Specific Recognition of Cr^{3+} in Physiological Condition by allyl substituted appendage Rhodamine and Its Cell-Imaging Studies

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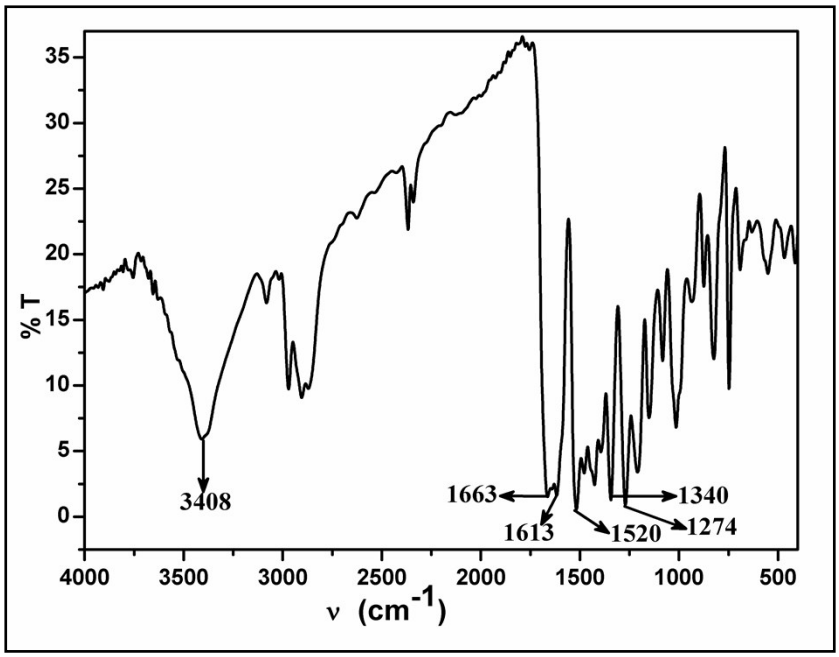

