Electronic Supplementary Information

Specific detection and determination of cysteine by a luminescent

samarium macrocycle-based fluorescence probe platform

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Experimental Section

Materials and Instrumentations

All starting materials under the 99% purity were commercially purchased from the TCI Shanghai Company and directly used without any further purifications.

¹H NMR spectrum was recorded on Bruker DPX 400 MHz spectrometer at room temperature, with TMS as internal standard using CDCl₃ as deuterated solvent. The electrospray ionization mass spectra (ESI-MS) were measured by a ThermoFisher Scientific LCQ-Fleet mass spectrometer in a scan range of 500-2000 amu. The FT-IR spectra were recorded from 4000 to 400 cm⁻¹ on a Nicolet FT-IR 170X spectrophotometer with 1 cm⁻¹ resolution. Samples were dried and grinded with KBr to obtain pellet for recording FT-IR. UV-vis were monitored by а Shimadzu UV-3150 double-beam spectra spectrophotometer between a wavelength range of 250-550 nm. Fluorescence measurements in this work were determined from 500 to 750 nm on the HORIBA JOBIN YVON FluoroMax-4 fluorometer equipped with a R928P PMT emission detector in the visible region, and the slits of 5/5 nm.



Scheme S1. Synthesis route of the dialdehyde H_2Q_n and complex Sm-2_n.

Syntheses of H₂Q_n

The dialdehyde H₂Q_n was synthesized by previous procedures¹ except that 4-fluorobenzylamine (0.313 g, 2.50 mmol) and 5-chloro-3-bromomethyl-2hydroxybenzaldehyde (1.248 g, 5.00 mmol) was used here, and H₂Q_n was finally obtained in the yield of 68 % (0.785 g) by silica gel column chromatography using ethyl acetate/petroleum ether ($\nu/\nu = 1$:5) as the eluent. Mp: 185–186 °C. ¹H NMR (400 MHz, CDCl₃): δ 11.40 (s, 2H), 10.01 (s, 2H), 7.51 (s, 2H), 7.43 (s, 2H), 7.33 (s, 2H), 7.06 (s, 2H), 3.74 (s, 4H), 3.70 (s, 2H). ¹³C NMR (400 MHz, CDCl₃): δ (ppm) 193.17, 163.60, 158.78, 136.47, 132.63, 130.93, 130.92, 127.32, 124.30, 122.01, 115.68, 58.19, 53.26. Main FT-IR absorptions (KBr pellets, cm⁻¹): 2924 (w), 2851 (w), 1660 (s, -CH=O), 1602(m), 1458 (s), 1239 (m), 1017(w), 744 (w), 680(w). UV-vis spectrum, λ/nm ($\varepsilon/L \cdot mol^{-1} \cdot cm^{-1}$) in CH₃OH: 342 (9550).

Syntheses of Sm-2_n [Sm(HL2_n)(NO₃)₂]

Upon reported template synthesis method¹ with Sm(NO₃)₃·6H₂O (0.045 g, 0.10 mmol) as the template reagent, the targeted yellow-green product Sm-2_n could be finally obtained by use of dialdehyde H₂Q_n (0.046 g, 0.10 mmol) and diamine 1,2-bis(2-aminoethoxy)ethane (0.015 g, 0.10 mmol). Yield: 70 %, (0.059 g). ESI-MS (positive mode, m/z): 1033.42 {Sm-2_n+5CH₃OH+Na}⁺ and 981.50 {Sm-2_n+3CH₃OH+2H₂O}⁺. Main FT-IR absorptions (KBr pellets, cm⁻¹): 2907 (w), 1638 (s, CH=N), 1385 (s, N=O), 1290 (m), 1064 (m), 774 (m). UV-vis spectrum, λ /nm (ϵ /L·mol⁻¹·cm⁻¹) in CH₃OH: 359 (13758). After the slow evaporation in air at room temperature for six days, yellow-green single crystals

of complex Sm-2_n in prismatic shape were grown from its mixture of CH₃CN/CH₃OH (v/v = 1:4).



Scheme S2. The structures of used amino acids.

Cysteine sensing experiments

Complex Sm-2_n was firstly dispersed in MeOH (0.5 mM), and 0.6 ml of prepared Sm-2_n suspension was transferred to volumetric flasks, followed by the addition of 0.5 ml of amino acids (50 mM) and specific volumes of MeOH using a precise pipette to maintain the total volume of mixtures at 10 mL. At the same time, under the same volume (0.6 ml) of Sm-2_n (0.5 mM), different volumes of Cys (50 mM) and MeOH were added into volumetric flasks for titration experiments. Shake treatments were applied to these mixtures to keep uniform dispersion for latter spectral measurements. The final concentration of Sm-2_n in all samples remained at 30 μ M.

