Electronic Supplementary Material (ESI) for Analytical Methods

Supporting Information (ESI)

Thiophene anchored naphthalene derivative: Cr^{3+} selective turn-on fluorescent probe for living cell imaging

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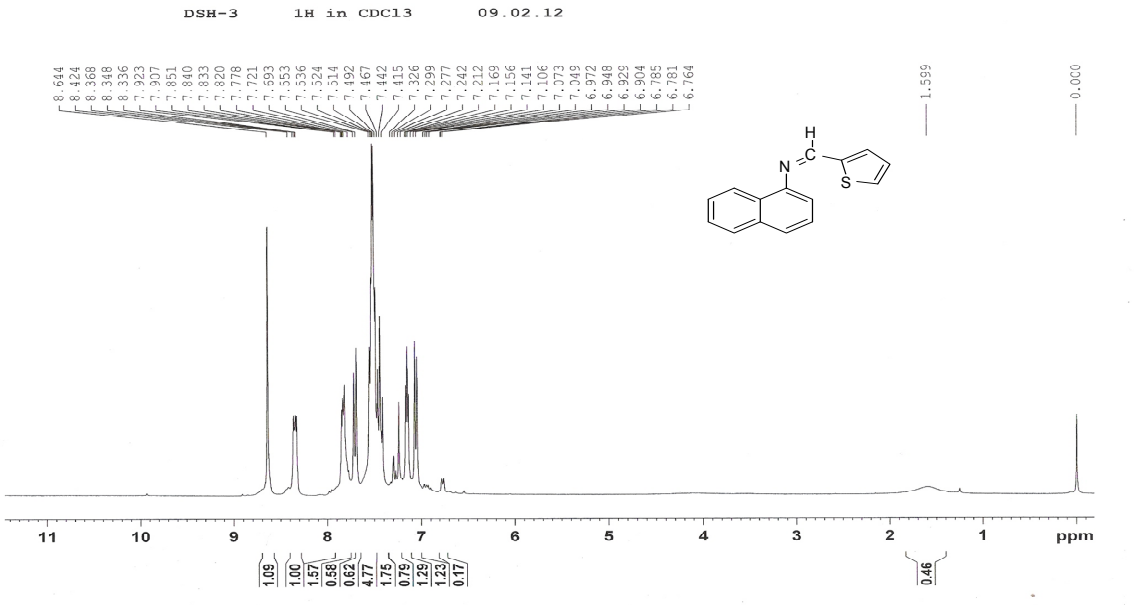

Fig. S1a. ^{1}H NMR spectrum of **L** in $CDCl_3$.

