# Electronic Supplementary Information (ESI)

# An Iron Carbonyl Approach to the Influenza Neuraminidase Inhibitor Oseltamivir

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**Spectra for the Synthesis of Oseltamivir:**



Also available is a separate ESI file containing all experimental procedures.

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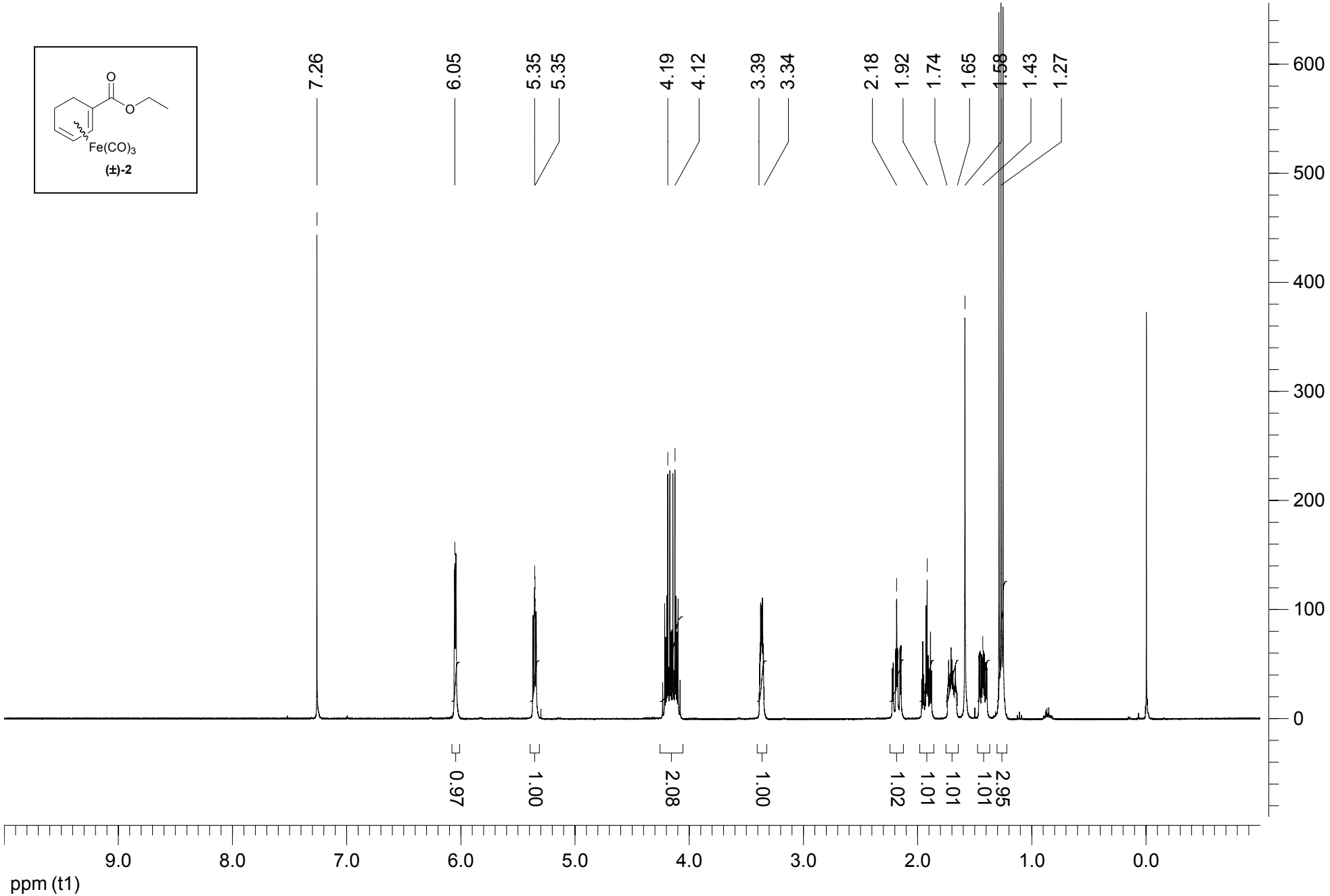
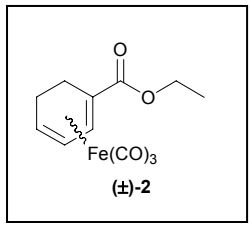
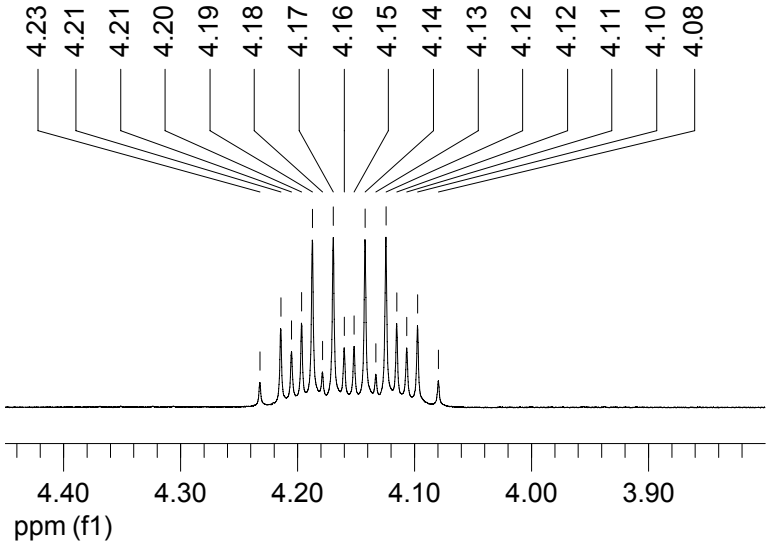
* Residual solvent was removed by high vacuum before further analysis
† The shown racemic sample was purified for characterisation, where as samples of the desired enantiomer were used crude in the next step and therefore not characterized.
‡ The shown racemic sample was purified for characterisation, where as samples of the desired enantiomer were of lower purity and therefore not characterized fully.
§ The signal at 1.8 ppm disappeared with high vacuum and was therefore attributed to H-bonded $H_2O$ in this sample.

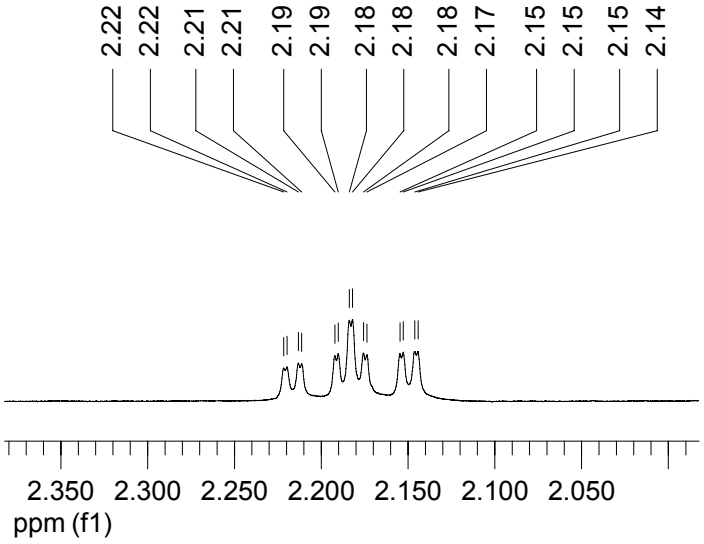
**Tricarbonyl(1-carboethoxycyclohexa-1,3-dienyl)iron ((±)-2): $^1$H NMR (400 MHz, $CDCl_3$)**

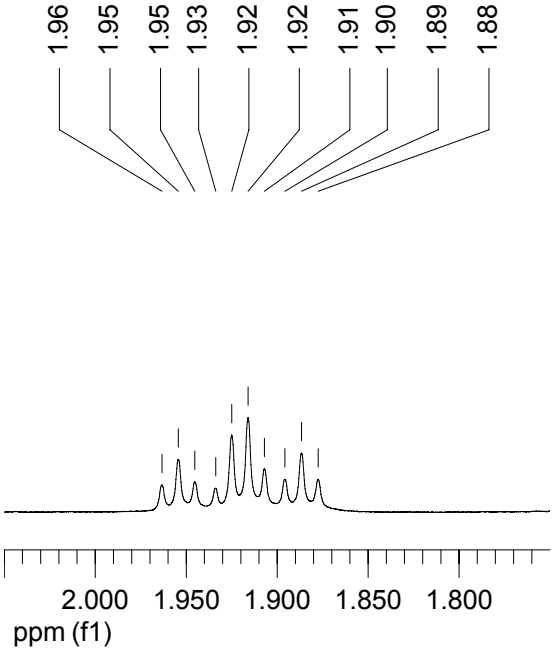


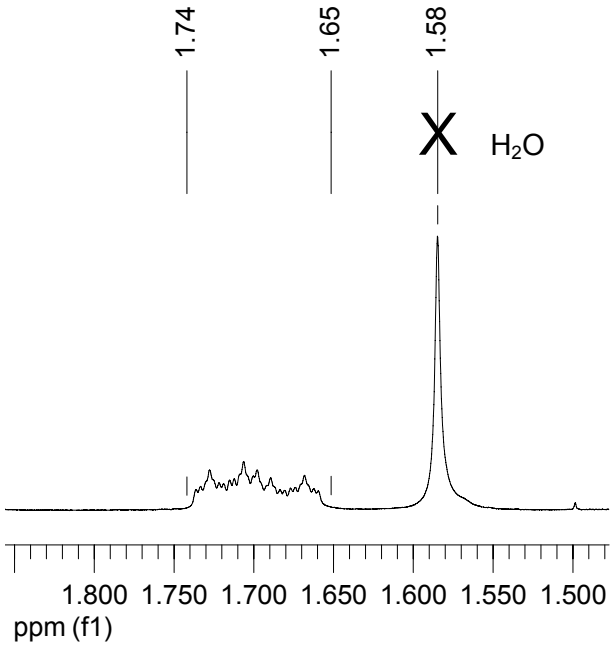
**Tricarbonyl(1-carboethoxycyclohexa-1,3-dienyl)iron ((±)-2): $^1$H NMR (400 MHz, $CDCl_3$)…….cont**

