

Electronic Supplementary Information (ESI)

First example of a heterobimetallic ‘Pd–Sn’ catalyst for direct activation of alcohol: Efficient allylation, benzylation and propargylation of arenes, heteroarenes, active methylenes and allyl-Si nucleophiles

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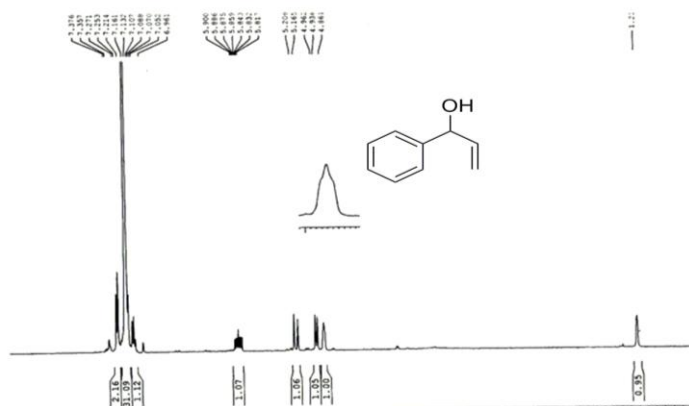
S-3. Spectra of the complexes and alkylated products

S-1. Study for substrate catalyst interaction

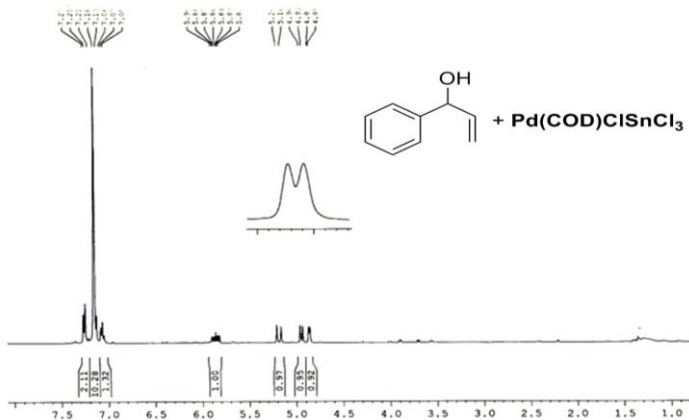
(a) Experimental procedure to study and observation for the interaction of alpha-allyl benzyl alcohol with [Pd-Sn] by ^1H NMR

To see the initial activation the spectrum of alpha-allyl benzyl alcohol **2b** (1.4 mg, 0.01 mmol) was recorded in C_6D_6 solvent at room temperature in the absence as well as in the presence of catalyst **1a** (4.75 mg, 0.01 mmol). In the absence of catalyst **1a** the alcohol **2b** shows an unresolved broad singlet at 4.86 ppm for allylic proton and a singlet at 1.21 ppm for -OH proton. Upon addition of the catalyst **1a**, the initial broad singlet of the allylic -CH proton of **2b** was converted to a well resolved doublet ($J=5.6$ Hz) at 5.45 ppm, while the peak for -OH proton almost vanishes.

^1H NMR (400MHz) of alpha allyl benzyl alcohol in C_6D_6

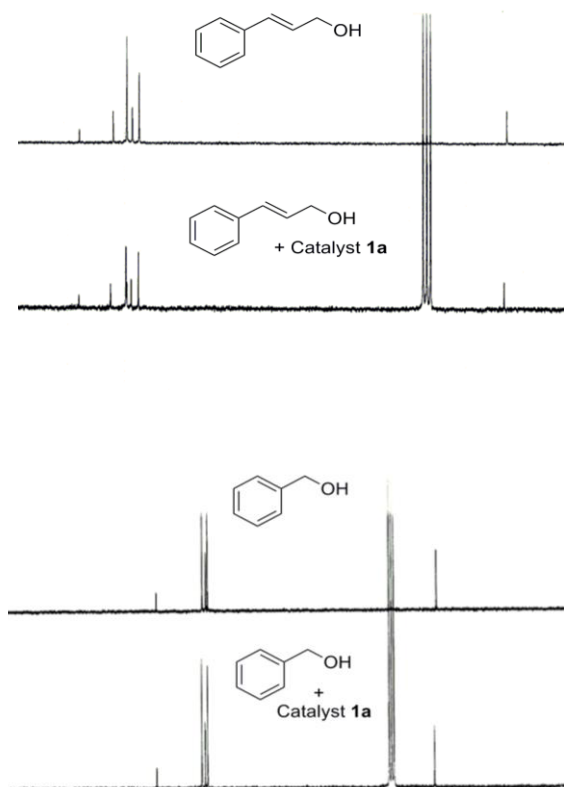


^1H NMR (400MHz) of alpha allyl benzyl alcohol and $\text{Pd}(\text{COD})\text{ClSnCl}_3$ in C_6D_6



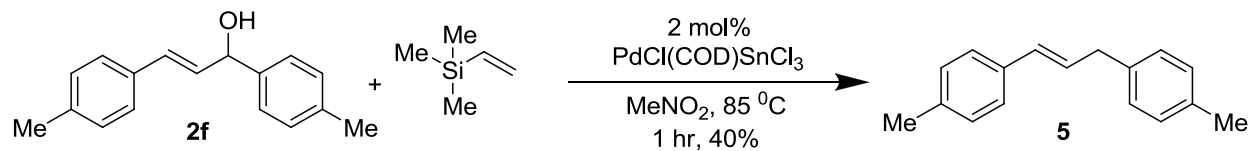
(b) Procedure for the *In situ* ^{13}C NMR study

^{13}C NMR of cinnamyl alcohol/benzyl alcohol was recorded at room temperature in the absence as well as in the presence of 1 eqv. of catalyst **1a** with respect to alcohol in CDCl_3 .



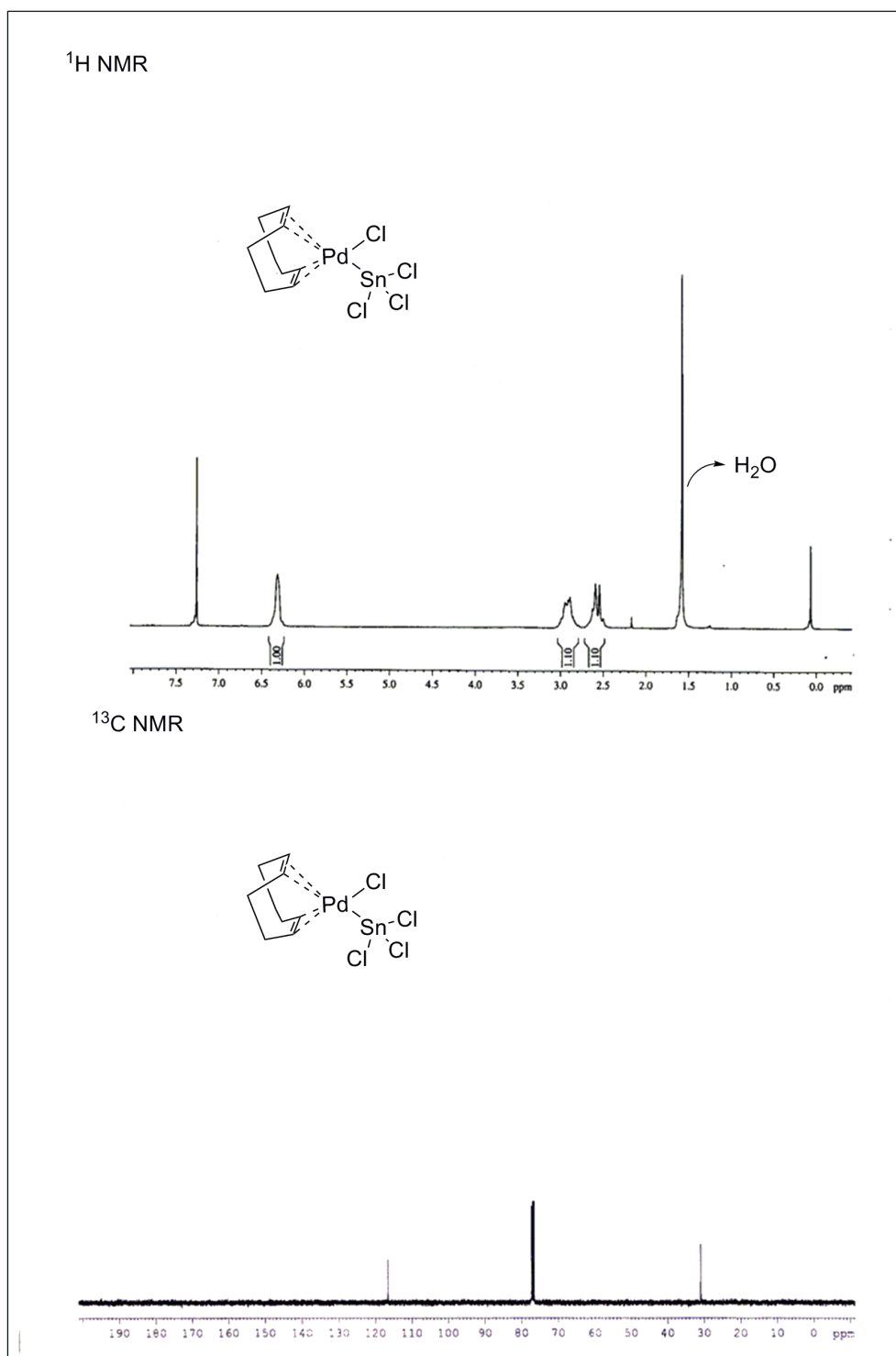
S-2. Reaction of Vinylsilane: Formation of reduced product (*E*)-1,3-di(*p*-tolyl)prop-2-en (**5**)

A mixture of allyl alcohol **2f** (1 mmol), vinyltrimethylsilane (2 mmol), and $[\text{Pd}(\text{COD})\text{Cl}(\text{SnCl}_3)]$ (2 mol %) in 2 mL of nitromethane was stirred at 85 °C for 1 hr. After that the reaction mixture was concentrated and purified by column chromatography to give 40% yield of **5**.

