Supporting Information

NIR luminescent detection of quercetin based on an octanuclear Zn(II)-Nd(III) salen nanocluster

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Contents

1. Synthesis of H_4L

H_4L 2,3-Dihydroxybenzaldehyde (20.0 mmol, 2.7624 g) was dissolved in 15 mL EtOH, and a solution of 4-methoxy-*o*-phenylenediamine (10.0 mmol,1.3817 g) in 20 mL EtOH was then added drop by drop. The resulting solution was stirred and heated under reflux for 5 h. It was allowed to cool and was then filtered. The solid was washed with EtOH (3 × 5 mL) and then dried in the air at room temperature to give red product. Yield (based on 4-Methoxy-O-Phenylenediamine): 3.630g (96%). Elemental analysis: Found: C, 66.63%; H, 4.77%; N, 7.43%; Calc. For $C_{21}H_{18}N_2O_5$: C, 66.66%; H, 4.79%; N, 7.40%. ^{1}H NMR (500 MHz, DMSO): 12.86 (2H), 9.22 (2H), 8.88 (2H), 7.46 (1H), 6.77 (2H), 6.92 (4H), 7.09 (2H), 3.87 (3H). IR (cm^{-1}): 1615 (m), 1456 (m), 1270 (m), 1158 (s), 1073 (s), 972 (w), 775 (m), 716(s) , 623(m).

2. The ^{1}H NMR spectrum of H_4L

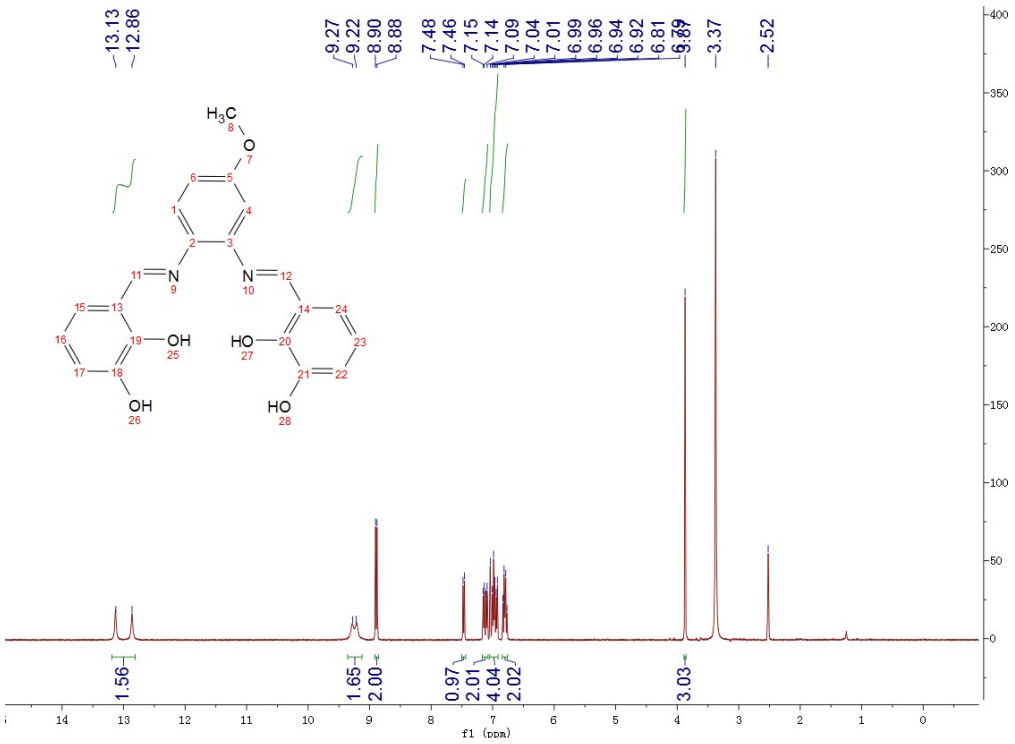


Figure S1. ^{1}H NMR spectrum of H_4L.

3. IR spectra of H_4L and 1

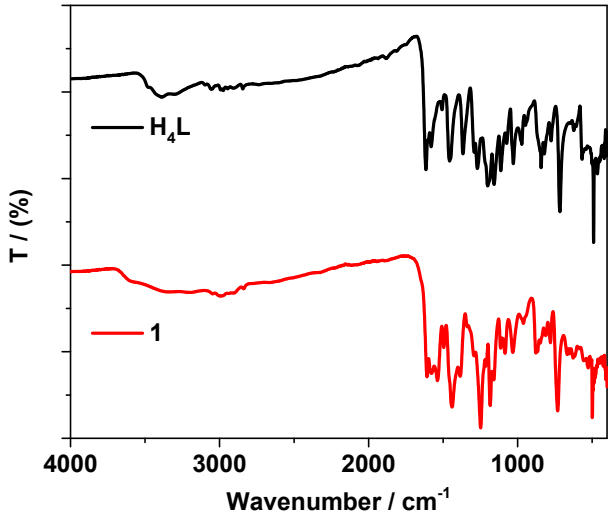


Figure S2. IR spectra of H_4L and **1**.

