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Construction of a terbium-based metal-organic framework for specific detection of MnO_4^- in aqueous media

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Table S1. Crystal data and structure refinement for SLX-3.

Identification code	SLX-3	
Empirical formula	$C_{34}H_{23}O_{10}Tb$	
Formula weight	750.44	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* -1	
Unit cell dimensions	a = 10.629(4) Å	α = 95.870(6)°
	b = 10.842(4) Å	β = 102.724(6)°
	c = 17.852(6) Å	γ = 97.703(6)°
Volume	1970.2(11) $Å^3$	
Z	2	
Density (calculated)	1.265 Mg/m^3	
Absorption coefficient	1.840 mm^{-1}	
F(000)	744	
Crystal size	0.290 x 0.220 x 0.180 mm^3	
Theta range for data collection	1.990 to 26.000°	
Index ranges	-13<=h<=13, -13<=k<=13, -21<=l<=22	
Reflections collected	18891	
Independent reflections	7620 [R(int) = 0.0364]	
Completeness to theta = 25.242°	98.3%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.719 and 0.623	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	7620/38/407	
Goodness-of-fit on F^2	1.075	
Final R indices [I>2sigma(I)]	R1 = 0.0418, wR2 = 0.1180	
R indices (all data)	R1 = 0.0467, wR2 = 0.1205	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.058 and -1.149 $e.Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for SLX-3.

Tb(1)-O(1)	2.285(4)
Tb(1)-O(5)	2.322(3)
Tb(1)-O(6)#1	2.335(3)
Tb(1)-O(2)#1	2.336(4)
Tb(1)-O(9)	2.361(5)
Tb(1)-O(3)#2	2.425(4)
Tb(1)-O(10)	2.459(4)
Tb(1)-O(4)#2	2.507(4)
Tb(1)-C(17)#2	2.807(5)
O(1)-C(1)	1.239(7)
O(2)-C(1)	1.244(7)
O(3)-C(17)	1.270(6)
O(4)-C(17)	1.231(6)
O(5)-C(18)	1.237(6)
O(6)-C(18)	1.258(6)
O(7)-C(34)	1.295(16)
O(7)-H(7)	0.9039
O(8)-C(34)	1.202(14)
O(9)-H(9A)	0.8500
O(9)-H(9C)	0.8500
O(10)-H(10A)	0.8500
O(10)-H(10C)	0.8500
C(1)-C(2)	1.490(8)
C(2)-C(3)	1.382(8)
C(2)-C(7)	1.403(8)
C(3)-C(4)	1.391(11)
C(3)-H(3)	0.9300
C(4)-C(5)	1.399(12)
C(4)-H(4)	0.9300
C(5)-C(6)	1.366(10)
C(5)-H(5)	0.9300
C(6)-C(7)	1.390(8)
C(6)-H(6)	0.9300
C(7)-C(8)	1.491(7)

C(8)-C(13)	1.365(8)
C(8)-C(9)	1.392(7)
C(9)-C(10)	1.362(7)
C(9)-H(9)	0.9300
C(10)-C(11)	1.390(7)
C(10)-H(10)	0.9300
C(11)-C(12)	1.388(7)
C(11)-C(14)	1.486(7)
C(12)-C(13)	1.400(7)
C(12)-H(12)	0.9300
C(13)-H(13)	0.9300
C(14)-C(15)	1.394(7)
C(14)-C(16)#3	1.399(6)
C(15)-C(16)	1.383(7)
C(15)-C(17)	1.515(6)
C(16)-H(16)	0.9300
C(18)-C(19)	1.510(6)
C(19)-C(20)	1.385(7)
C(19)-C(21)#4	1.408(6)
C(20)-C(21)	1.382(6)
C(20)-H(20)	0.9300
C(21)-C(22)	1.485(7)
C(22)-C(27)	1.375(8)
C(22)-C(23)	1.382(8)
C(23)-C(24)	1.381(9)
C(23)-H(23)	0.9300
C(24)-C(25)	1.332(11)
C(24)-H(24)	0.9300
C(25)-C(26)	1.403(11)
C(25)-C(28)	1.498(10)
C(26)-C(27)	1.379(9)
C(26)-H(26)	0.9300
C(27)-H(27)	0.9300
C(28)-C(29)	1.344(13)
C(28)-C(33)	1.432(13)
C(29)-C(30)	1.393(15)

