Electronic Supplementary Information

A visible-light-gated donor–acceptor Stenhouse adducts chemosensor: Synthesis, photochromism and naked-eye colorimetric/fluorimetric sensing for Al^{3+} and Zn^{2+}

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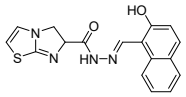
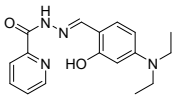
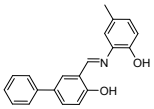
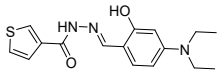
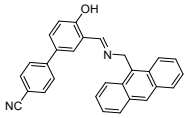
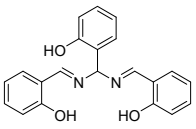
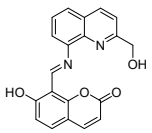
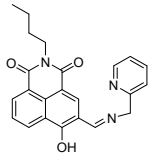
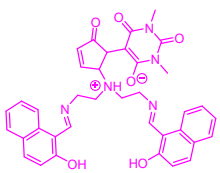
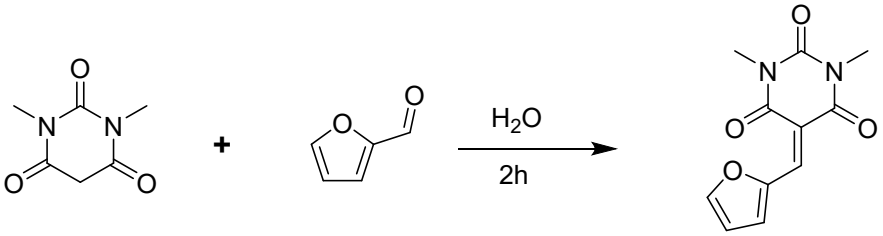
Section 1. Reported dual chemosensors for Al^{3+} & Zn^{2+} ions.

Table S1 Few parameters of dual chemosensors for Al^{3+} & Zn^{2+} ions.

Compound structure	Analyte	Detection Method	Solvent system	Reversibility	LOD(M)	Mechanism	Ref.
	Al^{3+}/Zn^{2+}	Fluorimetric	MeOH/H_2O	yes	$1.45\times10^{-7}(Al^{3+})$ $1.29\times10^{-7}(Zn^{2+})$	CHEF, C=N isomerizatin	40
	Al^{3+}/Zn^{2+}	Fluorimetric	MeOH/H_2O	-	$8.30\times10^{-8}(Al^{3+})$ $1.24\times10^{-7}(Zn^{2+})$	ESIPT	19
	Al^{3+}/Zn^{2+}	Fluorimetic	MeOH/H_2O	-	$2.24\times10^{-7}(Al^{3+})$ $4.10\times10^{-8}(Zn^{2+})$	ESIPT, C=N isomerization	41
	Al^{3+}/Zn^{2+}	Colorimetric Fluorimetric	DMSO/H_2O	-	$3.70\times10^{-9}(Al^{3+})$ $3.00\times10^{-8}(Zn^{2+})$	CHEF	18
	Al^{3+}/Zn^{2+}	Fluorimetric	EtOH/H_2O	-	$7.88\times10^{-8}(Al^{3+})$ $5.22\times10^{-8}(Zn^{2+})$	PET, C = N isomerization	42
	Al^{3+}/Zn^{2+}	Fluorimetric	MeOH	-	$1.00\times10^{-7}(Al^{3+})$ $4.98\times10^{-8}(Zn^{2+})$	CHEF, PET	43
	Al^{3+}/Zn^{2+}	Fluorimetric	MeOH/H_2O	-	$1.14\times10^{-8}(Al^{3+})$ $3.75\times10^{-8}(Zn^{2+})$	ICT	44
	Al^{3+}/Zn^{2+}	Fluorimetric	CH_3CN/H_2O	yes	$1.44\times10^{-5}(Al^{3+})$ $7.40\times10^{-5}(Zn^{2+})$	CHEF	45
	Al^{3+}/Zn^{2+}	Colorimetric Fluorimetric	DMSO	yes	$3.65\times10^{-7}(Al^{3+})$ $1.00\times10^{-7}(Zn^{2+})$	CHEF, PET	**This work**

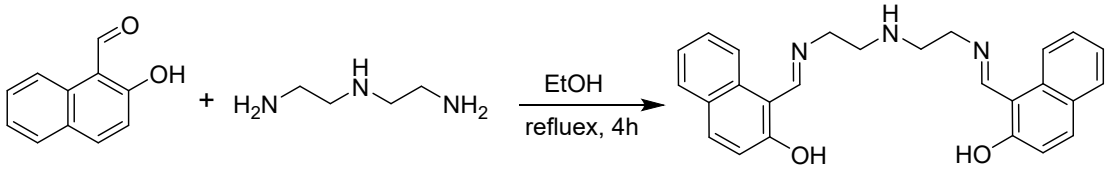
Section 2. Compound characterization

1. Synthesis of **1**



5-(furan-2-ylmethylene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-tone (1.56 g, 10 mmol) and 2-formaldehyde (1.15 g, 12 mmol) were put into 40 mL water in turn. The reaction solution was churned at 298K for 2 h. Thin Layer Chromatography (TLC) was employed to monitor the reaction. And yellow precipitates were collected by vacuum filtration. The filtered product was dissolved in (60mL) dichloromethane and washed successively with 30 mL saturated aqueous $NaHCO_3$, 30 mL H_2O and 30 mL saturated aqueous NaCl. The organic layers were combined and dried with anhydrous Na_2SO_4. Finally, filtration and rotary evaporation gave 2.19 g (90%) of **1** as a bright yellow powder.

2. Synthesis of **2**



2-hydroxy naphthaldehyde (1.00 g, 5.81 mmol) was added to 40mL methanol, and the mixture was dissolved with stirring at 323K. Then diethylenetriamine (0.314 mL, 2.91 mmol) was added to the reaction solution. The reflux reaction was continued for 4h and a yellow residue was formed. The crude product was recrystallized from methanol to obtain a pure product. Yield: 82% (1.28 g).

