

SUPPORTING INFORMATION

A New Highly Selective “off-on” Typical Chemosensor of Al³⁺, 1-((Z)-((E)-(3,5-dichloro-2-hydroxybenzylidene)hydrazono)methyl) naphthalene-2-ol, An experimental and In-Silico Study

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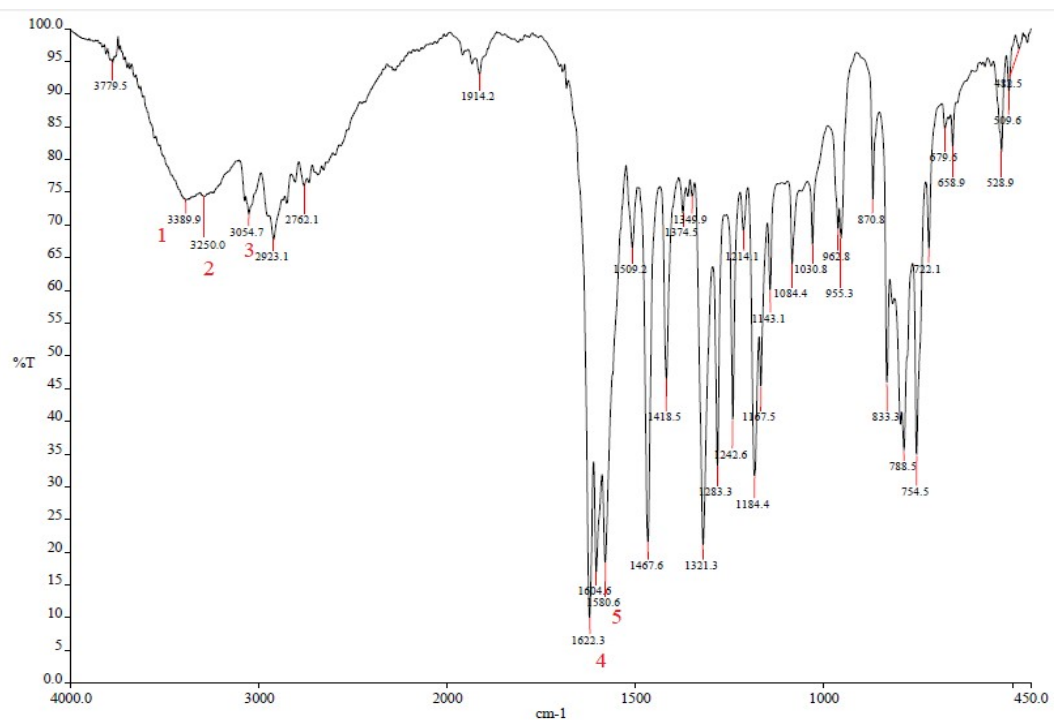


