Electronic Supplementary Information

Facile Synthesis of Mixed O, S or Se Substituted Hexabenzenes and Their Potential as Cu(II) ion Probe

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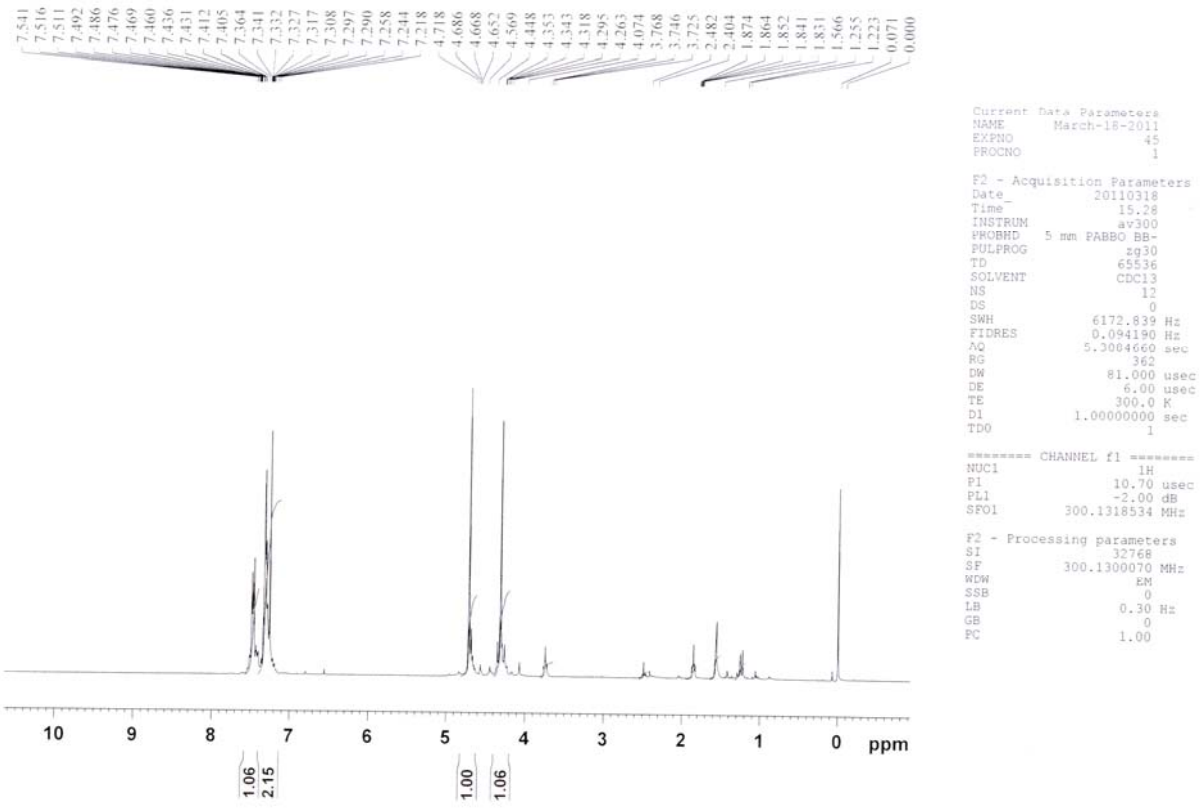