C(29)-H(29)	0.9300
C(33)-C(32)	1.386(14)
C(33)-C(34)	1.506(16)
C(31)-C(30)	1.341(18)
C(31)-C(32)	1.411(17)
C(31)-H(31)	0.9300
C(32)-H(32)	0.9300
C(30)-H(30)	0.9300
O(1)-Tb(1)-O(5)	79.69(14)
O(1)-Tb(1)-O(6)#1	76.49(16)
O(5)-Tb(1)-O(6)#1	125.35(13)
O(1)-Tb(1)-O(2)#1	123.70(16)
O(5)-Tb(1)-O(2)#1	79.50(14)
O(6)#1-Tb(1)-O(2)#1	74.45(14)
O(1)-Tb(1)-O(9)	80.6(2)
O(5)-Tb(1)-O(9)	83.69(16)
O(6)#1-Tb(1)-O(9)	137.83(18)
O(2)#1-Tb(1)-O(9)	146.64(19)
O(1)-Tb(1)-O(3)#2	137.47(14)
O(5)-Tb(1)-O(3)#2	142.30(13)
O(6)#1-Tb(1)-O(3)#2	79.38(15)
O(2)#1-Tb(1)-O(3)#2	81.53(15)
O(9)-Tb(1)-O(3)#2	95.02(19)
O(1)-Tb(1)-O(10)	142.89(18)
O(5)-Tb(1)-O(10)	71.40(15)
O(6)#1-Tb(1)-O(10)	139.72(18)
O(2)#1-Tb(1)-O(10)	73.71(17)
O(9)-Tb(1)-O(10)	73.7(2)
O(3)#2-Tb(1)-O(10)	72.12(15)
O(1)-Tb(1)-O(4)#2	86.20(14)
O(5)-Tb(1)-O(4)#2	154.80(14)
O(6)#1-Tb(1)-O(4)#2	70.20(13)
O(2)#1-Tb(1)-O(4)#2	125.61(13)
O(9)-Tb(1)-O(4)#2	73.41(16)
O(3)#2-Tb(1)-O(4)#2	52.60(13)
O(10)-Tb(1)-O(4)#2	110.77(14)

O(1)-Tb(1)-C(17)#2	110.96(15)
O(5)-Tb(1)-C(17)#2	163.70(13)
O(6)#1-Tb(1)-C(17)#2	70.31(14)
O(2)#1-Tb(1)-C(17)#2	102.96(14)
O(9)-Tb(1)-C(17)#2	85.93(16)
O(3)#2-Tb(1)-C(17)#2	26.85(14)
O(10)-Tb(1)-C(17)#2	93.63(15)
O(4)#2-Tb(1)-C(17)#2	26.01(14)
C(1)-O(1)-Tb(1)	165.3(4)
C(1)-O(2)-Tb(1)#1	126.6(4)
C(17)-O(3)-Tb(1)#5	93.6(3)
C(17)-O(4)-Tb(1)#5	90.7(3)
C(18)-O(5)-Tb(1)	139.7(3)
C(18)-O(6)-Tb(1)#1	140.3(3)
C(34)-O(7)-H(7)	119.5
Tb(1)-O(9)-H(9A)	109.2
Tb(1)-O(9)-H(9C)	109.4
H(9A)-O(9)-H(9C)	109.5
Tb(1)-O(10)-H(10A)	109.2
Tb(1)-O(10)-H(10C)	109.3
H(10A)-O(10)-H(10C)	109.5
O(1)-C(1)-O(2)	122.8(5)
O(1)-C(1)-C(2)	119.4(5)
O(2)-C(1)-C(2)	117.7(5)
C(3)-C(2)-C(7)	119.8(6)
C(3)-C(2)-C(1)	117.4(5)
C(7)-C(2)-C(1)	122.8(5)
C(2)-C(3)-C(4)	121.1(7)
C(2)-C(3)-H(3)	119.4
C(4)-C(3)-H(3)	119.4
C(3)-C(4)-C(5)	118.3(6)
C(3)-C(4)-H(4)	120.8
C(5)-C(4)-H(4)	120.8
C(6)-C(5)-C(4)	120.9(7)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.6

C(5)-C(6)-C(7)	120.9(7)
C(5)-C(6)-H(6)	119.5
C(7)-C(6)-H(6)	119.5
C(6)-C(7)-C(2)	118.9(5)
C(6)-C(7)-C(8)	119.4(5)
C(2)-C(7)-C(8)	121.6(5)
C(13)-C(8)-C(9)	118.7(5)
C(13)-C(8)-C(7)	122.2(5)
C(9)-C(8)-C(7)	119.1(5)
C(10)-C(9)-C(8)	120.5(5)
C(10)-C(9)-H(9)	119.8
C(8)-C(9)-H(9)	119.8
C(9)-C(10)-C(11)	121.7(5)
C(9)-C(10)-H(10)	119.1
C(11)-C(10)-H(10)	119.1
C(12)-C(11)-C(10)	117.9(5)
C(12)-C(11)-C(14)	123.5(4)
C(10)-C(11)-C(14)	118.5(4)
C(11)-C(12)-C(13)	120.0(5)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(8)-C(13)-C(12)	121.1(5)
C(8)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
C(15)-C(14)-C(16)#3	116.8(4)
C(15)-C(14)-C(11)	124.0(4)
C(16)#3-C(14)-C(11)	118.9(4)
C(16)-C(15)-C(14)	121.1(4)
C(16)-C(15)-C(17)	115.3(4)
C(14)-C(15)-C(17)	123.6(4)
C(15)-C(16)-C(14)#3	122.2(5)
C(15)-C(16)-H(16)	118.9
C(14)#3-C(16)-H(16)	118.9
O(4)-C(17)-O(3)	121.9(4)
O(4)-C(17)-C(15)	120.2(4)
O(3)-C(17)-C(15)	117.8(4)

