Supporting information for

A fast-response, fluorescent 'turn-on' chemosensor for selective detection of Cr^{3+}

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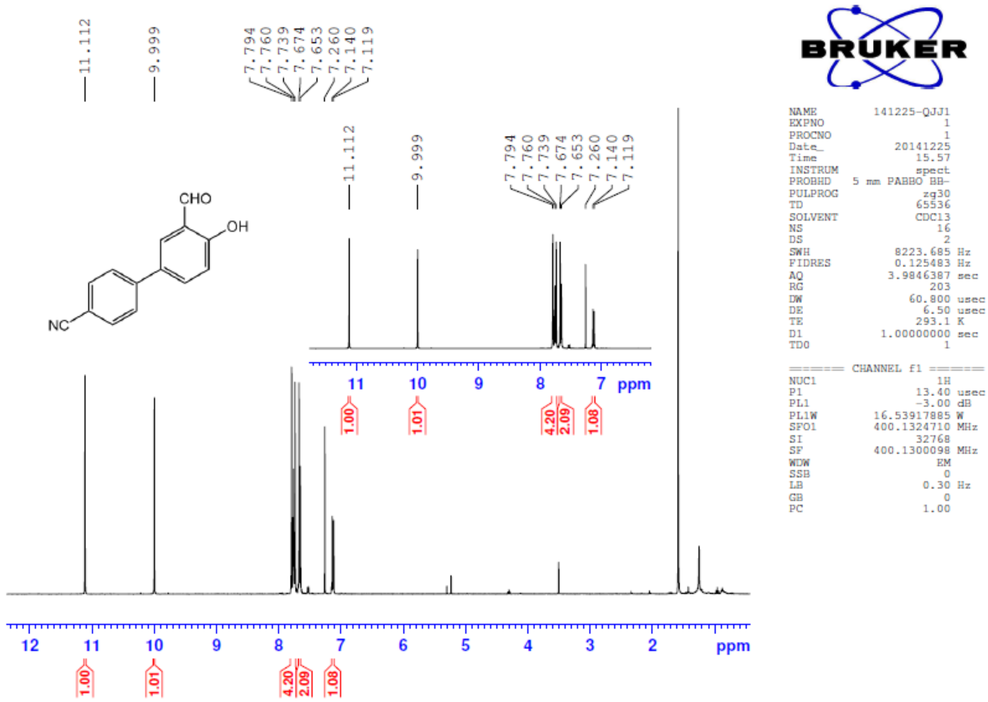