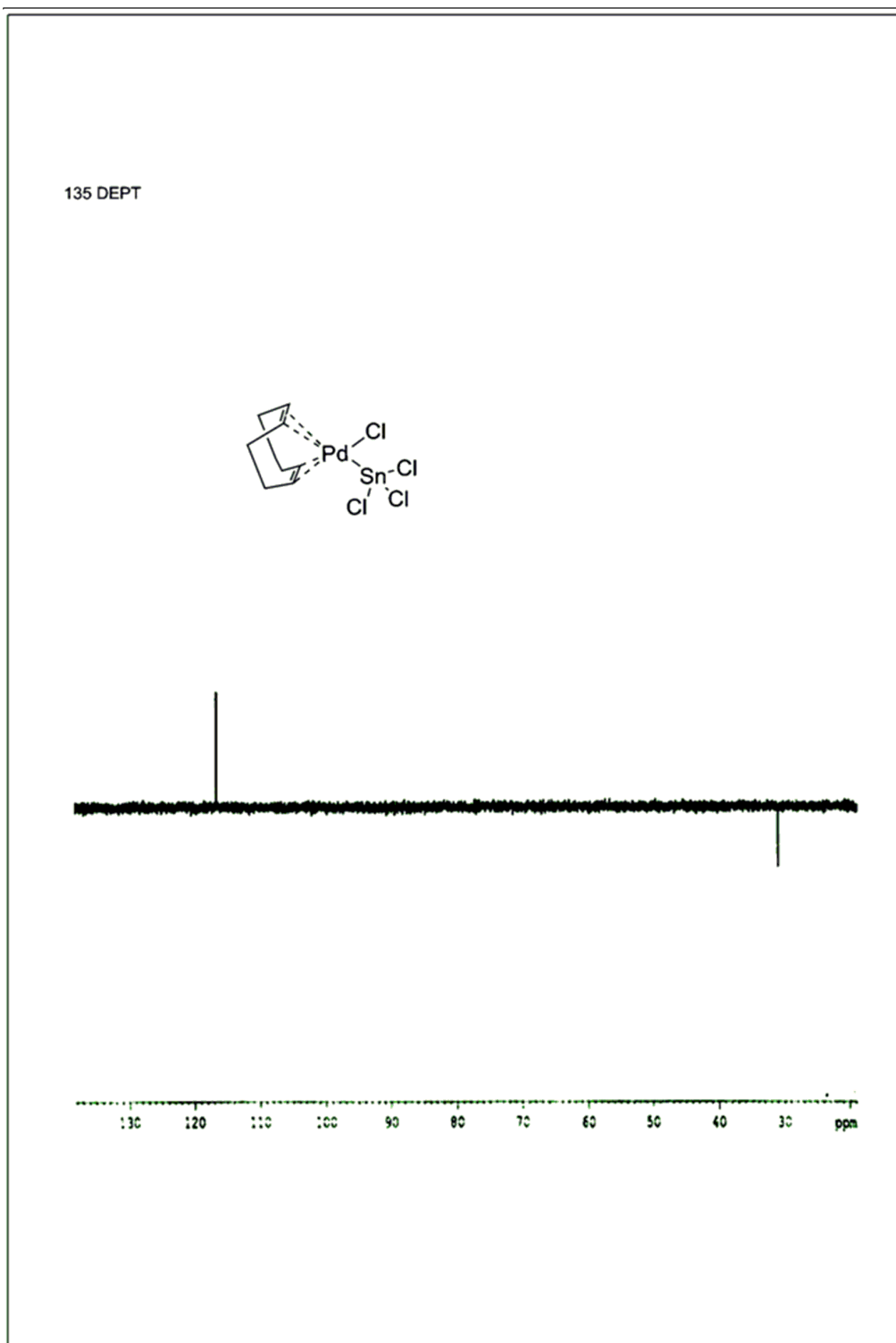


S-3. Spectra of complexes and alkylated products

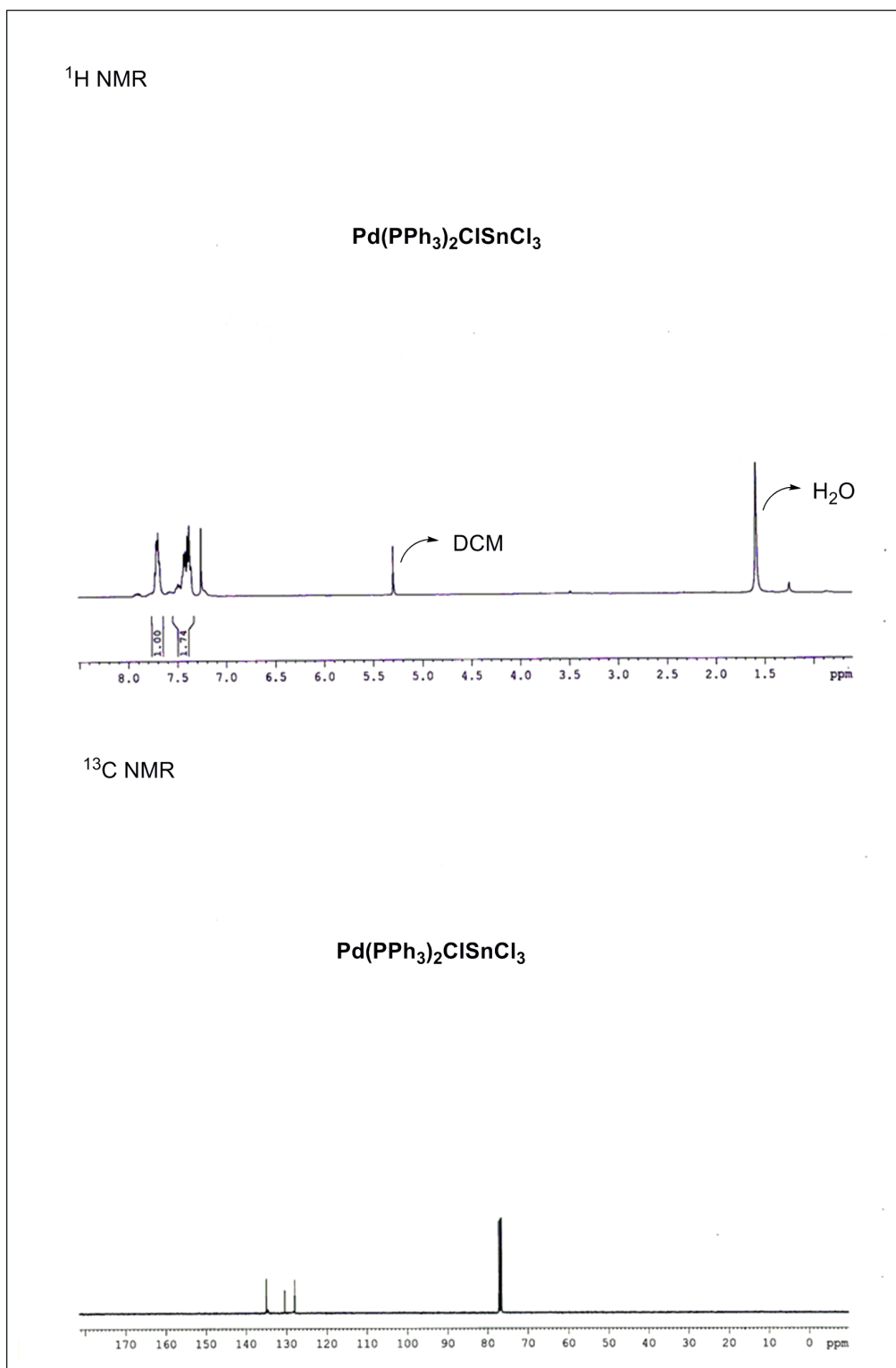
^1H and ^{13}C spectra of catalyst **1a**



