Fluorimetric detection of Mg^{2+} and DNA with 9-(alkoxyphenyl)benzo[*b*]quinolizinium derivatives

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Electronic Supplementary Information (ESI)

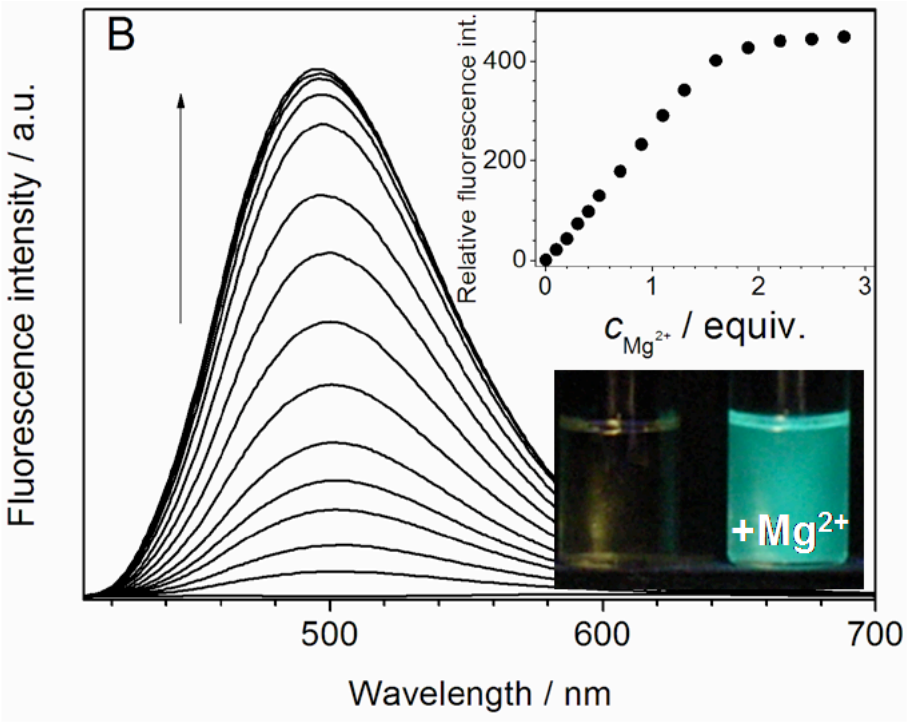

Fig. S1 (Fig. 3B in main manuscript) Spectrofluorimetric titration of Mg^{2+} to compound **2a** (c = 10 µM, λ_{ex} = 395 nm) in MeCN. The arrows indicate the changes of emission upon addition of Mg^{2+}. Insets: Plot of the emission intensity at 495 nm versus Mg^{2+} concentration, and picture of the emission color of **2a** in the absence and in the presence of Mg^{2+}.

