Supporting Information

Single Exited State Intramolecular Proton Transfer (ESIPT) containing Rhodol based chemodosimeter for both Hg^{2+} and OCl^-: ratiometric detection with live-cell imaging

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CONTENTS

1. Determination of fluorescence quantum yield:

Here, the quantum yield φ was measured by using the following equation,

$\varphi_x = \varphi_s (F_x / F_s)(A_s / A_x)(n_x^2/ n_s^2)$

Where, X & S indicate the unknown and standard solution respectively, φ = quantum yield,

F = area under the emission curve, A = absorbance at the excitation wave length,

n = index of refraction of the solvent. Here φ measurements were performed using rhodamine in ethanol as standard [φ = 0.96] (error ~ 10%). [Grabolle et al. 2009, Karstens et al. 1980, Arden et al. 1991]

The quantum yield of **STBR** itself is 0.02 which change into 0.55 with the addition of Hg^{2+} and 0.73 with the addition of hypochlorite.

2. Calculation of the detection limit:

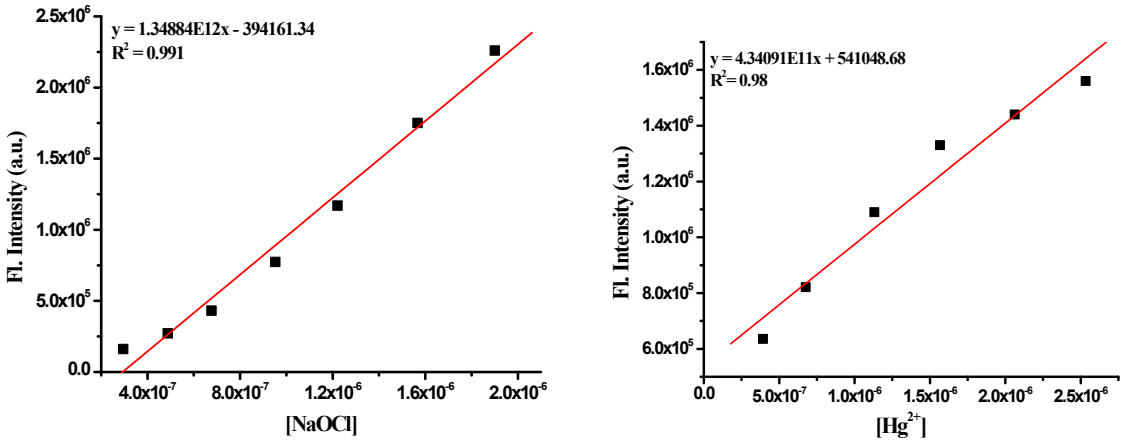


Figure S1: Fl. Intensity Vs. conc. of OCl^- and Hg^{2+} at 595 nm and 590 nm respectively.

The detection limit DL of **STBR** for Hg^{2+} and OCl^- was determined from the following equation [Zhu et al. 2008]:

DL = K* Sb1/S

Where K = 2 or 3 (we take 2 in this case); Sb1 is the standard deviation; S is the slope of the calibration curve.

From the graph we get slope = 4E + 11 for Hg^{2+} and 1E+12 for OCl^-, and Sb1 value is 82954.67249 for Hg^{2+} and 111416.0156 for OCl^-.

Thus using the formula we get the Detection Limit = 0.41 μM for Hg^{2+} and 0.22 μM for OCl^- i.e. STBR can detect Hg^{2+} and OCl^- in this ppm level.

