Supplementary Materials

Importance of the proximity and orientation of ligand-linkage to the design of cinnamate-GW9662 hybrid compounds as covalent PPARγ agonists

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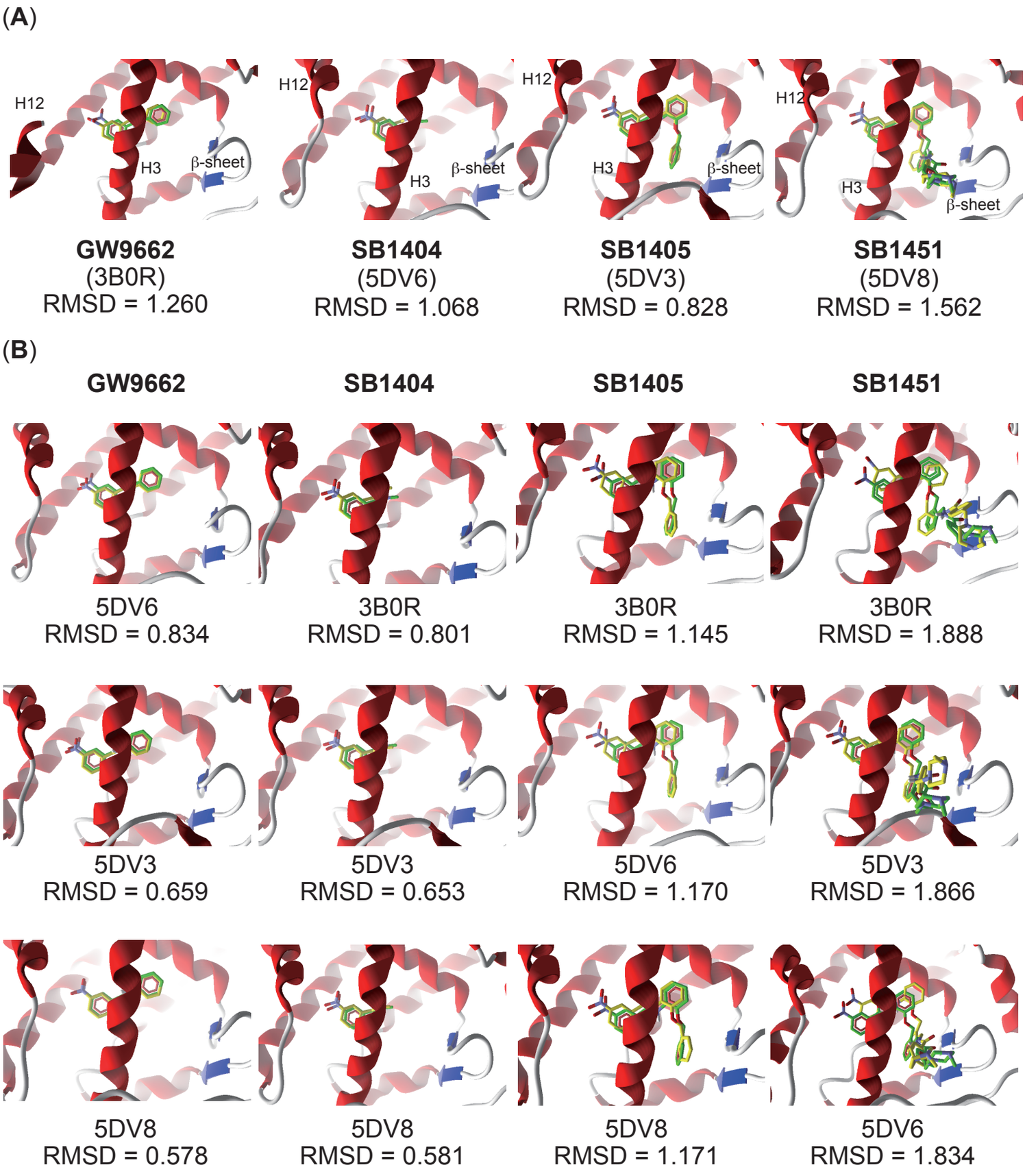
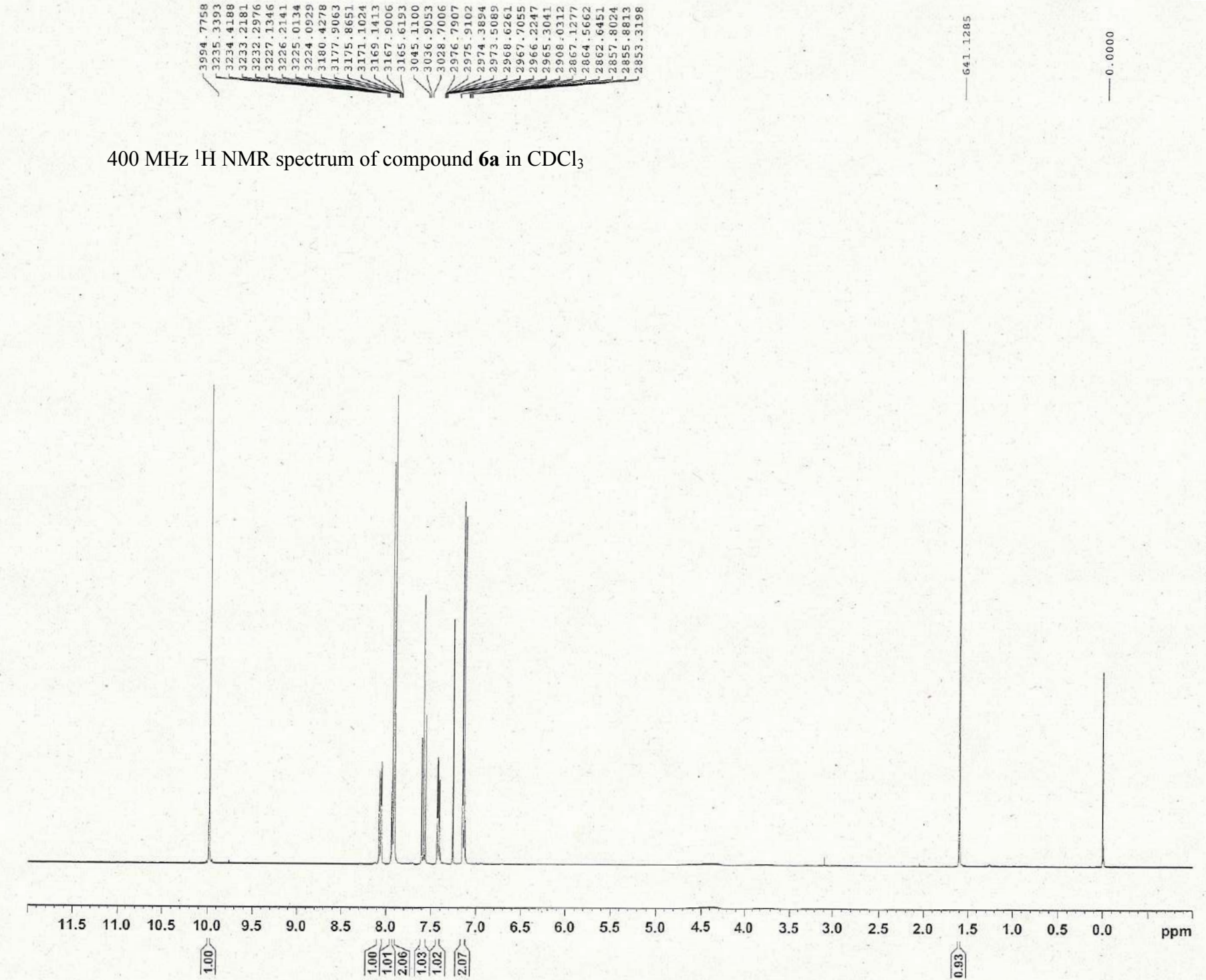
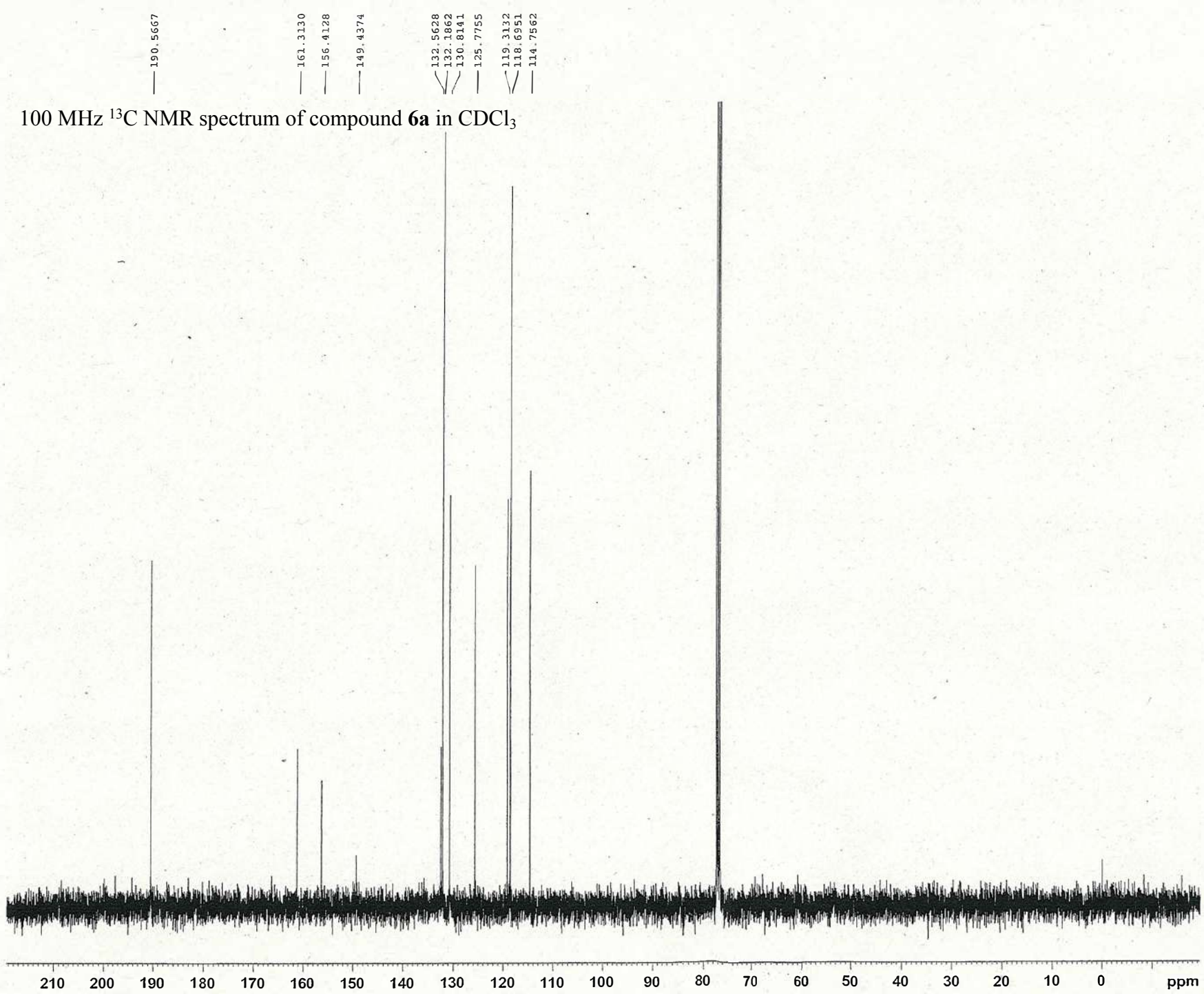


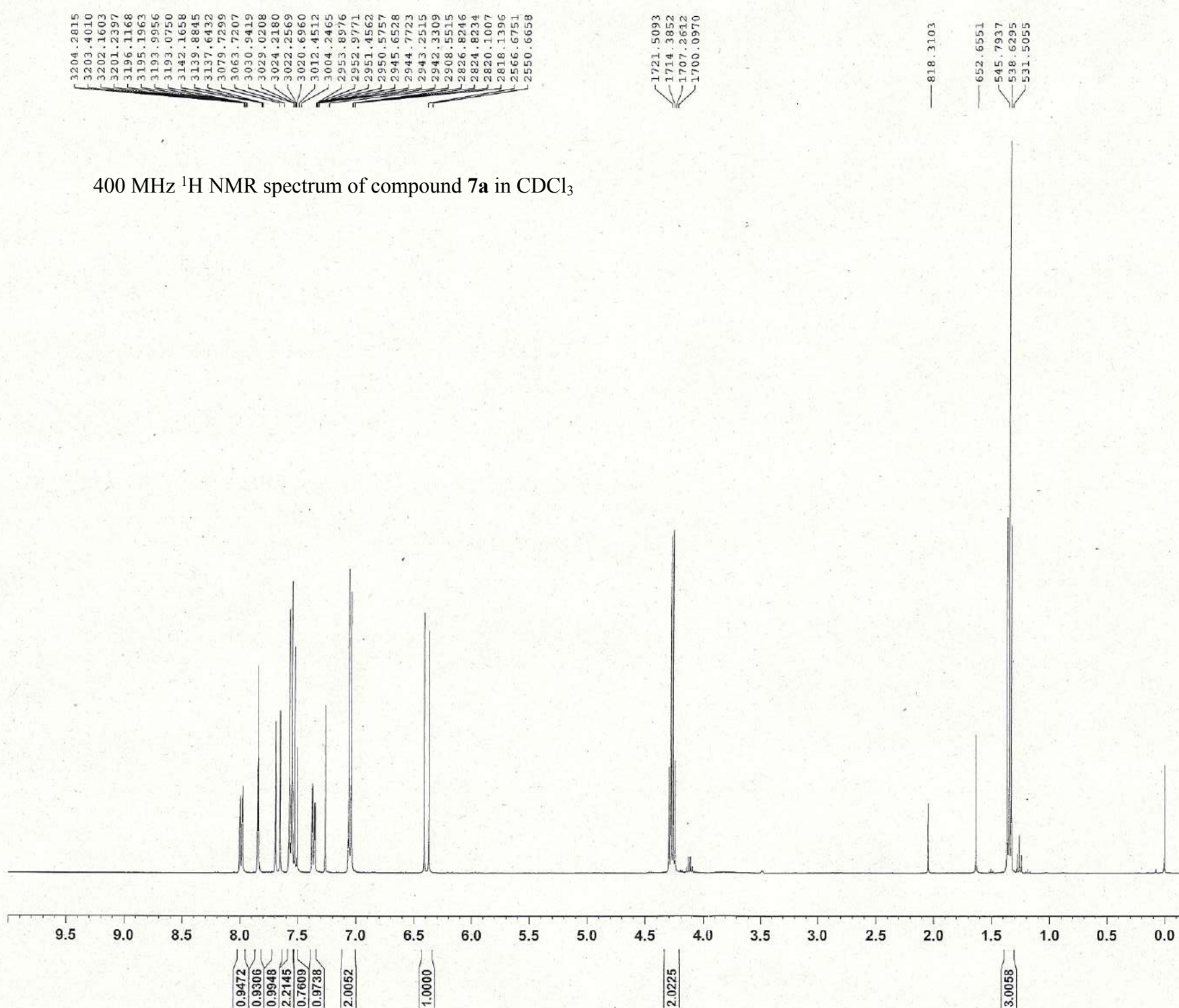
Supplemntary Figure 1. Validation of docking protocol. (A) The indicated ligands were docked into the original protein crystal structures. The reported binding manners and predicted docking poses were displayed in green and yellow, respectively. (B) The ligands were docked in the crystal structures other than originally reported structural data. The reported binding manners and predicted docking poses were displayed in green and yellow, respectively.



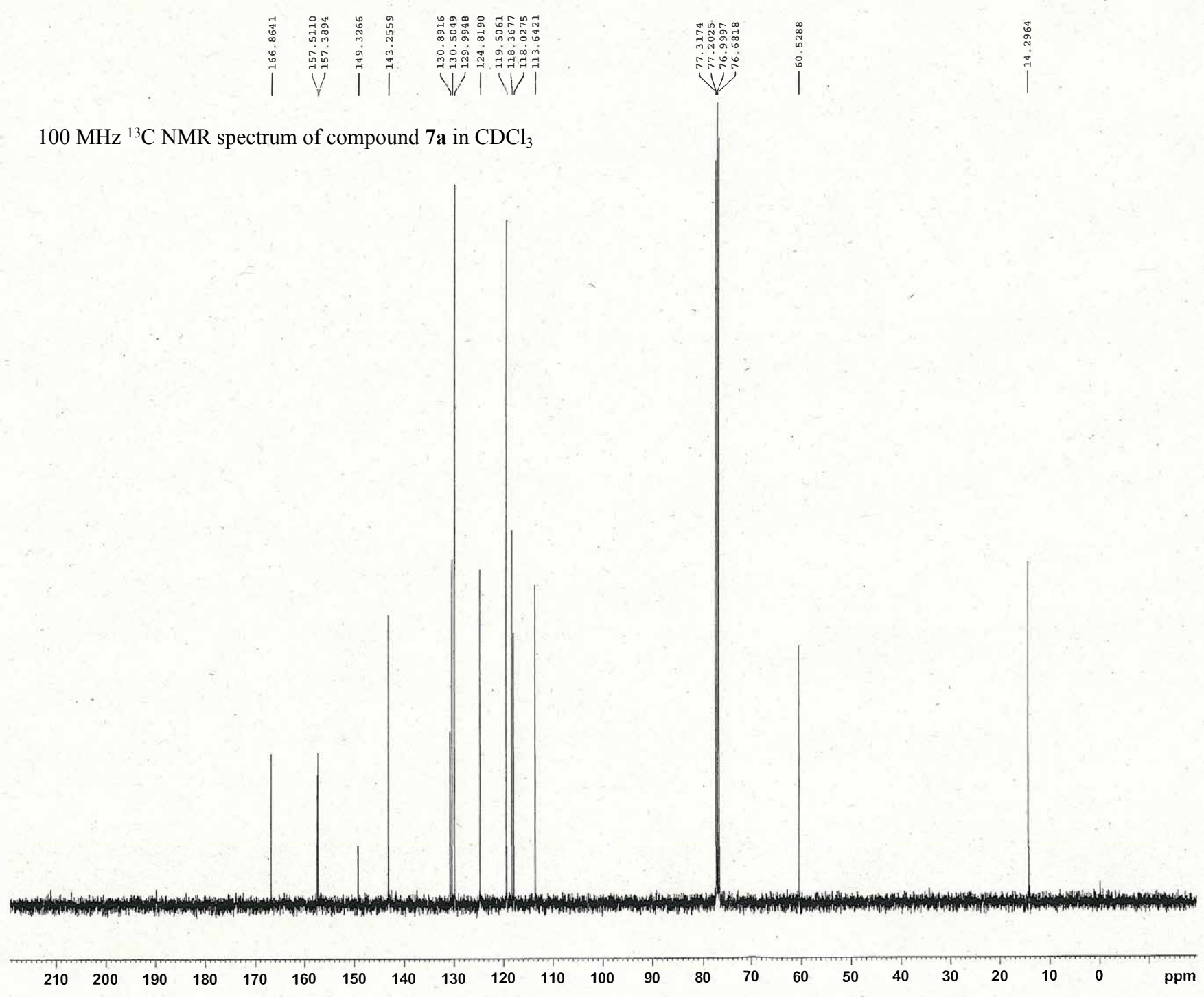
400 MHz ^{1}H NMR spectrum of compound **6a** in $CDCl_3$