Fig. SI 1. Infrared spectra of compound **3** in KBr pellet

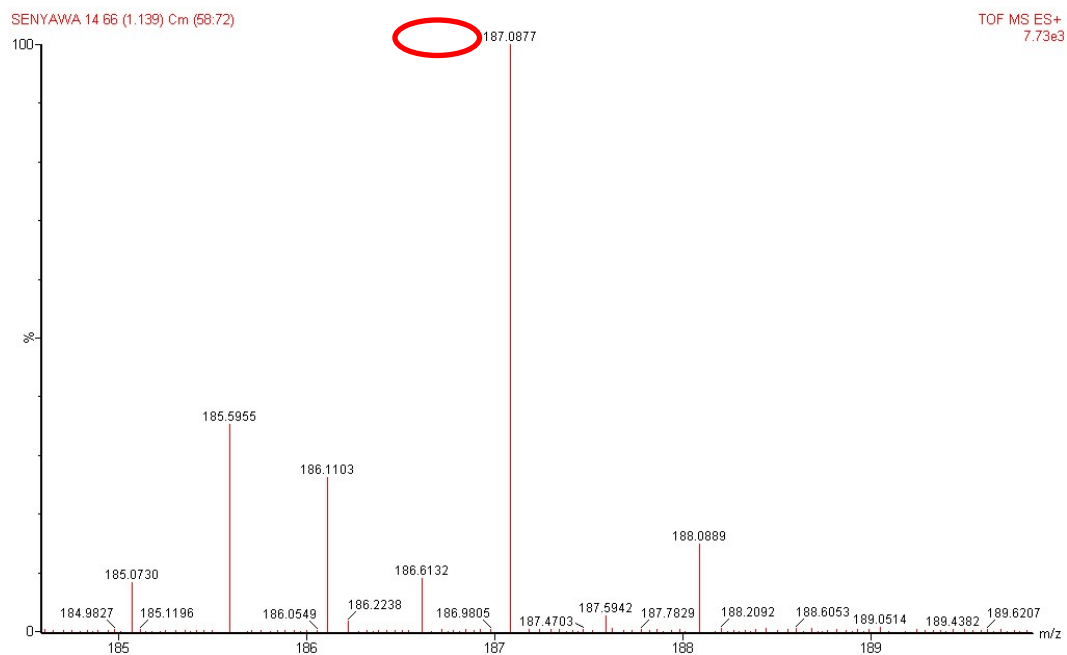


Fig. SI 2. ToF-HRMS spectra of compound **3** (ES⁺)