Fig.S1. ^{1}H NMR ($CDCl_3$) spectrum of **1.**

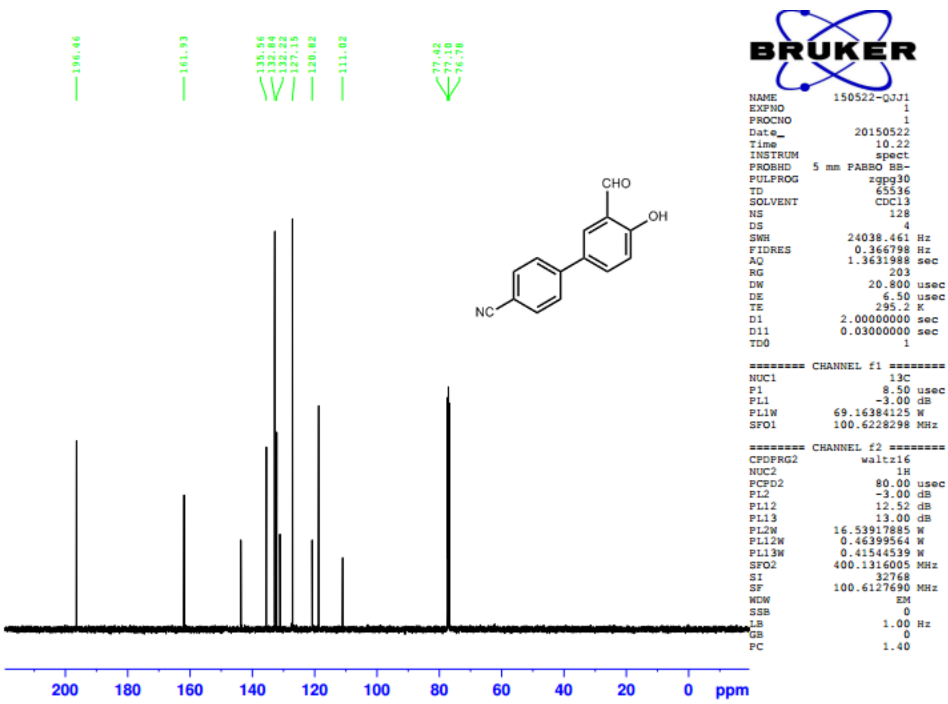


Fig.S2. ^{13}C NMR ($CDCl_3$) spectrum of **1.**

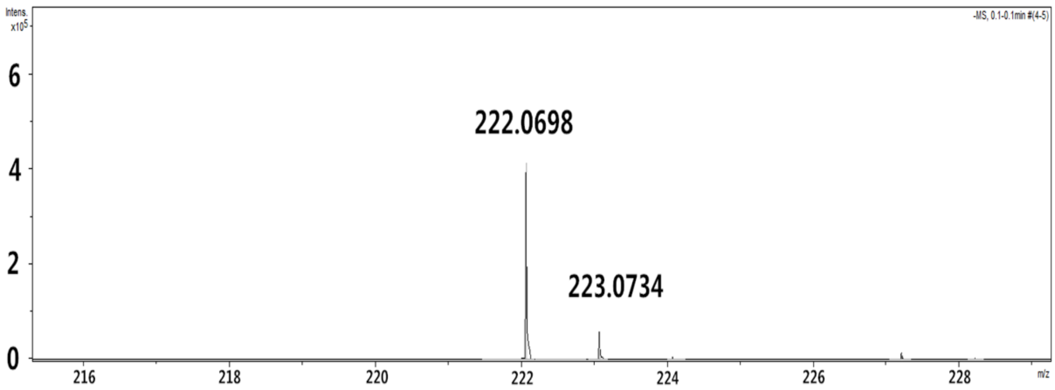


Fig.S3. ESI-MS spectrum of **1**.

