Electronic Supplementary Information

Rhodamine based fluorescent chemosensor for Al^{3+}: Is it possible to control metal ion selectivity of rhodamine-6G based chemosensor?

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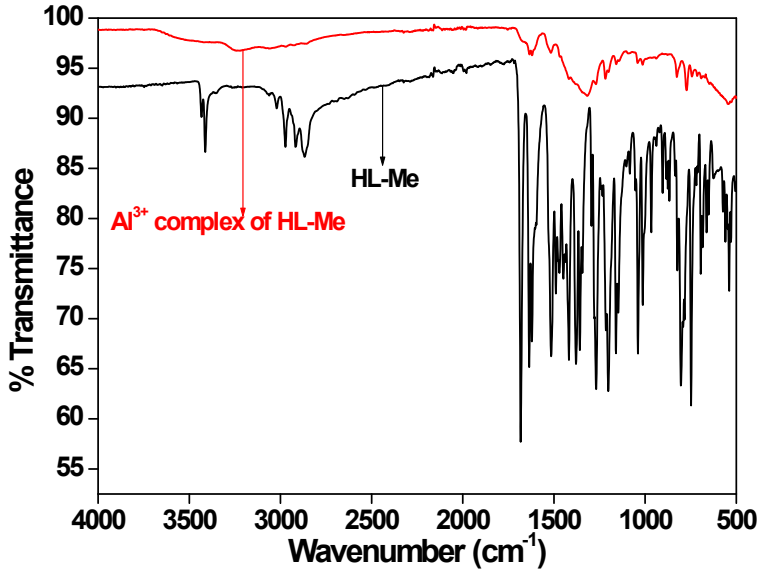