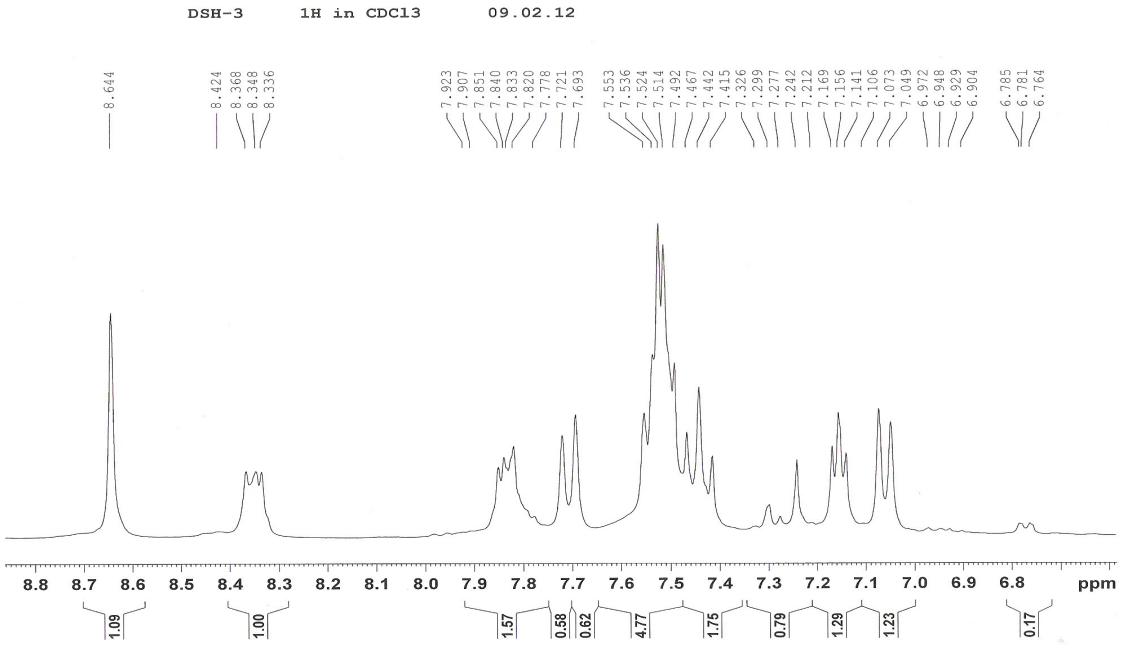

Fig. S1b. ^{1}H NMR spectrum (expanded to aromatic region) of **L** in $CDCl_3$.

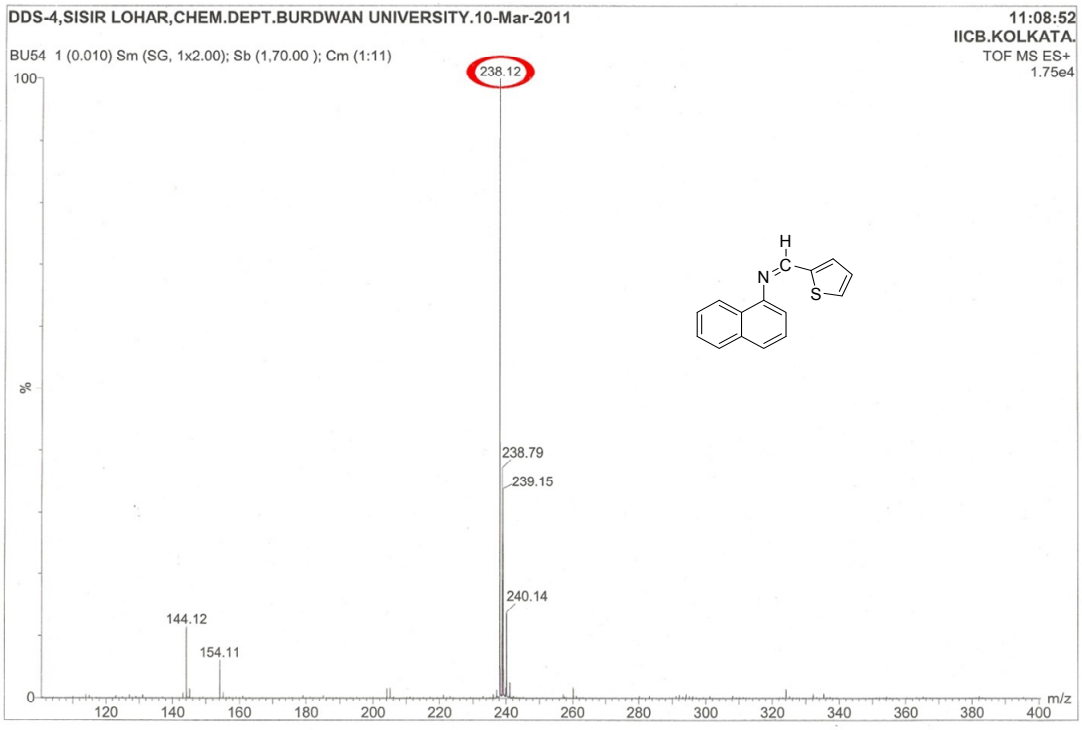

Fig. S2. Mass spectrum of **L** .