Fig. S1 ^{1}H NMR spectrum of **2a** in $CDCl_3$

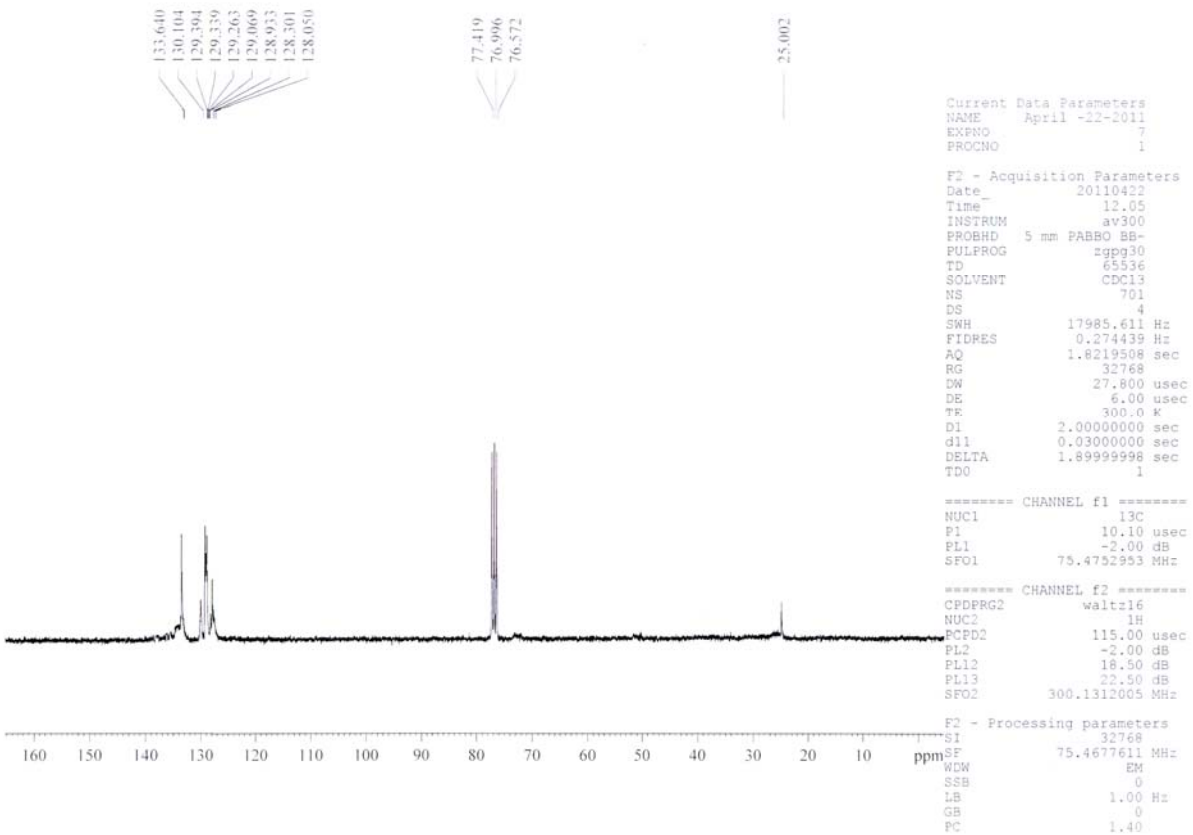

Fig. S2 $^{13}C[^{1}H]$ NMR spectrum of **2a** in $CDCl_3$

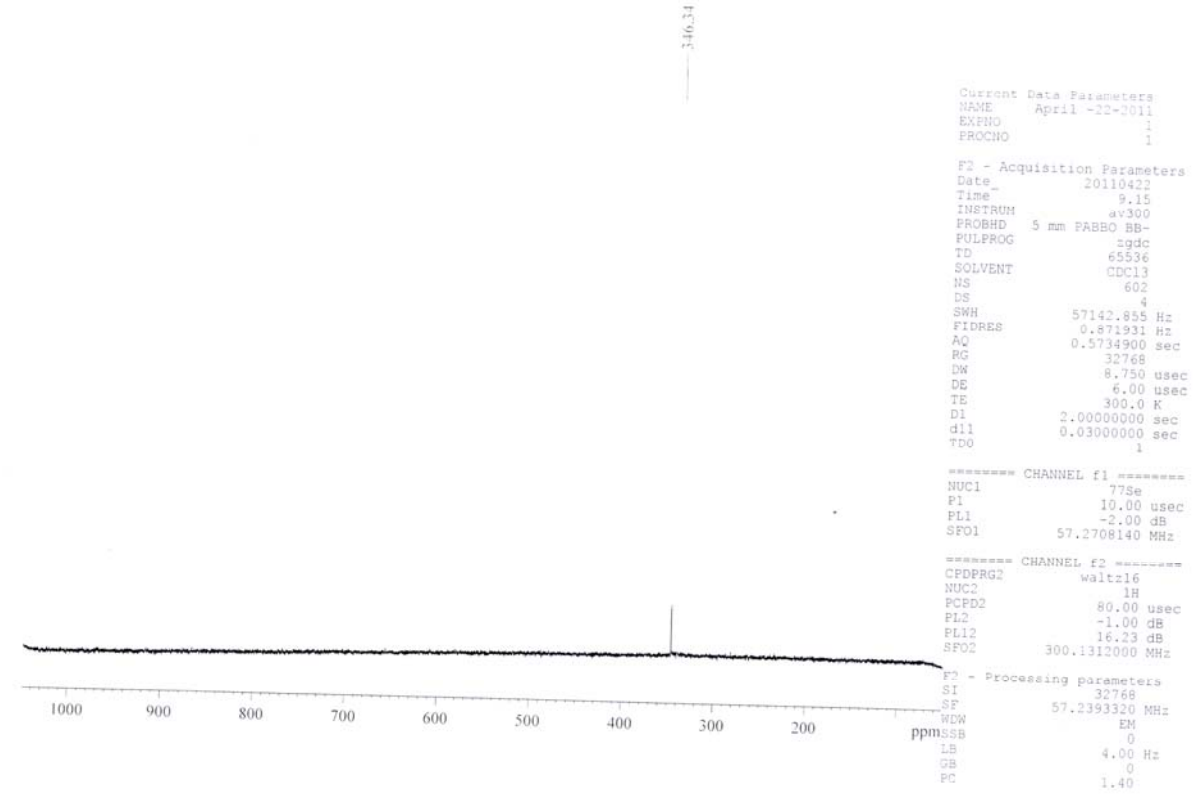

Fig. S3 ^{77}Se NMR spectrum of **2a** in $CDCl_3$

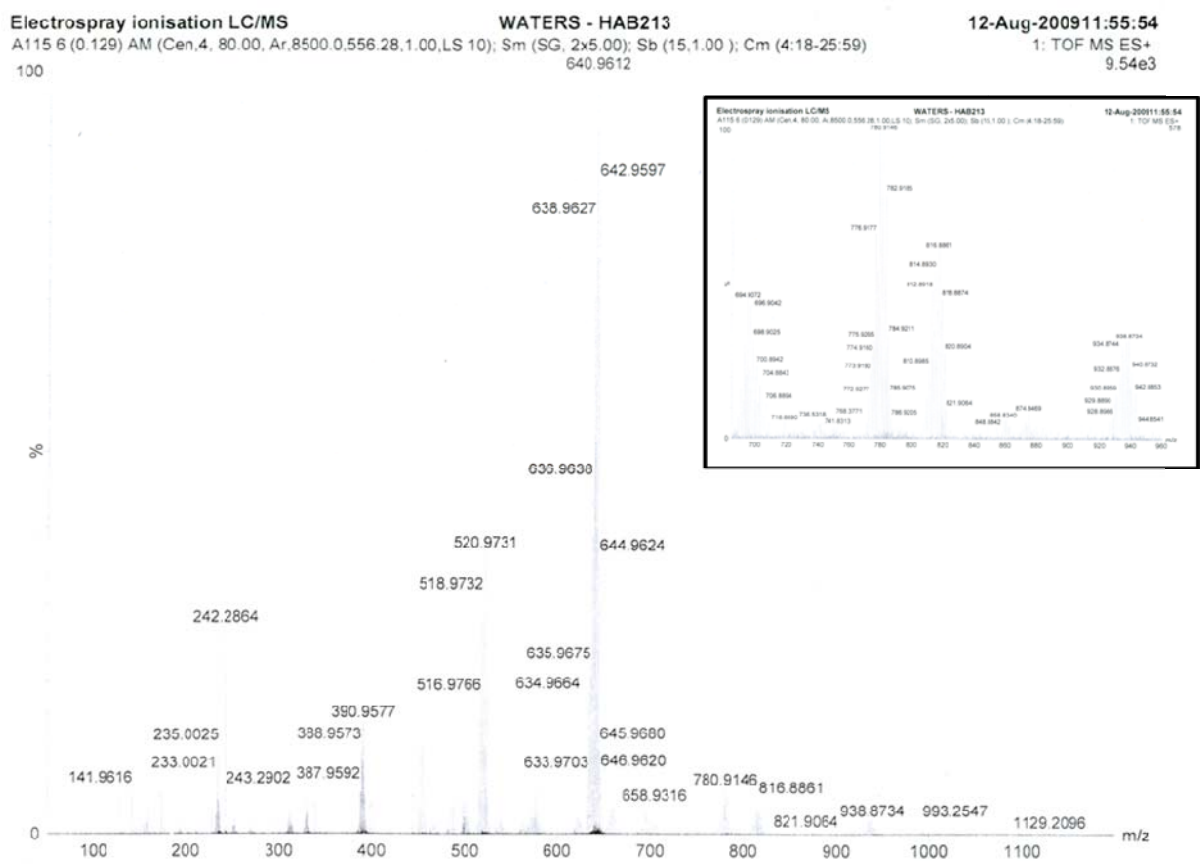

Fig. S4 ES-MS spectrum of **2a** (Inset: Expanded portion showing molecular ion peak)

