

Supporting Information

Electrophilic C–H Borylation and Related Reactions of B–H Boron Cations

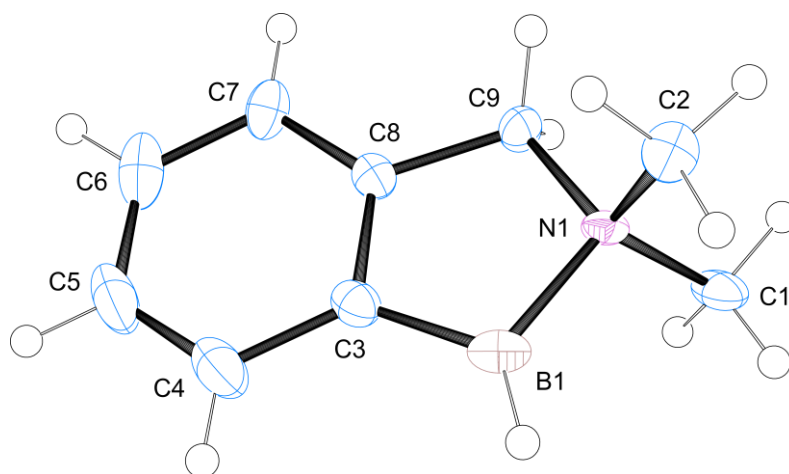
Aleksandrs Prokofjevs, Janis Jermaks, Alina Borovika, Jeff W. Kampf, and Edwin Vedejs*

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Preparation and X-Ray Crystallography Details of **6** ($[\text{HCB}_{11}\text{Cl}_{11}]^-$ Salt)

This procedure describes preparation of crystalline $[\textit{closo}\text{-HCB}_{11}\text{Cl}_{11}]^-$ salt of borenium **6** for the X-ray crystallographic study. Every possible effort was made to protect the reaction mixture from exposure to air and moisture. The reaction was performed under N_2 atmosphere in a glovebox. Disposable glassware flame-dried at the glass softening temperature was used. Toluene was distilled from CaH_2 , and subsequently dried with freshly activated molecular sieves in the glovebox. Hexanes were dried by passing through a column of activated alumina, followed by storing over freshly activated molecular sieves in the glovebox. In a dry 4 mL scintillation vial a mixture of solid $\text{Ph}_3\text{C}[\textit{closo}\text{-HCB}_{11}\text{Cl}_{11}]$ (95.0 mg, 0.124 mmol) and amine borane **37** (18.2 mg, 0.124 mmol) was layered with 1 mL of dry PhMe at rt. No substantial exotherm was observed, potentially due to the small scale of the reaction. The resulting two-layer mixture was stirred at rt for ca. 10-20 min, and the top layer containing Ph_3CH byproduct was removed and discarded. The bottom oily layer was washed with 2-3 portions of PhMe (~ 1mL), and then triturated with hexanes, inducing crystallization. X-ray quality crystals were obtained by layering CH_2Cl_2 solution of the product with hexanes at rt. X-ray crystallographic study confirmed the proposed B–H borenium structure of **6**.



A crystal of dimensions 0.23 x 0.19 x 0.19 mm was mounted on a Bruker SMART APEX CCD-based X-ray diffractometer equipped with a low temperature device and fine focus Mo-target X-ray tube ($\lambda = 0.71073 \text{ \AA}$) operated at 1500 W power (50 kV, 30 mA). The X-ray intensities were measured at 85(1) K; the detector was placed at a distance 5.055 cm from the crystal. A total of 5190 frames were collected with a scan width of 0.5° in θ and 0.45° in ϕ with an exposure time of 10 s/frame. The integration of the data yielded a total of 151618 reflections to a maximum 2θ value of 72.76° of which 6882 were independent and 5395 were greater than $2\sigma(I)$. The final cell constants (Table 1) were based

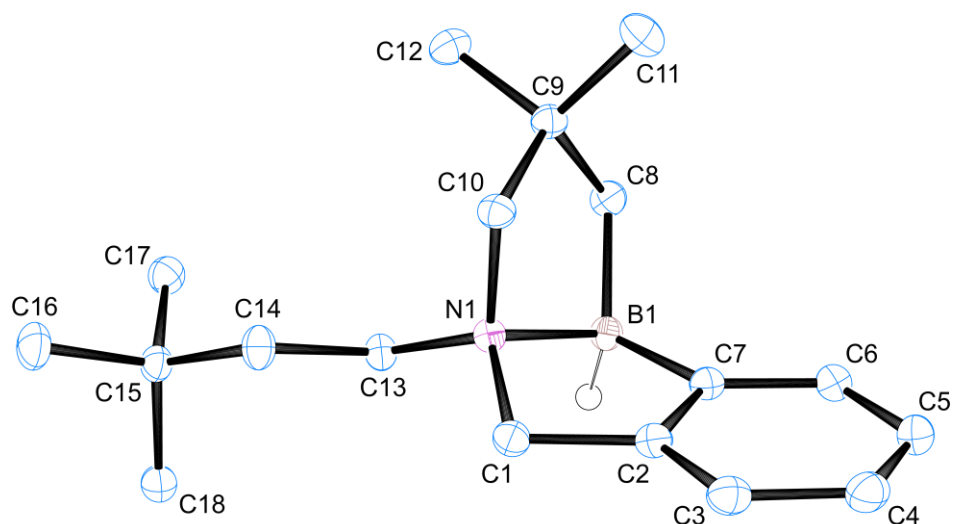
on the xyz centroids of 9701 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection; the data were processed with SADABS and corrected for absorption. The structure was solved and refined with the Bruker SHELXTL (version 2008/4) software package, using the space group Pbam with $Z = 4$ for the formula $C_{10}H_{14}B_{12}NCl_{11}$. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in a mix of idealized and refined positions. Both the borolidine cation and carba-closo-dodecaborate anion lie on mirror planes in the crystal lattice. The borolidine cation is disordered. Full matrix least-squares refinement based on F^2 converged at $R1 = 0.0398$ and $wR2 = 0.0923$ [based on $I > 2\sigma(I)$], $R1 = 0.0570$ and $wR2 = 0.1005$ for all data. Additional details are given as Supporting Information in a CIF file.