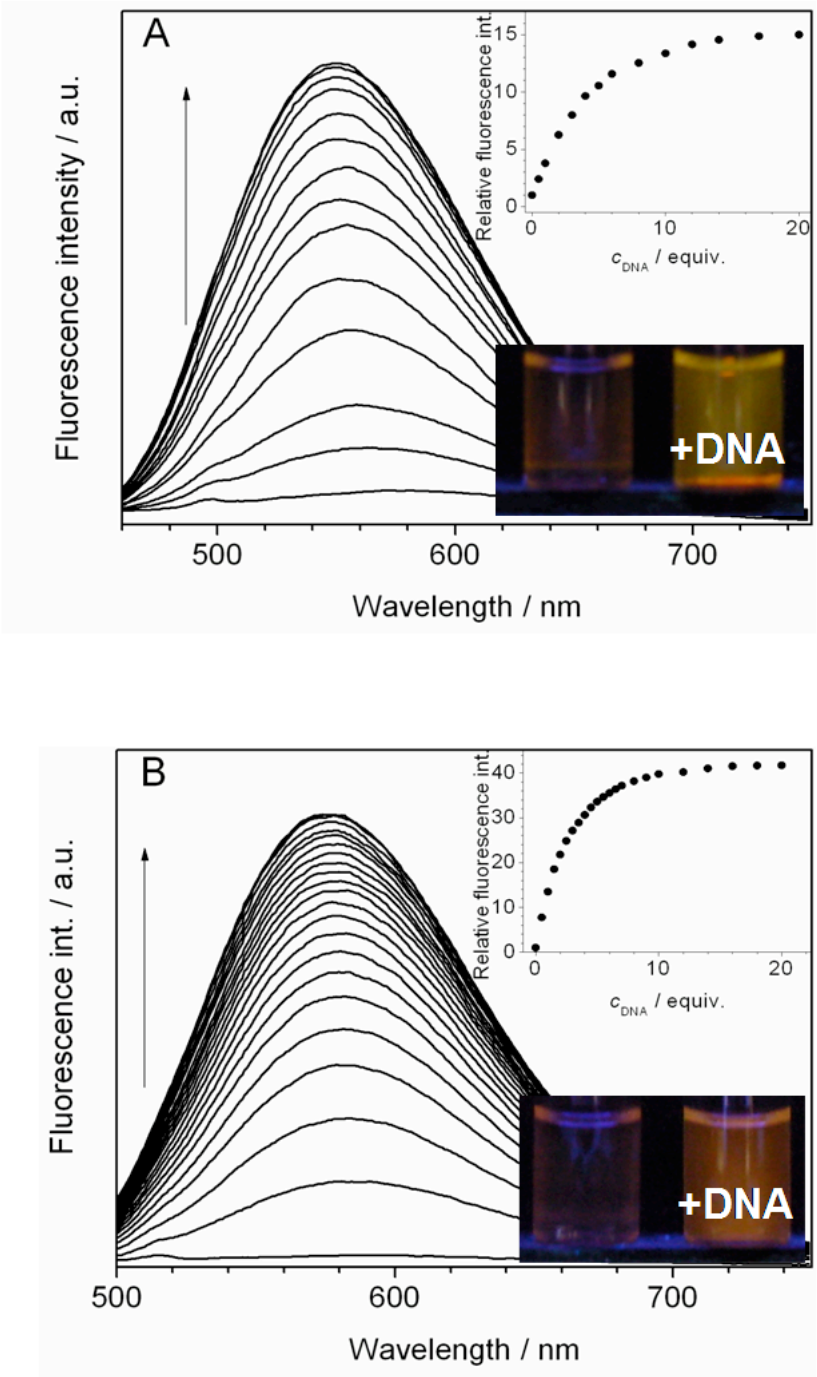

Fig. S2 (Fig. 6A and 6B in main manuscript) Spectrofluorimetric titrations of **2a** (A, λ_{ex} = 425 nm), **2b** (B, λ_{ex} = 438 nm) with ct DNA in BPE buffer (c = 10 μM). The arrows indicate the changes of the bands upon addition of ct DNA. Insets: plot of the relative emission intensity versus c_{DNA}, and picture of the emission color of **2a** and **2b** in the absence and in the presence of ct DNA.