3. Single crystal X-ray structure:

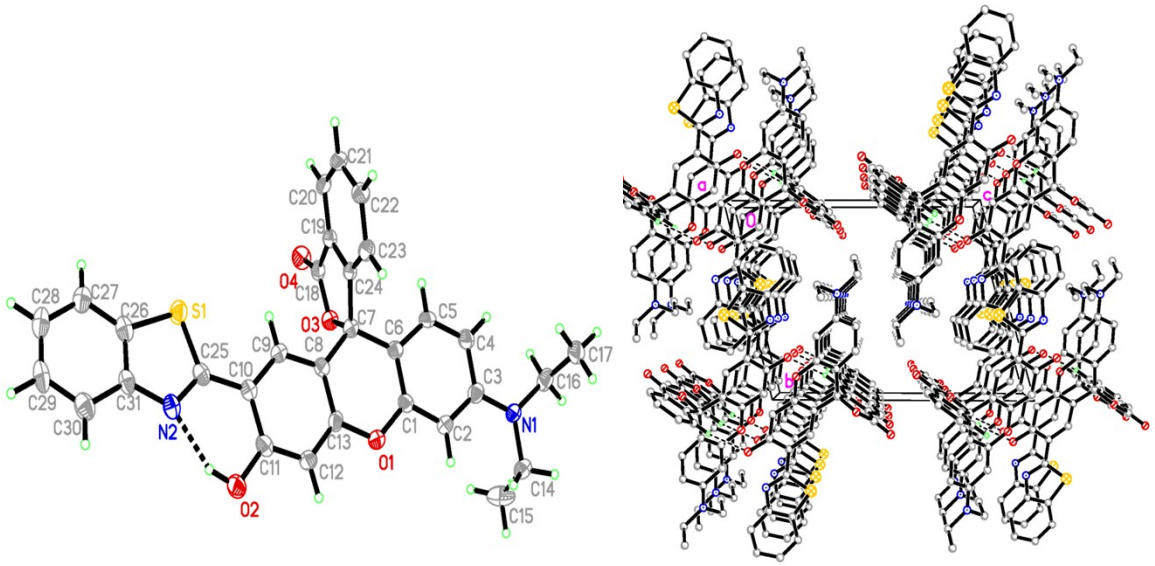


Figure S2: The molecular structure of ESIPT containing rhodol moiety, showing 50% probability displacement ellipsoids for non-H atoms and the atom-numbering scheme. The intramolecular hydrogen bond is shown as dashed line (left) and the crystal packing of ESIPT containing rhodol moiety, viewed along the *a*-axis. H atoms not involved in intermolecular interactions (dashed lines) have been omitted for clarity (right)

Table S1: Experimental details

Crystal data	CCDC 1420361
Chemical formula	$C_{31}H_{24}N_2O_4S$
M_r	520.58
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, *b*, *c* (Å)	7.742 (4), 11.180 (5), 15.075 (7)
