Supporting Information

An alternative to 'propylene/Leonard linker' for studying arene interactions in flexible pyrazolo[3,4-*d*]pyrimidine core based models both at molecular and supramolecular level

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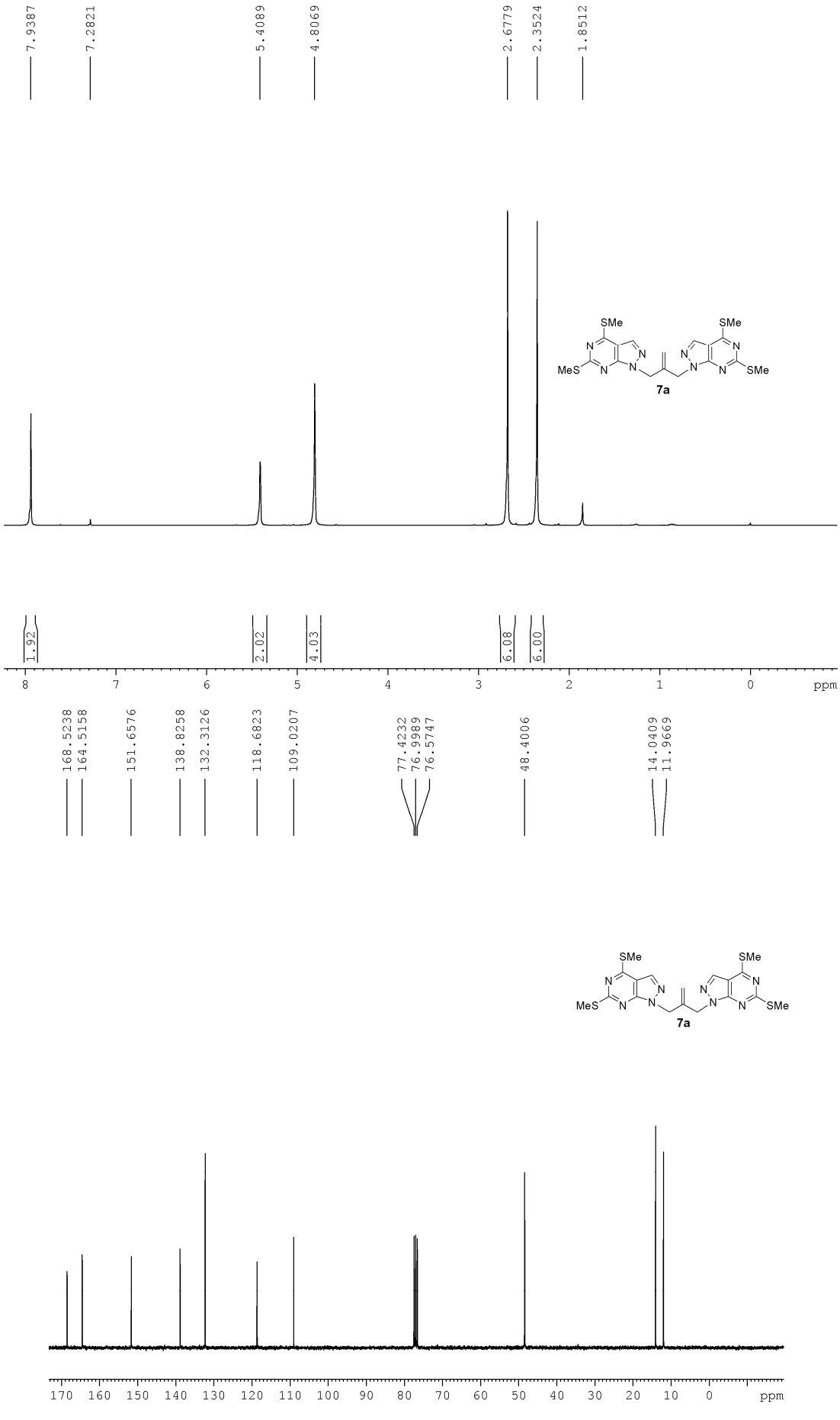