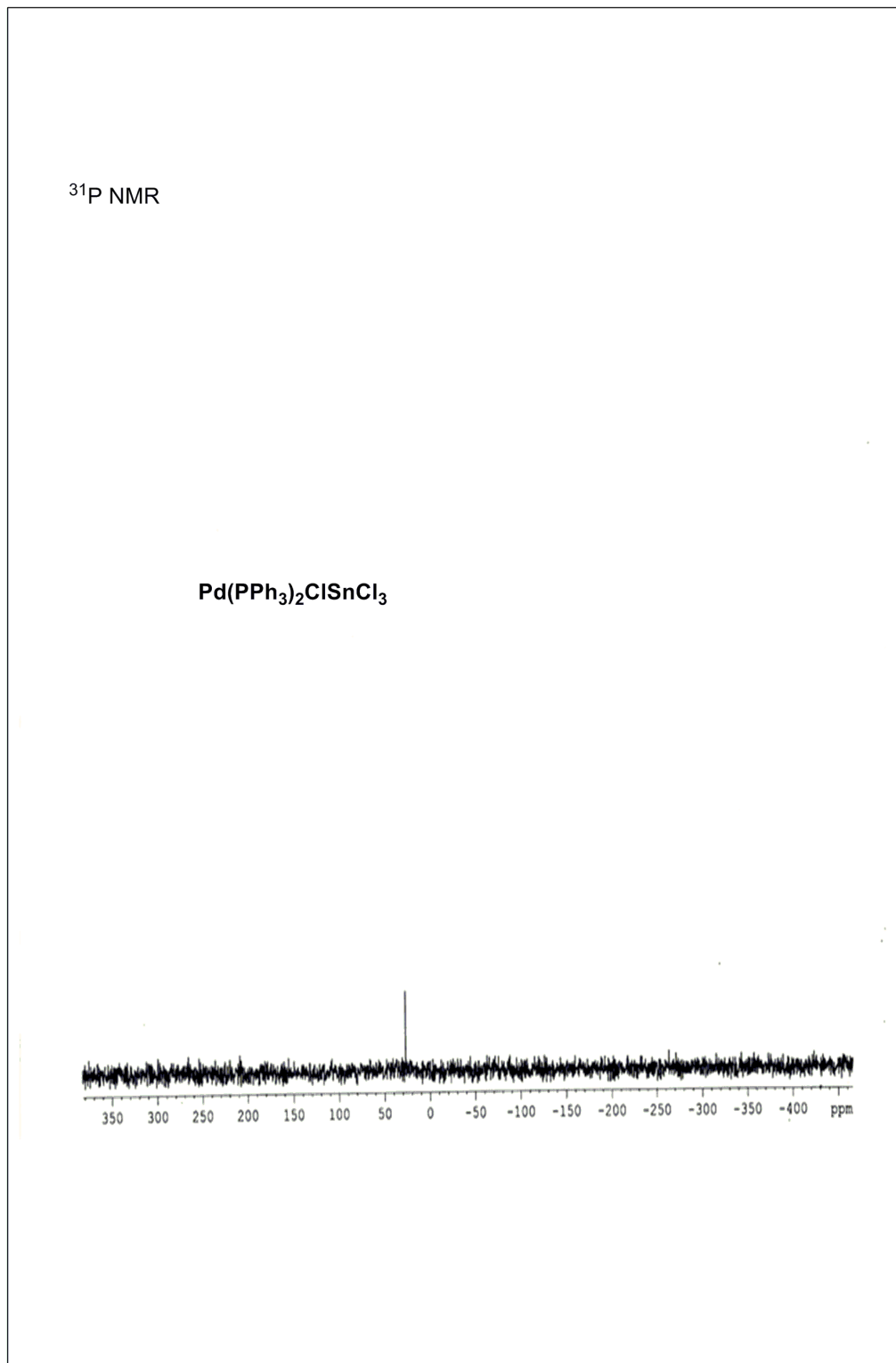
DEPT spectra of catalyst **1a**



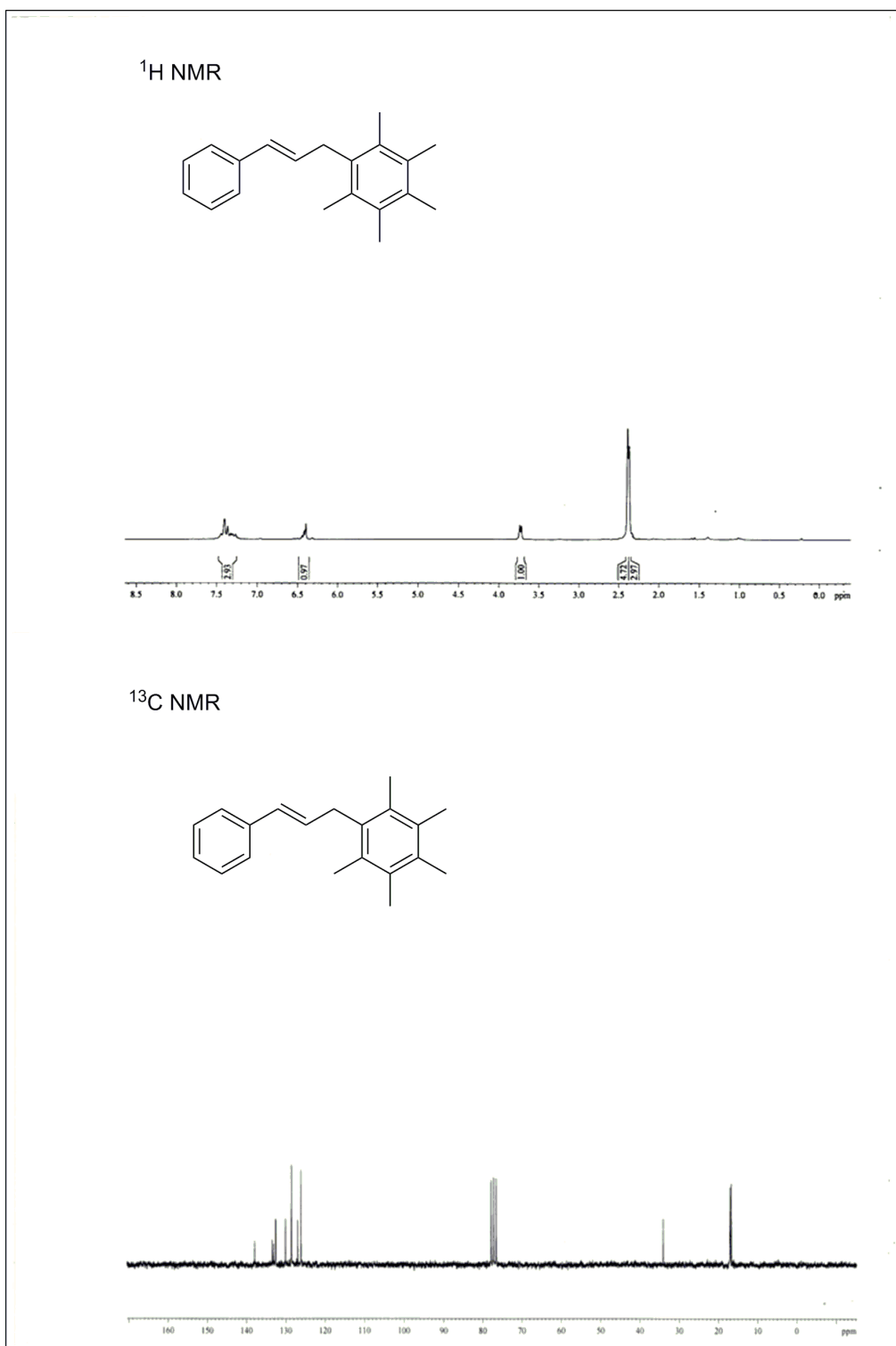
^1H and ^{13}C spectra of catalyst **1b**