O(4)-C(17)-Tb(1)#5	63.3(2)
O(3)-C(17)-Tb(1)#5	59.6(2)
C(15)-C(17)-Tb(1)#5	166.1(3)
O(5)-C(18)-O(6)	125.3(4)
O(5)-C(18)-C(19)	117.8(4)
O(6)-C(18)-C(19)	116.8(4)
C(20)-C(19)-C(21)#4	119.2(4)
C(20)-C(19)-C(18)	117.2(4)
C(21)#4-C(19)-C(18)	123.2(4)
C(21)-C(20)-C(19)	123.3(4)
C(21)-C(20)-H(20)	118.4
C(19)-C(20)-H(20)	118.4
C(20)-C(21)-C(19)#4	117.5(4)
C(20)-C(21)-C(22)	119.4(4)
C(19)#4-C(21)-C(22)	123.1(4)
C(27)-C(22)-C(23)	117.6(5)
C(27)-C(22)-C(21)	123.5(5)
C(23)-C(22)-C(21)	118.9(5)
C(24)-C(23)-C(22)	120.8(6)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	122.3(7)
C(25)-C(24)-H(24)	118.9
C(23)-C(24)-H(24)	118.8
C(24)-C(25)-C(26)	117.5(6)
C(24)-C(25)-C(28)	121.4(7)
C(26)-C(25)-C(28)	121.1(7)
C(27)-C(26)-C(25)	120.8(7)
C(27)-C(26)-H(26)	119.6
C(25)-C(26)-H(26)	119.7
C(22)-C(27)-C(26)	120.8(6)
C(22)-C(27)-H(27)	119.6
C(26)-C(27)-H(27)	119.6
C(29)-C(28)-C(33)	119.2(8)
C(29)-C(28)-C(25)	121.4(9)
C(33)-C(28)-C(25)	119.2(8)

C(28)-C(29)-C(30)	121.2(11)
C(28)-C(29)-H(29)	119.4
C(30)-C(29)-H(29)	119.3
C(32)-C(33)-C(28)	119.2(10)
C(32)-C(33)-C(34)	117.7(10)
C(28)-C(33)-C(34)	122.0(9)
O(8)-C(34)-O(7)	115.7(13)
O(8)-C(34)-C(33)	129.8(13)
O(7)-C(34)-C(33)	114.5(12)
C(30)-C(31)-C(32)	120.8(15)
C(30)-C(31)-H(31)	119.6
C(32)-C(31)-H(31)	119.6
C(33)-C(32)-C(31)	118.9(13)
C(33)-C(32)-H(32)	120.6
C(31)-C(32)-H(32)	120.5
C(31)-C(30)-C(29)	120.0(14)
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 x+1,y,z #3 -x,-y+3,-z+1

#4 -x+1,-y+1,-z+1 #5 x-1,y,z

Table S3. Torsion angles [°] for SLX-3.

Tb(1)-O(1)-C(1)-O(2)	-27.9(19)
Tb(1)-O(1)-C(1)-C(2)	148.8(14)
Tb(1)#1-O(2)-C(1)-O(1)	3.3(7)
Tb(1)#1-O(2)-C(1)-C(2)	-173.5(3)
O(1)-C(1)-C(2)-C(3)	-47.4(8)
O(2)-C(1)-C(2)-C(3)	129.5(6)
O(1)-C(1)-C(2)-C(7)	133.3(6)
O(2)-C(1)-C(2)-C(7)	-49.8(7)
C(7)-C(2)-C(3)-C(4)	2.9(10)
C(1)-C(2)-C(3)-C(4)	-176.5(7)
C(2)-C(3)-C(4)-C(5)	-1.7(12)