3. ^{1}H NMR spectra, ^{13}C NMR and HRMS spectra

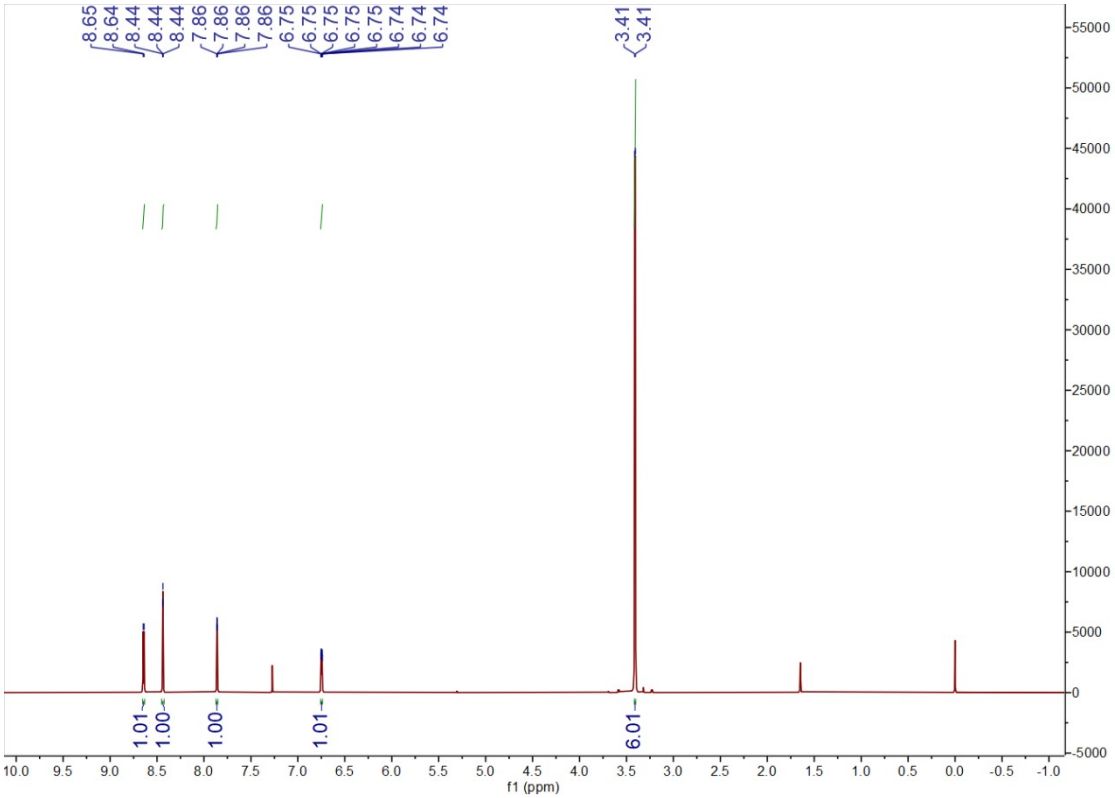


Fig. S1 ^{1}H NMR spectrum of compound **1**

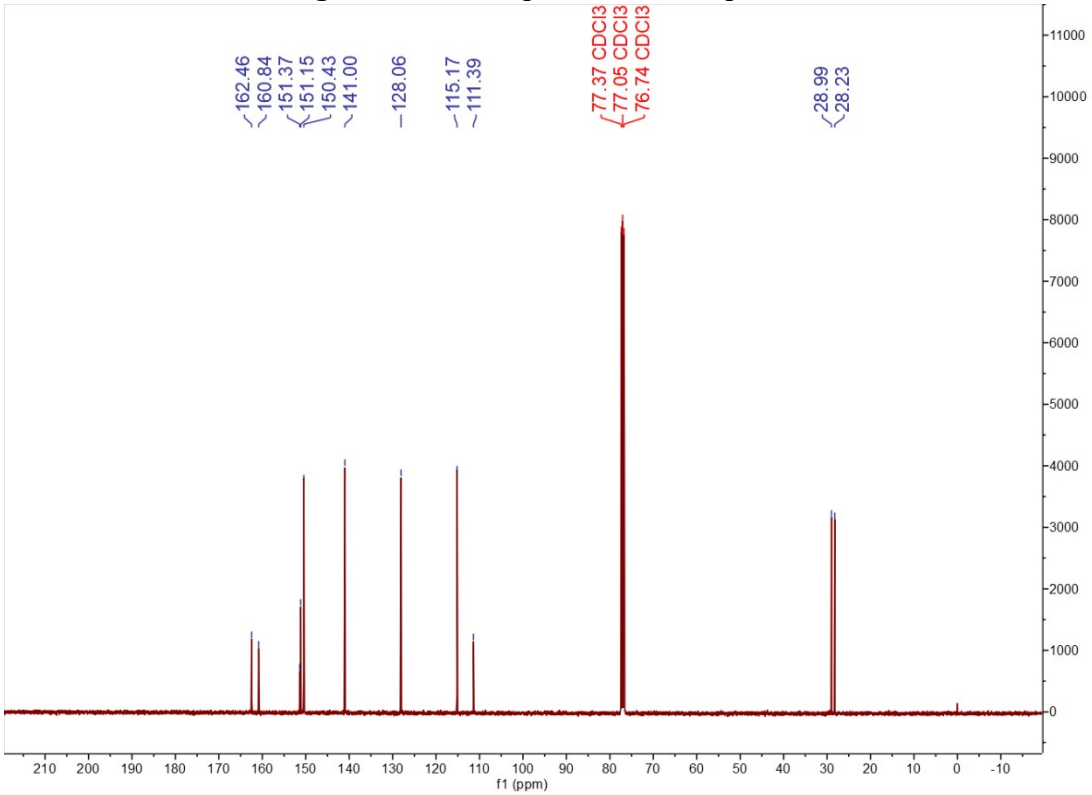


Fig. S2 ^{13}C NMR spectrum of compound **1**

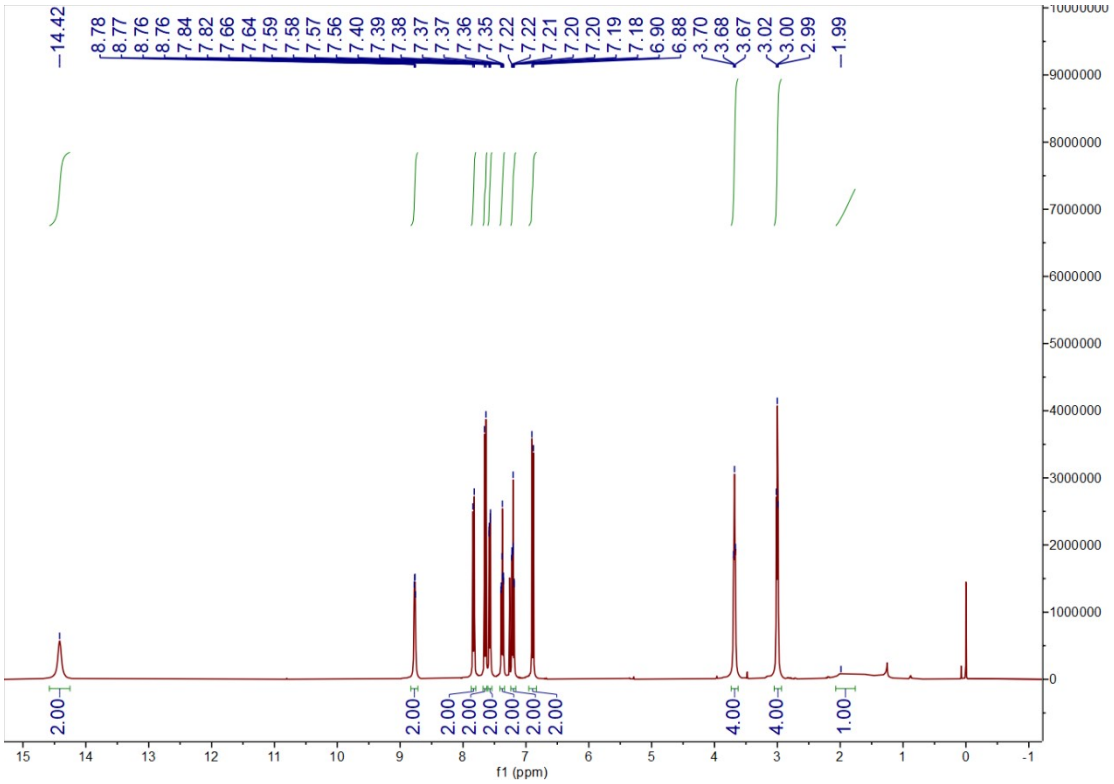


Fig. S3 ^{1}H NMR spectrum of compound **2**

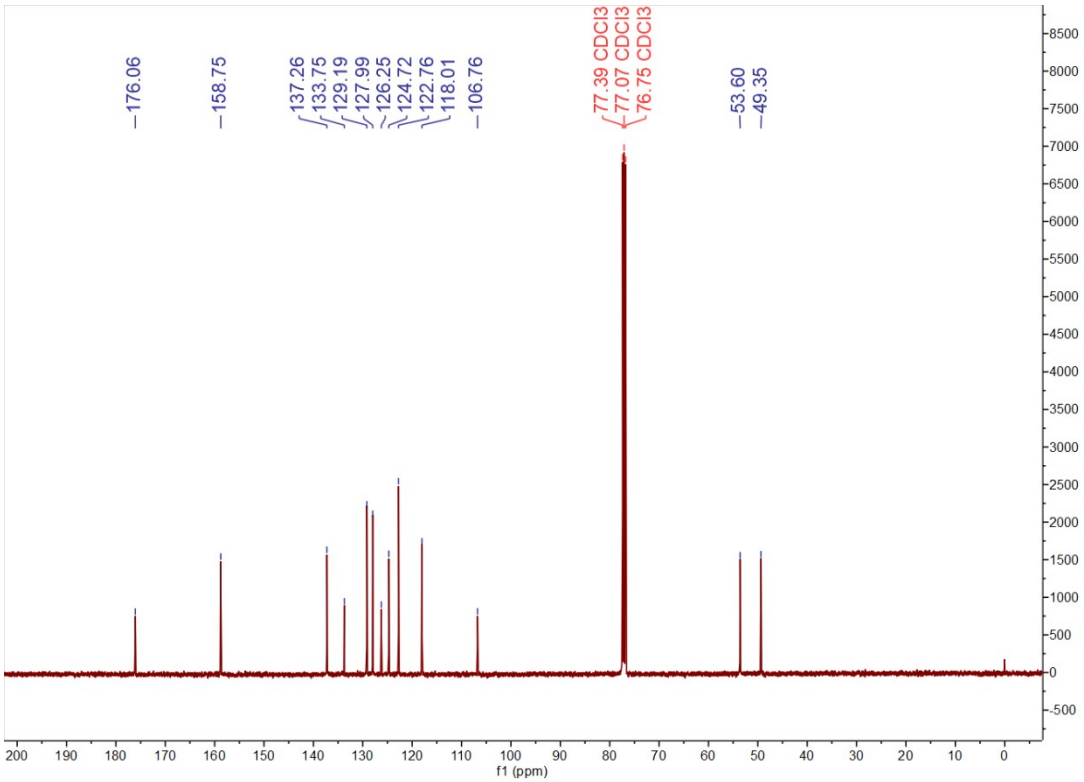


Fig. S4 C^{13} NMR spectrum of compound **2**

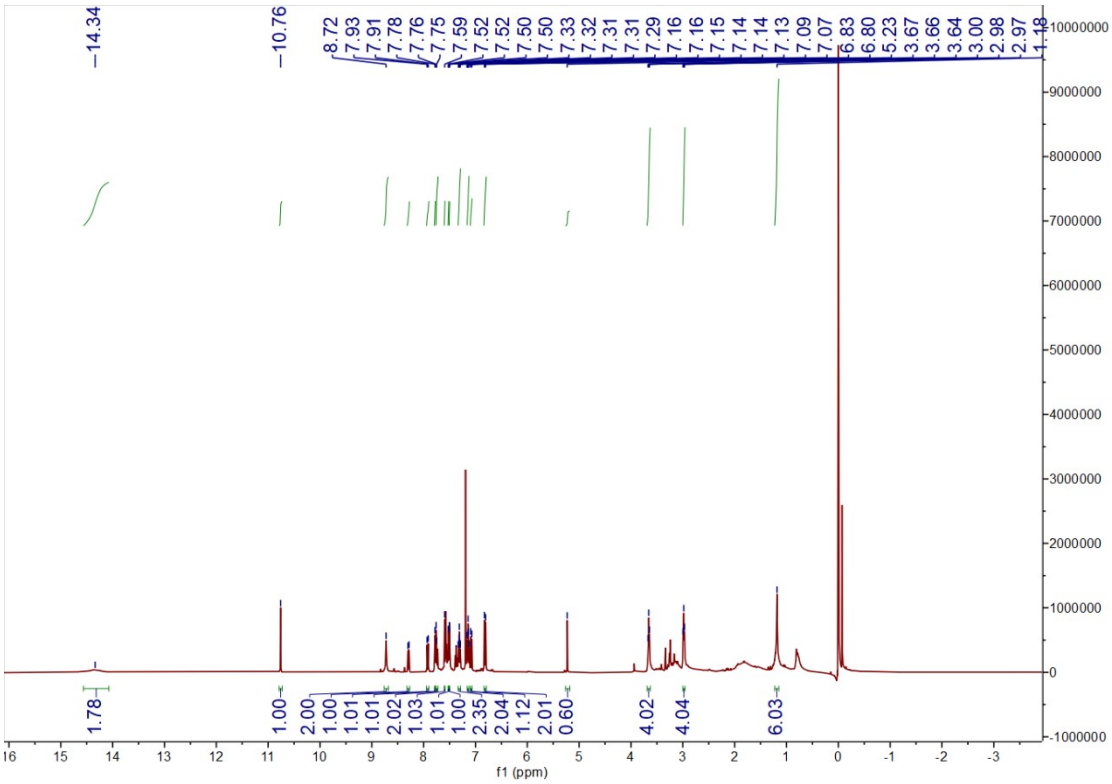


Fig. S5 ^{1}H NMR spectrum of **ND-O**

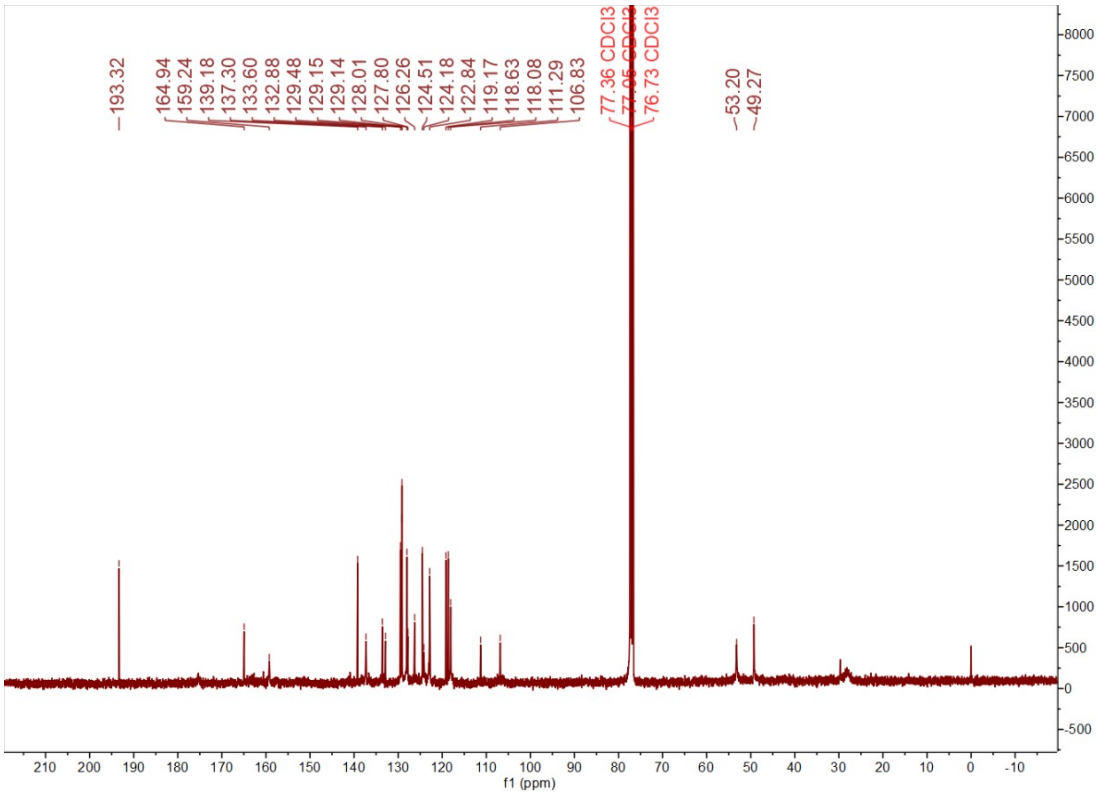


Fig. S6 C^{13} NMR spectrum of **ND-O**

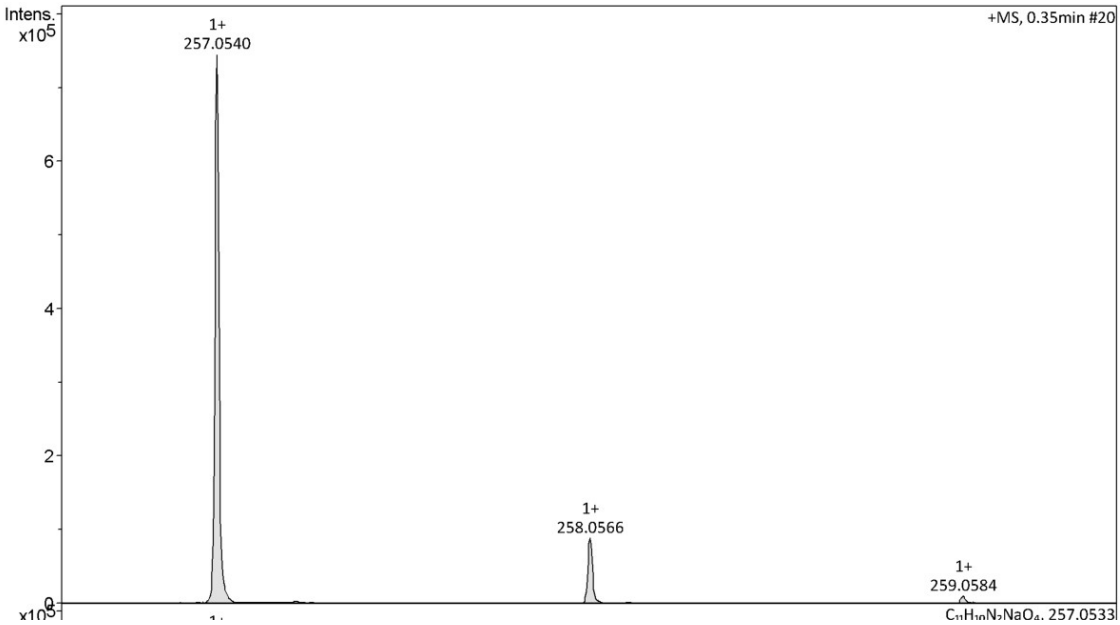


Fig. S7 HRMS spectrum of compound **1**

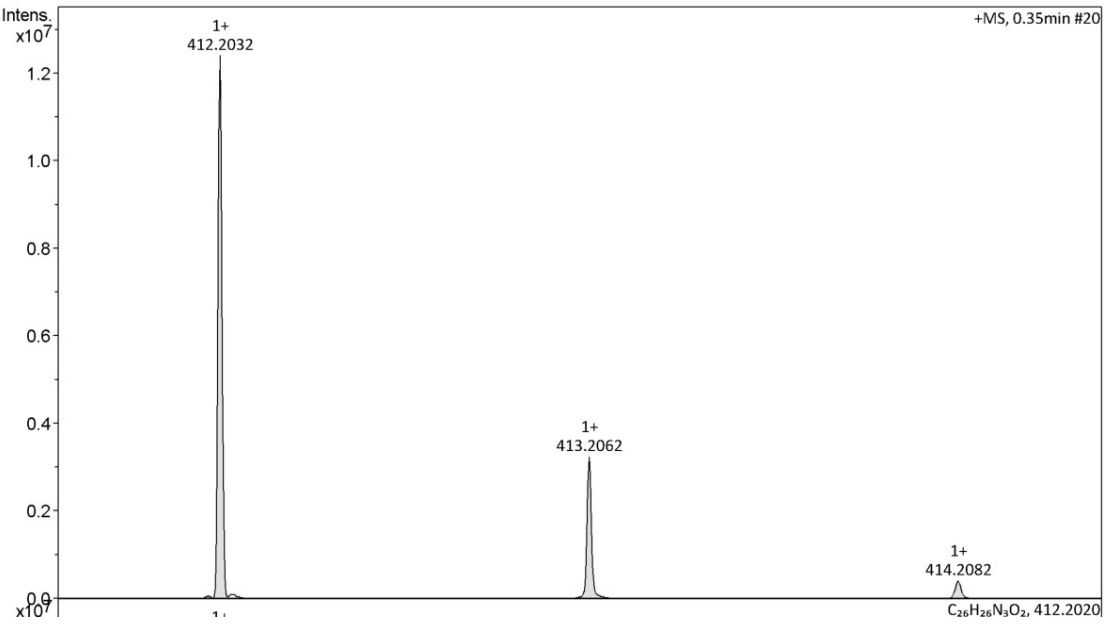


Fig. S8 HRMS spectrum of compound **2**