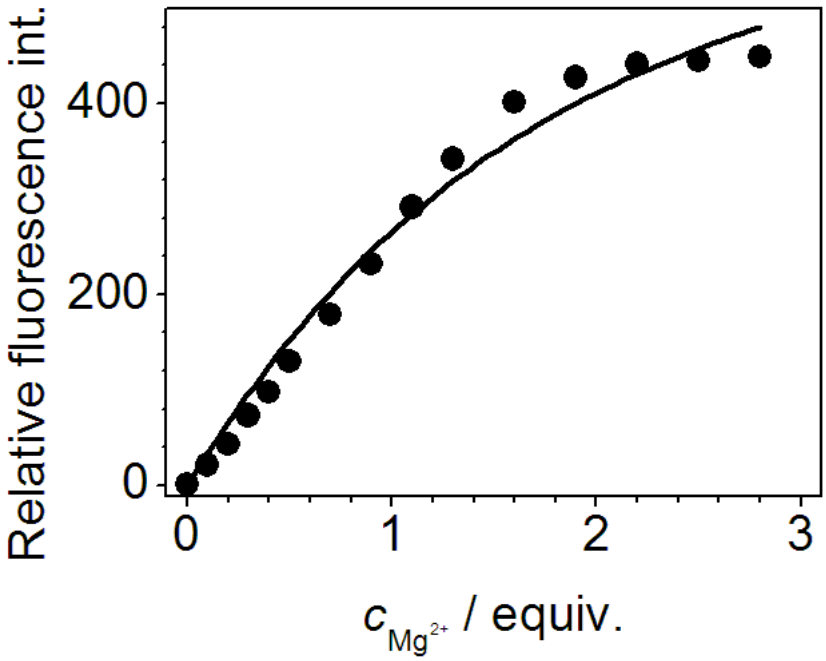

Fig. S3 Spectrofluorimetric titration of Mg^{2+} to compound **2a** (c = 10 μM, λ_{ex} = 395 nm) in MeCN; plot of the emission intensity versus Mg^{2+} concentration and fit of the experimental data to the theoretical model; numerical fit calculated for $K = 0.9 \times 10^5$ M^{-1}.

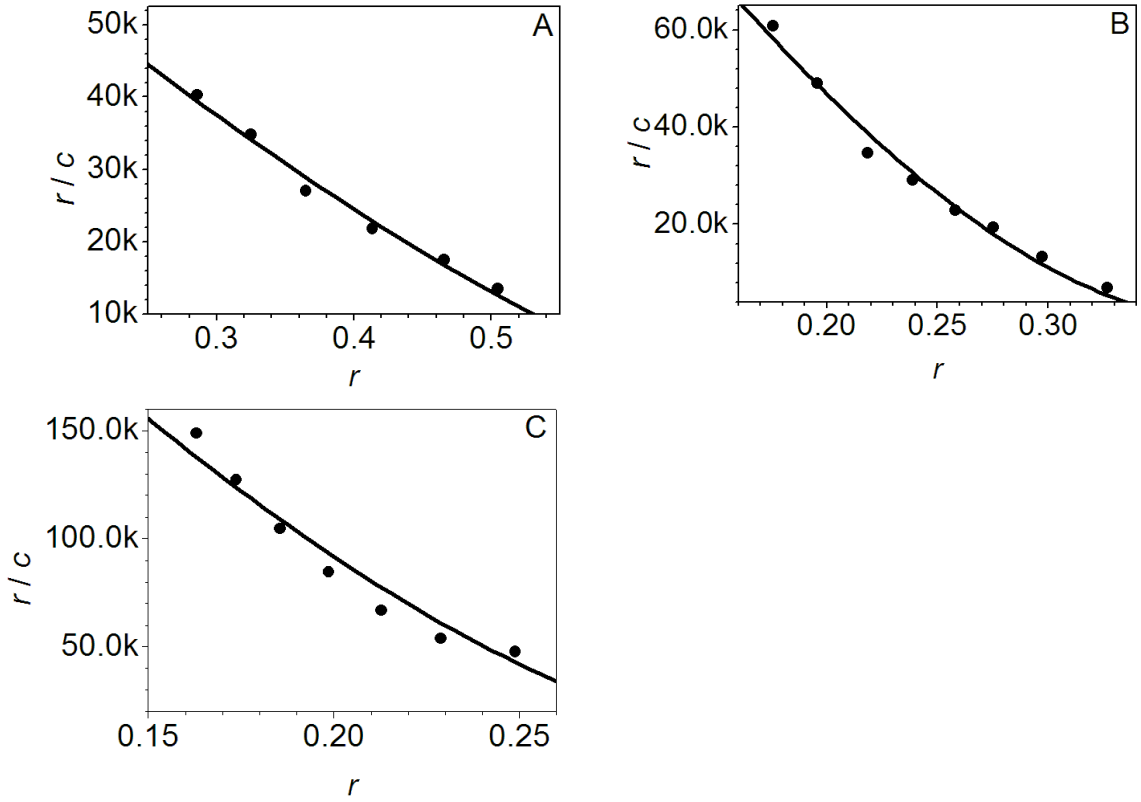

Fig. S4 Scatchard plots, *r*/*c* vs *r*; *r* = ligand-to-DNA ratio, obtained from spectrophotometric titrations of **2a** (A), **2b** (B) and **2c** with ct DNA in BPE buffer (*c* = 50 μM). The experimental data points were fitted to the model of McGhee and von Hippel.