Fig. S1. FT-IR spectrum of RD-3 in KBr disc

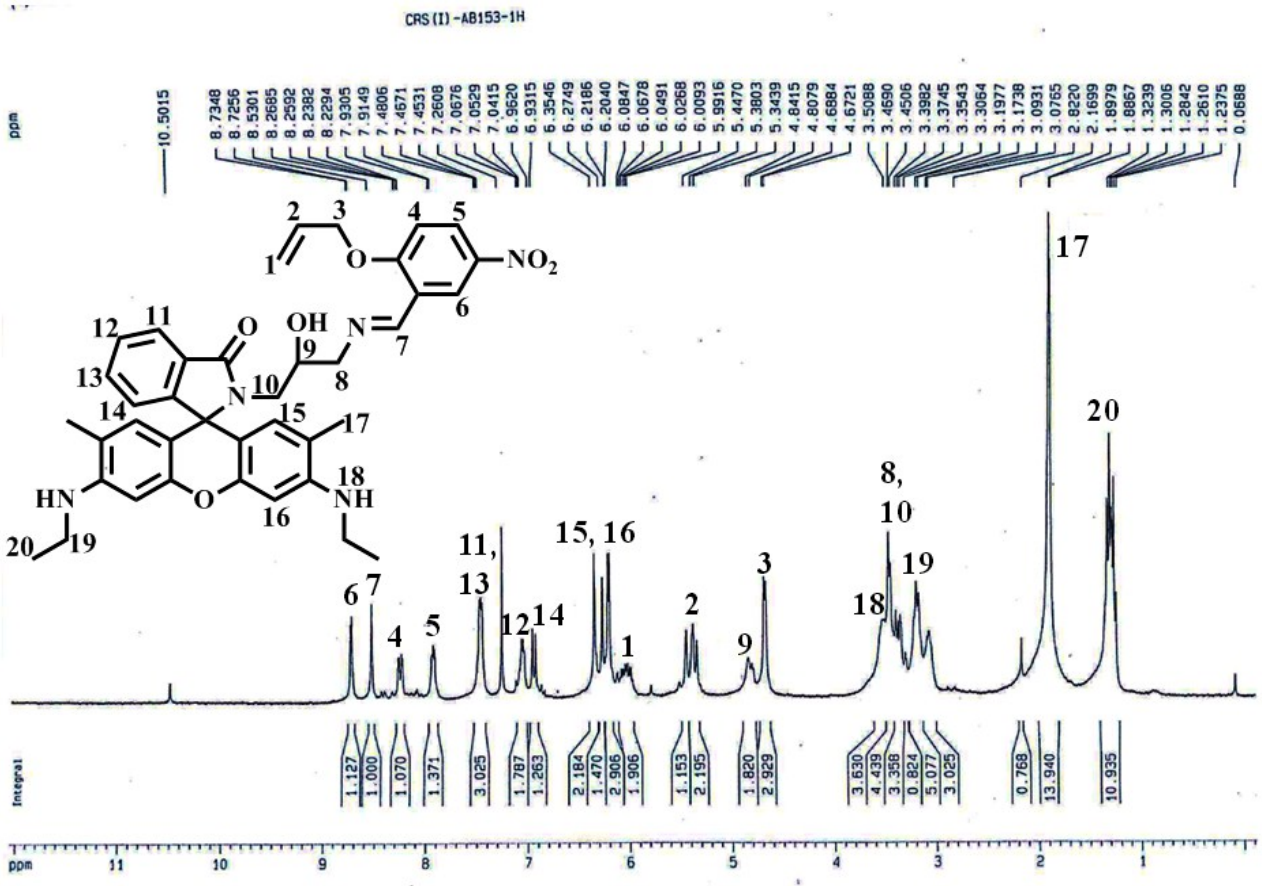

Fig. S2. ^{1}HNMR spectrum of RD-3 in $CDCl_3$

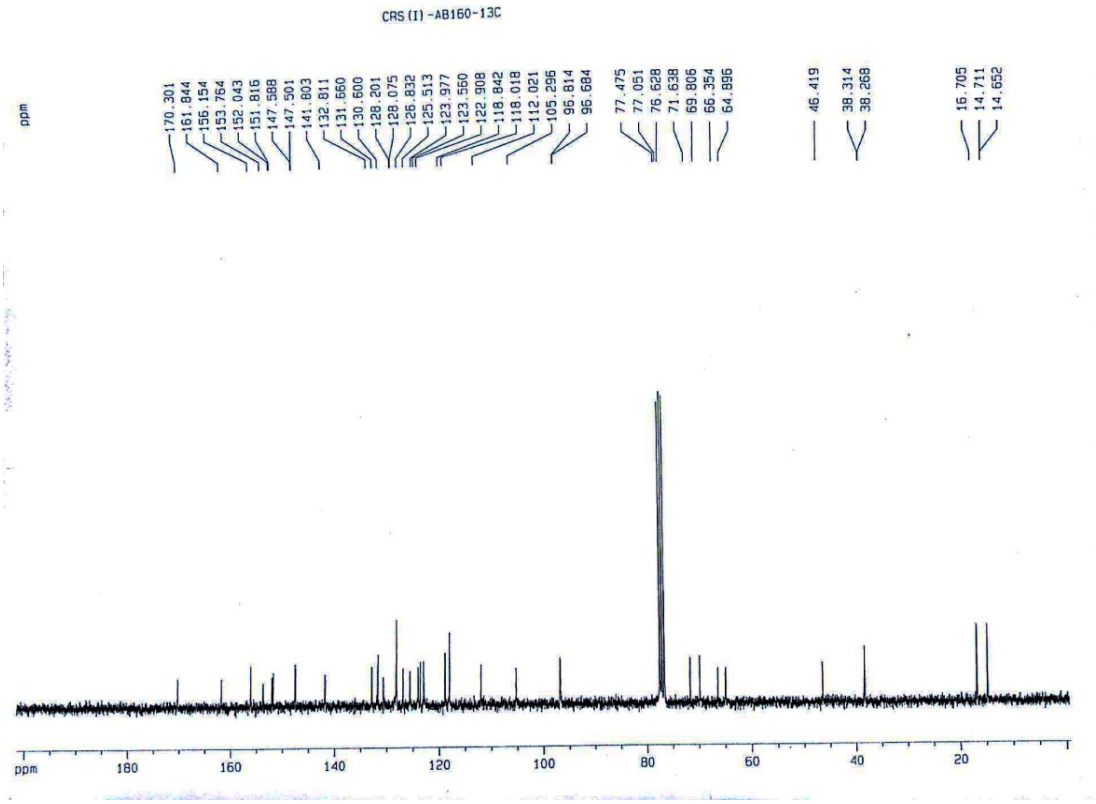

Fig. S3. ^{13}CNMR spectrum of RD-3 in $CDCl_3$

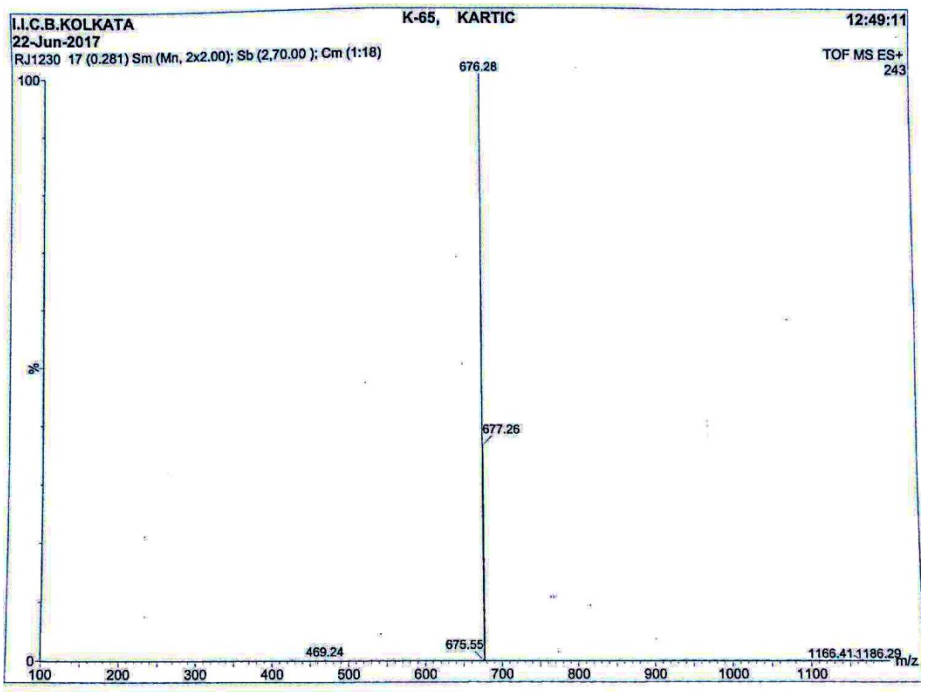

Fig. S4. Mass spectrum of RD-3

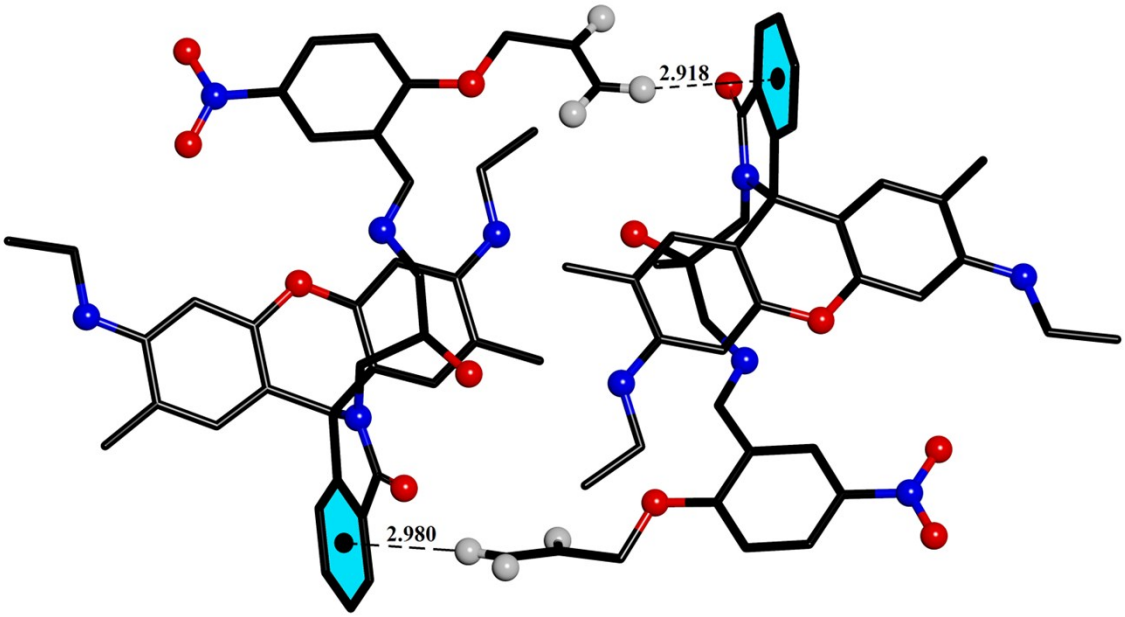