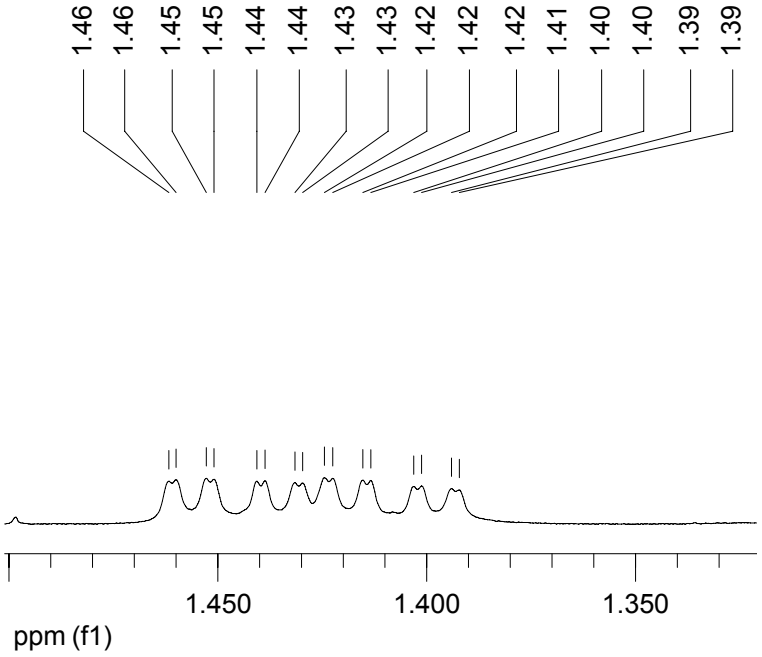


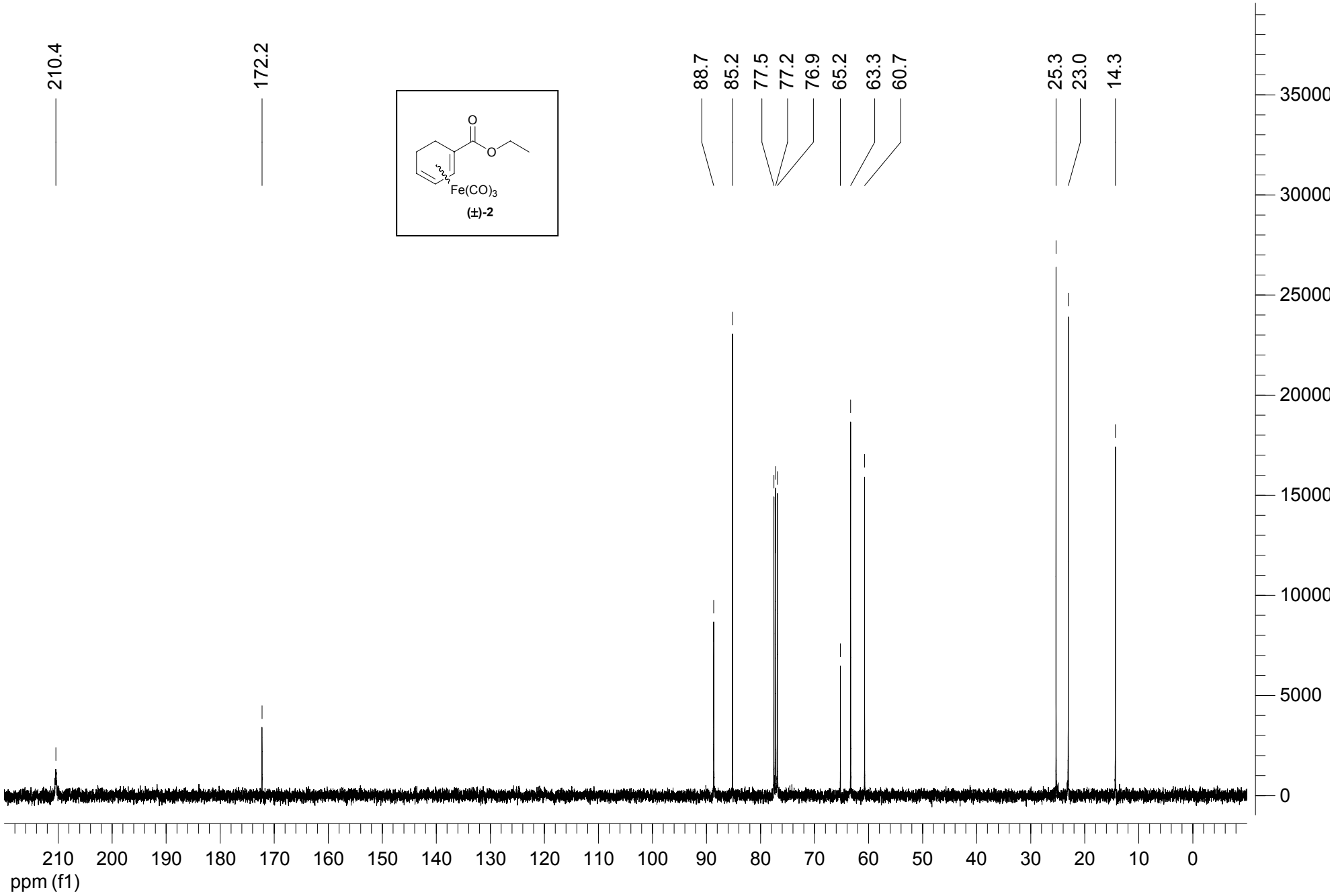



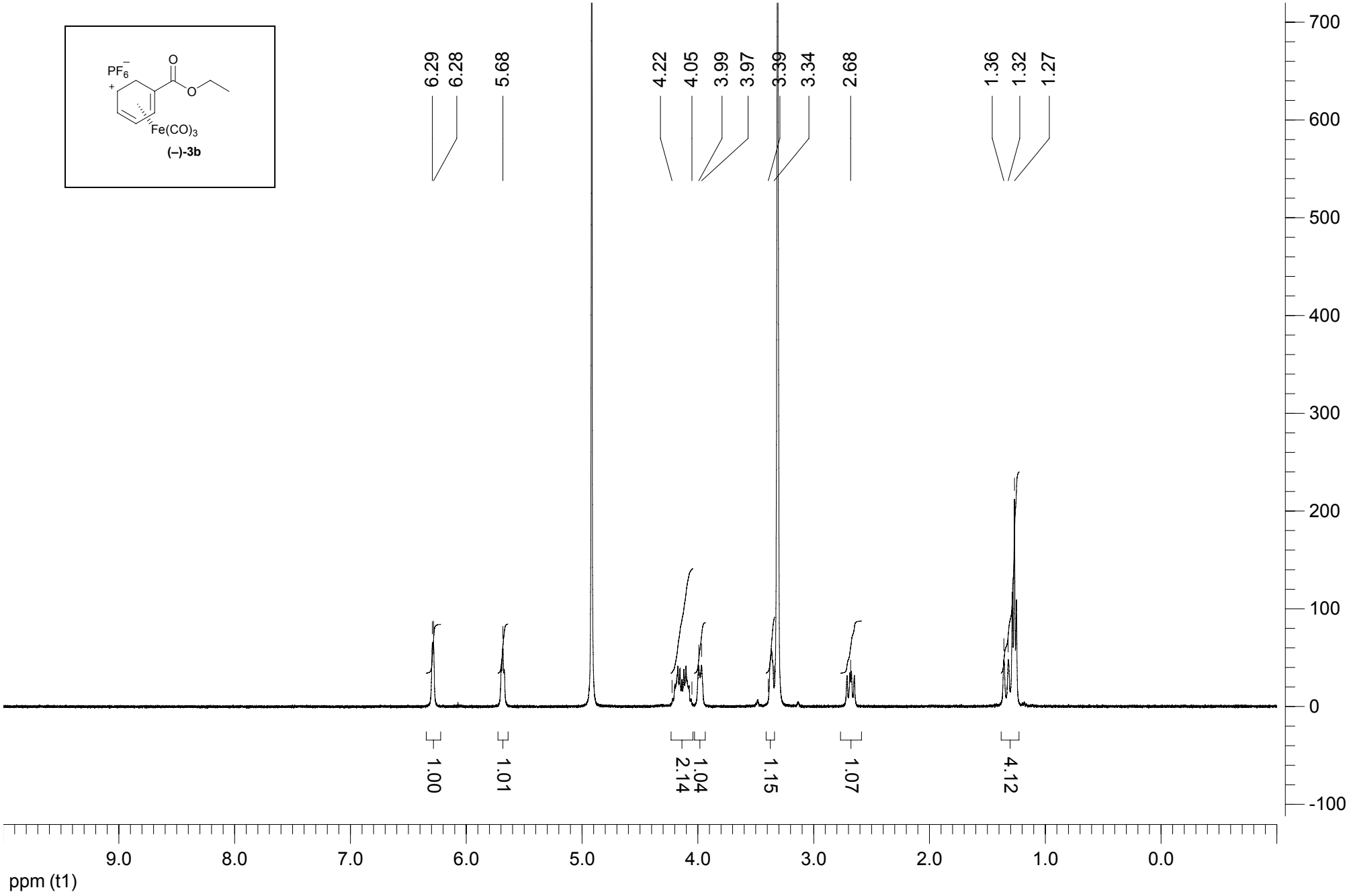



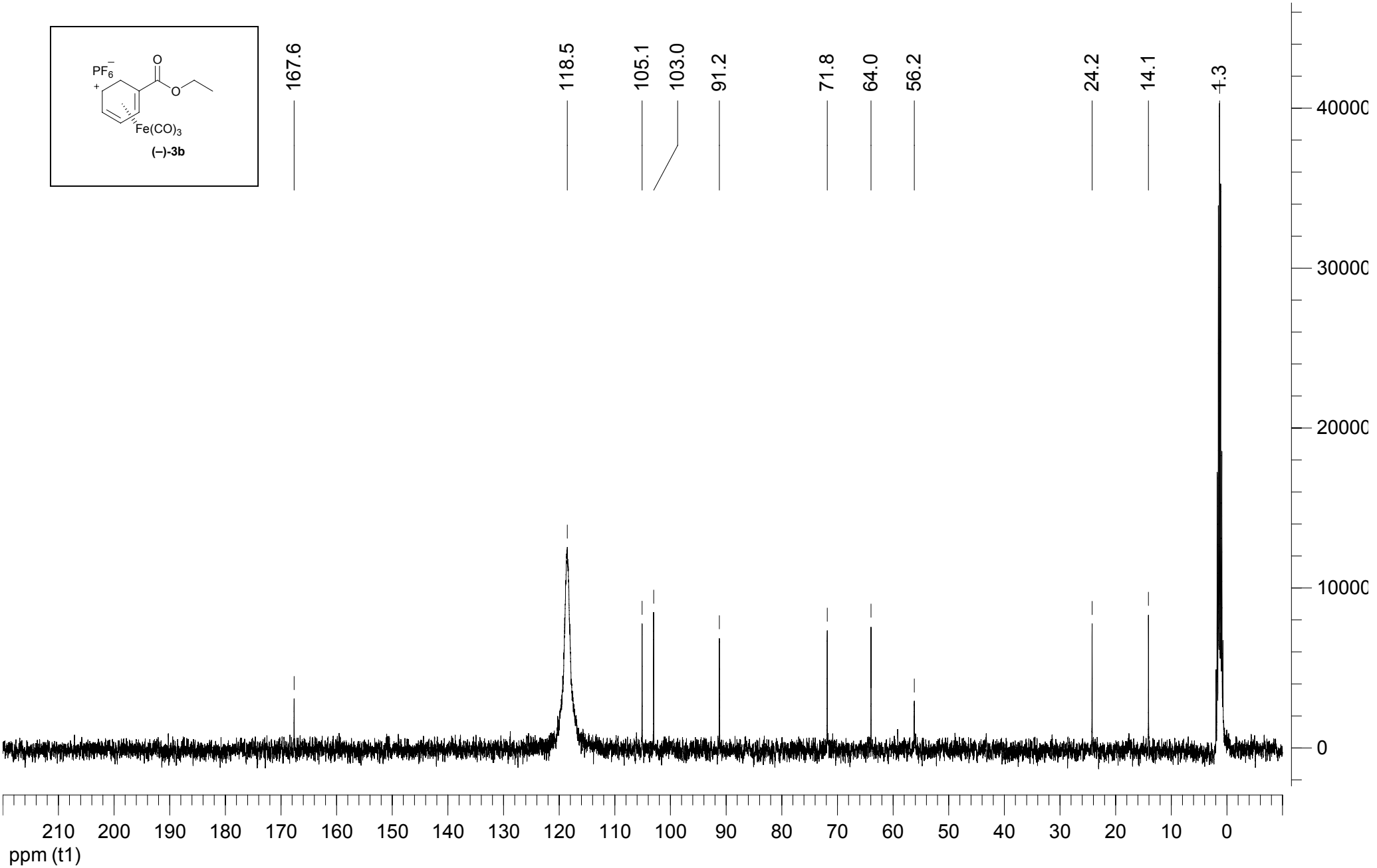
**Tricarbonyl(1-carboethoxycyclohexa-1,3-dienyl)iron ((±)-2) $^{13}$C NMR (100 MHz, $CDCl_3$)**



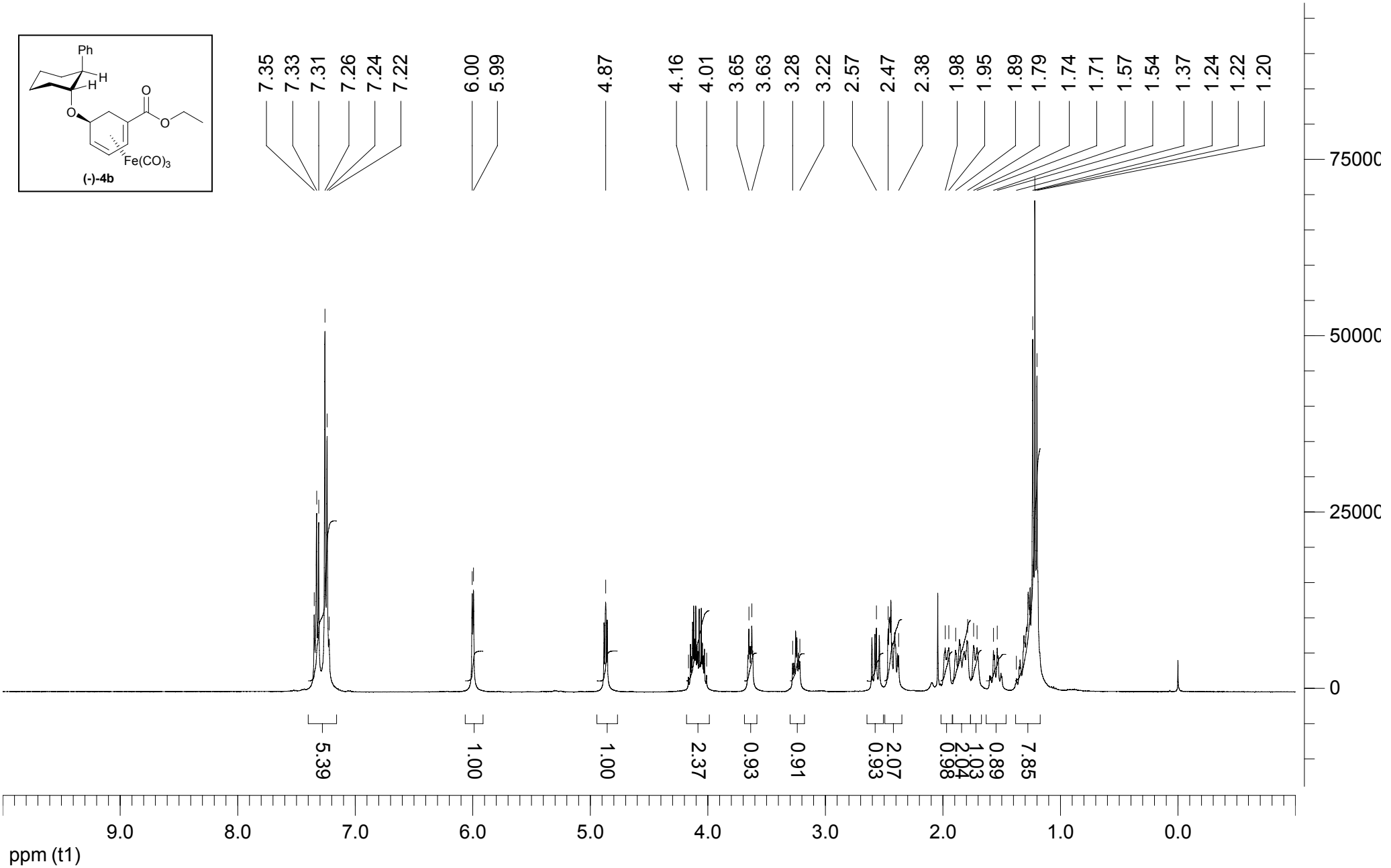
**Tricarbonyl(1-carboethoxycyclohexa-1,3-dienyl)iron hexafluorophosphate ((–)-3b): $^{1}$H NMR (400 MHz, $CD_3OD$)**