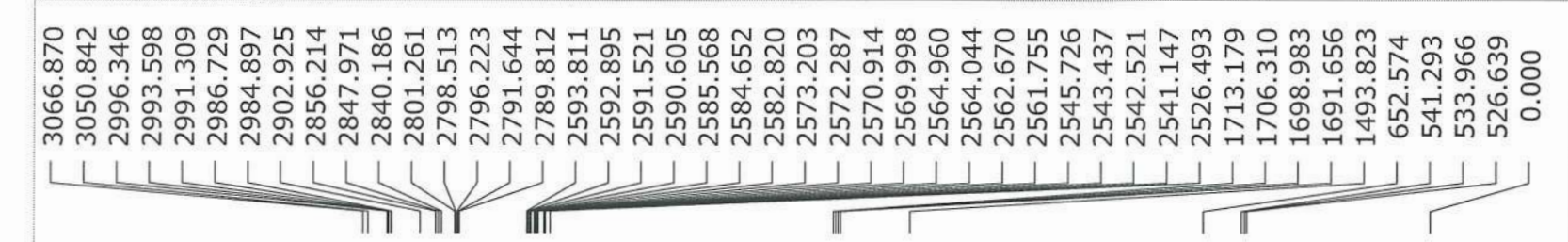
100 MHz ^{13}C NMR spectrum of compound **6a** in $CDCl_3$



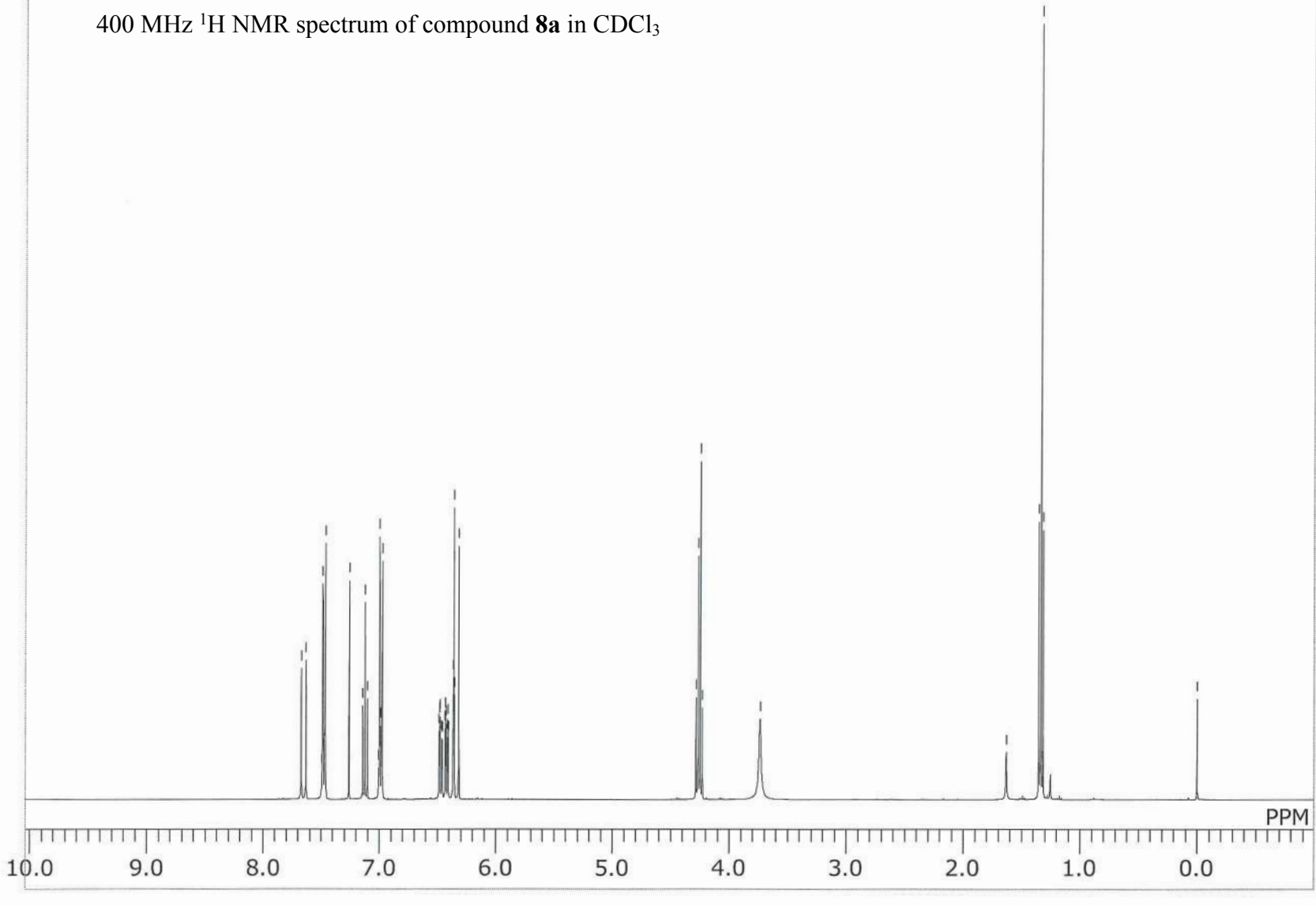
400 MHz ^{1}H NMR spectrum of compound **7a** in $CDCl_3$



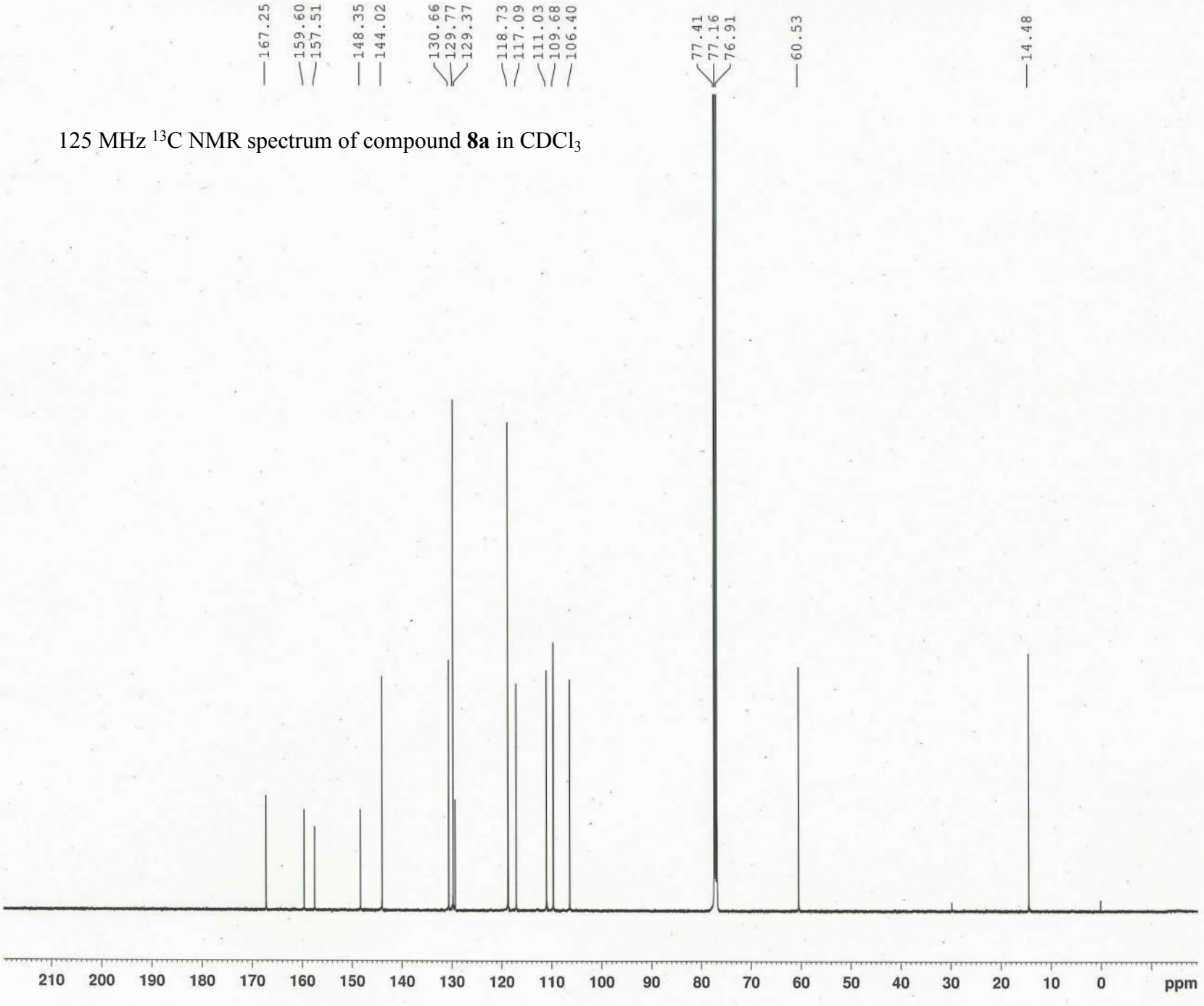
100 MHz ^{13}C NMR spectrum of compound **7a** in $CDCl_3$

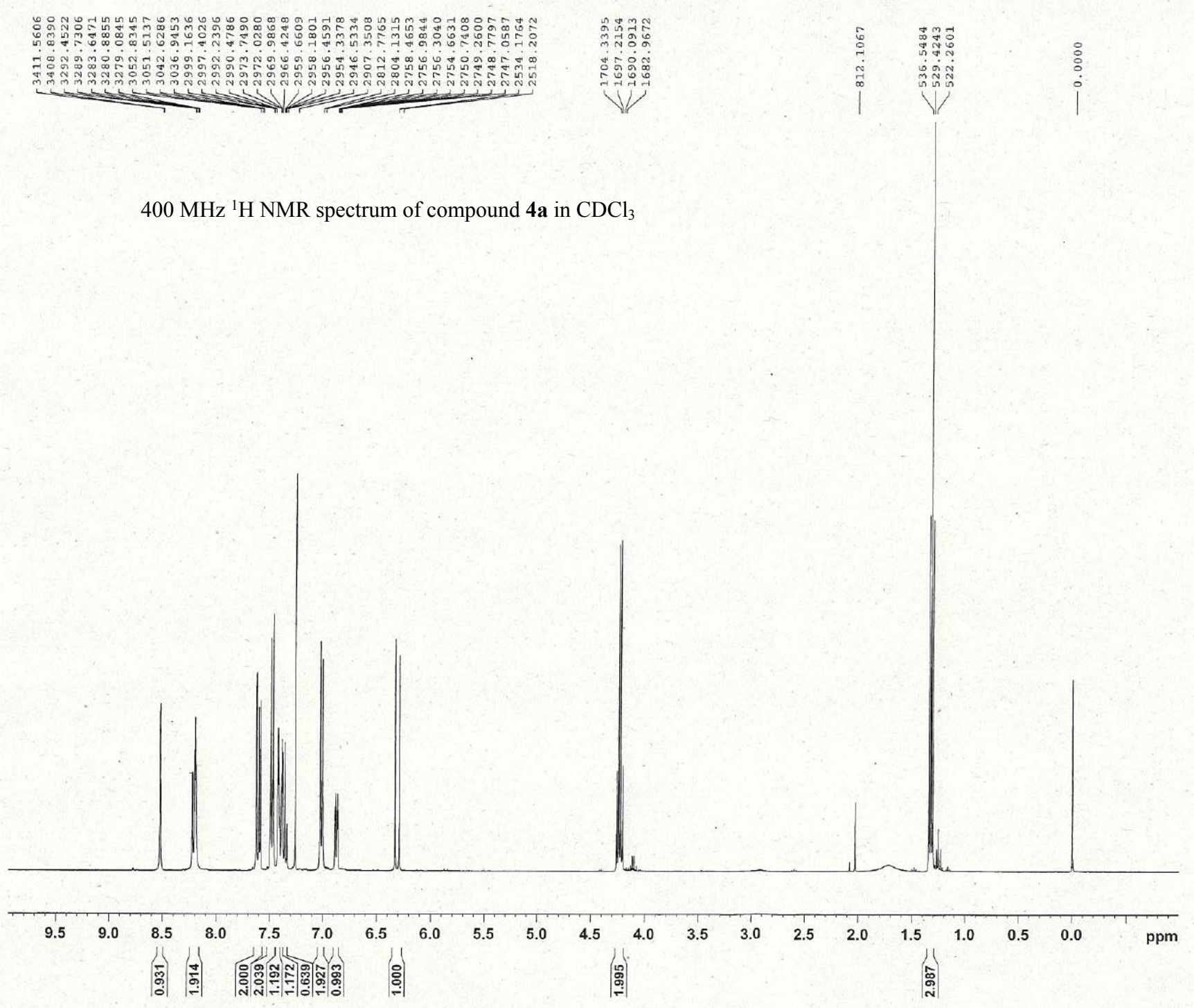


400 MHz ^{1}H NMR spectrum of compound **8a** in $CDCl_3$

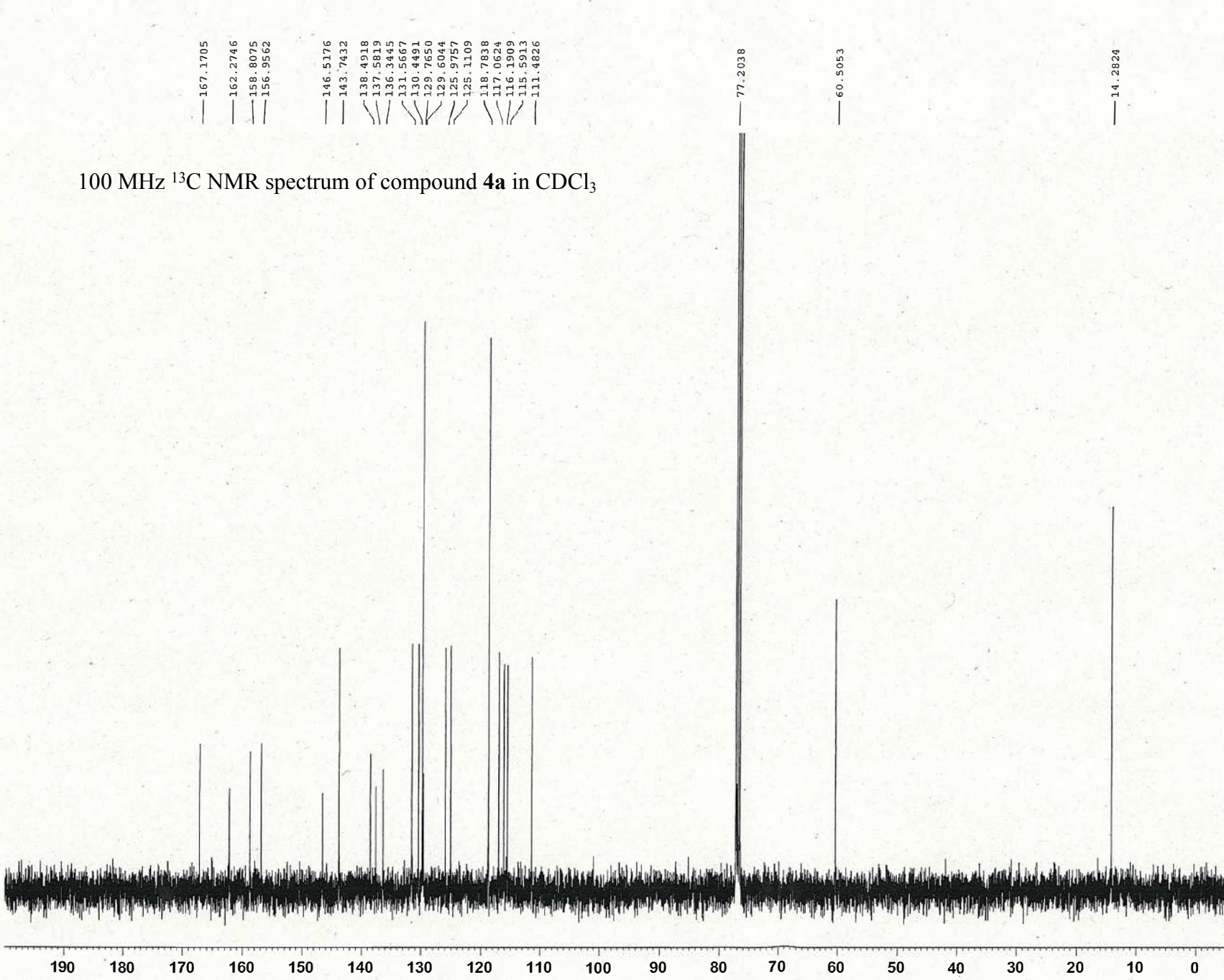


125 MHz ^{13}C NMR spectrum of compound **8a** in $CDCl_3$

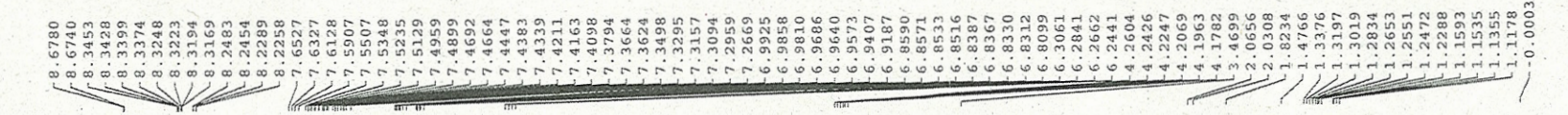




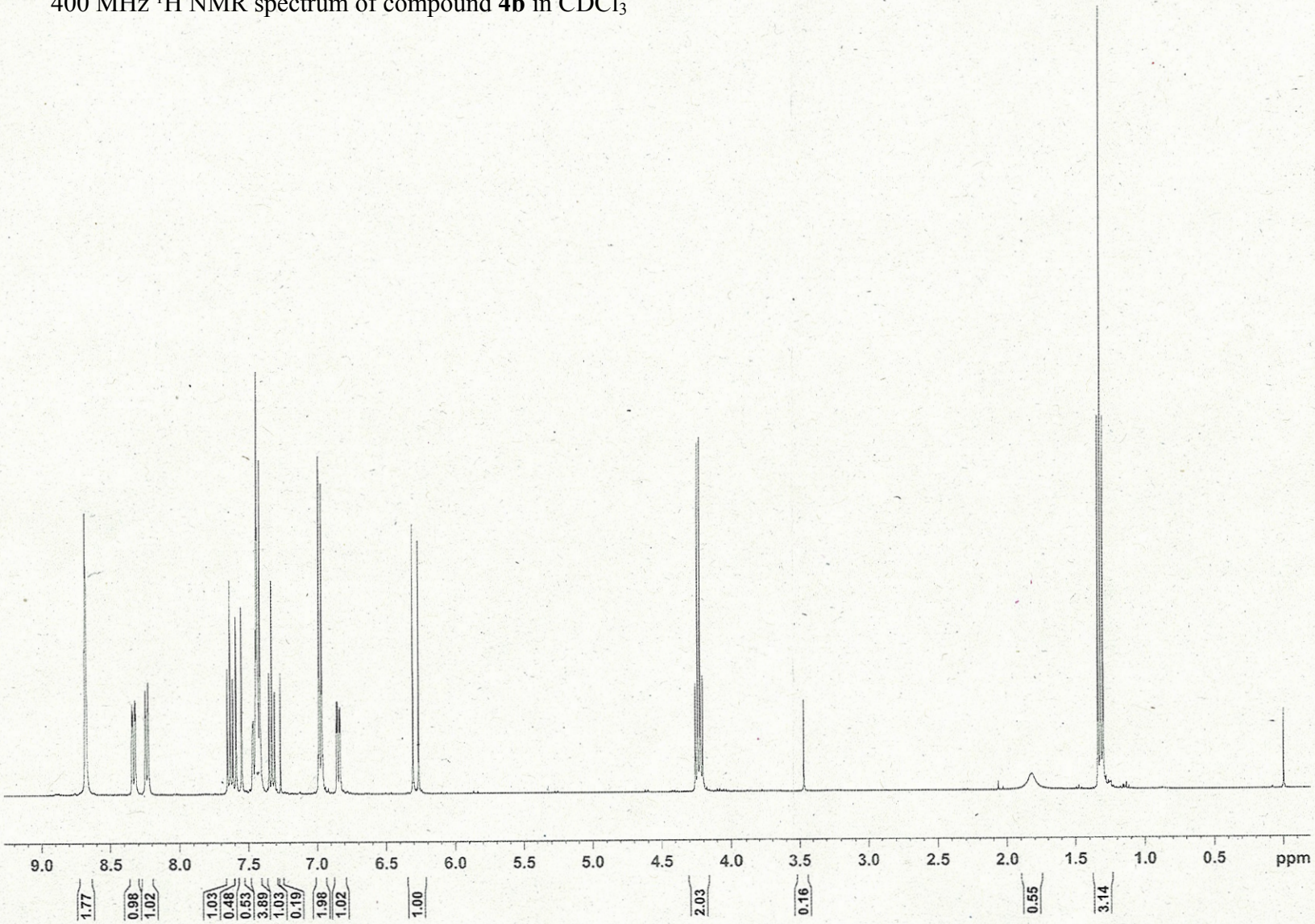
400 MHz ^{1}H NMR spectrum of compound **4a** in $CDCl_3$