Fig. s1: FT-IR spectra of HL-Me and its Al^{3+} complex

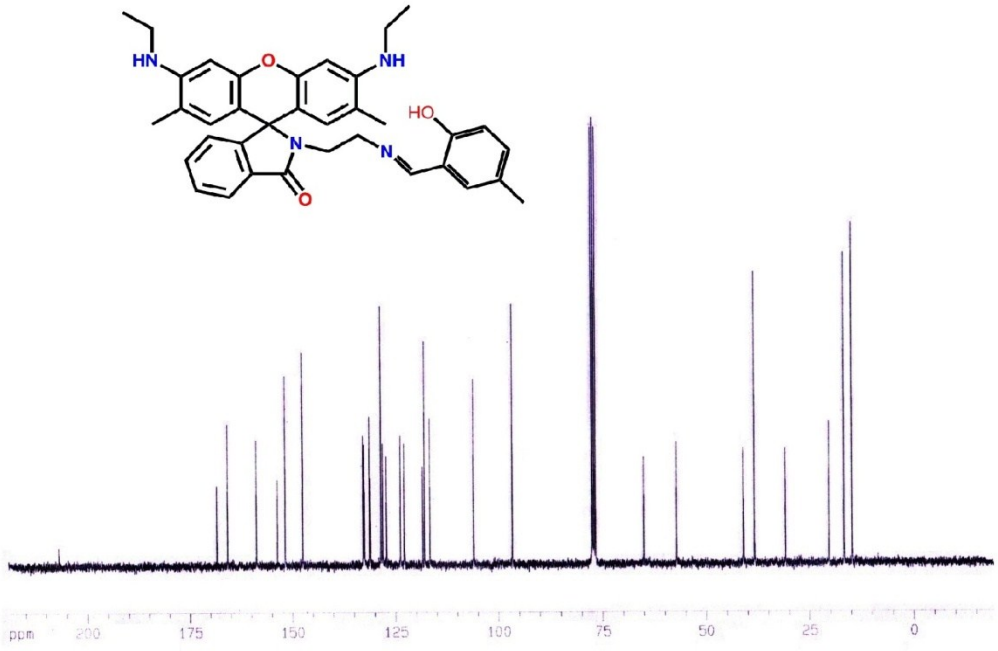

Fig. s2: ^{13}C NMR Spectrum of HL-Me in $CDCl_3$

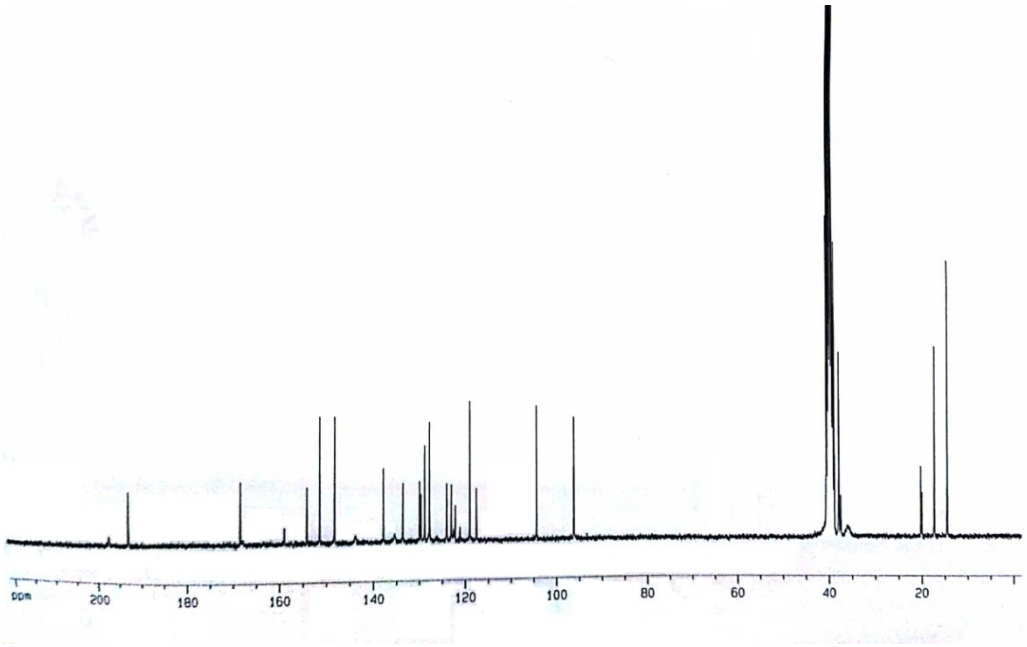

Fig. s3: ^{13}C NMR Spectrum of HL-Me in the presence of Al^{3+} ion in DMSO-d_6

Fig. s4: Mass spectrum of HL-Me in methanol