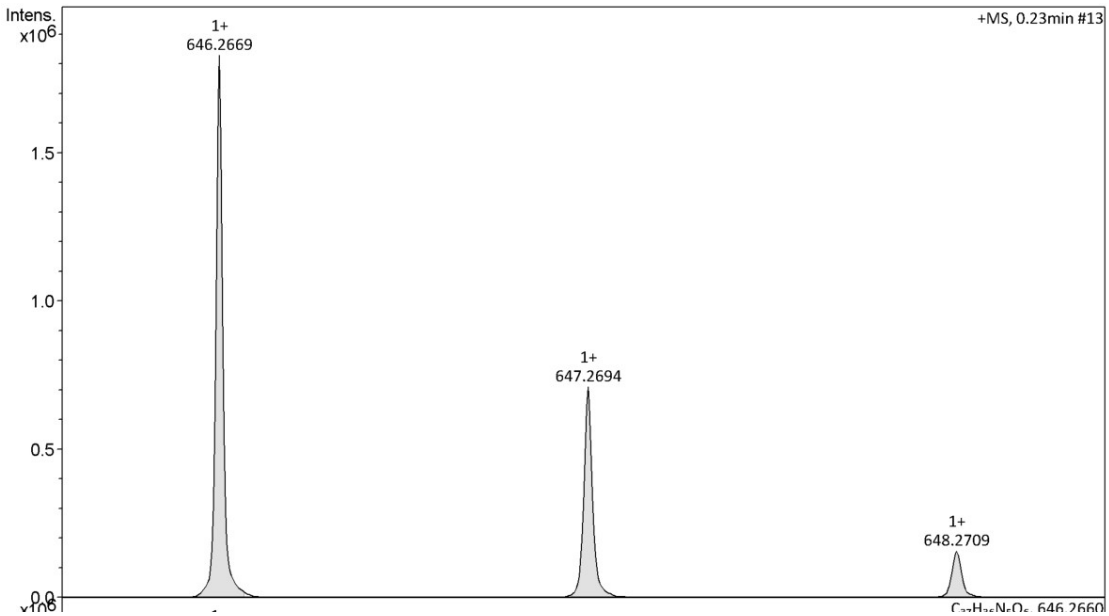


Fig. S9 HRMS spectrum of **ND-O**

Section 4. Photochromic properties study of ND-O

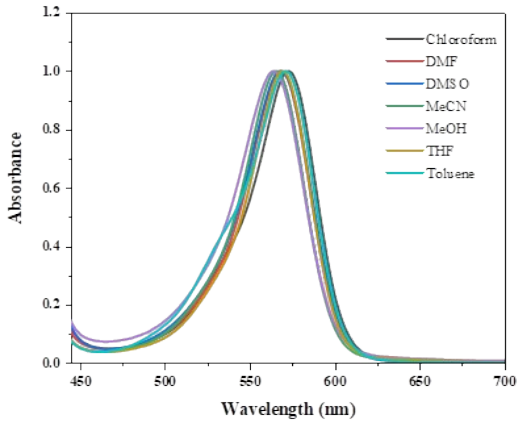


Fig. S10 The normalized UV absorption spectra of **ND-O** in various solvents

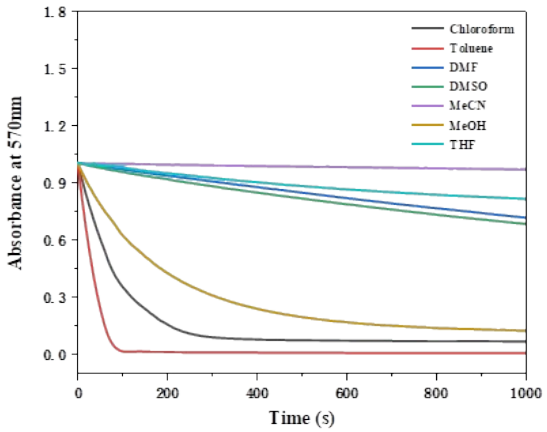


Fig. S11 The Solvent effect kinetics of **ND-O** in various solvents

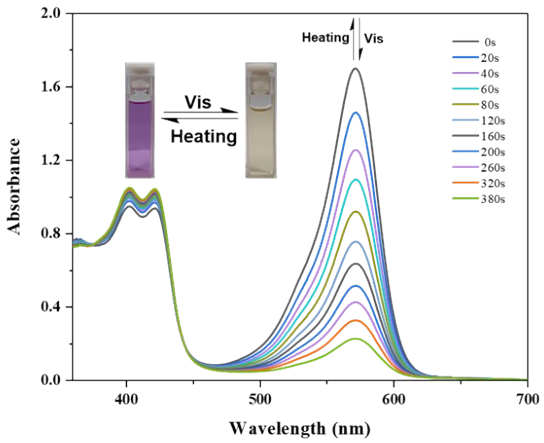


Fig. S12 The photochromism of **ND-O** in chloroform solution

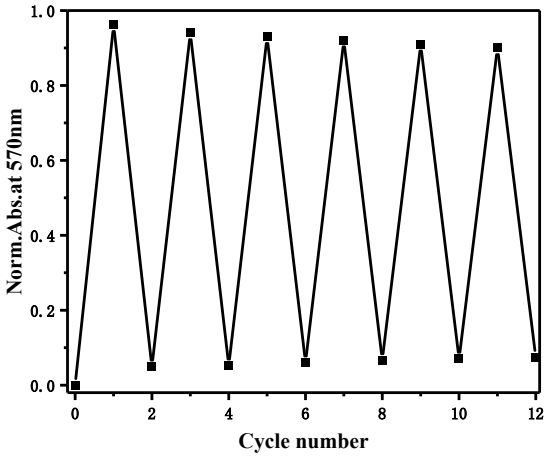


Fig. S13 The fatigue resistance ability of **ND-O**

Table S2: Fluorescence parameters of **ND-C** and **ND-C-Zn^{2+}**

Solvent (DMSO)	Quantum yield (φ)	Lifetime τ (ns)
ND-C	2.51%	5.31
ND-C-Zn^{2+}	4.49%	6.15