Fig. S1 ^{1}H and ^{13}C NMR Spectra of compound **7a** in $CDCl_3$

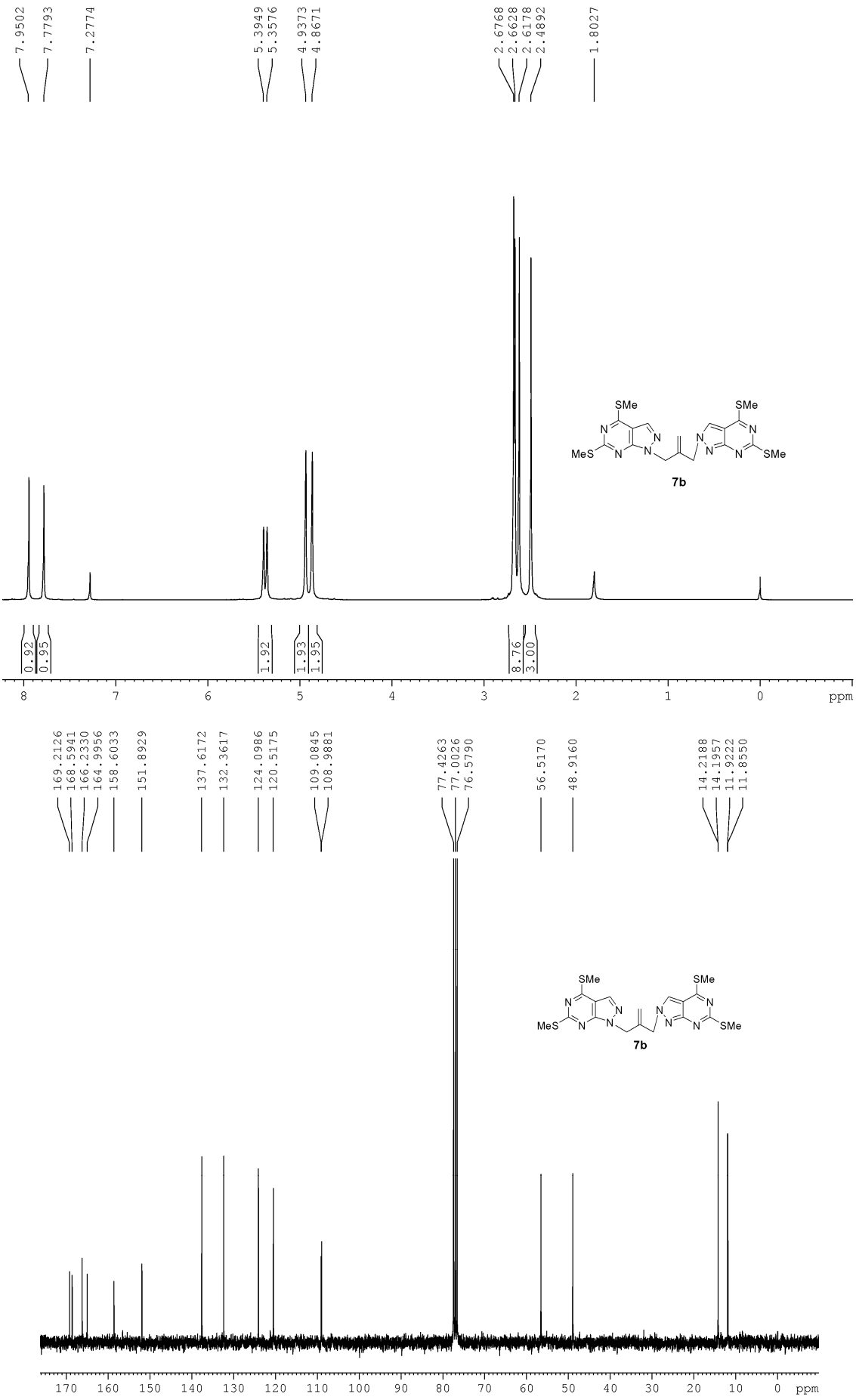


Fig. S2 ^{1}H and ^{13}C NMR Spectra of compound **7b** in $CDCl_3$

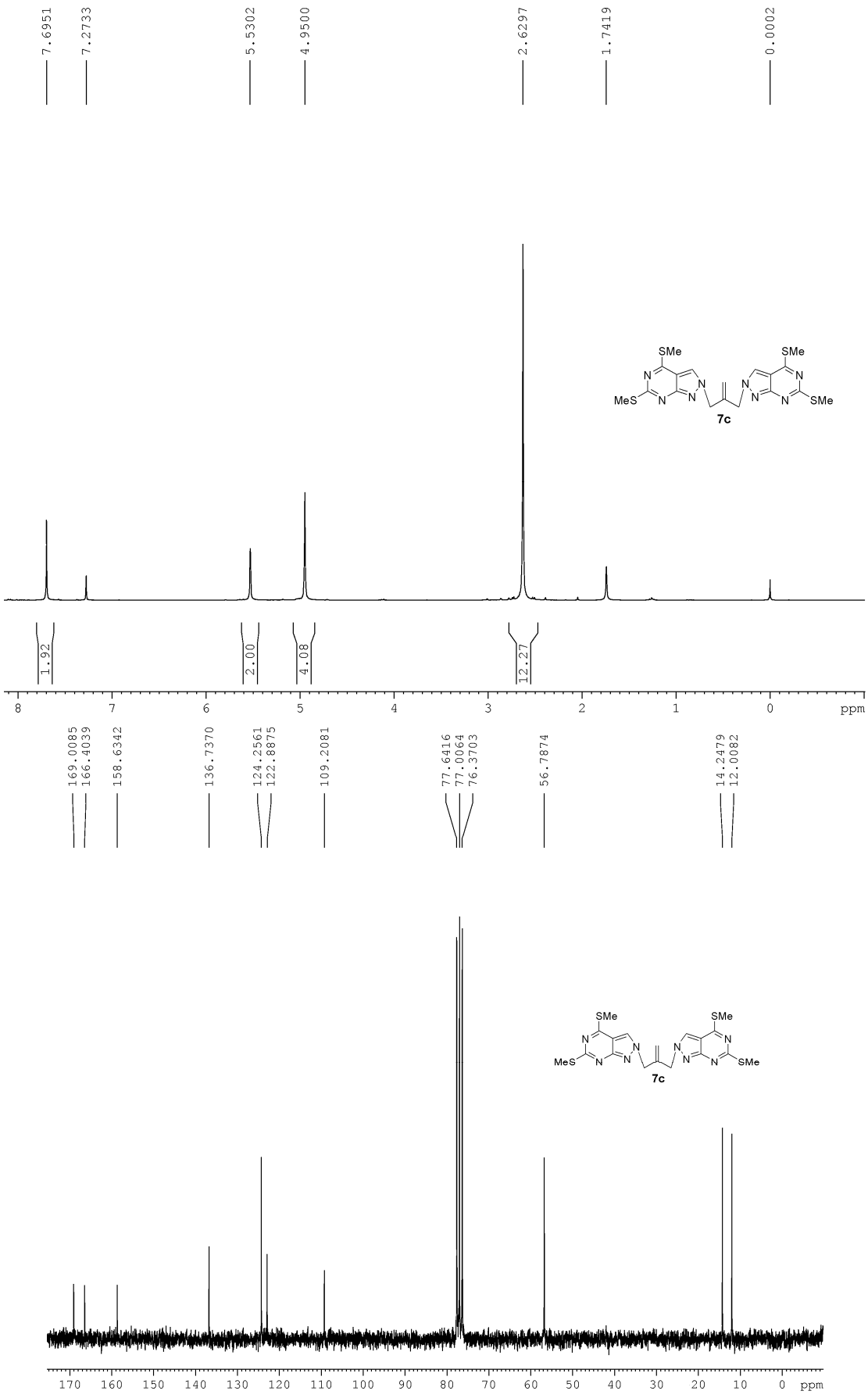


Fig. S3 ^{1}H and ^{13}C NMR Spectra of compound **7c** in $CDCl_3$

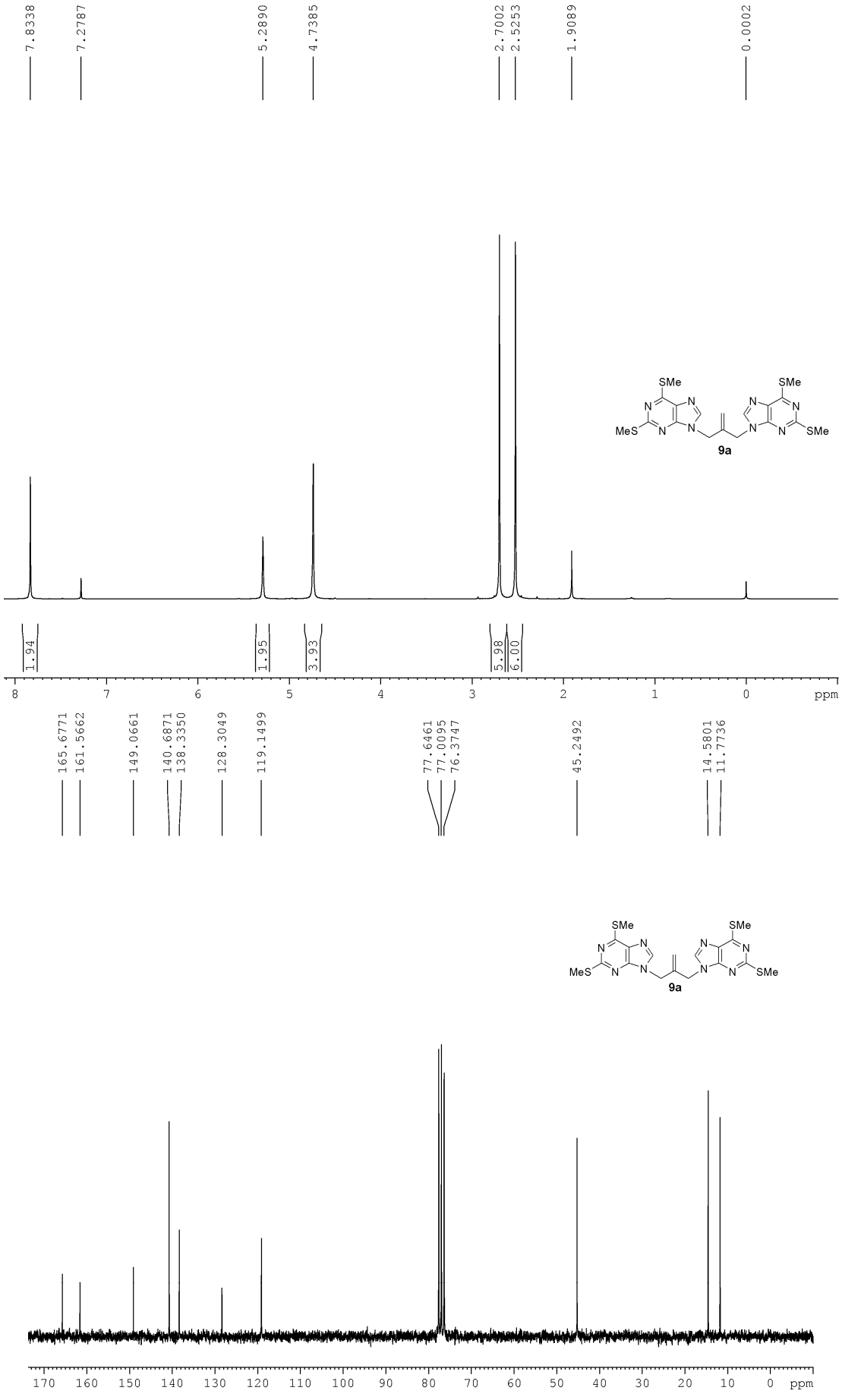


Fig. S4 ^{1}H and ^{13}C NMR Spectra of compound **9a** in $CDCl_3$

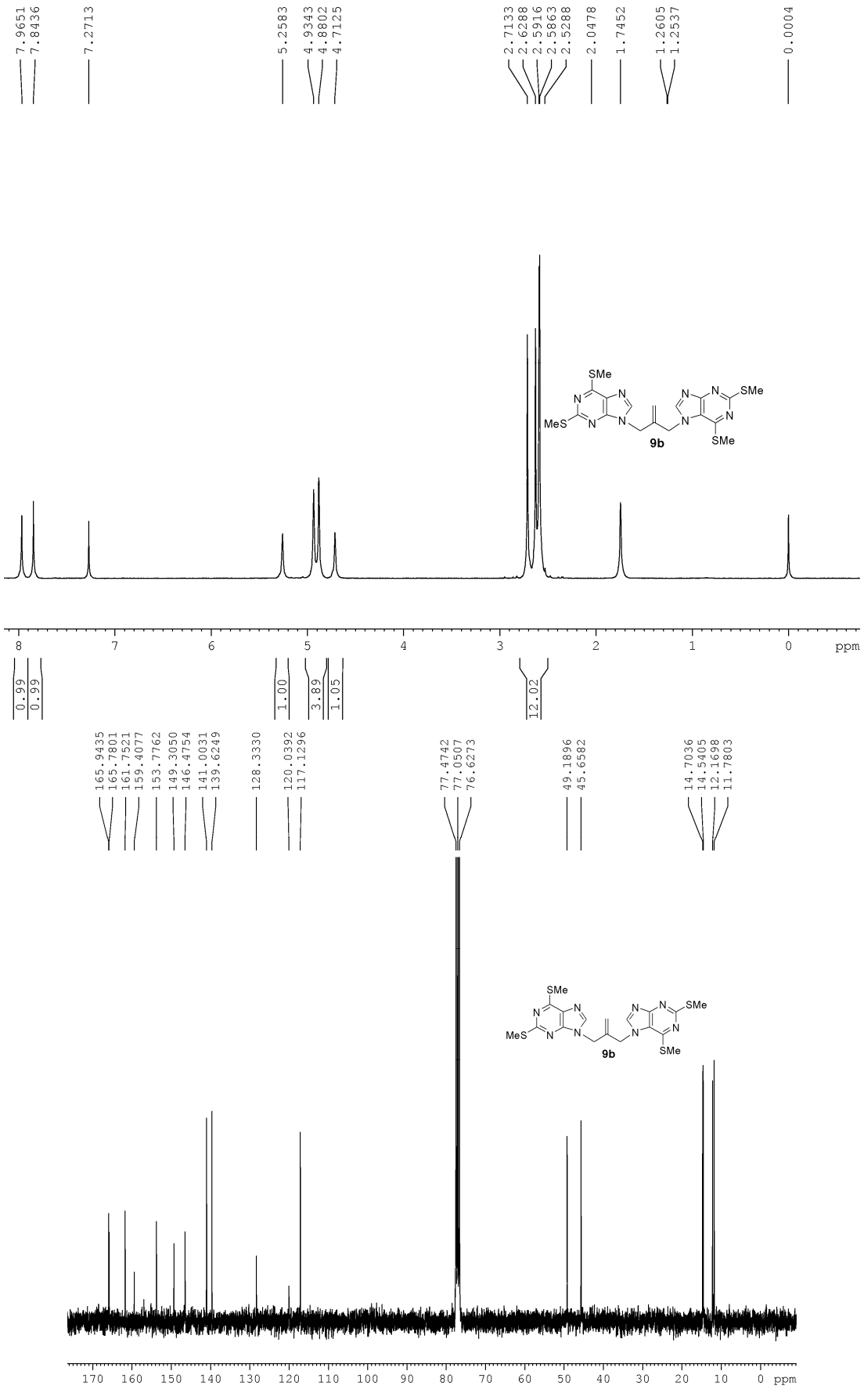