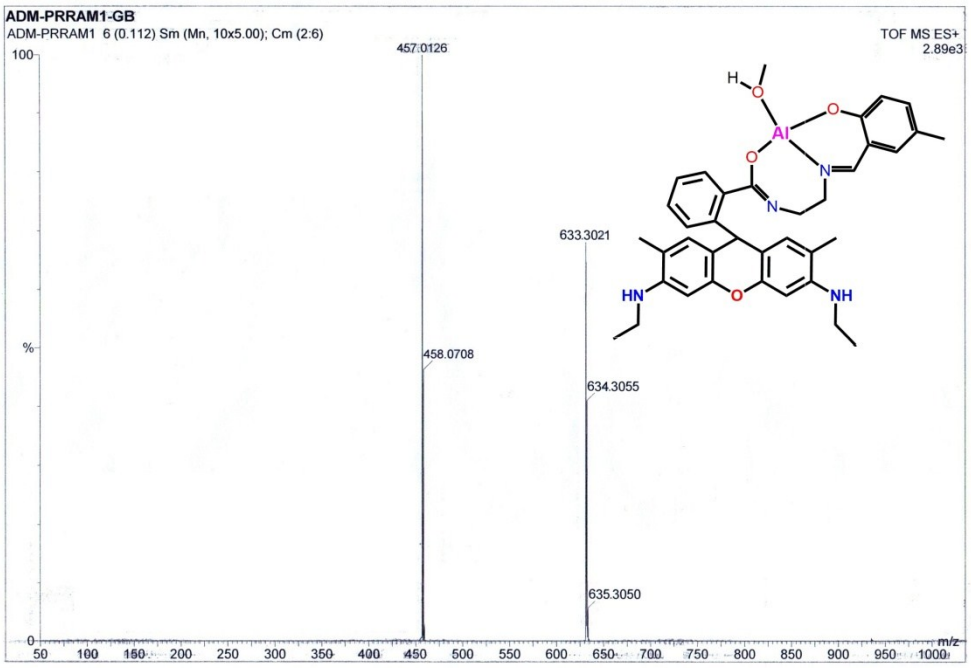

Fig. s5: Mass spectrum of HL-Me with Al^{3+} i.e. Al-(L-Me) complex in methanol

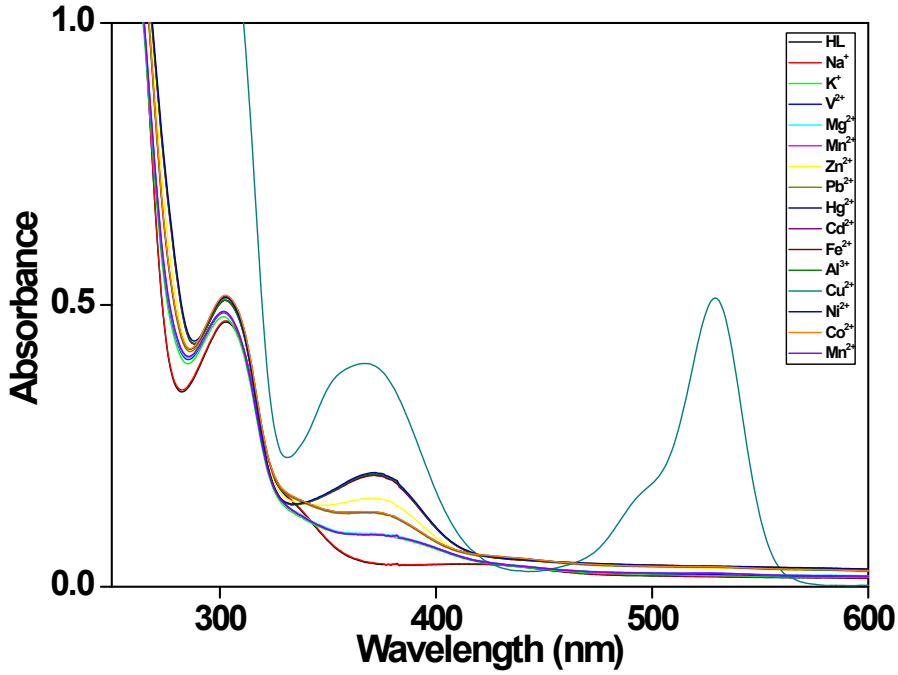

Fig. s6: Absorption spectra of HL-Me (40 μM) upon addition of in the presence of one equivalent of different metal ions in 10 mM HEPES buffer at pH 7.4 in H_2O/MeOH =1:9 (v/v) at 25 °C