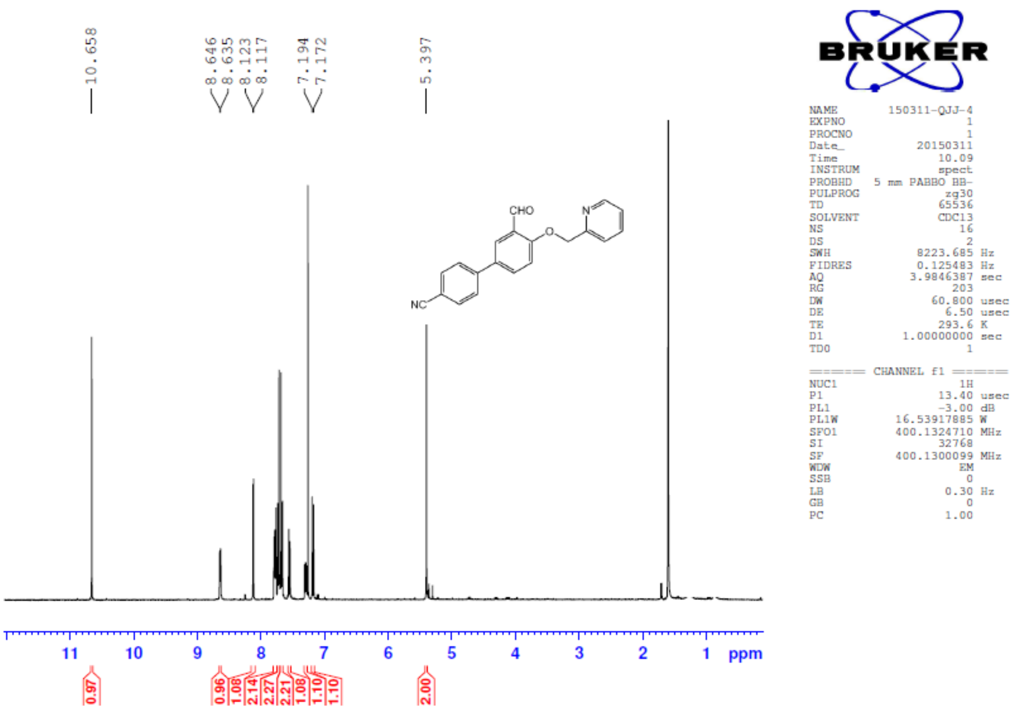


Fig.S4. ^{1}H NMR ($CDCl_3$) spectrum of **2.**

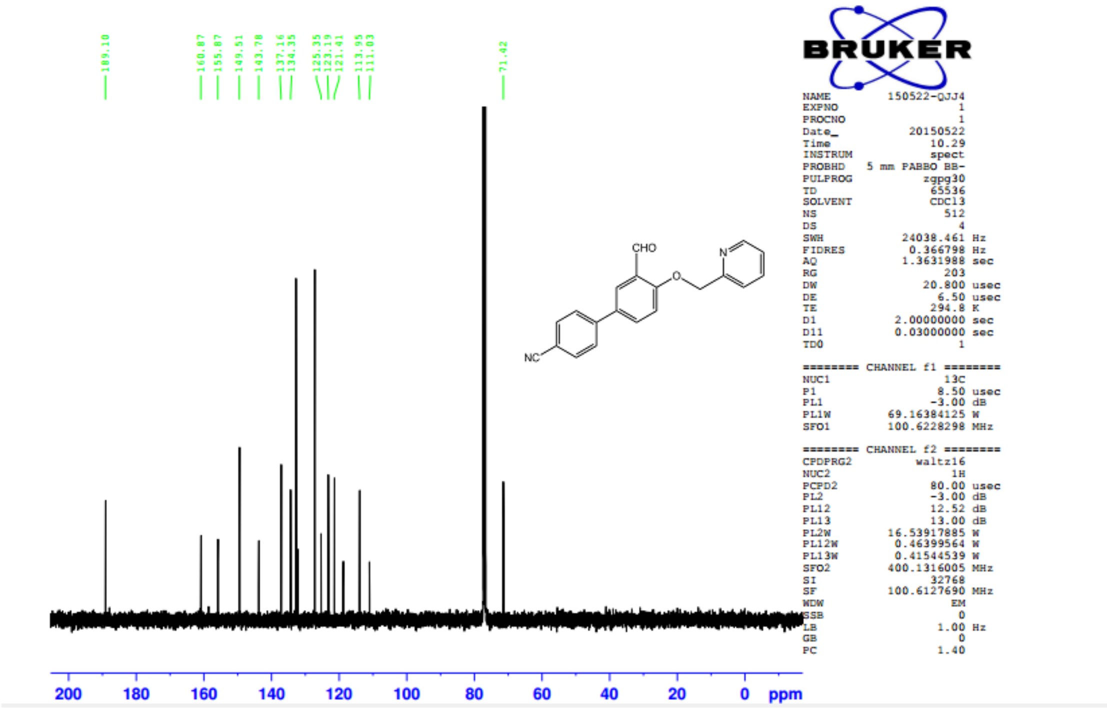


Fig.S5. ^{13}C NMR ($CDCl_3$) spectrum of **2.**

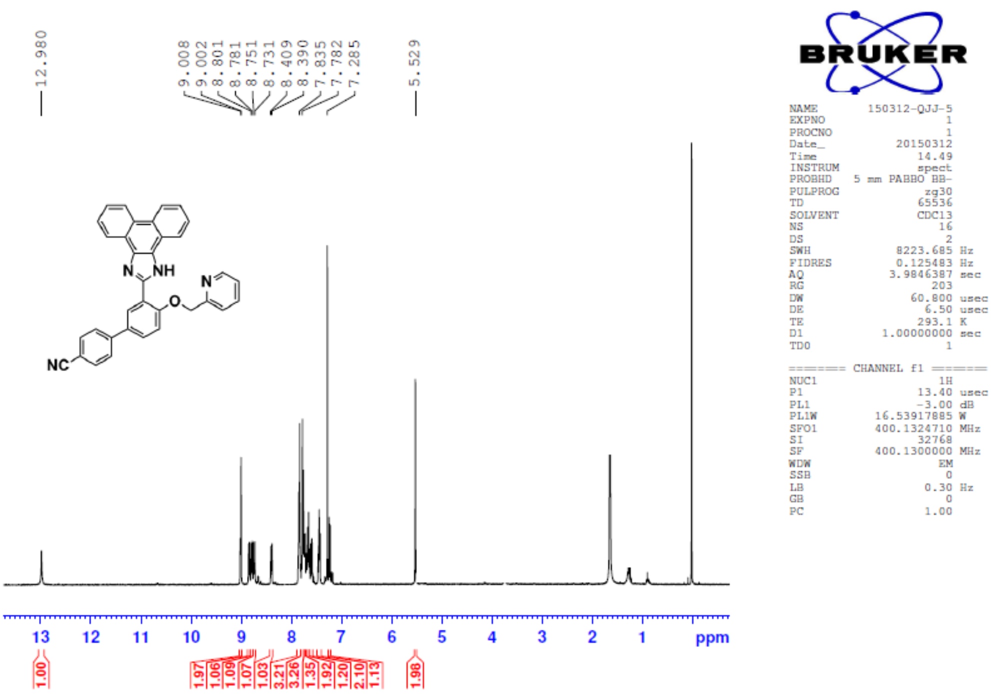