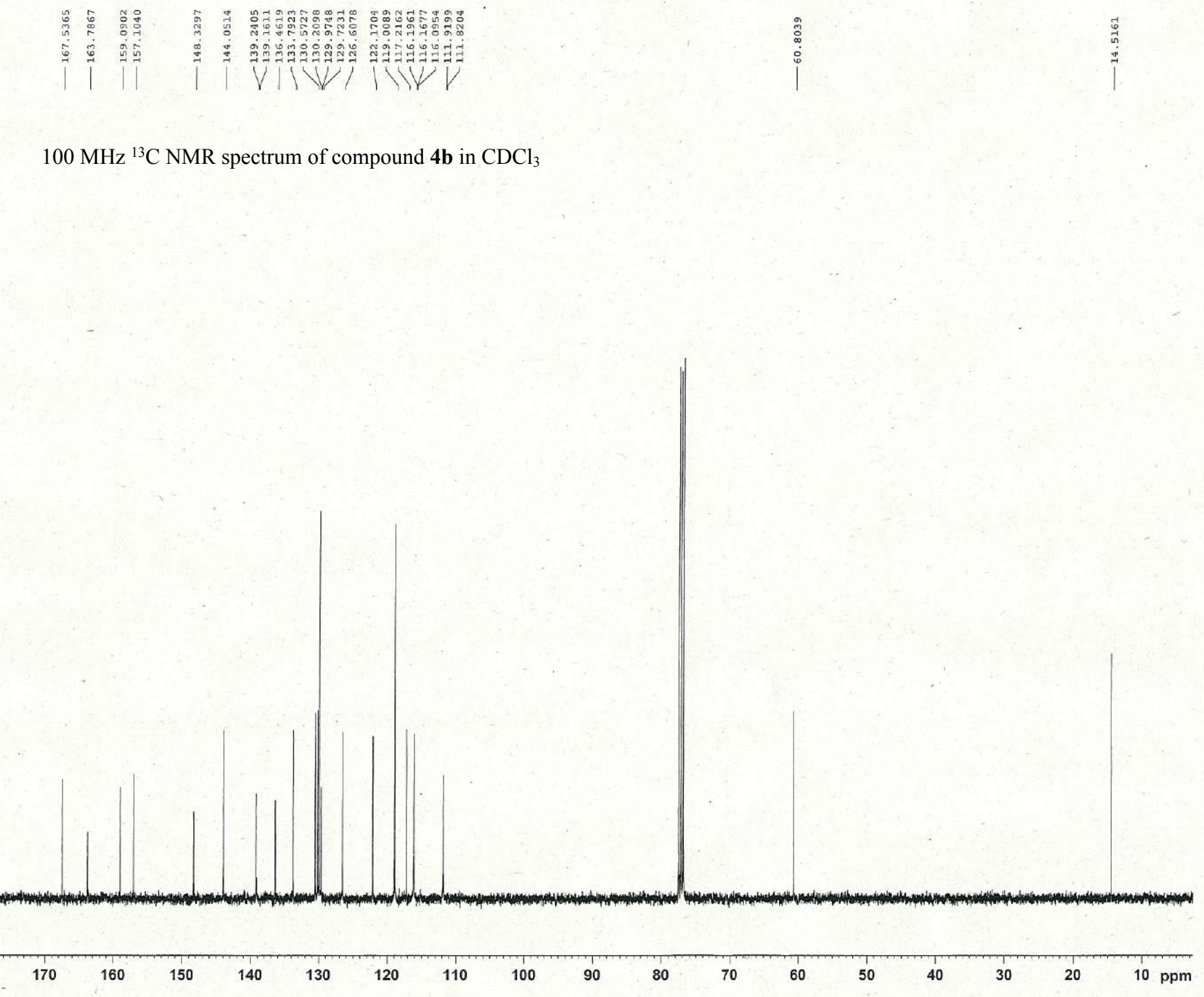


100 MHz ^{13}C NMR spectrum of compound **4a** in $CDCl_3$

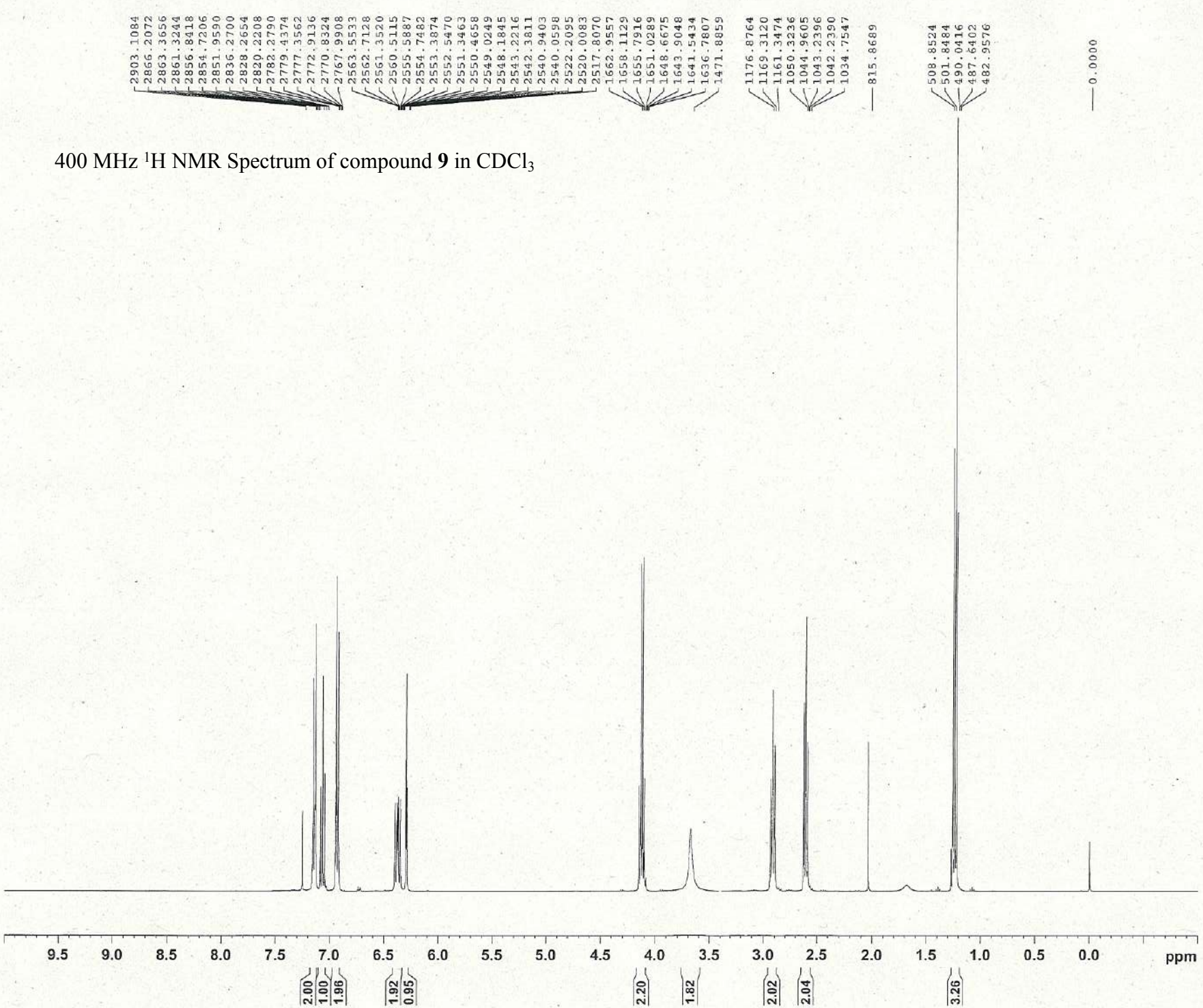


400 MHz ^{1}H NMR spectrum of compound **4b** in $CDCl_3$

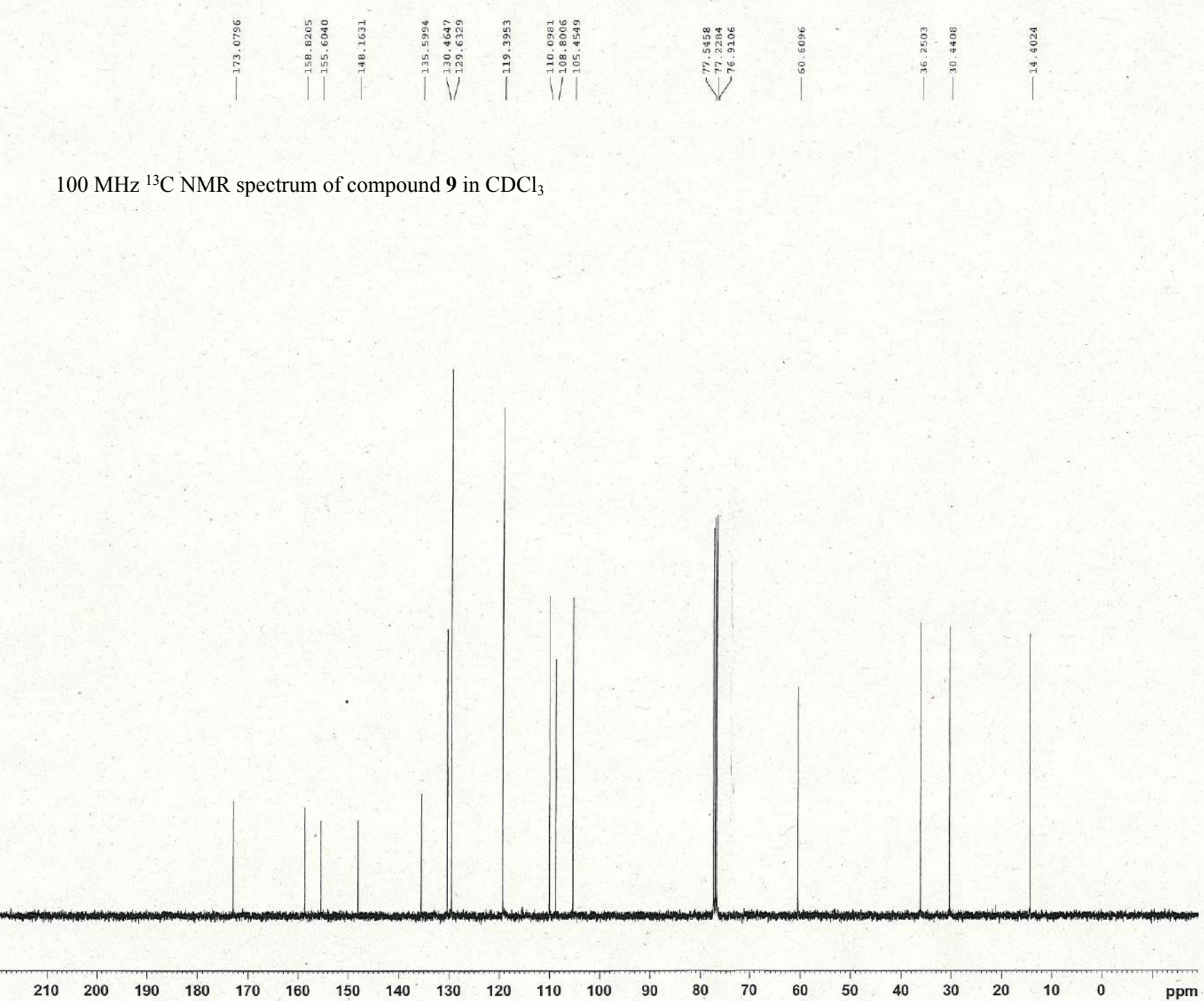




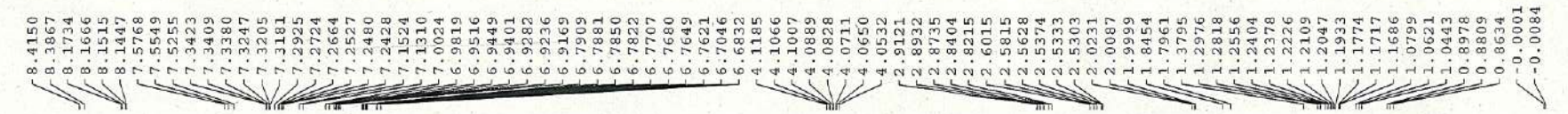
100 MHz ^{13}C NMR spectrum of compound **4b** in $CDCl_3$



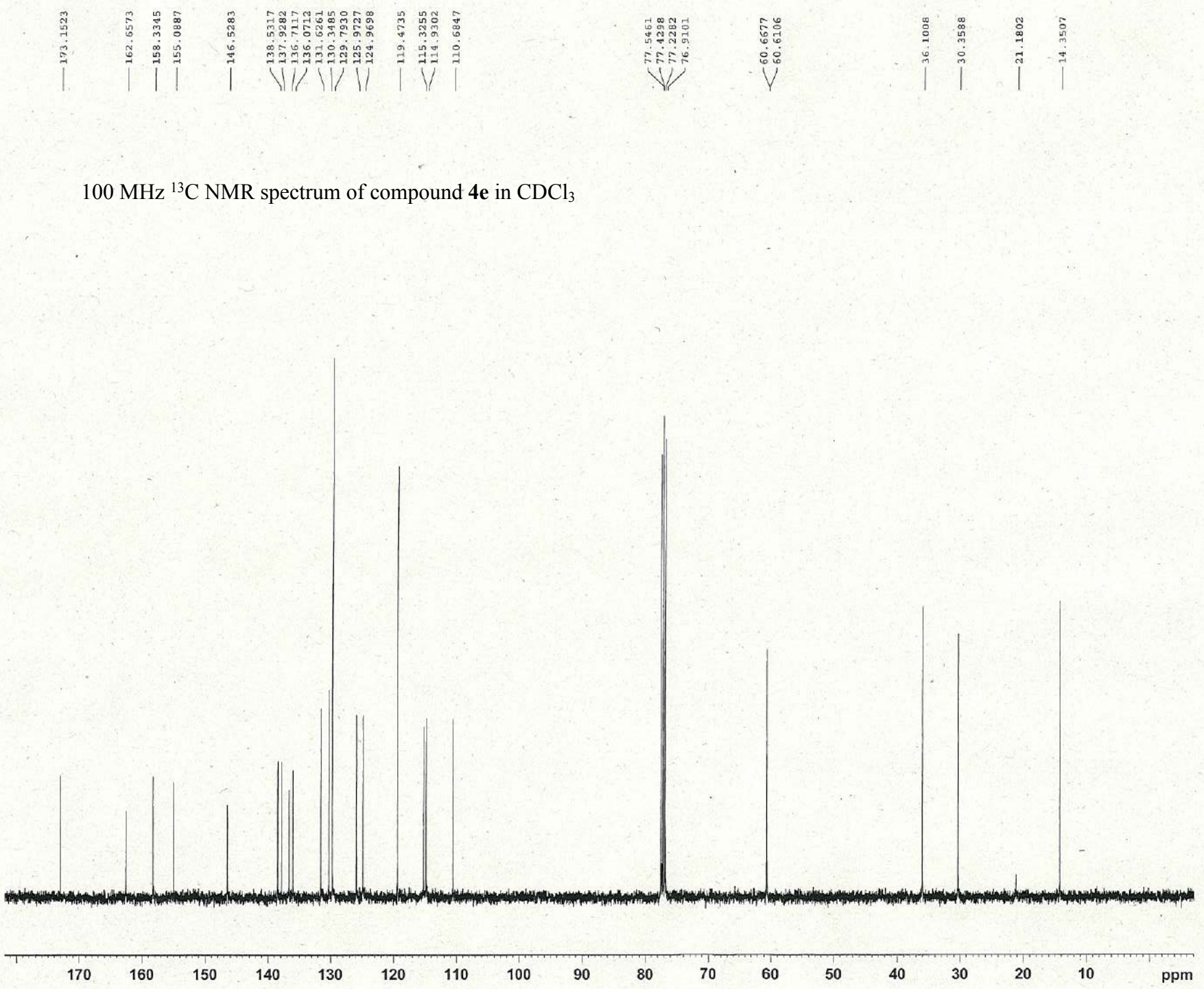
400 MHz ^{1}H NMR Spectrum of compound **9** in $CDCl_3$



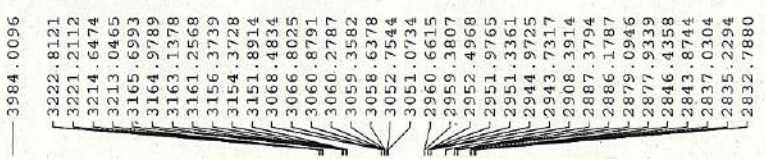
100 MHz ^{13}C NMR spectrum of compound **9** in $CDCl_3$