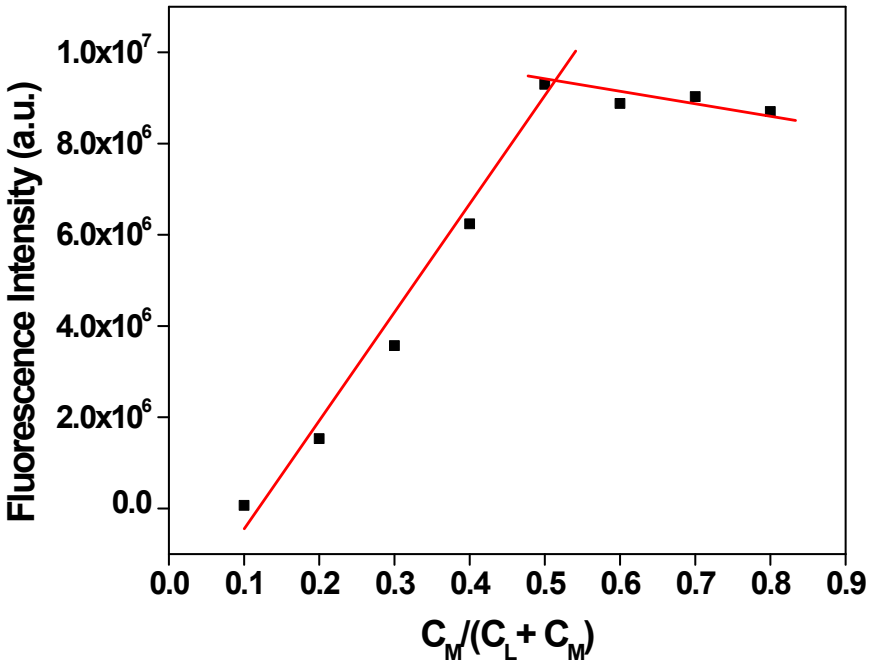

Fig. s7: Job's plot analysis of HL-Me shows formation of 1:1 complex with Al^{3+}

Determination of LOD of HL-Me:

Limit of detection (LOD) for our probe has been determined by 3σ method by the following equation: DL = K* Sb1/S

where K = 2 or 3 (3 in this case); here Sb1 is the standard deviation of the blank solution (Fig. s8); and S is the slope of the calibration curve obtained from Linear dynamic plot of F.I. vs $[Al^{3+}]$ M (Fig. s9).

Here Sb1= 331.61298, S=3.47518×10^{11}

LOD (Al^{3+}) = $(3 \times 331.61298)/ (3.47518 \times 10^{11})$ = 2.8627 nM

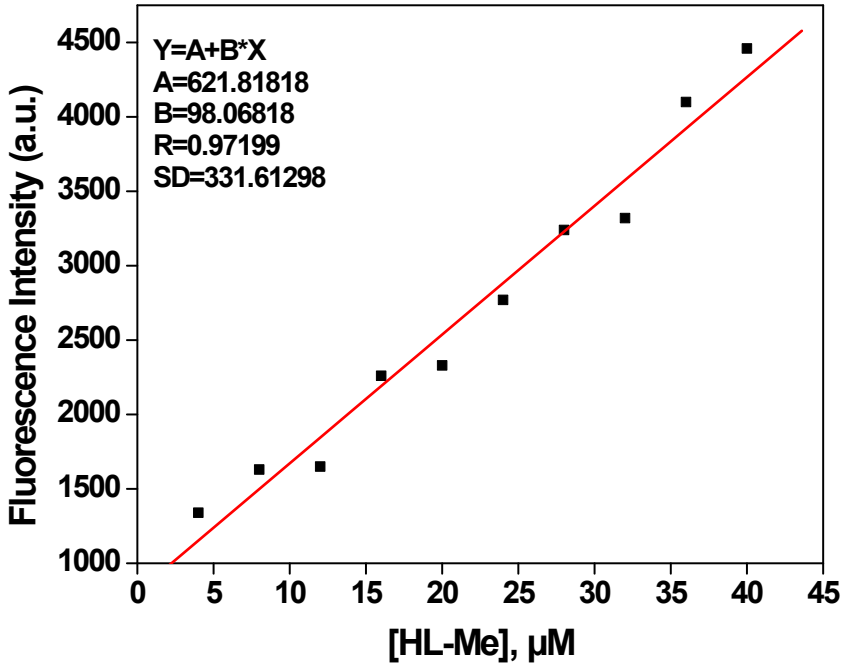

Fig. s8: Determination of Sb1 of the blank, HL-Me solution.