Fig.S6. ^{1}H NMR ($CDCl_3$) spectrum of **3.**

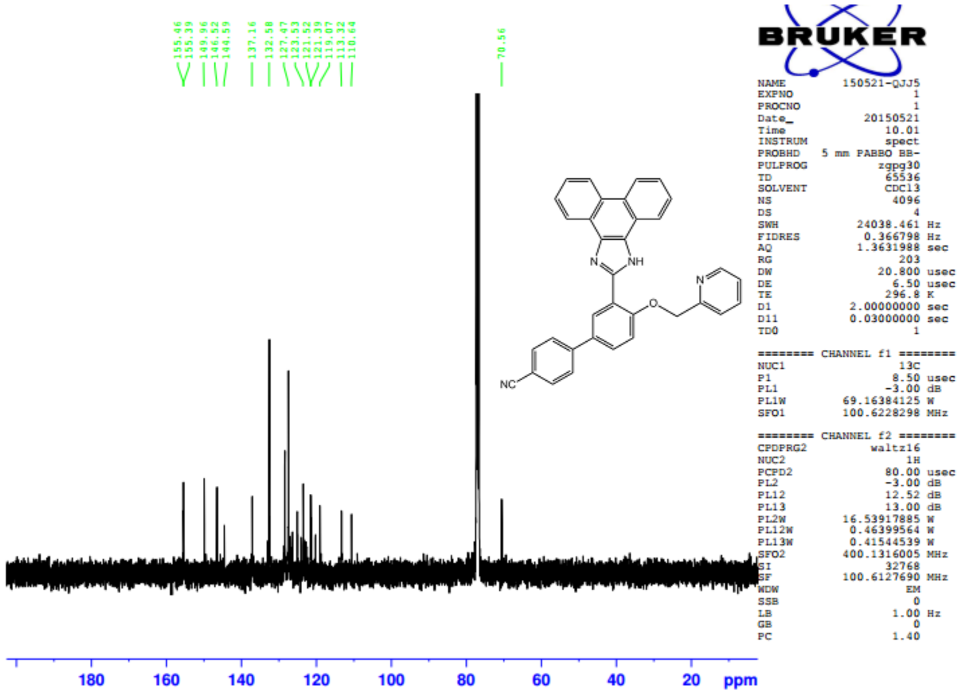


Fig.S7. ^{13}C NMR ($CDCl_3$) spectrum of **3.**

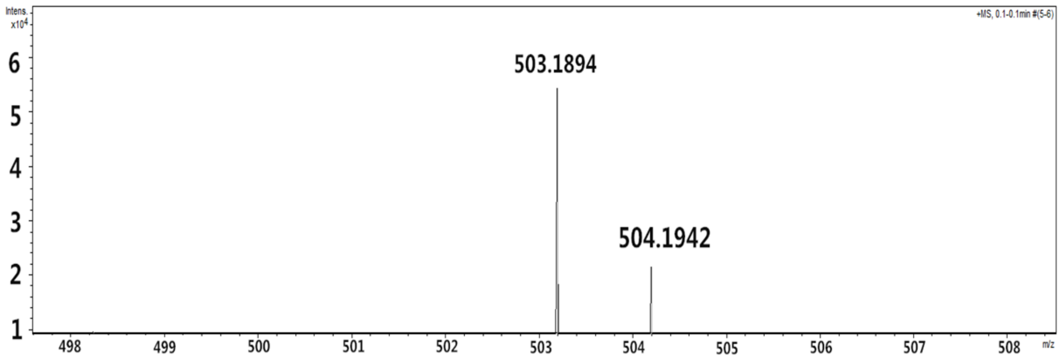


Fig.S8. ESI-MS spectrum of **3**.