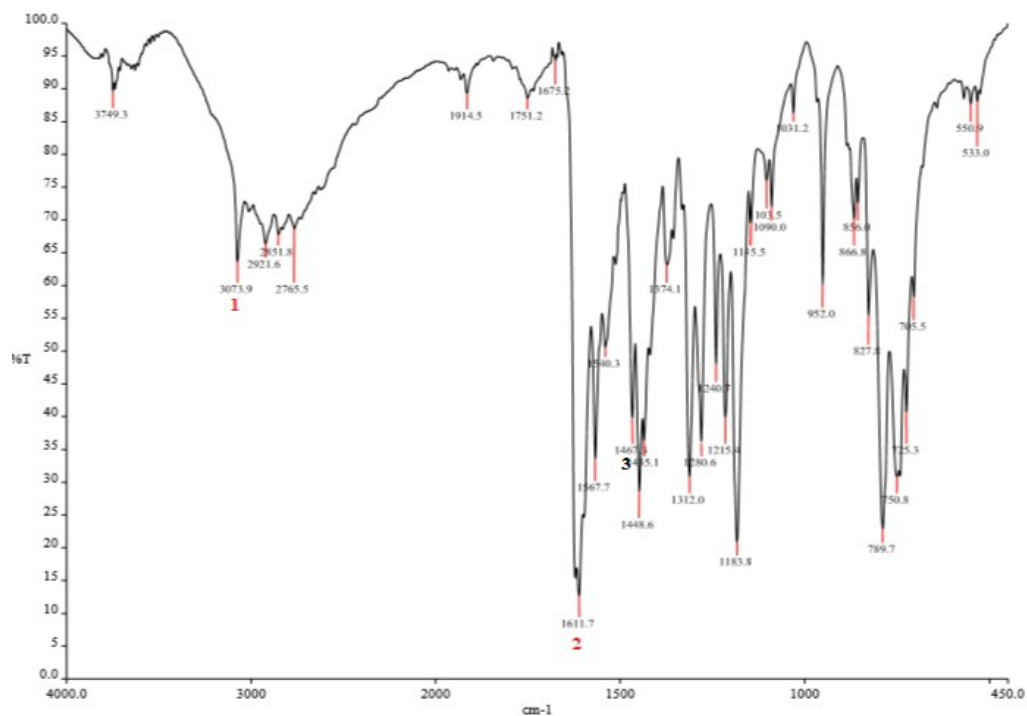


Fig. SI 3. Infrared spectra of compound **1** in KBr pellet

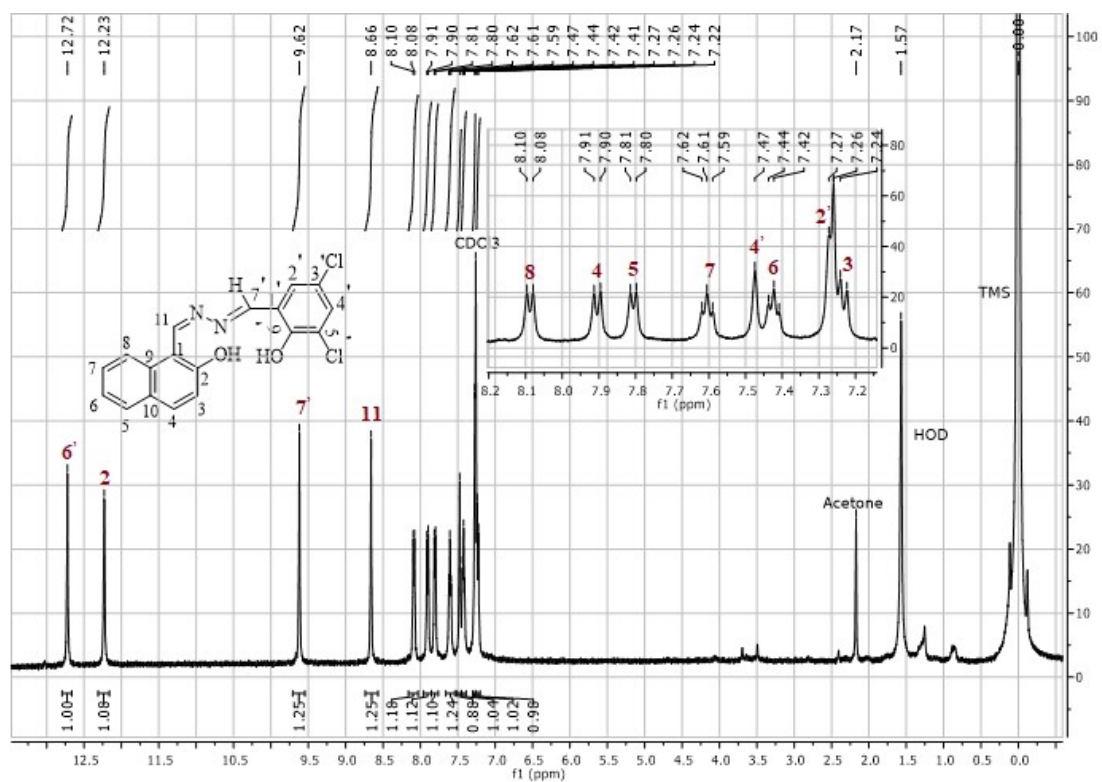


Fig. SI 4. $^1\text{H-NMR}$ spectra of compound **1** (500 MHz, CDCl_3)