Fig.S5. C-H-π interaction of RD-3

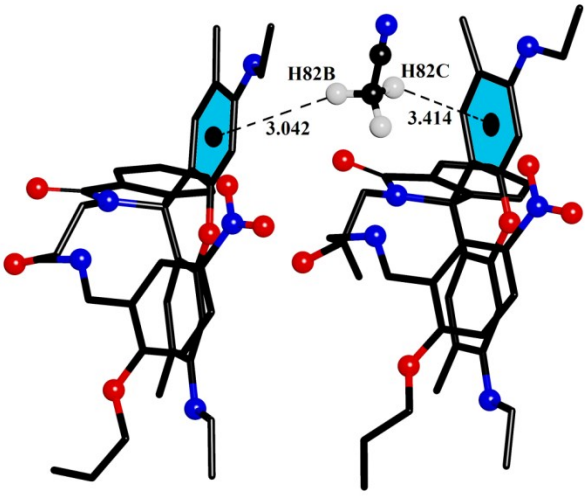

Fig.S6. Interaction of the probe(RD-3) with solvent molecule (CH_3CN)

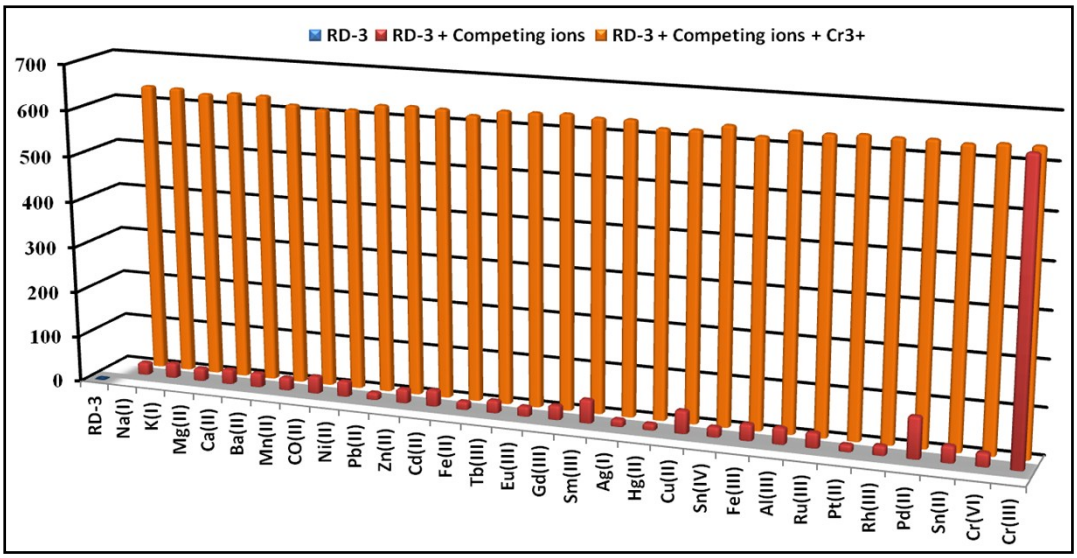

Fig. S7. Fluorescence intensity changes profiles of 50 μM RD-3 in CH_3CN/water (HEPES buffer, pH = 7.4; v/v, 1/4) in presence of selected metal ions for Cr^{3+}