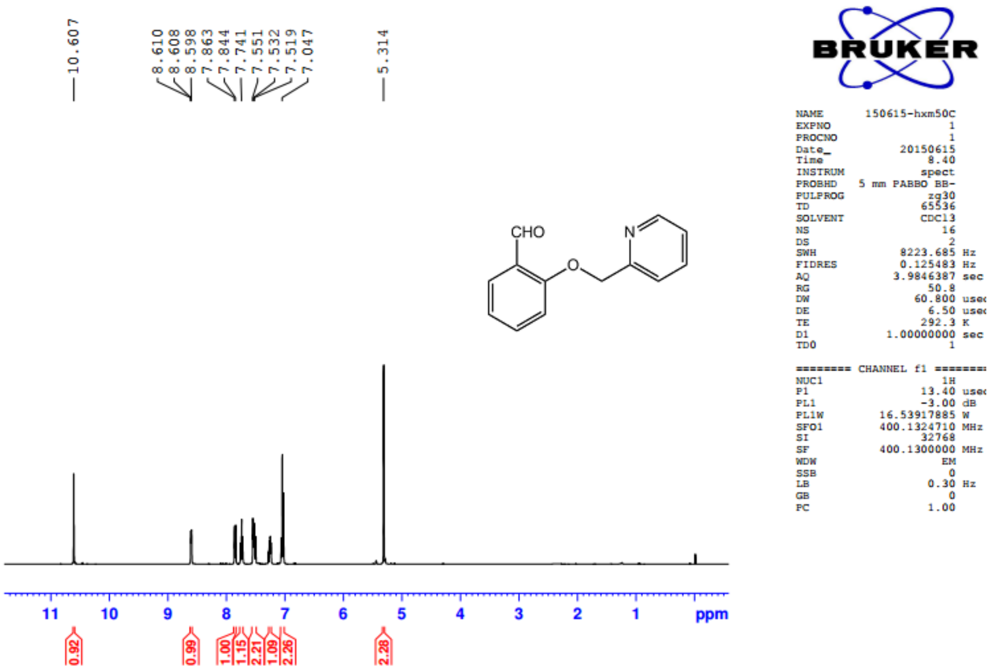


Fig.S9. ^{1}H NMR ($CDCl_3$) spectrum of **4.**

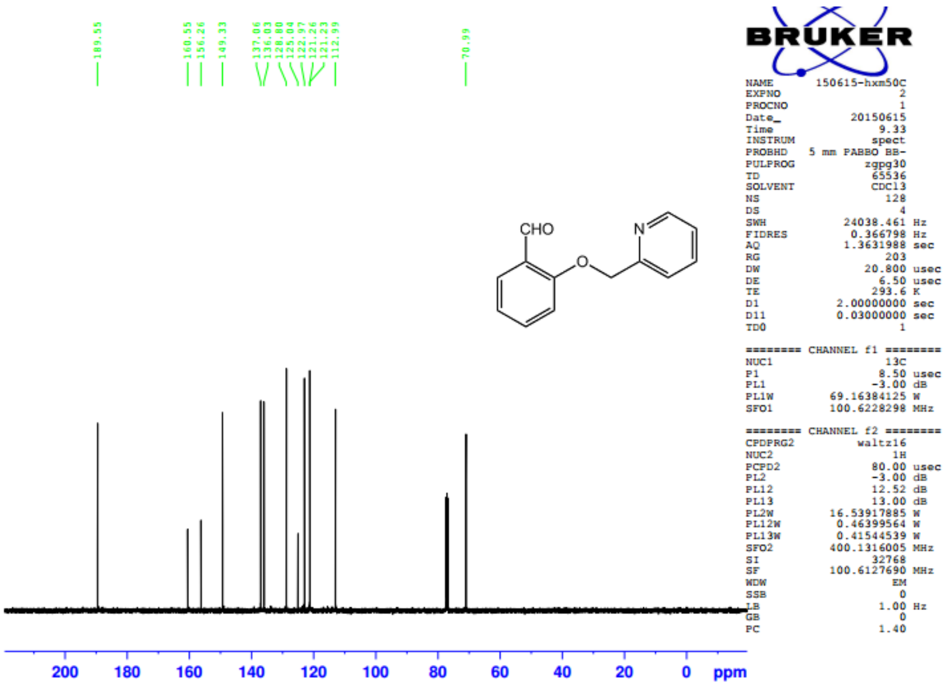


Fig.S10. ^{13}C NMR ($CDCl_3$) spectrum of **4.**

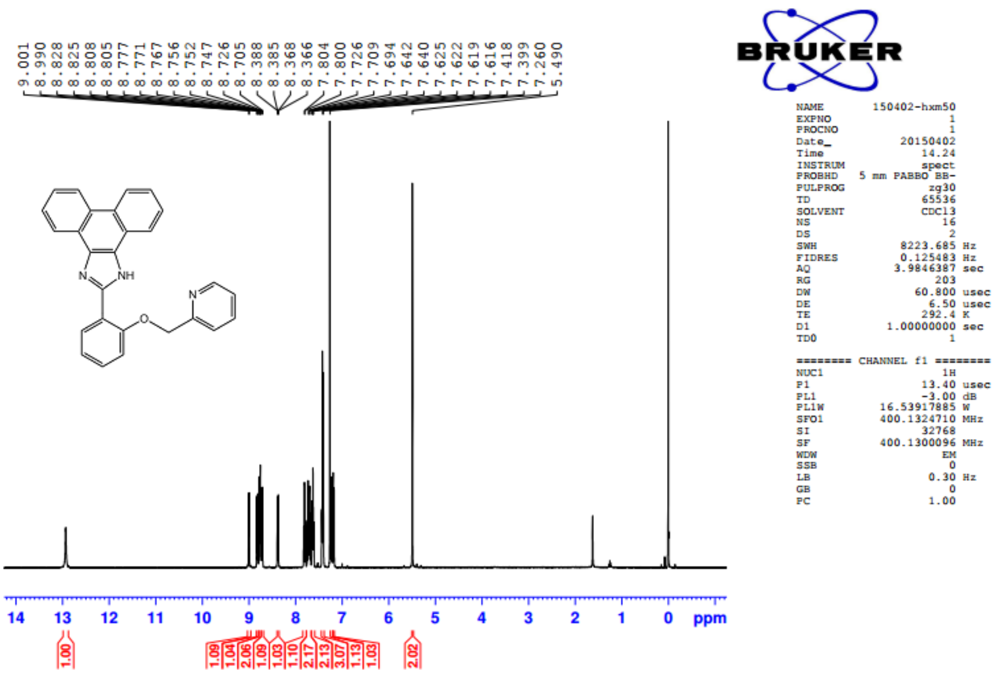


Fig.S11. ^{1}H NMR ($CDCl_3$) spectrum of **5.**

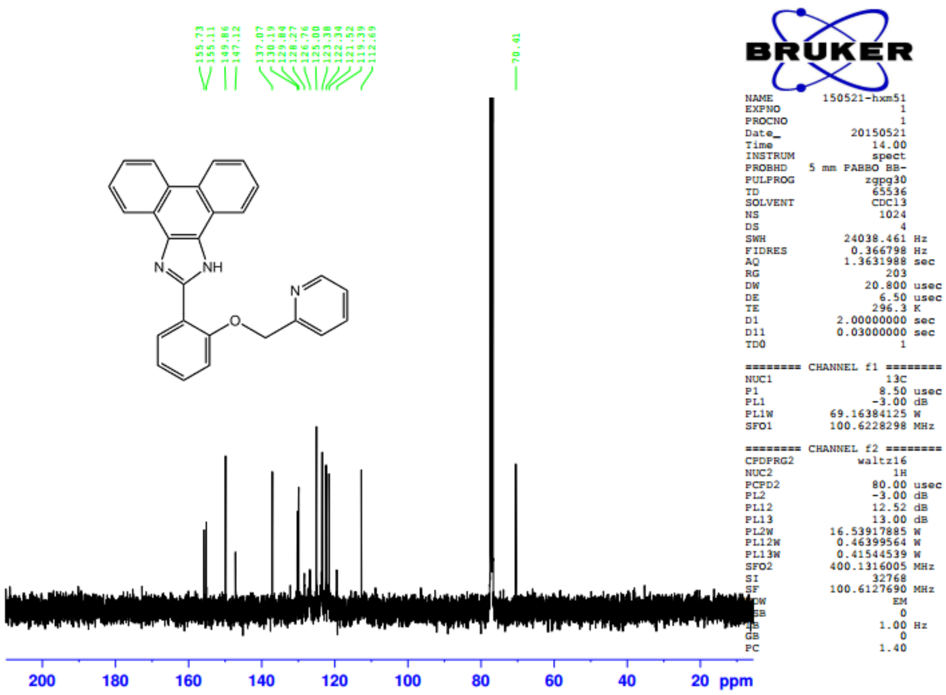