C(3)-C(4)-C(5)-C(6)	-0.9(14)
C(4)-C(5)-C(6)-C(7)	2.2(13)
C(5)-C(6)-C(7)-C(2)	-1.0(11)
C(5)-C(6)-C(7)-C(8)	-177.0(7)
C(3)-C(2)-C(7)-C(6)	-1.5(9)
C(1)-C(2)-C(7)-C(6)	177.8(6)
C(3)-C(2)-C(7)-C(8)	174.4(6)
C(1)-C(2)-C(7)-C(8)	-6.2(8)
C(6)-C(7)-C(8)-C(13)	-54.9(8)
C(2)-C(7)-C(8)-C(13)	129.2(6)
C(6)-C(7)-C(8)-C(9)	125.0(6)
C(2)-C(7)-C(8)-C(9)	-50.9(8)
C(13)-C(8)-C(9)-C(10)	-2.2(8)
C(7)-C(8)-C(9)-C(10)	177.9(5)
C(8)-C(9)-C(10)-C(11)	-0.5(9)
C(9)-C(10)-C(11)-C(12)	2.5(8)
C(9)-C(10)-C(11)-C(14)	-175.3(5)
C(10)-C(11)-C(12)-C(13)	-1.9(8)
C(14)-C(11)-C(12)-C(13)	175.8(5)
C(9)-C(8)-C(13)-C(12)	2.8(9)
C(7)-C(8)-C(13)-C(12)	-177.3(5)
C(11)-C(12)-C(13)-C(8)	-0.7(9)
C(12)-C(11)-C(14)-C(15)	-45.7(8)
C(10)-C(11)-C(14)-C(15)	132.1(5)
C(12)-C(11)-C(14)-C(16)#3	140.6(5)
C(10)-C(11)-C(14)-C(16)#3	-41.7(7)
C(16)#3-C(14)-C(15)-C(16)	0.6(8)
C(11)-C(14)-C(15)-C(16)	-173.2(5)
C(16)#3-C(14)-C(15)-C(17)	-177.7(5)
C(11)-C(14)-C(15)-C(17)	8.5(8)
C(14)-C(15)-C(16)-C(14)#3	-0.7(9)
C(17)-C(15)-C(16)-C(14)#3	177.8(5)
Tb(1)#5-O(4)-C(17)-O(3)	-11.1(5)
Tb(1)#5-O(4)-C(17)-C(15)	164.7(4)
Tb(1)#5-O(3)-C(17)-O(4)	11.5(5)
Tb(1)#5-O(3)-C(17)-C(15)	-164.4(4)

C(16)-C(15)-C(17)-O(4)	-97.5(6)
C(14)-C(15)-C(17)-O(4)	80.9(6)
C(16)-C(15)-C(17)-O(3)	78.4(6)
C(14)-C(15)-C(17)-O(3)	-103.2(6)
C(16)-C(15)-C(17)-Tb(1)#5	3.2(17)
C(14)-C(15)-C(17)-Tb(1)#5	-178.4(12)
Tb(1)-O(5)-C(18)-O(6)	-12.2(9)
Tb(1)-O(5)-C(18)-C(19)	164.1(4)
Tb(1)#1-O(6)-C(18)-O(5)	43.0(8)
Tb(1)#1-O(6)-C(18)-C(19)	-133.4(4)
O(5)-C(18)-C(19)-C(20)	-129.5(5)
O(6)-C(18)-C(19)-C(20)	47.2(6)
O(5)-C(18)-C(19)-C(21)#4	43.7(7)
O(6)-C(18)-C(19)-C(21)#4	-139.7(5)
C(21)#4-C(19)-C(20)-C(21)	-0.8(8)
C(18)-C(19)-C(20)-C(21)	172.6(4)
C(19)-C(20)-C(21)-C(19)#4	0.8(8)
C(19)-C(20)-C(21)-C(22)	-178.9(5)
C(20)-C(21)-C(22)-C(27)	134.7(5)
C(19)#4-C(21)-C(22)-C(27)	-44.9(7)
C(20)-C(21)-C(22)-C(23)	-45.3(7)
C(19)#4-C(21)-C(22)-C(23)	135.1(6)
C(27)-C(22)-C(23)-C(24)	2.4(10)
C(21)-C(22)-C(23)-C(24)	-177.6(6)
C(22)-C(23)-C(24)-C(25)	-0.1(12)
C(23)-C(24)-C(25)-C(26)	-3.9(12)
C(23)-C(24)-C(25)-C(28)	176.7(7)
C(24)-C(25)-C(26)-C(27)	5.8(11)
C(28)-C(25)-C(26)-C(27)	-174.9(7)
C(23)-C(22)-C(27)-C(26)	-0.5(9)
C(21)-C(22)-C(27)-C(26)	179.5(6)
C(25)-C(26)-C(27)-C(22)	-3.6(10)
C(24)-C(25)-C(28)-C(29)	130.2(11)
C(26)-C(25)-C(28)-C(29)	-49.1(12)
C(24)-C(25)-C(28)-C(33)	-43.8(11)
C(26)-C(25)-C(28)-C(33)	136.9(9)

C(33)-C(28)-C(29)-C(30)	-7(2)
C(25)-C(28)-C(29)-C(30)	179.0(13)
C(29)-C(28)-C(33)-C(32)	1.0(17)
C(25)-C(28)-C(33)-C(32)	175.2(10)
C(29)-C(28)-C(33)-C(34)	169.3(12)
C(25)-C(28)-C(33)-C(34)	-16.5(15)
C(32)-C(33)-C(34)-O(8)	122.4(16)
C(28)-C(33)-C(34)-O(8)	-46(2)
C(32)-C(33)-C(34)-O(7)	-55.4(19)
C(28)-C(33)-C(34)-O(7)	136.2(15)
C(28)-C(33)-C(32)-C(31)	2.0(18)
C(34)-C(33)-C(32)-C(31)	-166.8(12)
C(30)-C(31)-C(32)-C(33)	1(2)
C(32)-C(31)-C(30)-C(29)	-7(3)
C(28)-C(29)-C(30)-C(31)	10(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 x+1,y,z #3 -x,-y+3,-z+1