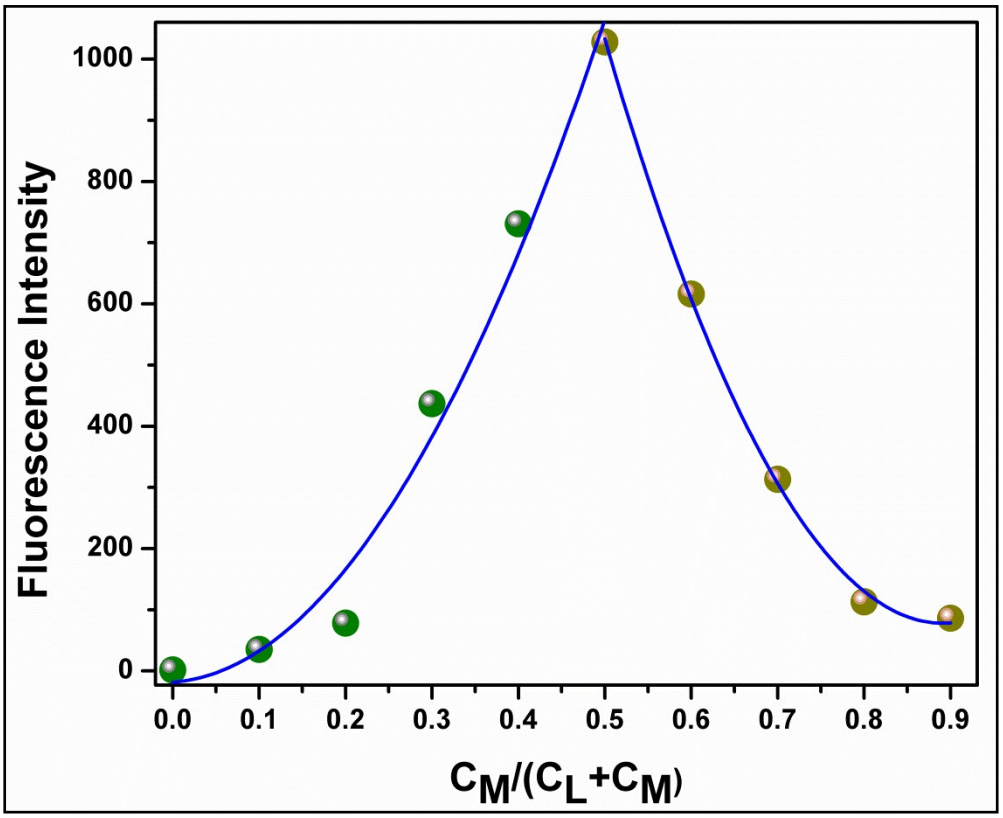

Fig.S8. The Job's plot shows 1:1 stoichiometry between [RD-3] and [Cr^{3+}]

Determination of the apparent binding constants

Benesi-Hildebrand equation is given as:

$$\frac{(F_{MAX} - F_O)}{F - F_O} = 1 + \frac{1}{K\sqrt{[M^{n+}]}}$$

F_0 is the fluorescence of HL in the absence of externally added Zn^{2+} and Al^{3+}, F is the fluorescence obtained at different $[Zn^{2+}]$ and $[Al^{3+}]$ (λ_{ex} = 372 nm and λ_{em} = 508 nm , 585 nm respectively) and with F_{max} is the fluorescence of HL at $[Zn^{2+}]$ and $[Al^{3+}]$ in large excess. K is the association constant