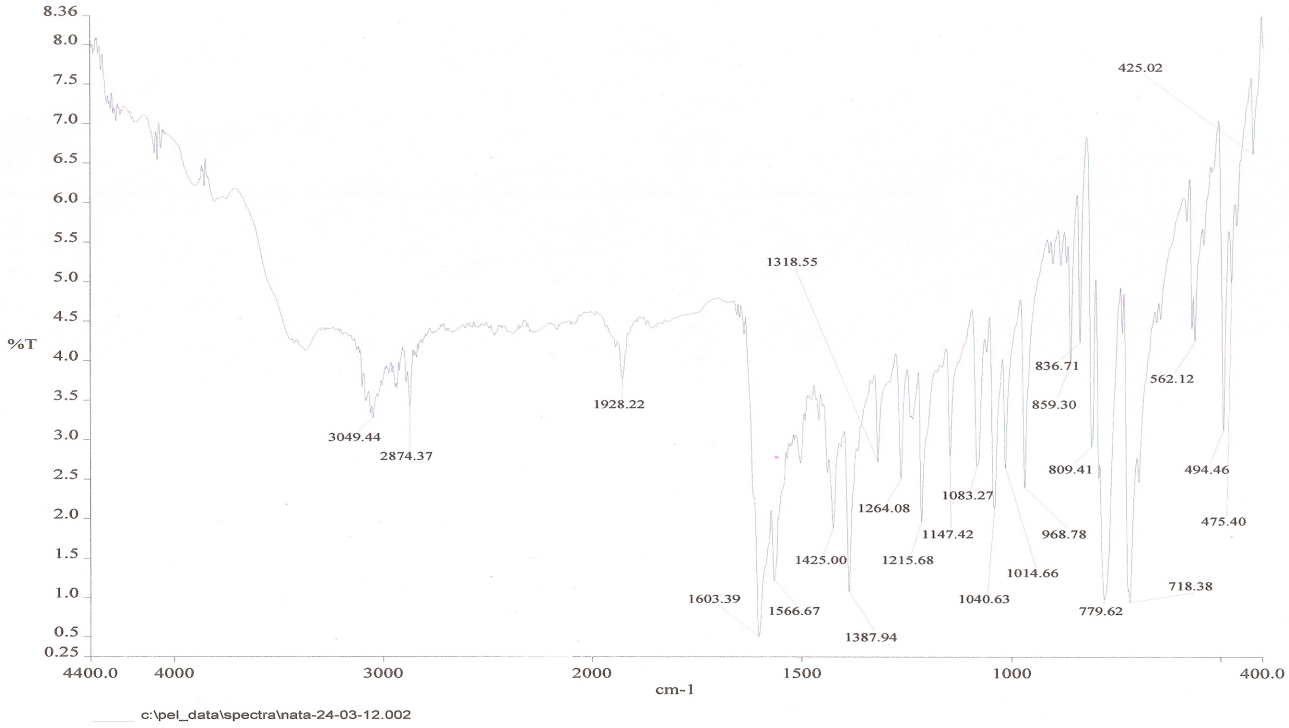

Fig. S3. FTIR spectrum of **L.**

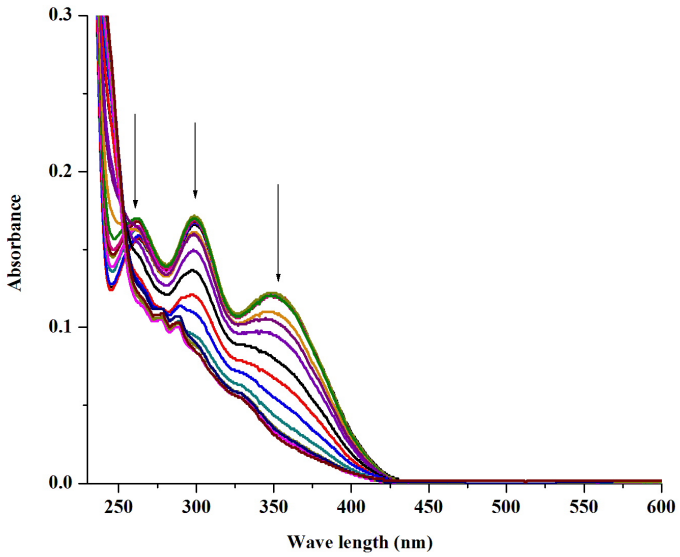

Fig . S4. UV-Vis spectral changes of **L** (10 μ M) with gradual addition of 0.1 to 5.5 times [Cr^{3+}] from top to bottom.