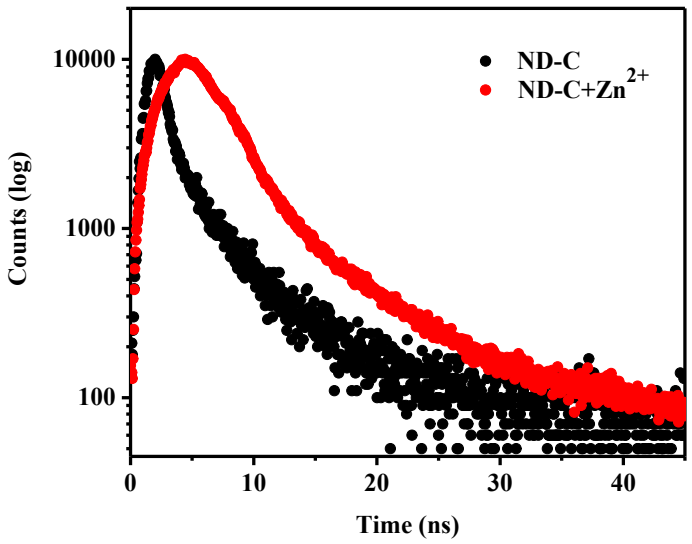


Fig. S14 Time-resolved fluorescence decay of **ND-C** and **ND-C-Zn^{2+}** (λ_{ex}= 380 nm)

Section 3. Colorimetric detection of Al^{3+} and fluorescence response of Zn^{2+}

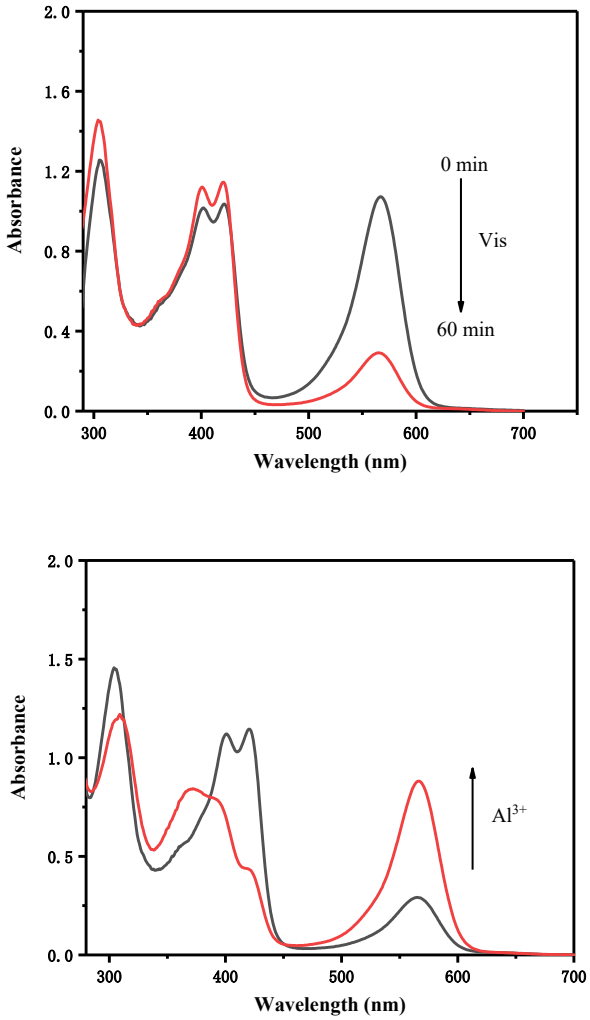
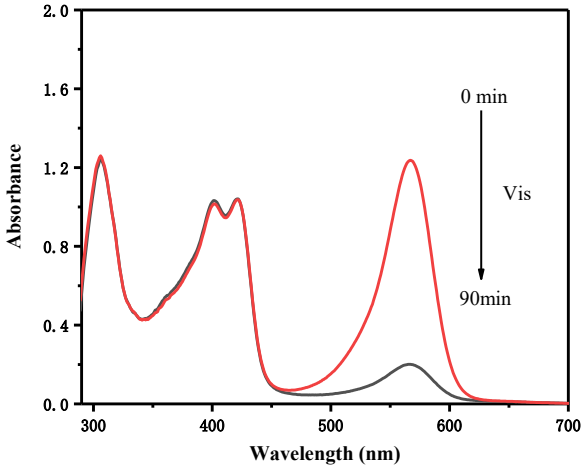


Fig. S15 The UV absorption spectra of visible light and aluminum ion added in DMF ([**ND-C**] = 0.1 mM)



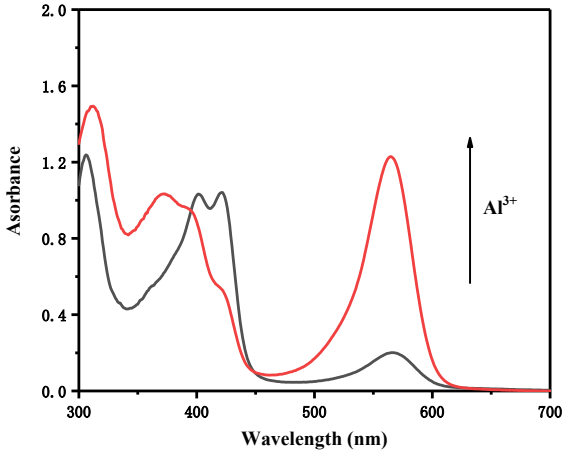
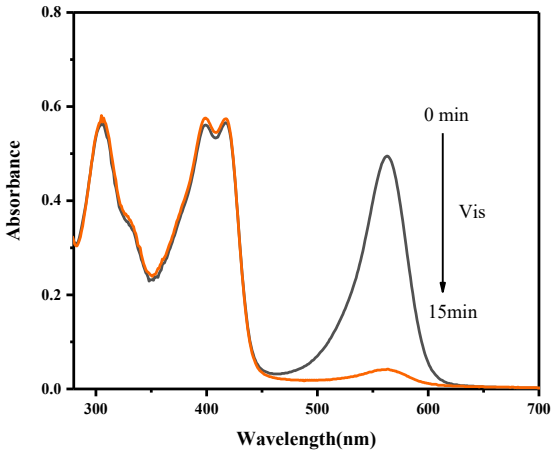


Fig. S16 The UV absorption spectra of visible light and aluminum ion added in DMSO ([**ND-C**] = 0.1 mM)



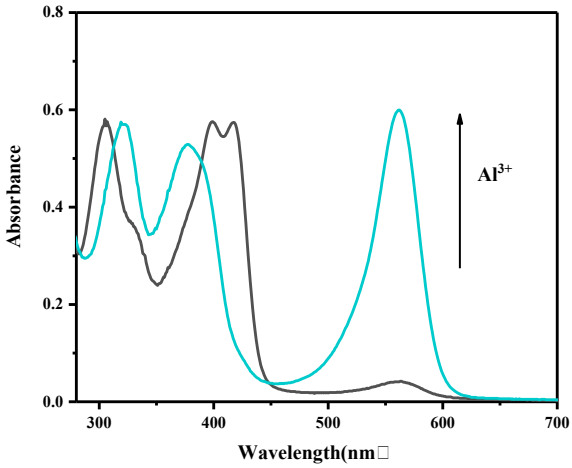


Fig. S17 The UV absorption spectra of visible light and aluminum ion added in methanol ([**ND-C**] = 0.1 mM)