4. Powder XRD patterns of 1

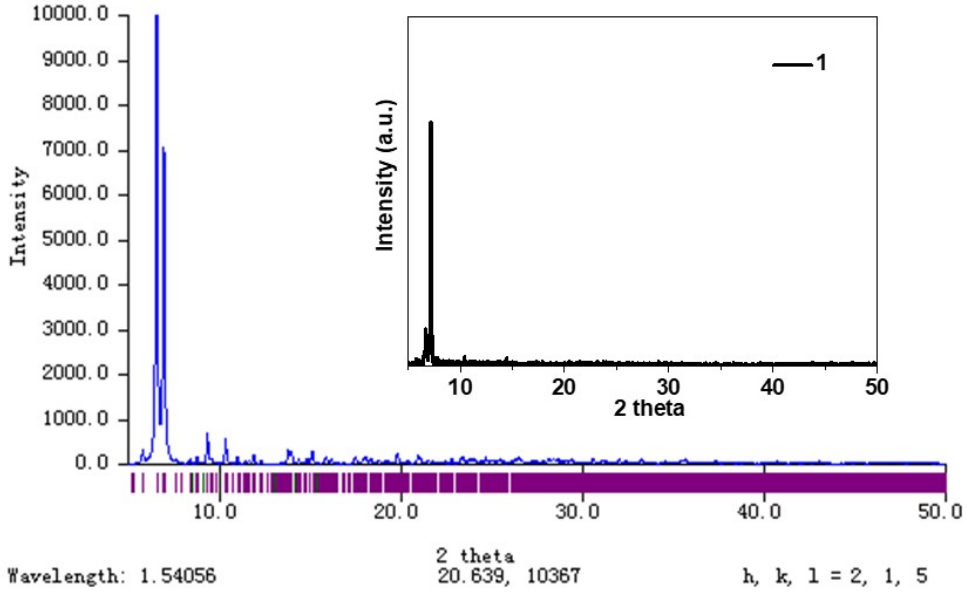


Figure S3. Powder XRD patterns of **1**.

5. The thermogravimetric analysis of 1

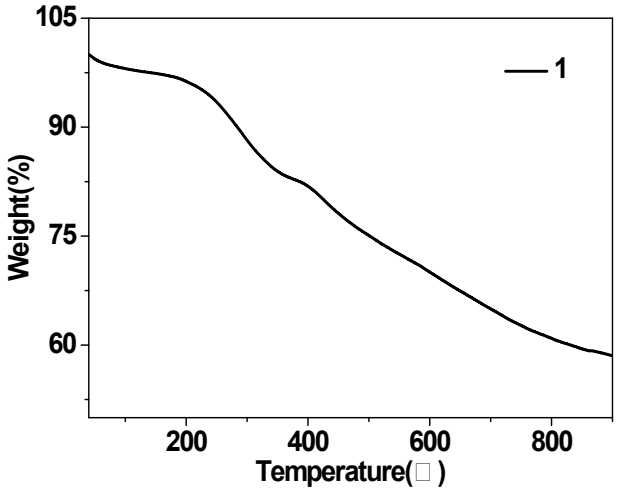


Figure S4. The thermogravimetric analysis of **1**.

6. The ^{1}H NMR spectrum of the Zn-La analogue

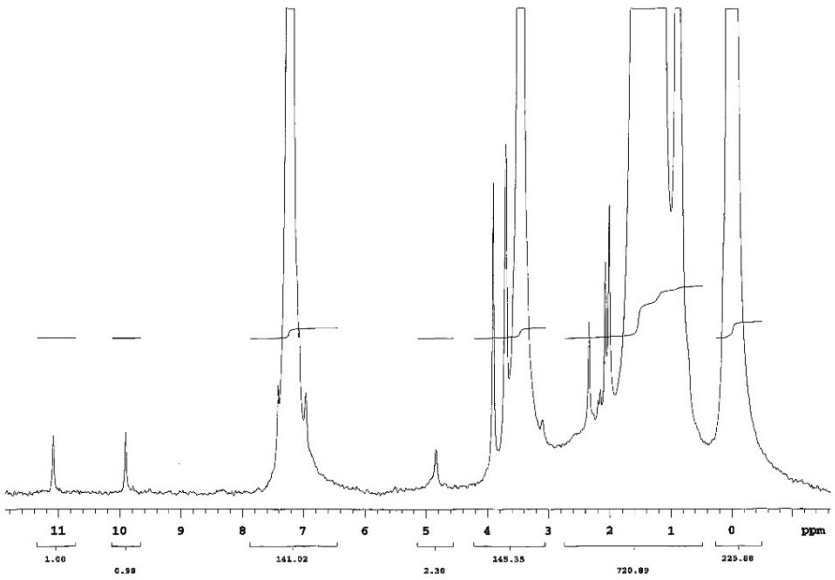


Figure S5. The ^{1}H NMR spectrum of the Zn-La analogue in CD_3OD.

