Supporting Information

Ratiometric fluorescent detection of dipicolinic acid as an anthrax biomarker based on a high-nuclearity Yb_{18} nanoring

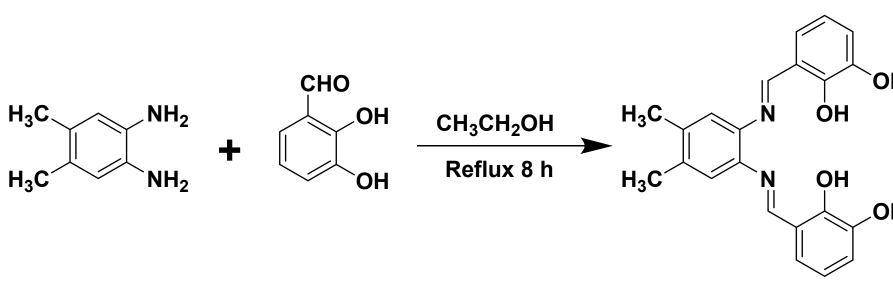
Yanan Ma, Xiaoping Yang,* Wenxin Hao, Ting Zhu, Chengri Wang, and Desmond Schipper

Contents

1. General Procedures

Photophysical Studies. Visible and NIR luminescence spectra were recorded on a FLS 980 fluorimeter. The light source for the spectra was a 450 W xenon arc lamp with continuous spectral distribution from 190 to 2600 nm. Liquid nitrogen cooled Ge PIN diode detector was used to detect the NIR emissions from 800 nm to 1700 nm. The quantum yields (Φ_{em}) were obtained by using an integrating sphere, according to eqn $\Phi_{em} = N_{em} / N_{abs}$, where N_{em} and N_{abs} are the numbers of emitted and absorbed photons, respectively. Systematic errors have been deducted through the standard instrument corrections.

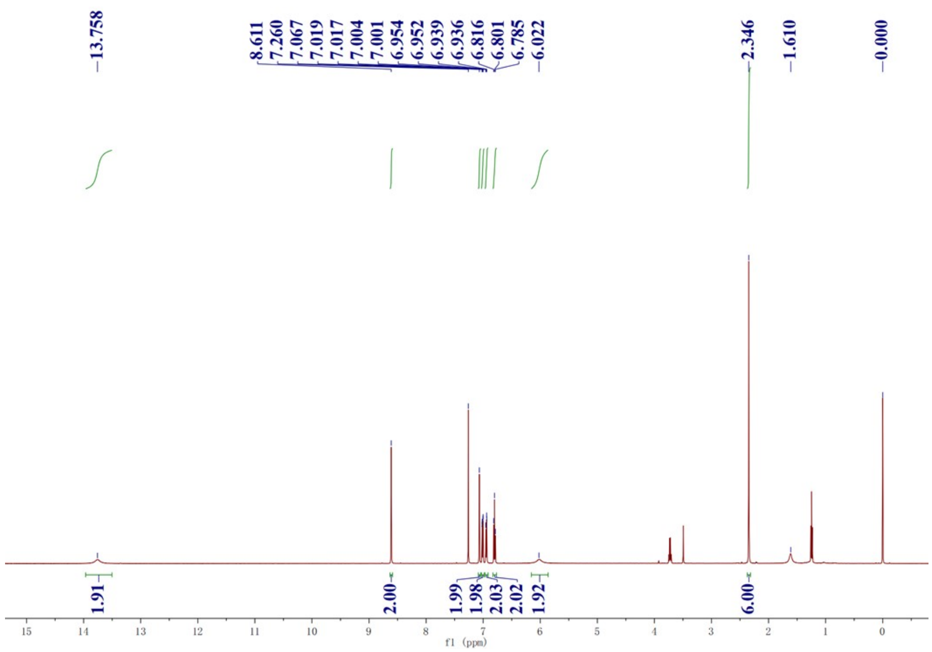
2. Synthesis of the ligand H_4L^1



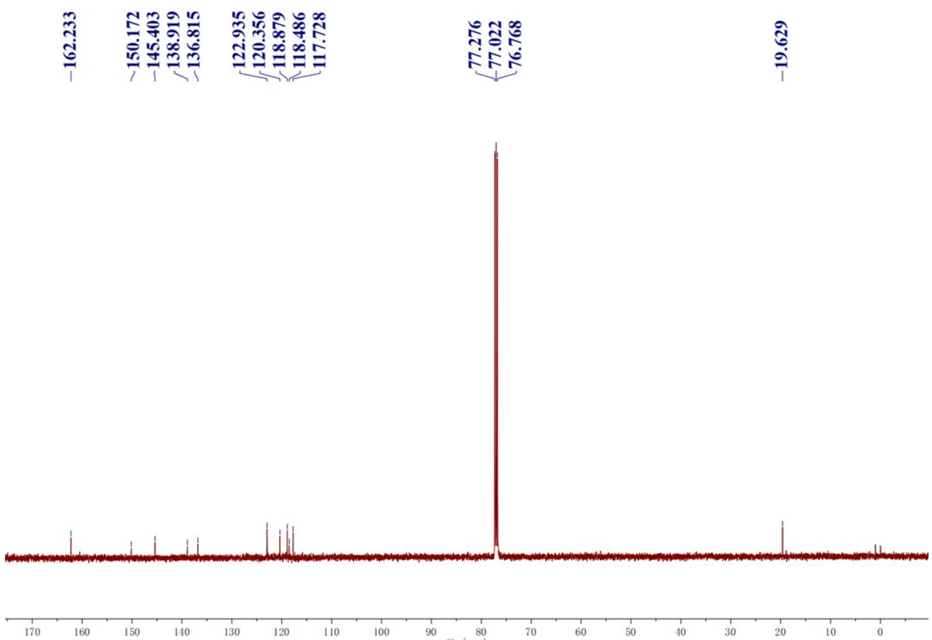
Scheme S1. Synthetic approach to H_4L^1.