Fig.S12. ^{13}C NMR ($CDCl_3$) spectrum of **5.**

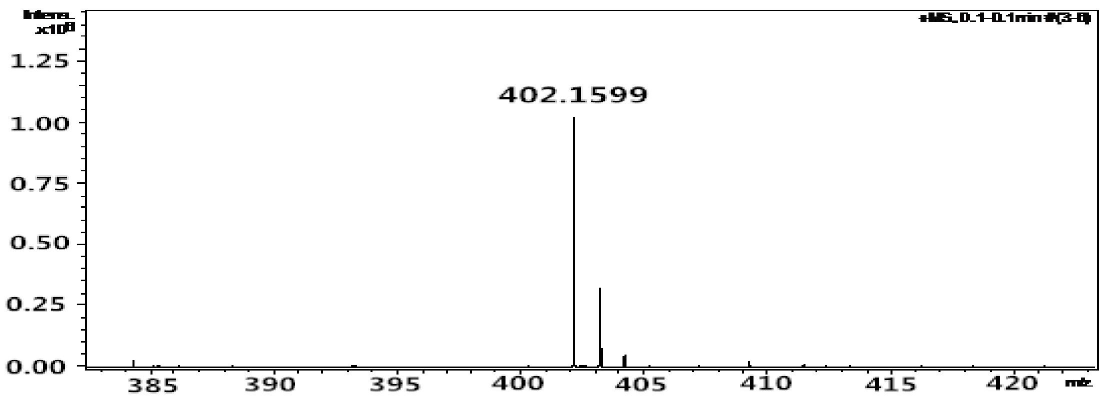


Fig.S13. ESI-MS spectrum of **5**.

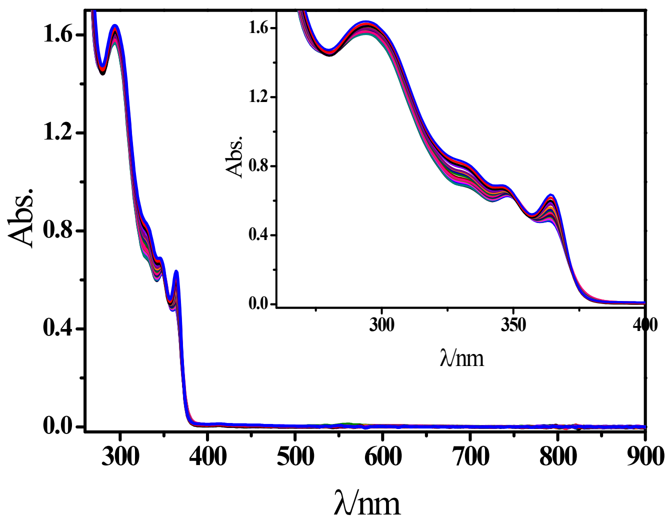


Fig. S14. Change of absorption spectra of sensor **3** (20 μM) upon the gradual addition of $CrCl_3$ (0 to 8 equiv.).