7. The mass spectrum of 1

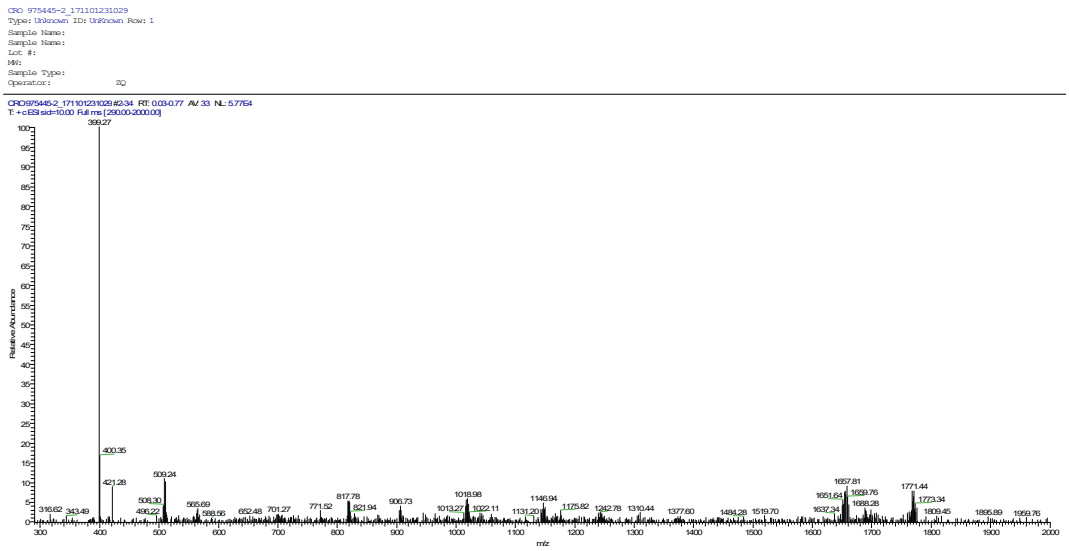


Figure S6. The mass spectrum (ESI) of **1** in MeOH.

8. UV-vis spectra of H_4L and 1

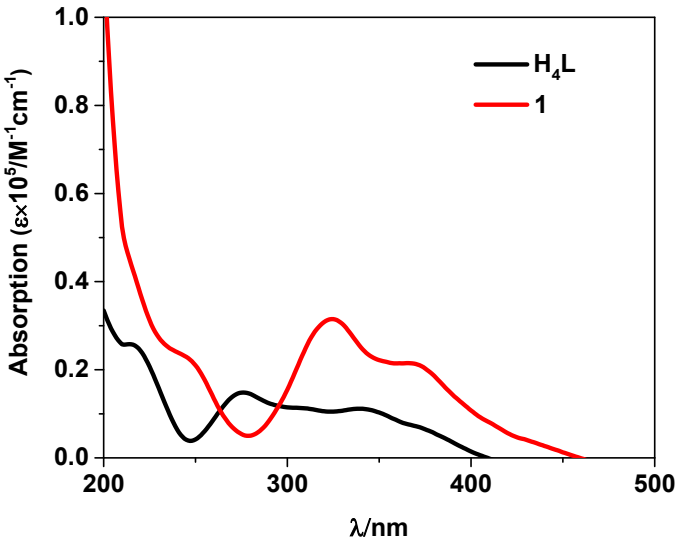


Figure S7. UV-vis absorption spectra of H_4L and **1** in CH_3CN (C = 10^{-6} mol/L).