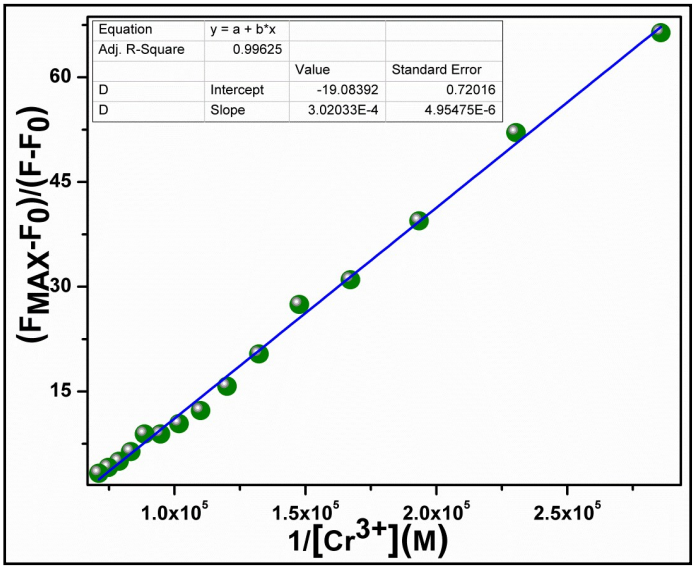

Fig.S9. Binding constant of Cr^{3+} with RD-3 in mixed aqueous media at pH 7.4

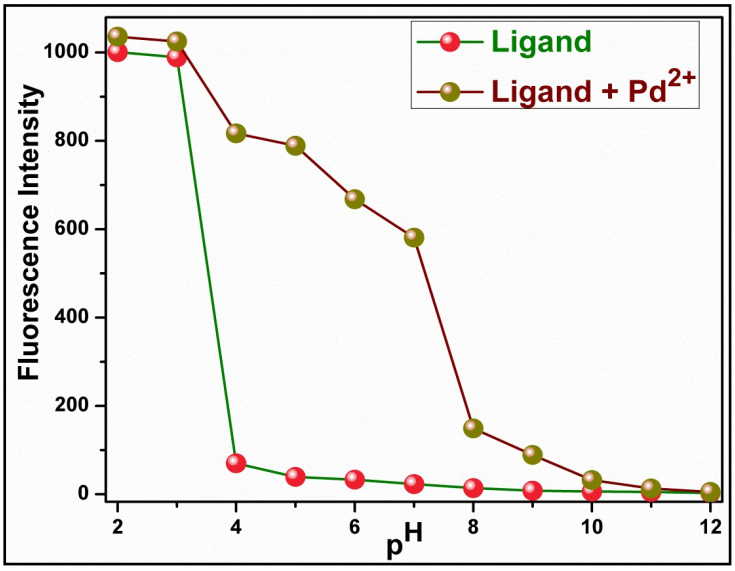

Fig. S10. Effect of pH on the fluorescence activity of Ligand (RD-3) and RD-3+Cr^{3+}

CH_3CN/water (v/v, 1/4)

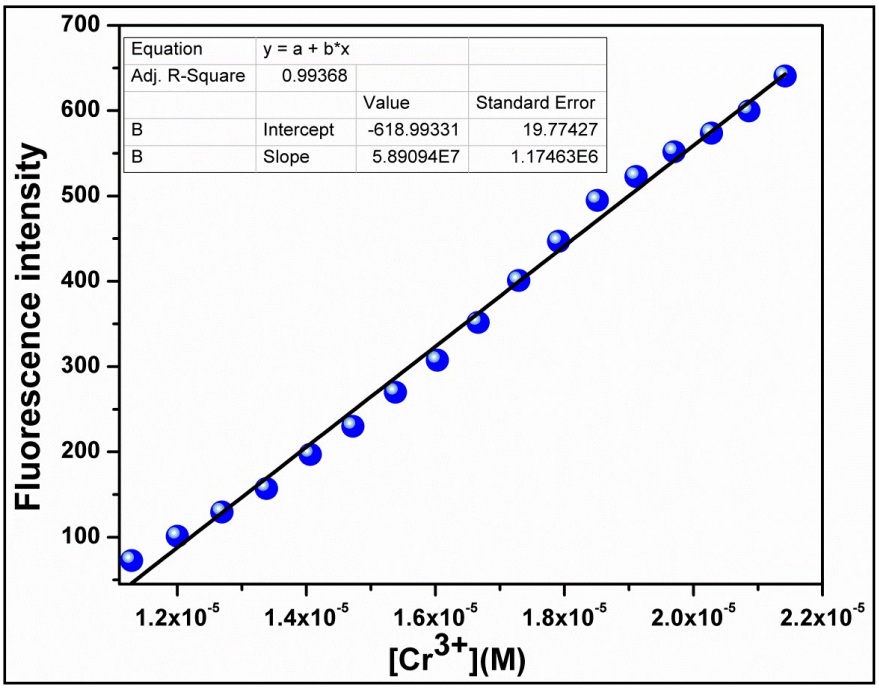

Fig. S11. The linear dynamic response of RD-3 for Cr^{3+} and the determination of the detection limit(LOD) of Cr^{3+}