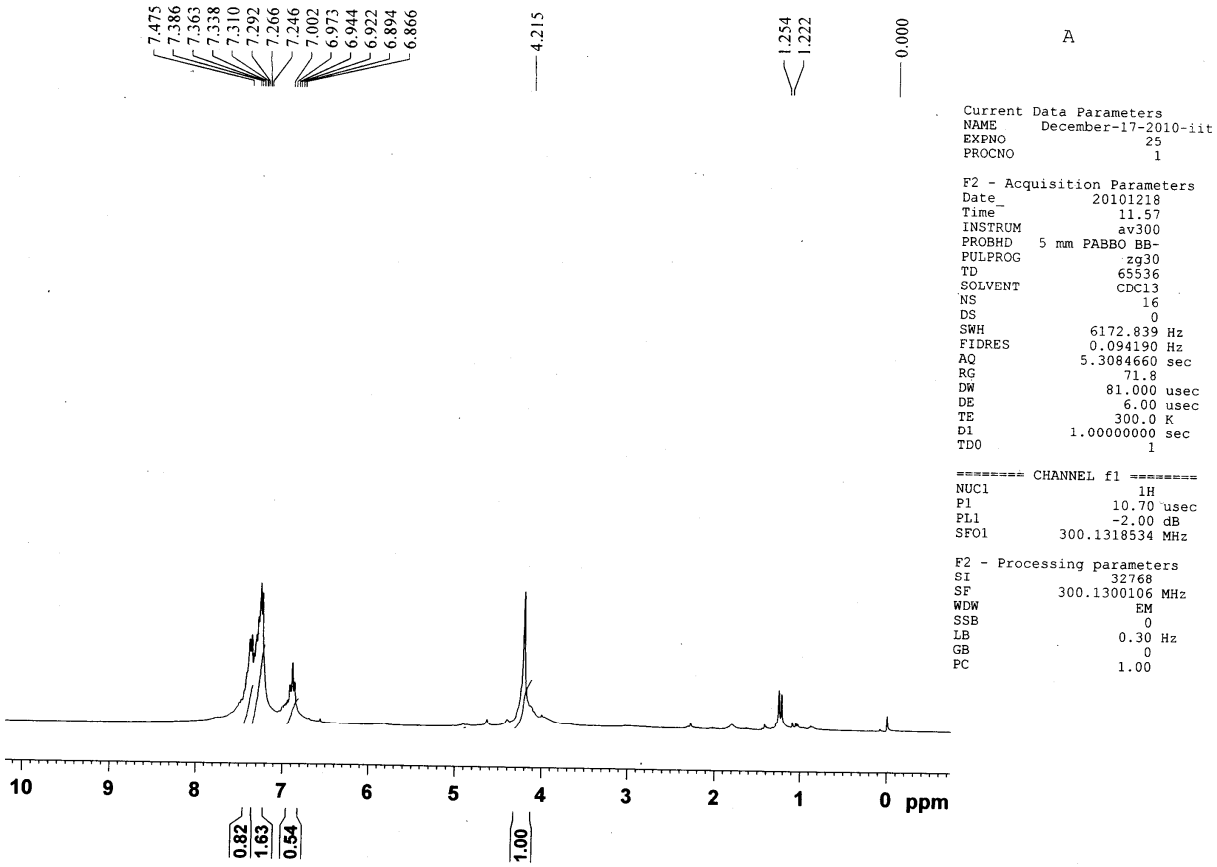

Fig. S5 ^{1}H NMR spectrum of **3a** in $CDCl_3$

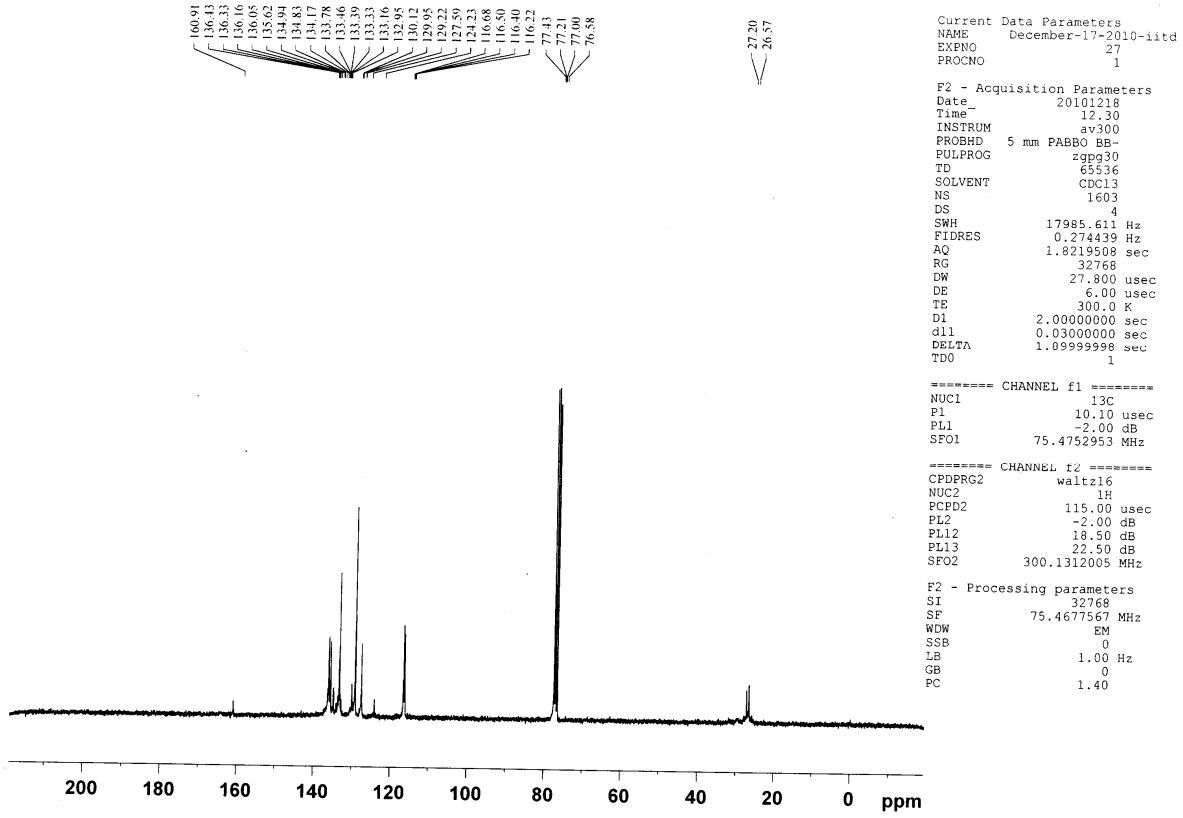

Fig. S6 ^{13}C[^{1}H] NMR spectrum of **3a** in $CDCl_3$

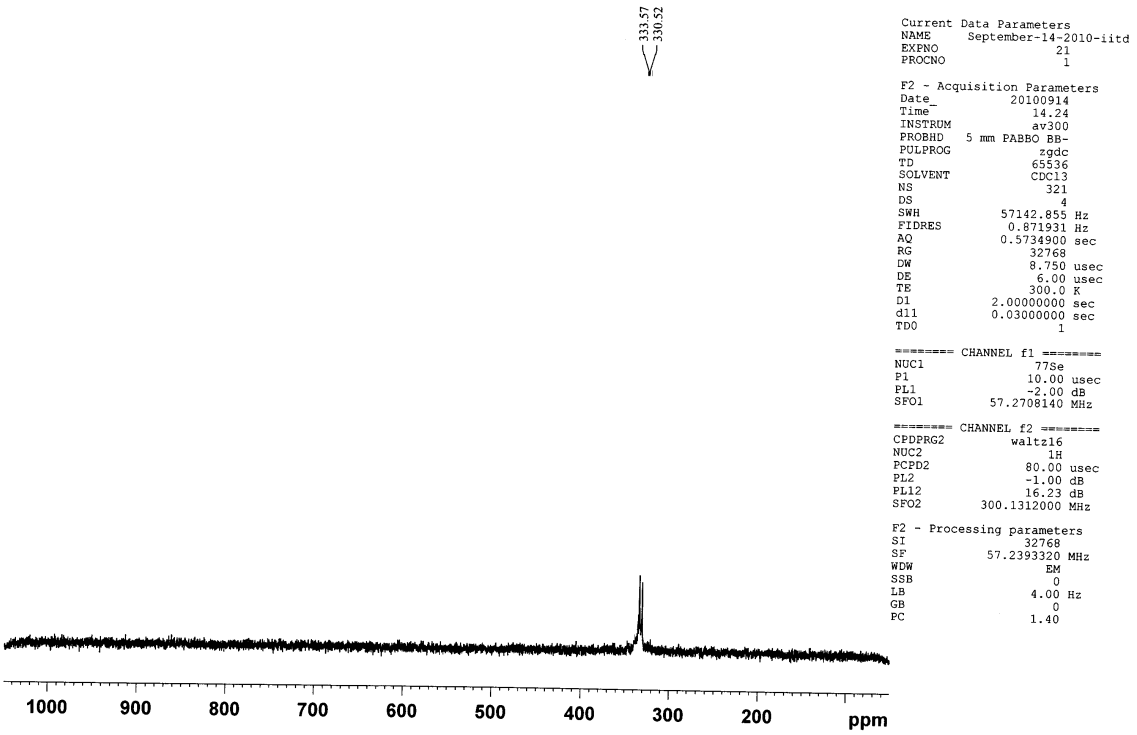

Fig. S7 ^{77}Se NMR spectrum of **3a** in $CDCl_3$

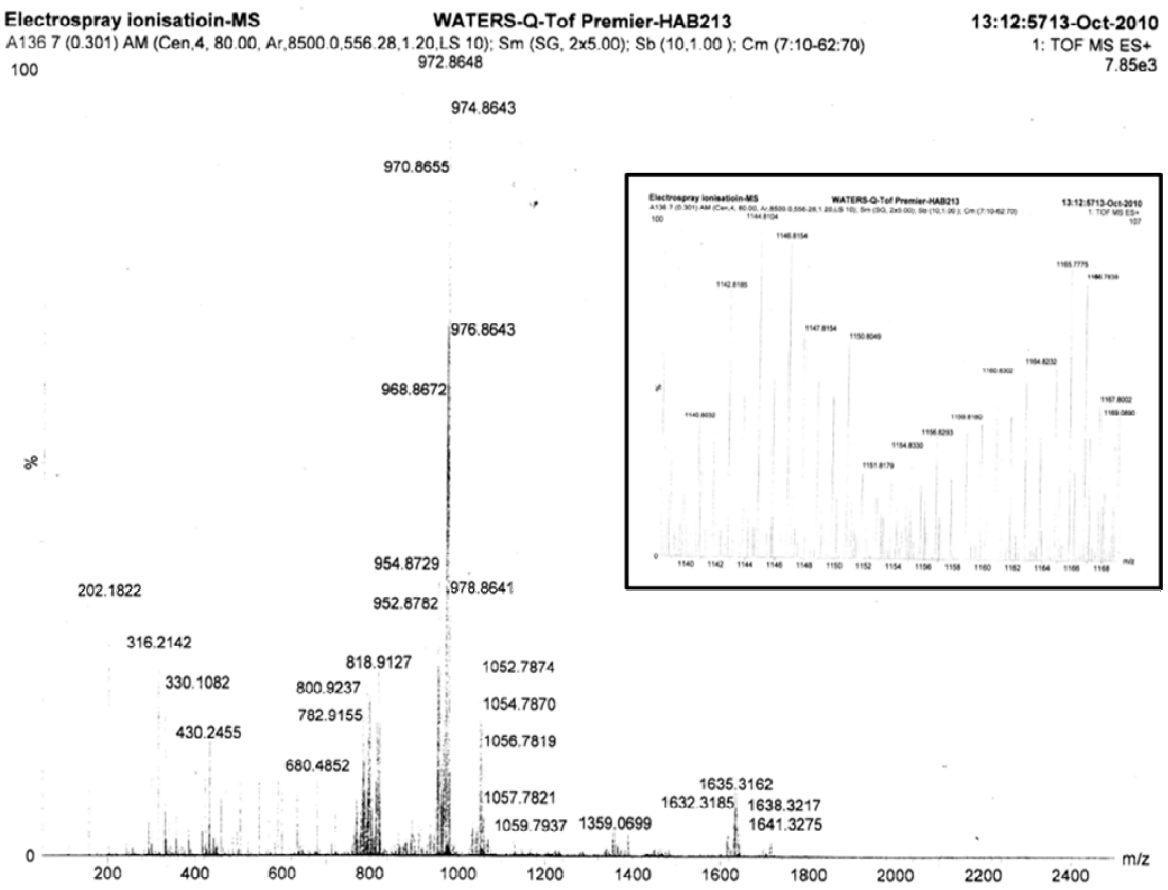

Fig. S8 ES-MS spectrum of **3a** (Inset: Expanded portion showing molecular ion peak)

