182.1 M^{-1}	Ethanol	*J. Mater. Chem. A*, 2013, 1, 8745-8752
$\{[Tb(L_1)_{1.5}(H_2O)]\cdot 3H_2O\}_n$ H_2L_1 = 2-(2-Hydroxy-propionylamino)-terephthalic acid	7.47×10^4 M^{-1}	H_2O	*Chem. Eur. J.*, 2015, 21, 15705–15712
$[Tb(BTB)H_2O]$ H_3BTB = 1,3,5-Benzenetrisbenzoic acid	3.25×10^{-2} ppm^{-1}	H_2O	*Dalton Trans*., 2015, 44 , 14594–14603
$[Y_{0.9}Tb_{0.1}(OBA)(Ox)_{0.5}(H_2O)_2]$ OBA = 4,4'- Oxybis(benzoic acid), Ox = Oxalate	3.19×10^4 M^{-1}	Acetonitrile	*RSC Adv.*, 2015, 5, 102076–102084
$[Tb(L)(OH)]\cdot x(solv)$ H_2L = 5-(4-carboxyphenyl)pyridine-2-carboxylate	7.73×10^{-2} ppm^{-1}	H_2O	*J. Mater. Chem. A*, 2015, 3, 12690–12697
$[Tb_2(H_2L)_3(H_2O)_2]\cdot 21H_2O$ $H_4L = 1,4\text{-}C_6H_4(CH(OH)(PO_3H_2))_2$	9.2×10^3 M^{-1}	Ethanol	*J. Mater. Chem. A*, 2017, 5, 1952–1956
$\{[Tb_2(L)_2(OH)(HCOO)]\cdot[H_2O]\}_n$ H_2L = 4'-(4-(3,5-dicarboxylphenoxy) phenyl)-4,2':6',4''-terpyridine	5.1×10^{-2} ppm^{-1}	H_2O	*Dalton Trans.*, 2017, 46, 15434–15442
$\{[Tb(L_1)(L_2)_{0.5}(NO_3)(DMF)].DMF\}_n$ L_1 = 1,10-phenanthroline (phen), L_2 = 3,3′,5,5′-azobenzene-tetra carboxylic acid	15.97 ppm^{-1} (5.67×10^5 M^{-1})	H_2O	**Present work**