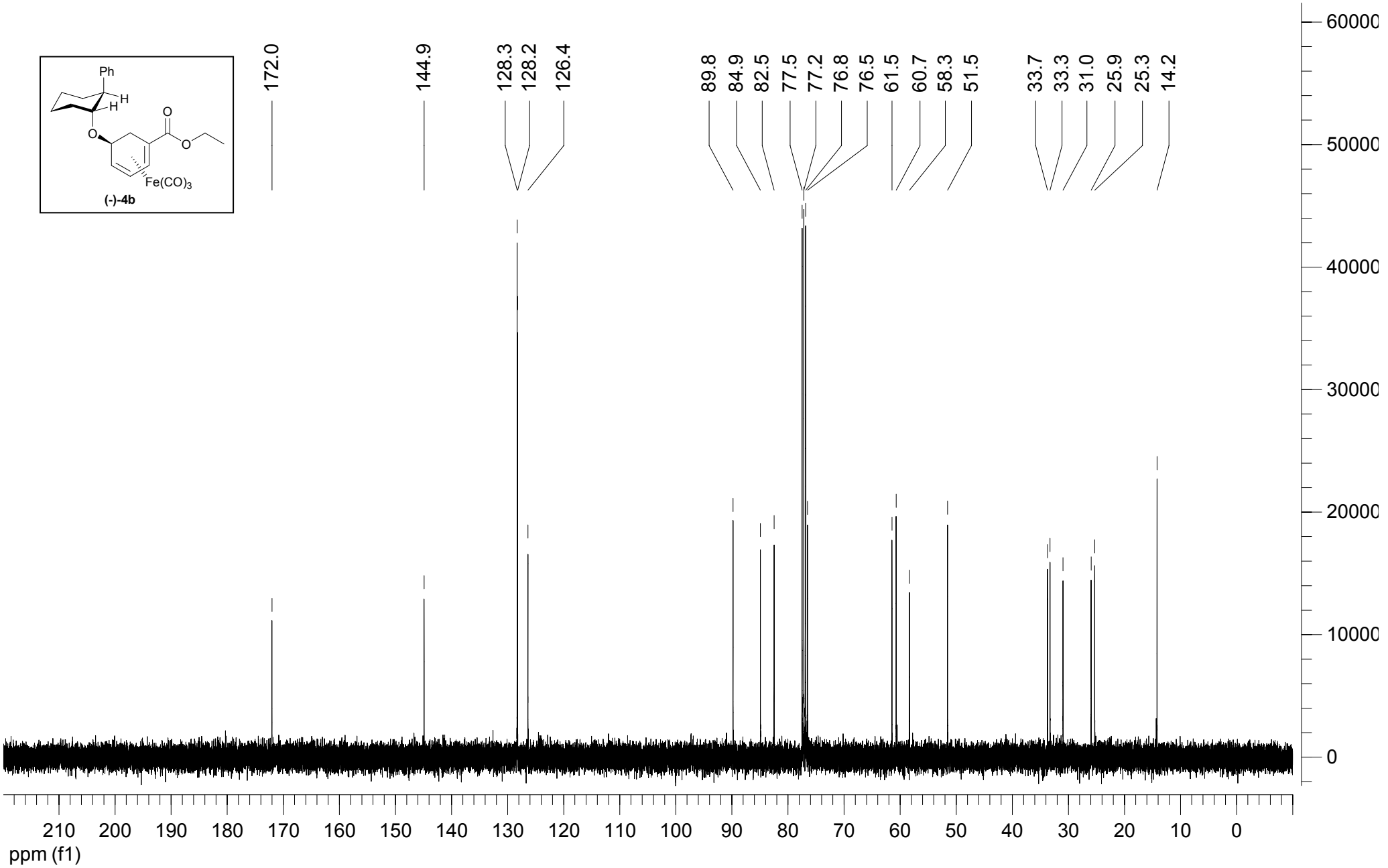
**Tricarbonyl(1-carboethoxycyclohexa-1,3-dienyl)iron hexafluorophosphate ((–)-3b): $^{13}$C NMR (100 MHz, $CD_3CN$)**



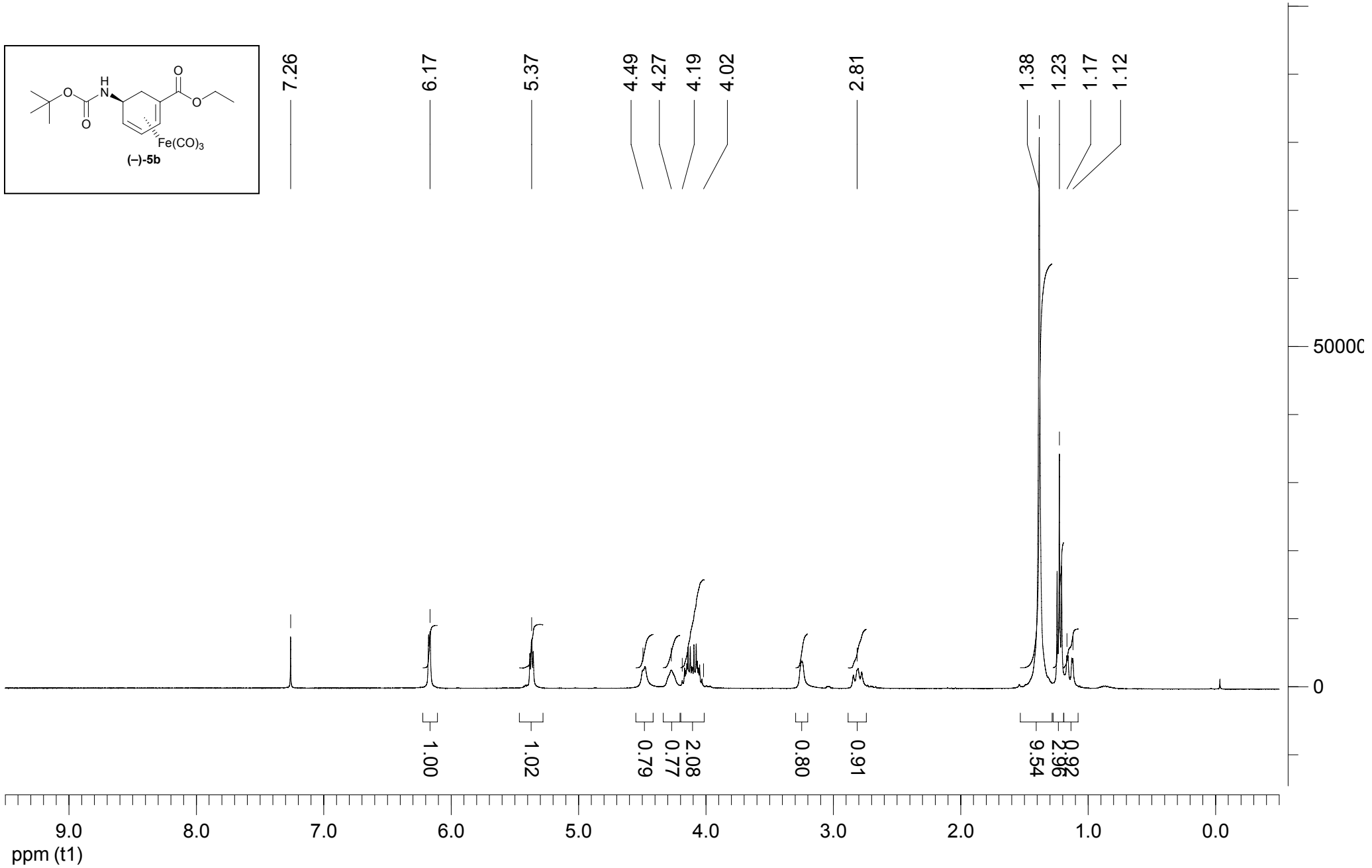
**Tricarbonyl[1-carboethoxy-5-[[(*1R,2S*)-*trans*-2-phenylcyclohexyl]oxy]cyclohexa-1,3-diene]iron ((–)-4b): $^{1}$H NMR (400 MHz, $CDCl_3$)***



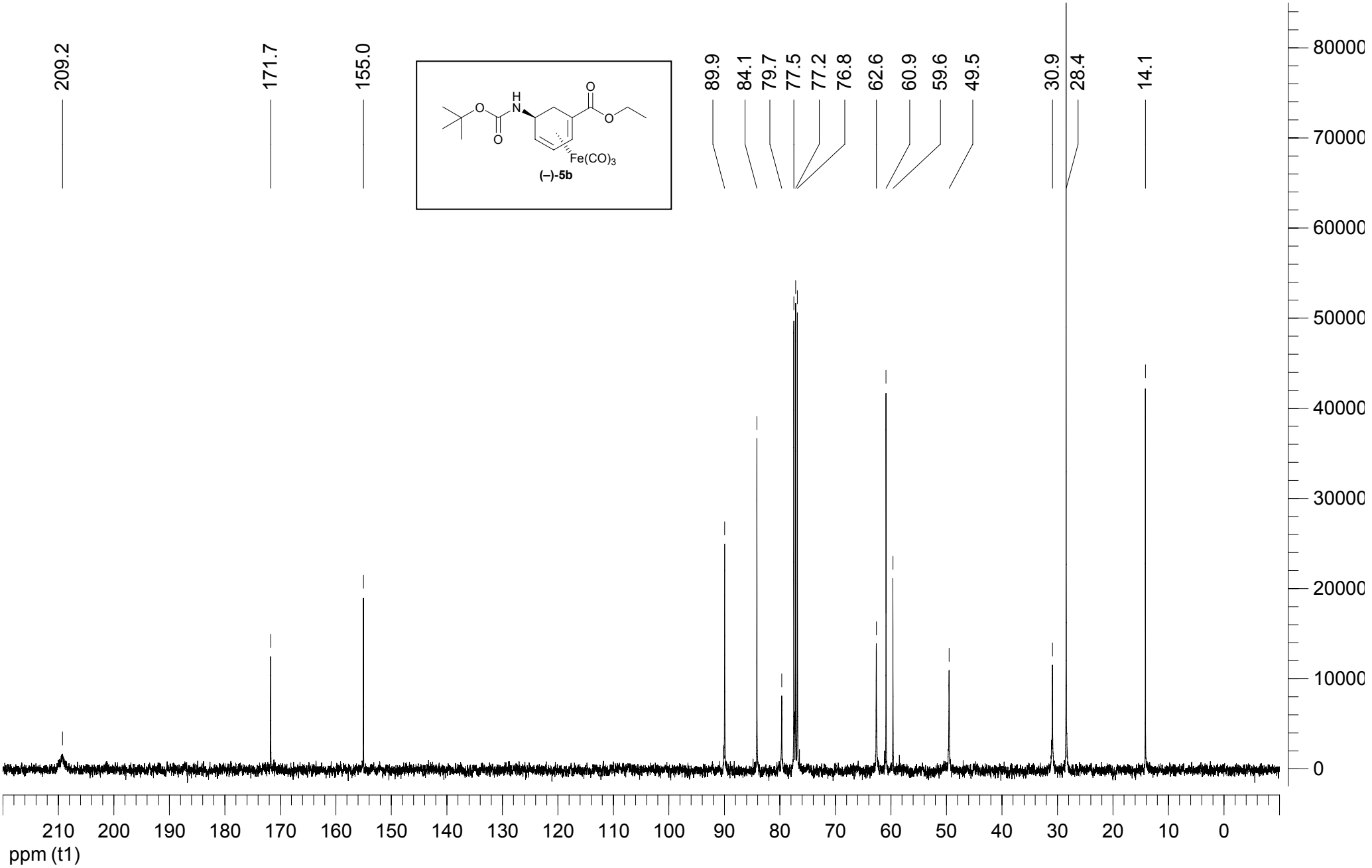
**Tricarbonyl[1-carboethoxy-5-[[(*1R,2S*)-*trans*-2-phenylcyclohexyl]oxy]cyclohexa-1,3-diene]iron ((–)-4b): $^{13}$C NMR (100 MHz, $CDCl_3$)**