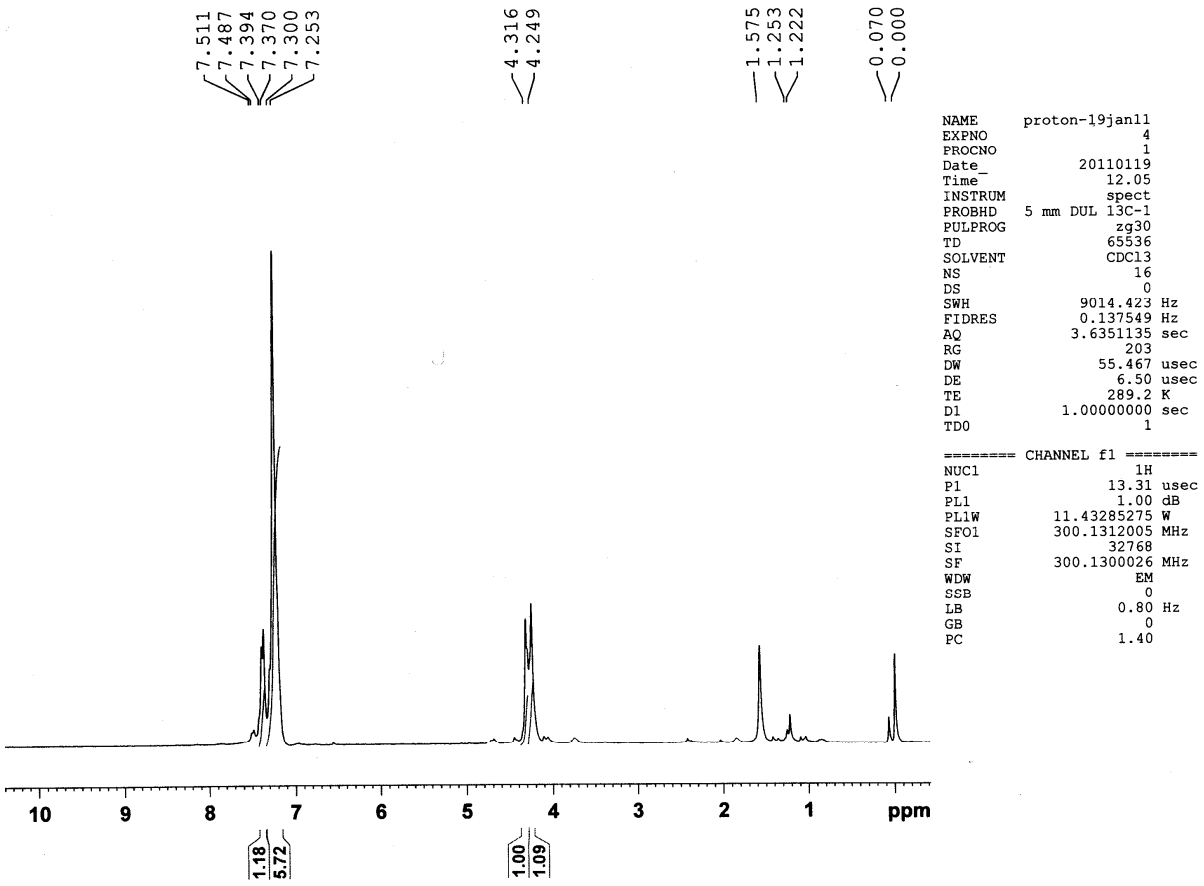

Fig. S9 ^{1}H NMR spectrum of **4a** in $CDCl_3$

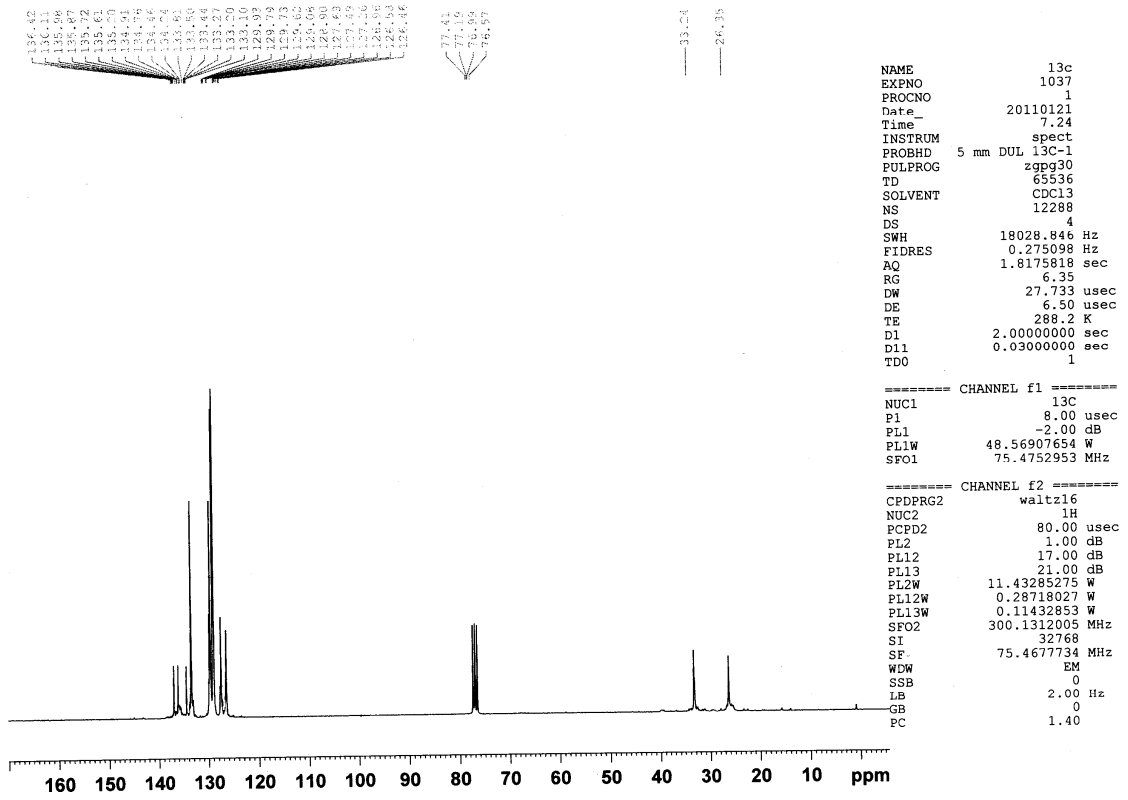

Fig. S10 $^{13}C[^{1}H]$ NMR spectrum of **4a** in $CDCl_3$