2,3-Dihydroxybenzaldehyde (20 mmol, 2.76 g) was dissolved in 30 mL EtOH, and a solution of 4,5-dimethyl-1,2-phenylenediamine (10 mmol, 1.36 g) in 40 mL EtOH was then added drop by drop. The resulting solution was stirred and heated under reflux for 6 h. It was allowed to cool and was then filtered in vacuum. The solid was washed with EtOH (3 × 5 mL) and then dried under vacuum to give red product. Yield (based on 4,5-Dimethyl-1,2-phenylenediamine): 3.27 g (87%).^{1}H NMR(δ_H, ppm, 500 MHz, $CDCl_3$-d_1): 13.7(s, 2H), 8.6(s, 2H), 7.0(s, 2H), 7.0(m, 2H) 6.9(m, 2H), 6.8(t, 2H), 2.3(s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$-d_1, δ): 162.2, 150.1, 145.4, 138.9, 136.8, 112.9, 120.3, 118.8, 118.4, 117.7, 19.6. IR (KBr, cm^{-1}): 1614(s), 1539(w), 1461(s), 1420(w), 1353(s), 1281(s), 1214(s), 1158(s), 1017(m), 876(m), 724(s).

3. ^{1}H NMR and ^{13}C NMR spectra of the ligand H_4L^1



(**a**)



(**b**)

Figure S1. (**a**) ^{1}H NMR of the ligand H_4L^1 in $CDCl_3$; (**b**) ^{13}C NMR of the ligand H_4L^1 in $CDCl_3$.

4. IR spectra of the ligand H_4L^1 and 1

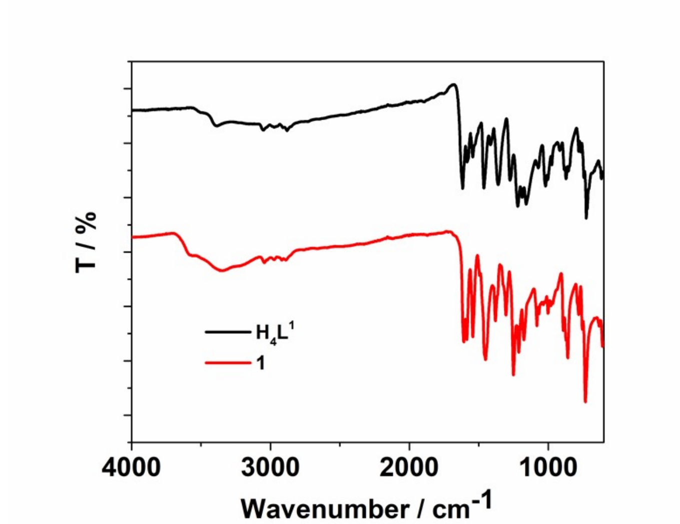


Figure S2. IR spectra of the ligand H_4L^1 and **1**.

5. The thermogravimetric analysis of 1

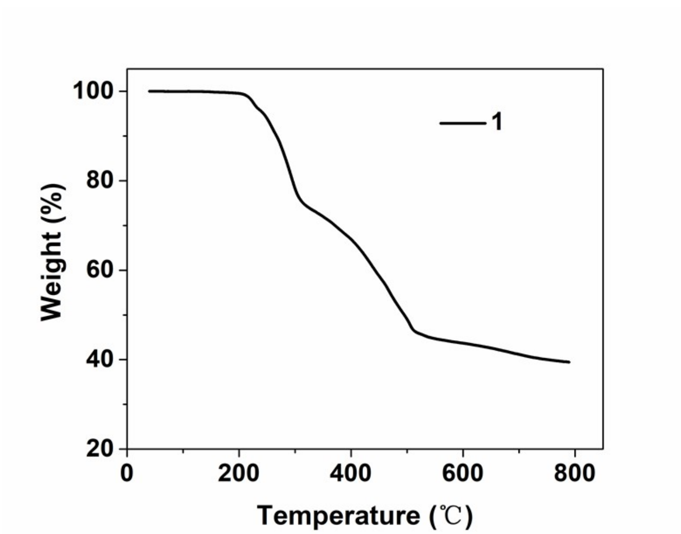


Figure S3. The thermogravimetric analysis of **1**.

6. Powder XRD pattern of 1

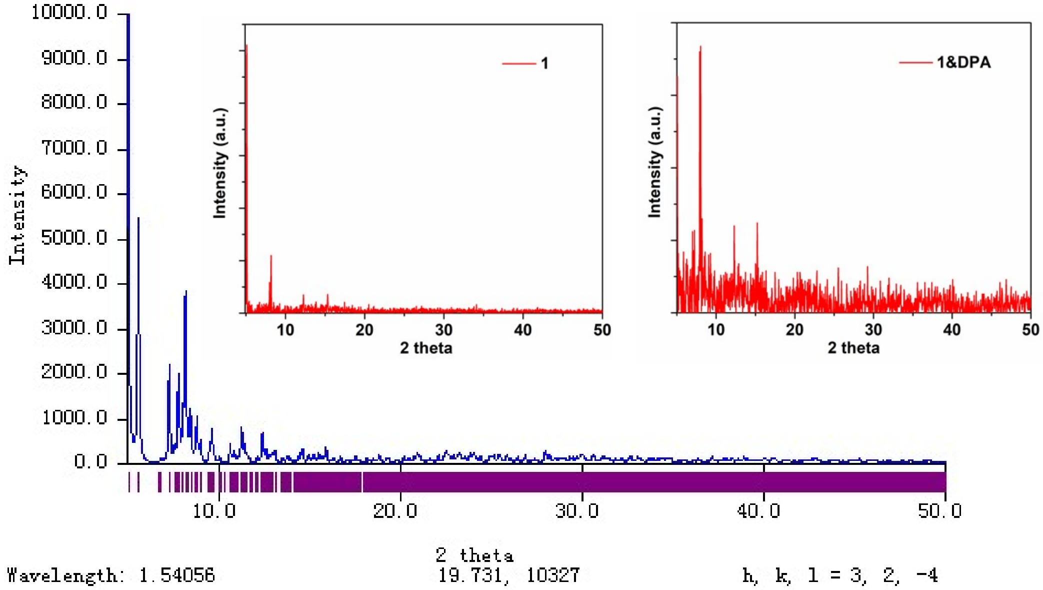


Figure S4. Powder XRD pattern of **1** before (left) and after (right) treated with DPA.