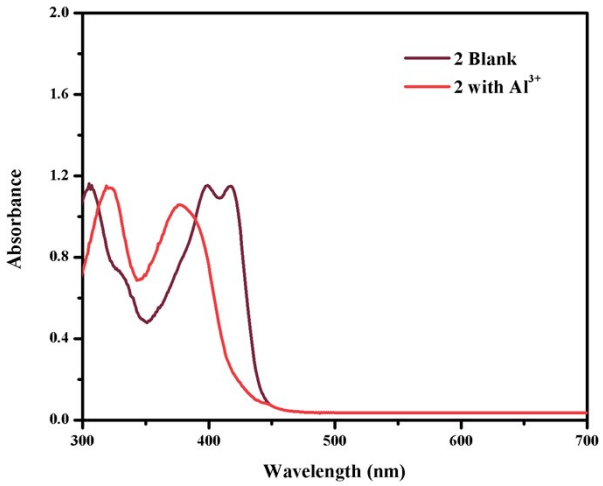


Fig. S18 The UV absorption spectra of **2** (20.0 μM) and in presence of 4eq. Al^{3+}

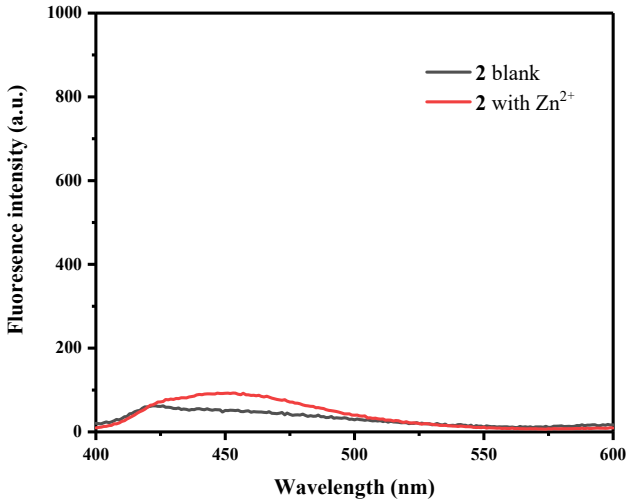


Fig. S19 Fluorescence spectra of **2** (20.0 μM) and in presence of 4eq. Zn^{2+}

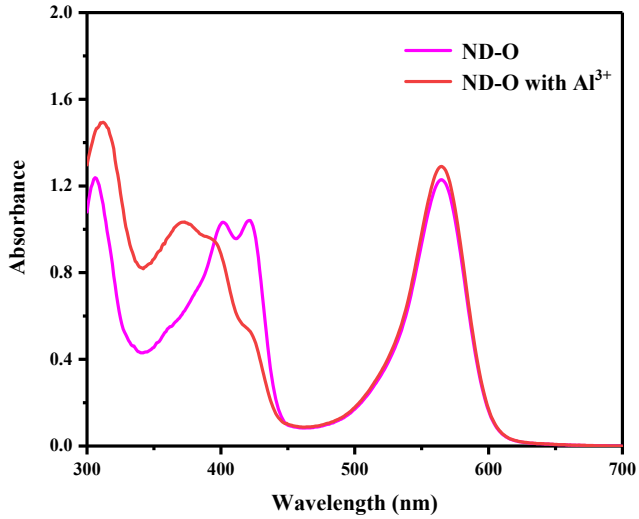


Fig. S20 The UV absorption spectra of **ND-O** (20.0 μM) and in presence of 4eq. Al^{3+}

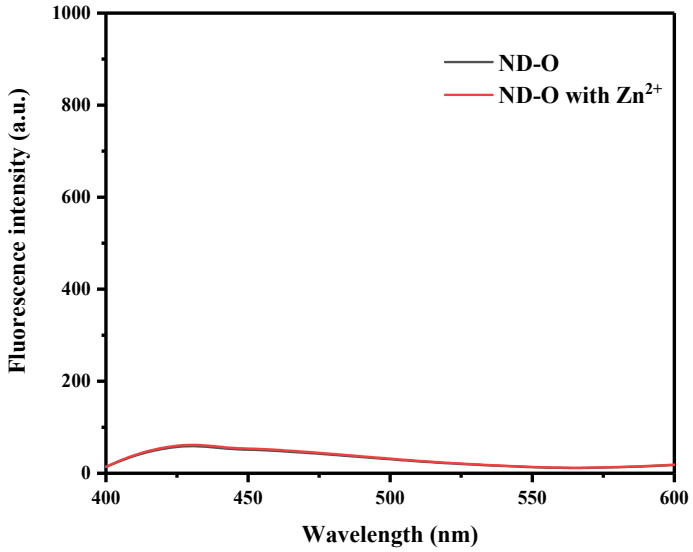


Fig. S21 Fluorescence spectra of **ND-O** (20.0 μM) and in presence of 4eq. Zn^{2+}

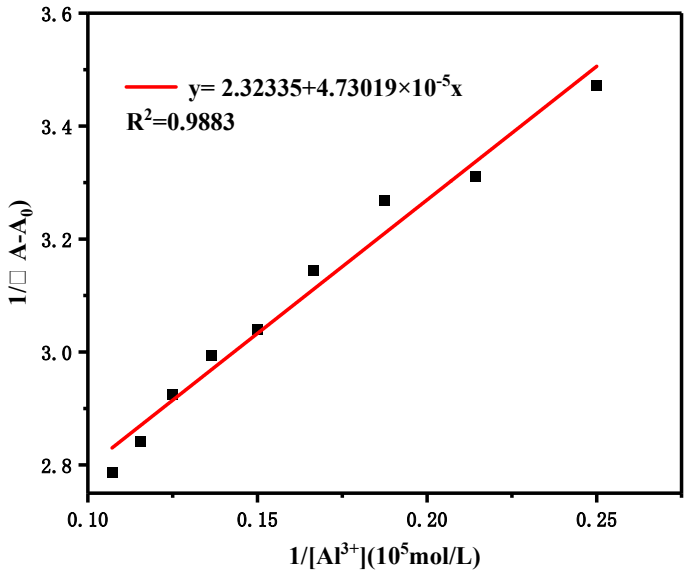


Fig. S22 Benesi–Hildebrand plot for calculation of binding constant between **ND-C** and Al^{3+}.

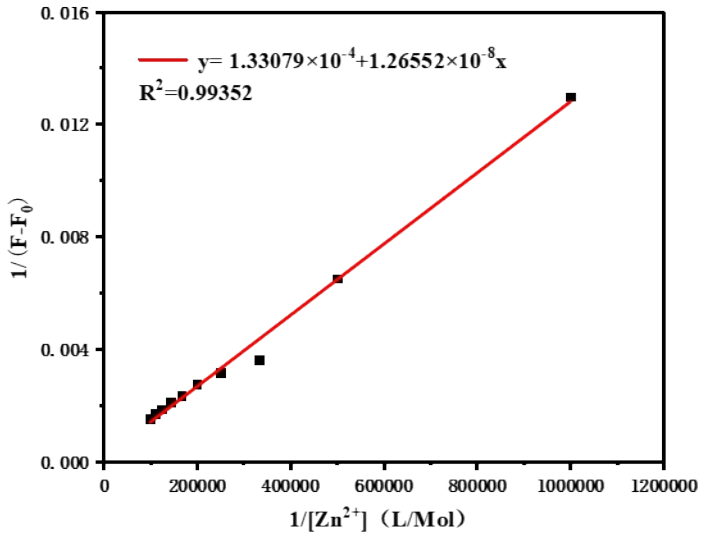


Fig. S23 Benesi-Hildebrant plot based on fluorescence intensity of **ND-C** with added Zn^{2+} concentrations in DMSO.