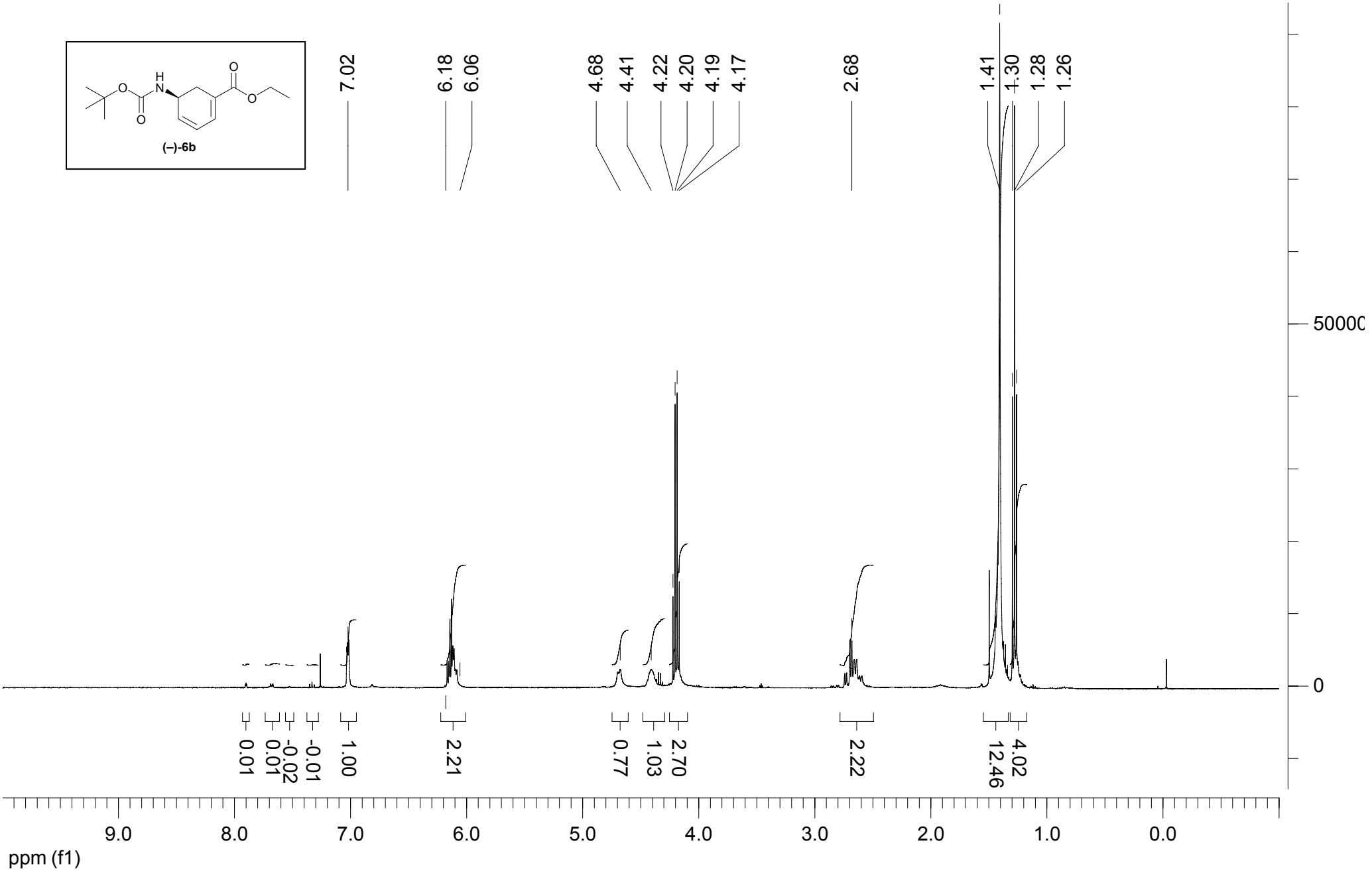
**Tricarbonyl[5-(*tert*-butoxycarbonylamino)-1-carboethoxycyclohexa-1,3-diene]iron ((–)-(5*S*)-5b): $^1$H NMR (400 MHz, $CDCl_3$)**



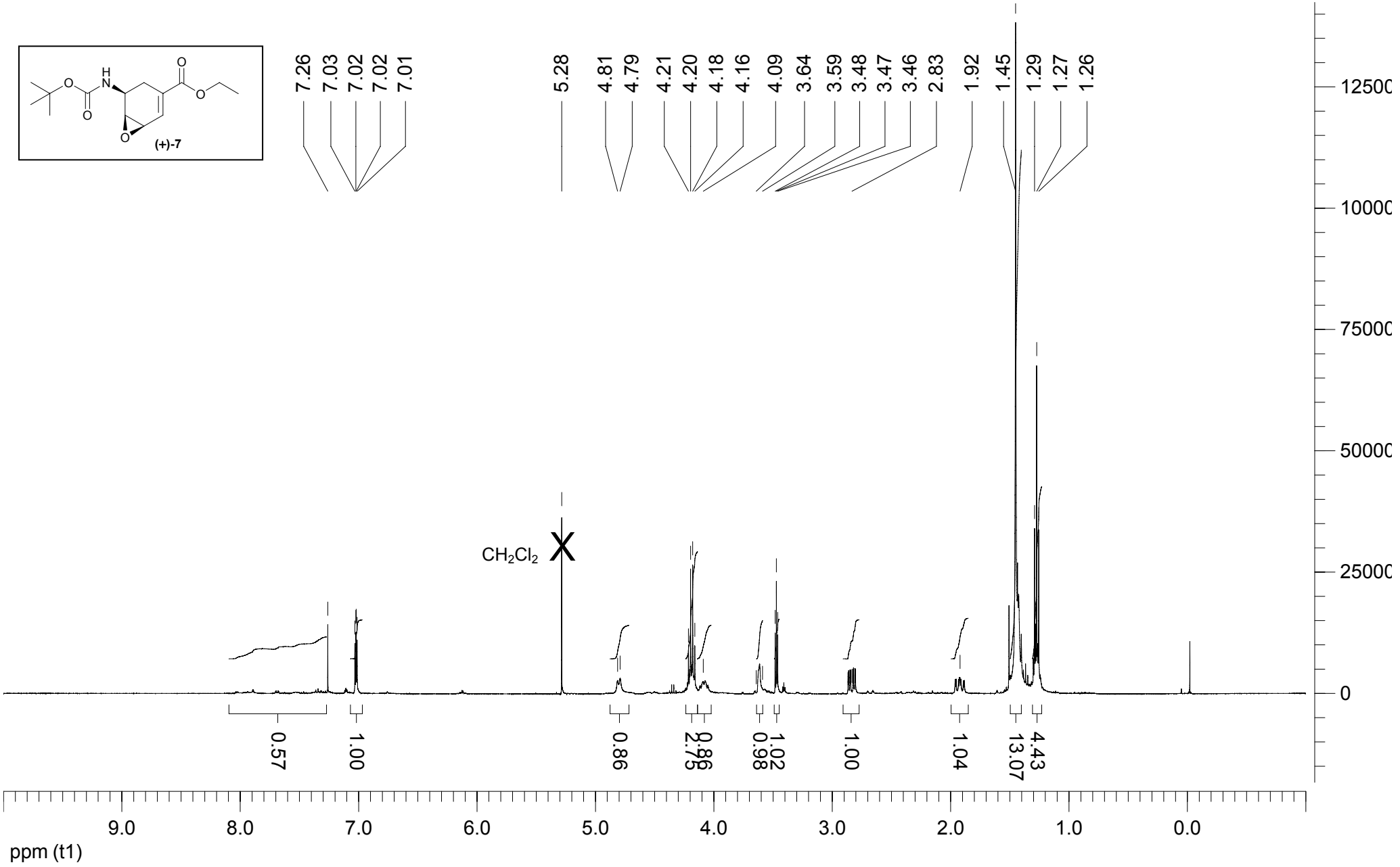
**Tricarbonyl[5-(*tert*-butoxycarbonylamino)-1-carboethoxycyclohexa-1,3-diene]iron ((–)-(5*S*)-5b): $^{13}$C NMR (100 MHz, $CDCl_3$)**