7. UV-vis absorption spectra of the ligand H_4L^1 and 1

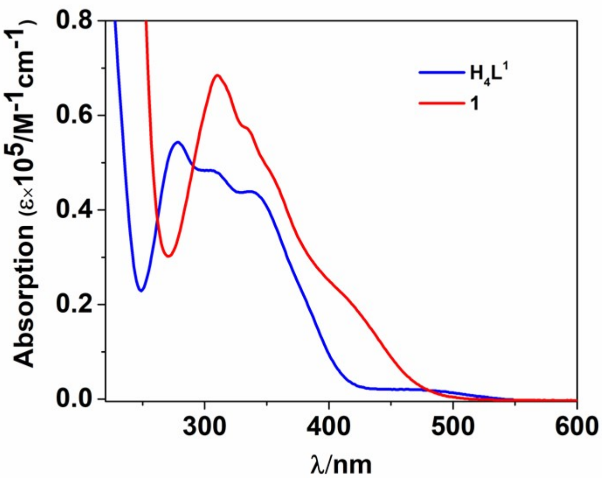


Figure S5. UV-vis absorption spectra of the ligand H_4L^1, **1** and **2** in CH_3CN.

8. The emission spectrum of the Gd(III) analogue at 77 K

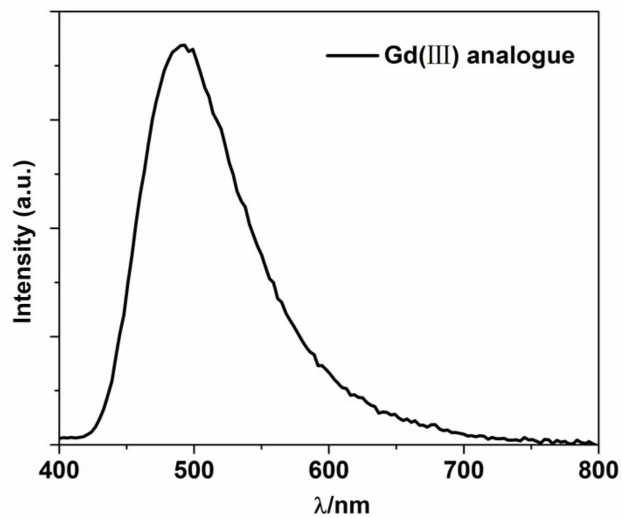
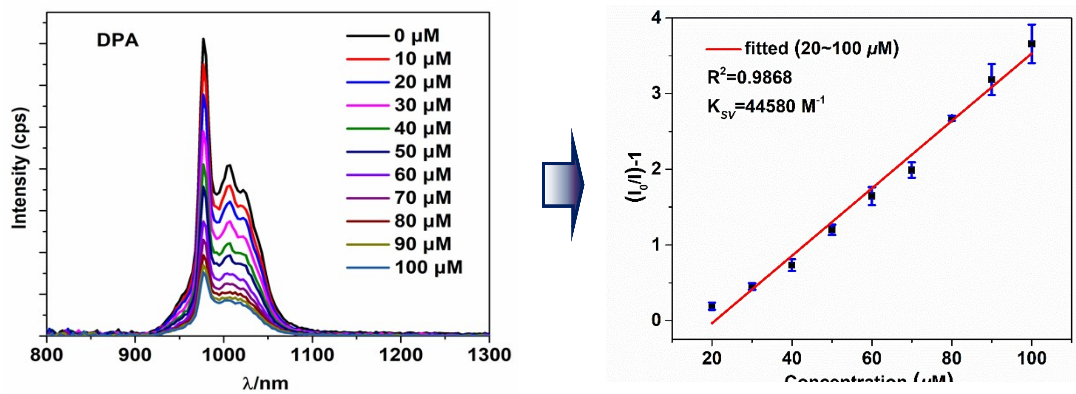
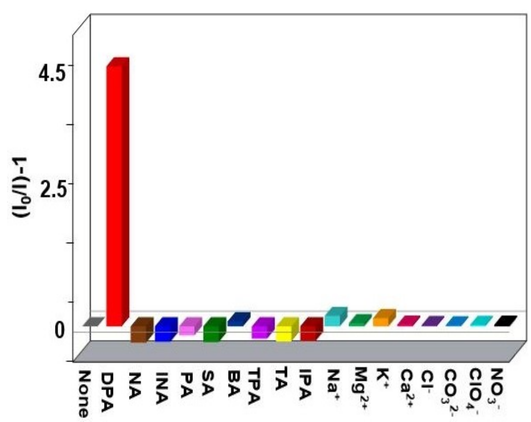


Figure S6. The emission spectrum of the Gd(III) analogue (10 μM) at 77 K in CH_3CN (λ_{ex} = 365 nm).

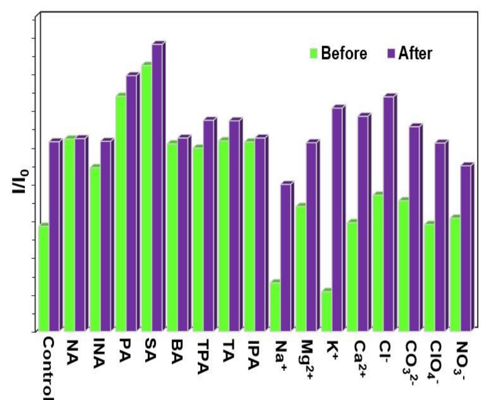
9. The fluorescent response of 1 to DPA and interferents



(a)