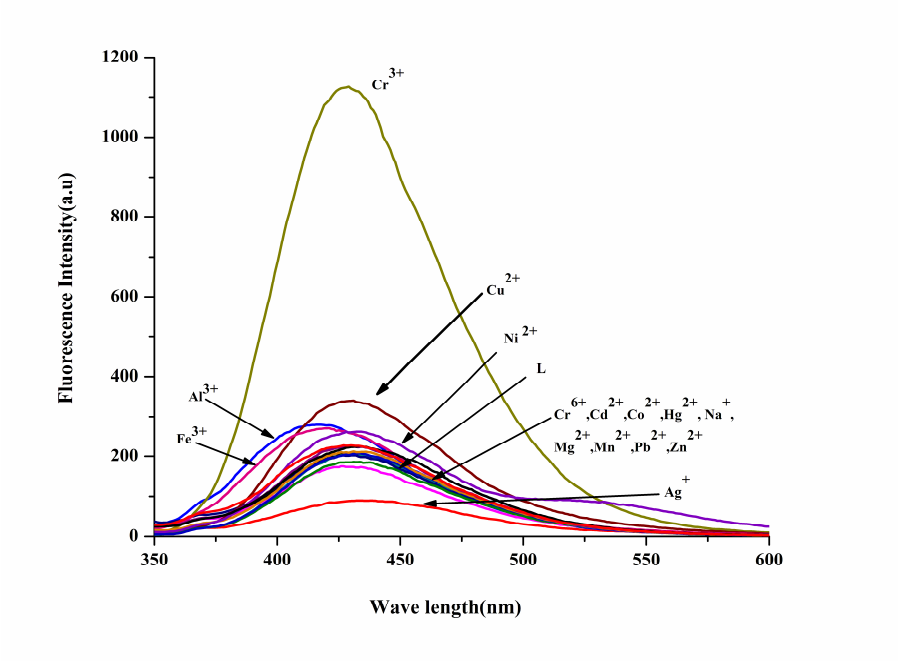

Fig. S5. Fluorescence spectra of **L** (10 μM), **L** + Cr^{3+} (45 μM) and **L** (10 μM) + M^{n+} (300 μM), where M^{n+} = Na^{+}, Mg^{2+}, Cr^{6+} ($Cr_2O_7^{2-}$), Mn^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Hg^{2+}, Pb^{2+}, Cd^{2+}, Ag^{+}, Al^{3+} (λ_{em}: 435 nm, λ_{ex}: 330 nm).

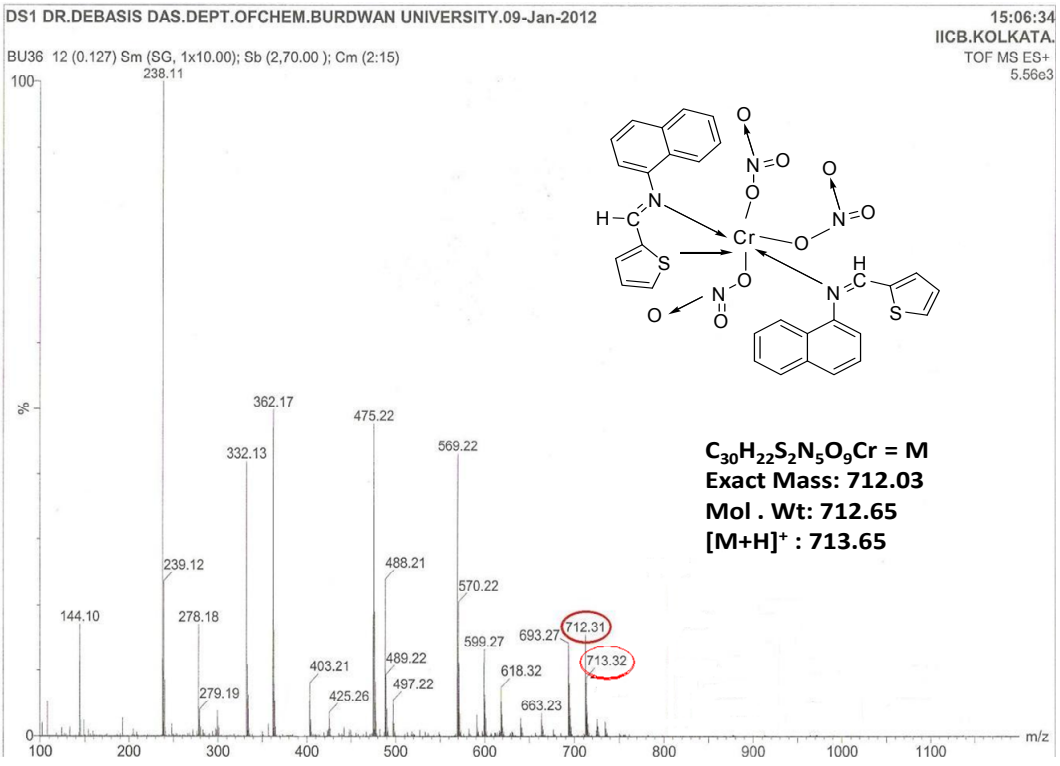

Fig. S6 Mass spectrum of **L**-Cr^{3+} complex.