The concentration of the DNA-bound ligand was calculated according to equation S1.

$$c_b = c_L \times \frac{A_f - A}{A_f - A_b} \qquad \text{(eq. S1)}$$

The bulk concentration of the ligand is c_L, A_f is the absorbance of the free ligand at a given wavelength, A_b is the absorbance of the bound ligand, and A is the absorbance at a given ligand-to-DNA ratio. The concentration of the unbound ligand (c) and he ratio of bound ligand molecules per DNA base pair (r) were determined according to equation S2 and S3.

$$c = c_L - c_b \qquad \text{(eq. S2)}$$

$$r = \frac{c_b}{c_{DNA}} \qquad \text{(eq. S1)}$$

The data were given as Scatchard plots, *r*/*c vs.* *r*, and numerically fitted to the neighbor exclusion model of McGhee and von Hippel (eq S4),[1] to deduce the binding constant *K*. The numerical fitting was performed using the Levenberg–Marquardt non-linear curve fitting algorithm implemented into calculus software.

$$\frac{r}{c} = K(1 - nr)\left(\frac{1 - nr}{1 - (n-1)r}\right)^{n-1} \qquad \text{(eq. S4)}$$

[1] J. D. McGhee and P. H. von Hippel, *J. Mol. Biol.*, 1974, **86**, 469–489.