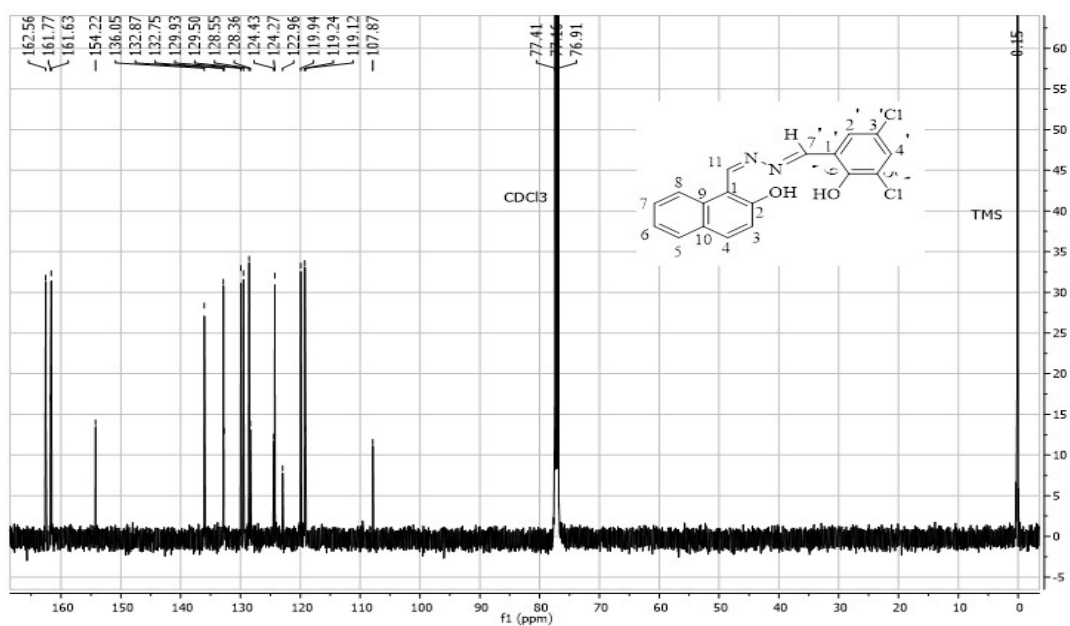


Fig. SI 5. ^{13}C -NMR spectra of compound 1 (125 MHz, CDCl_3)

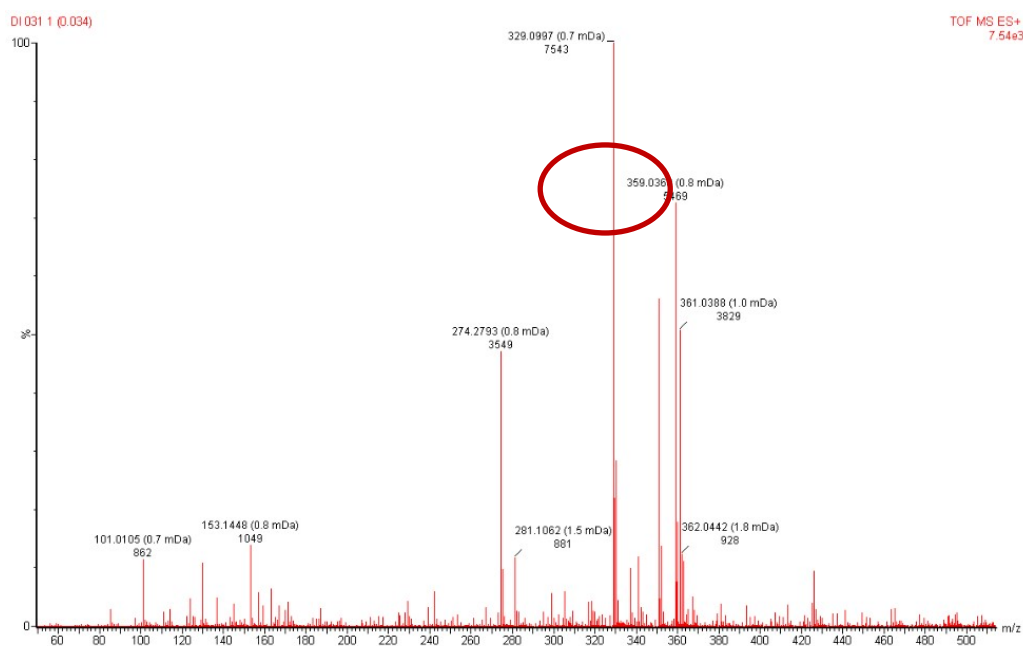


Fig. SI 6. ToF-HRMS spectra of compound 1 (ES^+)