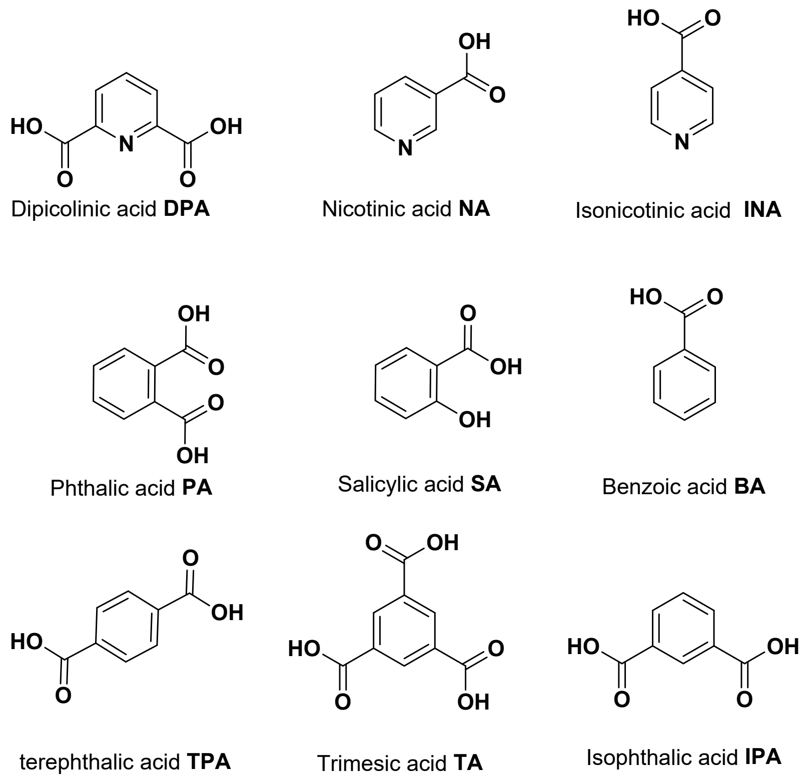
(b)



(c)

Figure S7. (a) NIR luminescent response and K_{sv} of **1** (7 μM) to the addition of DPA with different concentrations in CH_3CN (λ_{ex} = 368 nm); (b) NIR luminescent response of **1** (7 μM) to DPA and various carboxylic acids and ions (100 μM) in CH_3CN (λ_{ex} = 368 nm). (c) The ligand-centered emission (484 nm) quenching of **1** (7 μM) before and after the addition of DPA (100 μM) in the presence of other interferents (100 μM).

10. Chemical structures of DPA and carboxylic acids



Scheme S2. Chemical structures of various carboxylic acids.

11. UV-vis absorption spectra of the PDA and carboxylic acids

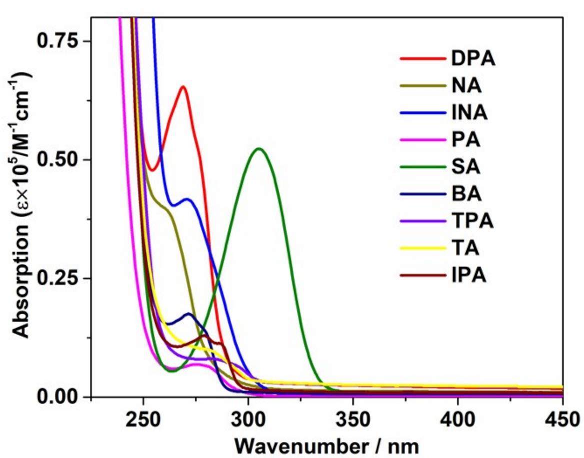


Figure S8. UV-vis absorption spectra of the carboxylic acids in CH_3CN (c = 10 μM).

12. UV-vis titration of 1 to the addition of DPA

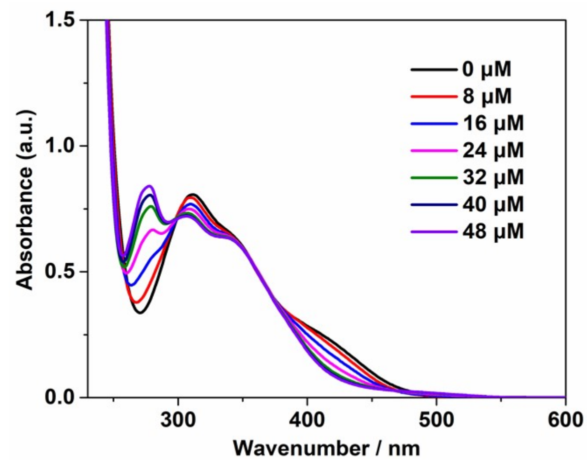


Figure S9. UV-vis titration of **1** (10 μM) with the addition of DPA in CH_3CN.

13. The NIR emission lifetimes of 1

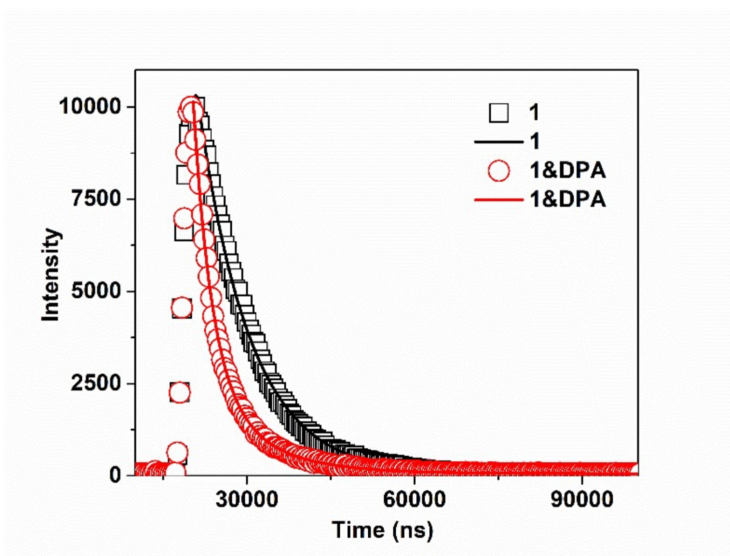


Figure S10. The NIR emission lifetimes of **1** with (red line) and without (black line) the addition of DPA (100 μM) in CH_3CN

14. The visible emission spectrum of DPA

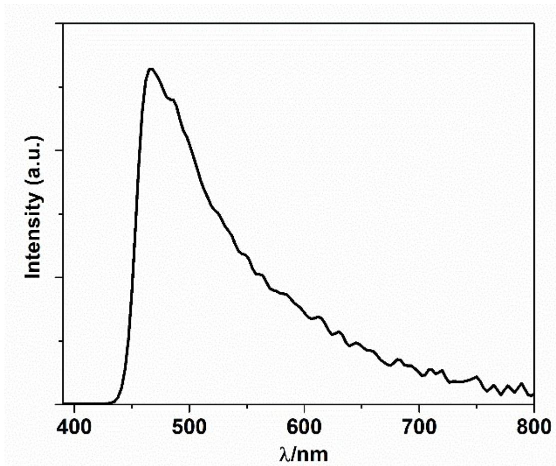


Figure S11. The visible emission spectrum of DPA (15 μM) in CH_3CN. (λ_{ex}=368 nm)

15. X-Ray Crystallography

X-ray data of **1** were collected on a Smart APEX CCD diffractometer in the θ–2θ mode with monochromated Mo Kα radiation at 190 K. The structures were solved by direct method using SHELX 97 program.[1] An empirical absorption correction was applied using SADABS program. The non-hydrogen atoms in the structures were refined anisotropically. All hydrogen atoms were calculated by geometrical methods and refined isotropically. The data can be obtained from www.ccdc.cam.ac.uk/data_request/cif (CCDC number: 2022305). The structure refinements of **1** are listed in Table S1, and selected bond lengths and angles are shown in Table S2.