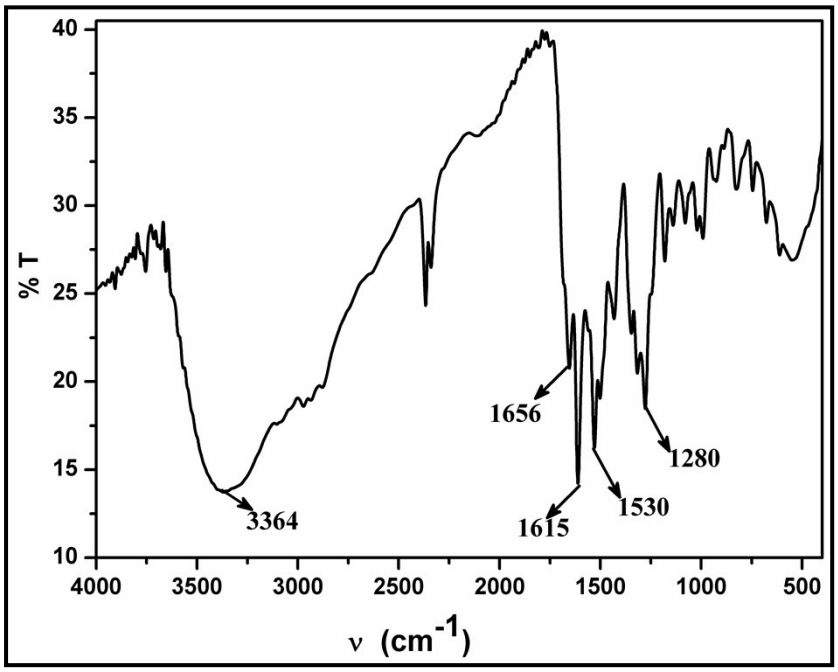

Fig. S12. FT-IR spectrum of Cr-Complex in KBr disc

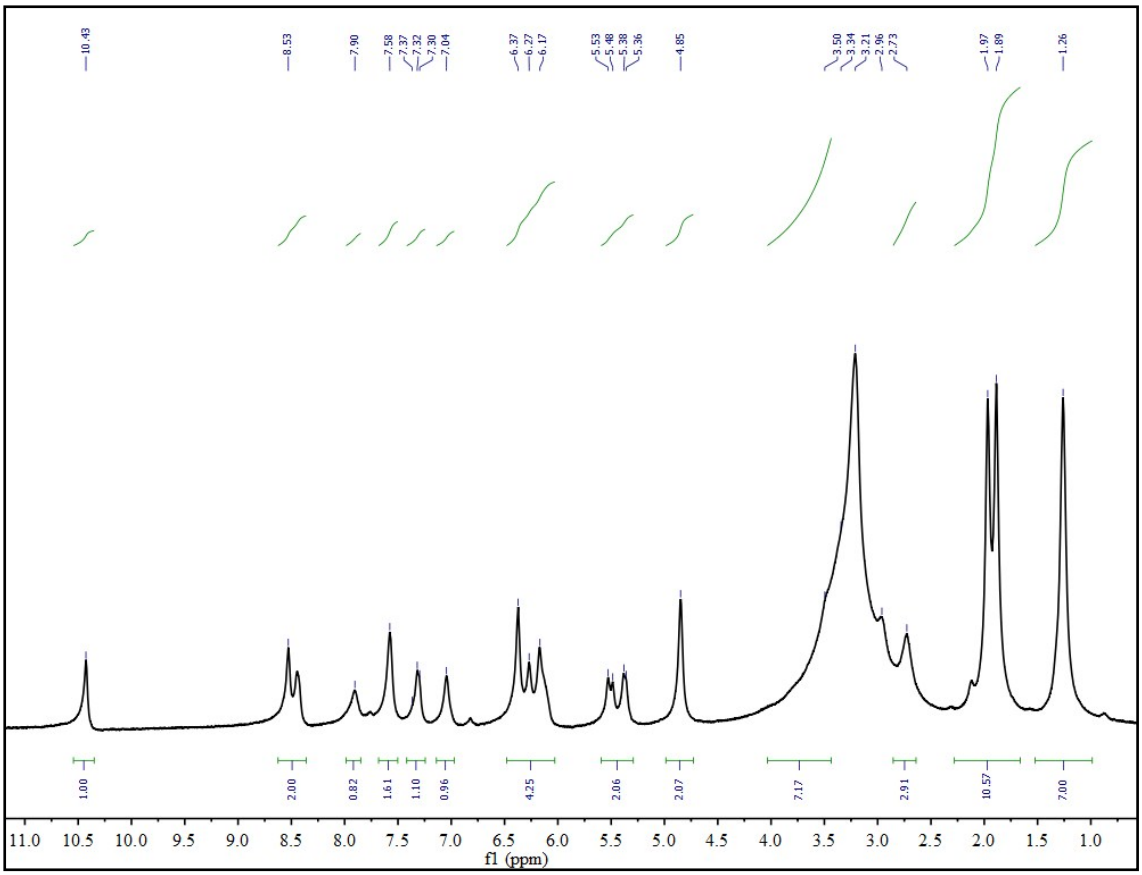

Fig. S13. [1]HNMR spectrum of Chromium Complex in CD_3CN

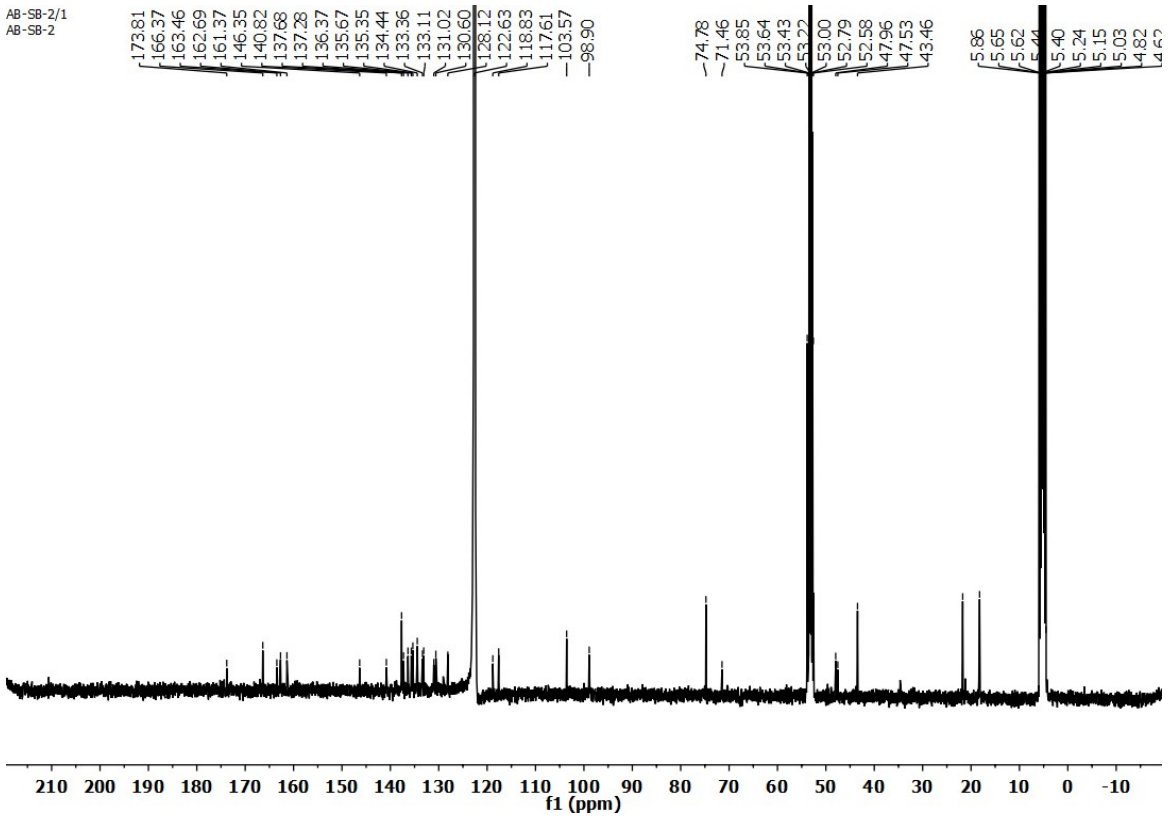

Fig. S14. [13]CNMR (400MHZ) spectrum of Cr-Complex in CD_3CN- CD_3OD

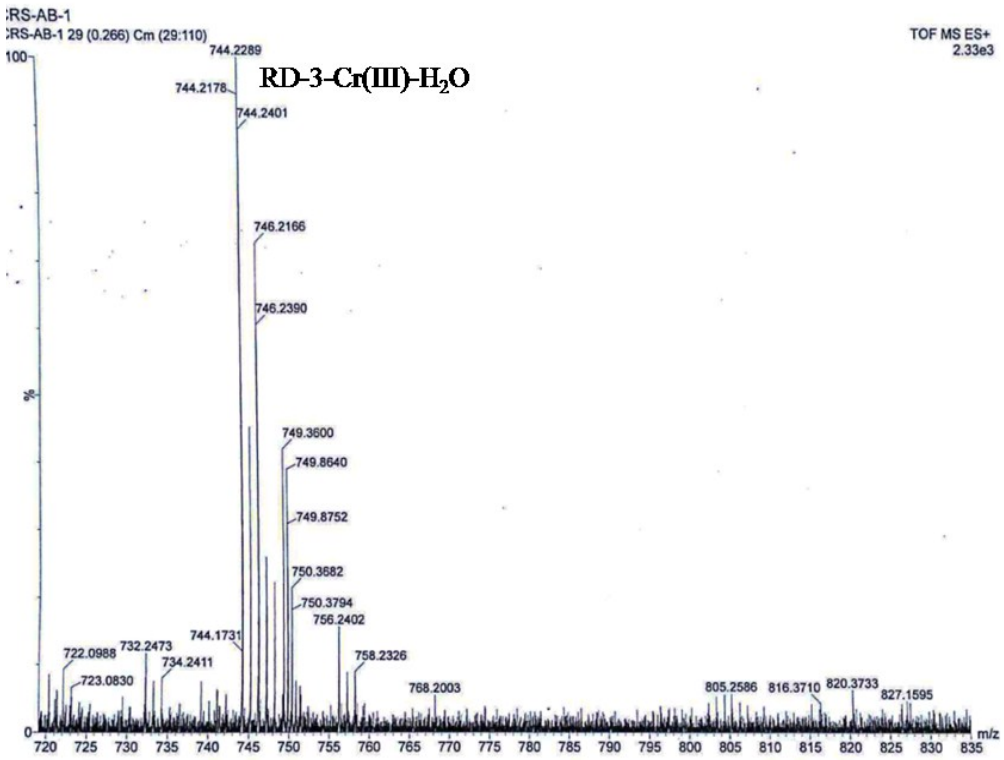

Fig. S15. Mass spectrum of Cr-Complex

Table S1. Bond parameters of RD-3

Bond Distance (Å)		Bond angle (°)	
N(67)-C(68) C(64)-N(67)	1.271 1.454	C(64)-N(67)-C(68)	121.39
C(72)-O(79) O(79)-C(80)	1.353 1.437	C(72)-O(79)-C(80)	119.90
C(30)-N(31) N(31)-C(34)	1.364 1.463	C(30)-N(31)-C(34)	124.15
C(18)-N(31) C(18)-C(19)	1.499 1.528	C(19)-C(18)-N(31)	100.38

Table S2. Bond parameters of Chromium Complex

Bond Distance (Å)		Bond angle (°)	