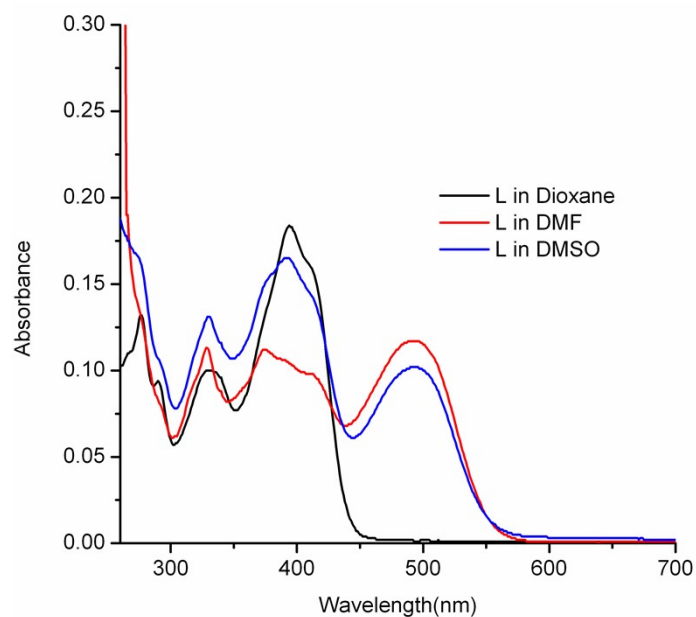


Fig. SI 7. UV/Vis spectra of compound **1 (L)** at various aprotic solvents ($c_{tot} 5 \times 10^{-5}$ mole dm^{-3})

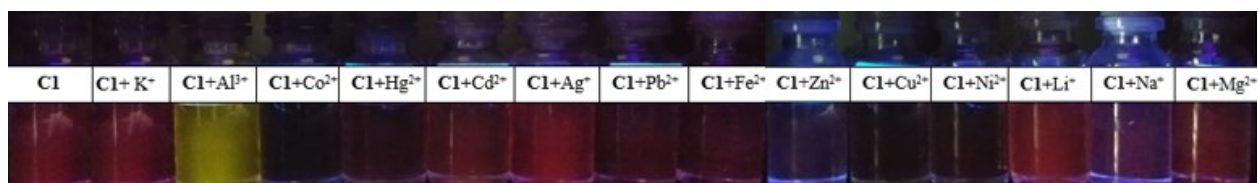


Fig SI 8. Fluorescence changes of compounds **1 (C1)** induced by various metal ions in DMSO under UV light 365 nm. (1:1, mole ratio, $c_{total} 10^{-5}$ mole dm^{-3})

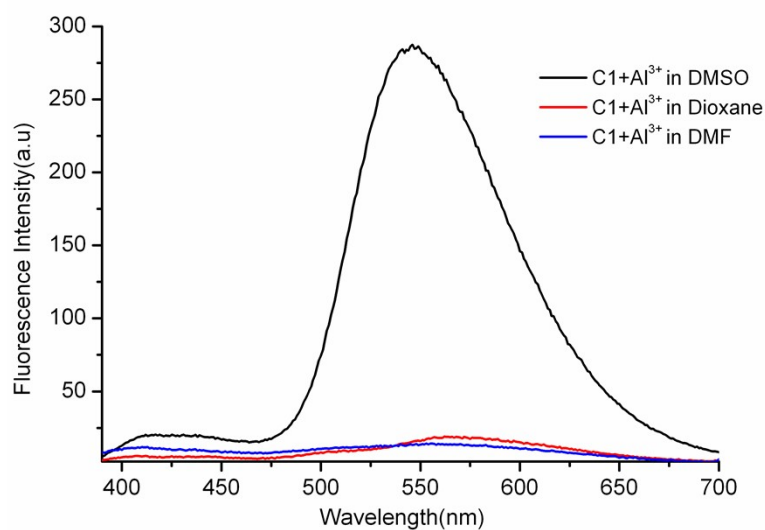


Fig SI 9. Emission spectra of compound **1 (C1)** with the addition of Al^{3+} in DMSO, DMF, and dioxane (1:1, mole ratio, $c_{total} 10^{-5}$ mol dm^{-3} , $\lambda_{ex} 360$ nm)