Fig. S5 ^{1}H and ^{13}C NMR Spectra of compound **9b** in $CDCl_3$

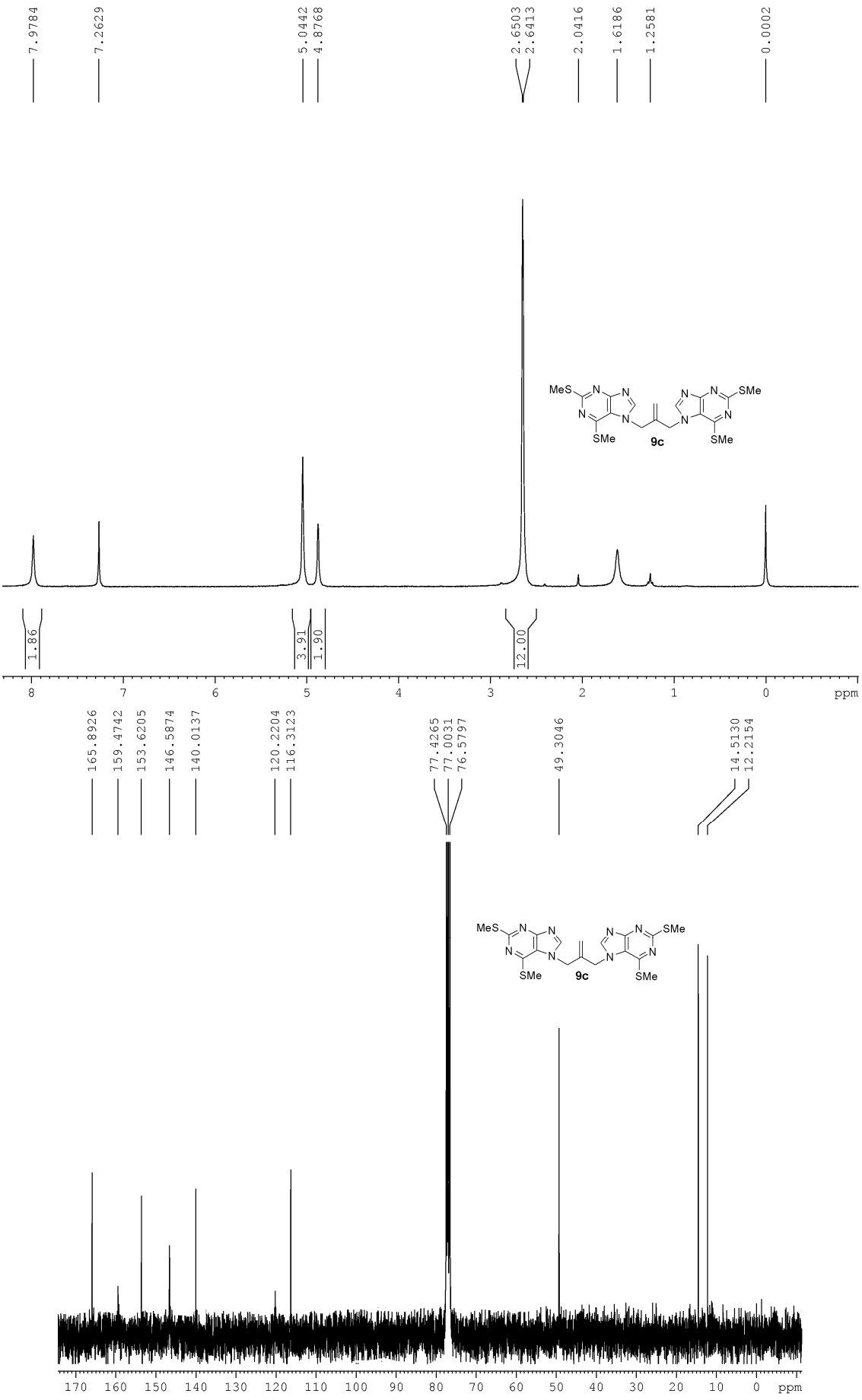


Fig. S6 ^{1}H and ^{13}C NMR Spectra of compound **9c** in $CDCl_3$

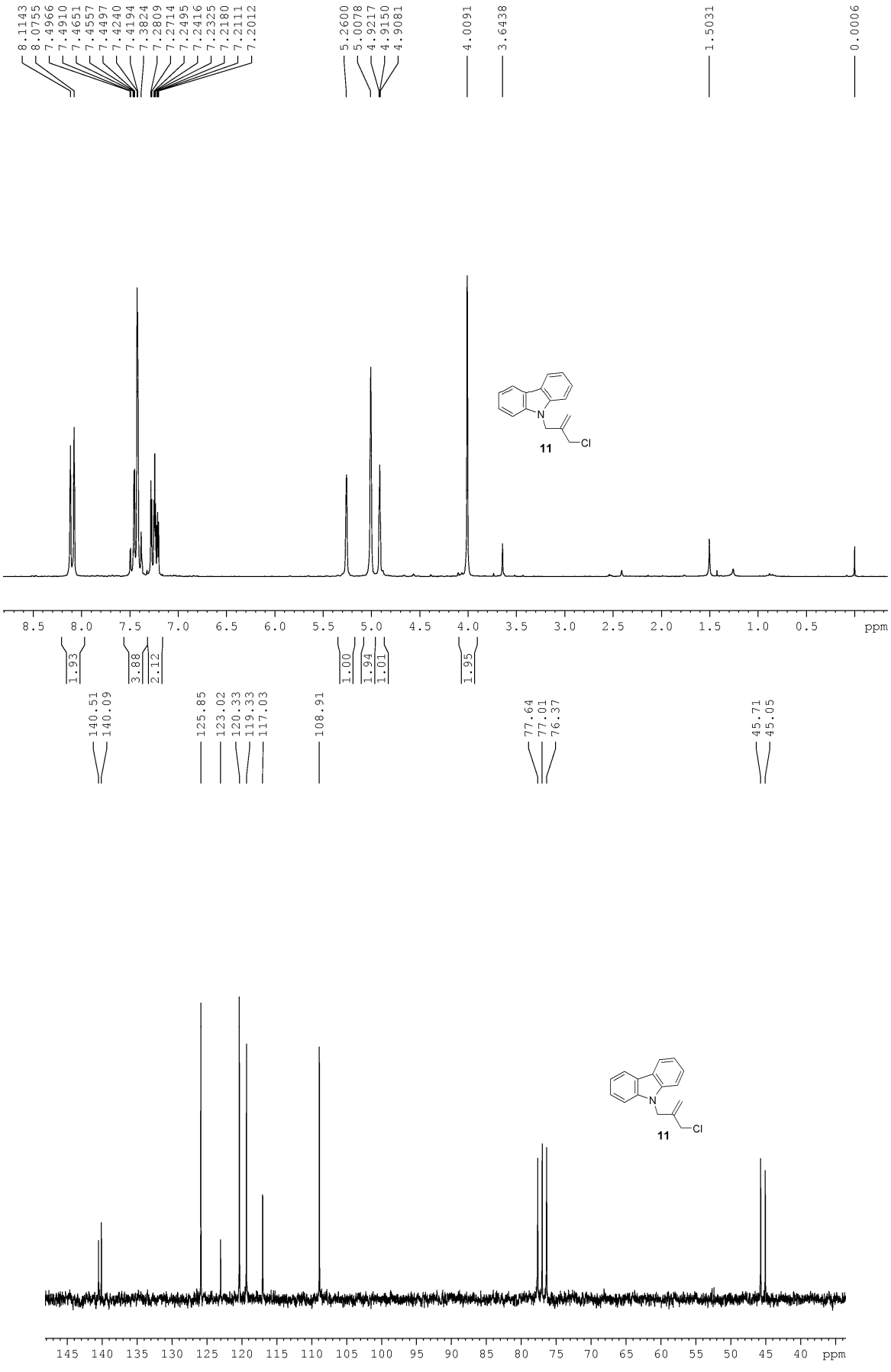


Fig. S7 ^{1}H and ^{13}C NMR Spectra of compound **11** in $CDCl_3$

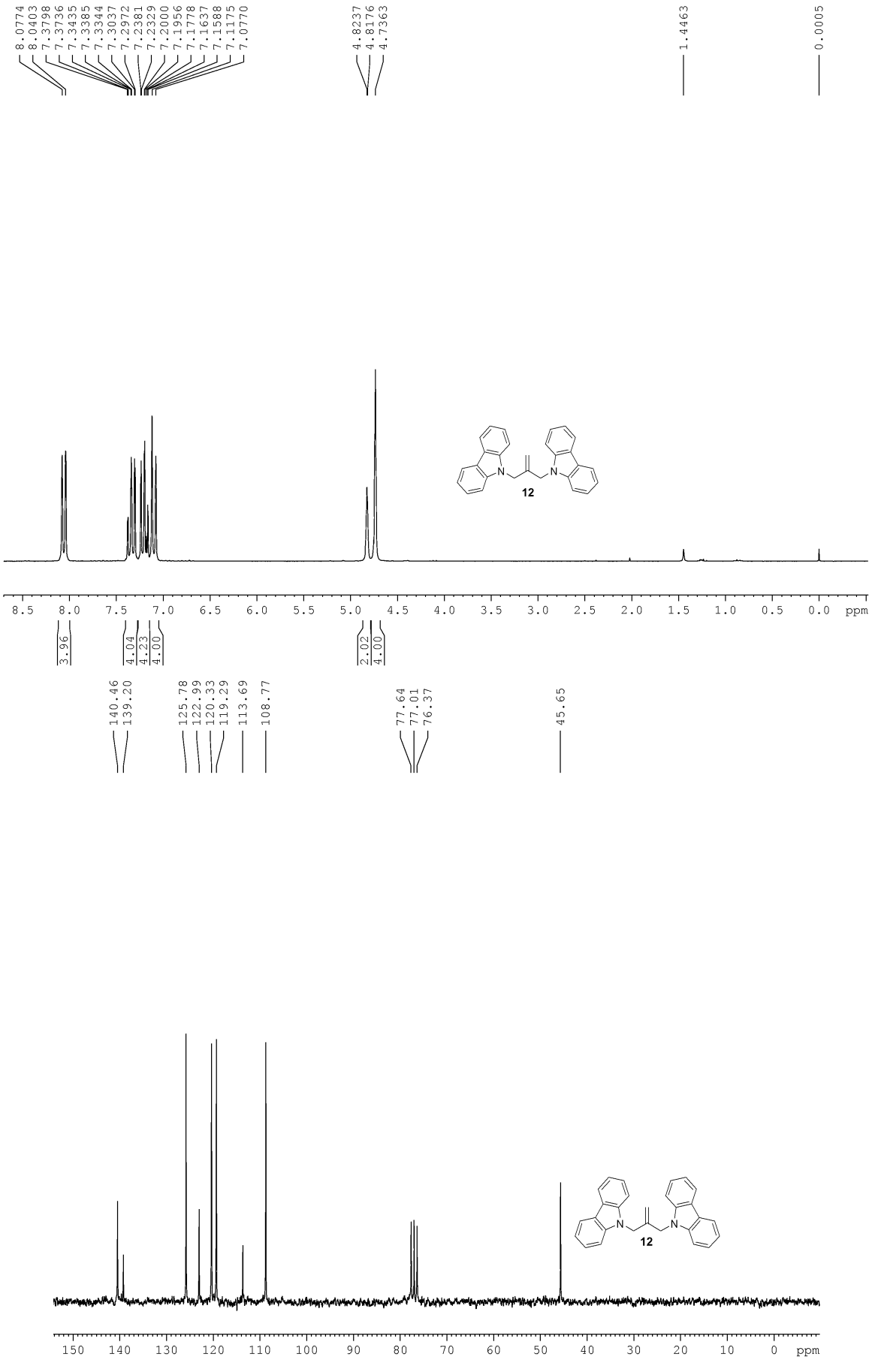


Fig. S8 ^{1}H and ^{13}C NMR Spectra of compound **12** in $CDCl_3$