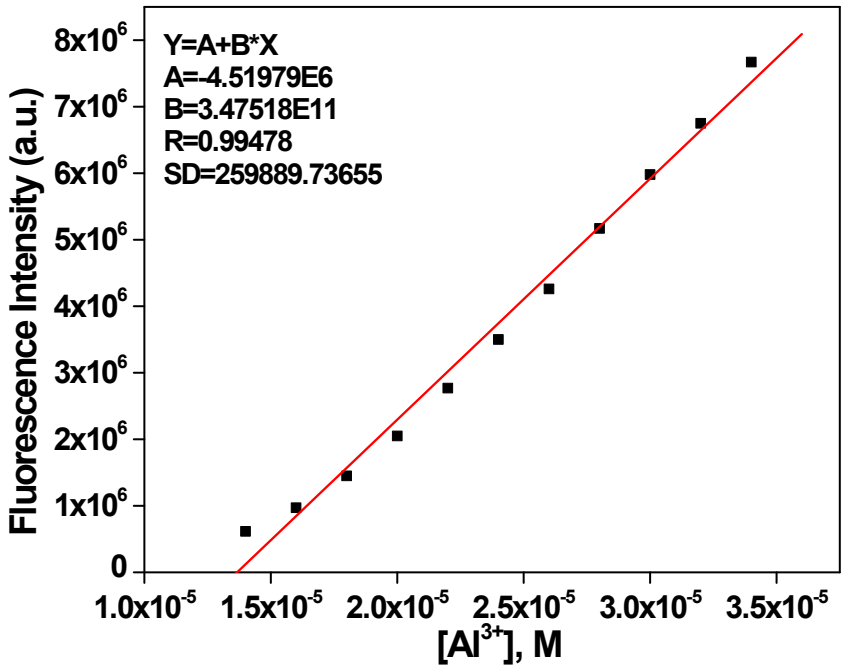

Fig. s9: Linear dynamic plot of F.I. (at 552 nm) vs. [Al^{3+}] for the determination of S (slope); [HL-Me] = 40 µM

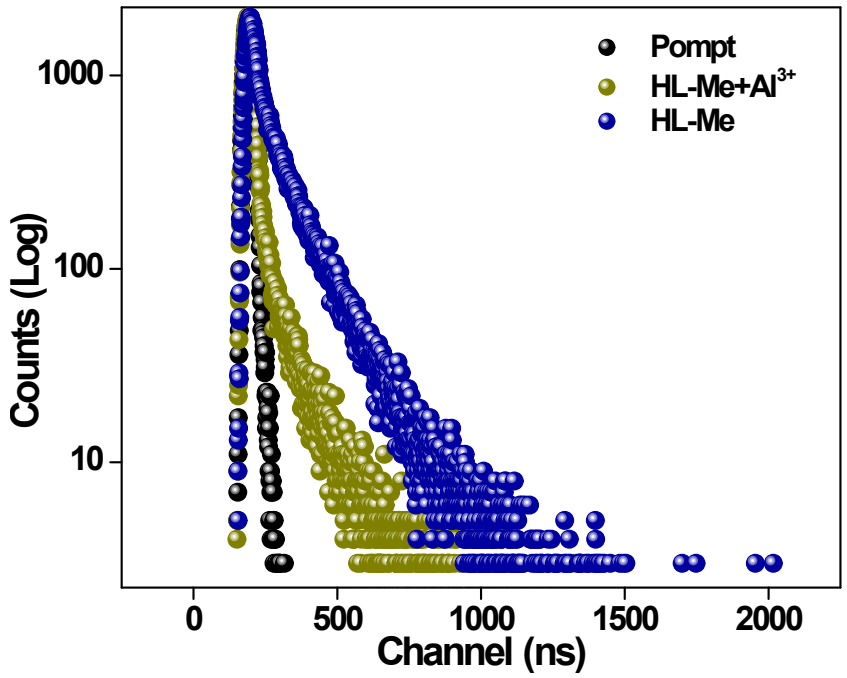

Fig. s10: Excited state fluorescence decay behavior of HL-Me and its complex with Al^{3+} ion in 10 mM HEPES buffer at pH 7.4 in H_2O:MeOH (1:9, *v/v*) at room temperature.