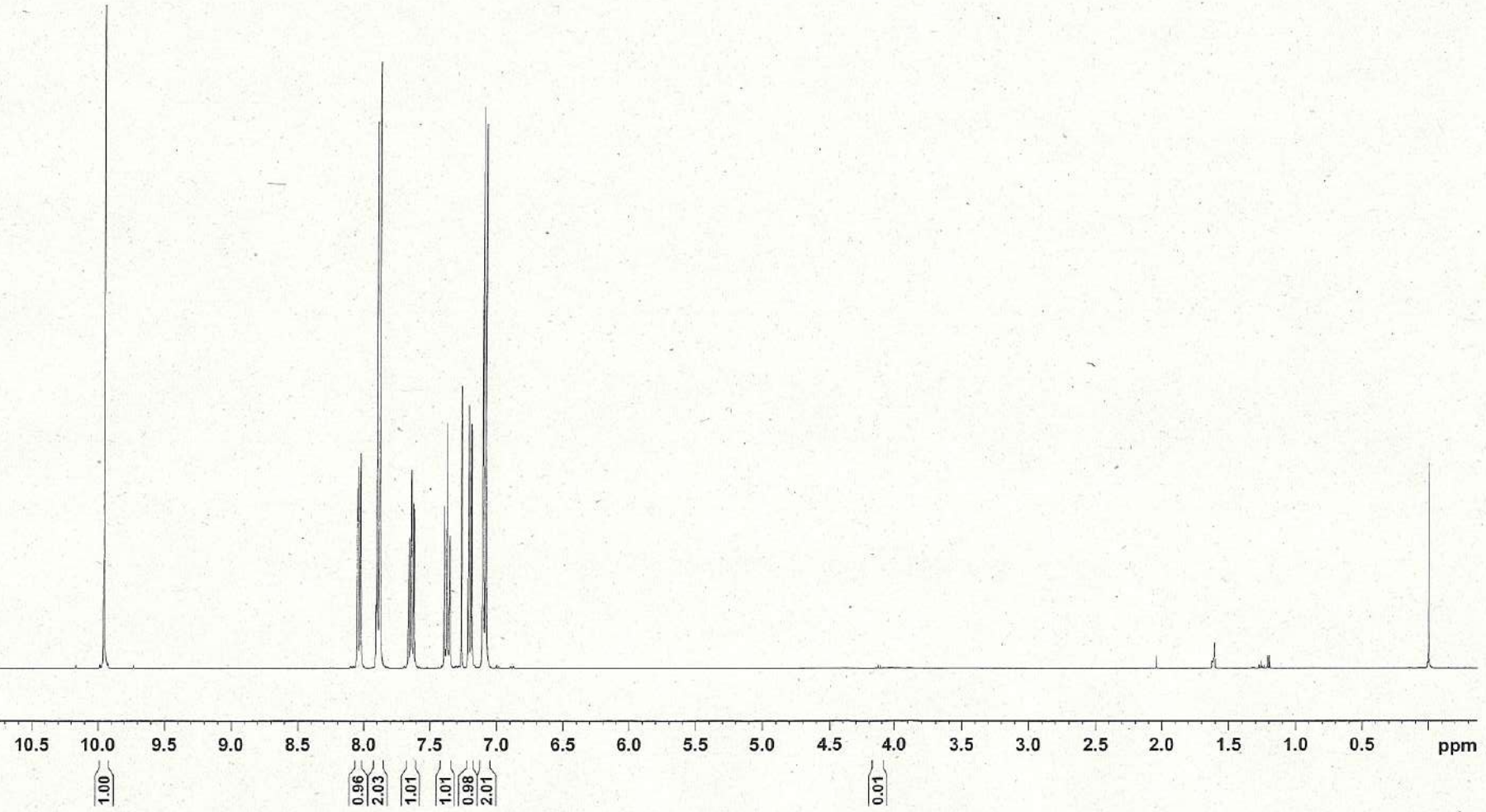
400 MHz ^{1}H NMR Spectrum of compound **4e** in $CDCl_3$

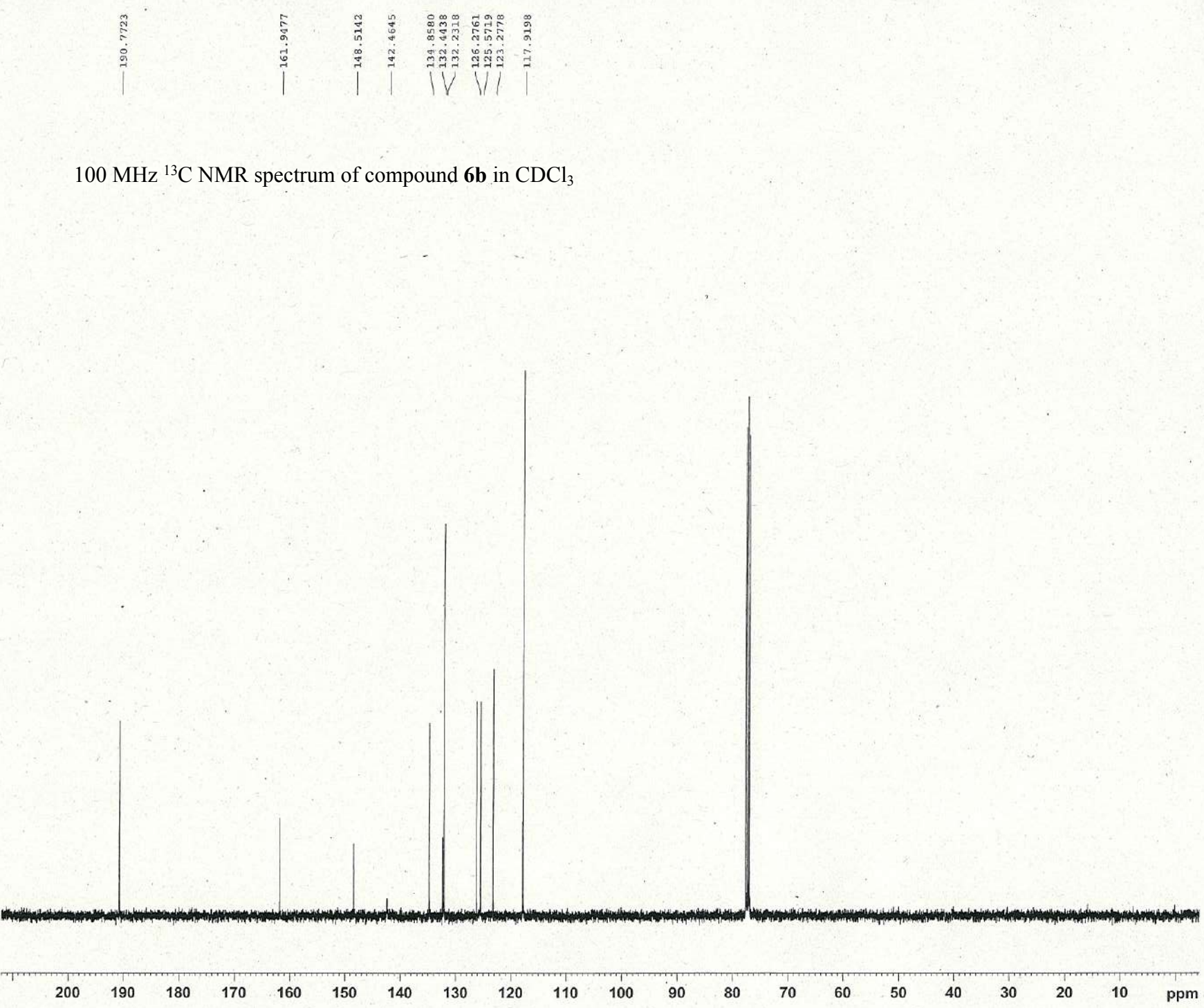


100 MHz ^{13}C NMR spectrum of compound **4e** in $CDCl_3$

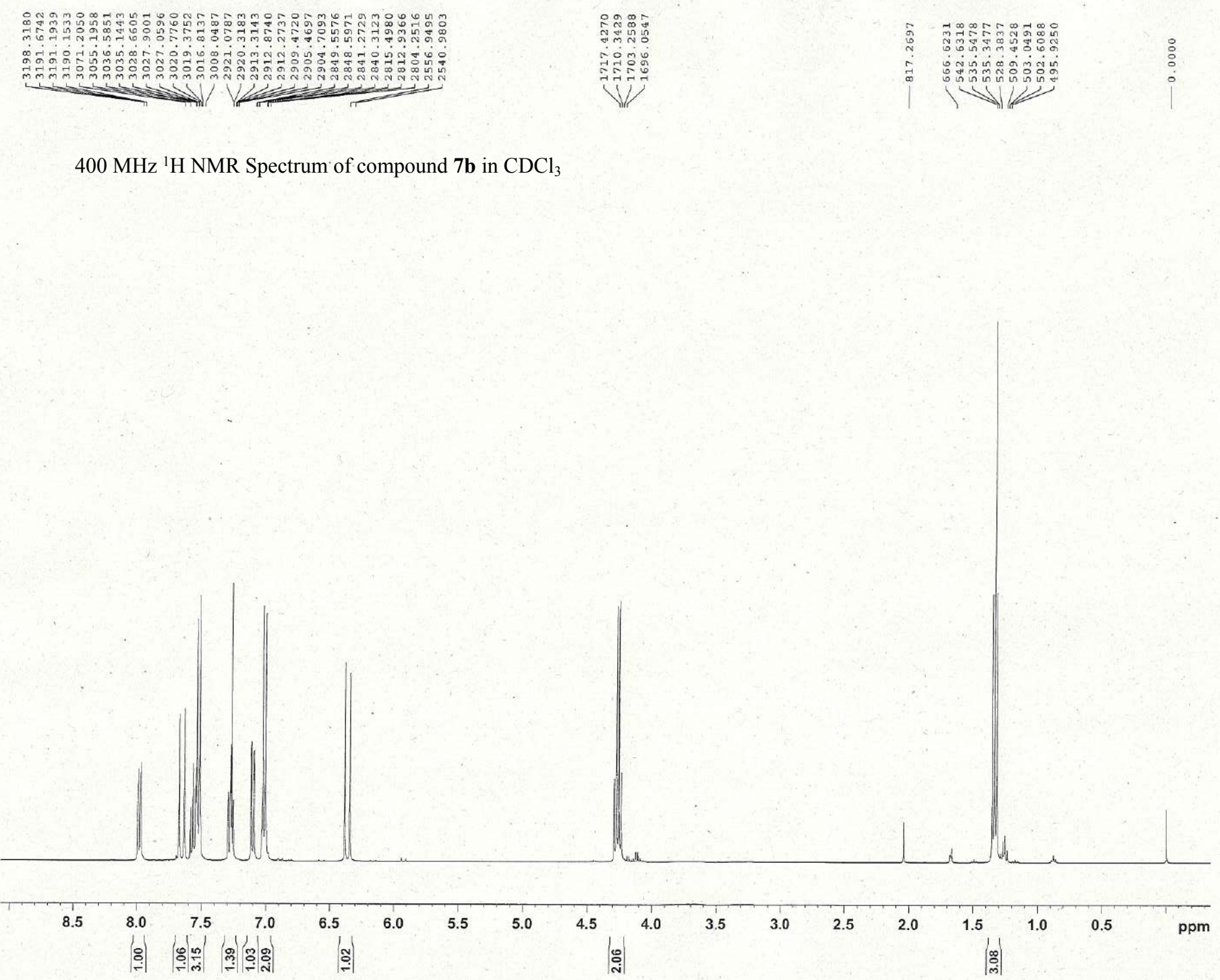


400 MHz ^{1}H NMR Spectrum of compound **6b** in $CDCl_3$

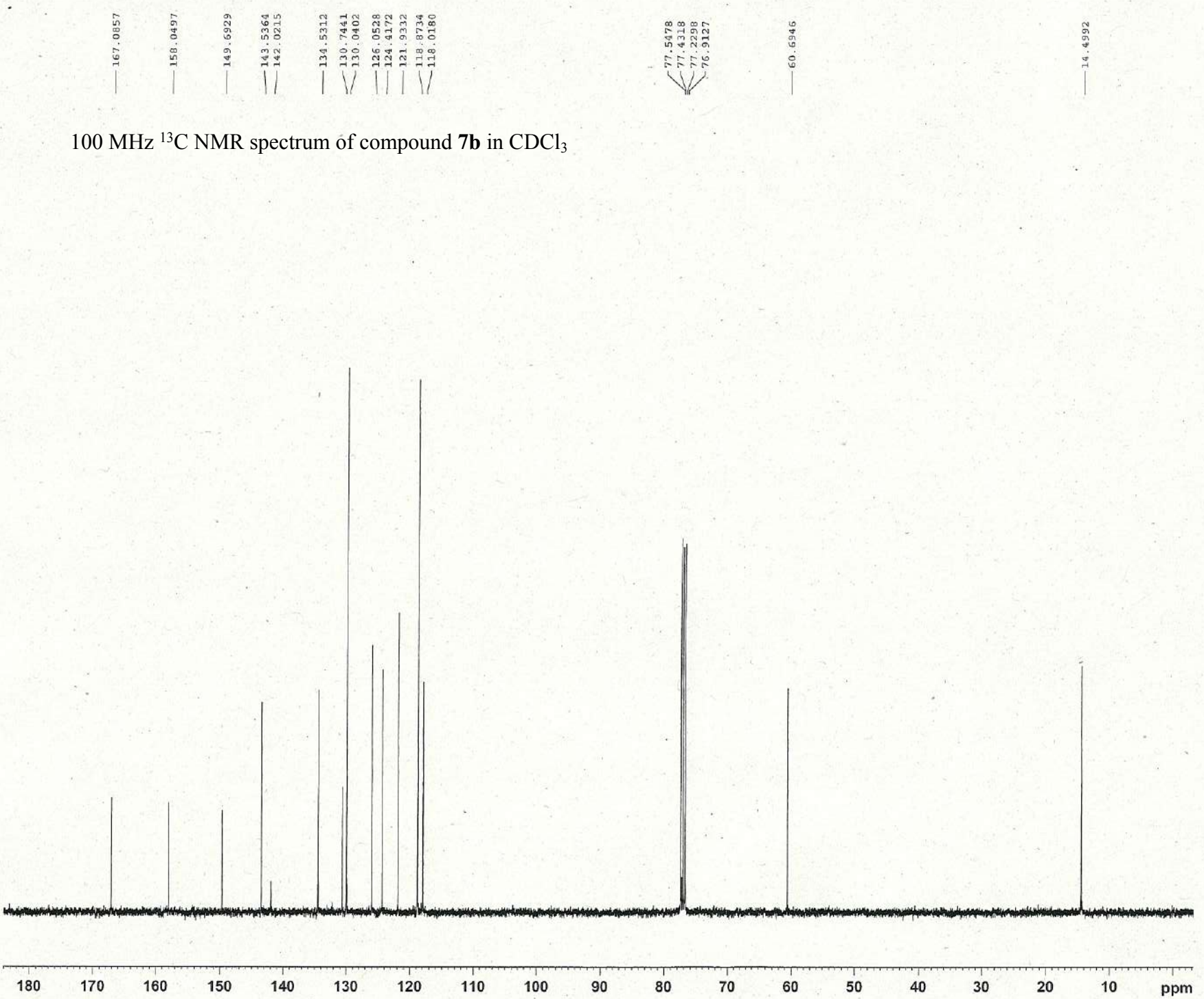




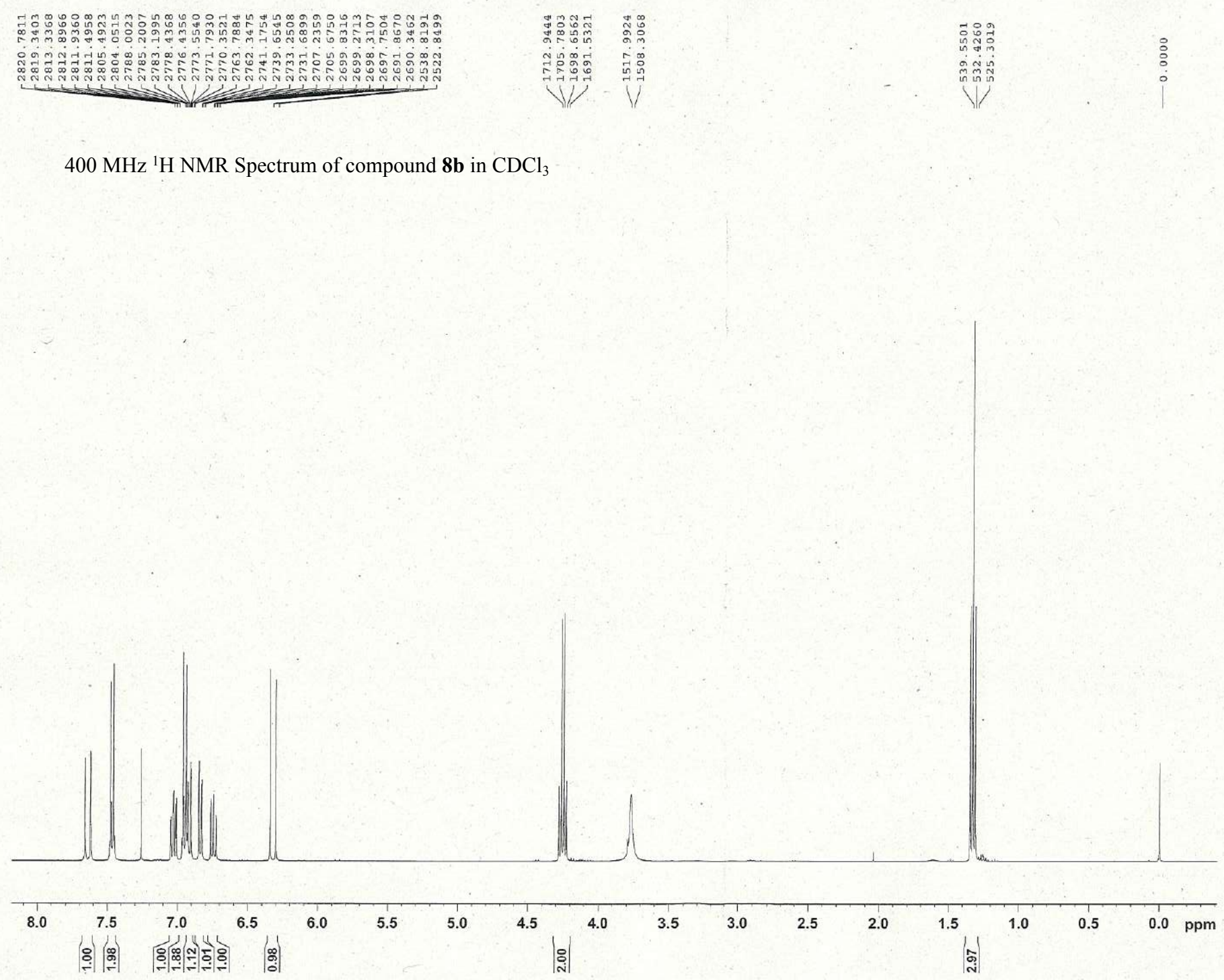
100 MHz ^{13}C NMR spectrum of compound **6b** in $CDCl_3$



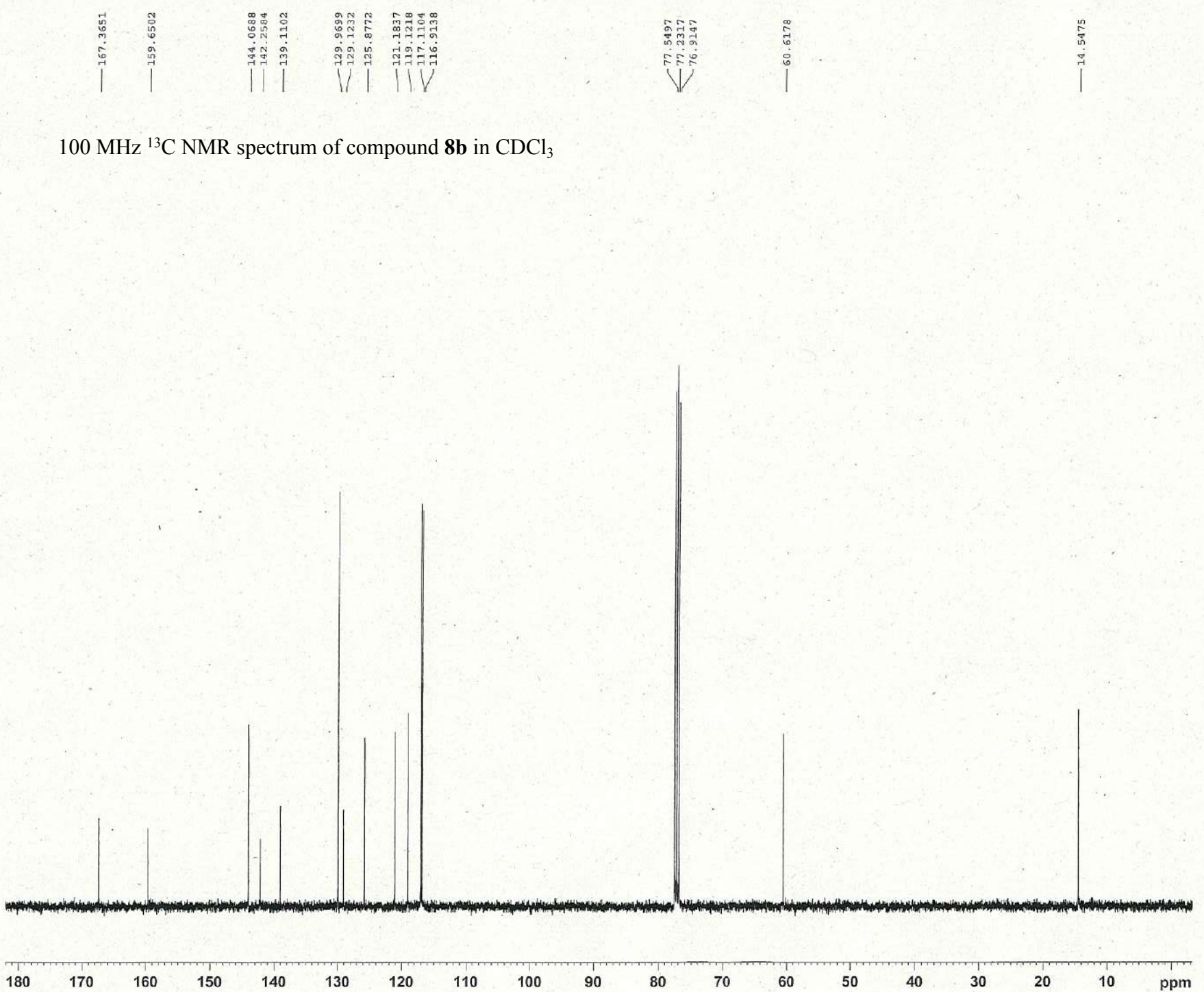
400 MHz ^{1}H NMR Spectrum of compound **7b** in $CDCl_3$