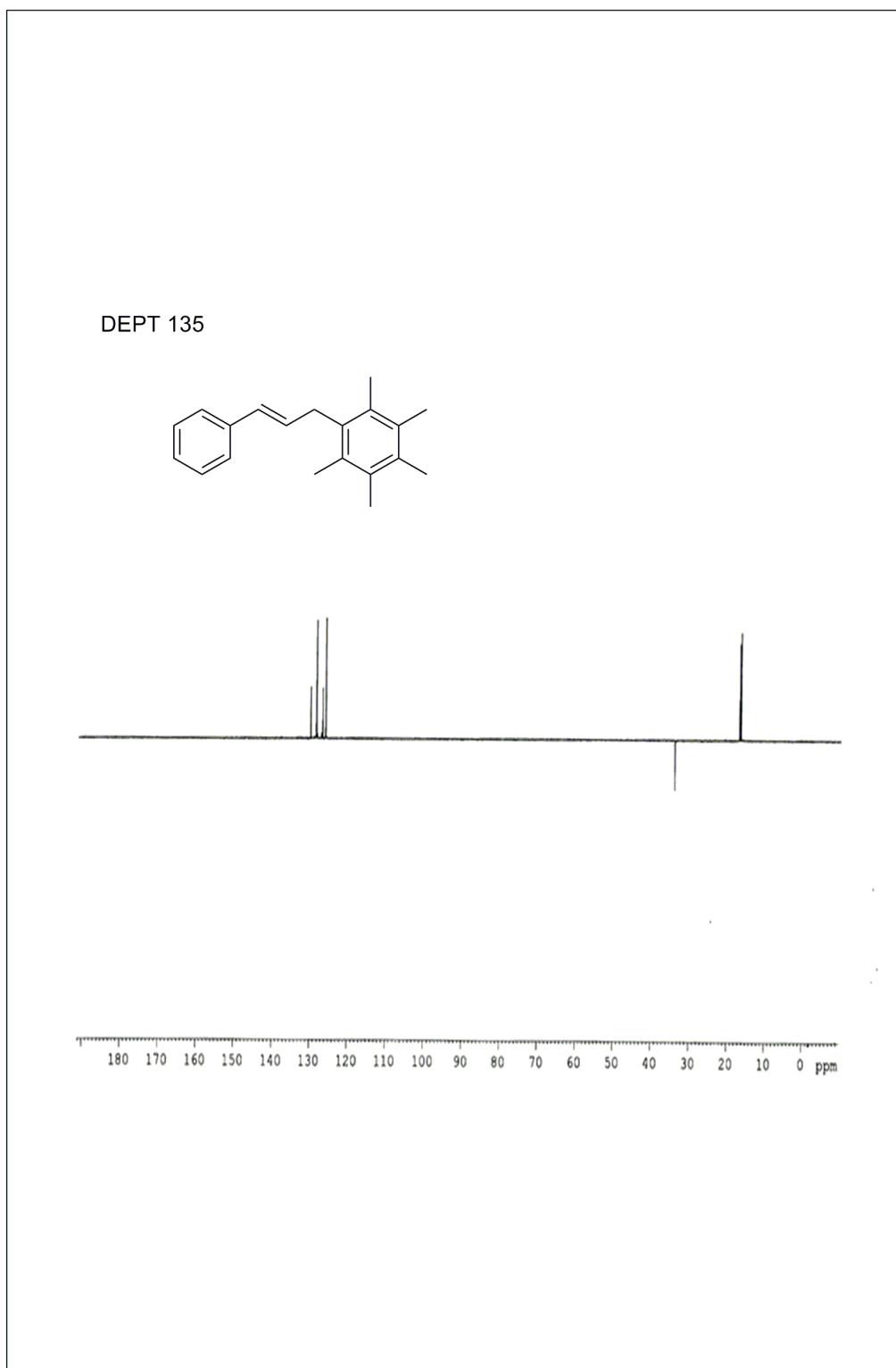
^{31}P spectra of catalyst **1b**



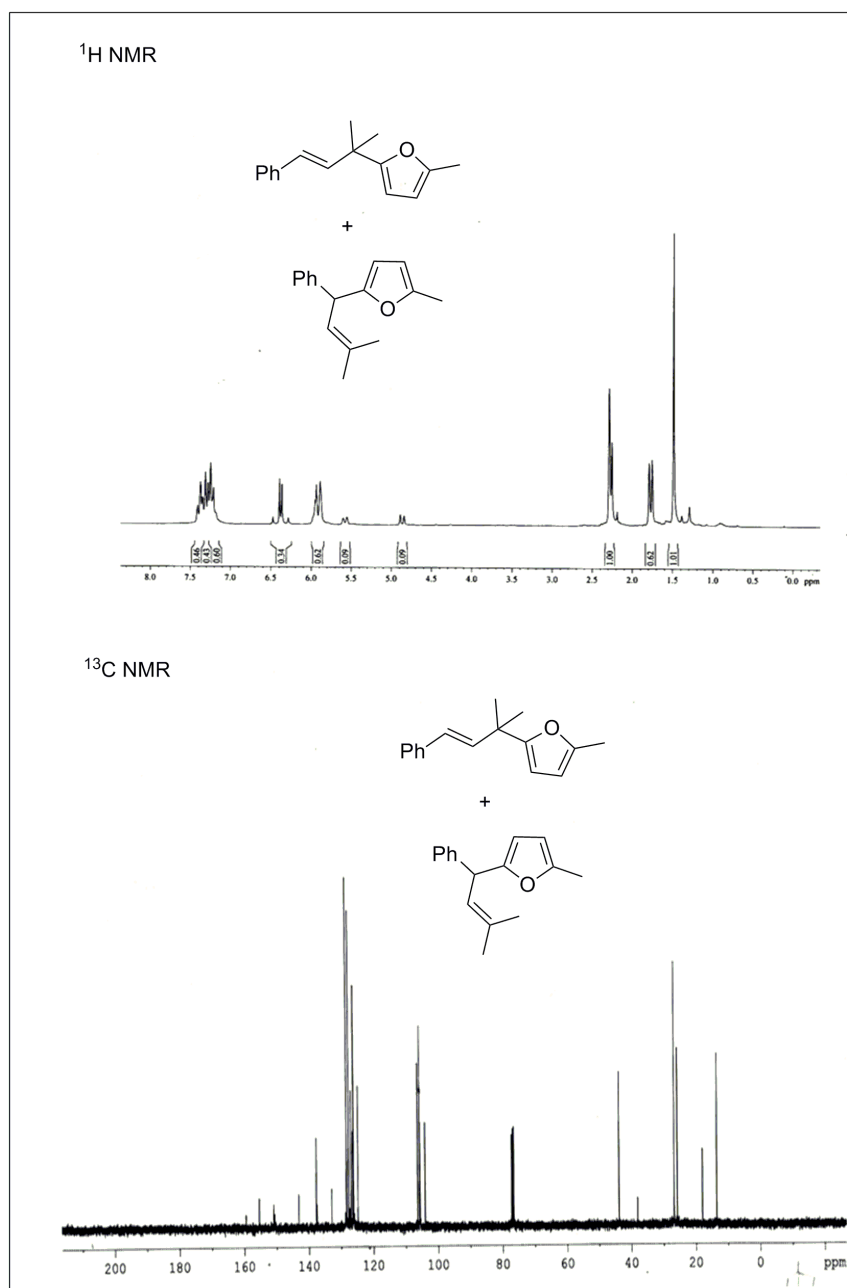
^1H and ^{13}C spectra of compound **4b'**