#4 -x+1,-y+1,-z+1 #5 x-1,y,z

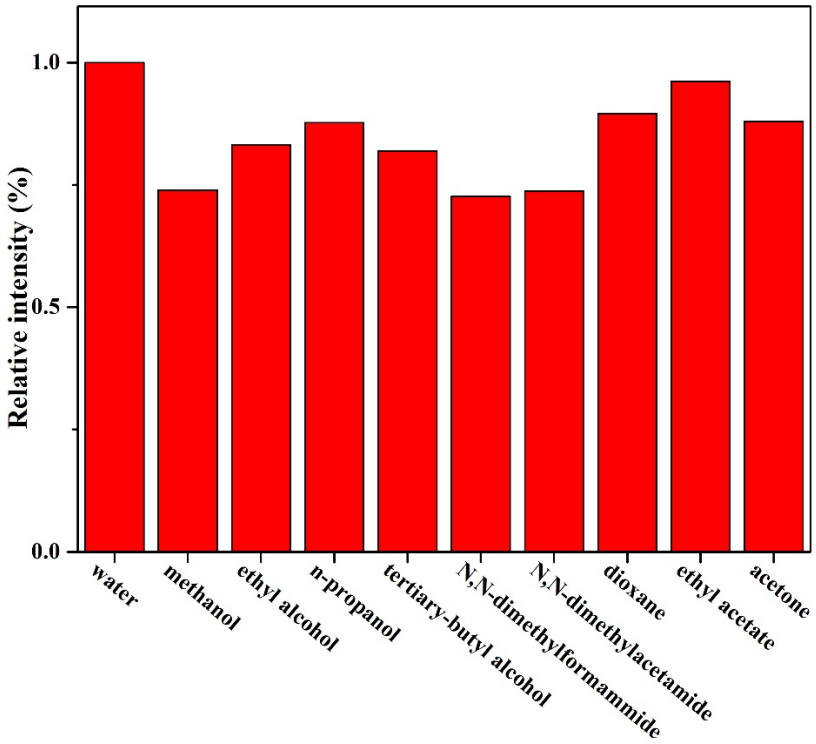

Fig. S1 The fluorescence intensity of SLX-3 in different solutions.

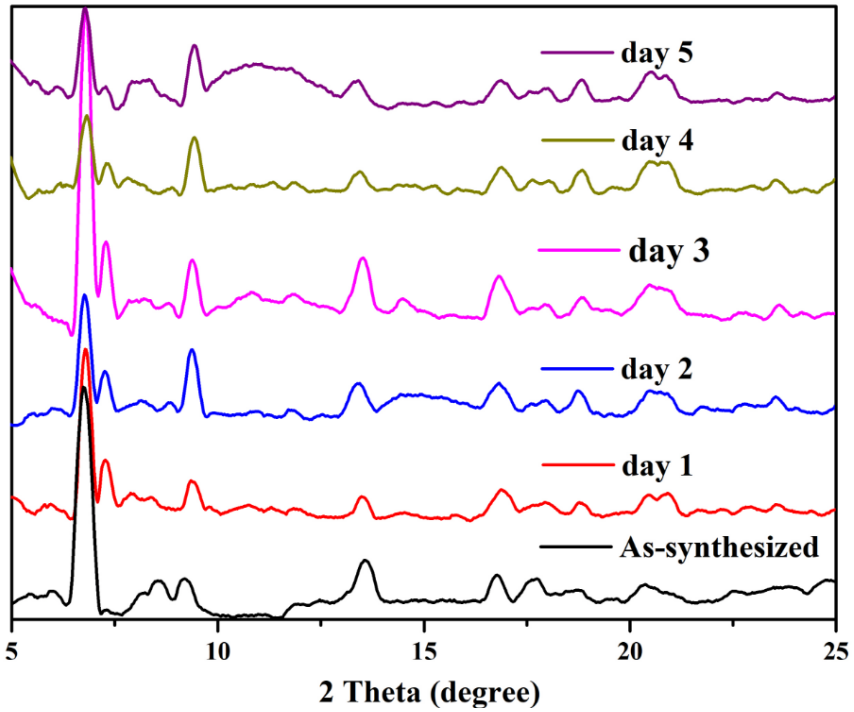

Fig. S2 PXRD spectra of SLX-3 placed in water for different days (room temperature, 2theta: 5-25 degree)