Cr-O(29) Cr-O(62)	1.823 1.782	O(29)-Cr-O(62)	103.62
Cr-O(91)	1.782	O(29)-Cr-O(91) O(62)-Cr-O(91)	127.31 121.83
O(29)-C(30) C(30)-N(31)	1.395 1.283	O(29)-C(30)- N(31)	124.11
C(32)-O(62) C(32)-C(34)	1.457 1.556	O(62)-C(32)-C(34)	109.52
N(66)-C(67) C(63)-N(66)	1.286 1.467	C(63)-N(66)-C(67)	122.53

Table S3. Composition and energy of MOs Chromium Complex

Orbital	Energy(eV)	Composition	
		Metal	Ligand
LUMO+10	-0.39	1	99
LUMO+9	-0.57	2	98
LUMO+8	-0.7	40	60
LUMO+7	-0.72	16	84
LUMO+6	-0.77	18	82
LUMO+5	-1.03	1	99
LUMO+4	-1.74	12	88
LUMO+3	-1.81	2	98
LUMO+2	-1.95	56	44
LUMO+1	-2.8	0	100
LUMO	-3.13	43	57
HOMO	-3.85	46	54
HOMO-1	-6.1	0	100
HOMO-2	-6.74	6	94
HOMO-3	-6.9	4	96
HOMO-4	-6.96	1	99
HOMO-5	-7.07	0	100
HOMO-6	-7.18	39	61
HOMO-7	-7.2	16	84
HOMO-8	-7.38	5	95
HOMO-9	-7.54	2	98
HOMO-10	-7.58	0	100