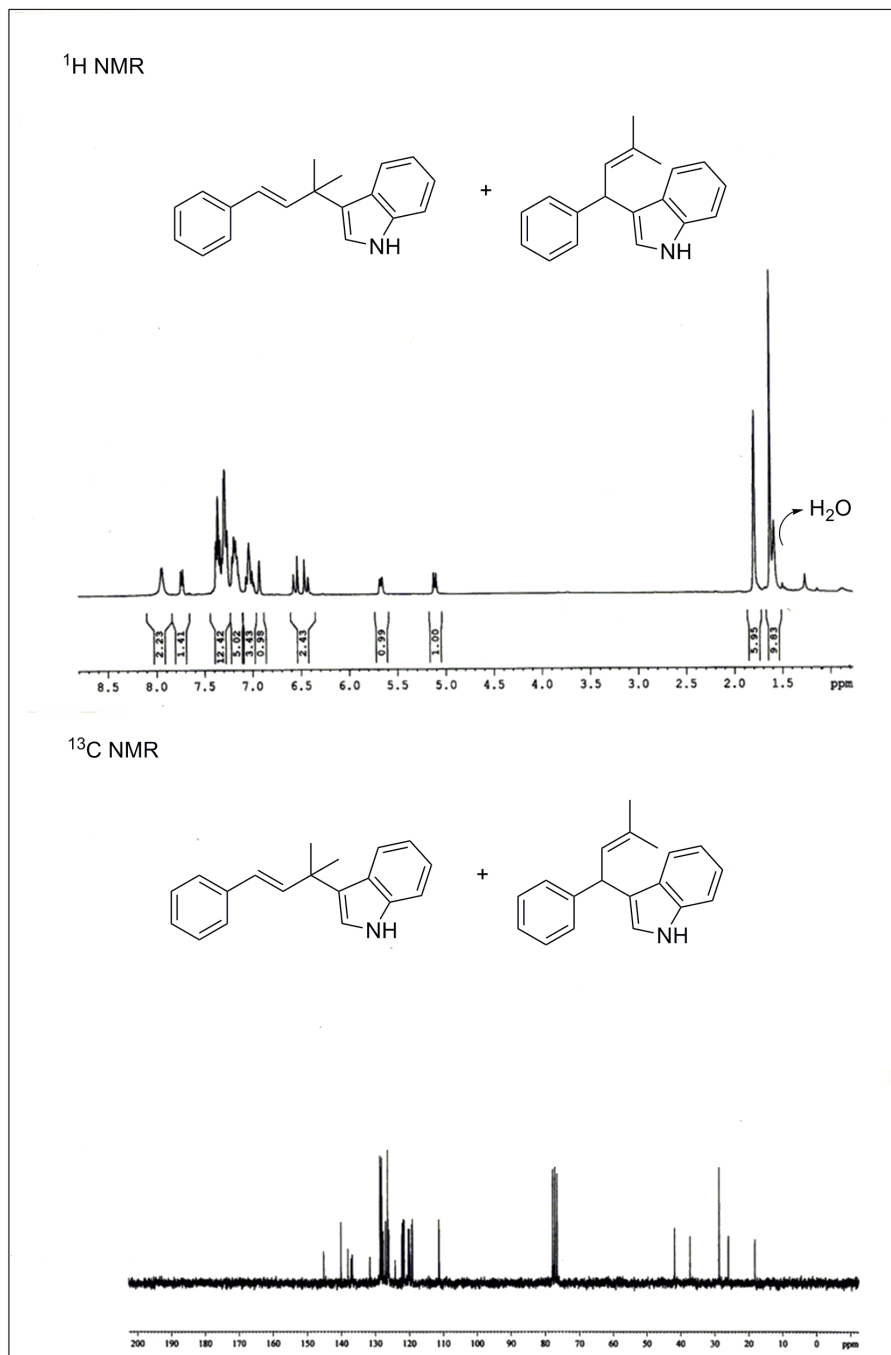
DEPT spectra of compound **4b'**



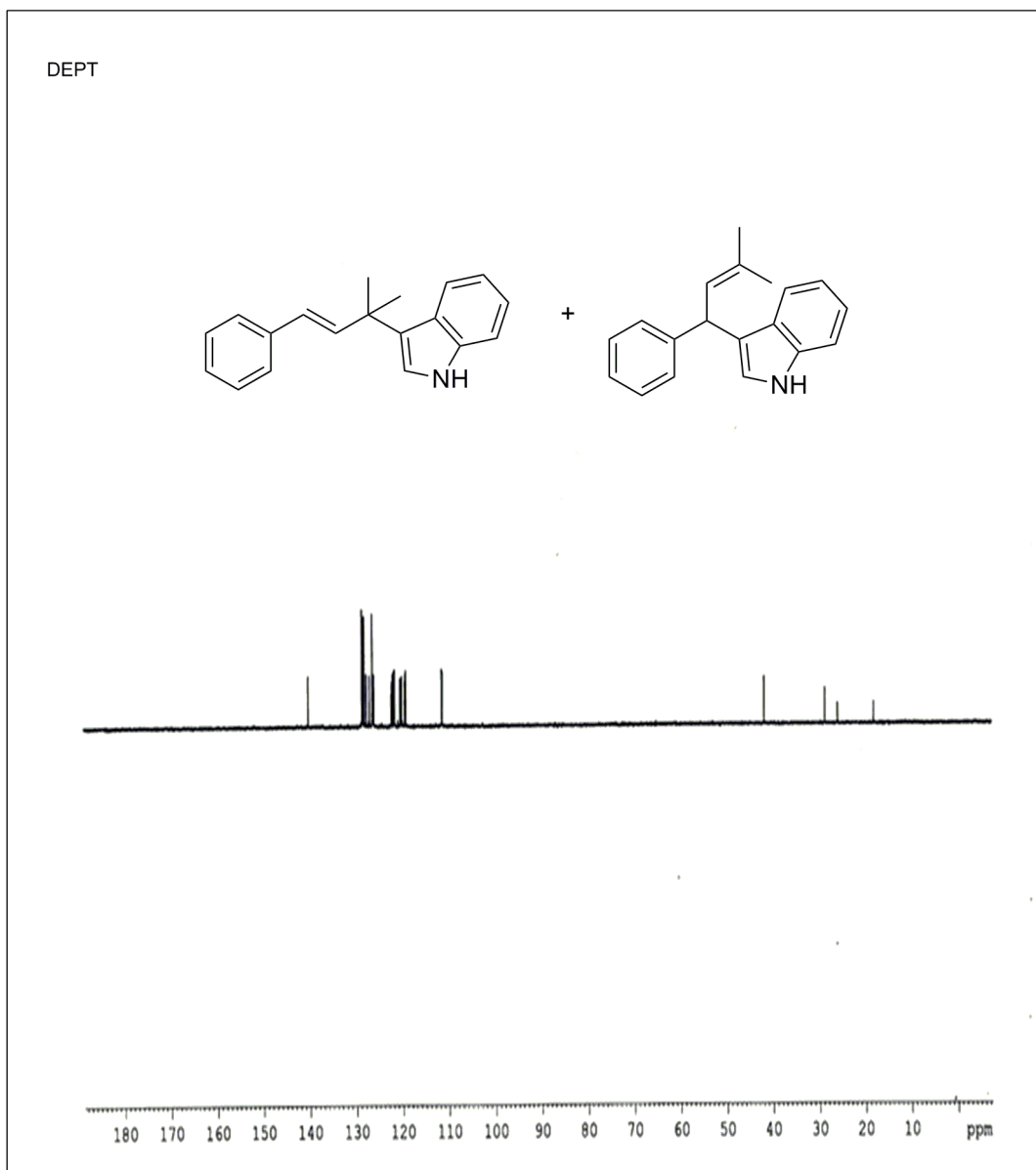
^1H and ^{13}C spectra of compound **4f** and **4f'**



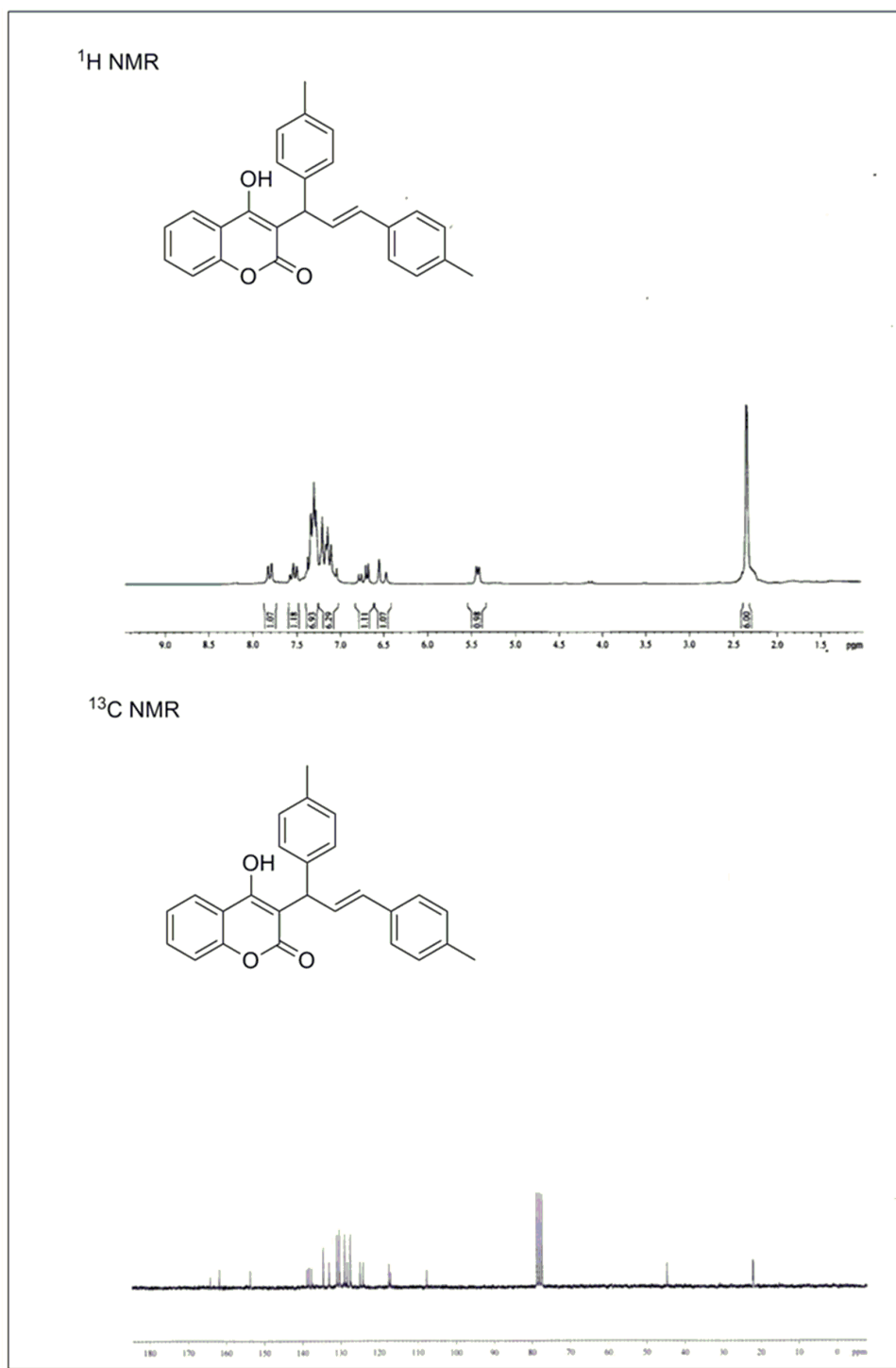
^1H and ^{13}C spectra of compound **4h** and **4h'**