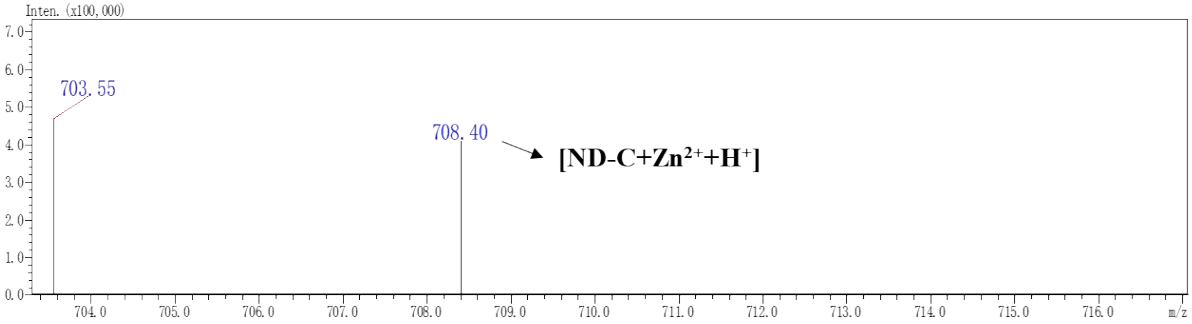


Fig. S24 ESI-MS spectra of **ND-C+Zn^{2+}**

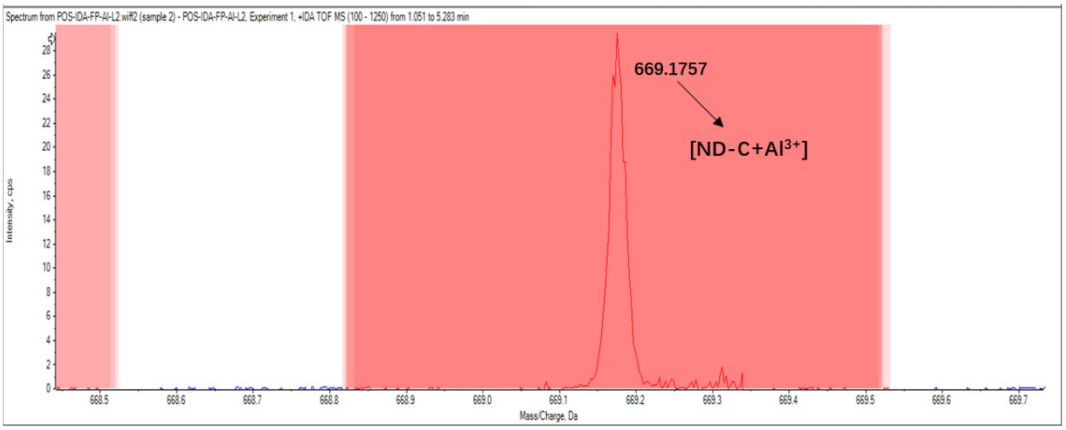


Fig. S25 HRMS spectra of **ND-C+Al^{3+}**

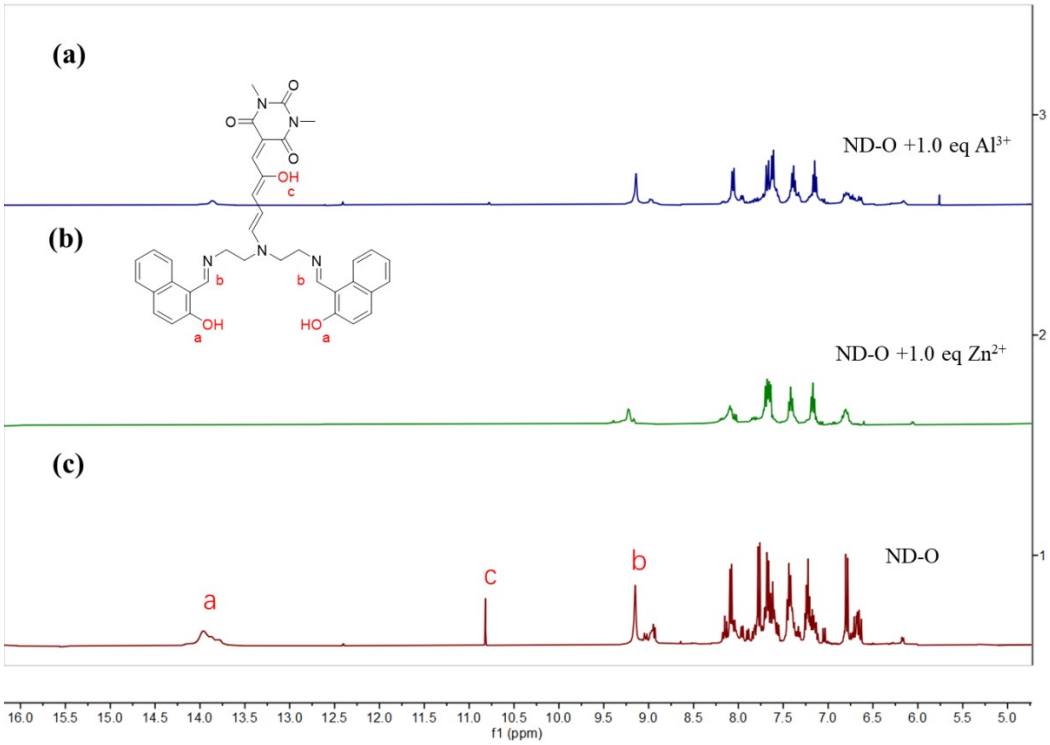


Fig. S26 ^{1}H NMR spectra in DMSO-d_6 of (a) **ND-O** in presence of 1.0 eq. Al^{3+}; (b) **ND-O** in presence of 1.0 eq. Zn^{2+}; (c) **ND-O**.

Section 5. Crystal data and structure refinement for 1 and 2

5.1 Experimental

Single crystals of $C_{11}H_{10}N_2O_4$(**1**) and $C_{26}H_{26}N_3O_2$(**2**) were measured. the suitable crystal of $C_{11}H_{10}N_2O_4$(**1**) and $C_{26}H_{26}N_3O_2$(**2**) was selected and measured on a XtaLAB Synergy R, HyPix diffractometer. The crystal was kept at 169.99(11) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

[1] Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.

[2] Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.

[3] Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

5.2 Structures of crystal 1

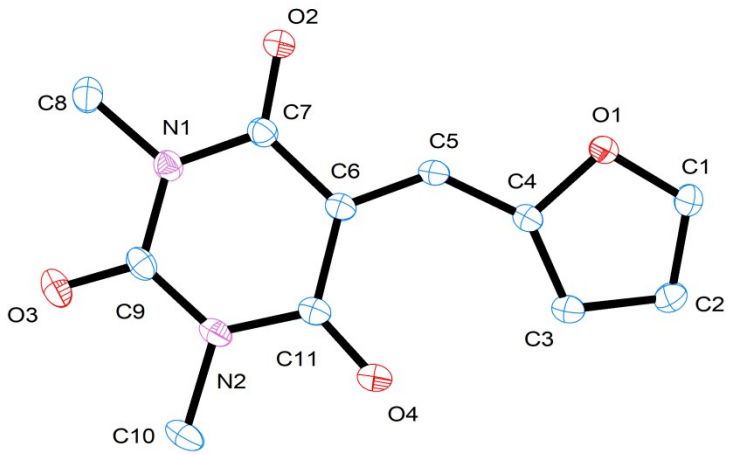


Fig. S27 ORTEP drawings for compound **1**, thermal ellipsoids are drawn at the 30% probability level, and H atoms are omitted for clarity.

5.3 Crystal data and structure refinement for 1

Single crystal **1** CCDC number: 2110023

Table S3 Crystal data and structure refinement for 1.

Identification code	**1**
Empirical formula	$C_{11}H_{10}N_2O_4$
Formula weight	234.21
Temperature/K	169.99(11)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.8240(3)
b/Å	6.1616(2)
c/Å	13.2002(3)
α/°	90
β/°	99.354(2)
γ/°	90
Volume/Å^3	1029.16(5)
Z	4
ρ_{calc}g/cm^3	1.512
μ/mm^{-1}	0.994
F(000)	488.0
Crystal size/mm^3	0.15 × 0.1 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.916 to 149.606
Index ranges	-15 ≤ h ≤ 16, -7 ≤ k ≤ 7, -16 ≤ l ≤ 13
Reflections collected	6441
Independent reflections	2025 [R_{int} = 0.0257, R_{sigma} = 0.0279]
Data/restraints/parameters	2025/0/156
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0419, wR_2 = 0.1101
Final R indexes [all data]	R_1 = 0.0454, wR_2 = 0.1132
Largest diff. peak/hole / e Å^{-3}	0.21/-0.26

Table S4 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	3822.7(8)	-186.9(17)	4345.1(8)	33.0(3)
O3	2563.4(9)	10397.1(18)	7013.3(9)	41.3(3)
O2	5003.7(8)	5271(2)	6688.8(9)	43.0(3)
O4	1513.4(8)	4803.4(19)	4878.1(9)	42.4(3)
N1	3813.3(9)	7913(2)	6798.5(9)	29.4(3)
N2	2057.8(9)	7666(2)	5899.8(9)	30.8(3)
C5	3647.0(10)	3033(2)	5230.2(10)	26.7(3)
C6	3317.3(10)	4862(2)	5657.8(10)	27.0(3)
C4	3153.8(10)	1521(2)	4489.2(10)	26.4(3)
C3	2218.6(11)	1222(2)	3837.2(11)	30.4(3)
C11	2235.5(11)	5713(2)	5434.6(11)	29.3(3)
C7	4111.1(11)	5982(2)	6411.5(11)	29.4(3)
C9	2793.6(11)	8755(2)	6600.4(11)	30.1(3)
C1	3288.6(12)	-1490(2)	3618.3(11)	33.1(3)
C2	2310.0(11)	-700(3)	3279.5(11)	32.8(3)
C8	4557.6(13)	9052(3)	7577.2(13)	41.5(4)
C10	992.6(12)	8599(3)	5708.0(13)	41.7(4)

Table S5 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	27.8(5)	34.9(6)	34.3(5)	-8.0(4)	-0.9(4)	7.3(4)
O3	49.2(7)	34.2(6)	42.6(6)	-4.6(5)	14.2(5)	10.9(5)
O2	28.2(6)	44.9(7)	52.3(7)	-16.1(5)	-4.2(5)	8.9(5)
O4	24.9(5)	45.2(7)	55.0(7)	-9.6(5)	0.0(5)	6.2(4)
N1	28.8(6)	29.6(6)	31.2(6)	-1.7(5)	8.8(5)	0.9(5)
N2	27.8(6)	34.7(7)	30.7(6)	3.8(5)	7.0(5)	10.8(5)
C5	21.1(6)	31.3(7)	27.3(7)	2.3(6)	2.8(5)	3.9(5)
C6	23.9(7)	29.7(7)	28.1(7)	2.3(5)	6.0(5)	2.7(5)
C4	25.3(6)	28.6(7)	25.9(6)	2.3(5)	5.5(5)	4.7(5)
C3	26.1(7)	34.8(8)	29.9(7)	3.0(6)	3.5(5)	3.8(6)
C11	25.3(7)	33.2(7)	30.1(7)	3.1(6)	6.3(5)	4.1(6)
C7	26.9(7)	31.9(7)	30.1(7)	-0.7(6)	6.7(5)	2.8(6)
C9	35.5(8)	28.7(7)	28.4(7)	3.3(5)	12.7(6)	5.9(6)
C1	35.0(7)	32.6(7)	30.7(7)	-7.2(6)	1.8(6)	1.8(6)
C2	30.6(7)	37.6(8)	28.5(7)	-1.1(6)	-0.4(5)	-1.7(6)
C8	38.4(8)	40.6(9)	45.5(9)	-14.0(7)	6.7(7)	-1.4(7)
C10	33.0(8)	44.9(9)	48.1(9)	4.7(7)	9.0(7)	18.1(7)

Table S6 Bond Lengths for 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C4	1.3903(17)	N2	C9	1.383(2)
O1	C1	1.3493(17)	N2	C10	1.4656(18)
O3	C9	1.2084(18)	C5	C6	1.3581(19)
O2	C7	1.2248(18)	C5	C4	1.4225(19)
O4	C11	1.2208(18)	C6	C11	1.4675(18)
N1	C7	1.3732(18)	C6	C7	1.474(2)
N1	C9	1.3915(18)	C4	C3	1.3703(19)
N1	C8	1.4632(19)	C3	C2	1.409(2)
N2	C11	1.3865(19)	C1	C2	1.353(2)