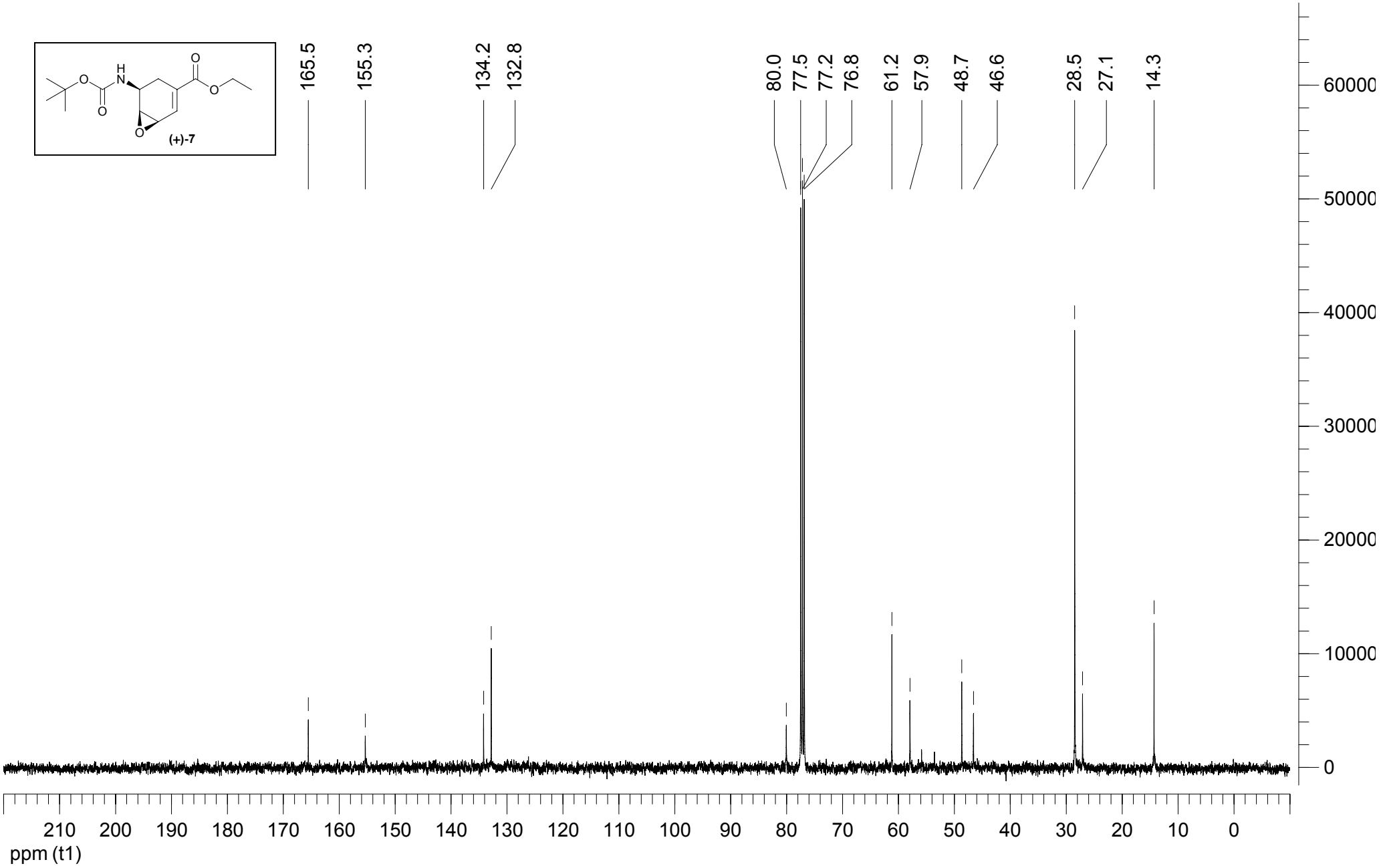
**Ethyl 5-(*tert*-Butoxycarbonylamino)-cyclohexa-1,3-diene-1-carboxylate ((–)-(5*S*)-6b): Crude $^{1}$H NMR (400 MHz, $CDCl_3$)**



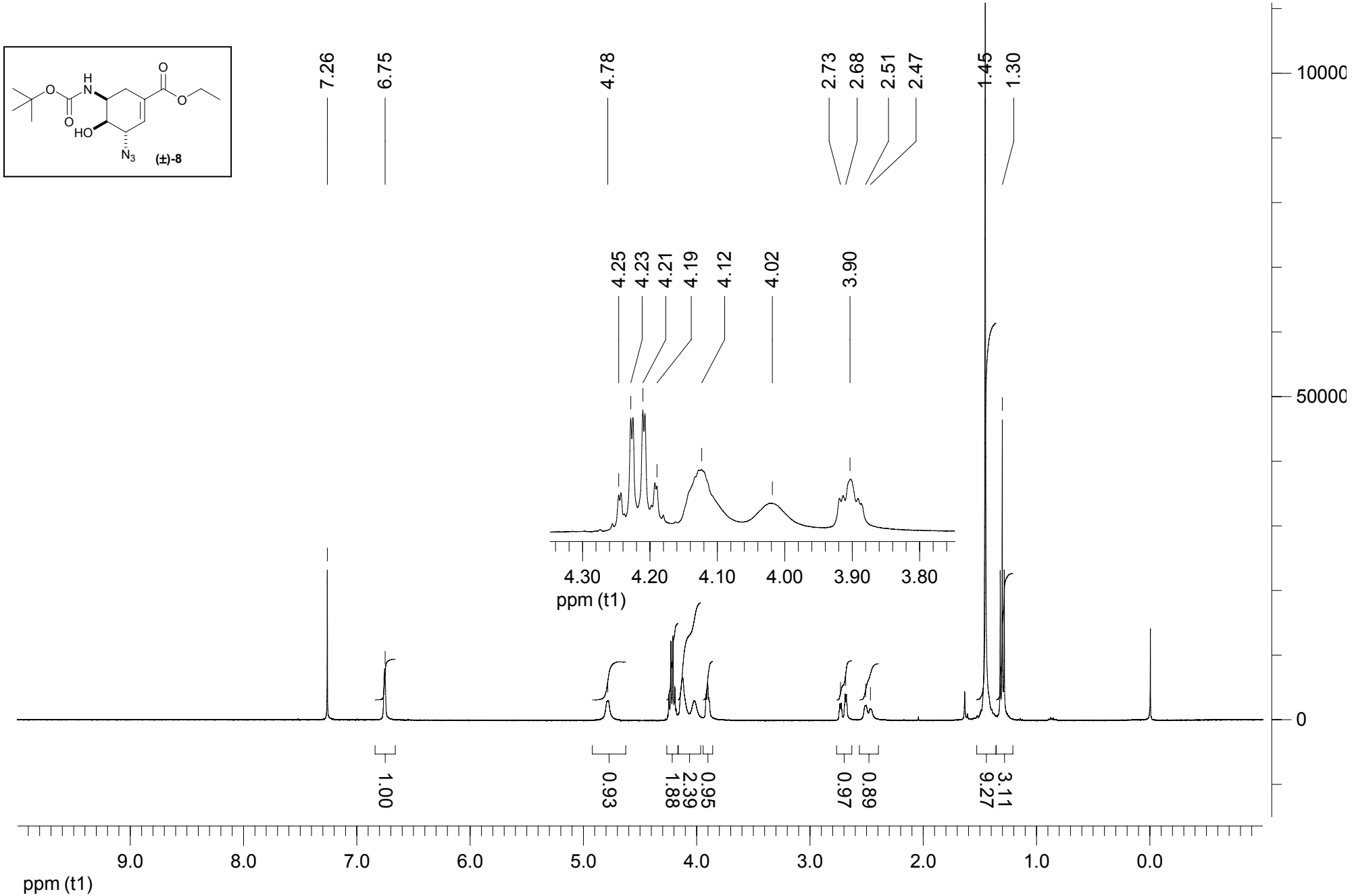
**Ethyl 5-(*tert*-Butoxycarbonylamino)-3,4-epoxy-cyclohexa-1-ene-1-carboxylate ((+)-(*3R,4S,5S*)-7): Crude $^1$H NMR (400 MHz, $CDCl_3$)**



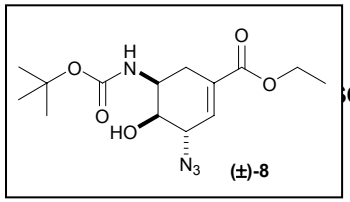
**Ethyl 5-(*tert*-Butoxycarbonylamino)-3,4-epoxy-cyclohexa-1-ene-1-carboxylate ((+)-(*3R,4S,5S*)-7): Crude $^{13}$C NMR (100 MHz, $CDCl_3$)**