Ref. (1) G. H. Sheldrick, SHELX 97, *A software package for the solution and refinement of X-ray data*; University of Göttingen: Göttingen, Germany, **1997**.

Table S1. Crystal data and structure refinements for **1**.

	1
Formula	$C_{252}H_{278}N_{16}O_{104}Yb_{18}$
Fw	8309.62
Crystal system	Triclinic
Space group	P-1
a [Å]	21.7568(17)
b [Å]	23.689(2)
c [Å]	24.8453(19)
α [deg]	97.103(2)
β [deg]	110.9060(10)
γ [deg]	114.890(2)
V / [Å^3]	10268.9(14)
d / [g/cm^3]	1.344
Z	1
T [K]	190(1)
F(000)	3994
μ, mm^{-1}	4.115
θ rang, deg	1.00-25.00
reflns meads	42386
reflns used	35714
params	1732
R1[a], wR2[a] [$I > 2\sigma(I)$]	0.0916, 0.1414
R1, wR2 (all data)	0.2042, 0.2303
Quality of fit	1.155

[a] $R1 = \Sigma|F_o| - |F_c|\Sigma|F_o|$. $wR2 = [\Sigma w[(F_o^2 - F_c^2)^2]/\Sigma|[w(F_o^2)^2]]^{1/2}$. $w=1/[\sigma^2(F_o^2)+(0.075P)^2]$, where $P = [\max(F_o^2,0)+2F_c^2]/3$.

Table S2. Selected Bond Lengths (Å) and angles (◦) for **1**.

Yb(1)-O(30)	2.285(17)	Yb(6)-O(40)	2.83(2)
Yb(1)-O(25)	2.360(16)	Yb(7)-O(11)	2.404(18)
Yb(1)-O(31)	2.419(18)	Yb(7)-O(10)	2.41(2)
Yb(1)-O(13)	2.426(16)	Yb(7)-O(16)	2.456(18)
Yb(1)-O(1)	2.433(17)	Yb(7)-O(48)	2.48(3)
Yb(1)-O(24)	2.46(2)	Yb(7)-O(15)	2.50(2)
Yb(1)-O(22)	2.51(2)	Yb(7)-O(44)	2.575(19)
Yb(1)-O(23)	2.59(2)	Yb(7)-O(45)	2.595(19)
Yb(2)-O(1)	2.328(19)	Yb(7)-N(5)	2.72(3)
Yb(2)-O(2)	2.426(16)	Yb(7)-N(6)	2.77(3)
Yb(2)-O(5)	2.448(14)	Yb(8)-O(15)#1	2.380(19)
Yb(2)-O(31)	2.483(15)	Yb(8)-O(17)	2.410(19)
Yb(2)-O(26)	2.52(2)	Yb(8)-O(11)#1	2.466(19)
Yb(2)-O(32)	2.545(18)	Yb(8)-O(47)	2.471(17)
Yb(2)-O(28)	2.570(19)	Yb(8)-O(14)	2.502(17)
Yb(2)-O(27)	2.58(2)	Yb(8)-O(12)	2.55(2)
Yb(2)-O(25)	2.600(18)	Yb(8)-N(8)	2.60(2)
Yb(3)-O(5)	2.407(15)	Yb(8)-N(7)	2.63(3)
Yb(3)-O(3)	2.423(17)	Yb(8)-O(18)	2.63(2)
Yb(3)-O(2)	2.46(2)	Yb(9)-O(14)	2.350(18)
Yb(3)-O(46)	2.495(17)	Yb(9)-O(13)	2.352(16)
Yb(3)-O(32)	2.576(18)	Yb(9)-O(17)	2.394(18)
Yb(3)-O(34)	2.59(2)	Yb(9)-O(21)	2.455(19)
Yb(3)-O(6)	2.629(17)	Yb(9)-O(23)	2.519(19)
Yb(3)-N(1)	2.64(2)	Yb(9)-O(19)	2.529(19)
Yb(3)-N(2)	2.67(2)	Yb(9)-O(47)	2.561(17)
Yb(4)-O(6)	2.375(16)	Yb(9)-O(20)	2.56(2)
Yb(4)-O(4)	2.393(16)	Yb(9)-O(22)	2.72(2)
Yb(4)-O(36)	2.440(19)	O(30)-Yb(1)-O(25)	132.4(7)
Yb(4)-O(7)	2.488(16)	O(30)-Yb(1)-O(31)	67.0(6)
Yb(4)-O(3)	2.488(15)	O(25)-Yb(1)-O(31)	73.4(6)
Yb(4)-O(35)	2.51(2)	O(30)-Yb(1)-O(13)	84.5(6)
Yb(4)-N(3)	2.65(3)	O(25)-Yb(1)-O(13)	82.2(6)
Yb(4)-O(33)	2.687(17)	O(31)-Yb(1)-O(13)	106.3(5)
Yb(4)-N(4)	2.75(2)	O(30)-Yb(1)-O(1)	117.3(7)
Yb(5)-O(8)	2.415(18)	O(25)-Yb(1)-O(1)	66.8(6)
Yb(5)-O(7)	2.418(19)	O(31)-Yb(1)-O(1)	67.4(6)
Yb(5)-O(4)	2.435(14)	O(13)-Yb(1)-O(1)	148.9(6)
Yb(5)-O(9)	2.474(18)	O(30)-Yb(1)-O(24)	81.3(7)
Yb(5)-O(33)	2.498(17)	O(25)-Yb(1)-O(24)	144.5(6)
Yb(5)-O(39)	2.52(2)	O(31)-Yb(1)-O(24)	122.6(6)
Yb(5)-O(37)	2.59(3)	O(13)-Yb(1)-O(24)	117.2(7)
Yb(5)-O(38)	2.579(19)	O(1)-Yb(1)-O(24)	89.3(7)
Yb(5)-O(40)	2.64(2)	O(30)-Yb(1)-O(22)	138.9(7)
Yb(6)-O(43)	2.39(2)	O(25)-Yb(1)-O(22)	79.0(7)
Yb(6)-O(38)	2.42(2)	O(31)-Yb(1)-O(22)	152.1(6)
Yb(6)-O(9)	2.429(18)	O(13)-Yb(1)-O(22)	73.4(6)
Yb(6)-O(10)	2.44(2)	O(1)-Yb(1)-O(22)	98.1(7)
Yb(6)-O(16)	2.44(2)	O(24)-Yb(1)-O(22)	78.9(7)
Yb(6)-O(42)	2.50(2)	O(30)-Yb(1)-O(23)	72.2(7)
Yb(6)-O(45)	2.549(16)	O(25)-Yb(1)-O(23)	138.4(6)
Yb(6)-O(41)	2.59(3)	O(31)-Yb(1)-O(23)	139.0(5)