α, β, γ (°)	73.813 (11), 85.765 (12), 80.157 (10)
V (Å^3)	1234.1 (10)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.17
Crystal size (mm)	0.22 × 0.19 × 0.05
Data collection	

Diffractometer	Bruker *SMART APEX* II DUO CCD area-detector diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.962, 0.991
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20730, 4965, 3123
R_{int}	0.076
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.623
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.132, 1.03
No. of reflections	4965
No. of parameters	349
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.28

Table 5B.2

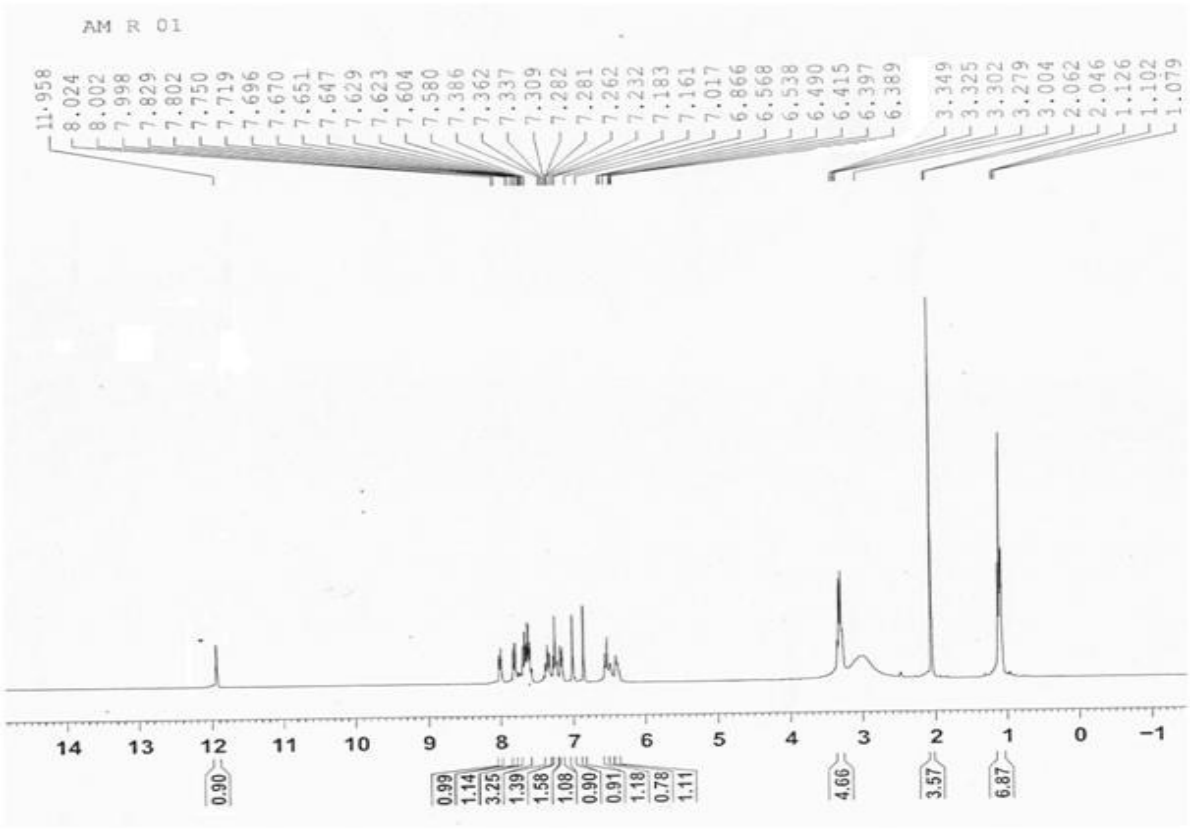
Hydrogen-bond geometry (Å, º)