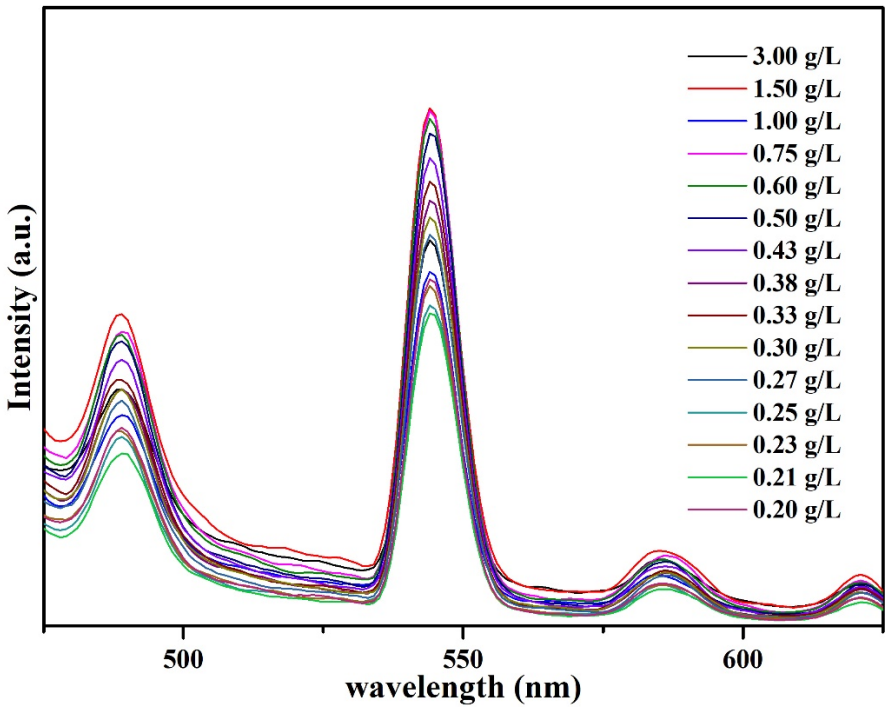

Fig. S3 Emission spectra of SLX-3 aqueous suspension in different concentration.

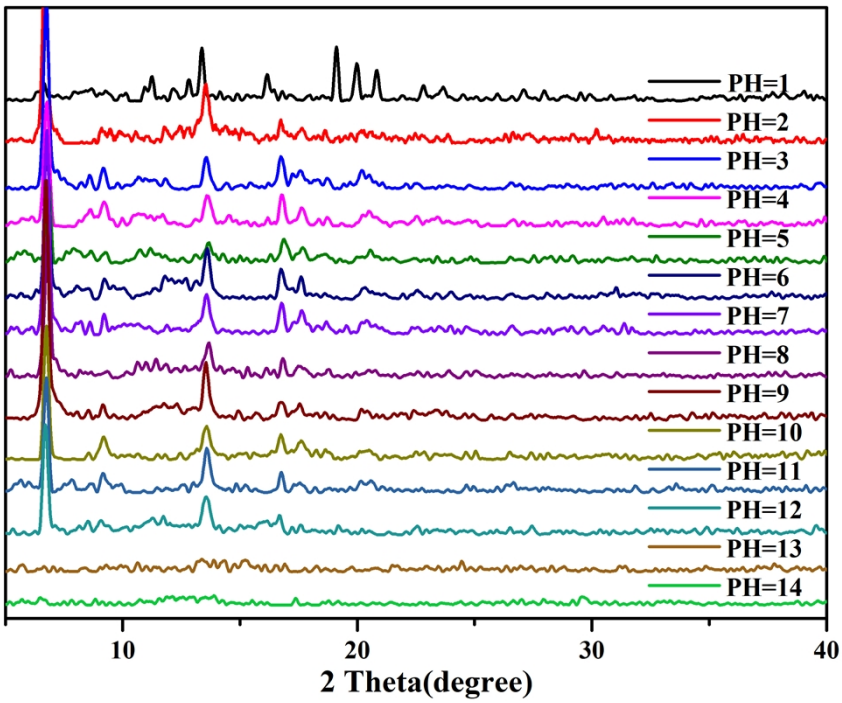

Fig. S4 PXRD spectra of SLX-3 soaked into different pH solutions (room temperature, 2theta: 5-40 degree)