9. The NIR luminescence lifetime of 1

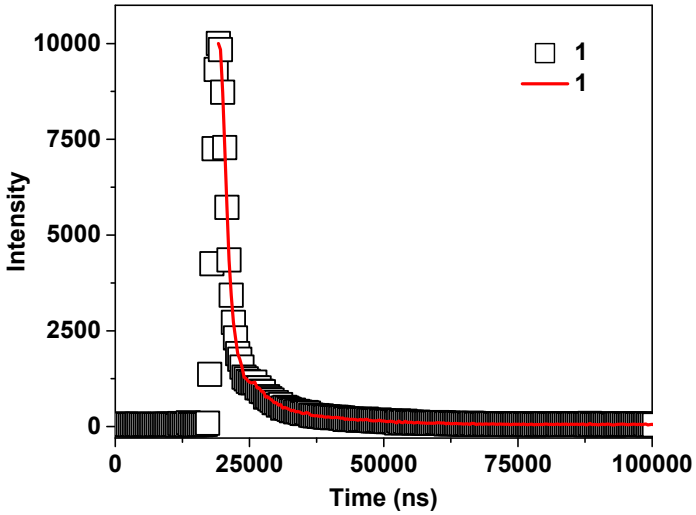
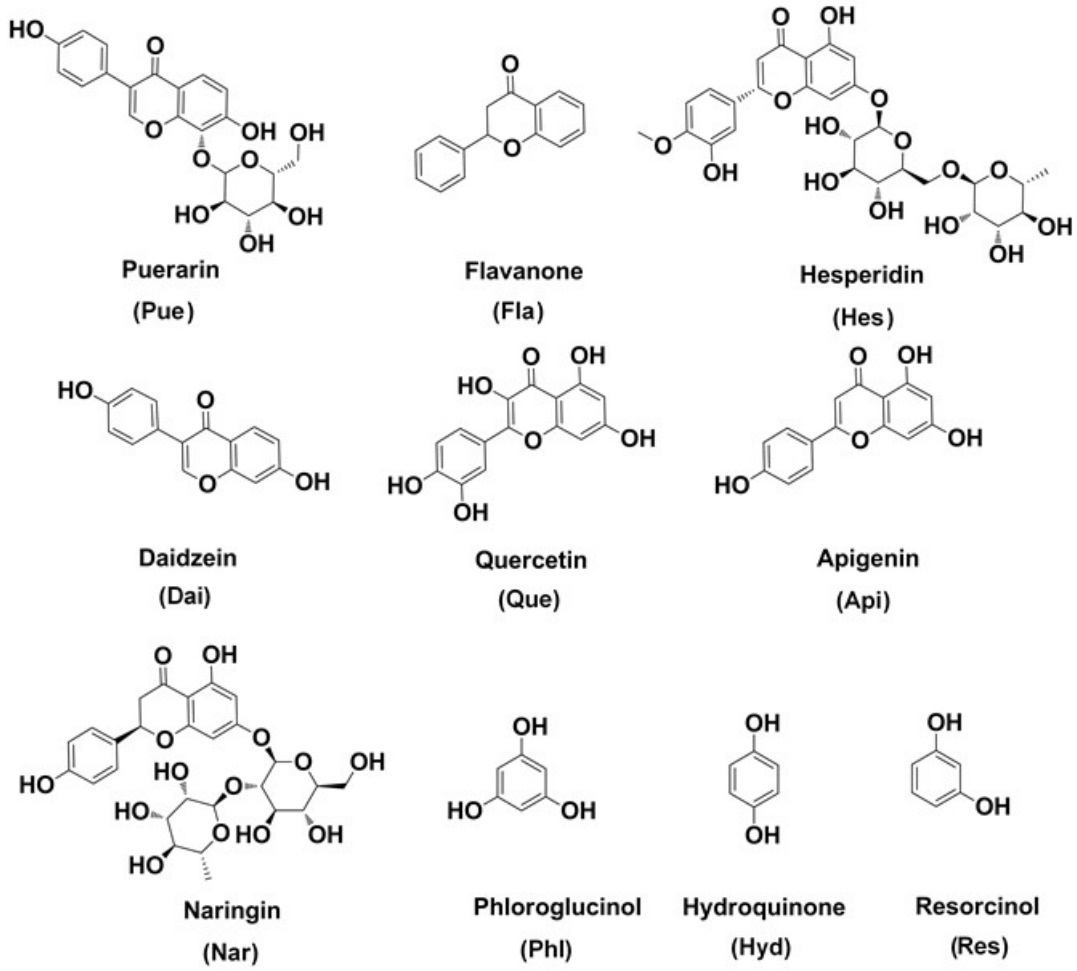


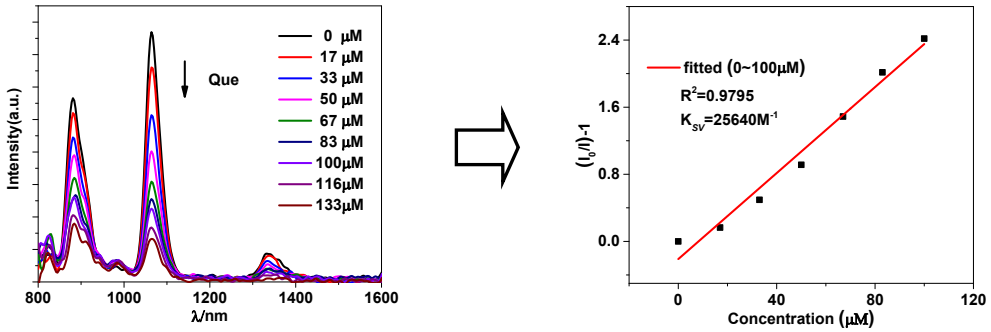
Figure S8. The NIR luminescence lifetime of **1** (30 μM) in CH_3CN.

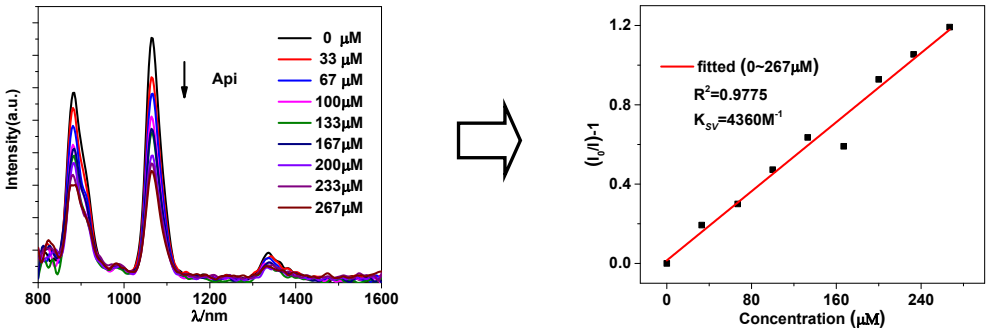
10. Chemical structures of Que and biomolecules