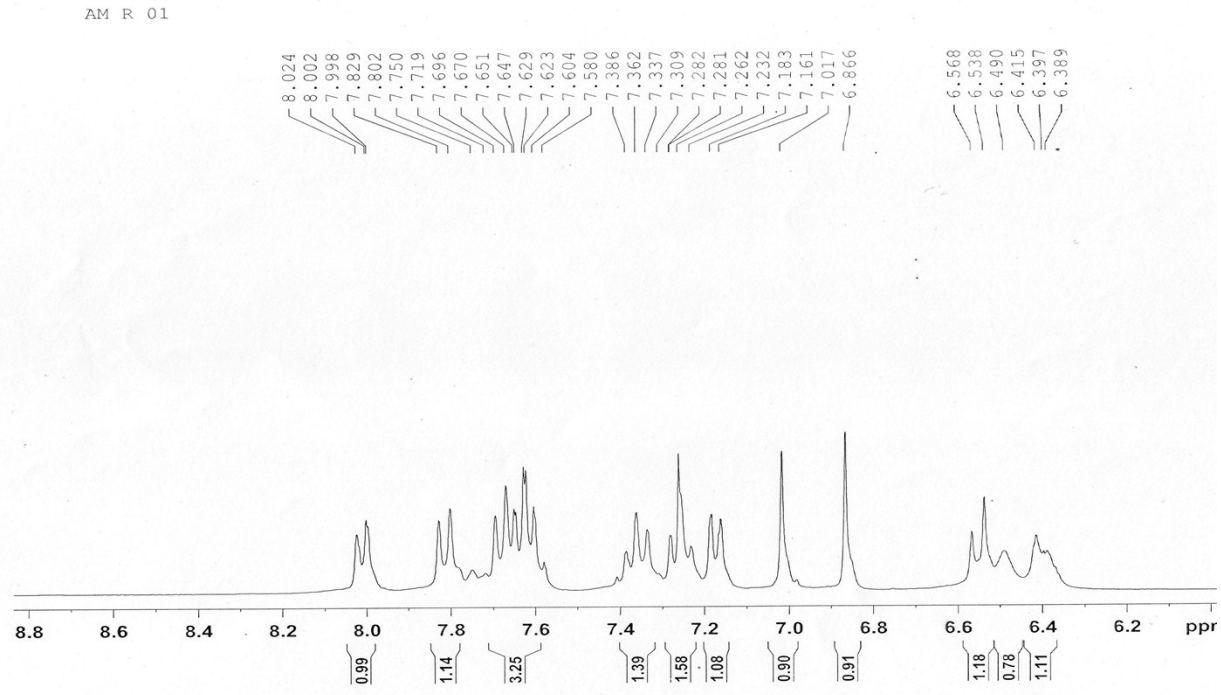
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O2*···N2	0.90 (3)	1.81 (3)	2.629 (3)	150 (3)
C23—H23*A*···O2^{i}	0.95	2.41	3.321 (4)	160

Symmetry code: (i) −*x*+1, −*y*, −*z*.