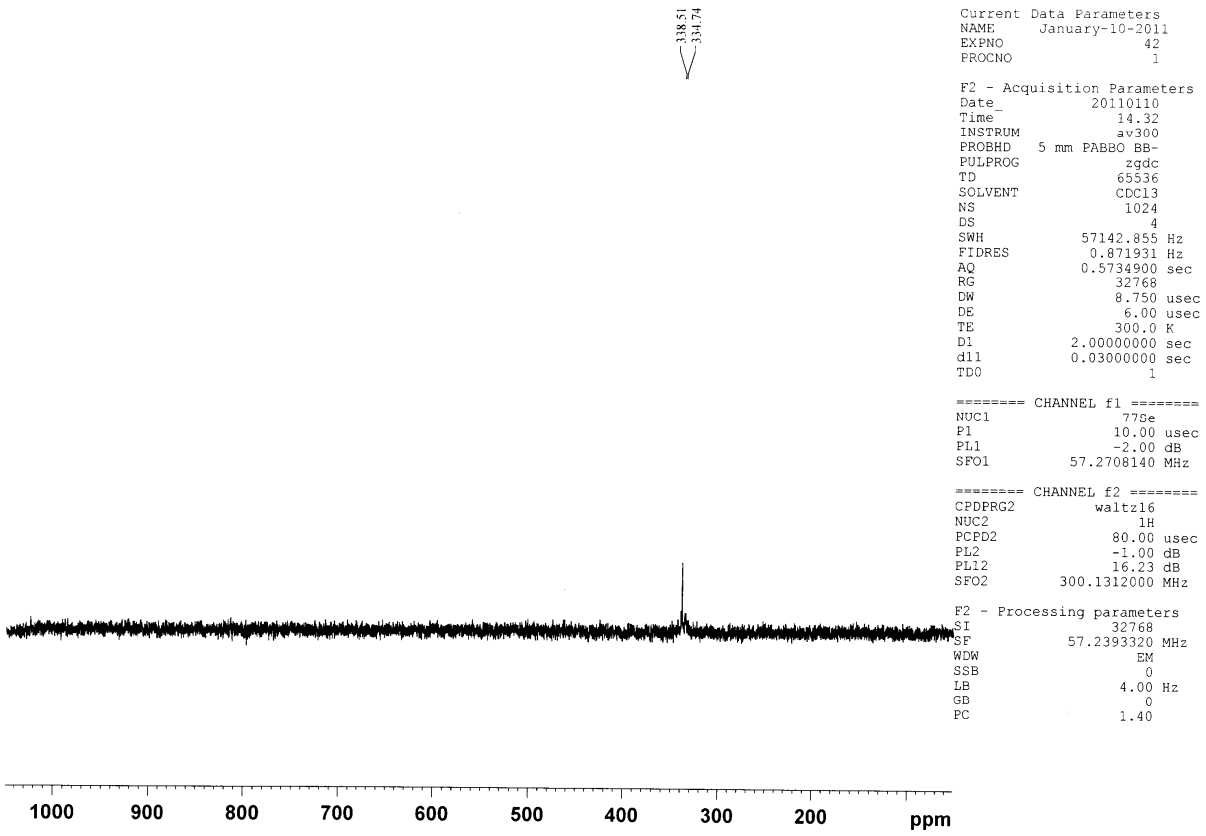

Fig. S11 ^{77}Se NMR spectrum of **4a** in $CDCl_3$

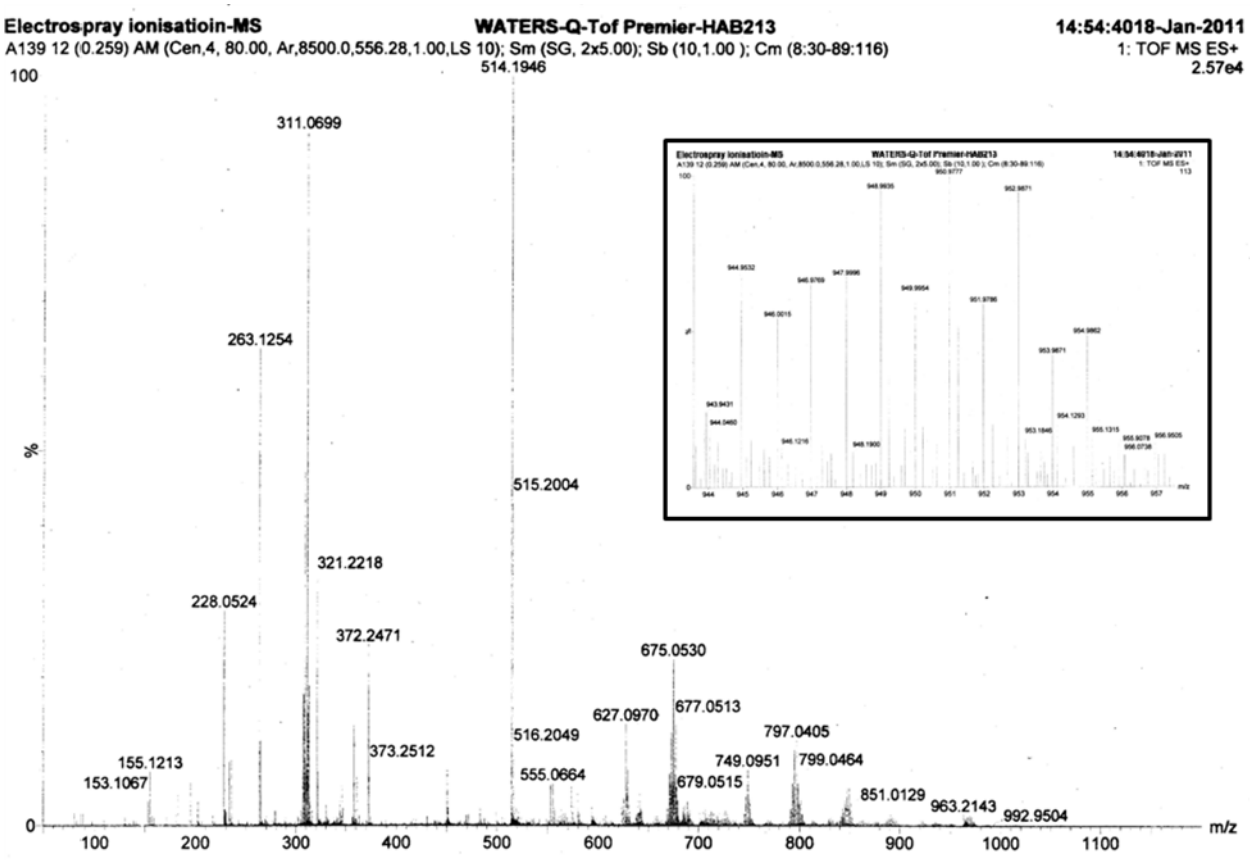

Fig. S12 ES-MS spectrum of **4a** (Inset: Expanded portion showing molecular ion peak)