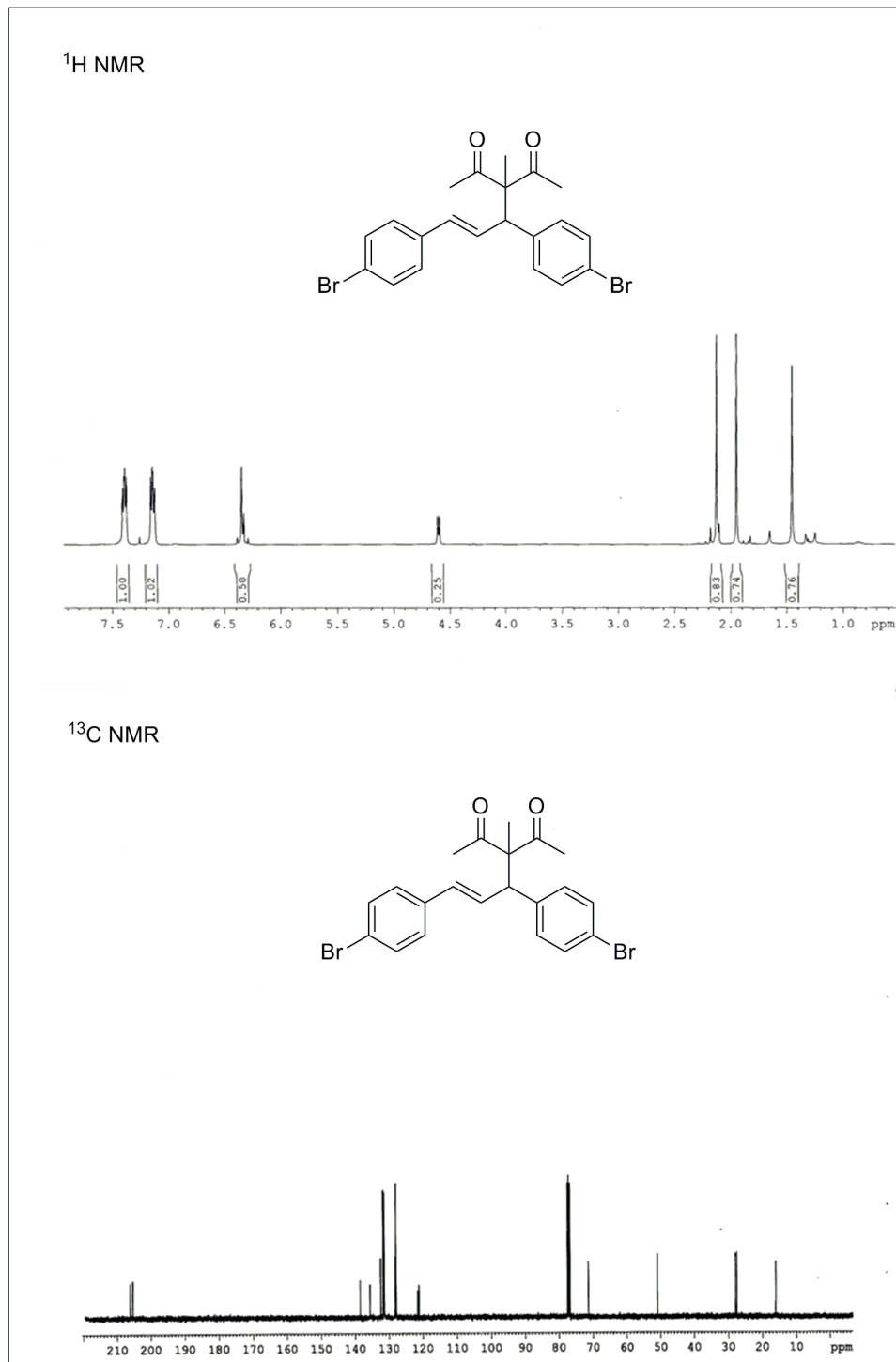
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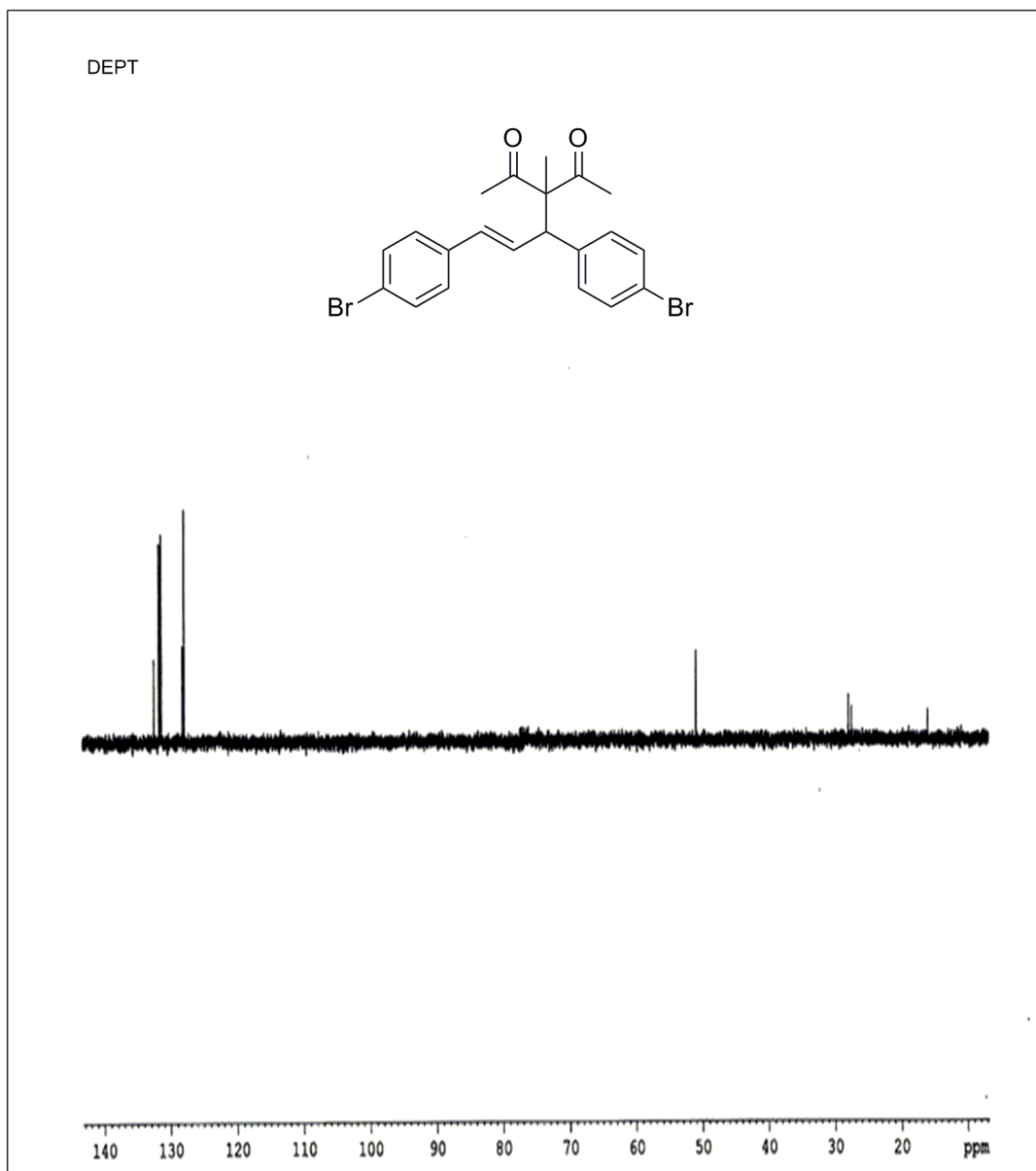
^1H and ^{13}C spectra of compound **4j**



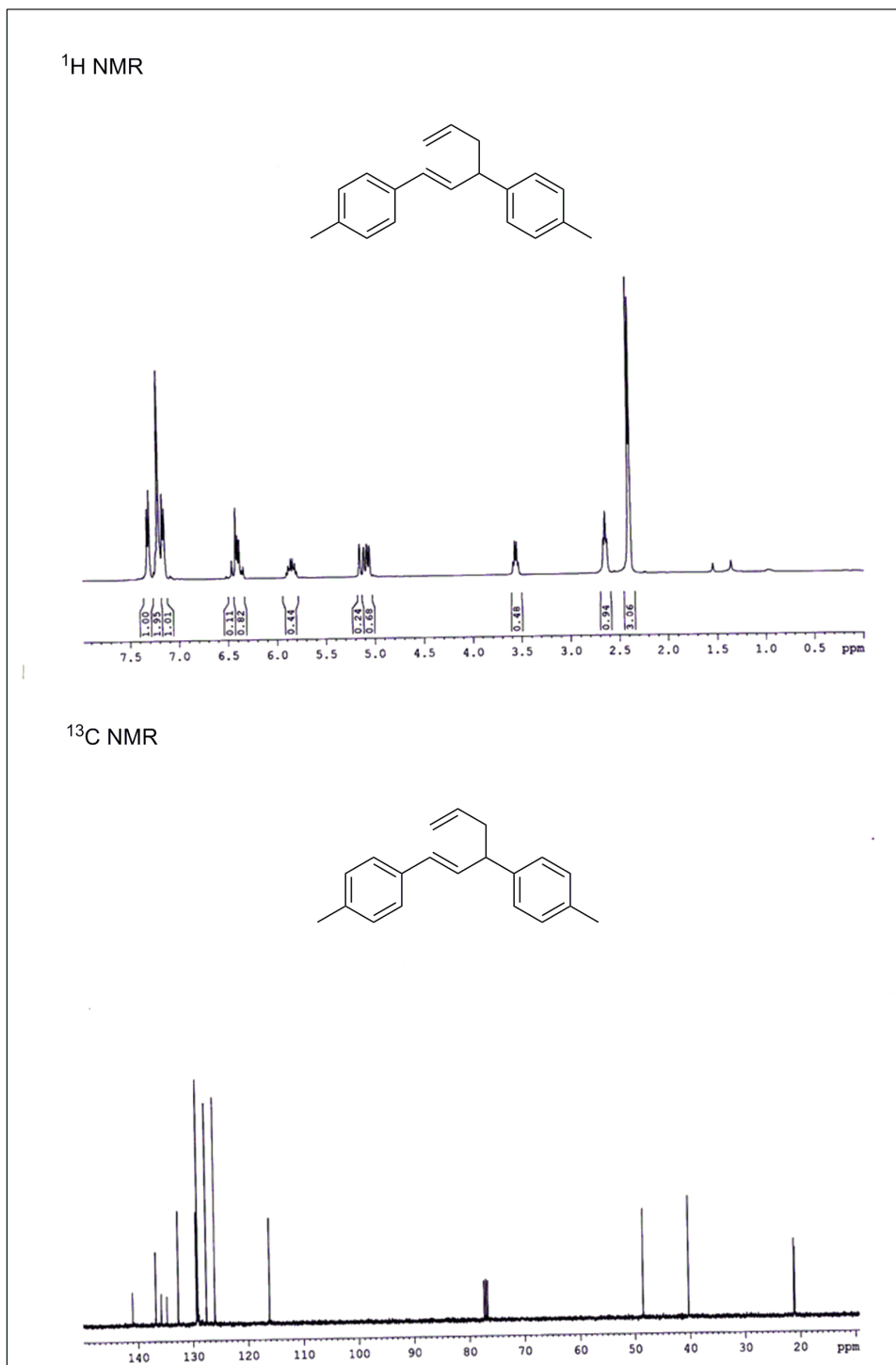
^1H and ^{13}C spectra of compound **4k**