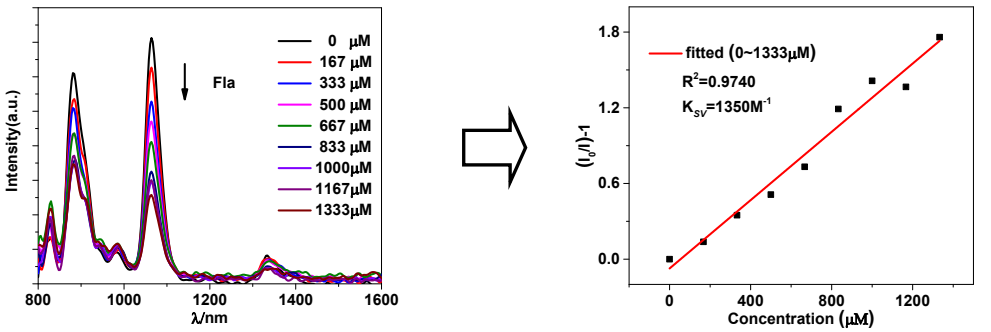


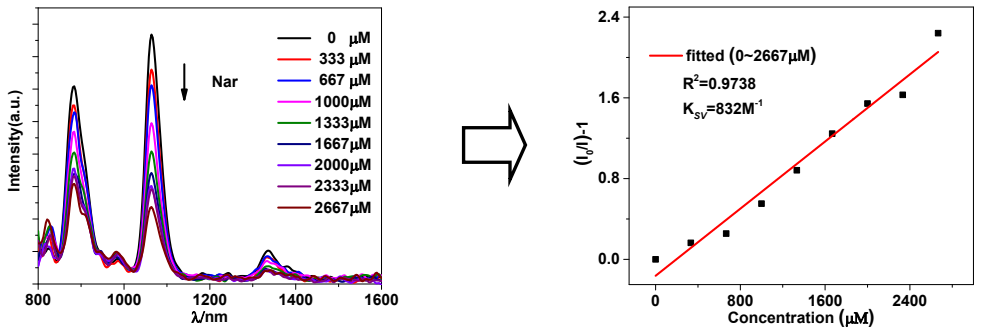
Scheme S1. Chemical structures of Que and biomolecules.

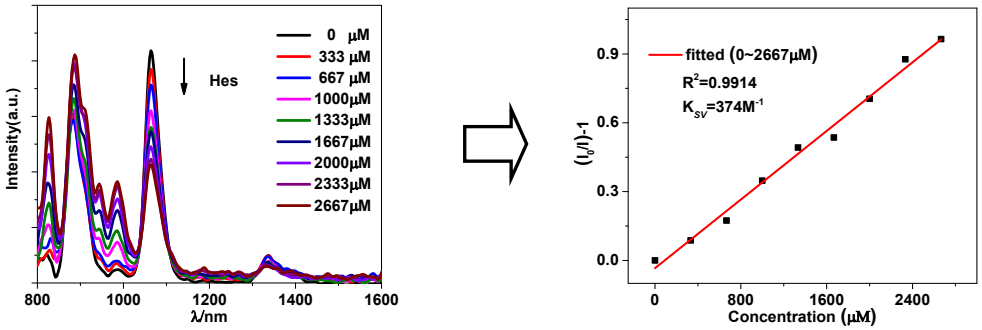
11. NIR luminescent sensing of 1 to Que and biomolecules