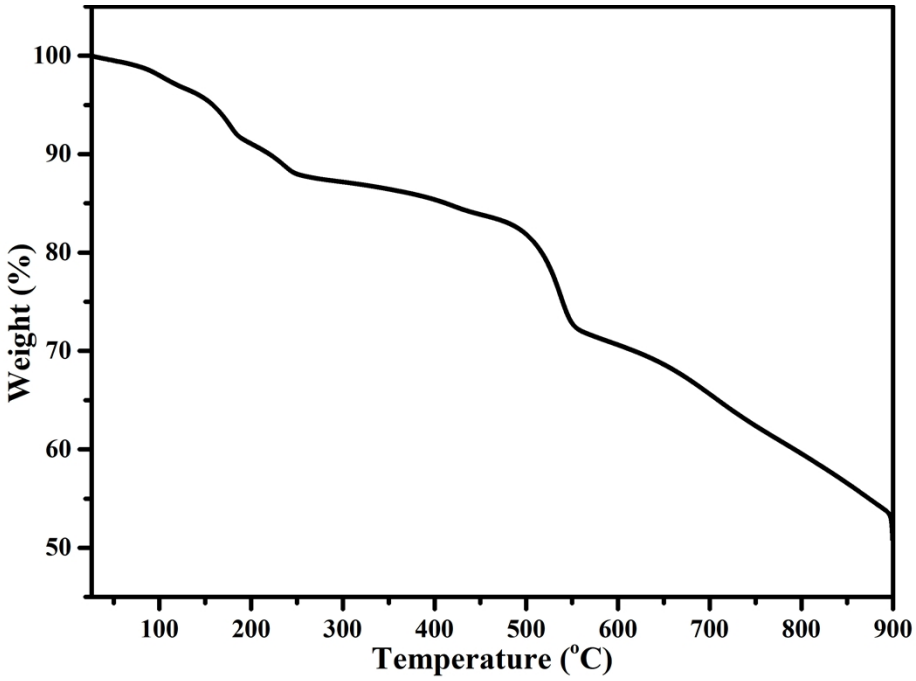

Fig. S5 TGA curve of SLX-3.

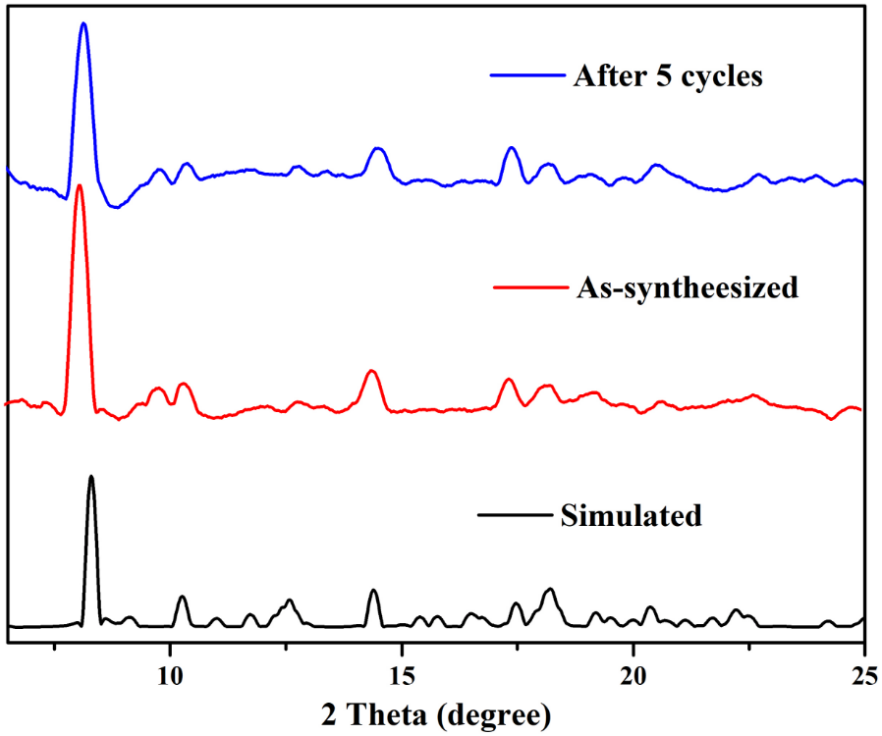

Fig. S6 PXRD spectra of SLX-3 after five cycles of use.

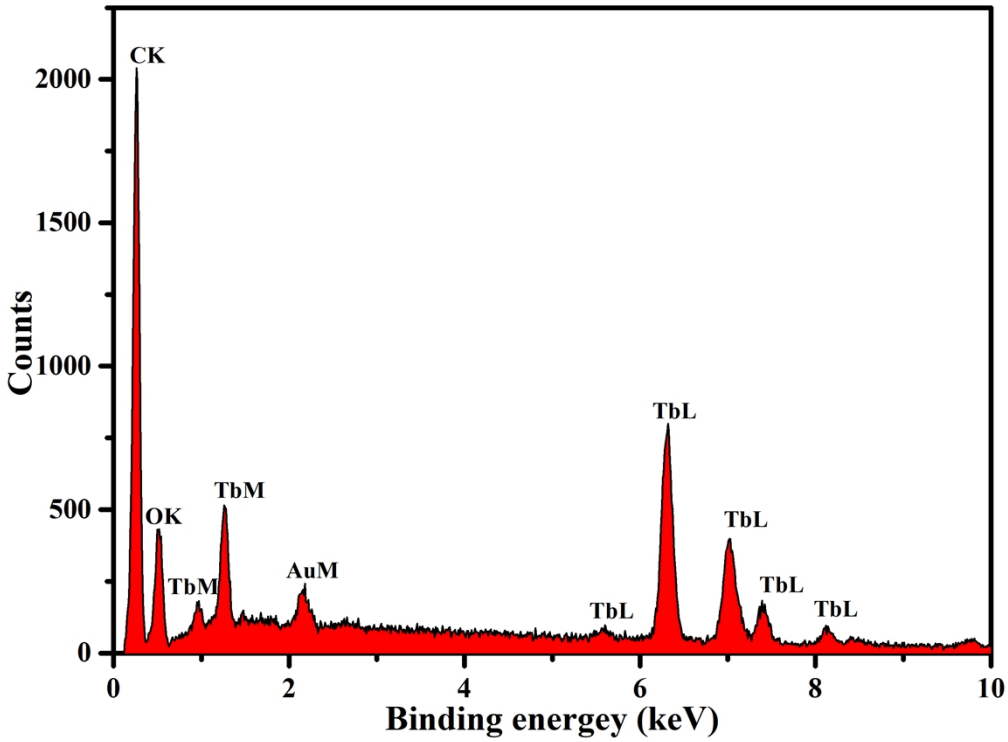

Fig. S7 SEM-EDS of recovered SLX-3 after the sensing of MnO_4^-.