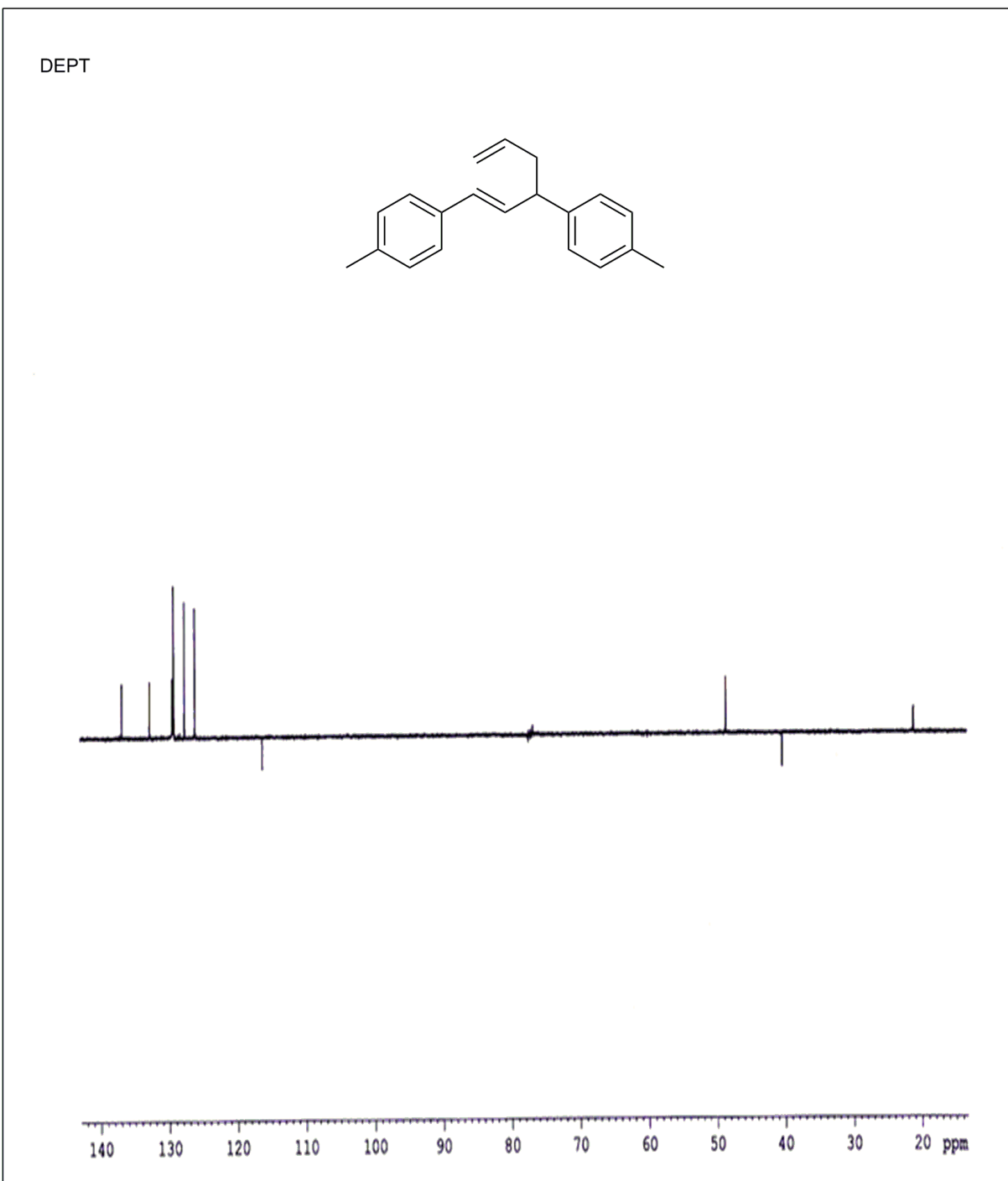
DEPT spectra of compound **4k**



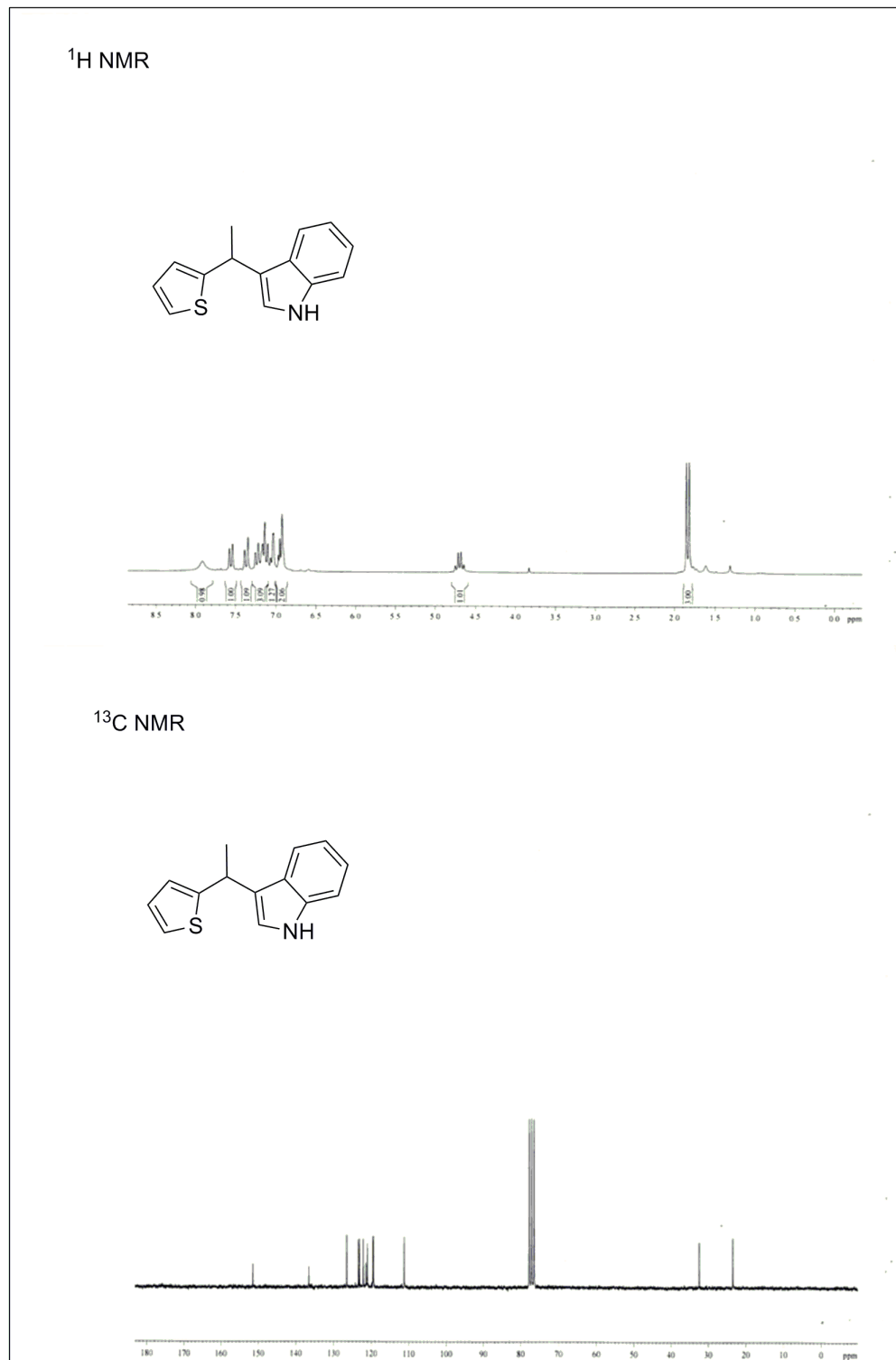
^1H and ^{13}C spectra of compound **4I**