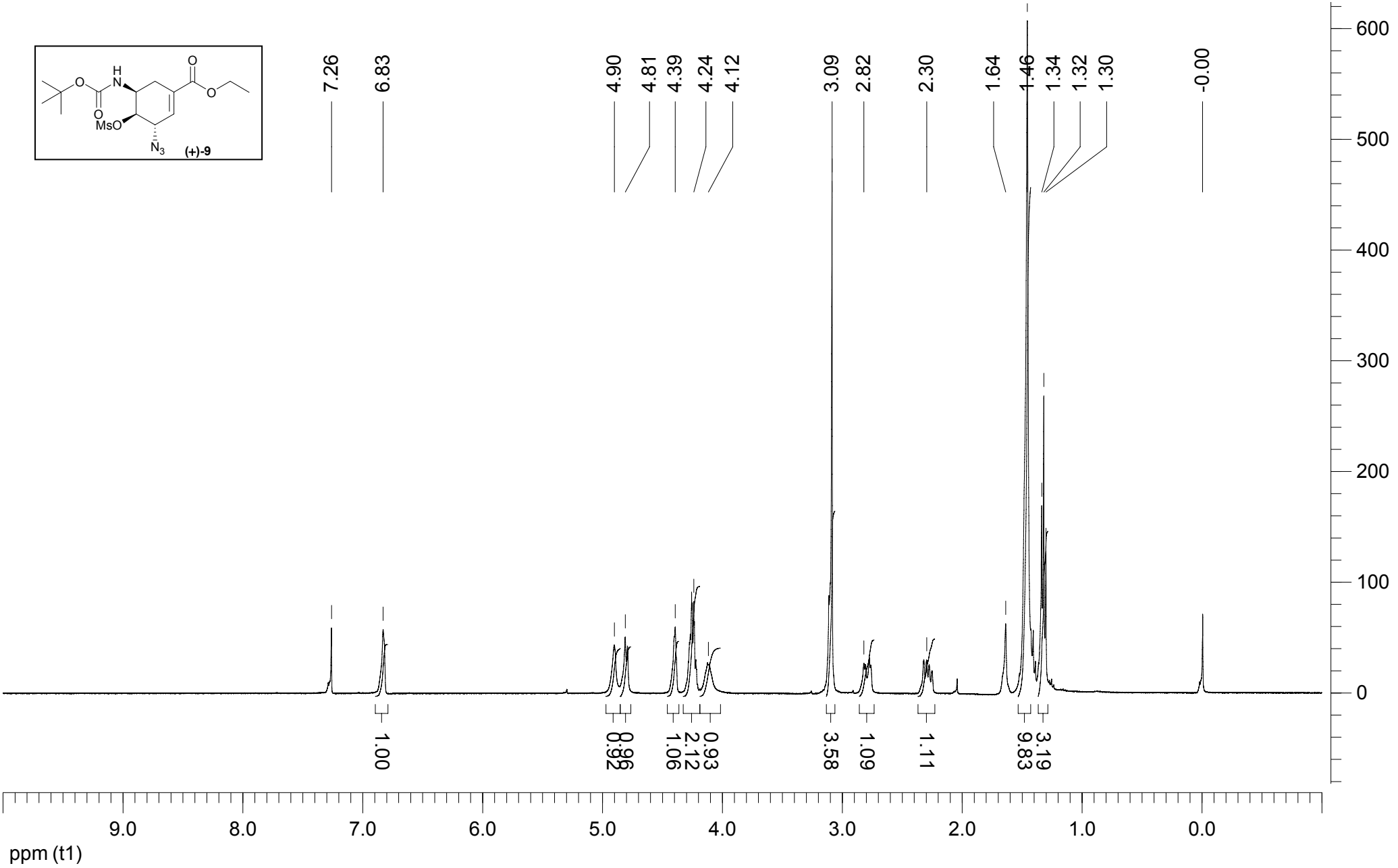
**Ethyl 3-Azido-5-(*tert*-butoxycarbonylamino)-4-hydroxy-cyclohexa-1-ene-1-carboxylate ((±)-8):† $^1$H NMR (400 MHz, $CDCl_3$)**



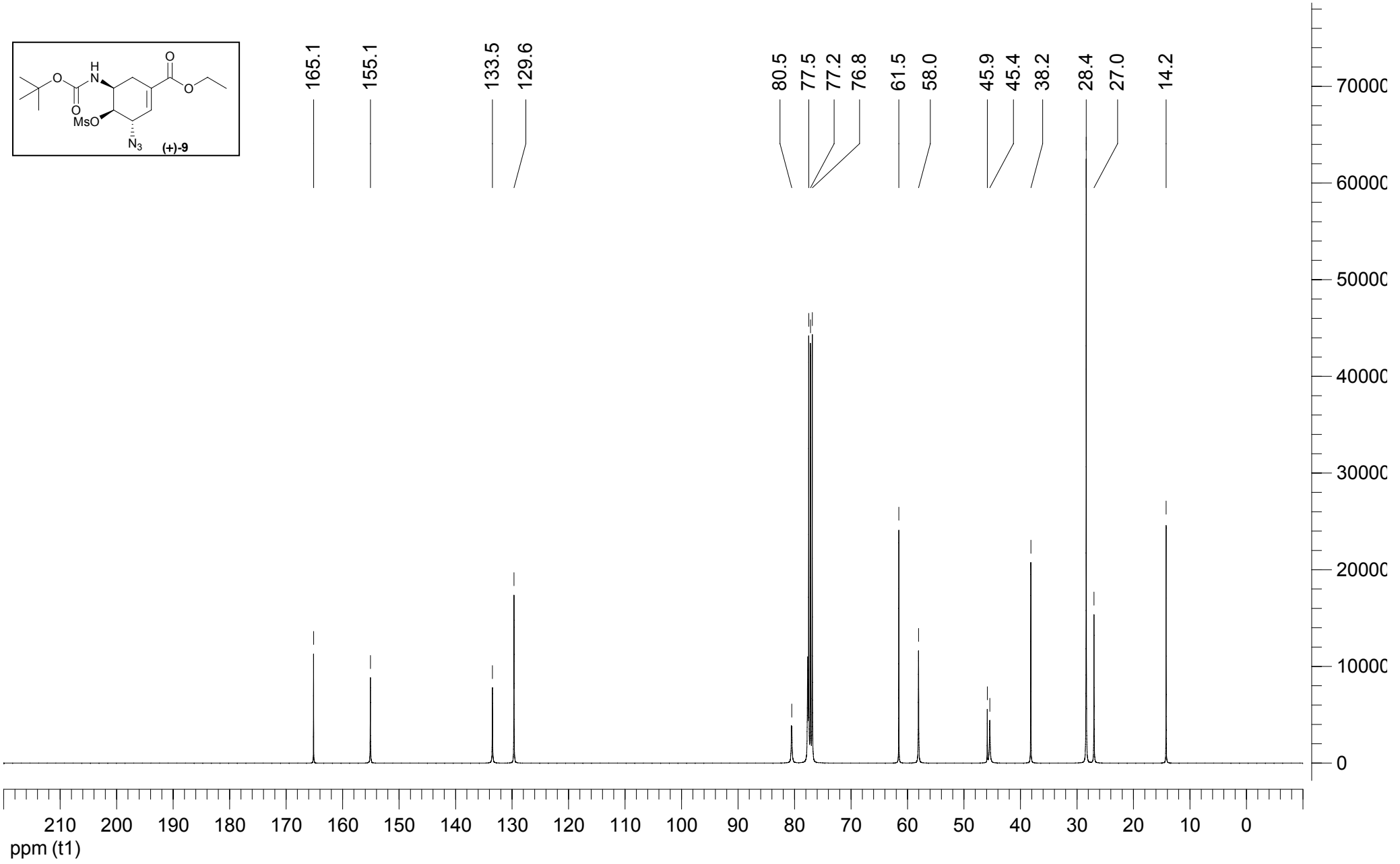
**Ethyl 3-Azido-5-(*tert*-butoxycarbonylamino)-4-hydroxy-cyclohexa-1-ene-1-carboxylate ((±)-8):† $^{13}$C NMR (100 MHz, $CDCl_3$)**



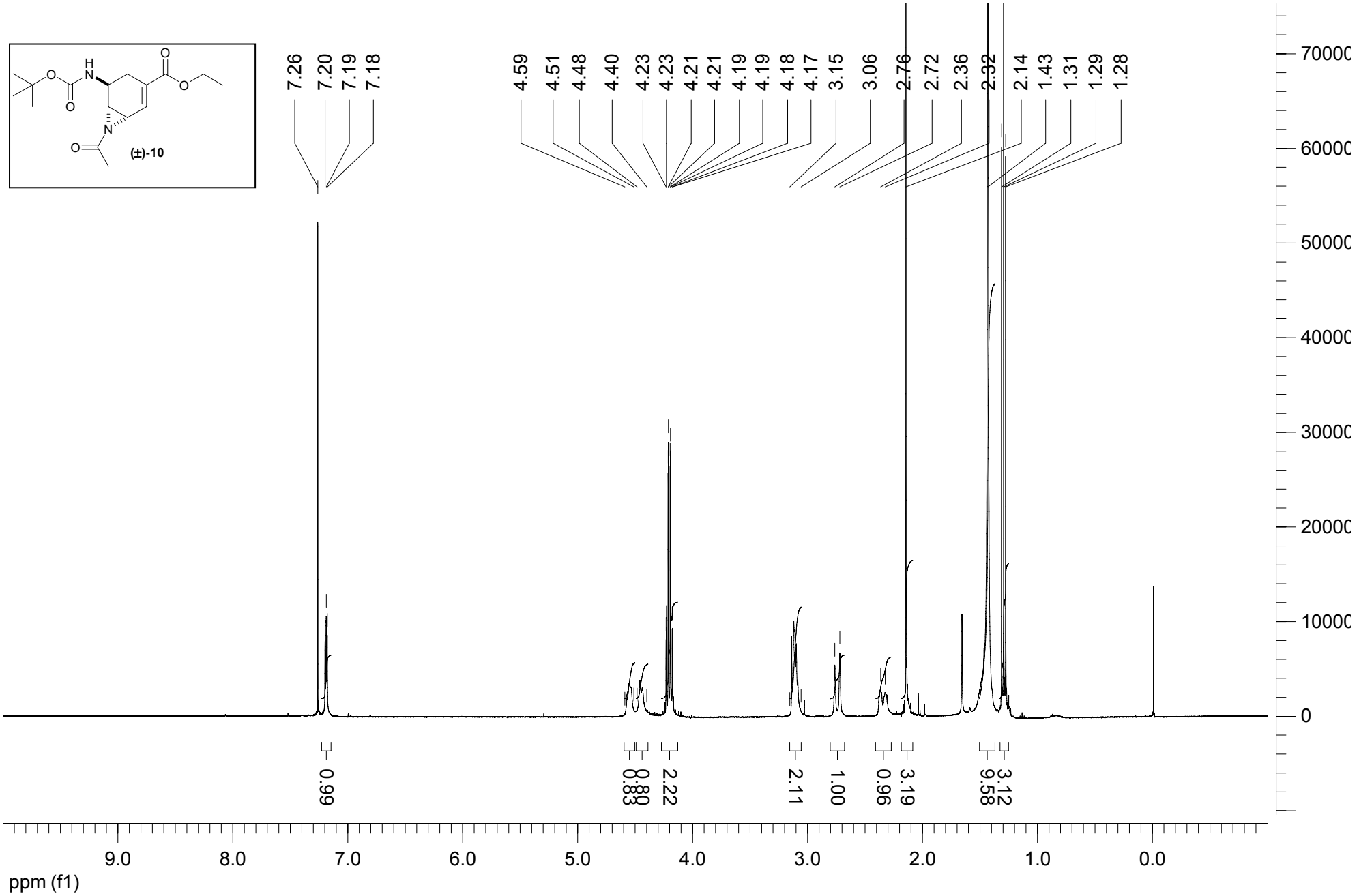
**Ethyl 3-Azido-5-(*tert*-butoxycarbonylamino)-4-[(methylsulfonyl)oxy]-cyclohexa-1-ene-1-carboxylate ((+)-(*3S,4S,5S*)-9): $^1$H NMR (400 MHz, $CDCl_3$)***