O(13)-Yb(1)-O(23)	65.6(6)
O(1)-Yb(1)-O(23)	139.5(6)
O(24)-Yb(1)-O(23)	51.7(7)
O(22)-Yb(1)-O(23)	67.3(7)
O(1)-Yb(2)-O(2)	65.2(6)
O(1)-Yb(2)-O(5)	128.8(6)
O(2)-Yb(2)-O(5)	64.5(6)
O(1)-Yb(2)-O(31)	68.0(6)
O(2)-Yb(2)-O(31)	125.7(5)
O(5)-Yb(2)-O(31)	158.0(5)
O(1)-Yb(2)-O(26)	86.0(7)
O(2)-Yb(2)-O(26)	85.3(7)
O(5)-Yb(2)-O(26)	81.0(6)
O(31)-Yb(2)-O(26)	117.2(6)
O(1)-Yb(2)-O(32)	98.2(6)
O(2)-Yb(2)-O(32)	67.4(6)
O(5)-Yb(2)-O(32)	70.8(5)
O(31)-Yb(2)-O(32)	94.3(5)
O(26)-Yb(2)-O(32)	147.0(7)
O(1)-Yb(2)-O(28)	146.5(6)
O(2)-Yb(2)-O(28)	128.6(6)
O(5)-Yb(2)-O(28)	77.4(5)
O(31)-Yb(2)-O(28)	82.1(6)
O(26)-Yb(2)-O(28)	122.4(7)
O(32)-Yb(2)-O(28)	68.4(6)
O(1)-Yb(2)-O(27)	134.8(6)
O(2)-Yb(2)-O(27)	150.4(6)
O(5)-Yb(2)-O(27)	89.5(6)
O(31)-Yb(2)-O(27)	83.6(6)
O(26)-Yb(2)-O(27)	76.4(7)
O(32)-Yb(2)-O(27)	119.0(6)
O(28)-Yb(2)-O(27)	50.9(6)
O(1)-Yb(2)-O(25)	64.5(6)
O(2)-Yb(2)-O(25)	111.9(6)
O(5)-Yb(2)-O(25)	129.2(5)
O(31)-Yb(2)-O(25)	68.3(5)
O(26)-Yb(2)-O(25)	49.0(6)
O(32)-Yb(2)-O(25)	158.7(6)
O(28)-Yb(2)-O(25)	118.8(6)
O(27)-Yb(2)-O(25)	72.8(6)
O(5)-Yb(3)-O(3)	126.7(5)
O(5)-Yb(3)-O(2)	64.6(5)
O(3)-Yb(3)-O(2)	144.0(5)
O(5)-Yb(3)-O(46)	72.3(6)
O(3)-Yb(3)-O(46)	101.4(6)
O(2)-Yb(3)-O(46)	114.3(6)
O(5)-Yb(3)-O(32)	70.9(5)
O(3)-Yb(3)-O(32)	84.5(5)
O(2)-Yb(3)-O(32)	66.4(5)
O(46)-Yb(3)-O(32)	137.7(6)
O(5)-Yb(3)-O(34)	136.3(6)
O(3)-Yb(3)-O(34)	73.8(6)
O(2)-Yb(3)-O(34)	77.9(6)
O(46)-Yb(3)-O(34)	148.0(6)
O(32)-Yb(3)-O(34)	74.1(6)
O(5)-Yb(3)-O(6)	65.1(5)
O(3)-Yb(3)-O(6)	62.4(5)
O(2)-Yb(3)-O(6)	122.3(5)
O(46)-Yb(3)-O(6)	74.1(6)
O(32)-Yb(3)-O(6)	72.0(5)
O(34)-Yb(3)-O(6)	126.1(6)
O(5)-Yb(3)-N(1)	103.4(6)
O(3)-Yb(3)-N(1)	127.2(6)
O(2)-Yb(3)-N(1)	68.4(6)
O(46)-Yb(3)-N(1)	76.8(6)
O(32)-Yb(3)-N(1)	131.9(6)
O(34)-Yb(3)-N(1)	81.3(6)
O(6)-Yb(3)-N(1)	150.8(6)
O(5)-Yb(3)-N(2)	141.2(6)
O(3)-Yb(3)-N(2)	69.6(6)
O(2)-Yb(3)-N(2)	126.1(7)
O(46)-Yb(3)-N(2)	69.7(7)
O(32)-Yb(3)-N(2)	147.1(7)
O(34)-Yb(3)-N(2)	79.2(7)
O(6)-Yb(3)-N(2)	110.7(6)
N(1)-Yb(3)-N(2)	60.3(7)
O(6)-Yb(4)-O(4)	130.0(5)
O(6)-Yb(4)-O(36)	95.9(6)
O(4)-Yb(4)-O(36)	73.9(6)
O(6)-Yb(4)-O(7)	150.4(6)
O(4)-Yb(4)-O(7)	64.3(5)
O(36)-Yb(4)-O(7)	113.7(7)
O(6)-Yb(4)-O(3)	65.3(6)
O(4)-Yb(4)-O(3)	64.8(5)
O(36)-Yb(4)-O(3)	75.2(6)
O(7)-Yb(4)-O(3)	122.4(6)
O(6)-Yb(4)-O(35)	78.1(6)
O(4)-Yb(4)-O(35)	137.1(6)
O(36)-Yb(4)-O(35)	142.9(7)
O(7)-Yb(4)-O(35)	77.1(6)
O(3)-Yb(4)-O(35)	130.9(7)
O(6)-Yb(4)-N(3)	66.9(8)
O(4)-Yb(4)-N(3)	138.4(8)
O(36)-Yb(4)-N(3)	66.0(8)
O(7)-Yb(4)-N(3)	122.7(8)
O(3)-Yb(4)-N(3)	112.9(7)
O(35)-Yb(4)-N(3)	78.2(8)
O(6)-Yb(4)-O(33)	95.8(5)
O(4)-Yb(4)-O(33)	69.2(5)
O(36)-Yb(4)-O(33)	139.8(6)
O(7)-Yb(4)-O(33)	62.9(5)
O(3)-Yb(4)-O(33)	75.3(4)
O(35)-Yb(4)-O(33)	77.3(6)
N(3)-Yb(4)-O(33)	152.5(8)
O(6)-Yb(4)-N(4)	122.7(7)
O(4)-Yb(4)-N(4)	102.6(7)
O(36)-Yb(4)-N(4)	76.5(7)
O(7)-Yb(4)-N(4)	66.1(6)