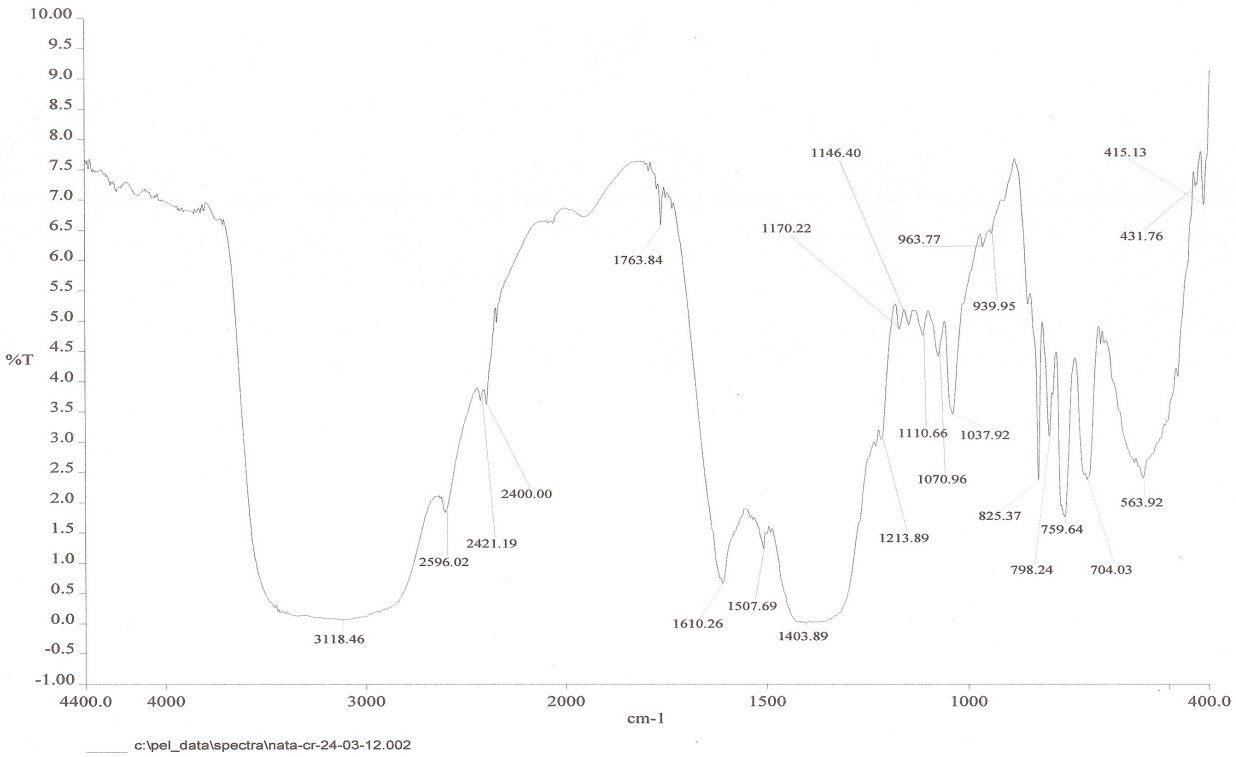

Fig. S7 FTIR spectrum of **L**-Cr^{3+} complex.

Table S1. Bond lengths of **L**

Bond	**Length (A°)**	**Bond**	**Length (A°)**
C_1 C_2	1.377(3)	C_8 C_9	1.371(3)
C_1 N_1	1.415(2)	C_8 H_8	0.9500
C_1 C_{10}	1.429(2)	C_9 C_{10}	1.421(3)
C_2 C_3	1.403(3)	C_9 H_9	0.9500
C_2 H_2	0.9500	C_{11} N_1	1.281(2)
C_3 C_4	1.367(3)	C_{11} C_{12}	1.445(3)
C_3 H_3	0.9500	C_{11} H_{11}	0.9500
C_4 C_5	1.417(3)	C_{12} C_{13}	1.374(3)
C_4 H_4	0.9500	C_{12} S_1	1.7268(19)
C_5 C_6	1.413(3)	C_{13} C_{14}	1.408(3)
C_5 C_{10}	1.428(3)	C_{13} H_{13}	0.9500
C_6 C_7	1.361(3)	C_{14} C_{15}	1.356(3)
C_6 H_6	0.9500	C_{14} H_{14}	0.9500
C_7 C_8.	1.413(3)	C_{15} S_1	1.7194(19)
C_7 H_7	0.9500	C_{15} H_{15}	0.9500