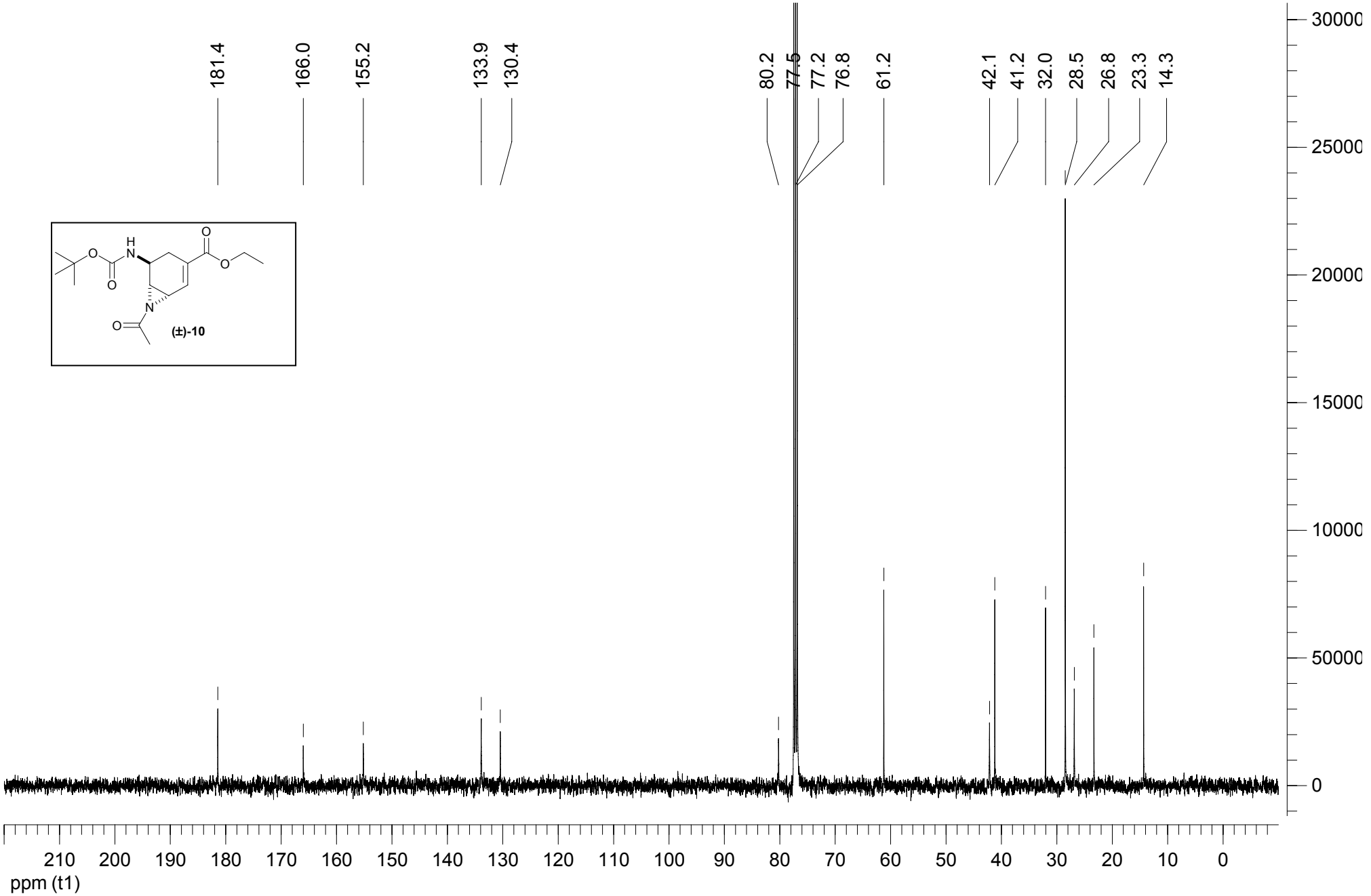
**Ethyl 3-Azido-5-(*tert*-butoxycarbonylamino)-4-[(methylsulfonyl)oxy]-cyclohexa-1-ene-1-carboxylate ((+)-(*3S,4S,5S*)-9): $^{13}$C NMR (100 MHz, $CDCl_3$)**



**Ethyl 3-(*N*-Acetylaziridinyl)-5-(*tert*-butoxycarbonylamino)-cyclohexa-1-ene-1-carboxylate ((±)-10):‡ $^1$H NMR (400 MHz, $CDCl_3$)**

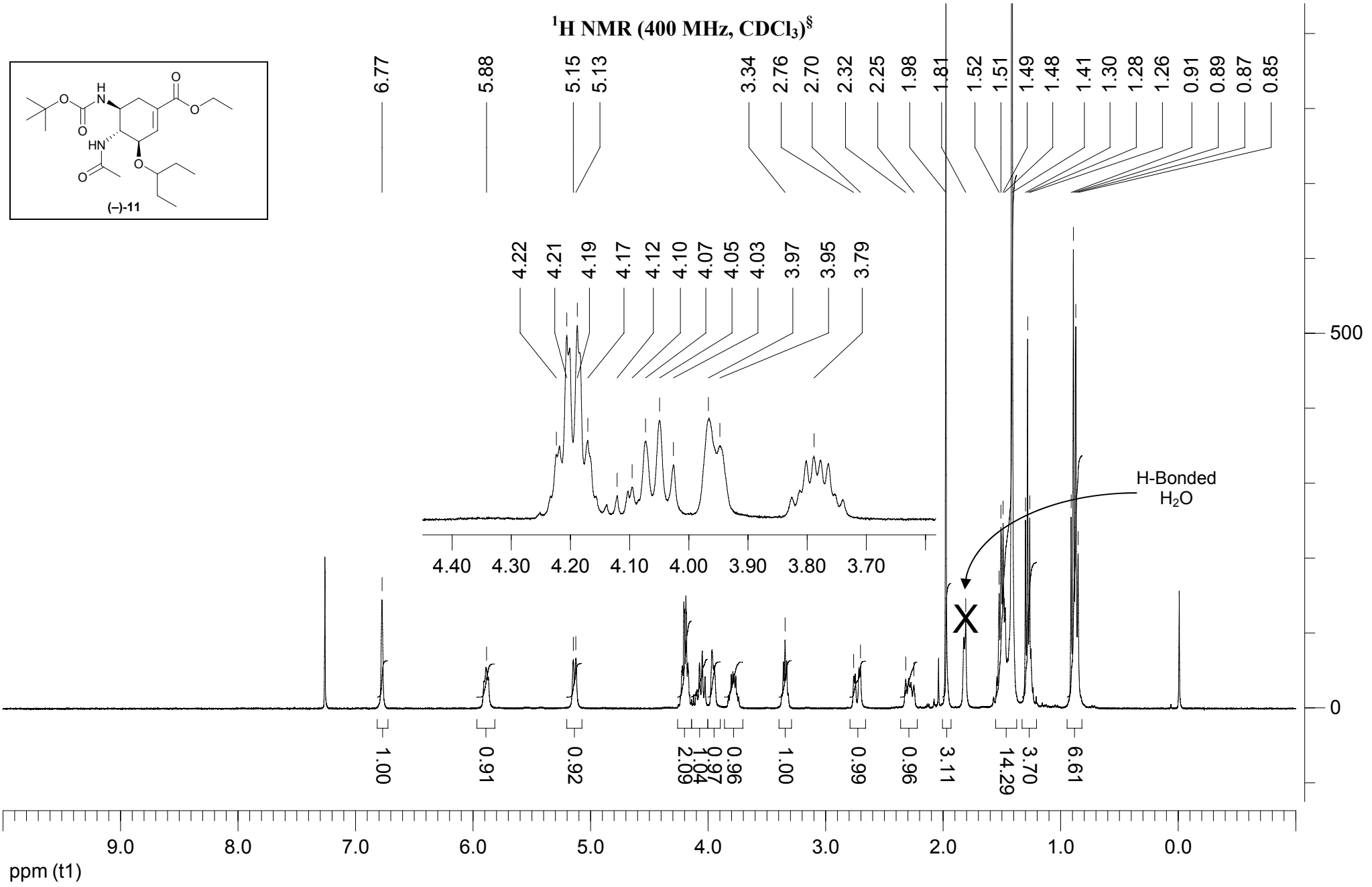


**Ethyl 3-(*N*-Acetylaziridinyl)-5-(*tert*-butoxycarbonylamino)-cyclohexa-1-ene-1-carboxylate ((±)-10):‡ $^{13}$H NMR (100 MHz, $CDCl_3$)**



**Ethyl 4-Acetylamino-5-(*tert*-butoxycarbonylamino)-3-(1-ethylpropoxy)-cyclohexa-1-ene-1-carboxylate ((–)-(*3R,4R,5S*)-11):**

**$^1$H NMR (400 MHz, $CDCl_3$)[§]**



**Ethyl 4-Acetylamino-5-(*tert*-butoxycarbonylamino)-3-(1-ethylpropoxy)-cyclohexa-1-ene-1-carboxylate ((–)-(*3R,4R,5S*)-11):**

**$^{13}$C NMR (100 MHz, $CDCl_3$)**