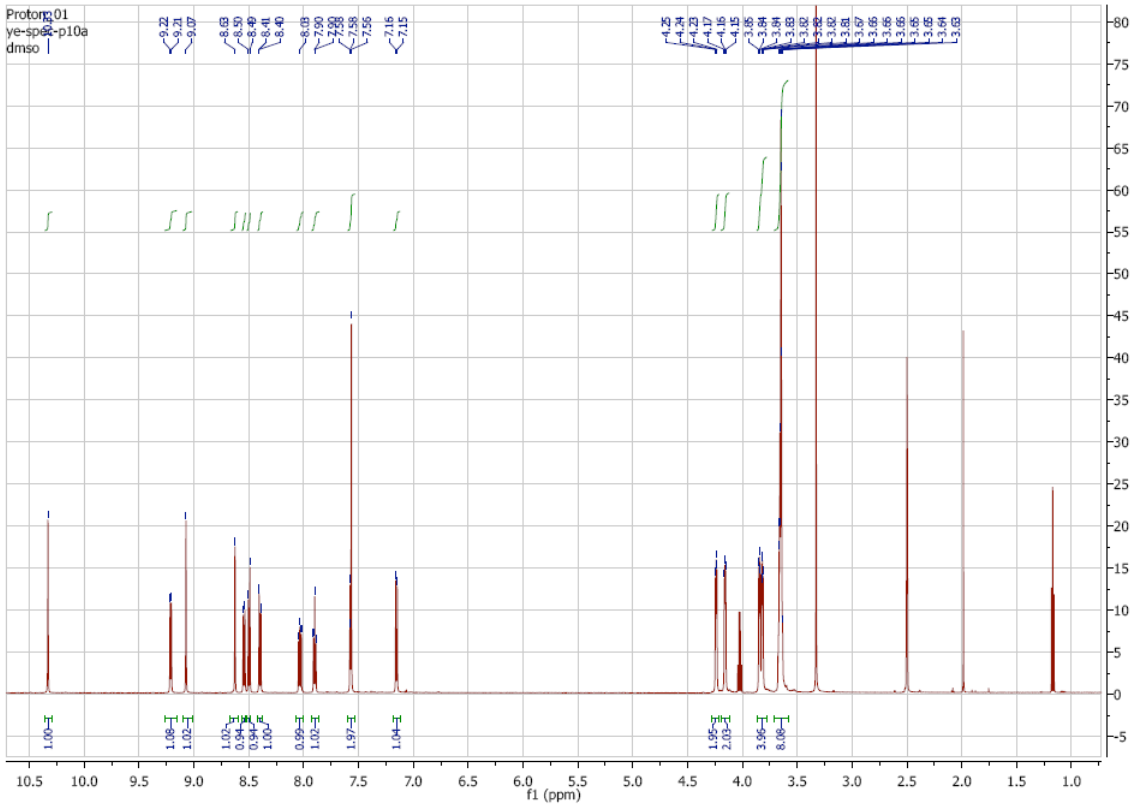

Fig. S5 ^{1}H-NMR spectrum of **2a** in [D_6]DMSO

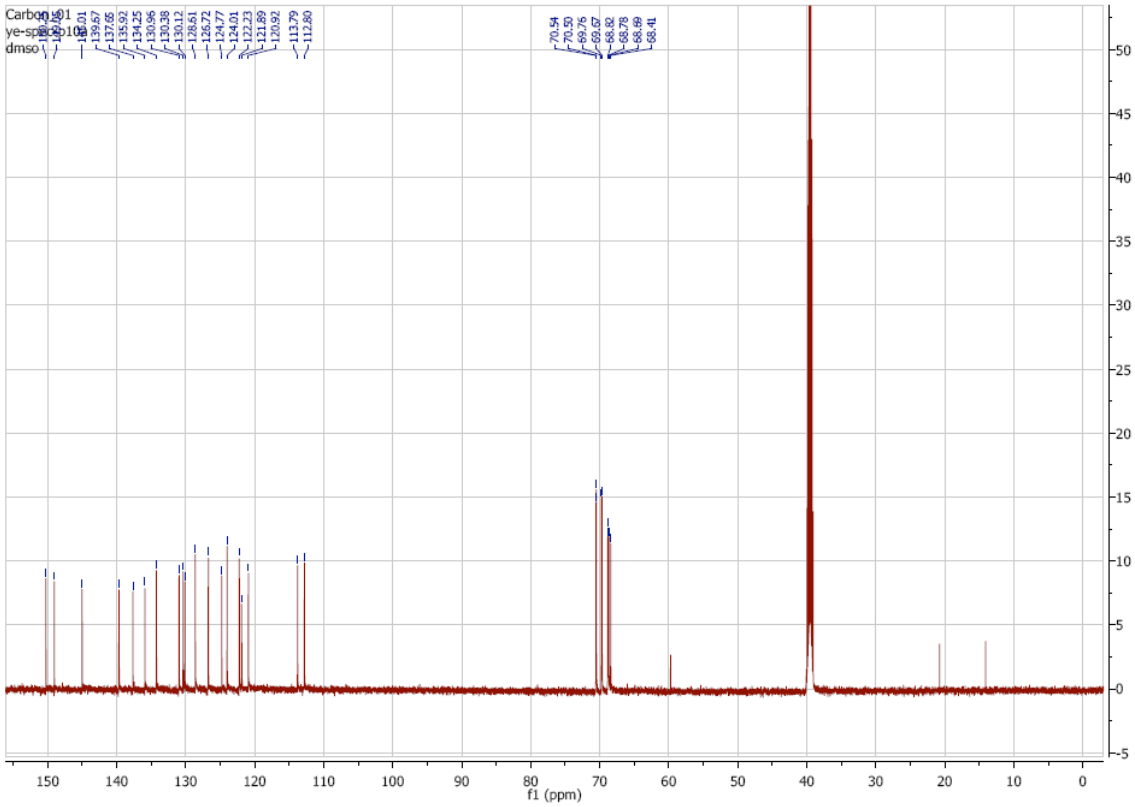