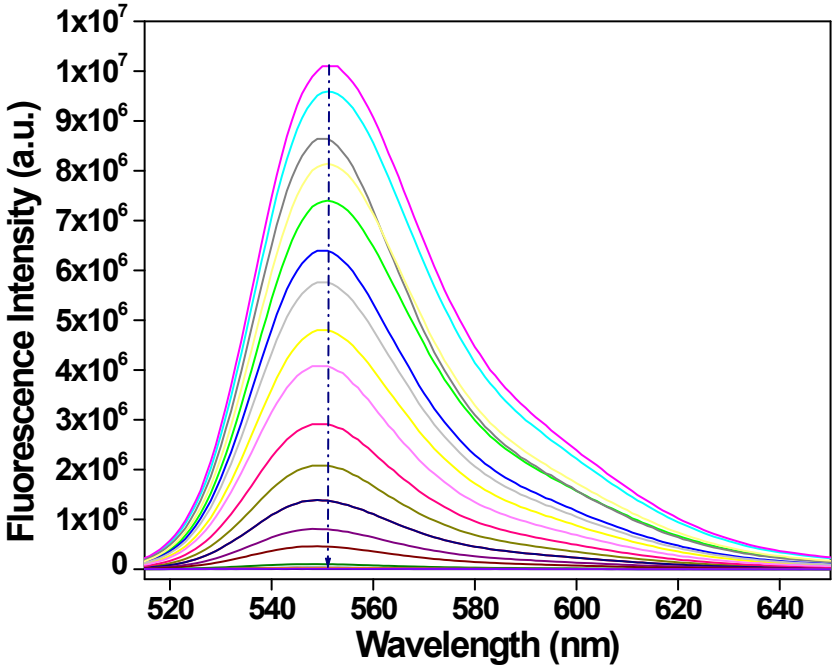

Fig. s11: Fluorescence spectra of Al-L-Me complex (40 μM) upon addition of (0-44 μM) AsO_4^{3-} ion in 10 mM HEPES buffer at pH 7.4 in H_2O/MeOH =1:9 (v/v) at 25 °C.

Table s1: Crystal data of HL-Me

Formula	$C_{36}\ H_{38}\ N_4\ O_3$
formula weight	574.70
crystal system	monoclinic
space group	P21/n
a/Å	12.7536(5)
b/Å	16.6911(6)
c/Å	14.2331(5)
α/°	90.00
β/°	95.369(2)
γ/°	90.00
V/Å^3	3016.53(19)
Z	4
Dc/g cm^{-3}	1.265
μ/mm^{-1}	0.081
F(000)	1224
θ range/°	1.9-28.1
reflections collected	27355
unique reflections	7301
reflections I > 2σ(I)	4613
R_{int}	0.031
goodness-of-fit (F2)	0.94
R_1 (I > 2σ(I))[a]	0.0475
wR_2 (I > 2σ(I))[a]	0.1529
Δρ max/min/e Å^3	-0.21, 0.16

Table s2: Selected bond lengths (in Å) and selected bond angles (°) of HL-Me

N3-C21	1.447(2)	O3-C29	1.351(2)
N3-C20	1.366(2)	C19-C20	1.479(2)
N3-C13	1.504(2)	C21-C22	1.519(2)
N4-C23	1.271(2)	C13-C14	1.522(2)
N4-C22	1.450(2)	C14-C19	1.381(2)
O2-C20	1.224(2)	C24-C29	1.397(2)
C22-N4-C23	119.0(1)	N4-C22-C21	110.3(1)
C20-N3-C21	123.1(1)	N4-C23-C24	122.1(2)
C21-N3-C13	122.3(1)	O2-C20-N3	125.6(1)
C13-N3-O20	113.7(1)	O3-C29-C24	122.2(2)