Table S7 Bond Angles for 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	O1	C4	107.13(11)	C3	C4	C5	140.01(13)
C7	N1	C9	124.25(12)	C4	C3	C2	107.63(12)
C7	N1	C8	119.19(12)	O4	C11	N2	120.12(12)
C9	N1	C8	116.04(12)	O4	C11	C6	123.82(13)
C11	N2	C10	118.65(13)	N2	C11	C6	116.06(13)
C9	N2	C11	125.02(12)	O2	C7	N1	120.11(13)
C9	N2	C10	116.16(13)	O2	C7	C6	122.93(13)
C6	C5	C4	134.06(12)	N1	C7	C6	116.96(12)
C5	C6	C11	124.13(13)	O3	C9	N1	121.22(14)
C5	C6	C7	116.19(12)	O3	C9	N2	121.18(13)
C11	C6	C7	119.65(12)	N2	C9	N1	117.59(12)
O1	C4	C5	112.00(11)	O1	C1	C2	110.94(13)
C3	C4	O1	107.97(12)	C1	C2	C3	106.33(13)

Table S8 Torsion Angles for 1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C4	C3	C2	-0.09(15)	C7	N1	C9	N2	-5.8(2)
O1	C1	C2	C3	-0.53(17)	C7	C6	C11	O4	-174.61(14)
C5	C6	C11	O4	3.5(2)	C7	C6	C11	N2	5.30(19)
C5	C6	C11	N2	-176.55(12)	C9	N1	C7	O2	-174.12(14)
C5	C6	C7	O2	-3.8(2)	C9	N1	C7	C6	6.4(2)
C5	C6	C7	N1	175.63(12)	C9	N2	C11	O4	175.04(13)
C5	C4	C3	C2	177.82(17)	C9	N2	C11	C6	-4.9(2)
C6	C5	C4	O1	-176.64(14)	C1	O1	C4	C5	-178.78(12)
C6	C5	C4	C3	5.5(3)	C1	O1	C4	C3	-0.23(15)
C4	O1	C1	C2	0.48(16)	C8	N1	C7	O2	-2.8(2)
C4	C5	C6	C11	2.3(2)	C8	N1	C7	C6	177.77(12)
C4	C5	C6	C7	-179.46(14)	C8	N1	C9	O3	3.8(2)
C4	C3	C2	C1	0.37(17)	C8	N1	C9	N2	-177.37(12)
C11	N2	C9	O3	-176.19(13)	C10	N2	C11	O4	0.0(2)
C11	N2	C9	N1	5.0(2)	C10	N2	C11	C6	-179.92(12)
C11	C6	C7	O2	174.46(14)	C10	N2	C9	O3	-1.0(2)
C11	C6	C7	N1	-6.07(19)	C10	N2	C9	N1	-179.89(12)
C7	N1	C9	O3	175.39(13)					

Table S9 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 1.

Atom	*x*	*y*	*z*	U(eq)
H5	4349.39	2695.42	5475.76	32
H3	1630.02	2123.19	3774.12	36
H1	3557.45	-2761.54	3381.99	40
H2	1799.14	-1304.51	2778.16	39
H8A	4384.55	8760.1	8244.72	62
H8B	4513.89	10584.47	7446.69	62
H8C	5262.66	8557.68	7550.93	62
H10A	1024.92	10047.83	5447.55	63
H10B	708.66	8634.25	6337.37	63
H10C	546.51	7725.64	5213.41	63

5.4 Structures of crystal 2

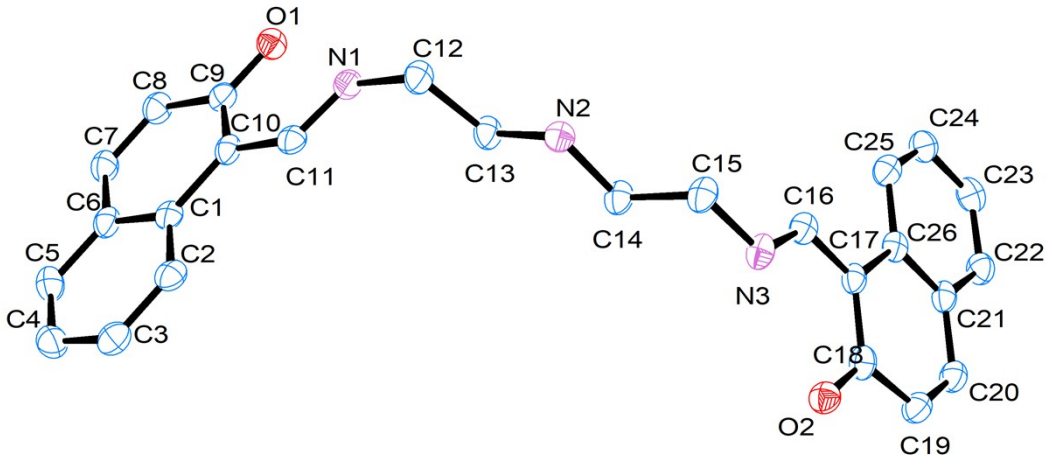


Fig. S28 ORTEP drawings for compound **2**, thermal ellipsoids are drawn at the 30% probability level, and H atoms are omitted for clarity.

5.5 Crystal data and structure refinement for 2.

Single crystal **2** CCDC number: 2110020

Table S10 Crystal data and structure refinement for 2

Identification code	**2**
Empirical formula	$C_{26}H_{26}N_3O_2$
Formula weight	412.50
Temperature/K	169.99(13)
Crystal system	monoclinic
Space group	C2
a/Å	37.4048(8)
b/Å	4.46170(10)
c/Å	15.4153(4)
α/°	90
β/°	96.692(2)
γ/°	90
Volume/Å^3	2555.12(10)
Z	4
ρ_{calc}g/cm^3	1.072
μ/mm^{-1}	0.545
F(000)	876.0
Crystal size/mm^3	0.15 × 0.1 × 0.06
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	4.758 to 150.212
Index ranges	-45 ≤ h ≤ 46, -5 ≤ k ≤ 4, -19 ≤ l ≤ 19
Reflections collected	16644
Independent reflections	4549 [R_{int} = 0.0296, R_{sigma} = 0.0255]
Data/restraints/parameters	4549/1/281
Goodness-of-fit on F^2	1.075
Final R indexes [I>=2σ (I)]	R_1 = 0.0769, wR_2 = 0.2305
Final R indexes [all data]	R_1 = 0.0817, wR_2 = 0.2360
Largest diff. peak/hole / e Å^{-3}	0.39/-0.29
Flack parameter	0.30(13)

Table S11 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	3836.8(8)	-4544(9)	1997(2)	45.4(8)
O002	6148.5(10)	14660(10)	3206(2)	53.4(9)
N2	5000	-9731(13)	0	38.7(11)
N1	4128.1(10)	-7782(10)	841(3)	44.2(9)
N006	5900.3(11)	17883(10)	4351(3)	46.5(10)
N00A	5000	19847(16)	5000	48.4(14)
C00B	6689.9(12)	13463(13)	5342(3)	42.4(11)
C00C	6411.9(12)	14611(12)	4679(3)	39.9(10)
C10	3612.7(11)	-4677(11)	486(3)	38.0(10)
C1	3346.9(11)	-3523(10)	-209(3)	37.0(9)
C00F	6158.0(11)	16737(12)	4910(3)	40.2(10)
C6	3075.2(12)	-1502(12)	16(3)	42.3(11)
C9	3606.5(12)	-3733(13)	1377(3)	44.5(11)
C00I	6395.1(13)	13668(11)	3794(3)	43.0(11)
C11	3878.8(12)	-6682(12)	281(3)	39.9(10)
C00K	6940.5(12)	11423(12)	5066(3)	43.0(11)
C2	3342.3(13)	-4198(12)	-1096(3)	44.5(11)
C7	3073.0(13)	-691(13)	913(3)	45.9(11)
C00N	6658.6(14)	11578(13)	3560(3)	49.4(12)
C12	4410.5(12)	-9799(13)	588(4)	45.8(11)
C5	2819.7(13)	-343(14)	-632(3)	49.5(13)
C00Q	6918.1(13)	10551(13)	4167(3)	46.9(11)
C00R	6721.3(14)	14313(14)	6228(3)	50.3(13)
C00S	6989.5(14)	13183(15)	6807(3)	52.5(13)
C8	3318.4(13)	-1799(13)	1549(3)	46.8(11)
C00U	7213.0(13)	10257(13)	5687(3)	47.4(11)
C13	4726.5(12)	-7930(12)	343(3)	44.4(11)
C00W	5619.2(13)	19803(13)	4596(4)	46.8(12)
C00X	7240.1(14)	11078(15)	6547(4)	54.9(14)
C00Y	5302.4(12)	17881(13)	4800(4)	46.6(12)
C3	3093.8(14)	-3017(14)	-1724(3)	50.1(12)
C4	2825.9(14)	-1118(14)	-1496(4)	52.3(13)