O(3)-Yb(4)-N(4)	151.2(6)	O(16)-Yb(6)-O(42)	73.8(7)
O(35)-Yb(4)-N(4)	76.5(8)	O(43)-Yb(6)-O(45)	143.8(8)
N(3)-Yb(4)-N(4)	58.2(8)	O(38)-Yb(6)-O(45)	84.5(6)
O(33)-Yb(4)-N(4)	126.4(5)	O(9)-Yb(6)-O(45)	95.8(6)
O(8)-Yb(5)-O(7)	63.0(5)	O(10)-Yb(6)-O(45)	67.6(7)
O(8)-Yb(5)-O(4)	127.8(5)	O(16)-Yb(6)-O(45)	69.9(6)
O(7)-Yb(5)-O(4)	64.8(5)	O(42)-Yb(6)-O(45)	70.4(7)
O(8)-Yb(5)-O(9)	93.9(6)	O(43)-Yb(6)-O(41)	72.8(9)
O(7)-Yb(5)-O(9)	88.5(6)	O(38)-Yb(6)-O(41)	93.1(8)
O(4)-Yb(5)-O(9)	85.3(6)	O(9)-Yb(6)-O(41)	138.7(7)
O(8)-Yb(5)-O(33)	87.4(5)	O(10)-Yb(6)-O(41)	143.3(8)
O(7)-Yb(5)-O(33)	66.8(6)	O(16)-Yb(6)-O(41)	84.6(7)
O(4)-Yb(5)-O(33)	71.8(5)	O(42)-Yb(6)-O(41)	51.3(8)
O(9)-Yb(5)-O(33)	151.6(6)	O(45)-Yb(6)-O(41)	121.0(7)
O(8)-Yb(5)-O(39)	141.0(6)	O(43)-Yb(6)-O(40)	68.3(8)
O(7)-Yb(5)-O(39)	130.6(6)	O(38)-Yb(6)-O(40)	62.2(6)
O(4)-Yb(5)-O(39)	77.5(6)	O(9)-Yb(6)-O(40)	68.4(6)
O(9)-Yb(5)-O(39)	119.9(6)	O(10)-Yb(6)-O(40)	124.6(6)
O(33)-Yb(5)-O(39)	72.1(6)	O(16)-Yb(6)-O(40)	143.5(6)
O(8)-Yb(5)-O(37)	75.5(6)	O(42)-Yb(6)-O(40)	107.2(7)
O(7)-Yb(5)-O(37)	132.8(6)	O(45)-Yb(6)-O(40)	146.1(6)
O(4)-Yb(5)-O(37)	148.5(6)	O(41)-Yb(6)-O(40)	70.4(7)
O(9)-Yb(5)-O(37)	117.0(6)	O(11)-Yb(7)-O(10)	146.4(7)
O(33)-Yb(5)-O(37)	90.8(6)	O(11)-Yb(7)-O(16)	127.3(6)
O(39)-Yb(5)-O(37)	72.1(7)	O(10)-Yb(7)-O(16)	64.6(7)
O(8)-Yb(5)-O(38)	79.6(6)	O(11)-Yb(7)-O(48)	104.8(8)
O(7)-Yb(5)-O(38)	134.0(6)	O(10)-Yb(7)-O(48)	108.8(8)
O(4)-Yb(5)-O(38)	143.6(6)	O(16)-Yb(7)-O(48)	74.2(8)
O(9)-Yb(5)-O(38)	67.4(6)	O(11)-Yb(7)-O(15)	64.0(6)
O(33)-Yb(5)-O(38)	140.2(6)	O(10)-Yb(7)-O(15)	124.6(7)
O(39)-Yb(5)-O(38)	95.2(6)	O(16)-Yb(7)-O(15)	64.7(6)
O(37)-Yb(5)-O(38)	49.6(6)	O(48)-Yb(7)-O(15)	76.9(8)
O(8)-Yb(5)-O(40)	142.7(6)	O(11)-Yb(7)-O(44)	72.0(6)
O(7)-Yb(5)-O(40)	145.9(7)	O(10)-Yb(7)-O(44)	79.9(6)
O(4)-Yb(5)-O(40)	86.0(6)	O(16)-Yb(7)-O(44)	135.9(7)
O(9)-Yb(5)-O(40)	71.1(7)	O(48)-Yb(7)-O(44)	145.5(8)
O(33)-Yb(5)-O(40)	122.1(6)	O(15)-Yb(7)-O(44)	126.5(6)
O(39)-Yb(5)-O(40)	50.8(7)	O(11)-Yb(7)-O(45)	87.1(6)
O(37)-Yb(5)-O(40)	81.3(7)	O(10)-Yb(7)-O(45)	67.3(6)
O(38)-Yb(5)-O(40)	63.2(6)	O(16)-Yb(7)-O(45)	69.0(6)
O(43)-Yb(6)-O(38)	130.4(7)	O(48)-Yb(7)-O(45)	140.6(7)
O(43)-Yb(6)-O(9)	88.9(7)	O(15)-Yb(7)-O(45)	75.1(6)
O(38)-Yb(6)-O(9)	70.7(7)	O(44)-Yb(7)-O(45)	73.9(6)
O(43)-Yb(6)-O(10)	82.4(8)	O(11)-Yb(7)-N(5)	126.6(8)
O(38)-Yb(6)-O(10)	123.6(7)	O(10)-Yb(7)-N(5)	66.9(8)
O(9)-Yb(6)-O(10)	65.0(6)	O(16)-Yb(7)-N(5)	102.9(8)
O(43)-Yb(6)-O(16)	79.3(7)	O(48)-Yb(7)-N(5)	69.4(9)
O(38)-Yb(6)-O(16)	148.1(6)	O(15)-Yb(7)-N(5)	146.2(8)
O(9)-Yb(6)-O(16)	128.9(6)	O(44)-Yb(7)-N(5)	84.9(8)
O(10)-Yb(6)-O(16)	64.2(6)	O(45)-Yb(7)-N(5)	132.1(7)
O(43)-Yb(6)-O(42)	119.0(8)	O(11)-Yb(7)-N(6)	68.1(7)
O(38)-Yb(6)-O(42)	79.9(7)	O(10)-Yb(7)-N(6)	123.1(7)
O(9)-Yb(6)-O(42)	148.8(7)	O(16)-Yb(7)-N(6)	144.5(7)
O(10)-Yb(6)-O(42)	128.2(7)	O(48)-Yb(7)-N(6)	70.6(9)