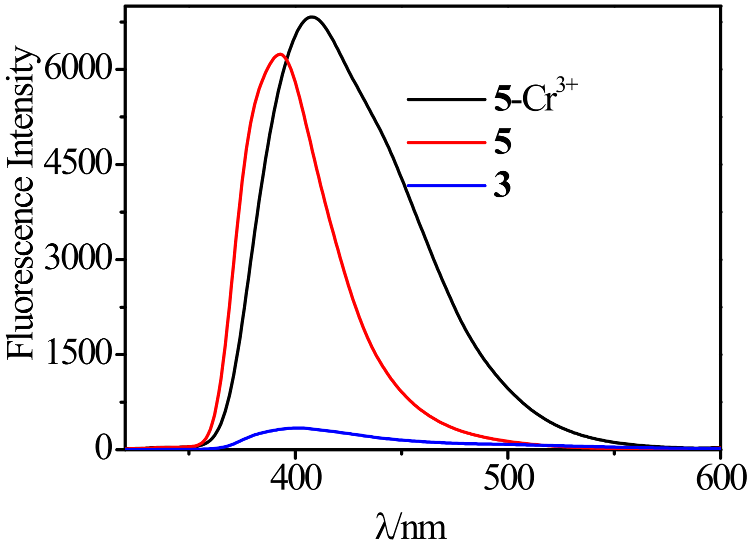
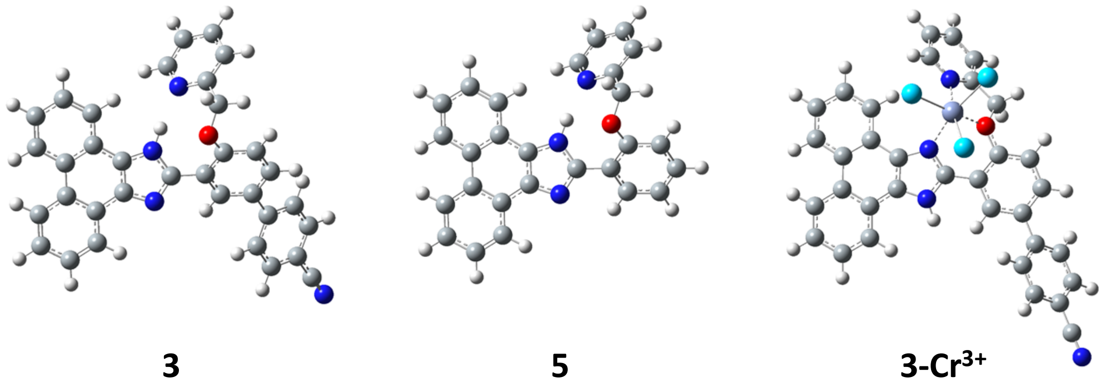


Fig. S15. Fluorescence responses for **3** (blue line, 20 μM, λ_{ex} = 300 nm), **5** (red line) and the complex **5**-Cr^{3+} (black line) in DMF-H_2O (1:1, v/v, HEPES, 20 mM, pH 7.0, λ_{ex} = 300 nm).



3 **5** **3-Cr^{3+}**

Fig. S16. DFT-optimized geometries for **3**, **5**, and **3**-$CrCl_3$ in DMF solution.

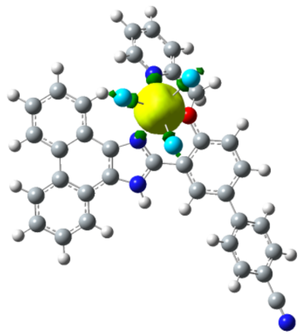


Fig. S17. The spin density for **3**-$CrCl_3$ calculated by DFT in DMF solution.

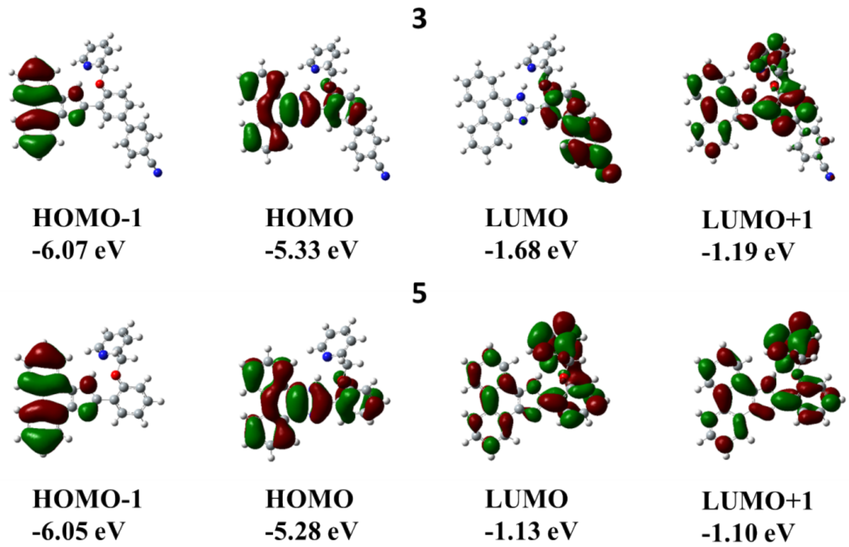


Fig. S18. DFT-calculated frontier molecular orbitals for **3** and **5** in DMF solution.

Table S1 the LOD calculation of **3**.

K = 3	
S = 6.77 × 10^7	The slope of the calibration curve (see Fig. 2 in the text).
Sb = 0.388	The standard deviation of the blank solution
LOD = *K*×*Sb*/*S* = 3 × 0.388 / 6.77 × 10^7 = 1.72 × 10^{-8}	

Table S2 Comparison of **3** with other Cr^{3+} selective fluorescenct chemosensors.