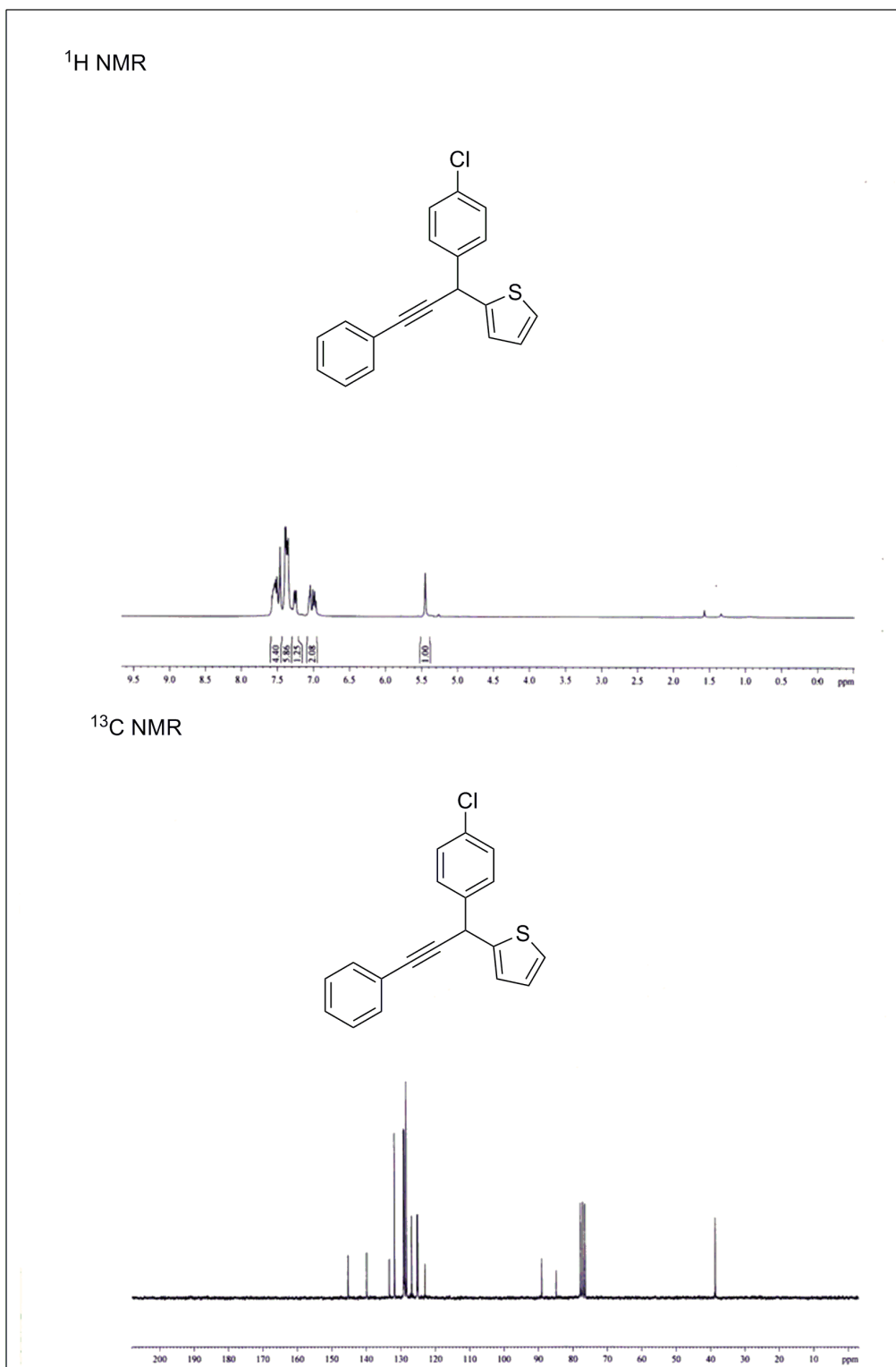
DEPT spectra of compound **41**



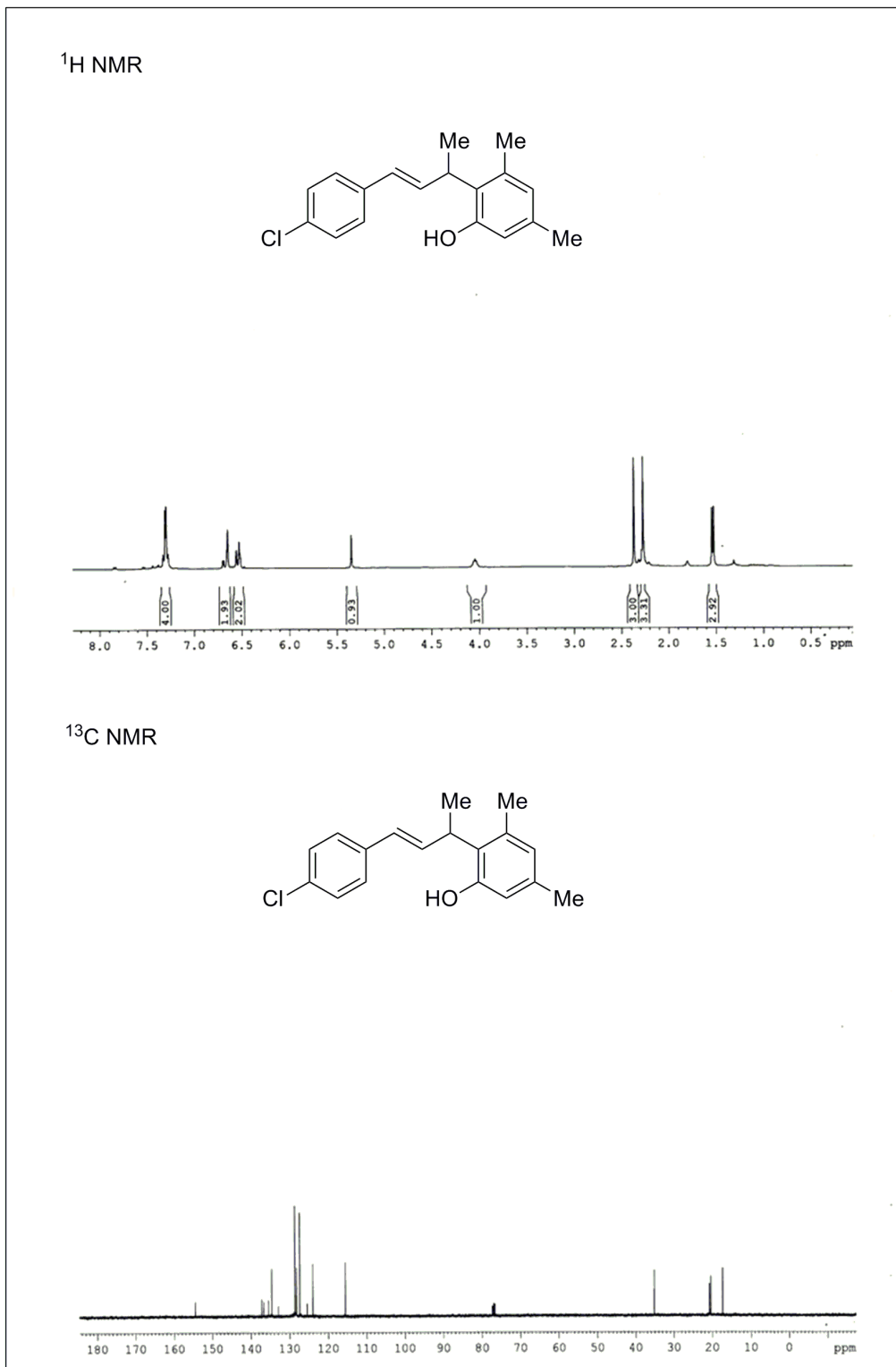
^1H and ^{13}C spectra of compound **4o**



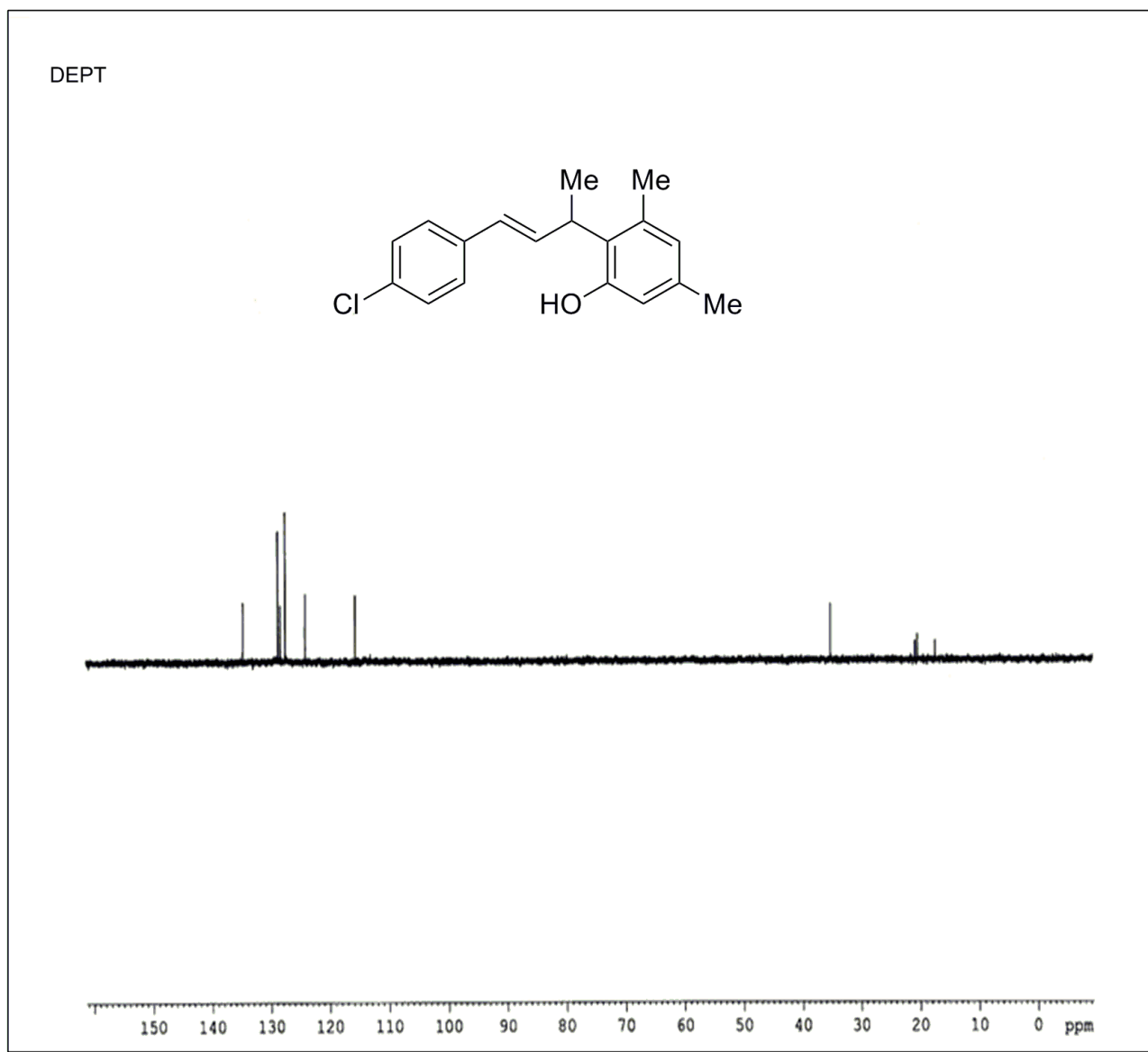
^1H and ^{13}C spectra of compound **4t**



^1H and ^{13}C spectra of compound **4v**



DEPT of compound **4v**



^1H and ^{13}C spectra of compound **4z**