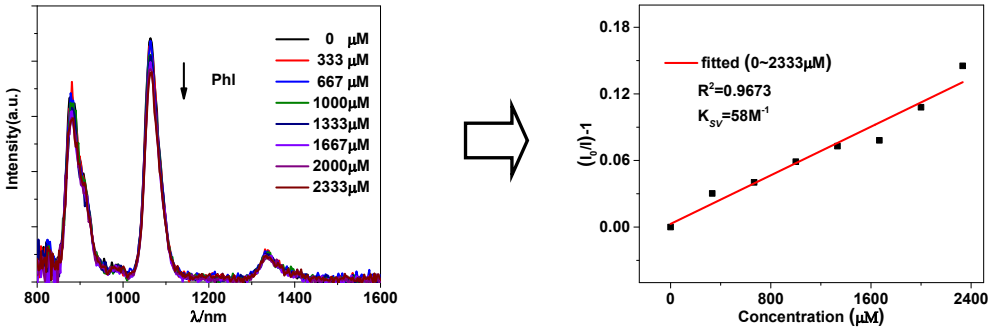


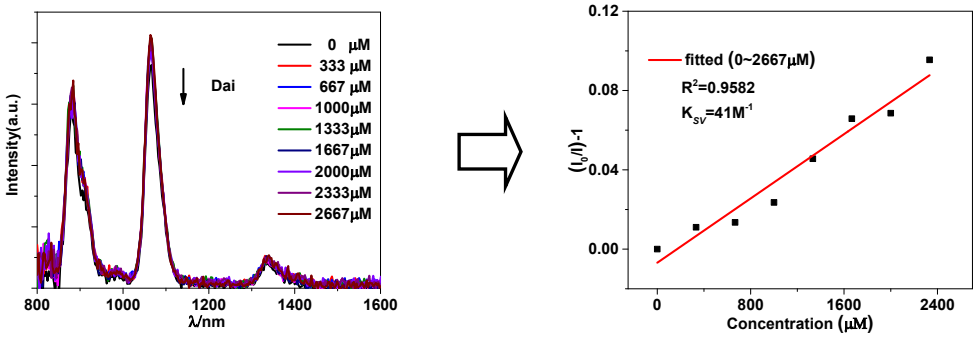


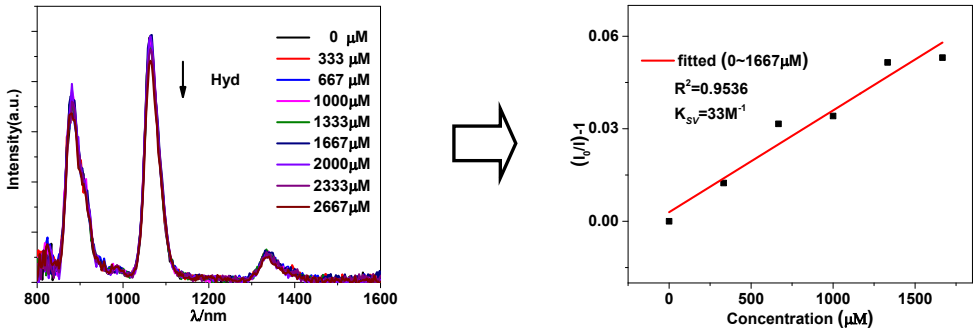





Intensity(a.u.)
λ/nm
Hes
0 μM
333 μM
667 μM
1000μM
1333μM
1667μM
2000μM
2333μM
2667μM
fitted (0~2667μM)
R²=0.9914
K_SV=374M⁻¹
(I₀/I)-1
Concentration (μM)


Intensity(a.u.)
λ/nm
Phl
0 μM
333 μM
667 μM
1000μM
1333μM
1667μM
2000μM
2333μM
fitted (0~2333μM)
R²=0.9673
K_SV=58M⁻¹
(I₀/I)-1
Concentration (μM)


Intensity(a.u.)
λ/nm
Dai
0 μM
333 μM
667 μM
1000μM
1333μM
1667μM
2000μM
2333μM
2667μM
fitted (0~2667μM)
R²=0.9582
K_SV=41M⁻¹
(I₀/I)-1
Concentration (μM)


Intensity(a.u.)
λ/nm
Hyd
0 μM
333 μM
667 μM
1000μM
1333μM
1667μM
2000μM
2333μM
2667μM
fitted (0~1667μM)
R²=0.9536
K_SV=33M⁻¹
(I₀/I)-1
Concentration (μM)

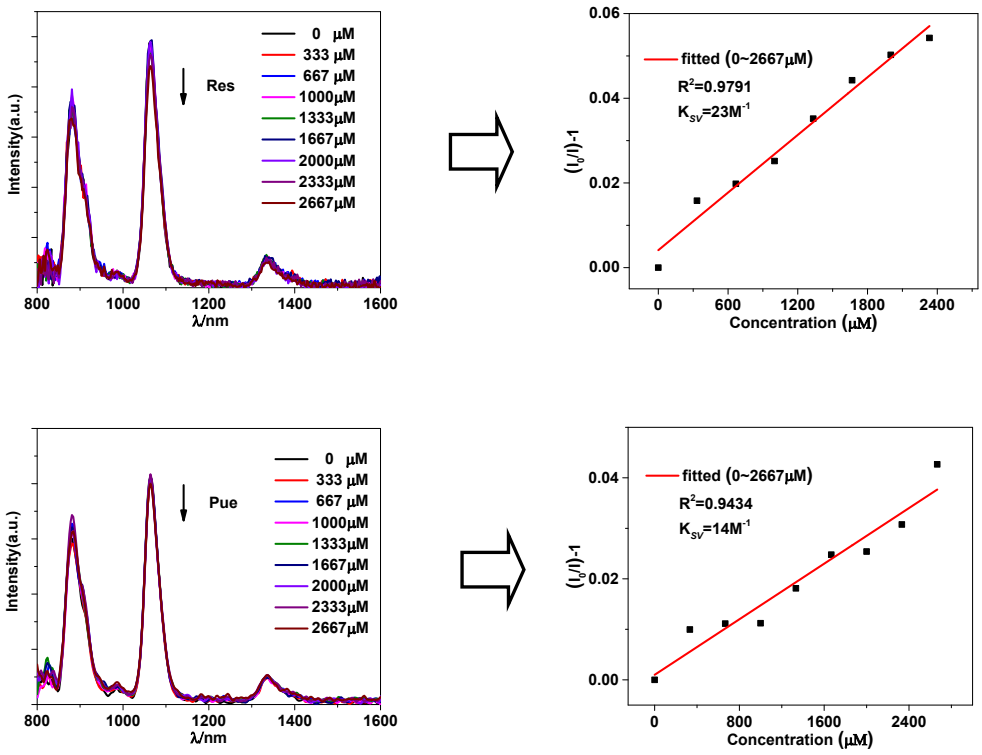


Figure S9. NIR luminescent sensing of **1** (30 μM) to Que and biomolecules in CH_3CN (λ_{ex} = 370 nm).