Table S12 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	45.4(17)	40(2)	51.5(17)	-1.7(15)	8.3(14)	4.0(16)
O002	55(2)	49(2)	55.0(18)	-8.1(17)	1.0(15)	9.2(18)
N2	43(3)	23(3)	51(3)	0	8(2)	0
N1	38.5(18)	40(2)	56(2)	9.2(19)	13.1(16)	3.4(19)
N006	43(2)	39(3)	59(2)	-1.3(19)	9.4(17)	1.2(19)
N00A	37(3)	38(4)	71(4)	0	10(2)	0
C00B	32.2(19)	45(3)	51(2)	3(2)	10.2(18)	-5(2)
C00C	35(2)	38(3)	48(2)	-1(2)	10.9(17)	-3(2)
C10	31.8(19)	31(2)	53(2)	0.1(19)	10.1(17)	-3.5(19)
C1	37(2)	20(2)	55(2)	4.8(18)	10.5(18)	-2.8(18)
C00F	30.5(18)	36(3)	55(2)	-1(2)	10.0(17)	-3.9(18)
C6	34(2)	36(3)	58(3)	2(2)	9.9(19)	-4(2)
C9	39(2)	44(3)	52(2)	8(2)	10.1(19)	-4(2)
C00I	44(2)	30(3)	56(3)	-4(2)	8(2)	-3(2)
C11	41(2)	30(2)	50(2)	5.0(19)	10.6(18)	-2.3(19)
C00K	38(2)	37(3)	56(2)	1(2)	13.3(19)	-4(2)
C2	47(2)	34(3)	55(2)	4(2)	15(2)	-1(2)
C7	38(2)	44(3)	56(3)	-1(2)	10.5(19)	4(2)
C00N	51(3)	41(3)	59(3)	-2(2)	19(2)	-3(2)
C12	42(2)	32(3)	66(3)	3(2)	15(2)	7(2)
C5	37(2)	49(3)	62(3)	-2(2)	4(2)	6(2)
C00Q	41(2)	38(3)	64(3)	-4(2)	16(2)	0(2)
C00R	43(2)	55(3)	55(3)	1(3)	14(2)	4(2)
C00S	46(2)	58(4)	53(3)	0(2)	2(2)	-9(3)
C8	45(2)	45(3)	52(2)	-3(2)	13.8(19)	3(2)
C00U	41(2)	35(3)	68(3)	4(2)	14(2)	0(2)
C13	38(2)	33(3)	63(3)	1(2)	10.8(19)	5(2)
C00W	38(2)	37(3)	67(3)	7(2)	12(2)	2(2)
C00X	48(3)	51(4)	64(3)	10(3)	0(2)	-4(2)
C00Y	38(2)	32(3)	70(3)	-4(2)	8(2)	-2(2)
C3	51(3)	45(3)	56(3)	1(2)	11(2)	-11(2)
C4	45(2)	49(3)	61(3)	9(2)	-4(2)	-4(2)

Table S13 Bond Lengths for 2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C9	1.263(6)	C1	C6	1.431(6)
O002	C00I	1.293(6)	C1	C2	1.399(7)
N2	C13	1.448(6)	C6	C7	1.431(7)
N2	C13[1]	1.448(6)	C6	C5	1.399(7)
N1	C11	1.292(6)	C9	C8	1.429(7)
N1	C12	1.474(6)	C00I	C00N	1.433(7)
N006	C00F	1.319(6)	C00K	C00Q	1.433(7)
N006	C00W	1.441(7)	C00K	C00U	1.413(7)
N00A	C00Y	1.491(6)	C2	C3	1.367(7)
N00A	C00Y[2]	1.492(6)	C7	C8	1.355(7)
C00B	C00C	1.462(7)	C00N	C00Q	1.347(8)
C00B	C00K	1.407(7)	C12	C13	1.530(7)
C00B	C00R	1.410(7)	C5	C4	1.379(8)
C00C	C00F	1.417(7)	C00R	C00S	1.359(8)
C00C	C00I	1.423(7)	C00S	C00X	1.417(9)
C10	C1	1.467(6)	C00U	C00X	1.369(8)
C10	C9	1.438(7)	C00W	C00Y	1.525(7)
C10	C11	1.402(7)	C3	C4	1.388(8)

[1]1-X,+Y,-Z; [2]1-X,+Y,1-Z

Table S14 Bond Angles for 2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C13	N2	C13[1]	112.6(6)	O002	C00I	C00C	121.2(5)
C11	N1	C12	122.6(4)	O002	C00I	C00N	120.1(4)
C00F	N006	C00W	124.0(4)	C00C	C00I	C00N	118.6(4)
C00Y	N00A	C00Y[2]	107.9(6)	N1	C11	C10	124.6(4)
C00K	C00B	C00C	117.4(4)	C00B	C00K	C00Q	120.1(5)
C00K	C00B	C00R	118.9(5)	C00B	C00K	C00U	119.1(5)
C00R	C00B	C00C	123.7(5)	C00U	C00K	C00Q	120.8(5)
C00F	C00C	C00B	120.2(4)	C3	C2	C1	122.6(5)
C00F	C00C	C00I	118.9(4)	C8	C7	C6	121.8(5)
C00I	C00C	C00B	121.0(4)	C00Q	C00N	C00I	120.5(5)
C9	C10	C1	120.6(4)	N1	C12	C13	109.3(4)
C11	C10	C1	119.9(4)	C4	C5	C6	120.7(5)
C11	C10	C9	119.5(4)	C00N	C00Q	C00K	122.4(5)
C6	C1	C10	119.0(4)	C00S	C00R	C00B	120.5(5)
C2	C1	C10	124.6(4)	C00R	C00S	C00X	121.5(5)
C2	C1	C6	116.4(4)	C7	C8	C9	123.2(5)
N006	C00F	C00C	123.8(4)	C00X	C00U	C00K	121.6(5)
C7	C6	C1	118.5(4)	N2	C13	C12	112.8(4)
C5	C6	C1	120.4(5)	N006	C00W	C00Y	109.2(4)
C5	C6	C7	121.1(5)	C00U	C00X	C00S	118.3(5)
O1	C9	C10	123.6(4)	N00A	C00Y	C00W	109.8(4)
O1	C9	C8	119.6(4)	C2	C3	C4	120.5(5)
C8	C9	C10	116.7(4)	C5	C4	C3	119.4(5)

[1]1-X,+Y,-Z; [2]1-X,+Y,1-Z

Table S15 Torsion Angles for 2.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C9	C8	C7	176.1(5)	C9	C10	C1	C6	-1.6(6)
O002	C00I	C00N	C00Q	179.5(5)	C9	C10	C1	C2	176.8(5)
N1	C12	C13	N2	-174.0(4)	C9	C10	C11	N1	-0.3(7)
N006	C00W	C00Y	N00A	-176.4(4)	C00I	C00C	C00F	N006	1.0(7)
C00B	C00C	C00F	N006	179.8(5)	C00I	C00N	C00Q	C00K	1.3(8)
C00B	C00C	C00I	O002	179.5(5)	C11	N1	C12	C13	87.7(6)
C00B	C00C	C00I	C00N	-0.4(7)	C11	C10	C1	C6	179.4(4)
C00B	C00K	C00Q	C00N	-1.1(8)	C11	C10	C1	C2	-2.3(7)
C00B	C00K	C00U	C00X	-0.4(8)	C11	C10	C9	O1	2.2(7)
C00B	C00R	C00S	C00X	-1.4(9)	C11	C10	C9	C8	-177.1(5)
C00C	C00B	C00K	C00Q	0.1(7)	C00K	C00B	C00C	C00F	-178.2(4)
C00C	C00B	C00K	C00U	-179.9(5)	C00K	C00B	C00C	C00I	0.6(7)
C00C	C00B	C00R	C00S	-179.2(5)	C00K	C00B	C00R	C00S	0.1(8)
C00C	C00I	C00N	C00Q	-0.5(8)	C00K	C00U	C00X	C00S	-0.9(9)
C10	C1	C6	C7	-0.2(7)	C2	C1	C6	C7	-178.7(5)
C10	C1	C6	C5	179.5(5)	C2	C1	C6	C5	1.0(7)
C10	C1	C2	C3	-178.5(5)	C2	C3	C4	C5	2.3(8)
C10	C9	C8	C7	-4.6(8)	C7	C6	C5	C4	179.5(5)
C1	C10	C9	O1	-176.9(4)	C12	N1	C11	C10	-177.7(4)
C1	C10	C9	C8	3.8(7)	C5	C6	C7	C8	179.9(5)
C1	C10	C11	N1	178.7(4)	C00Q	C00K	C00U	C00X	179.6(5)
C1	C6	C7	C8	-0.4(8)	C00R	C00B	C00C	C00F	1.1(8)
C1	C6	C5	C4	-0.2(8)	C00R	C00B	C00C	C00I	179.8(5)
C1	C2	C3	C4	-1.5(8)	C00R	C00B	C00K	C00Q	-179.1(5)
C00F	N006	C00W	C00Y	-89.2(6)	C00R	C00B	C00K	C00U	0.8(7)
C00F	C00C	C00I	O002	-1.7(7)	C00R	C00S	C00X	C00U	1.9(9)
C00F	C00C	C00I	C00N	178.3(5)	C00U	C00K	C00Q	C00N	178.9(5)
C6	C1	C2	C3	-0.1(7)	C13[1]	N2	C13	C12	172.0(5)
C6	C7	C8	C9	3.0(9)	C00W	N006	C00F	C00C	173.3(5)
C6	C5	C4	C3	-1.4(9)	C00Y[2]	N00A	C00Y	C00W	-179.7(5)

[1]1-X,+Y,-Z; [2]1-X,+Y,1-Z

Table S16 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2.

Atom	*x*	*y*	*z*	U(eq)
H2A	4895.87	-10905.74	-422.79	46
H2B	5104.12	-10905.8	422.78	46
H1	4129.43	-7319.61	1383.12	53
H006	5900.19	17458.95	3806.69	56
H00A	4929.17	21013.5	4543.8	58
H00B	5070.84	21013.55	5456.18	58
H00F	6173.88	17360.02	5488.98	48
H11	3875.59	-7261.89	-299.33	48
H2	3515.3	-5501.91	-1265.89	53
H7	2898.43	631.62	1064.9	55
H00N	6650.4	10926.03	2985.05	59
H12A	4314.47	-11020.56	94.86	55
H12B	4491.78	-11122.14	1070.47	55
H5	2643.77	963.46	-479.16	59
H00Q	7088.78	9227.58	3995.49	56
H00R	6557.2	15658.02	6418.41	60
H00S	7009.04	13806.59	7385.92	63
H8	3298.4	-1275.58	2124.82	56
H00U	7377.92	8899.79	5505.92	57
H13A	4637.12	-6453.92	-90.81	53
H13B	4834.31	-6861.71	856.18	53
H00C	5542.02	21173.22	4122.65	56
H00D	5708.68	20975.52	5105.52	56
H00X	7418.4	10274.48	6951.66	66
H00E	5223.38	16613.62	4303.47	56
H00G	5376.35	16599.01	5297.14	56
H3	3104.34	-3489.22	-2307.96	60
H4	2652.17	-375.5	-1922.97	63