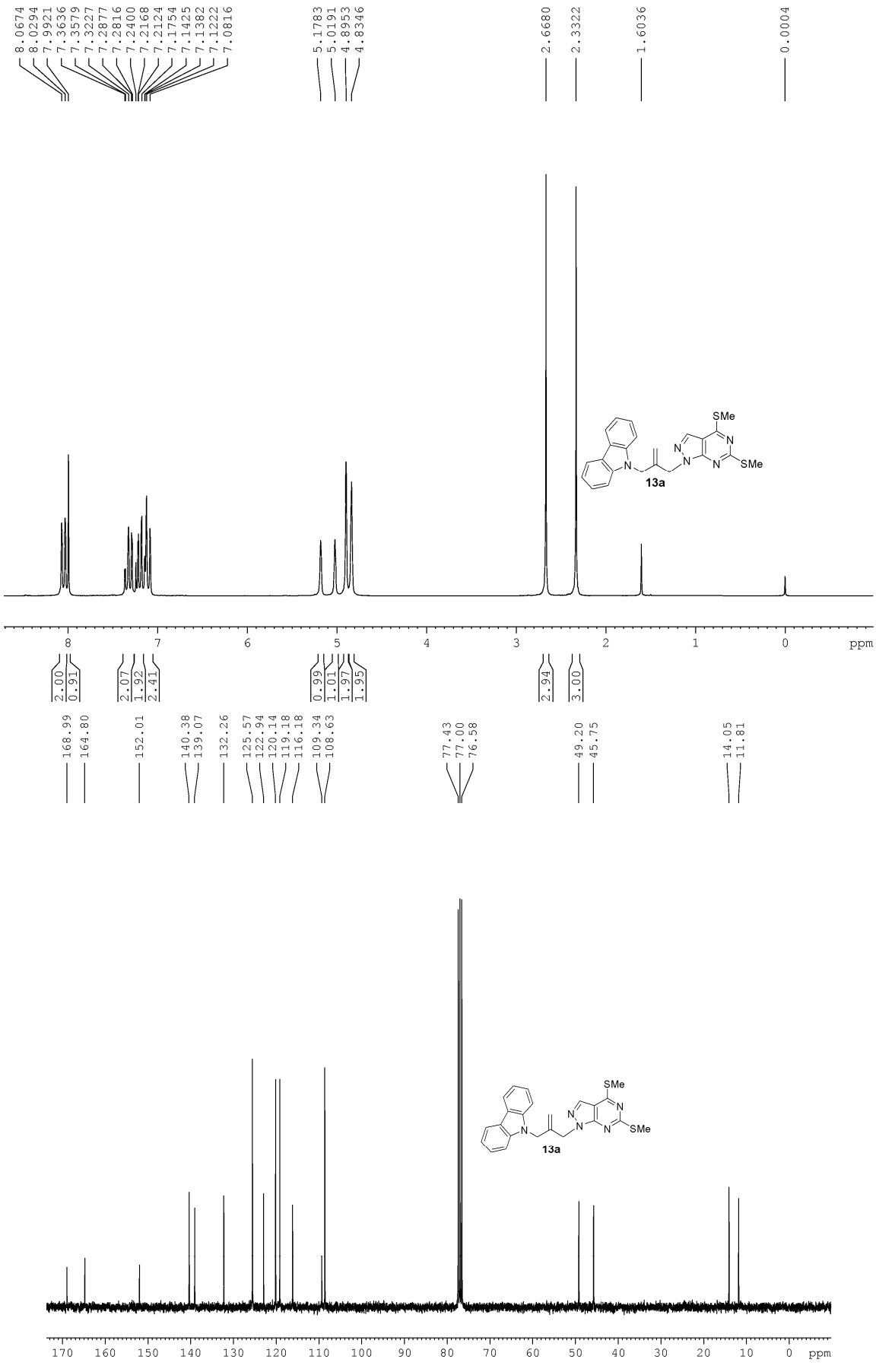


Fig. S9 ^{1}H and ^{13}C NMR Spectra of compound **13a** in $CDCl_3$

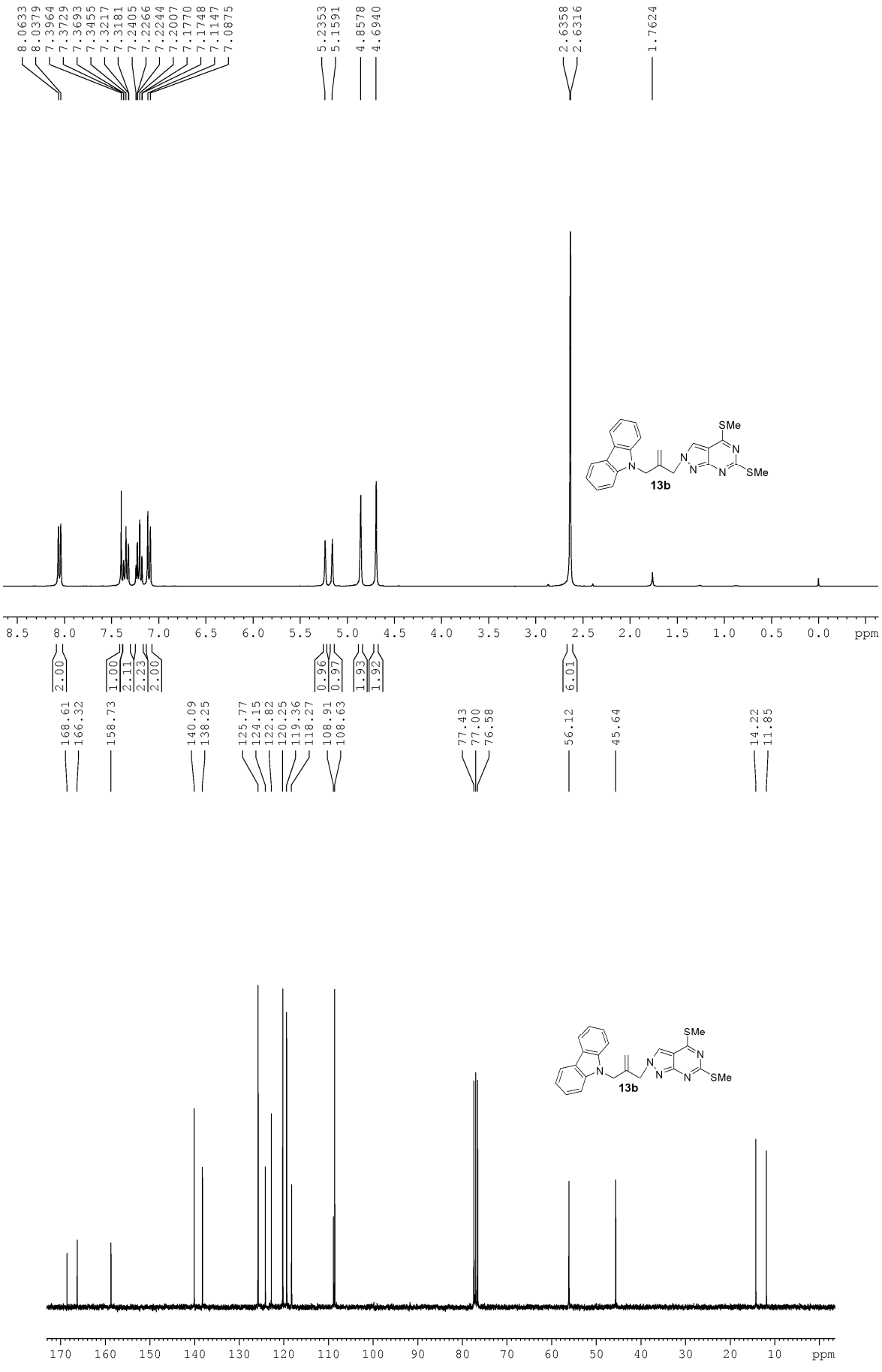


Fig. S10 ^{1}H and ^{13}C NMR Spectra of compound **13b** in $CDCl_3$

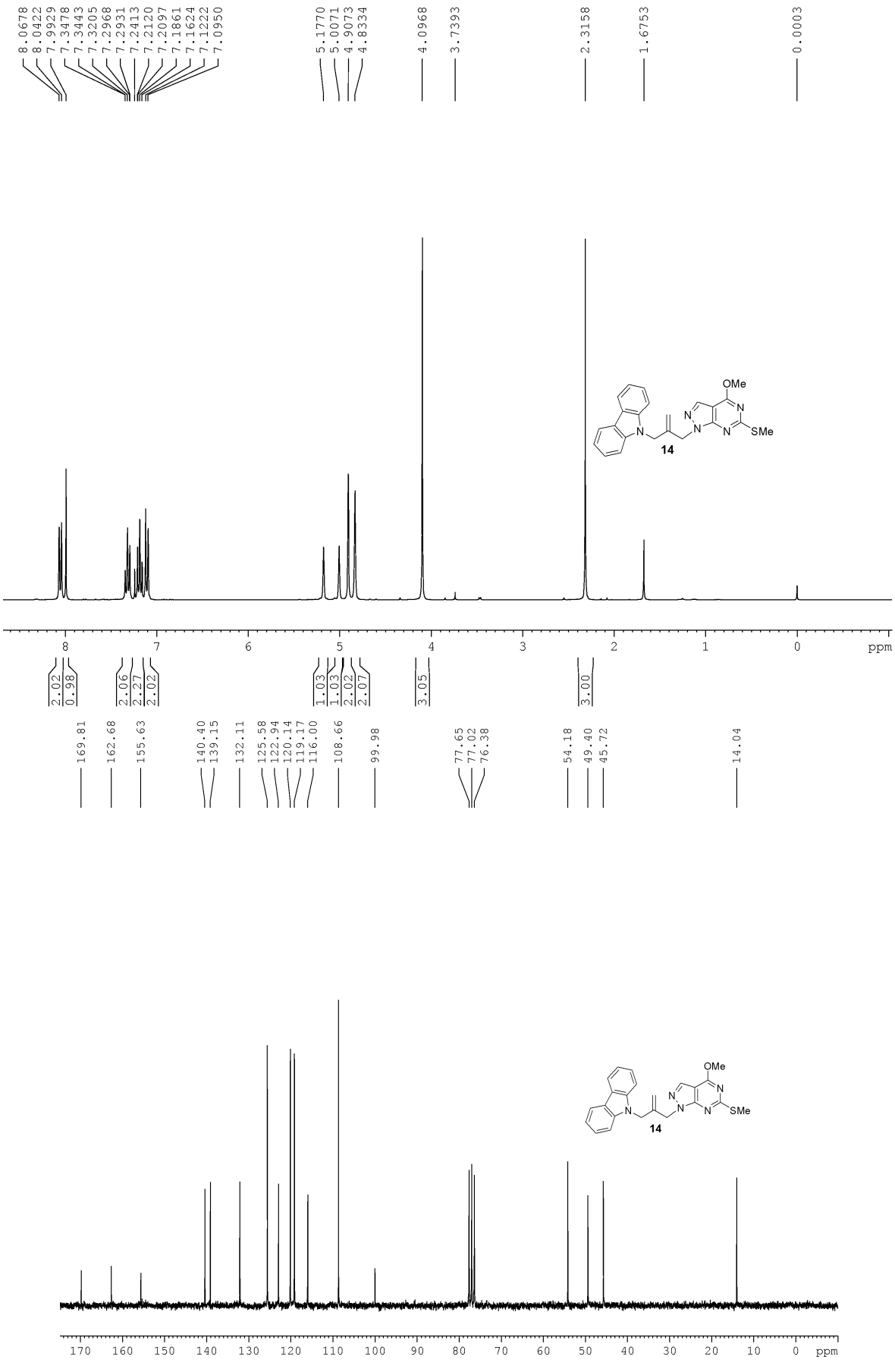


Fig. S11 ^{1}H and ^{13}C NMR Spectra of compound **14** in $CDCl_3$

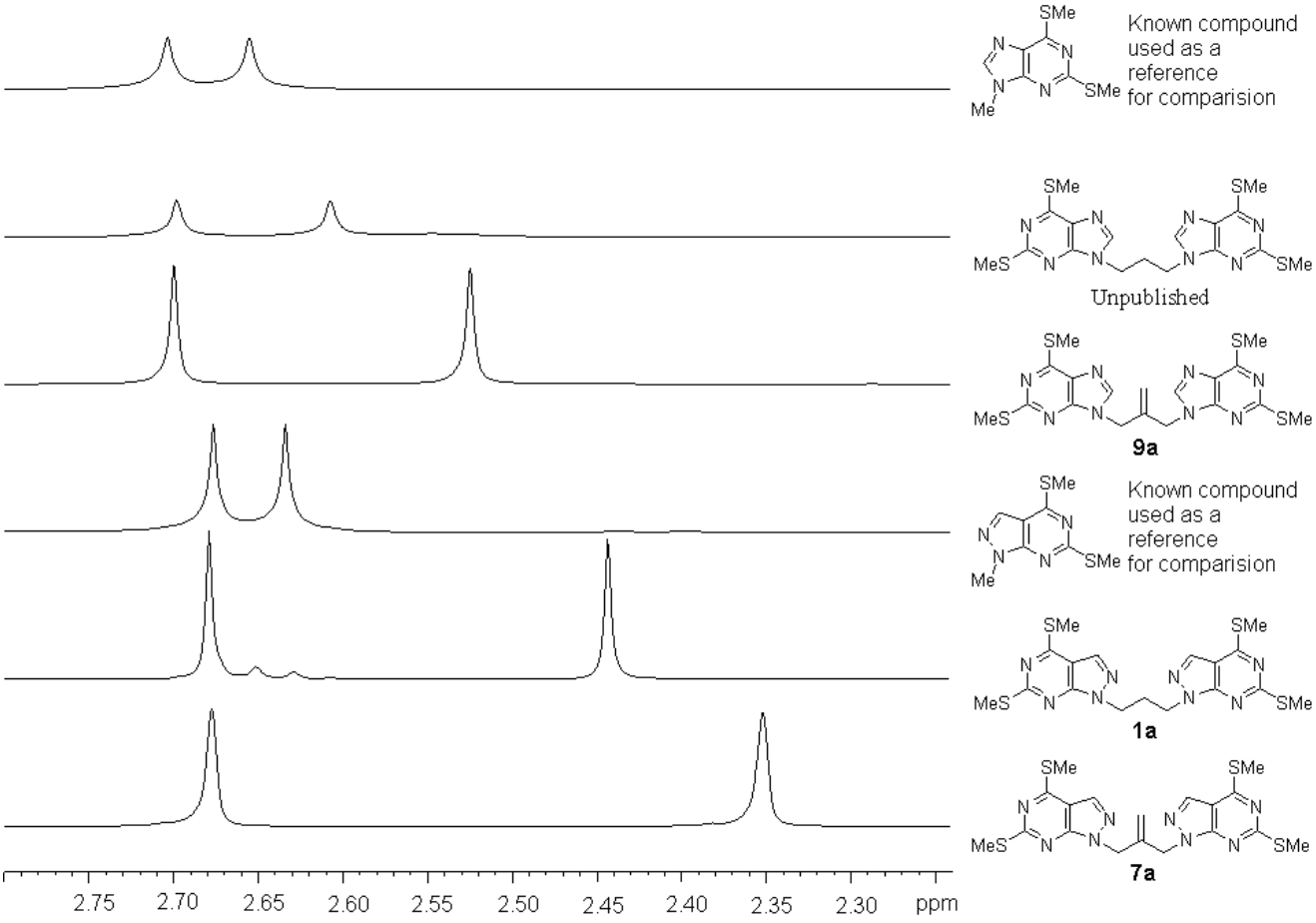
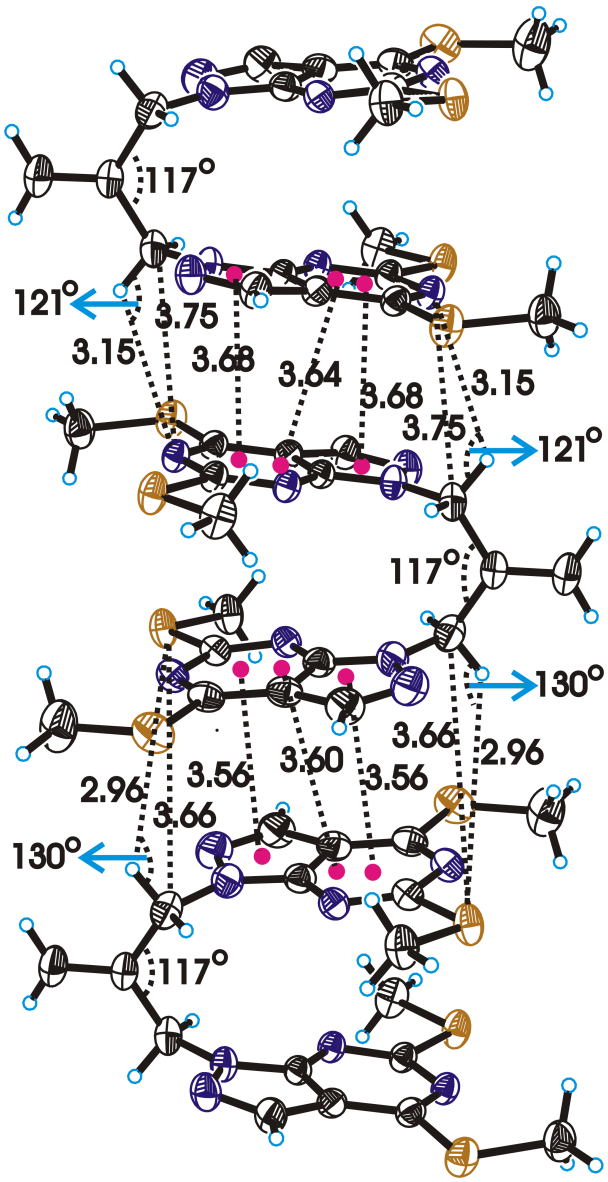
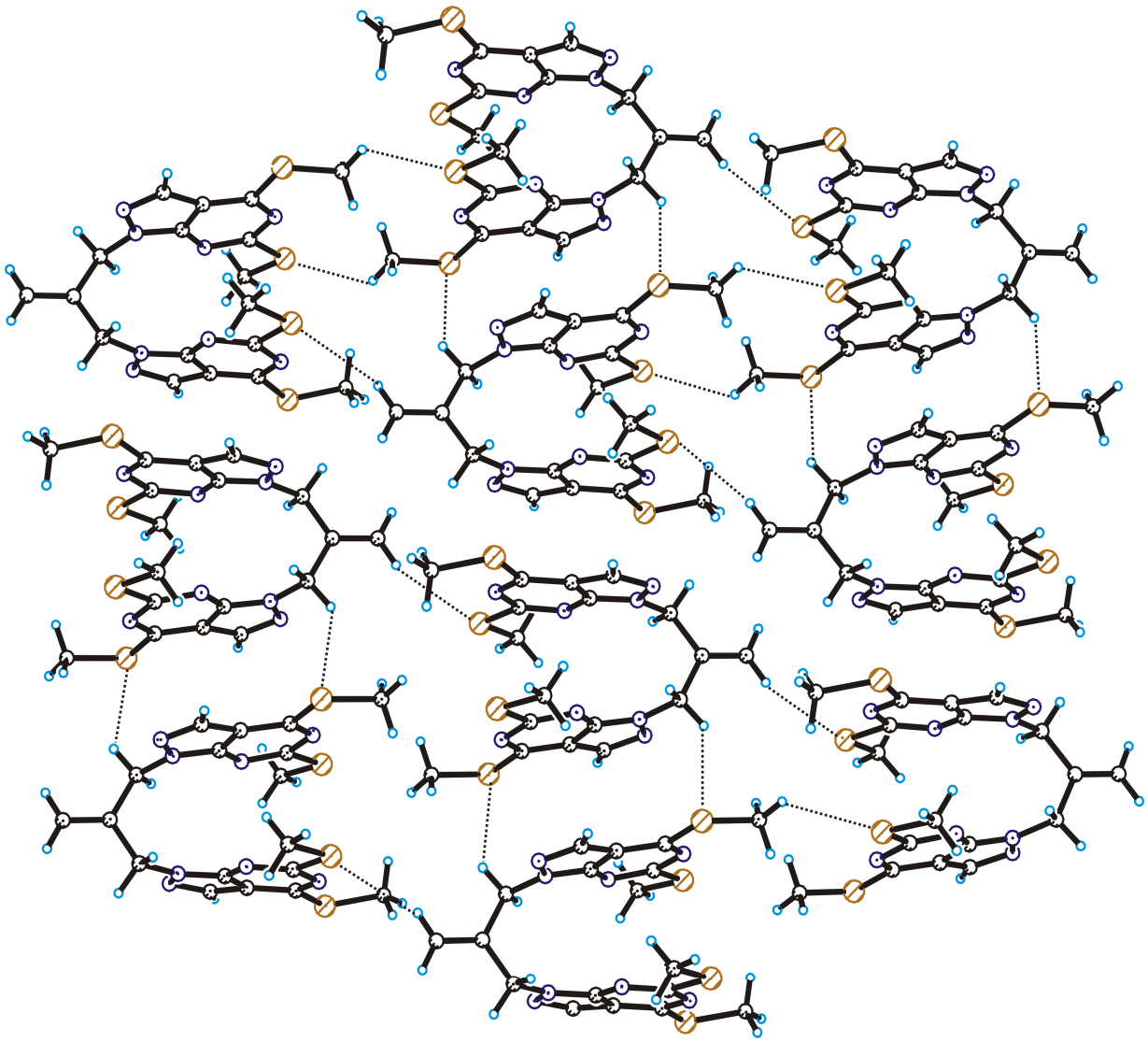


Fig. S12 Stack plot of ^{1}H NMRs of SMe region of selected compounds



One folded molecule is stacked between two adjacent molecules at each face by different interactions. One side by π–π interactions = Cg(5)…Cg(6) = 3.56 Å; Cg(9)…Cg(9) = 3.64 Å. C-H…S dimern = 2.96 Å, 3.66 Å, 130°. Other side by π–π interactions = Cg(5)…Cg(6) = 3.68 Å; Cg(9)…Cg(9) = 3.64 Å. C-H…N dimern. = 3.15 Å, 3.75 Å, 121°. This pattern keeps on repeating to form an infinite vertical stack. This pattern is different from that of corresponding propylene linker compound.

Fig. S13 Part of the vertical columns of **7a** formed as a result of π-π and C-H…S interactions (at 30% probability level).



CH…S interaction (SCH_3...SCH_3) = 2.97 Å, 3.66 Å, 130°
CH…S interaction (NCH_2...SCH_3) = 2.96 Å, 3.66 Å, 130°

Fig. S14 Network formed by C-H…S interaction in **7a**.