O(15)-Yb(7)-N(6)	110.9(7)	N(8)-Yb(8)-O(18)	79.9(7)
O(44)-Yb(7)-N(6)	76.8(7)	N(7)-Yb(8)-O(18)	68.1(8)
O(45)-Yb(7)-N(6)	146.2(7)	O(14)-Yb(9)-O(13)	66.2(6)
N(5)-Yb(7)-N(6)	59.9(8)	O(14)-Yb(9)-O(17)	65.0(7)
O(15)#1-Yb(8)-O(17)	129.8(7)	O(13)-Yb(9)-O(17)	131.0(6)
O(15)#1-Yb(8)-O(11)#1	64.9(7)	O(14)-Yb(9)-O(21)	84.5(6)
O(17)-Yb(8)-O(11)#1	65.6(6)	O(13)-Yb(9)-O(21)	96.3(6)
O(15)#1-Yb(8)-O(47)	88.7(6)	O(17)-Yb(9)-O(21)	83.8(7)
O(17)-Yb(8)-O(47)	70.7(6)	O(14)-Yb(9)-O(23)	132.7(7)
O(11)#1-Yb(8)-O(47)	74.0(6)	O(13)-Yb(9)-O(23)	67.9(6)
O(15)#1-Yb(8)-O(14)	146.9(6)	O(17)-Yb(9)-O(23)	156.1(6)
O(17)-Yb(8)-O(14)	62.5(6)	O(21)-Yb(9)-O(23)	111.1(7)
O(11)#1-Yb(8)-O(14)	121.6(6)	O(14)-Yb(9)-O(19)	130.2(6)
O(47)-Yb(8)-O(14)	65.4(6)	O(13)-Yb(9)-O(19)	134.7(6)
O(15)#1-Yb(8)-O(12)	73.8(7)	O(17)-Yb(9)-O(19)	77.7(7)
O(17)-Yb(8)-O(12)	137.4(7)	O(21)-Yb(9)-O(19)	124.3(7)
O(11)#1-Yb(8)-O(12)	128.7(6)	O(23)-Yb(9)-O(19)	78.4(7)
O(47)-Yb(8)-O(12)	76.0(7)	O(14)-Yb(9)-O(47)	66.2(5)
O(14)-Yb(8)-O(12)	79.9(6)	O(13)-Yb(9)-O(47)	86.9(5)
O(15)#1-Yb(8)-N(8)	123.0(7)	O(17)-Yb(9)-O(47)	69.5(6)
O(17)-Yb(8)-N(8)	104.7(7)	O(21)-Yb(9)-O(47)	146.4(7)
O(11)#1-Yb(8)-N(8)	152.5(6)	O(23)-Yb(9)-O(47)	101.1(6)
O(47)-Yb(8)-N(8)	129.0(6)	O(19)-Yb(9)-O(47)	70.5(6)
O(14)-Yb(8)-N(8)	68.1(6)	O(14)-Yb(9)-O(20)	148.9(7)
O(12)-Yb(8)-N(8)	76.5(7)	O(13)-Yb(9)-O(20)	139.8(6)
O(15)#1-Yb(8)-N(7)	69.2(8)	O(17)-Yb(9)-O(20)	88.2(7)
O(17)-Yb(8)-N(7)	138.5(7)	O(21)-Yb(9)-O(20)	76.8(7)
O(11)#1-Yb(8)-N(7)	111.0(8)	O(23)-Yb(9)-O(20)	77.8(7)
O(47)-Yb(8)-N(7)	150.5(7)	O(19)-Yb(9)-O(20)	50.9(6)
O(14)-Yb(8)-N(7)	125.1(8)	O(47)-Yb(9)-O(20)	120.7(6)
O(12)-Yb(8)-N(7)	79.1(8)	O(14)-Yb(9)-O(22)	108.2(6)
N(8)-Yb(8)-N(7)	57.9(8)	O(13)-Yb(9)-O(22)	70.7(6)
O(15)#1-Yb(8)-O(18)	100.0(7)	O(17)-Yb(9)-O(22)	130.4(6)
O(17)-Yb(8)-O(18)	72.0(6)	O(21)-Yb(9)-O(22)	47.0(7)
O(11)#1-Yb(8)-O(18)	72.6(7)	O(23)-Yb(9)-O(22)	65.2(6)
O(47)-Yb(8)-O(18)	137.6(7)	O(19)-Yb(9)-O(22)	121.2(7)
O(14)-Yb(8)-O(18)	112.9(7)	O(47)-Yb(9)-O(22)	156.7(6)
O(12)-Yb(8)-O(18)	146.3(7)	O(20)-Yb(9)-O(22)	76.5(6)