Crystal structure determination and refinement

The single-crystal sample of complex Sm-2_n was covered with glue and mounted on glass fiber for data collection. Crystallographic data were collected at 293(2) K on a Bruker SMART 1K CCD diffractometer, using graphite mono-chromated MoK α radiation ($\lambda = 0.71073$ Å). Absorption corrections were performed to all data and the structure was solved by direct method and refined by full-matrix least-squares method on F_{obs}² by using the SHELXTL-PC software package.² All non-H atoms were anisotropically refined and all hydrogen atoms were inserted in the calculated positions assigned fixed isotropic thermal parameters and allowed to ride on their respective parent atoms. A summary of the crystal data, experimental details and refinement results for $\mathbf{Sm-2_n}$ was listed in Table S1. Selected bond lengths and bond angles of $\mathbf{Sm-2_n}$ were tabulated in Table S2, and hydrogen-bonding parameters were shown in Table S3. CCDC nos. 2012636 for disalicylaldehyde $\mathbf{Sm-2_n}$ contains the supplementary crystallographic data in this work. This datum could be acquired free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK; fax: [+44]1223-336-033; or deposit @ccdc.cam.ac.uk).

References

K. Zhang, M.-L. Lin, C.-C. Feng, P.-P. Nie, Z.-R. Yang, T.-T. Chen, L.-F. Zhang, S. Ma, Y.-J. Shen, Z.-Y. Lu, *Polyhedron* 2019, **173**, 114133.
 G. M. Sheldrick, SHELXTL (Version 6.10). Software Reference Manual; Madison,

Wisconsin (USA): Bruker AXS, Inc.: 2000.

Tables

Table S1.	Crystal o	data and	structural	refinements	for co	mplex Sm-2 _n .
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Complex	Sm-2 _n
Empirical formula	$C_{29}H_{29}Cl_2FN_5O_{10}Sm$
Formula weight	847.82
Temperature / K	293
Wavelength / Å	0.71073
Crystal Size (mm)	0.15×0.21×0.26
Crystal system	Triclinic
Space group	$P\bar{1}$
<i>a</i> / Å	19.968(6)
b / Å	8.587(3)
<i>c</i> / Å	19.820(6)
α/°	90
β/°	92.046(9)
γ / °	90
$V/Å^3$	3396.3(2)
$Z / D_{\text{calcd}} (g / \text{cm}^3)$	4 / 1.658
<i>F</i> (000)	1692
μ / mm^{-1}	1.953
h_{\min} / h_{\max}	-26 / 25
k_{\min} / k_{\max}	-10 / 11
l_{\min} / l_{\max}	-25 / 25
Data / parameters	7713 / 433
$R_1, \mathrm{w}R_2 [I > 2\sigma(I)]^a$	$R_1 = 0.0894, wR_2 = 0.1914$
R_1 , w R_2 (all data) ^{<i>a</i>}	$R_1 = 0.1194, wR_2 = 0.2050$
S	1.09
Max/min $\Delta \rho/e \text{ Å}^{-3}$	4.13 / -2.26

^{*a*} $R_1 = \Sigma ||Fo| - |Fc|| / \Sigma |Fo|, wR_2 = [\Sigma [w(Fo^2 - Fc^2)^2] / \Sigma w(Fo^2)^2]^{1/2}$

Table S2. Selected bond distances	s (Å) and angles (°) in complex Sm-	2 _n .

Bond distances	Bond distances		Bond angles			
Sm-2 _n						
Sm1–O1	2.343(6)	O1–Sm1–O2	113.5(2)			
Sm1–O2	2.649(7)	O1–Sm1–O3	139.5(3)			
Sm1–O3	2.688(8)	O1–Sm1–O4	69.0(2)			

Sm1–O4	2.338(8)	01–Sm1–O5	92.5(3)
Sm1–O5	2.588(8)	01–Sm1–O6	134.0(2)
Sm1-O6	2.531(8)	O1–Sm1–O8	73.7(3)
Sm1–O8	2.621(11)	O1–Sm1–O9	68.9(3)
Sm1–O9	2.627(12)	O1–Sm1–N2	68.1(2)
Sm1–N2	2.646(8)	O1–Sm1–N3	134.8(3)
Sm1–N3	2.693(10)	O2–Sm1–O3	60.0(2)
		O2–Sm1–O4	177.5(2)
		O2–Sm1–O5	110.1(3)
		O2–Sm1–O6	68.5(2)
		O2–Sm1–O8	108.4(3)
		O2–Sm1–O9	67.8(3)
		O2–Sm1–N2	62.3(2)
		O2-Sm1-N3	111.4(3)
		O3–Sm1–O4	118.4(3)
		O3–Sm1–O5	127.9(3)
		O3–Sm1–O6	83.6(3)
		O3–Sm1–O8	71.9(3)
		O3–Sm1–O9	72.5(3)
		O3–Sm1–N2	122.3(3)
		O3–Sm1–N3	63.6(3)
		O4–Sm1–O5	69.1(3)
		O4–Sm1–O6	109.6(2)
		O4–Sm1–O8	72.4(3)
		O4–Sm1–O9	114.0(3)
		O4–Sm1–N2	119.1(3)
		O4–Sm1–N3	66.2(3)
		O5–Sm1–O6	49.7(3)
		O5–Sm1–O8	141.5(3)
		O5–Sm1–O9	156.7(4)
		O5–Sm1–N2	71.8(3)
		O5–Sm1–N3	77.4(3)
		O6–Sm1–O8	152.0(3)
		O6–Sm1–O9	136.2(3)
		O6–Sm1–N2	74.6(2)
		O6-Sm1-N3	69.5(3)
		O8–Sm1–O9	48.3(4)