12. The visible emission response of 1 to Que

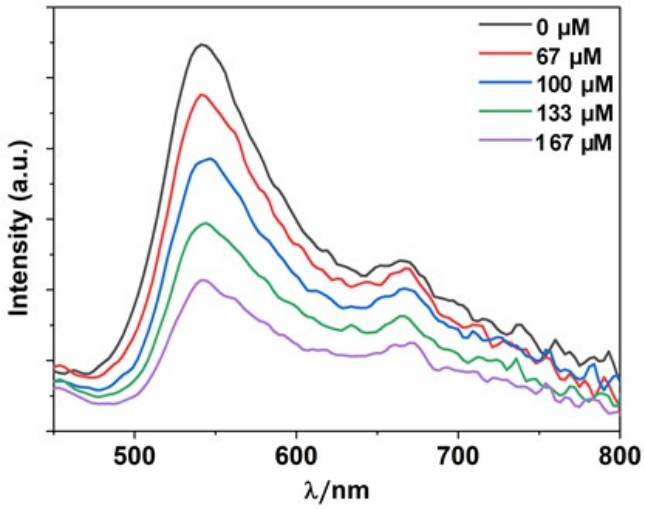


Figure S10. The quenching of visible ligand-centered emission of **1** (30 μM) to the addition of Que with different concentrations in CH_3CN.

13. X-Ray Crystallography

Table S1. Selected bond lengths (Å) and angles (°) for **1**.

Nd(1)-O(22)	2.28(3)	Zn(6)-O(17)	1.98(2)
Nd(1)-O(6)	2.31(2)	Zn(6)-O(21)	1.98(2)
Nd(1)-O(20)	2.34(2)	Zn(6)-N(8)	2.07(3)
Nd(1)-O(7)	2.355(18)	Zn(6)-O(19)	2.08(2)
Nd(1)-O(19)	2.384(19)	Zn(6)-N(7)	2.14(3)
Nd(1)-O(25)	2.37(3)	O(22)-Nd(1)-O(6)	85.2(9)
Nd(1)-O(10)	2.408(18)	O(22)-Nd(1)-O(20)	143.3(8)
Nd(1)-O(9)	2.460(17)	O(6)-Nd(1)-O(20)	99.3(7)
Nd(1)-C(83)	3.09(3)	O(22)-Nd(1)-O(7)	135.1(8)
Nd(2)-O(15)	2.31(2)	O(6)-Nd(1)-O(7)	67.2(7)
Nd(2)-O(1)	2.335(18)	O(20)-Nd(1)-O(7)	78.2(6)
Nd(2)-O(24)	2.34(2)	O(22)-Nd(1)-O(19)	77.8(8)
Nd(2)-O(11)	2.356(19)	O(6)-Nd(1)-O(19)	87.8(7)
Nd(2)-O(14)	2.43(2)	O(20)-Nd(1)-O(19)	66.1(6)
Nd(2)-O(2)	2.427(19)	O(7)-Nd(1)-O(19)	132.4(7)
Nd(2)-O(26)	2.47(2)	O(22)-Nd(1)-O(25)	72.3(9)
Nd(2)-O(12)	2.52(2)	O(6)-Nd(1)-O(25)	89.6(8)
Zn(1)-O(4)	2.01(2)	O(20)-Nd(1)-O(25)	143.6(8)
Zn(1)-O(23)	1.99(2)	O(7)-Nd(1)-O(25)	72.8(8)
Zn(1)-O(2)	2.033(19)	O(19)-Nd(1)-O(25)	150.0(8)
Zn(1)-N(1)	2.06(3)	O(22)-Nd(1)-O(10)	80.4(8)
Zn(1)-N(2)	2.18(3)	O(6)-Nd(1)-O(10)	162.9(7)
Zn(2)-O(11)	1.94(2)	O(20)-Nd(1)-O(10)	87.1(6)
Zn(2)-O(20)	1.96(2)	O(7)-Nd(1)-O(10)	129.8(7)
Zn(2)-O(5)	2.024(17)	O(19)-Nd(1)-O(10)	80.2(7)
Zn(2)-O(4)	2.06(2)	O(25)-Nd(1)-O(10)	94.7(7)
Zn(3)-O(7)	1.97(2)	O(22)-Nd(1)-O(9)	130.1(8)
Zn(3)-N(4)	1.99(3)	O(6)-Nd(1)-O(9)	133.4(7)
Zn(3)-O(5)	2.019(17)	O(20)-Nd(1)-O(9)	71.0(7)
Zn(3)-O(9)	2.056(18)	O(7)-Nd(1)-O(9)	66.2(6)
Zn(3)-N(3)	2.08(2)	O(19)-Nd(1)-O(9)	124.4(6)
Zn(4)-O(14)	1.96(2)	O(25)-Nd(1)-O(9)	77.3(7)
Zn(4)-O(16)	2.00(2)	O(10)-Nd(1)-O(9)	63.6(6)
Zn(4)-O(12)	2.024(19)	O(15)-Nd(2)-O(1)	97.5(7)
Zn(4)-N(6)	2.03(2)	O(15)-Nd(2)-O(24)	81.8(8)
Zn(4)-N(5)	2.06(2)	O(1)-Nd(2)-O(24)	142.3(8)
Zn(5)-O(10)	1.907(17)	O(15)-Nd(2)-O(11)	163.1(7)
Zn(5)-O(1)	1.965(17)	O(1)-Nd(2)-O(11)	90.1(7)
Zn(5)-O(16)	2.05(2)	O(24)-Nd(2)-O(11)	83.0(8)
Zn(5)-O(17)	2.09(2)	O(15)-Nd(2)-O(14)	67.6(8)