Sensor type	Selectivity	LOD	Ka	Ref.
Turn on	Cr^{3+} in aqueous methanol	0.15 μM	1.027 × 10^3 M^{-1}	[1]
Turn on	Cr^{3+} in CH_3CN–HEPES buffer (4:6, v/v, 0.02 M)	1 μM	8 × 10^4 M^{-1}	[2]
Turn on	Cr^{3+} in THF/H_2O (85/15, v/v)	0.20 μM	2.4 × 10^4 M^{-1}	[3]
Turn on	Cr^{3+} in ethanol-water (2:1, v/v) solution	1 μM	9.9 × 10^3 M^{-1}	[4]
Turn on	Cr^{3+} and PO_4^{3-} in methanol	2 μM	4 × 10^5 M^{-1}	[5]
Turn on	Al^{3+},Cr^{3+},Fe^{3+},$Ga^{3+}$and In^{3+} in methanol	1.6 μM	---	[6]
Turn on	Cr^{3+} and Hg^{2+} in acetonitrile:	5.6 ppm	2.0 ×10^3 M^{-1}	[7]

	aqueous HEPES buffer Cr^{3+} and Hg^{2+} (3:2, v/v) solution			
Turn on	Cr^{3+} and Hg^{2+} in CH_3CN-HEPES buffer (1 mM, pH = 7.2; 1:1, v/v)	0.14 ppb	1.38×10^5 M^{-1}	[8]
Turn on	Cr^{3+} and Fe^{3+} in aqueous solution	25 µM	1.75×10^3 M^{-1}	[9]
Turn off	Cr^{3+} in ethanol–water solution (9:1, v/v at pH = 7.4)	0.10 µM	1.4×10^4 M^{-1}	[10]
Turn off	Cr^{3+} and Cr^{6+} using unmodified gold nanoparticles	5 ppb	---	[11]
Turn off	$Cr^{3+}$and Cr^{6+} in environmental water samples	2.5 µg/L	---	[12]
Turn off	Cr^{3+} in water	0.03 µM	---	[13]
Turn off	Cr^{3+} in THF–H_2O (1:1, v/v) at pH = 7	0.23 µM	7.52×10^4 M^{-1}	[14]
Turn on	Cr^{3+}, Al^{3+} and Fe^{3+} in aqueous solution (8:2 = H_2O:EtOH).	0.2 µM	---	[15]
Turn on	Cr^{3+} in NaH_2PO_4/Na_2HPO_4 buffer solution (pH = 5.9)	0.1 µM (5.2 ppb)	9.24×10^{10} M^{-1}	[16]
Turn on	Cr^{3+} in buffered HEPES solution (pH = 7.0)	2.5×10^{-8} M	1.2×10^6 M^{-1}	[17]
Turn on	Cr^{3+} and Al^{3+} in MeOH/H_2O (3/7, v/v) buffered with HEPES.	2×10^{-8} M	$(2.38 \pm 0.14)10^3$ M^{-1}	[18]
Turn on	Cr^{3+} and F^- in CH_3CN-H_2O (9/1, v/v, pH = 7.0)	5.5×10^{-8} M	1.02×10^4 M^{-1}	[19]
Turn on	Cr^{3+} in Tris-HCl (10 mM, pH = 7.2) aqueous buffer solution	0.023 µM	---	[20]
Turn on	Cr^{3+} in CH_3CN–HEPES buffer solution (2:1, v/v, 0.5 mM, pH = 7.4)	0.14 nM	8.22×10^4 M^{-1}	[21]
Turn on	Cr^{3+} in THF and H_2O (1:99)	1 µM	---	[22]
Turn on	Cr^{3+} and Hg^{2+} in CH_3CN	2 µM	7.32×10^4 M^{-1}	[23]
Turn off	Cr^{6+} and Cr^{3+} in aqueous solution	26 nM	---	[24]
Turn on	Cr^{3+} in a methanol-H_2O (3:2, v/v, pH = 7.2)	7.5 ppb	1.03×10^4 M^{-1}	[25]
Turn on	Cr^{3+} in THF-water (v/v = 9/1) buffer solution	8.18×10^{-7} M	5.56×10^4 M^{-1}	[26]
Turn on	Cr^{3+} in MeOH-H_2O (3:2, v/v, pH = 7.4) solution	0.131 µM	1.96×10^3 M^{-1}	[27]
Turn on	Cr^{3+} in DMF/HEPES buffer (20 mM, pH = 7.0, 1:1, v/v)	17.2 nM (0.89 ppb)	4.44×10^3 M^{-1}	Present

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Table S3. TDDFT-calculated excitation energies and oscillator strengths for the lowest singlet excited states for **3** and **5** in DMF and water solutions.

	In DMF			**In water**		
	Energy (eV)	**Wavelength (nm)**	**Oscillator strength**	**Energy (eV)**	**Wavelength (nm)**	**Oscillator strength**
			3			
$\mathbf{S_1}$	3.2714	378.99	0.0275	3.2777	378.26	0.0262
$\mathbf{S_2}$	3.5899	345.37	0.5861	3.5989	344.50	0.5534
$\mathbf{S_3}$	3.7008	335.02	0.0206	3.7181	333.46	0.0136
			5			
$\mathbf{S_1}$	3.6088	343.56	0.3513	3.6163	342.85	0.3261
$\mathbf{S_2}$	3.6772	337.17	0.0120	3.6948	335.57	0.0073
$\mathbf{S_3}$	3.8287	323.83	0.2862	3.8373	323.10	0.2856