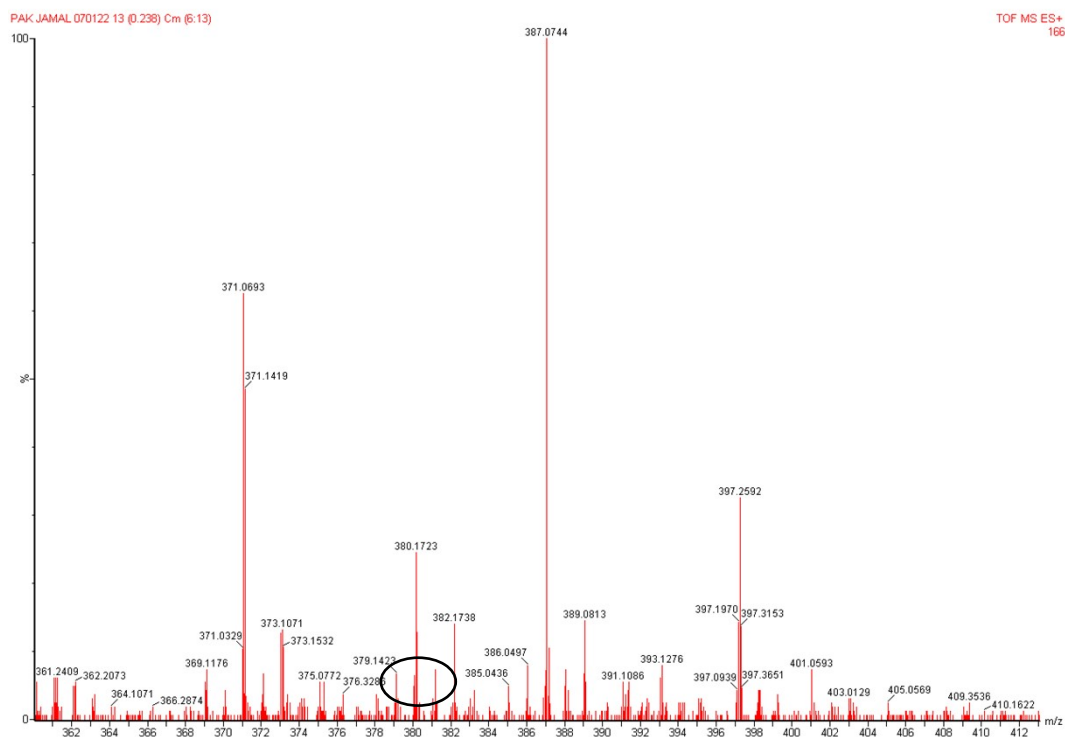


Fig. SI 10. ToF-HRMS spectra of compound **1**+Al³⁺ (ES⁺)

Table SI 1. Calculated imaginary frequency values of vibrated atoms of compound **1**

Mode	Frequency/cm ⁻¹	IR Intensity/km mol ⁻¹
1	17.68	0.5215
2	27.92	0.1514
3	61.16	0.4514
4	69.08	2.8846
5	112.06	3.8562
6	117.44	1.0852
7	131.91	0.2649
8	159.71	2.6537
9	175.11	1.7022
10	185.97	1.4276
11	190.67	22.5292
12	207.62	42.5277
13	216.14	16.5373
14	272.22	3.5125
15	284.81	18.1407
16	311.89	2.4789
17	324.8	8.3081
18	368	65.9319
19	370	6.6616
20	375.71	0.2988