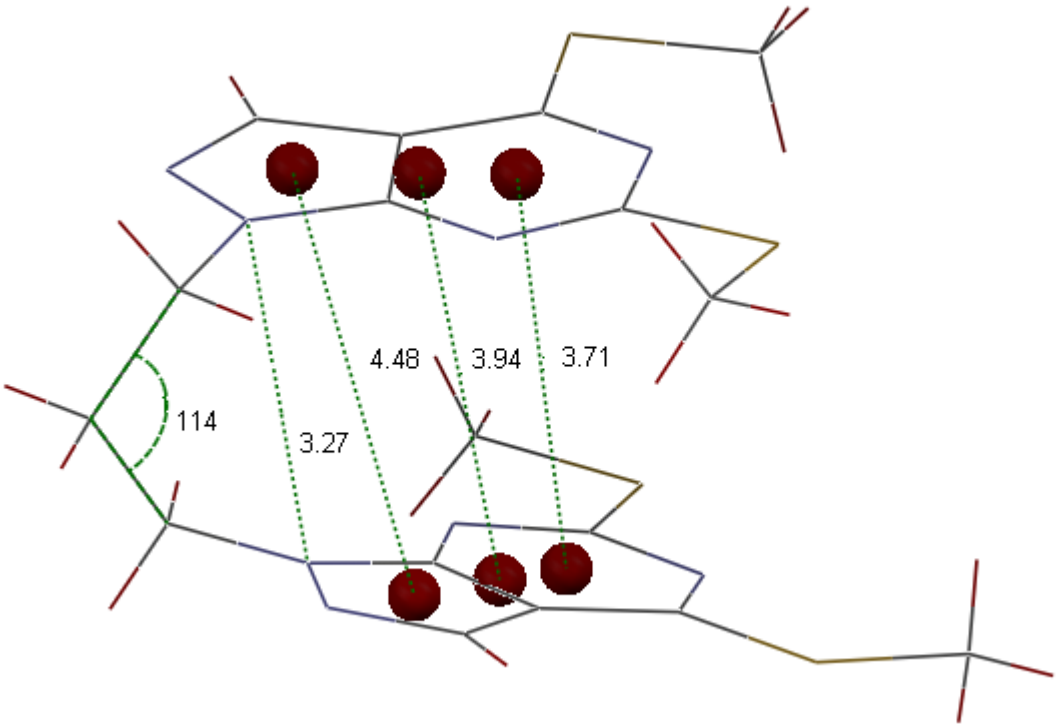
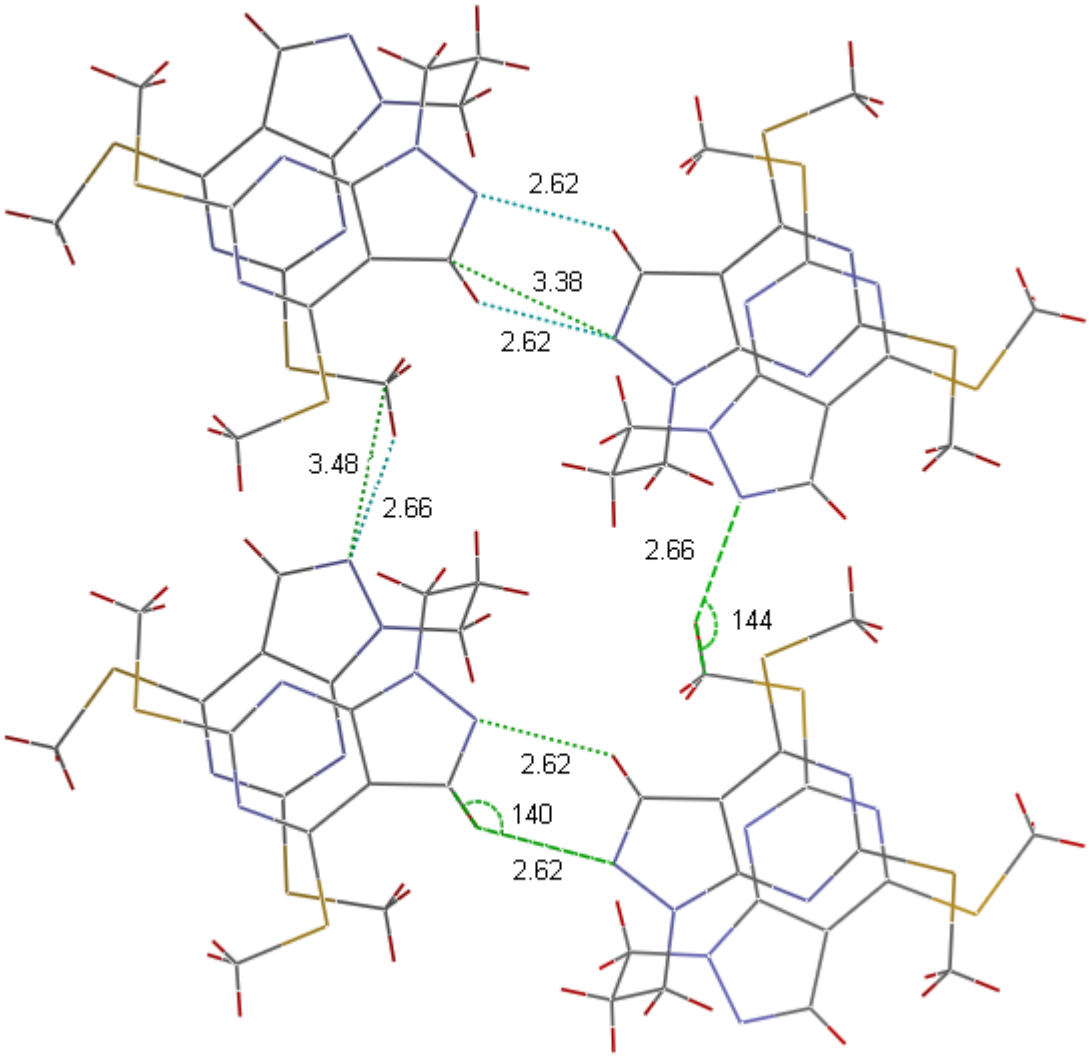
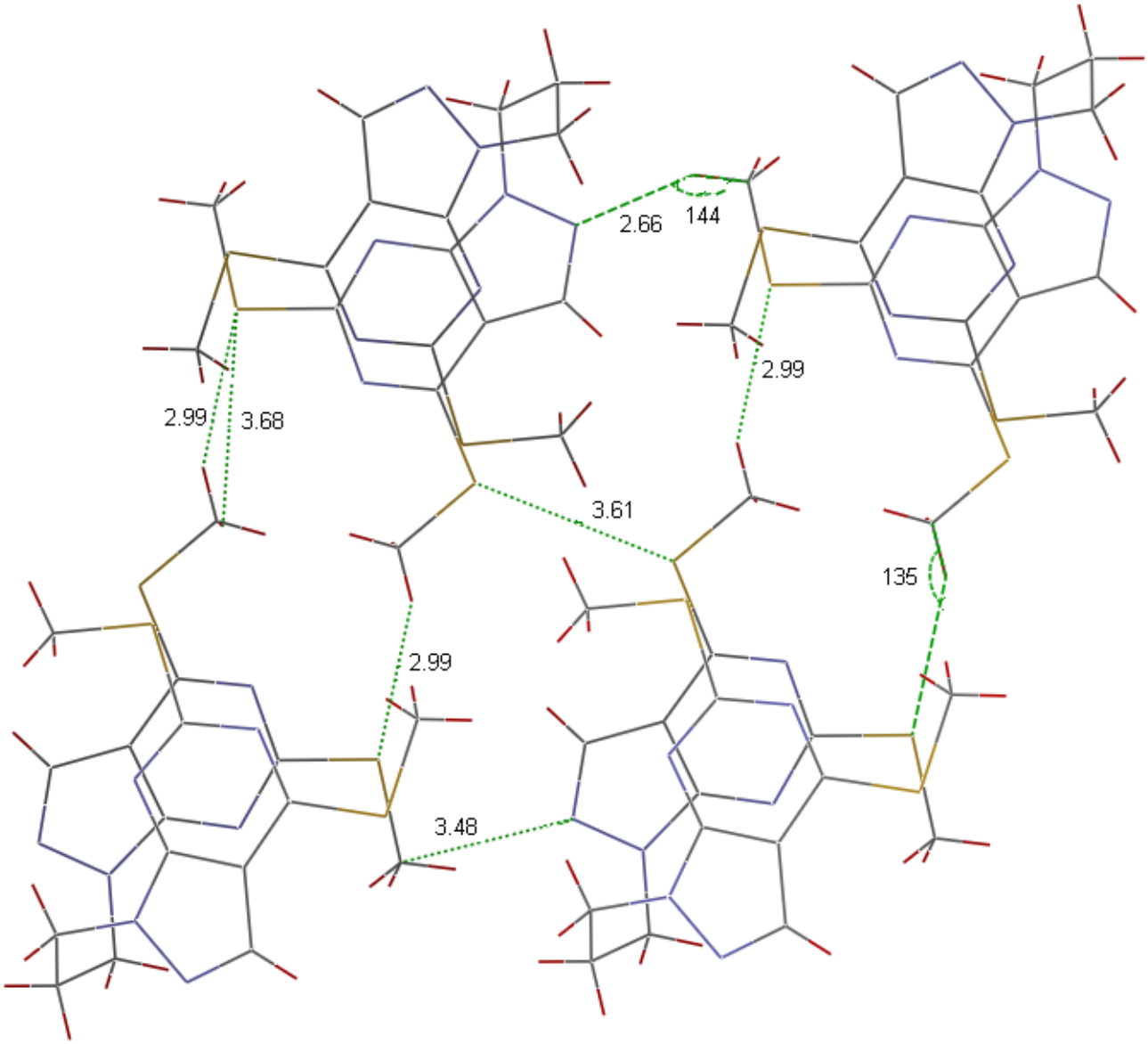


Fig. S15 Important distances and angle of **1a**.