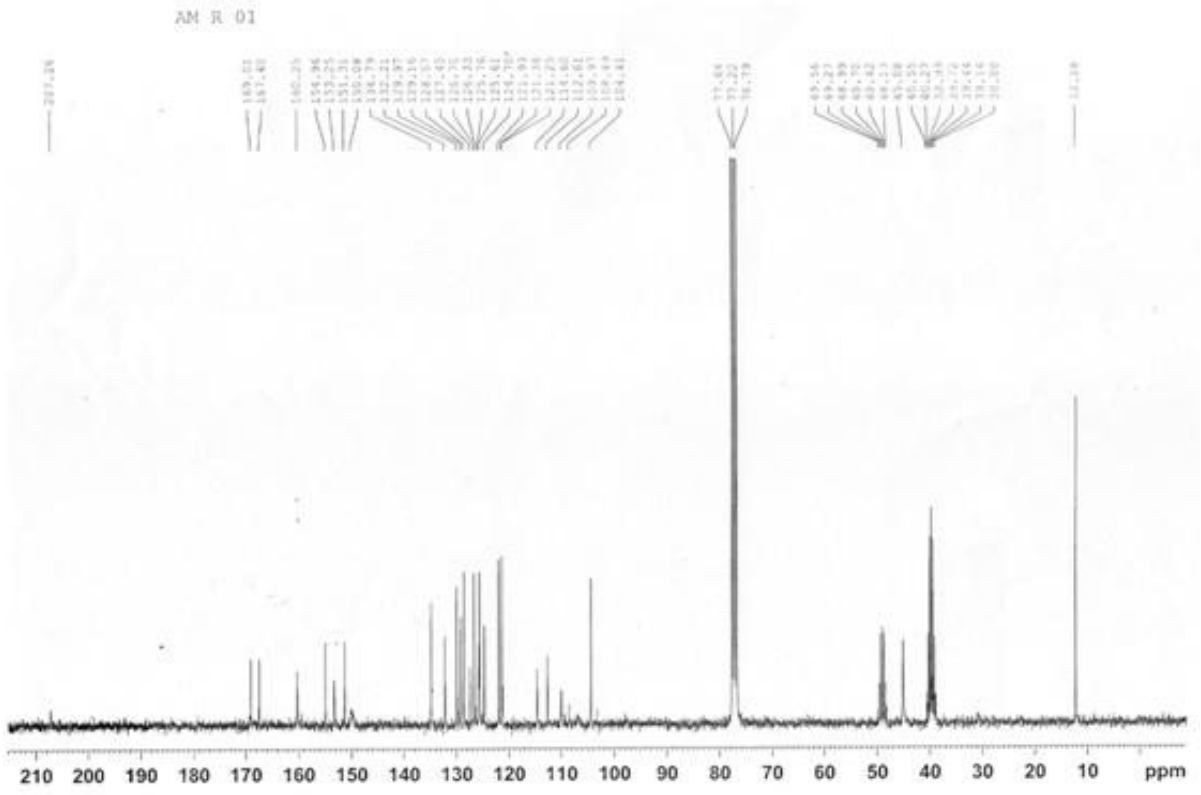
4. ^{1}H NMR, ^{13}C NMR and ESI MS spectra:

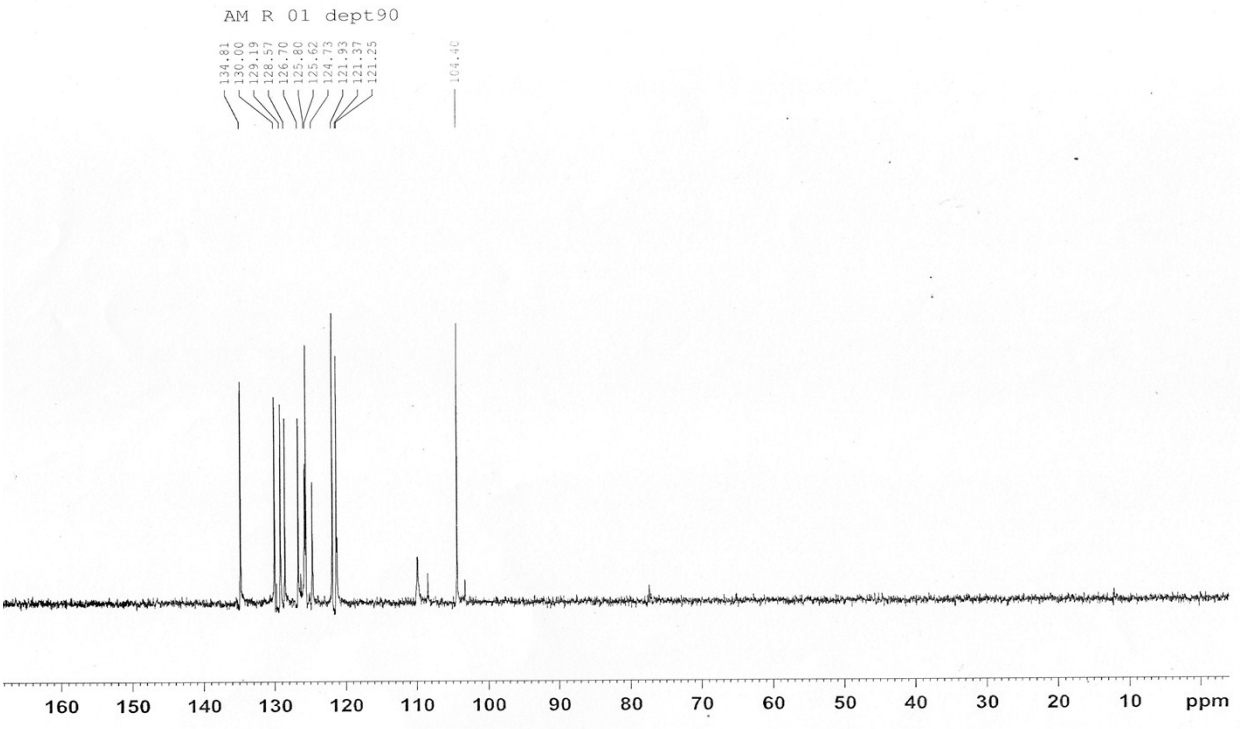
^{1}H NMR spectrum of Receptor i.e. STBR and its expansion:

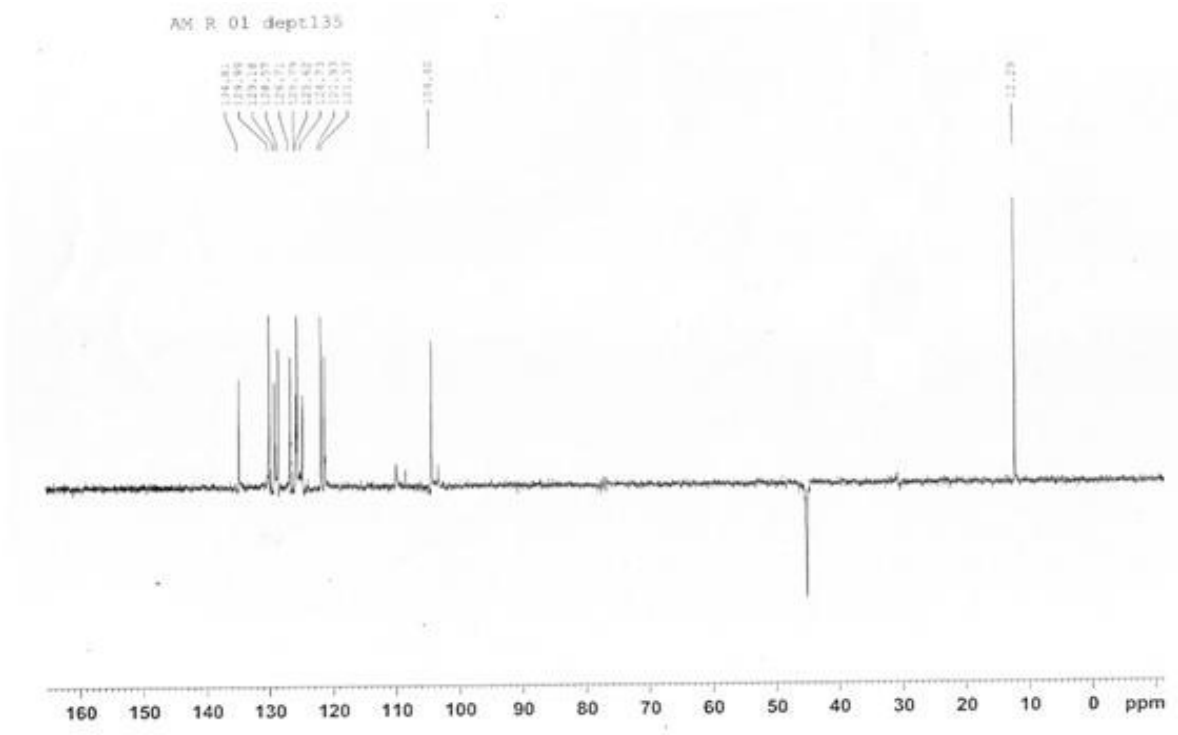




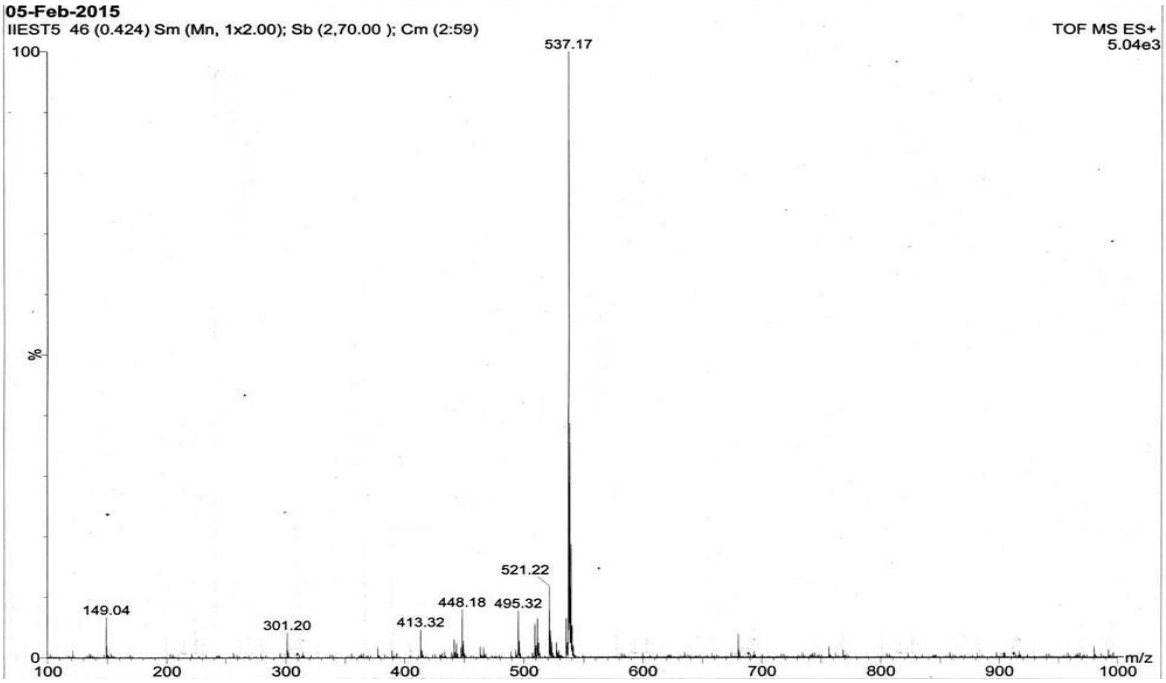
^{13}C NMR spectrum (with DEPT 90 and DEPT 135) of Receptor i.e. STBR:



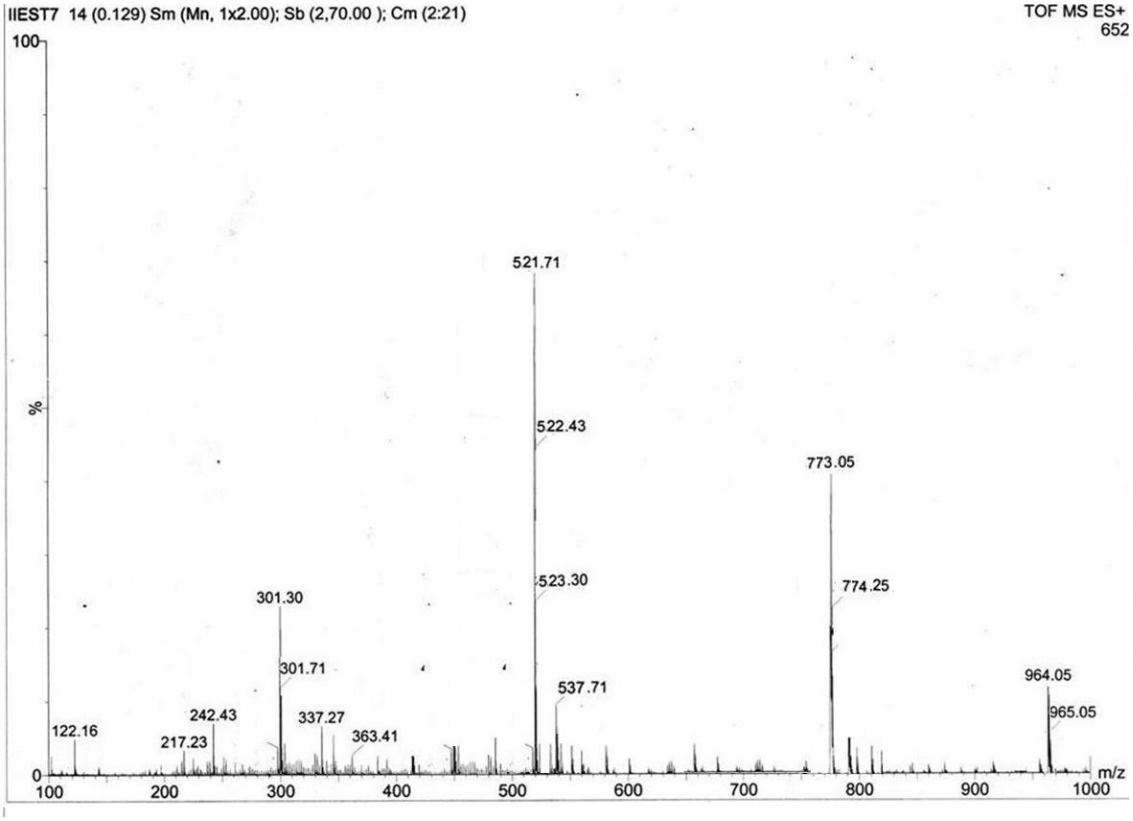




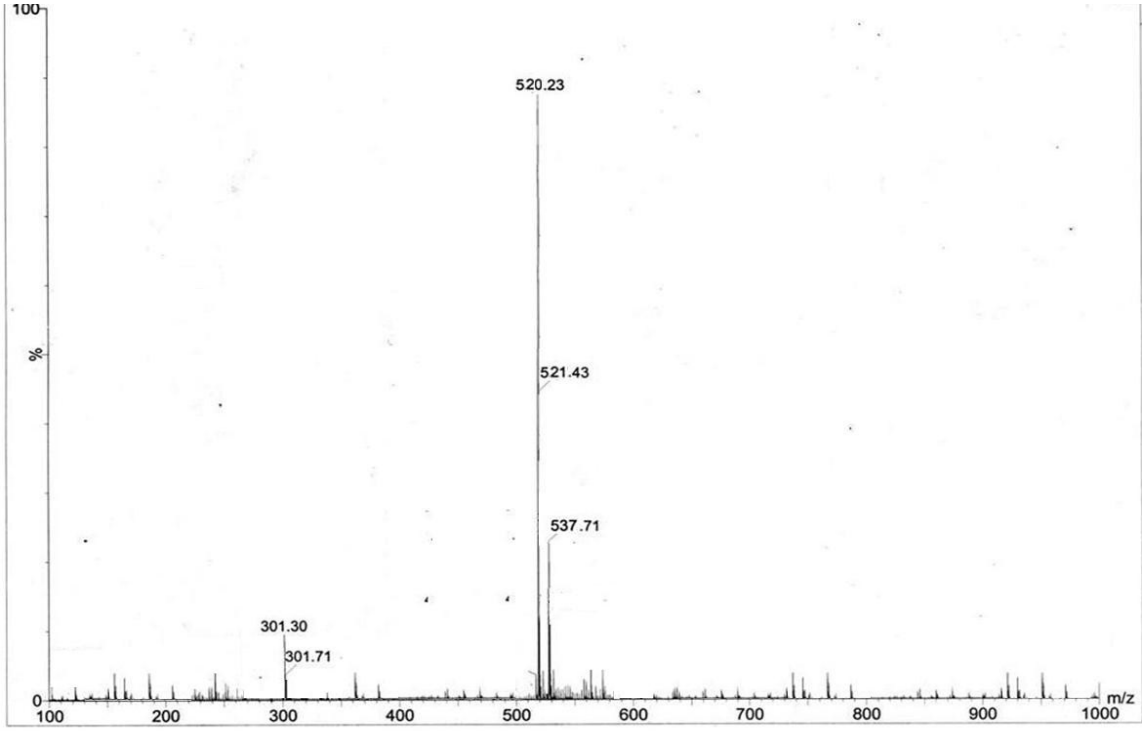
ESI MS spectra of Receptor i.e. STBR:



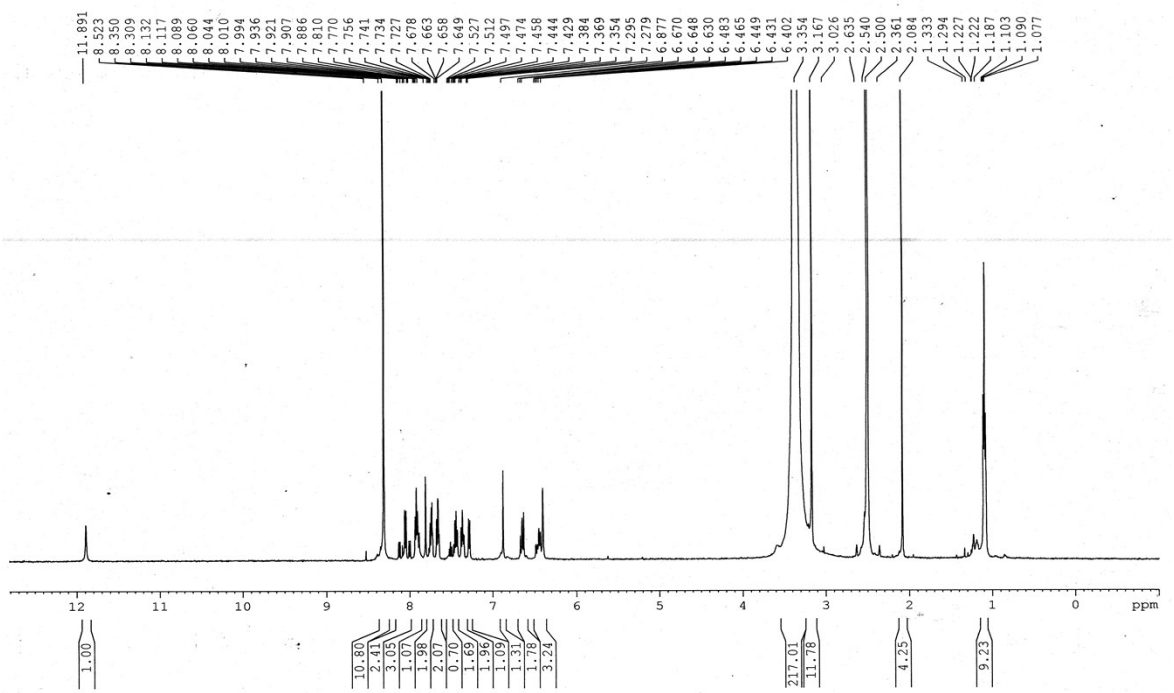
ESI MS spectra of Receptor i.e. STBR in presence of $HgCl_2$:



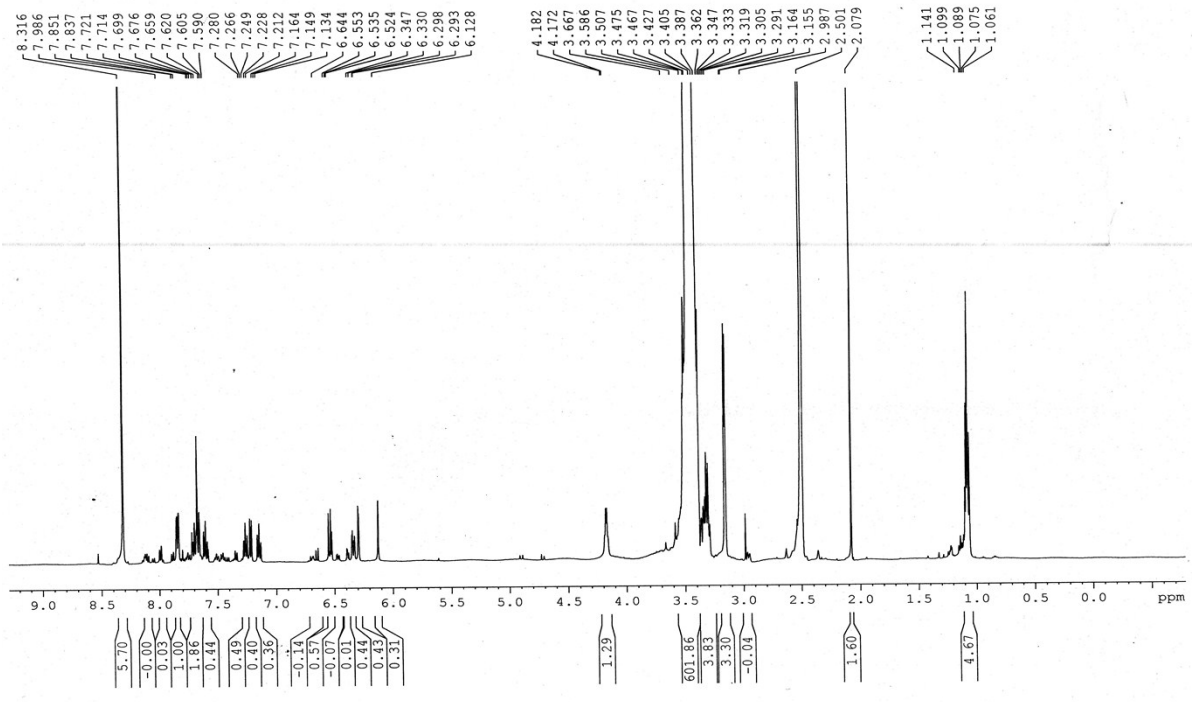
^{1}H NMR spectrum of Receptor i.e. STBR + OCl^- (as NaOCl Solution) in d_6-DMSO:



^{1}H NMR spectrum of Receptor i.e. STBR + Hg^{2+} (as $HgCl_2$) in d_6-DMSO:



^{1}H-NMR spectra of Receptor i.e. STBR in presence of NaOCl in d_6-DMSO:



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