Fig. S6 ^{13}C-NMR spectrum of **2a** in [D_6]DMSO

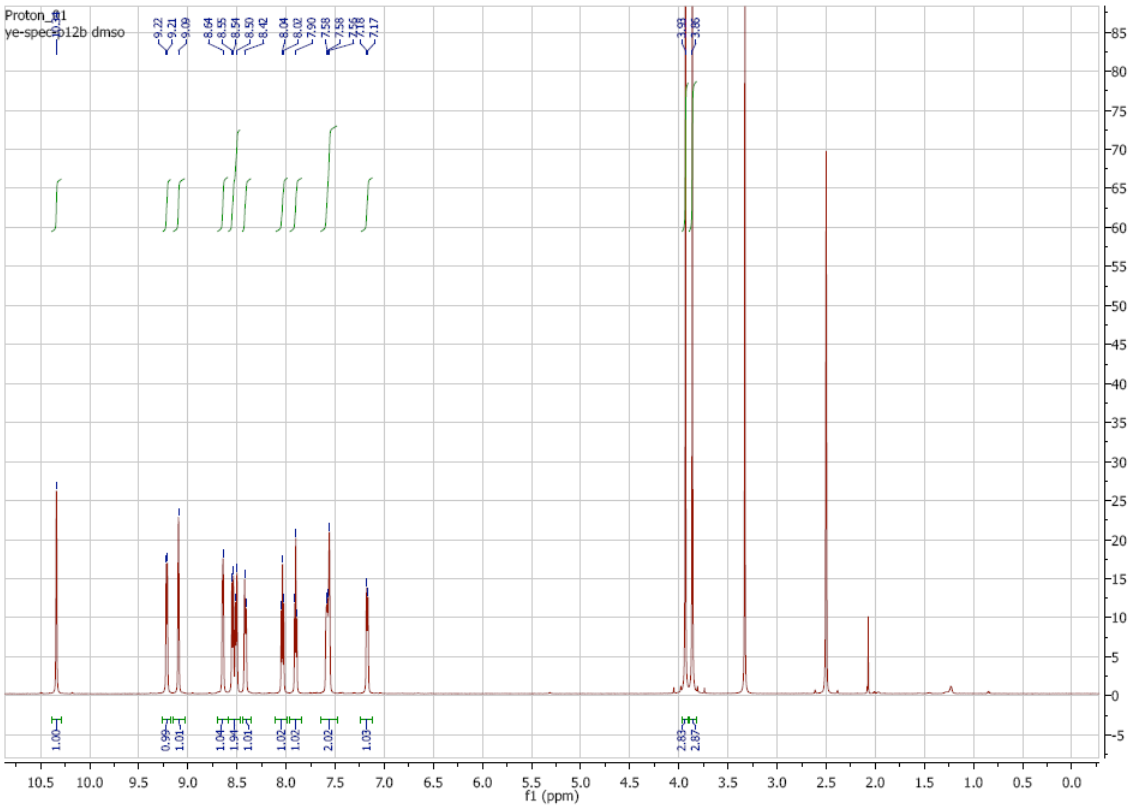

Fig. S7 ^{1}H-NMR spectrum of **2b** in [D_6]DMSO