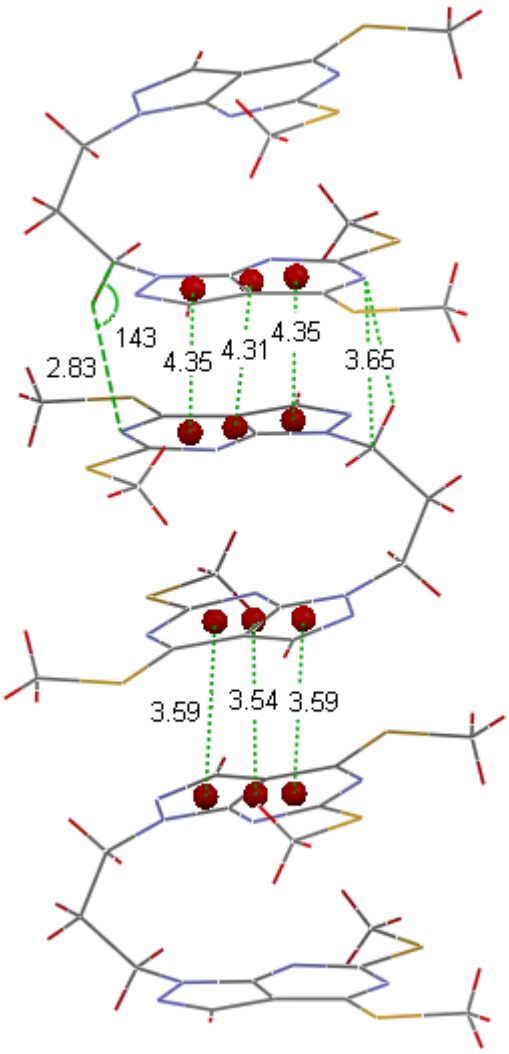
CH…N dimer = 2.62 Å, 3.38 Å, 140°
CH…N dimer = 2.66 Å, 3.48 Å, 144°

Fig. S16 CH…N interactions in **1a**.



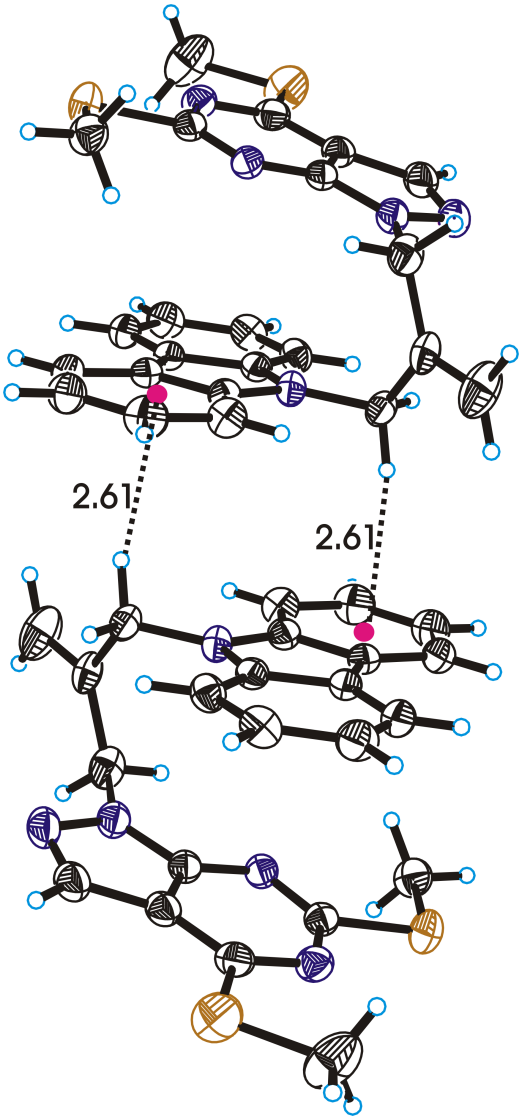
CH…S dimer = 2.99 Å, 3.73 Å, 135°;
CH…N dimer = 2.66 Å, 3.48 Å, 144°;
S…S dimer = 3.61 Å .

Fig. S17 CH…S, CH…N and S…S interactions in **1a**.



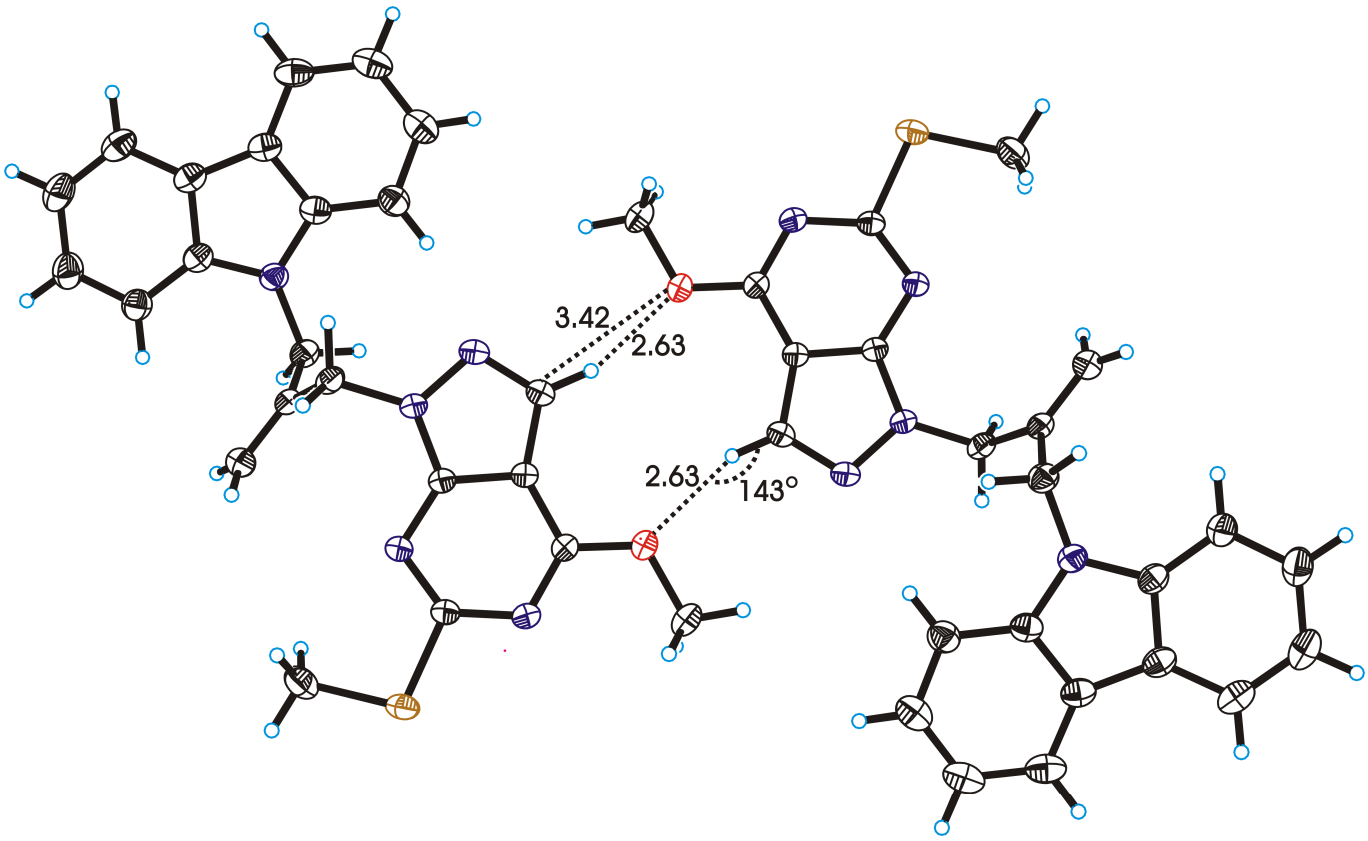
One folded molecule is stacked between two adjacent molecules at each face by different interactions.
One side by π–π interactions = Cg(5)…Cg(6) = 3.59 Å & 3.59 Å and Cg(9)…Cg(9) = 3.54 Å;
Other side by C-H…N dimern. = 2.84 Å, 3.65 Å, 143°.
Cg(5)…Cg(6) = 4.35 and Cg(9)…Cg(9) = 4.31
This pattern keeps on repeating to form infinite vertical stack.

Fig. S18 π–π and C-H…N interactions in **1a**.



C-H…π = 2.61 Å

Fig. S19 C-H…π dimerization in **13a** (at 30% probability level).



C-H...O = 2.63 Å, 3.42, 143º

Fig. S20 C-H...O dimerization in **14** (at 30% probability level).