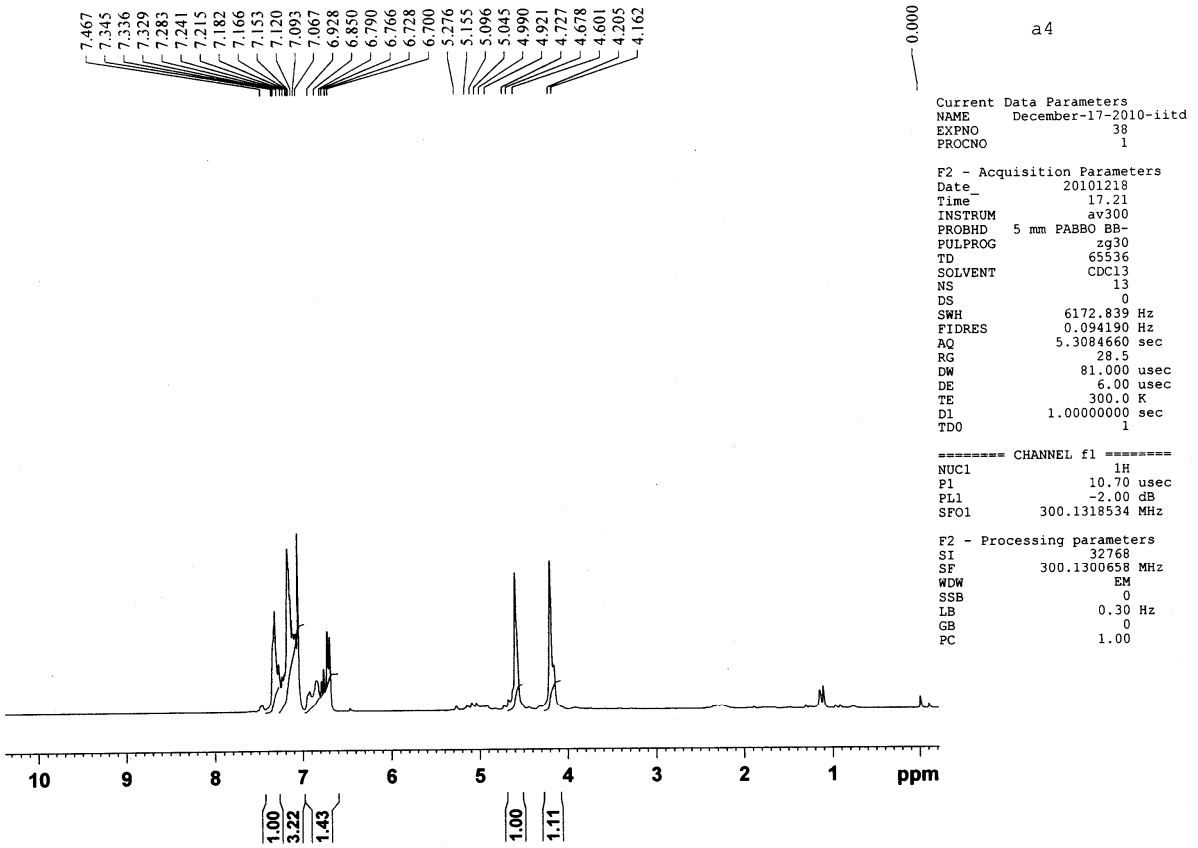

Fig. S13 ^{1}H NMR spectrum of **5a** in $CDCl_3$

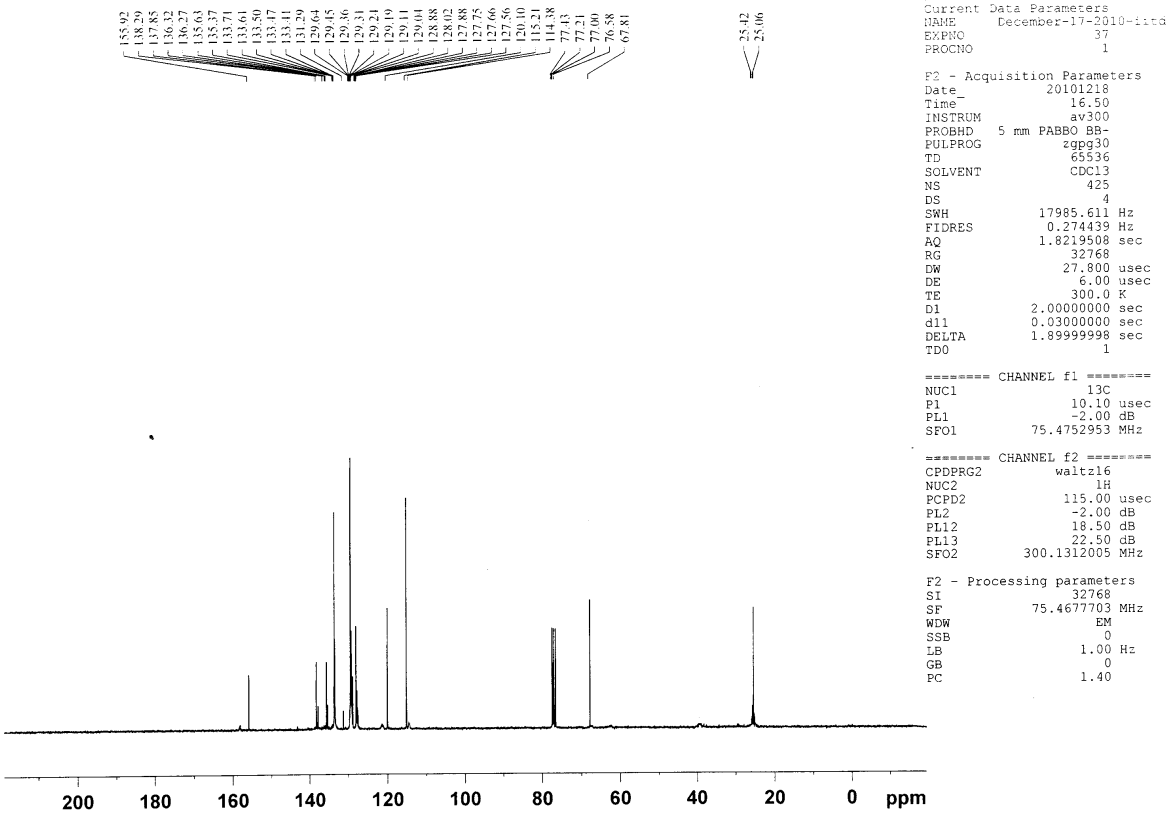

Fig. S14 $^{13}C[^{1}H]$ NMR spectrum of **5a** in $CDCl_3$