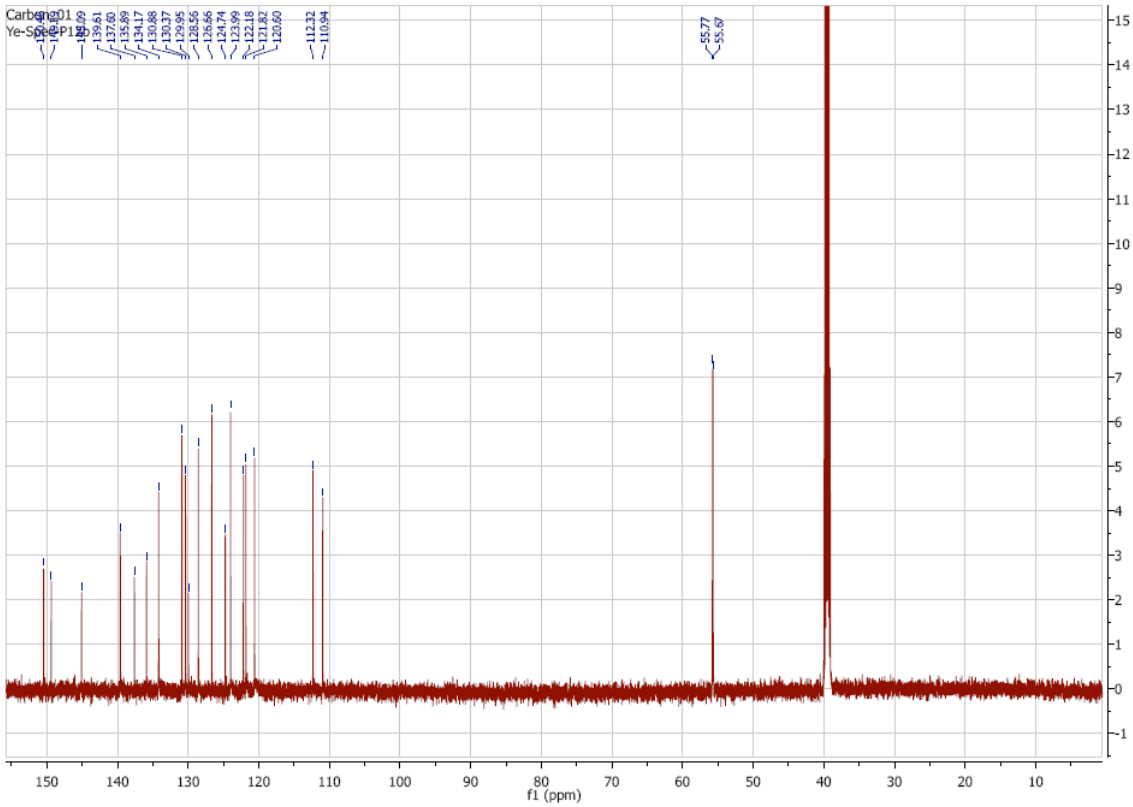

Fig. S8 ^{13}C-NMR spectrum of **2b** in [D_6]DMSO

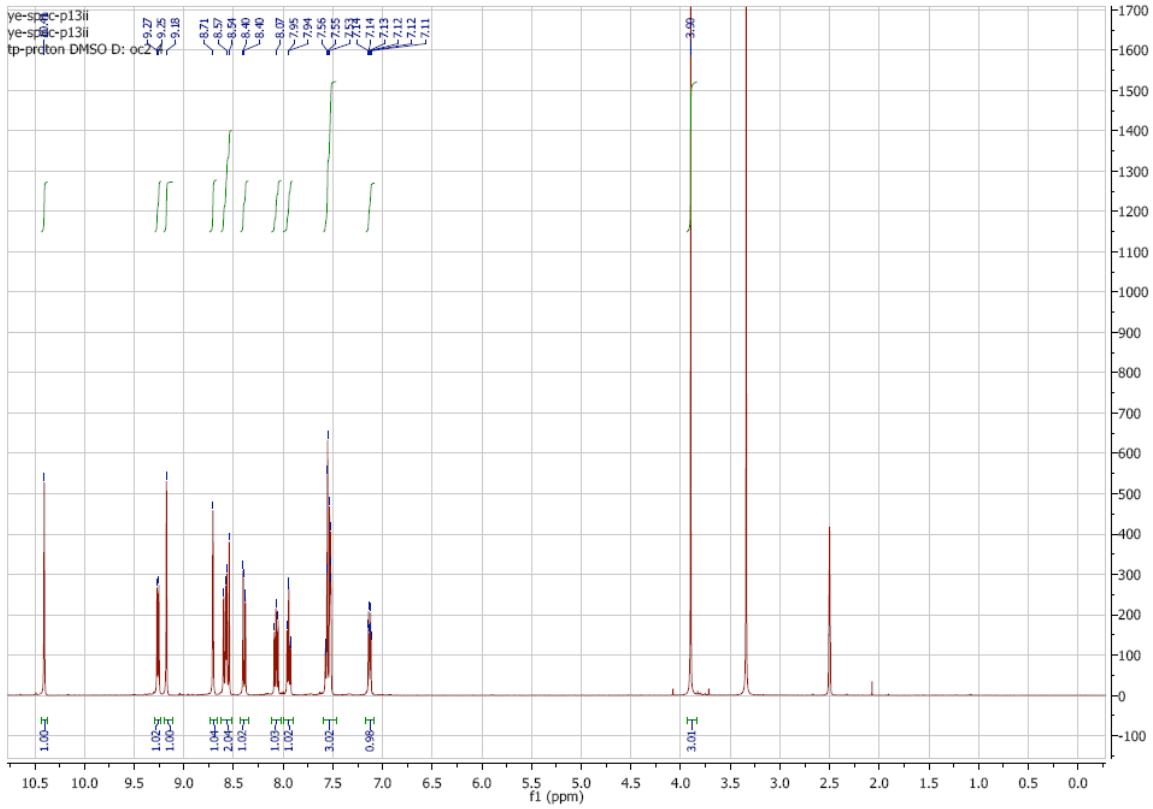