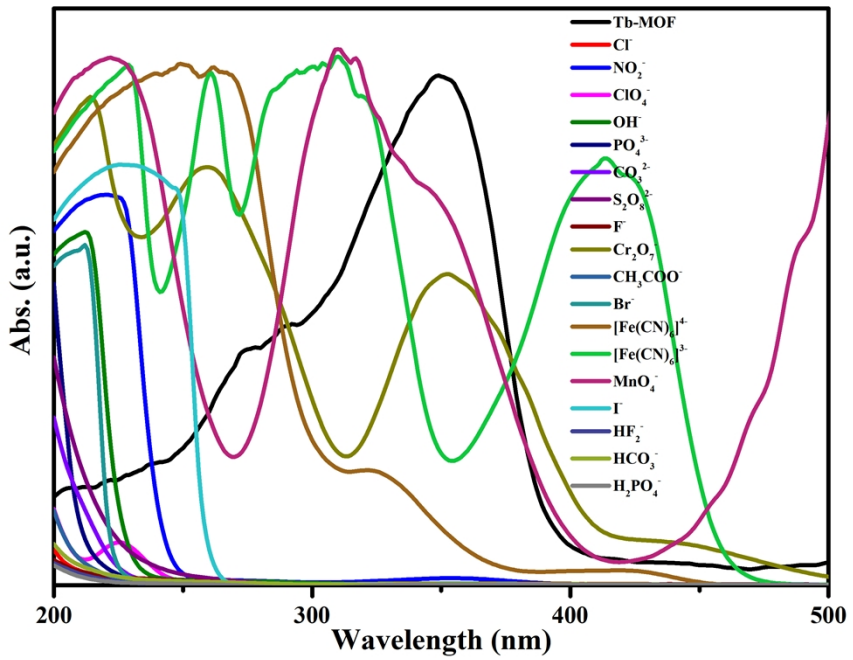

Fig. S8 Ultraviolet absorption spectrum of anion aqueous solutions.

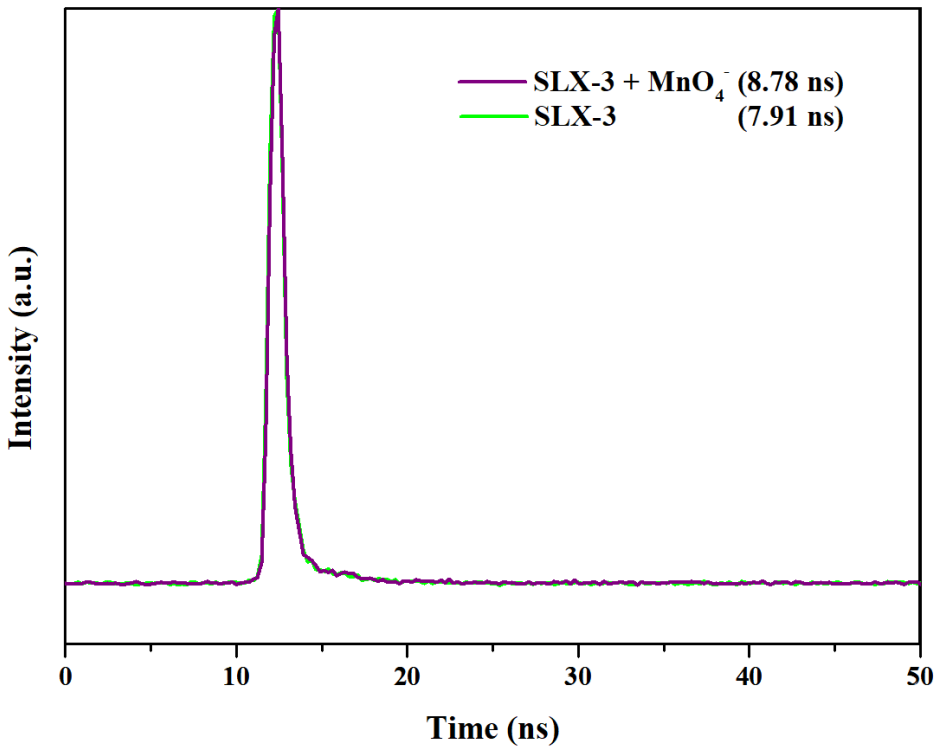

Fig. S9 Life time plots of sensor SLX-3 and its mixture with MnO_4^-.