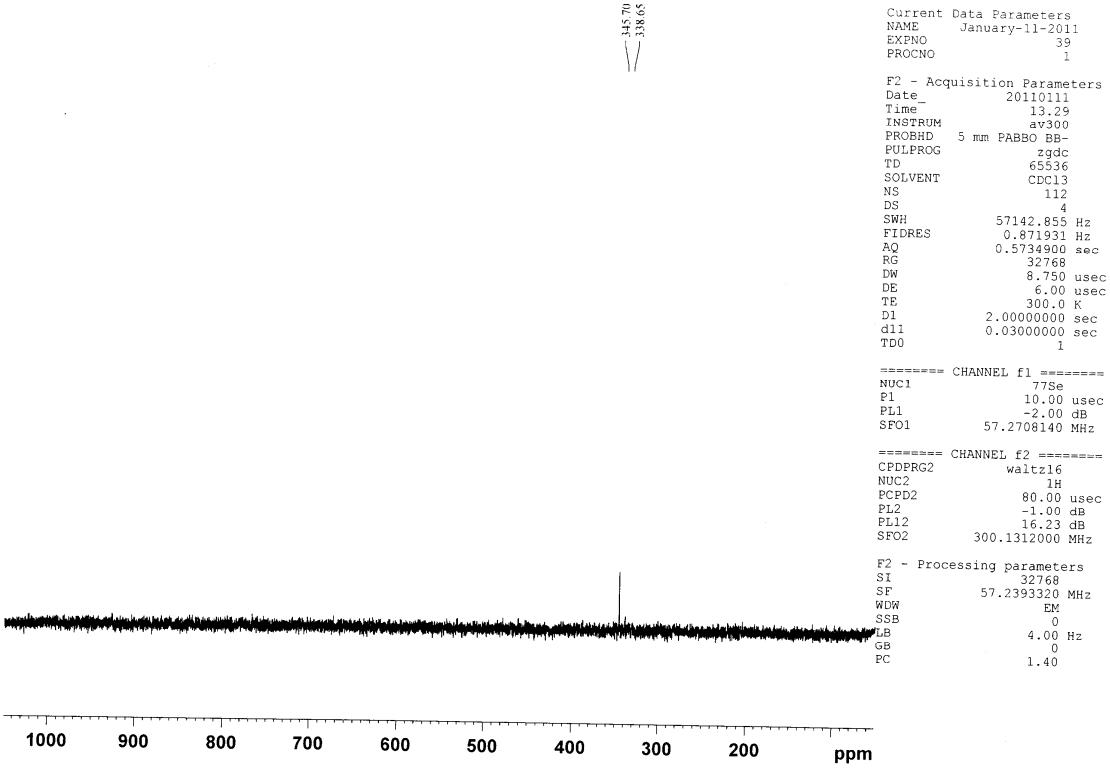

Fig. S15 ^{77}Se NMR spectrum of **5a** in $CDCl_3$

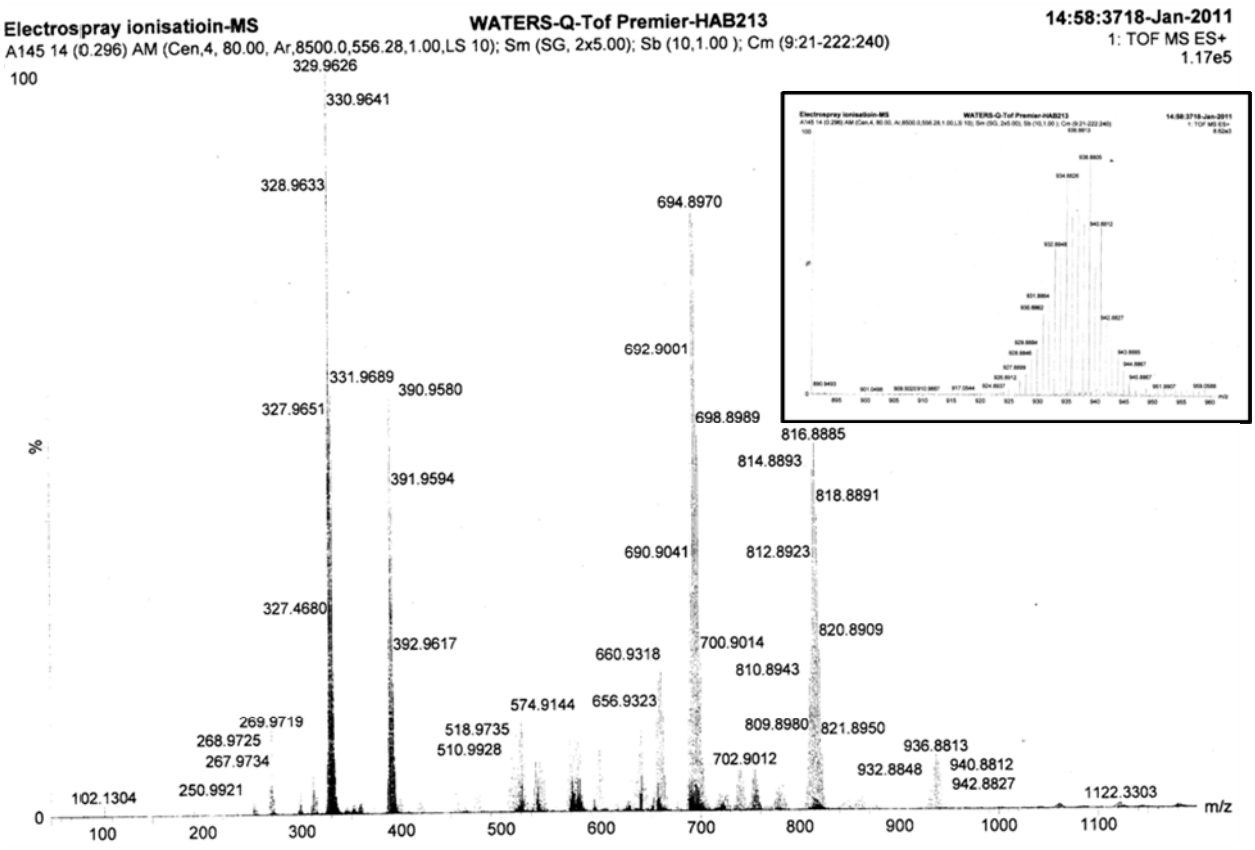

Fig. S16 ES-MS spectrum of **5a** (Inset: Expanded portion showing molecular ion peak)