Fig. S9 ^{1}H-NMR spectrum of **2c** in [D_6]DMSO

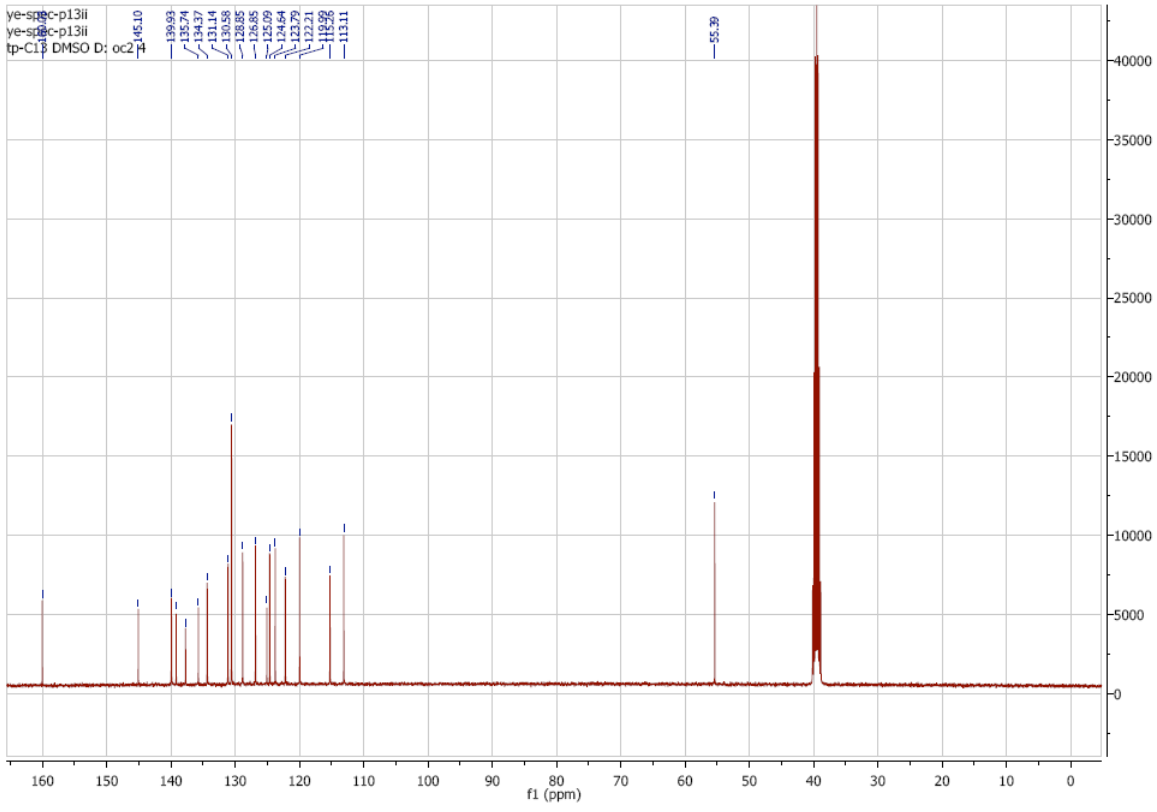

Fig. S10 ^{13}C-NMR spectrum of **2c** in [D_6]DMSO