O(1)-Nd(2)-O(14)	82.6(7)	O(7)-Zn(3)-N(4)	138.3(10)
O(24)-Nd(2)-O(14)	129.7(9)	O(7)-Zn(3)-O(5)	108.4(8)
O(11)-Nd(2)-O(14)	128.6(7)	N(4)-Zn(3)-O(5)	112.6(9)
O(15)-Nd(2)-O(2)	88.1(7)	O(7)-Zn(3)-O(9)	81.7(7)
O(1)-Nd(2)-O(2)	67.0(7)	N(4)-Zn(3)-O(9)	90.2(9)
O(24)-Nd(2)-O(2)	75.3(8)	O(5)-Zn(3)-O(9)	90.2(7)
O(11)-Nd(2)-O(2)	80.9(7)	O(7)-Zn(3)-N(3)	89.7(8)
O(14)-Nd(2)-O(2)	138.4(8)	N(4)-Zn(3)-N(3)	79.8(10)
O(15)-Nd(2)-O(26)	96.6(8)	O(5)-Zn(3)-N(3)	116.0(8)
O(1)-Nd(2)-O(26)	147.4(7)	O(9)-Zn(3)-N(3)	153.8(9)
O(24)-Nd(2)-O(26)	69.0(8)	O(14)-Zn(4)-O(16)	111.6(10)
O(11)-Nd(2)-O(26)	84.7(8)	O(14)-Zn(4)-O(12)	82.3(9)
O(14)-Nd(2)-O(26)	75.9(8)	O(16)-Zn(4)-O(12)	89.5(8)
O(2)-Nd(2)-O(26)	142.8(7)	O(14)-Zn(4)-N(6)	86.3(10)
O(15)-Nd(2)-O(12)	131.3(7)	O(16)-Zn(4)-N(6)	118.3(9)
O(1)-Nd(2)-O(12)	72.3(6)	O(12)-Zn(4)-N(6)	152.2(9)
O(24)-Nd(2)-O(12)	134.8(8)	O(14)-Zn(4)-N(5)	135.2(10)
O(11)-Nd(2)-O(12)	65.4(6)	O(16)-Zn(4)-N(5)	112.3(9)
O(14)-Nd(2)-O(12)	64.0(7)	O(12)-Zn(4)-N(5)	89.7(9)
O(2)-Nd(2)-O(12)	126.3(7)	N(6)-Zn(4)-N(5)	80.7(9)
O(26)-Nd(2)-O(12)	76.4(7)	O(10)-Zn(5)-O(1)	129.2(8)
O(4)-Zn(1)-O(23)	114.5(9)	O(10)-Zn(5)-O(16)	116.6(8)
O(4)-Zn(1)-O(2)	95.0(8)	O(1)-Zn(5)-O(16)	108.7(9)
O(23)-Zn(1)-O(2)	104.4(9)	O(10)-Zn(5)-O(17)	100.1(8)
O(4)-Zn(1)-N(1)	140.0(10)	O(1)-Zn(5)-O(17)	106.4(8)
O(23)-Zn(1)-N(1)	102.1(11)	O(16)-Zn(5)-O(17)	84.1(8)
O(2)-Zn(1)-N(1)	90.7(10)	O(17)-Zn(6)-O(21)	103.6(9)
O(4)-Zn(1)-N(2)	84.6(9)	O(17)-Zn(6)-N(8)	143.0(9)
O(23)-Zn(1)-N(2)	94.2(10)	O(21)-Zn(6)-N(8)	110.3(10)
O(2)-Zn(1)-N(2)	159.6(10)	O(17)-Zn(6)-O(19)	96.7(8)
N(1)-Zn(1)-N(2)	77.0(11)	O(21)-Zn(6)-O(19)	106.7(8)
O(11)-Zn(2)-O(20)	128.2(8)	N(8)-Zn(6)-O(19)	87.6(9)
O(11)-Zn(2)-O(5)	113.4(8)	O(17)-Zn(6)-N(7)	85.8(10)
O(20)-Zn(2)-O(5)	110.5(8)	O(21)-Zn(6)-N(7)	94.4(10)
O(11)-Zn(2)-O(4)	101.7(8)	N(8)-Zn(6)-N(7)	77.4(10)
O(20)-Zn(2)-O(4)	109.2(8)	O(19)-Zn(6)-N(7)	157.4(9)
O(5)-Zn(2)-O(4)	83.7(8)		