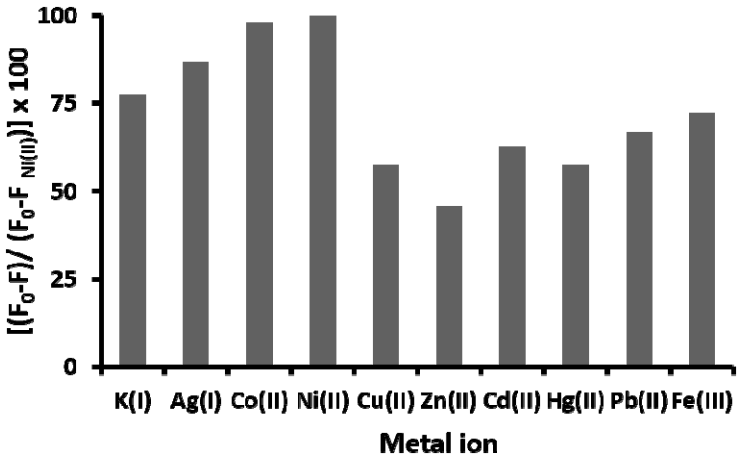

Fig. S17 Change ratio $\{[(F_0 - F)/(F_0-F_{Ni(II)})] \times 100\}$ of fluorescence intensity of '*oxo*' analogue $[(C_6H_5OCH_2)_6C_6]$ on addition of 15 equivalents of various tested metal ions with respect to change observed with Ni(II) which exhibited the largest change in fluorescence intensity.

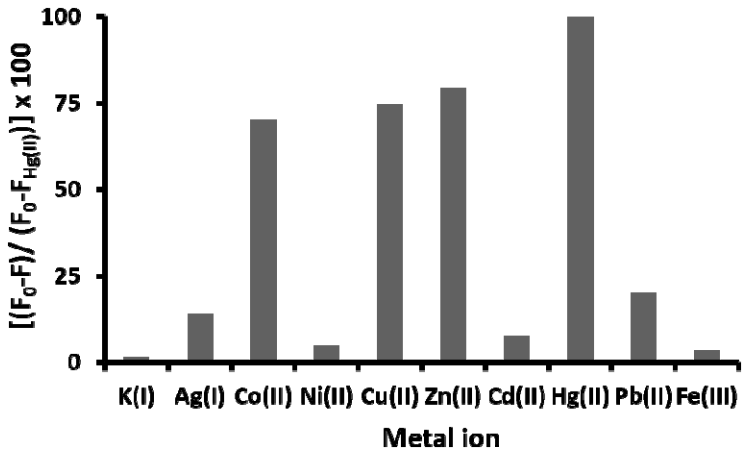

Fig. S18 Change ratio {[(F_0 - F)/(F_0-$F_{Hg(II)}$)] x 100} of fluorescence intensity of '*seleno*' analogue [$(C_6H_5SeCH_2)_6C_6$] on addition of 15 equivalents of various tested metal ions with respect to change observed with Hg(II) which exhibited the largest change in fluorescence intensity.

Detection limit calculations

The detection limit was calculated using the formula ($3\sigma/k$), where σ is the standard deviation and *k* is the slope of fluorescence intensity change with metal ion concentration.

In case of fluorescence changes obtained on addition of $Cu(NO_3)_2$ solution into species **5a**,

Slope k = 20558 AU/μM = 2.0558 x 10^{10} AU/M.

The Standard Deviation (σ) was calculated as 50.5

Therefore, detection limit = 7.4 x 10^{-9} M (7.4 nM).

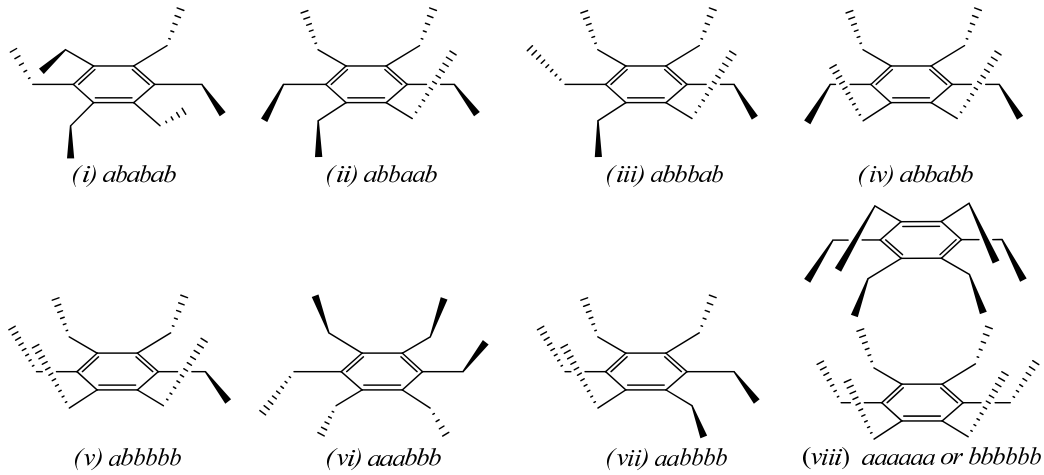

Chart S1 Various possible conformational isomers of hexa-substituted benzenes.

Table S1 Crystallographic data and refinement details for compounds **2a** and **3a**.

Compound	**2a**	**3a**
Empirical formula	C30 H27 Br1.09 Cl1.91 Se3	C48 H39 F3 Se6
Formula weight	779.38	1146.55
Temperature	298(2) K	295(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Orthorhombic	Triclinic
Space group	Pnma	P -1
a (Å)	15.970(2)	12.166(4)
b (Å)	13.690(4)	13.534(4)
c (Å)	14.857(1)	15.244(4)
α (°)	90	114.409(6)
β (°)	90	105.717(6)
γ (°)	90	91.805(6)
Z	4	2
D_{calc} (Mg/m^3)	1.594	1.754

F(000)	1519	1116
Theta range for data collection	1.87 to 28.23°	1.54 to 26.37°
Reflections collected	36785	12745
Independent reflections	4138	8675
R(int)	0.0983	0.0482
Completeness to theta = 25.00°	100 %	98.7 %
Data / restraints / parameters	4138 / 222 / 224	8675 / 0 / 502
Goodness-of-fit on F^2	1.094	0.972
Final R indices [I>2sigma(I)]	R1 = 0.0731, wR2 = 0.1267	R1 = 0.0705, wR2 = 0.1583
R indices (all data)	R1 = 0.1164, wR2 = 0.1416	R1 = 0.1532, wR2 = 0.1950