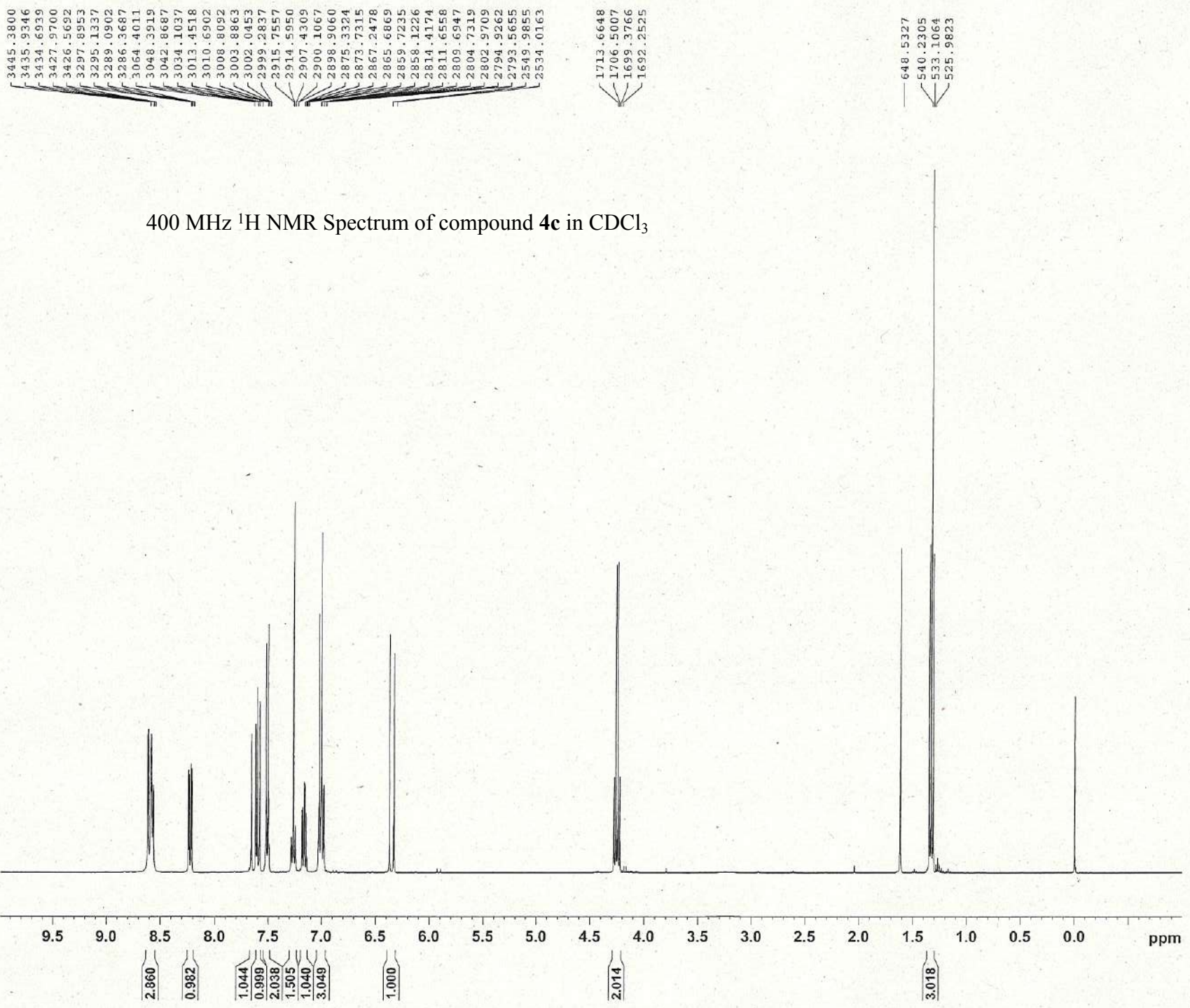
100 MHz ^{13}C NMR spectrum of compound **7b** in $CDCl_3$



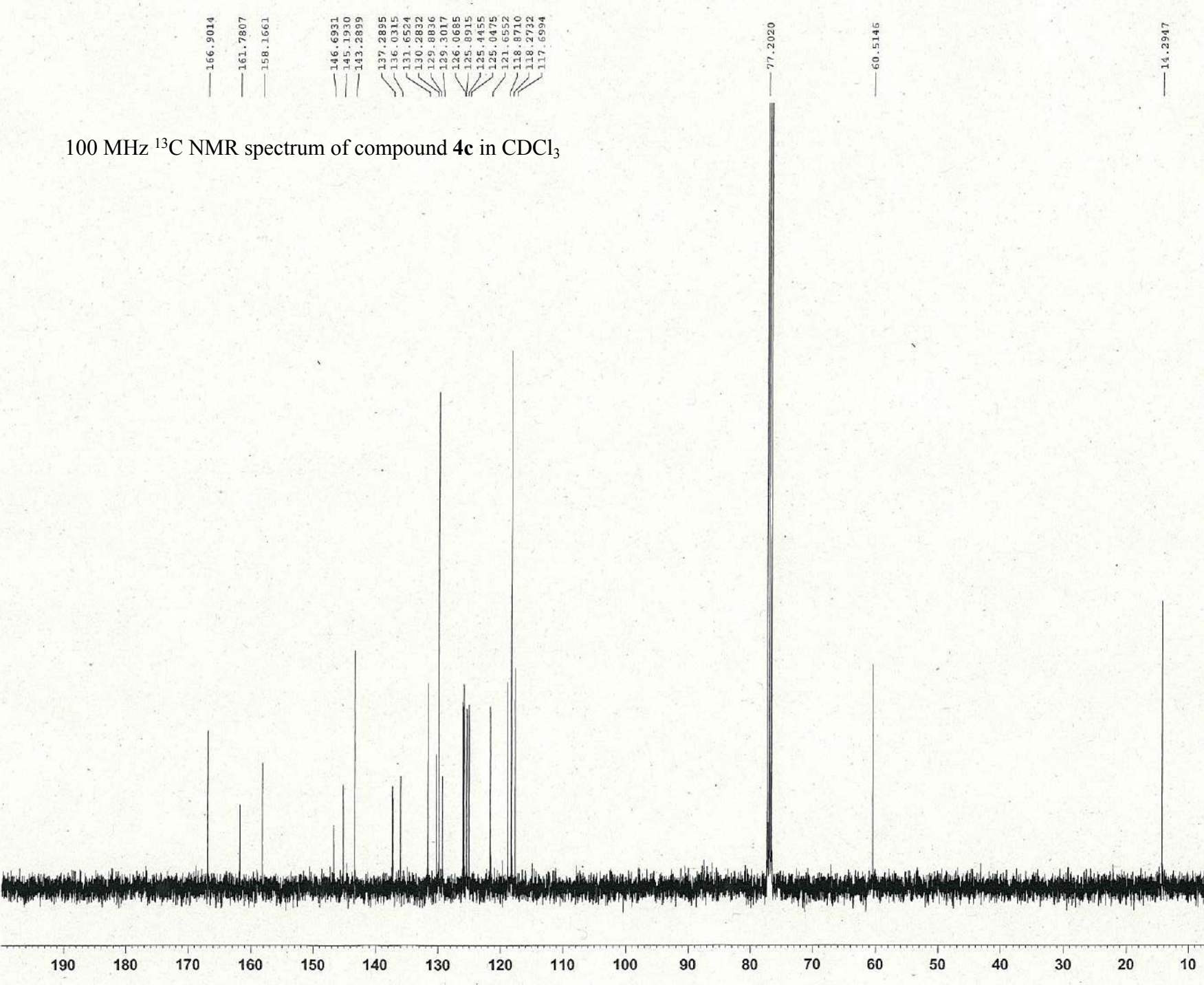
400 MHz ^{1}H NMR Spectrum of compound **8b** in $CDCl_3$



100 MHz ^{13}C NMR spectrum of compound **8b** in $CDCl_3$

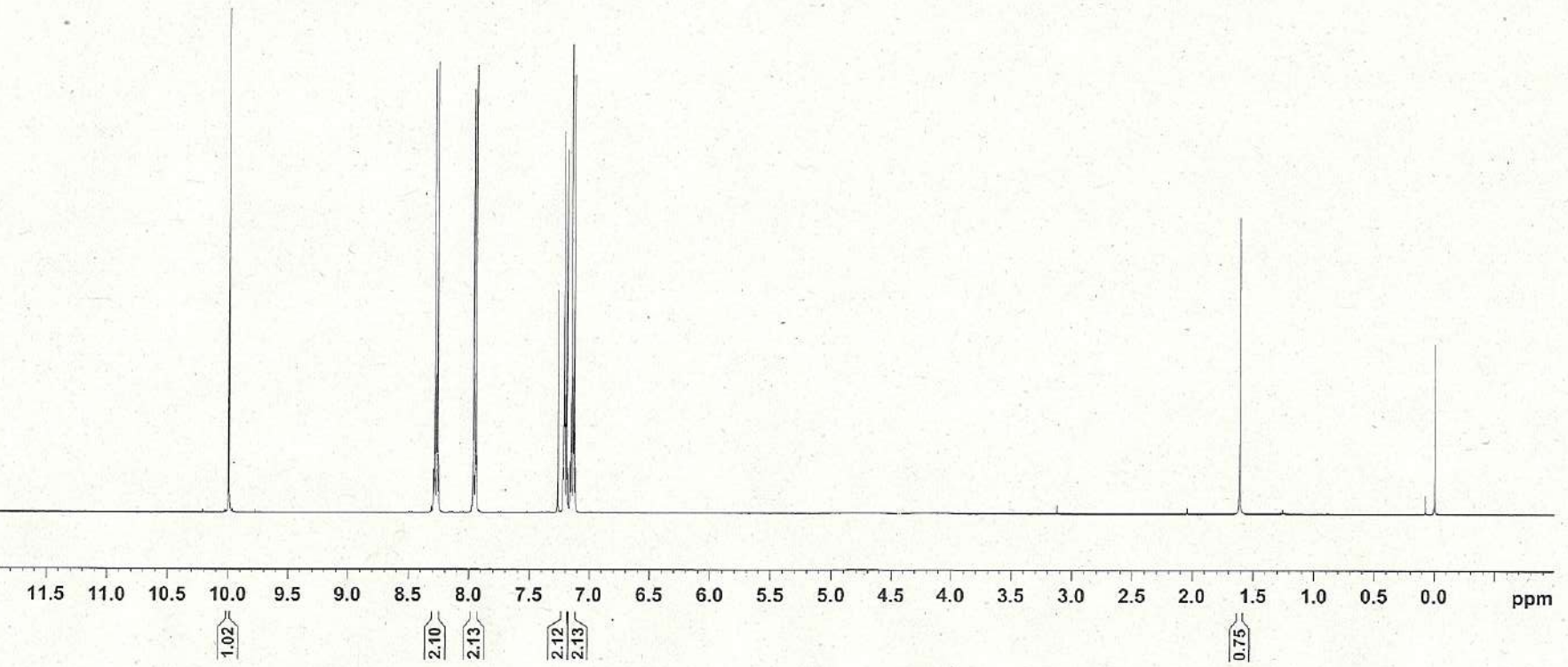


400 MHz ^{1}H NMR Spectrum of compound **4c** in $CDCl_3$



100 MHz ^{13}C NMR spectrum of compound **4c** in $CDCl_3$

400 MHz ^{1}H NMR Spectrum of compound **6c** in $CDCl_3$



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118.8197
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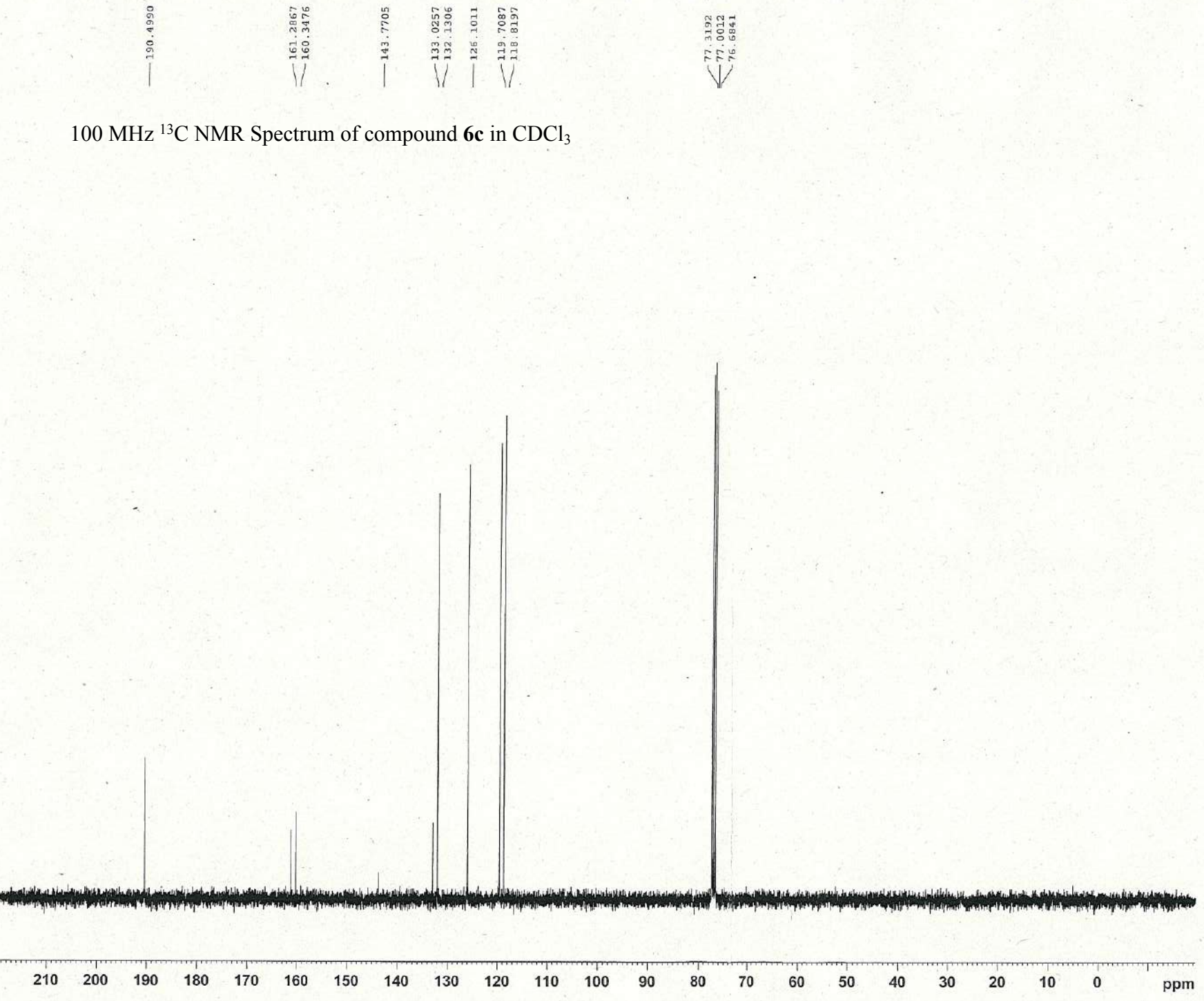
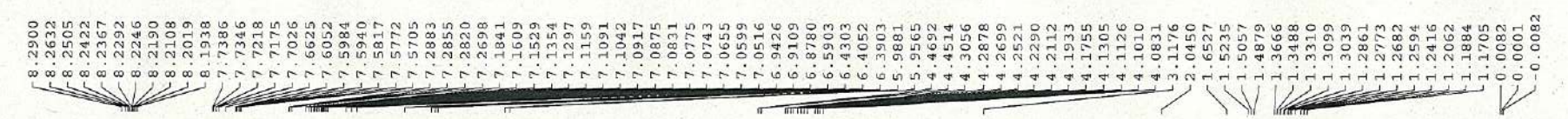
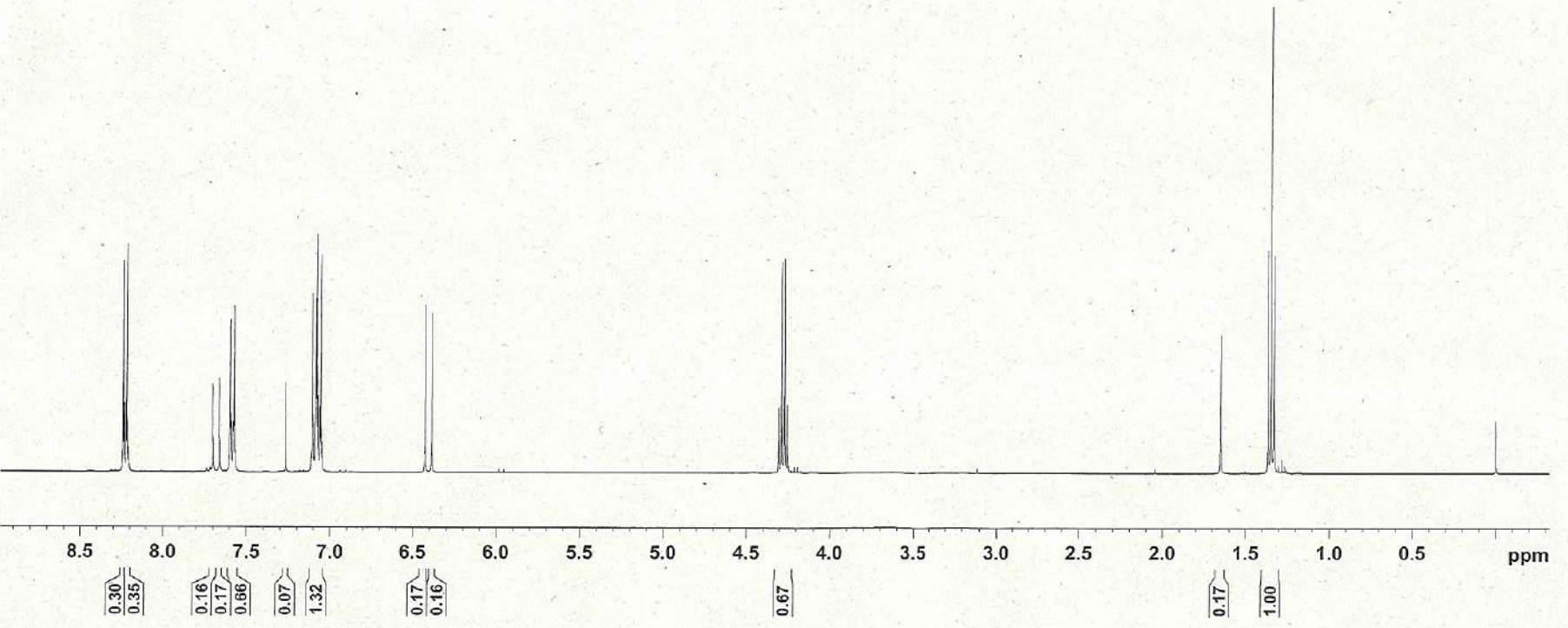
77.0012
76.6841