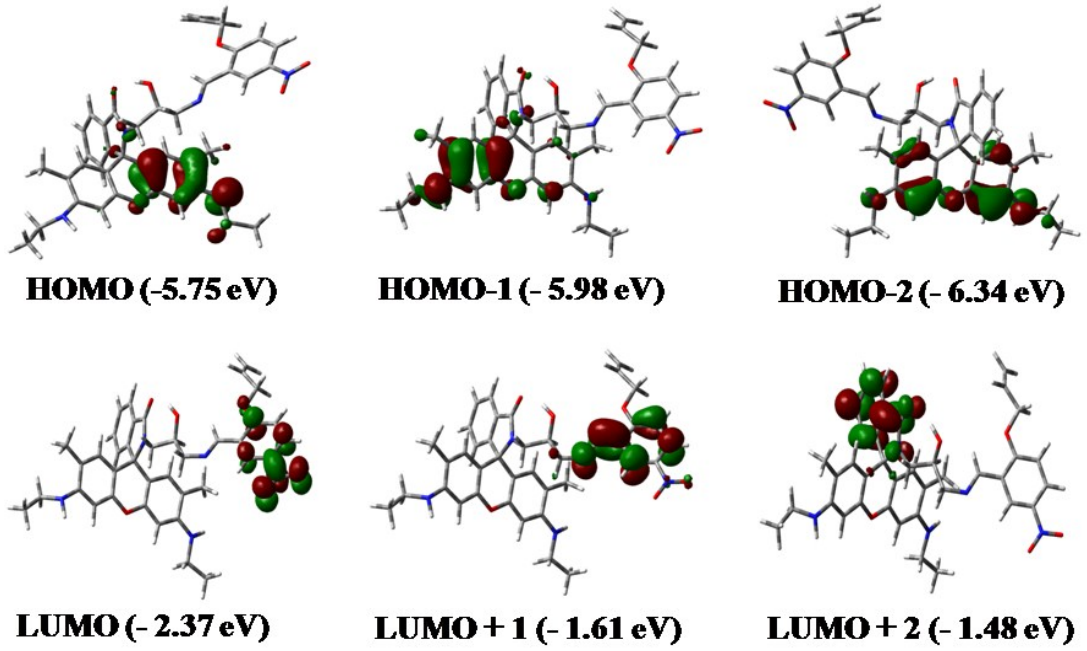

Fig. S16. Frontier molecular orbitals of RD-3

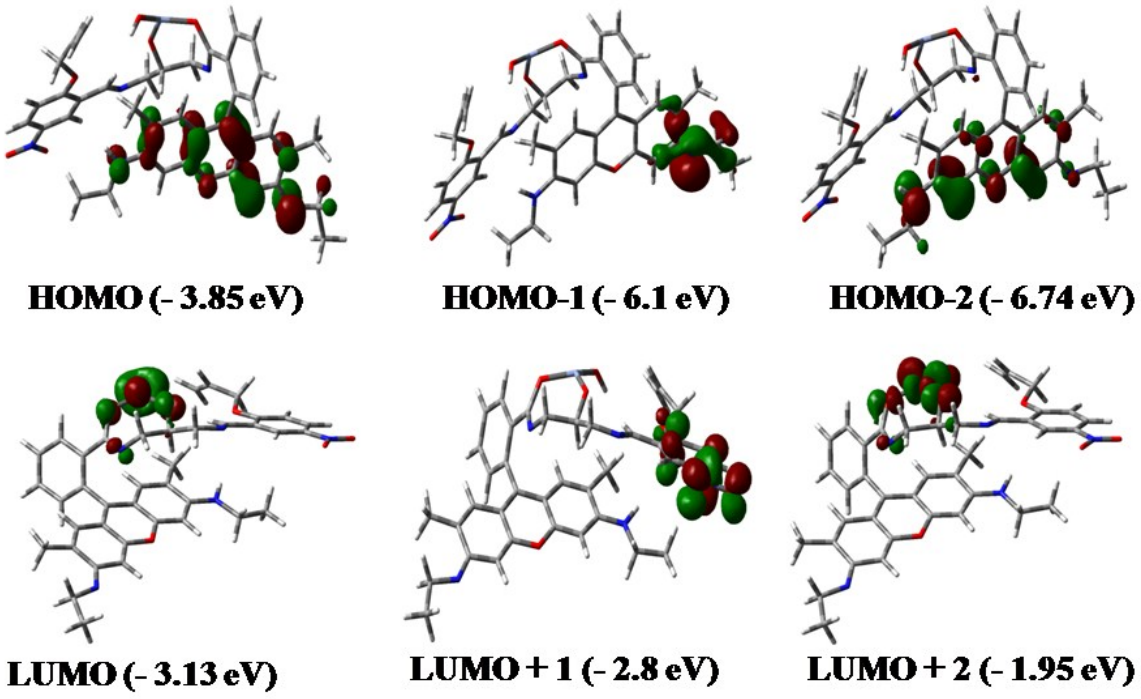

Fig. S17. Frontier molecular orbitals of Chromium Complex