	O8–Sm1–N2	130.1(3)
	O8–Sm1–N3	87.3(4)
	O9–Sm1–N2	87.8(3)
	O9–Sm1–N3	125.6(3)
	N2-Sm1-N3	142.6(3)

Table S3. Intramolecular hydrogen bonding parameters (Å, °) in complex $Sm-2_n$.

D–H···A	D–H	H···A	D····A	∠DHA
Sm-2 _n				
N1-H1…O1	0.98	2.10	2.858(10)	133
N1-H1O4	0.98	1.82	2.615(11)	136

Table S4. Bond distances $(d_{\text{Sm},j})$, bond valences $(v_{\text{Sm},j})$ and total lanthanide atom valence (V_{Sm}) in the crystal structure of complex Sm-2_n.

Compound	Atom	Donor type	$d_{\mathrm{Sm,j}}/\mathrm{\AA}$	$v_{\mathrm{Sm,j}}$	V _{Sm}
	01	HL2 _n -	2.343	0.464	
	02	HL2 _n -	2.649	0.203	
	03	HL2 _n -	2.688	0.183	
	04	HL2 _n -	2.338	0.470	
S1	05	NO ₃ -	2.588	0.239	2 802
5m1	06	NO ₃ -	2.531	0.279	2.803
	O8 N O9 N N2 HI	NO ₃ -	2.621	0.219	
		NO ₃ -	2.627	0.215	
		HL2 _n -	2.646	0.282	
	N3	HL2 _n -	2.693	0.249	

Figures



Fig. S1. ¹H NMR spectrum of dialdehyde H₂Q_n in CDCl₃.



Fig. S2. 13 C NMR spectrum of dialdehyde H_2Q_n in CDCl₃.



Fig. S3. FT-IR spectrum of dialdehyde H₂Q_n.



Fig. S4. FT-IR spectrum of macrocyclic Sm(III) complex Sm-2_n.



Fig. S5. UV-vis spectra of dialdehyde H_2Q_n (30 μ M) and macrocyclic Sm(III) complex Sm-2_n (30 μ M) in CH₃OH.



Fig. S6. X-ray crystal structure of complex $Sm-2_n$: white: hydrogen, gray: carbon, red: oxygen, blue: nitrogen, cyan: chlorine, green: fluorine, pink: samarium. For clarity, only the amide hydrogen (H1) related to hydrogen bonding interactions was kept. Insert: Description of distorted bicapped square antiprism coordination geometry of central Sm(III).



Fig. S7. ESI-MS (positive) of macrocyclic Sm(III) complex Sm-2_n together with the inserted experimental (**a** and **b**) and simulative (**c** and **d**, calculation for $[C_{32}H_{45}Cl_2FN_5O_{15}Sm]$ and $[C_{34}H_{49}Cl_2FN_5O_{15}NaSm]$, respectively) peaks of isotopic distribution corresponding to the peaks at m/z = 983.4966 and 1034.4214.



Fig. S8. Emission spectra of Sm(III) complex Sm-2_n ($\lambda_{ex} = 359$ nm, 30 μ M) in air over multiple time points, recorded in H₂O-CH₃OH (ν/ν , 1:19) at 298 K.



Fig. S9. Fluorescence spectra ($\lambda_{ex} = 359 \text{ nm}$) of complex **Sm-2**_n (30 µM) before and after the addition of various amino acids (2.5 mM) in 5% H₂O/CH₃OH (ν/ν) at 298 K.



Fig. S10. The time-dependent fluorescence spectra ($\lambda_{ex} = 359 \text{ nm}$) of complex Sm-2_n (15 μ M) mixed with Cys (1.25 mM) in 5% H₂O/CH₃OH (ν/ν) at 298 K.



Fig. S11. ESI-MS (negative) of probe complex Sm-2_n mixed with excessive Cys together with the inserted experimental (a) and simulative (b, calculation for $[C_{29}H_{24}Cl_2FN_3O_6S_2Sm]$) peaks of isotopic distribution corresponding to the peak at m/z = 817.1783.



Fig. S12. The ratio of G/(R+G+B) (**a**), G/(R+G+B) (**b**), R/G (**c**), R/B (**d**), and G/B (**e**) versus [Cys] in various Cys solutions (0–0.135 mM).

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Fig. S13. The RGB values of smartphone-based analysis for detecting Cys in the release capsule by probe $Sm-2_n$ impregnated test paper strips with five repetitions.