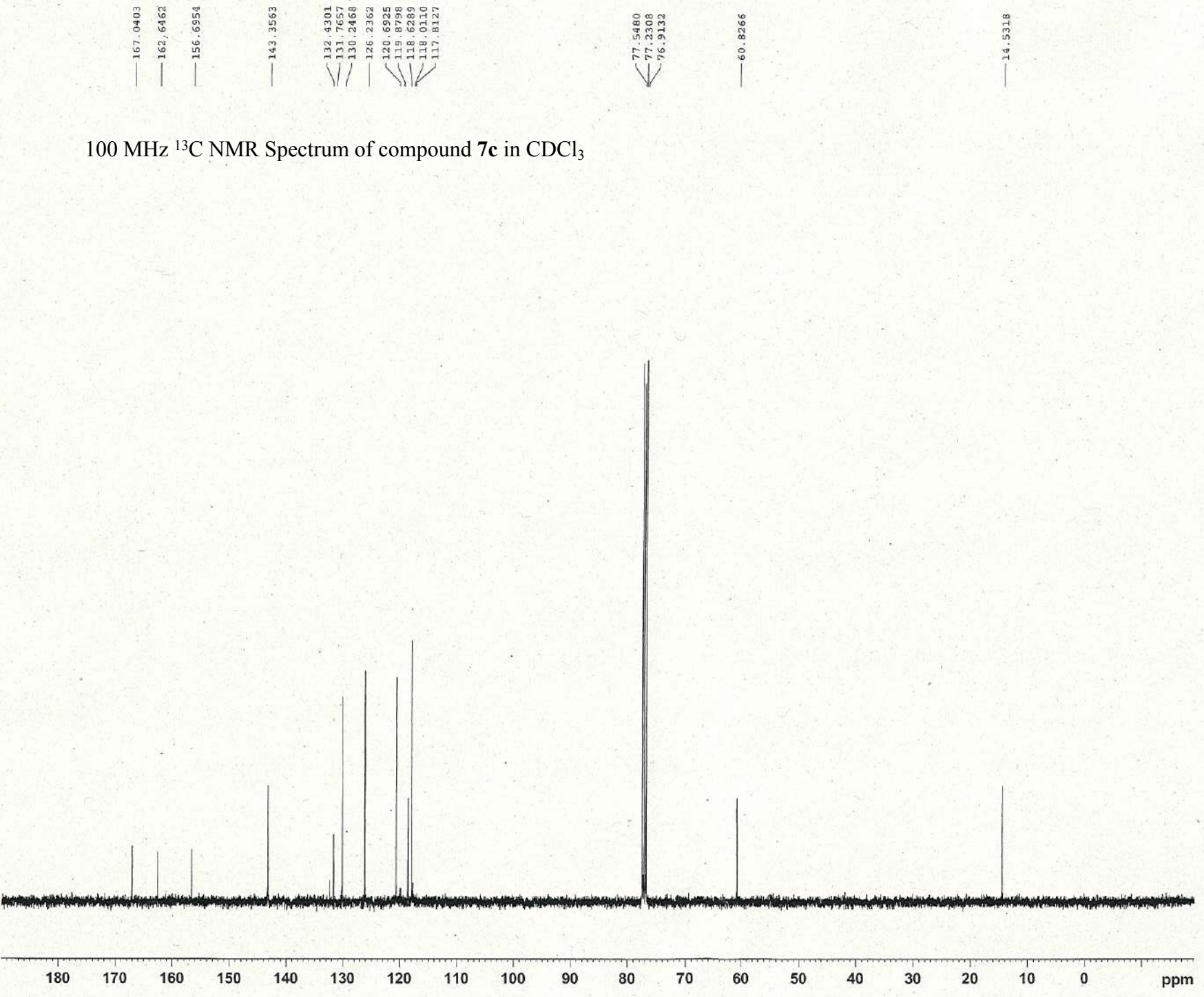
100 MHz ^{13}C NMR Spectrum of compound **6c** in $CDCl_3$



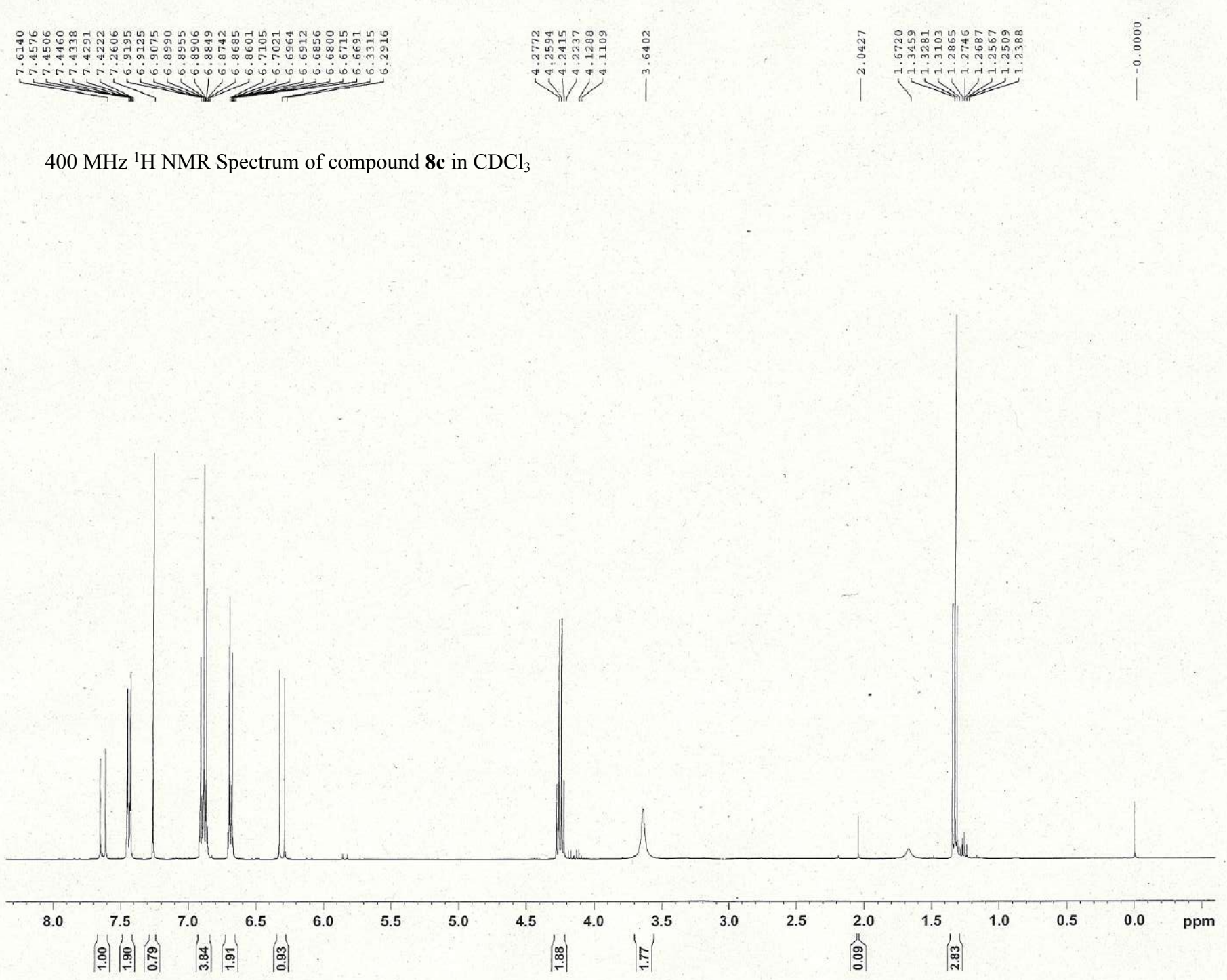


400 MHz ^{1}H NMR Spectrum of compound **7c** in $CDCl_3$

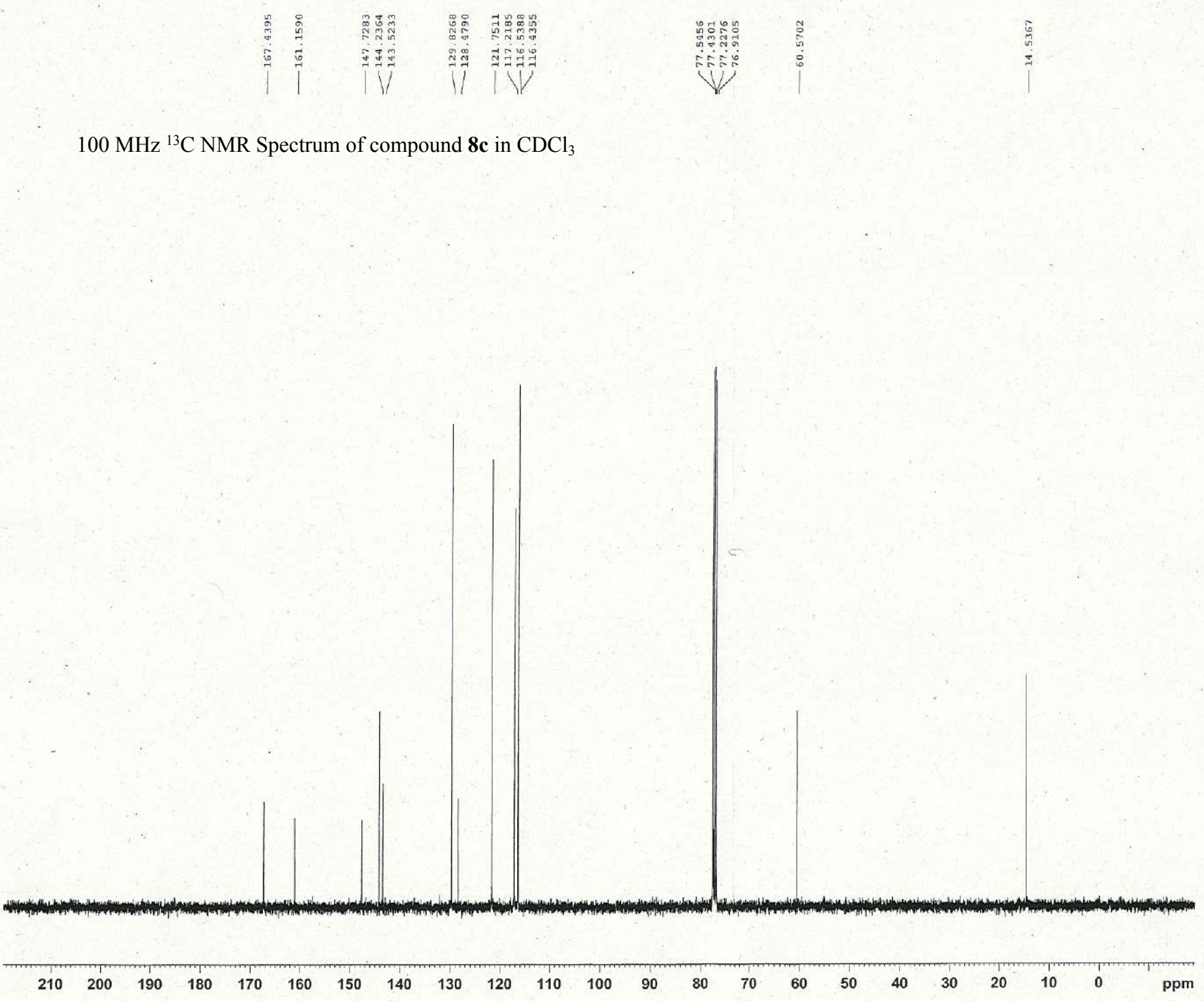




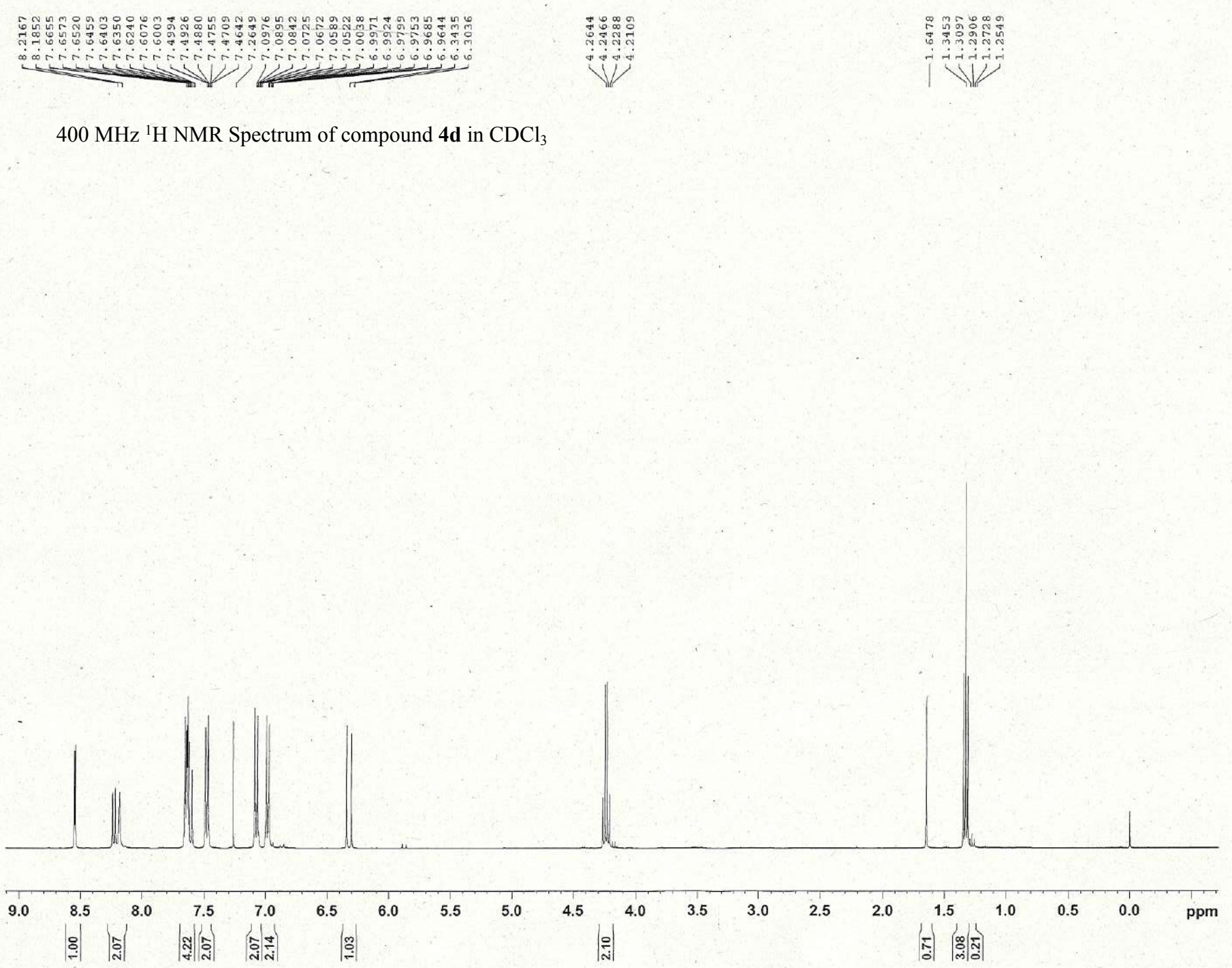
100 MHz ^{13}C NMR Spectrum of compound **7c** in $CDCl_3$



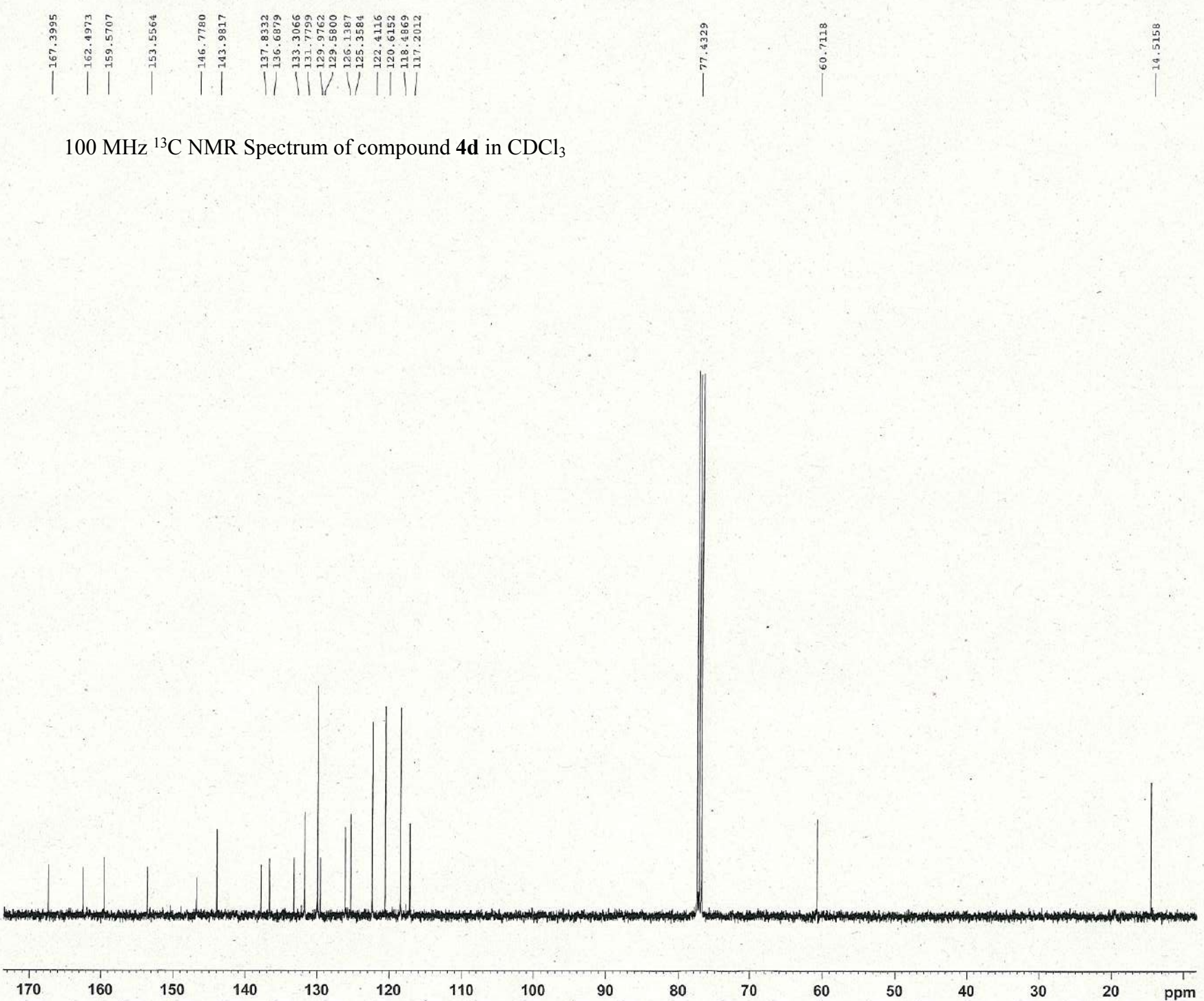
400 MHz ^{1}H NMR Spectrum of compound **8c** in $CDCl_3$