Table S2: Bond angles of **L**

Bond Angle	(°)	**Bond Angle**	(°)
$C_2\ C_1\ N_1$	123.11(16)	$C_7\ C_8\ H_8$	119.8
$C_2\ C_1\ C_{10}$	119.91(16)	$C_8\ C_9\ C_{10}$	120.47(19)
$N_1\ C_1\ C_{10}$	116.98(15)	$C_8\ C_9\ H_9$	119.8
$C_1\ C_2\ C_3$	120.67(17)	$C_{10}\ C_9\ H_9$	119.8
$C_1\ C_2\ H_2$	119.7	$C_9\ C_{10}\ C_5$	118.70(16)
$C_3\ C_2\ H_2$	119.7	$C_9\ C_{10}\ C_1$	122.50(17)
$C_4\ C_3\ C_2$	120.81(17)	$C_5\ C_{10}\ C_1$	118.80(16)
$C_4\ C_3\ H_3$	119.6	$N_1\ C_{11}\ C_{12}$	122.30(17)
$C_2\ C_3\ H_3$	119.6	$N_1\ C_{11}\ H_{11}$	118.8
$C_3\ C_4\ C_5$	120.54(18)	$C_{12}\ C_{11}H_{11}$	118.8
$C_3\ C_4\ H_4$	119.7	$C_{13}\ C_{12}\ C_{11}$	127.31(17)
$C_5\ C_4\ H_4$	119.7	$C_{13}\ C_{12}\ S_1$	111.43(14)
$C_6\ C_5\ C_4$	121.86(17)	$C_{11}\ C_{12}\ S_1$	121.16(14)
$C_6\ C_5\ C_{10}$	119.02(16)	$C_{12}\ C_{13}\ H_{13}$	123.7
$C_4\ C_5\ C_{10}$	119.11(17)	$C_{14}\ C_{13}\ H_{13}$	123.7
$C_7\ C_6\ C_5$	120.94(18)	$C_{15}\ C_{14}\ C_{13}$	112.69(17)
$C_7\ C_6\ H_6$	119.5	$C_{15}\ C_{14}\ H_{14}$	123.7
$C_5\ C_6\ H_6$	119.5	$C_{13}\ C_{14}\ H_{14}$	123.7
$C_6\ C_7\ C_8$	120.43(18)	$C_{14}\ C_{15}\ S_1$	112.38(15)
$C_6\ C_7\ H_7$	119.8	$C_{14}\ C_{15}\ H_{15}$	123.8
$C_8\ C_7\ H_7$	119.8	$S_1\ C_{15}\ H_{15}$	123.8
$C_9\ C_8\ C_7$	120.41(18)	$C_{11}\ N_1\ C_1$	118.28(15)
$C_9\ C_8\ H_8$	119.8	$C_{15}\ S_1\ C_{12}$	90.98(10)
$C_{12}\ C_{13}\ C_{14}$	112.53(18).		

General method of UV-Vis and fluorescence titration

Path length of the cells used for absorption and emission studies was 1 cm. For UV-vis and fluorescence titrations, stock solution of **L** (10 μM) was prepared in methanol water. Working solutions were prepared from their respective stock solutions. Fluorescence measurements were performed using 5 nm × 5 nm slit width.

Calculation of Quantum Yield

Fluorescence quantum yields (***Φ***) were estimated by integrating the area under the fluorescence curves using the equation[1],

$$\phi_{sample} = \phi_{ref} \times \frac{OD_{ref} \times A_{sample} \times \eta^2_{sample}}{OD_{sample} \times A_{ref} \times \eta^2_{ref}}$$

where, **A** was the area under the fluorescence spectral curve, **OD** was optical density of the compound at the excitation wavelength and **η** was the refractive indices [2] of the solvent. Anthracene was used as quantum yield standard (quantum yield is 0.27 in ethanol) [3] for measuring the quantum yields at 330 nm.

References

1. E. Austin and M. Gouterman, *Bioinorg . Chem.* , 1978, **9,** 281.

2. F. I. El - Dossoki, *J Chin . Chem. Soc* . , 2007, **54**, 1129 .

3. W. H. Melhuish , *J. Phys. Chem.*, 1961, **65,** 229.

Job's plot using fluorescence data

A series of solutions containing **L** and Cr^{3+} were prepared such that the total concentration of Cr^{3+} and **L** remain constant (10 μM) in all the sets. The mole fraction (X) of **L** was varied from 0.1 to 0.9. The fluorescence intensity at 435 nm was plotted against the mole fraction of **L**.