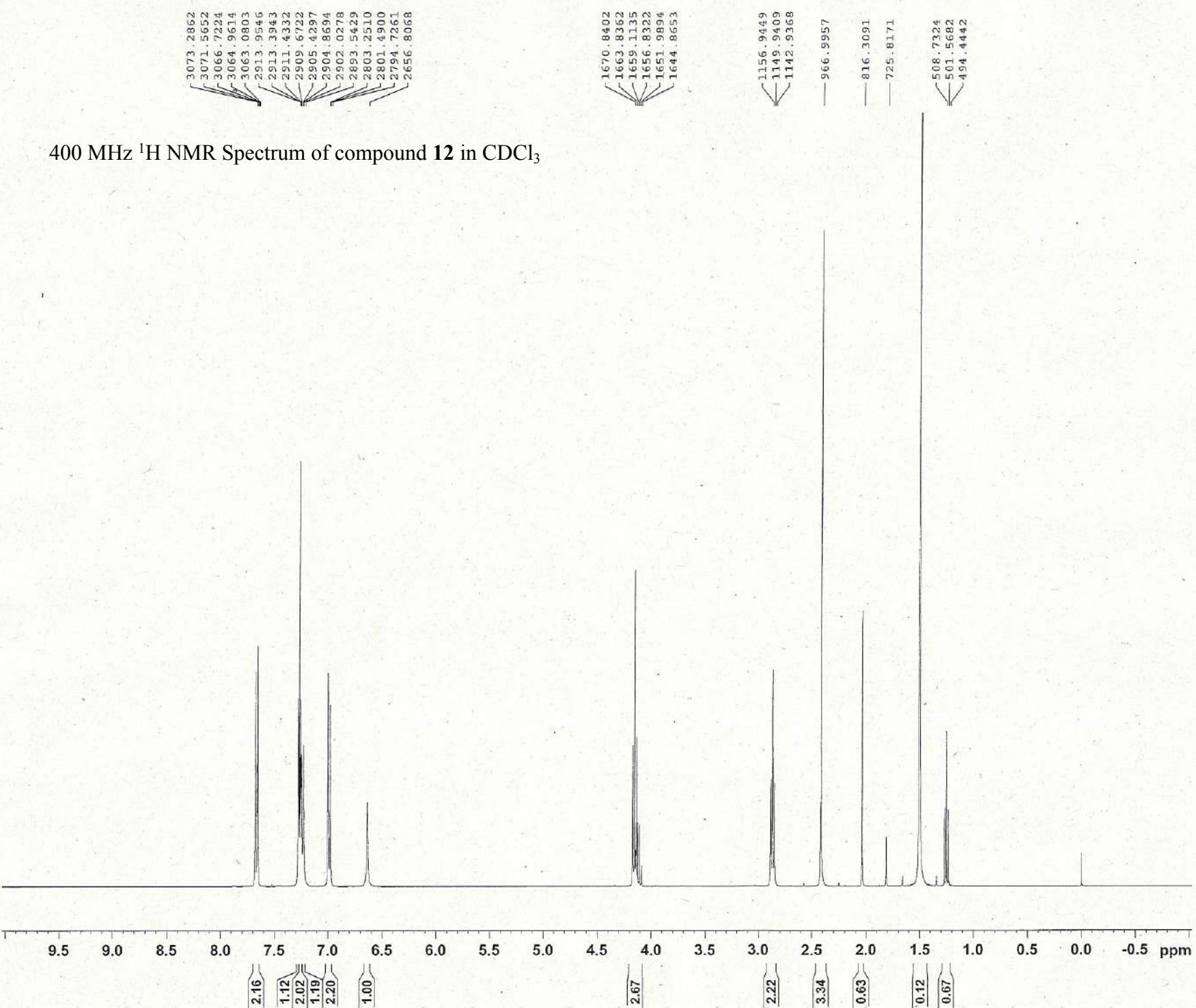
100 MHz ^{13}C NMR Spectrum of compound **8c** in $CDCl_3$



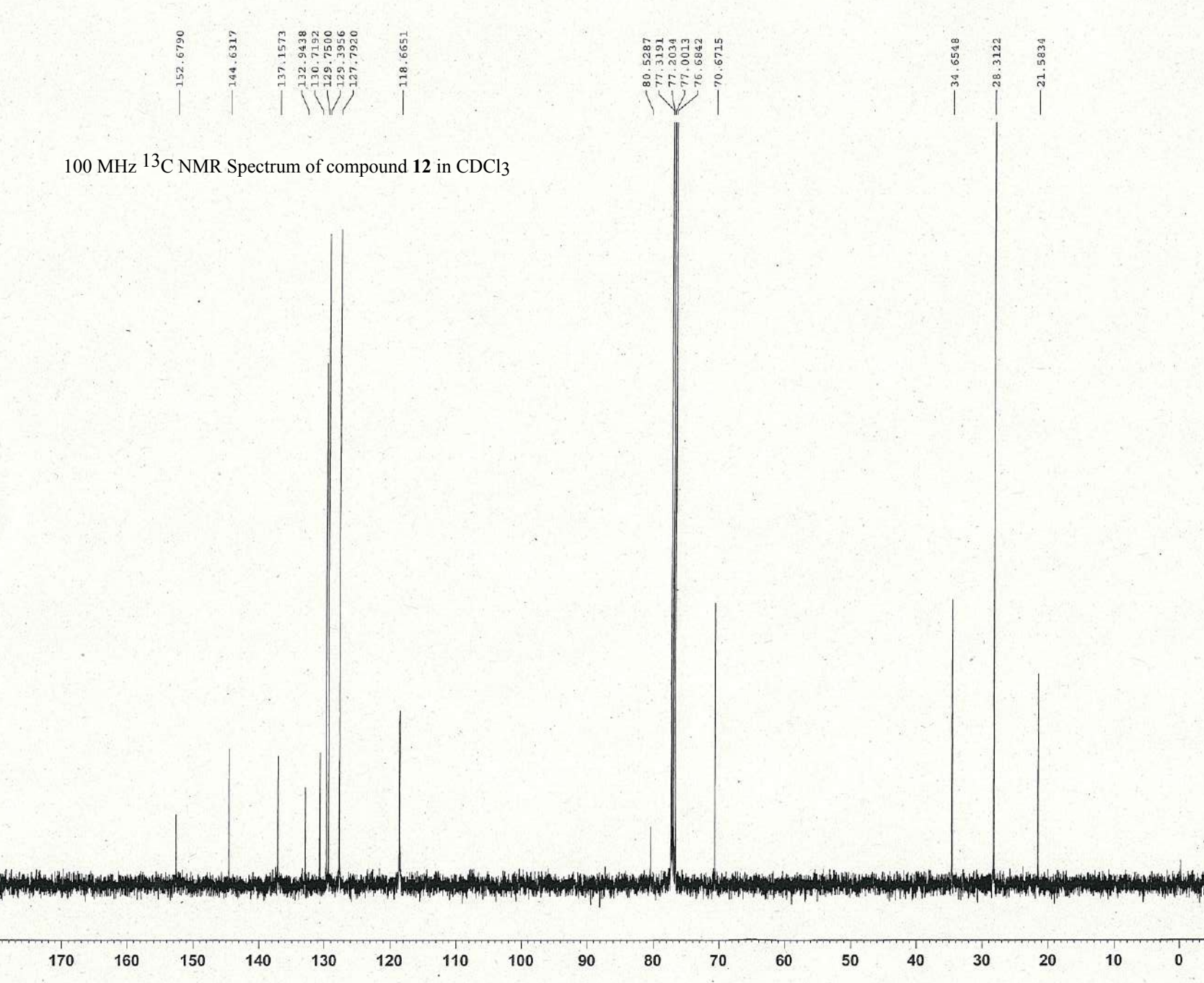
400 MHz ^{1}H NMR Spectrum of compound **4d** in $CDCl_3$



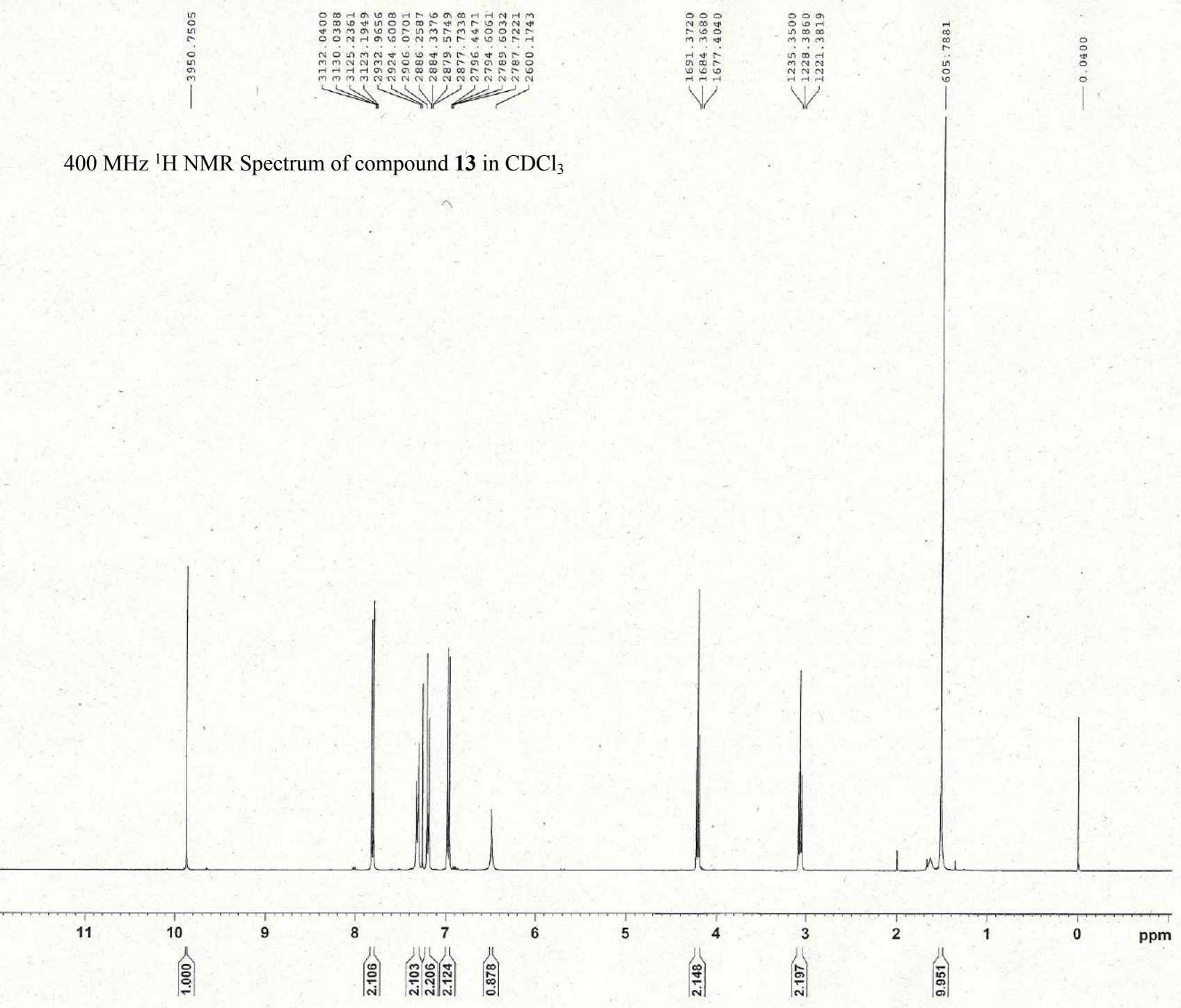
100 MHz ^{13}C NMR Spectrum of compound **4d** in $CDCl_3$



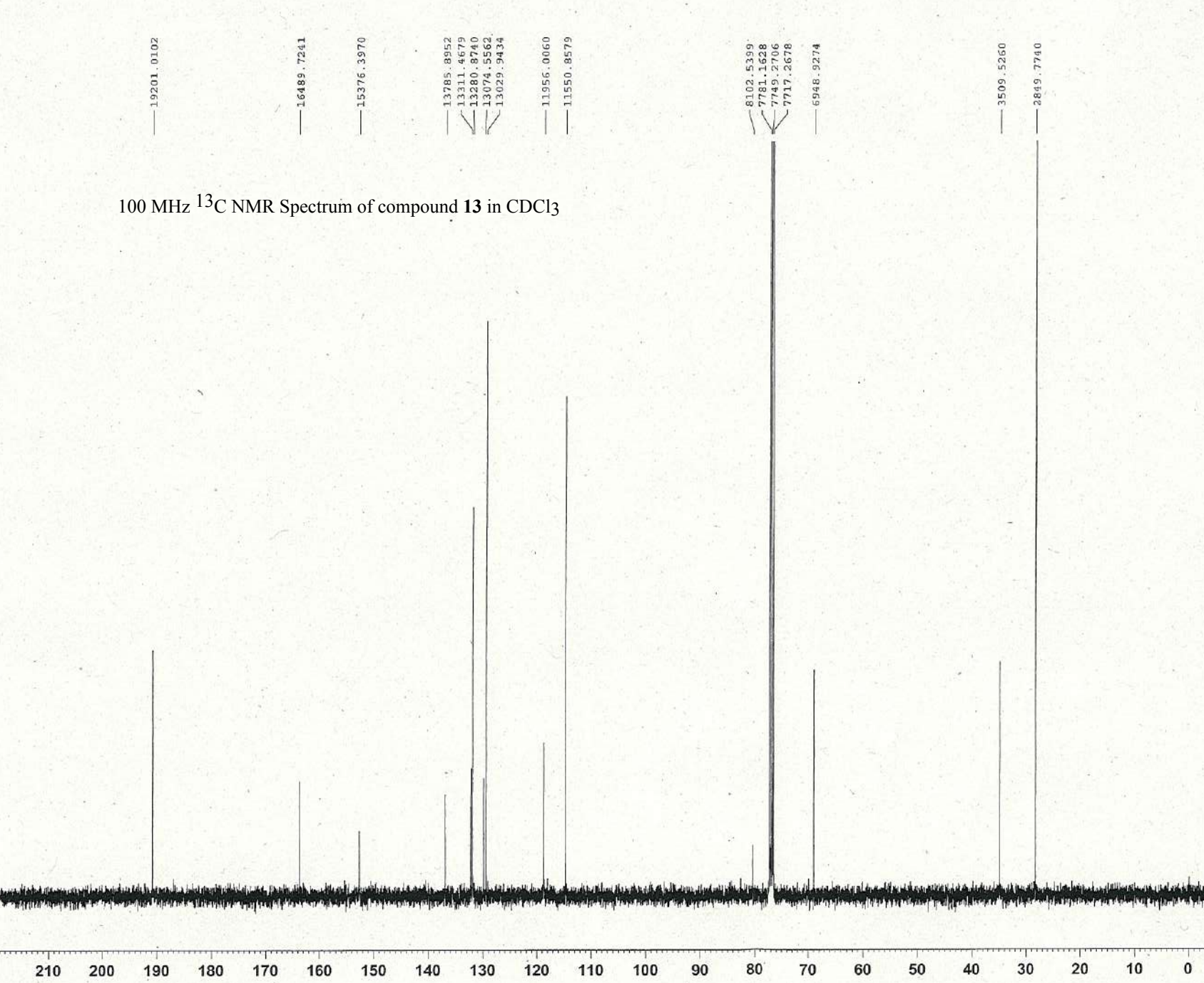
400 MHz ^{1}H NMR Spectrum of compound **12** in $CDCl_3$



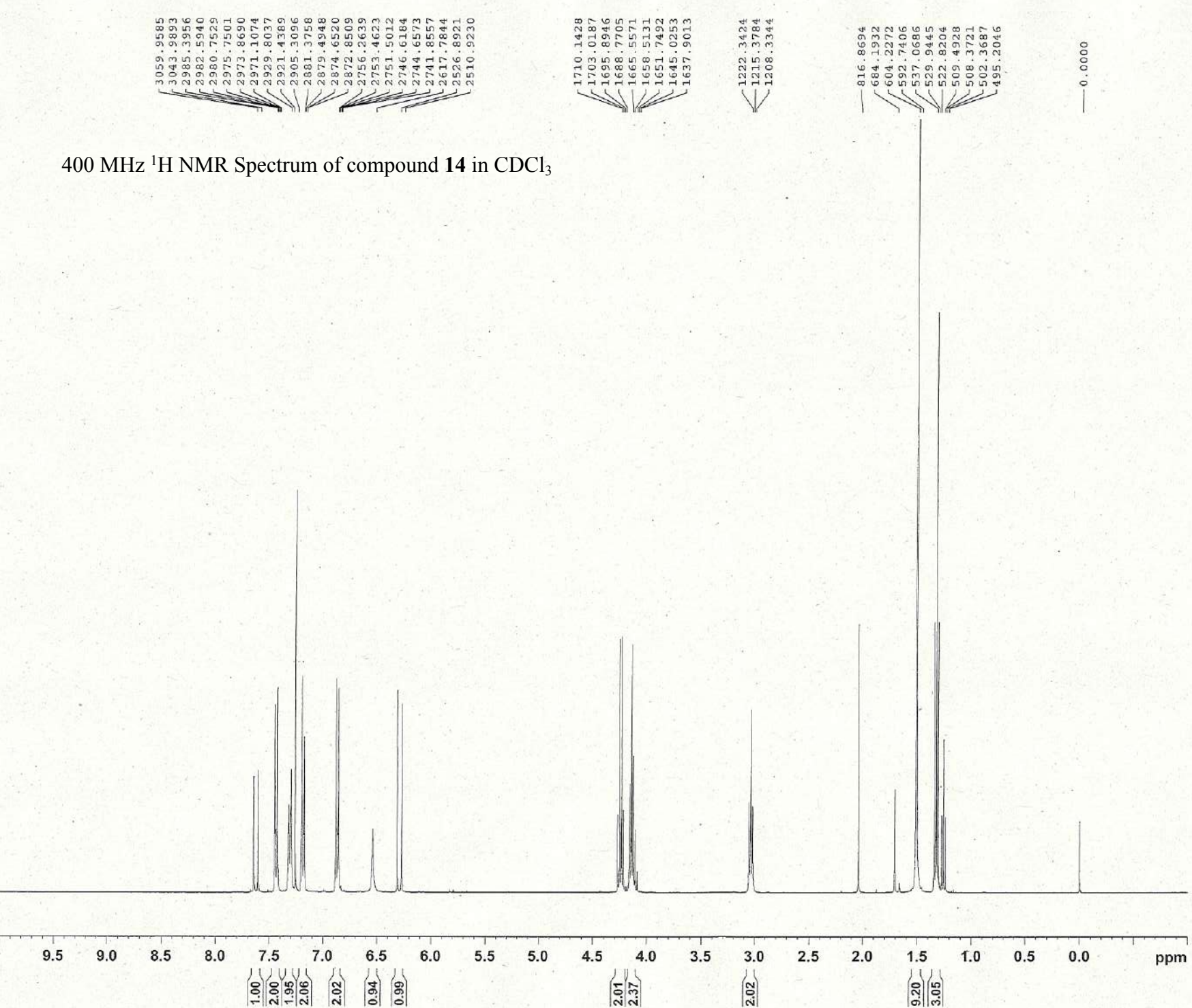
100 MHz ^{13}C NMR Spectrum of compound **12** in $CDCl_3$



400 MHz ^{1}H NMR Spectrum of compound **13** in $CDCl_3$

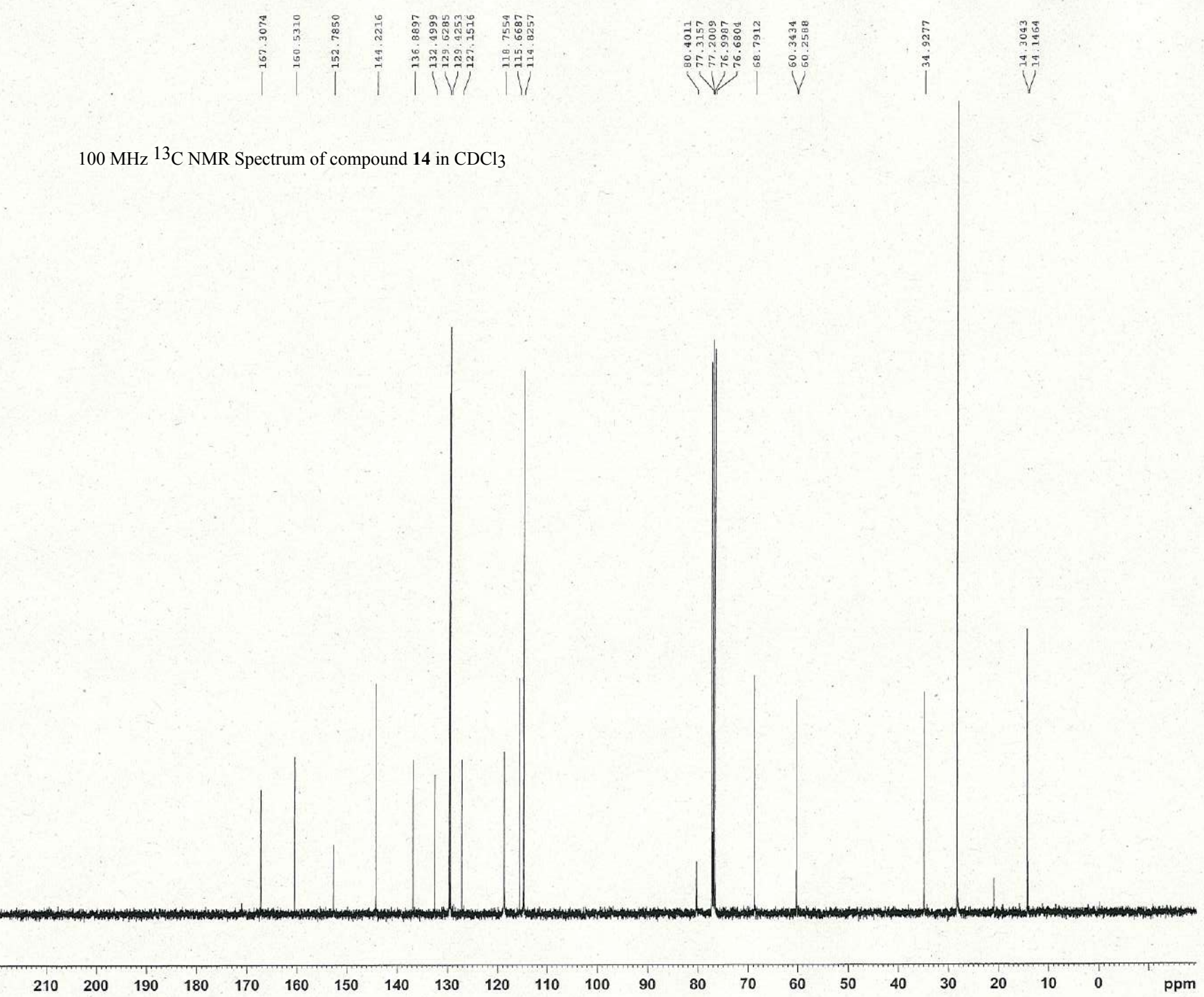


100 MHz ^{13}C NMR Spectrum of compound **13** in $CDCl_3$

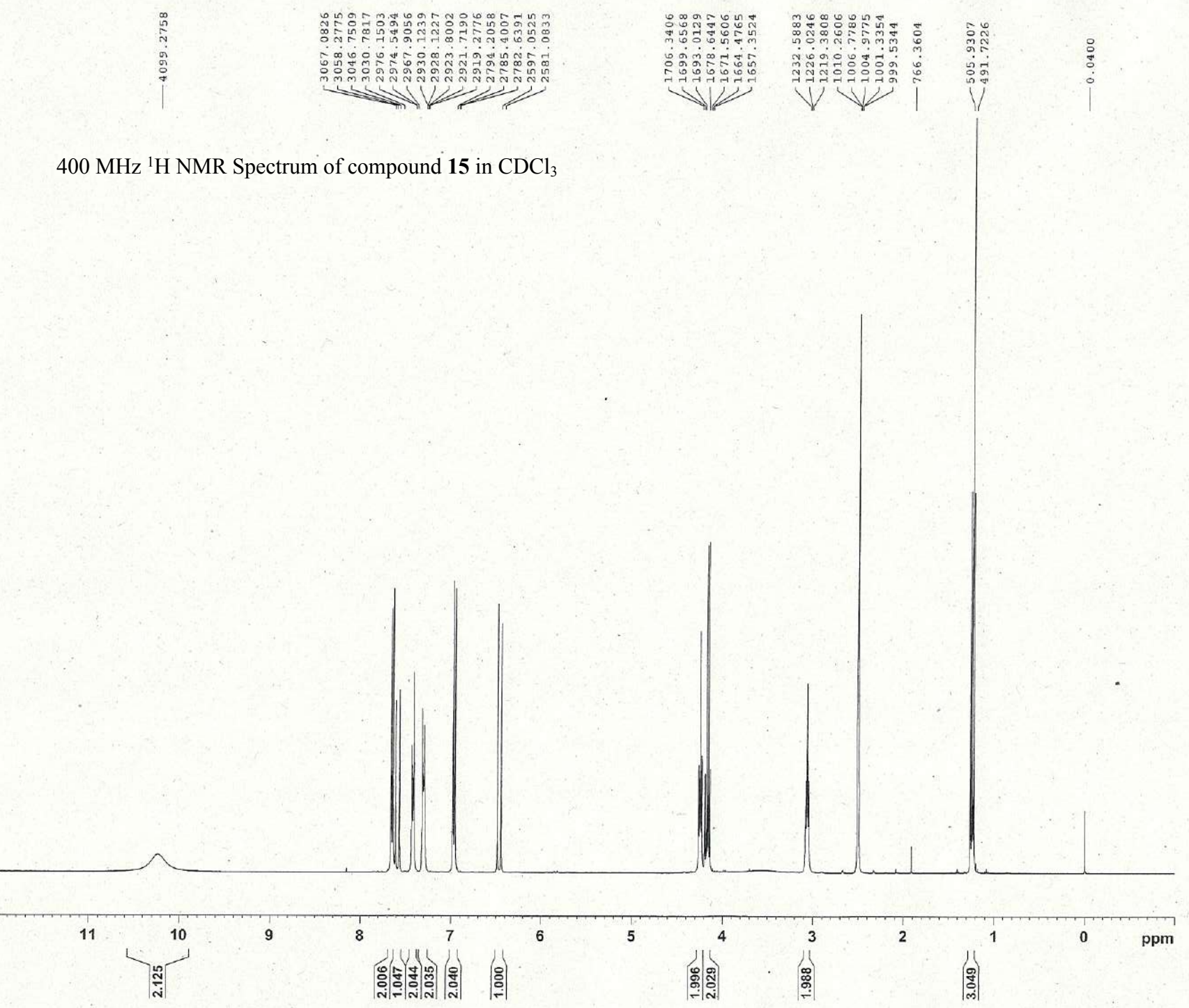


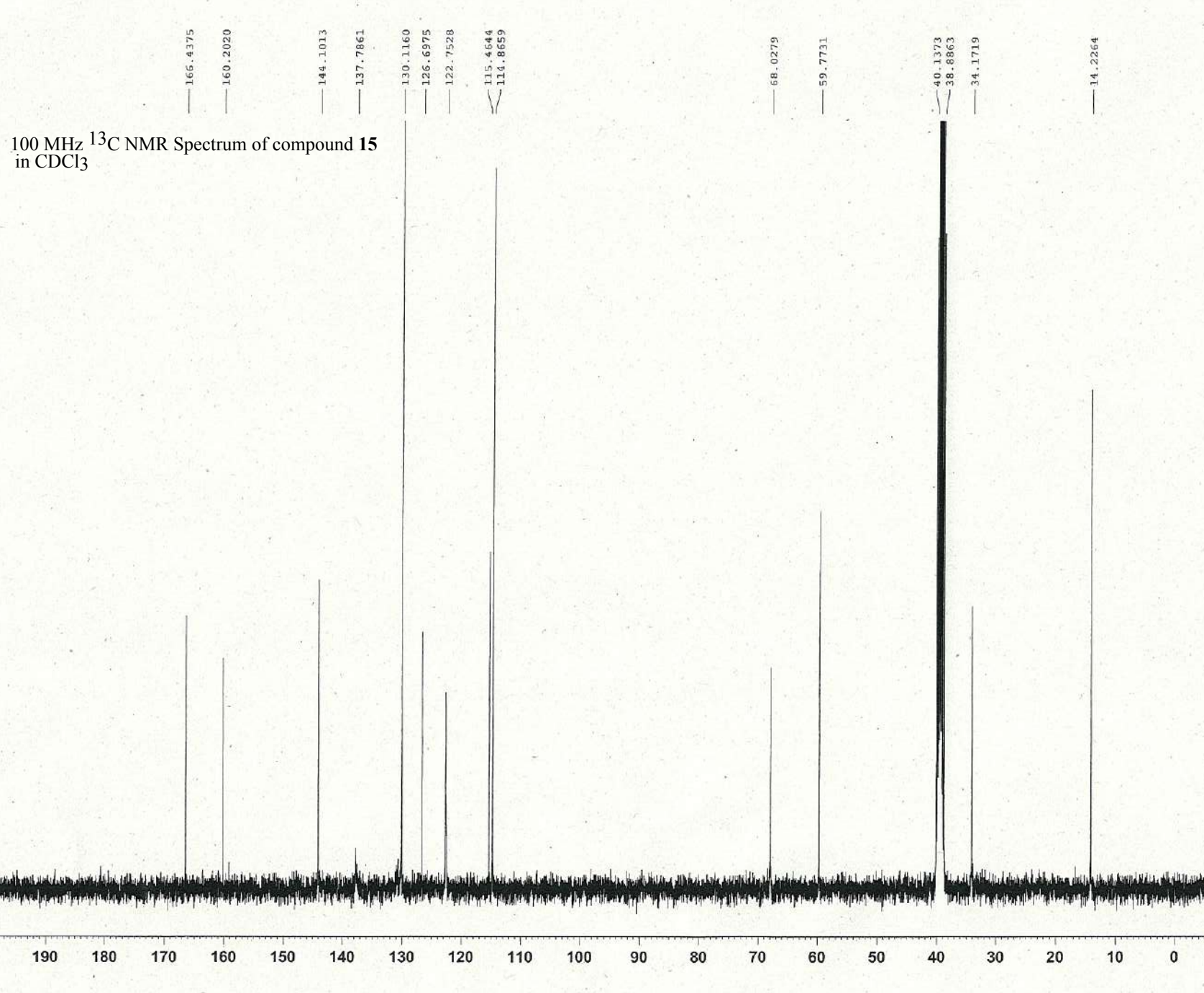
400 MHz ^{1}H NMR Spectrum of compound **14** in $CDCl_3$

100 MHz ^{13}C NMR Spectrum of compound **14** in $CDCl_3$



400 MHz ^{1}H NMR Spectrum of compound **15** in $CDCl_3$

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137.7861
130.1160
126.6975
122.7528
115.4644
114.8659
68.0279
59.7731
40.1373
38.8863
34.1719
14.2264
100 MHz ^{13}C NMR Spectrum of compound **15** in $CDCl_3$
190
180
170
160
150
140
130
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110
100
90
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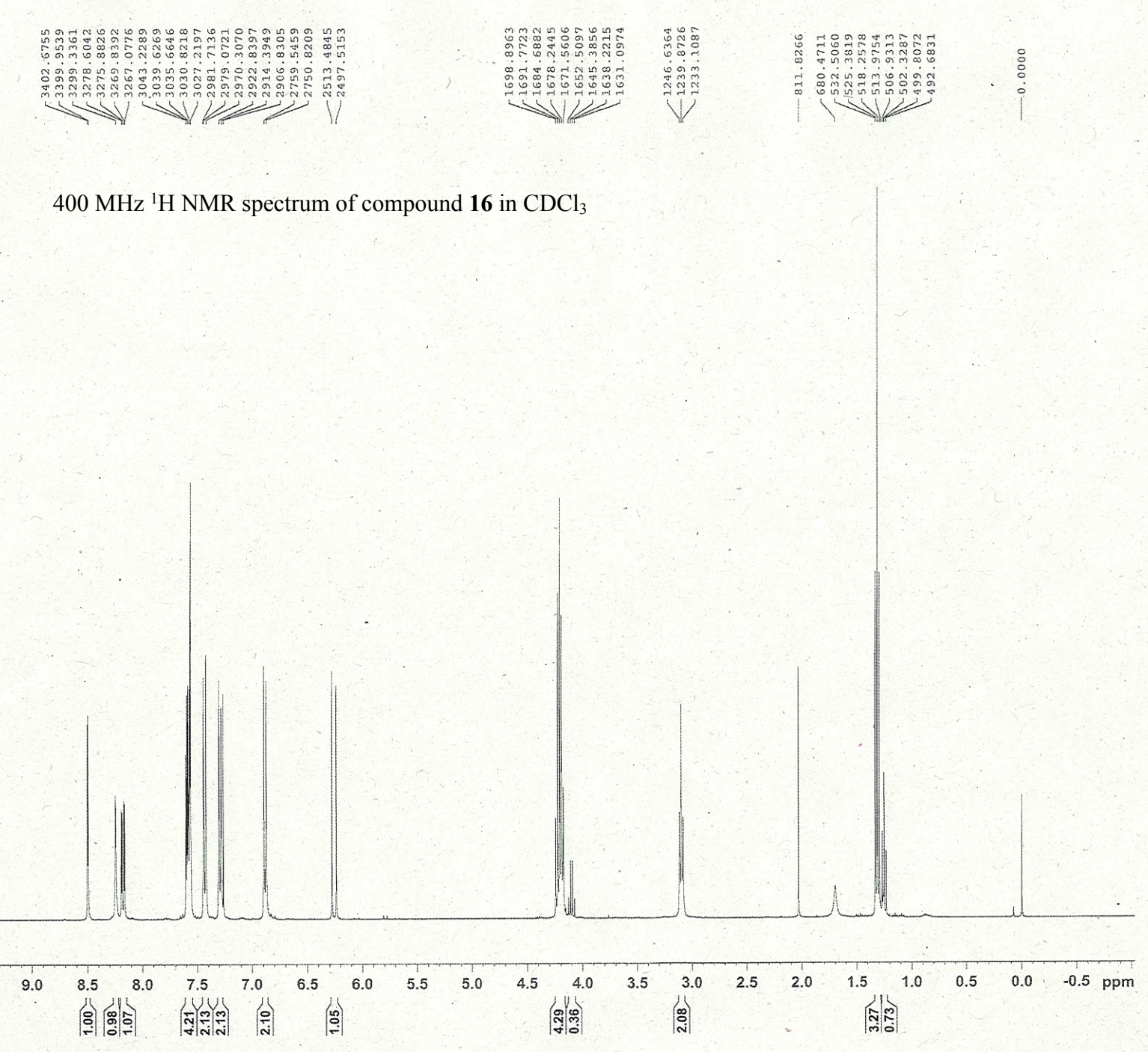
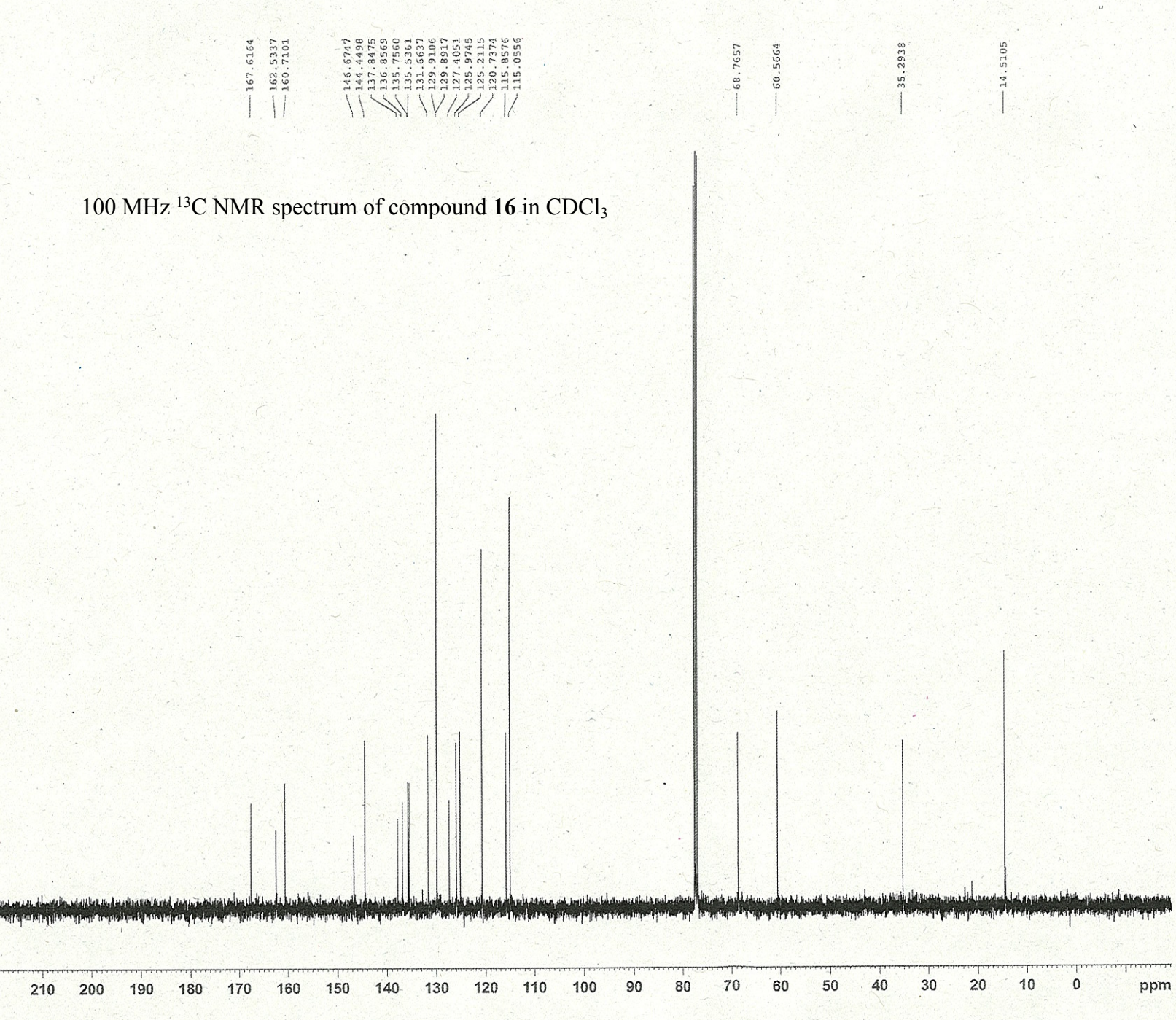


400 MHz ^{1}H NMR spectrum of compound **16** in $CDCl_3$



100 MHz ^{13}C NMR spectrum of compound **16** in $CDCl_3$