Sheldrick, G.M. SHELXTL, v. 2008/4; Bruker Analytical X-ray, Madison, WI, 2008.

Saint Plus, v. 7.60A, Bruker Analytical X-ray, Madison, WI, 2009.

Sheldrick, G.M. SADABS, v. 2008/1. Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen: Gottingen, Germany, 2008.

X-Ray Crystallography Details of **20**



Colorless plates of **20** were grown from a *n*-heptane solution at 23 °C. A crystal of dimensions 0.26x0.16x0.12 mm was mounted on a Bruker SMART APEX-I CCD-based X-ray diffractometer equipped with a low temperature device and fine focus Mo-target X-ray tube ($\lambda = 0.71073$ Å) operated at 1500 W power (50 kV, 30 mA). The X-ray intensities were measured at 85(1) K; the detector was placed at a distance 5.070 cm from the crystal. A total of 3615 frames were collected with a scan width

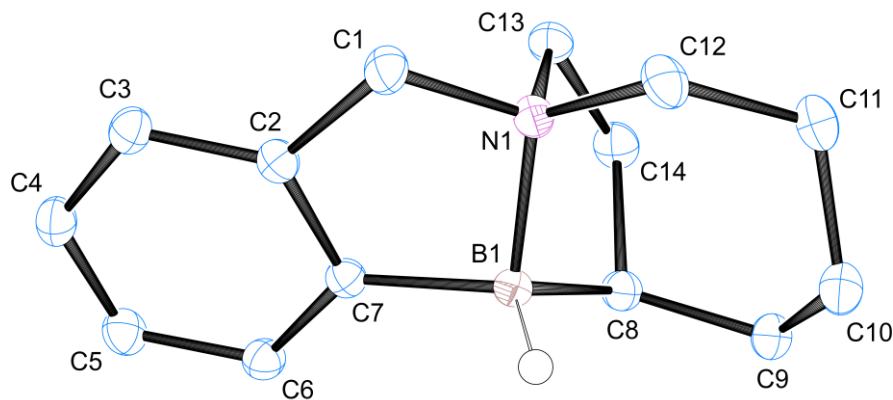
of 0.5° in θ and 0.45° in ϕ with an exposure time of 15 s/frame. The integration of the data yielded a total of 26822 reflections to a maximum 2θ value of 63.44° of which 5648 were independent and 4635 were greater than $2\sigma(I)$. The final cell constants (Table 1) were based on the xyz centroids of 9958 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection; the data were processed with SADABS and corrected for absorption. The structure was solved and refined with the Bruker SHELXTL (version 2008/4) software package, using the space group $P\bar{1}$ with $Z = 2$ for the formula $C_{18}H_{30}BN$. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in idealized or refined positions. Full matrix least-squares refinement based on F^2 converged at $R1 = 0.0474$ and $wR2 = 0.1235$ [based on $I > 2\sigma(I)$], $R1 = 0.0587$ and $wR2 = 0.1339$ for all data. Additional details are given as Supporting Information in a CIF file.

Sheldrick, G.M. SHELXTL, v. 2008/4; Bruker Analytical X-ray, Madison, WI, 2008.

Saint Plus, v. 7.60A, Bruker Analytical X-ray, Madison, WI, 2009.

Sheldrick, G.M. SADABS, v. 2008/1. Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen: Gottingen, Germany, 2008.

X-Ray Crystallography Details of **30**



Colorless needles of **30** were grown from a *n*-heptane solution at 23°C . A crystal of dimensions $0.20 \times 0.14 \times 0.08$ mm was mounted on a Bruker SMART APEX-I CCD-based X-ray diffractometer equipped with a low temperature device and fine focus Mo-target X-ray tube ($\lambda = 0.71073$ Å) operated at 1500 W power (50 kV, 30 mA). The X-ray intensities were measured at $85(1)$ K; the detector was placed at a distance 5.070 cm from the crystal. A total of 2487 frames were collected with a scan width of 0.5° in θ and 0.45° in ϕ with an exposure time of 30 s/frame. The integration of the data yielded a

total of 25403 reflections to a maximum 2θ value of 59.20° of which 3374 were independent and 2755 were greater than $2\sigma(I)$. The final cell constants (Table 1) were based on the xyz centroids of 8505 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection; the data were processed with SADABS and corrected for absorption. The structure was solved and refined with the Bruker SHELXTL (version 2008/4) software package, using the space group C2/c with $Z = 8$ for the formula $C_{14}H_{20}BN$. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in idealized and refined positions. Full matrix least-squares refinement based on F^2 converged at $R1 = 0.0518$ and $wR2 = 0.1338$ [based on $I > 2\sigma(I)$], $R1 = 0.0640$ and $wR2 = 0.1455$ for all data. Additional details are given as Supporting Information in a CIF file.

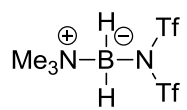
Sheldrick, G.M. SHELXTL, v. 2008/4; Bruker Analytical X-ray, Madison, WI, 2008.

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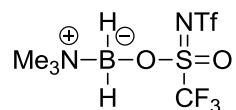
Sheldrick, G.M. SADABS, v. 2008/1. Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen: Gottingen, Germany, 2008.

NMR Spectra

^1H NMR (500 MHz),
 CD_2Cl_2

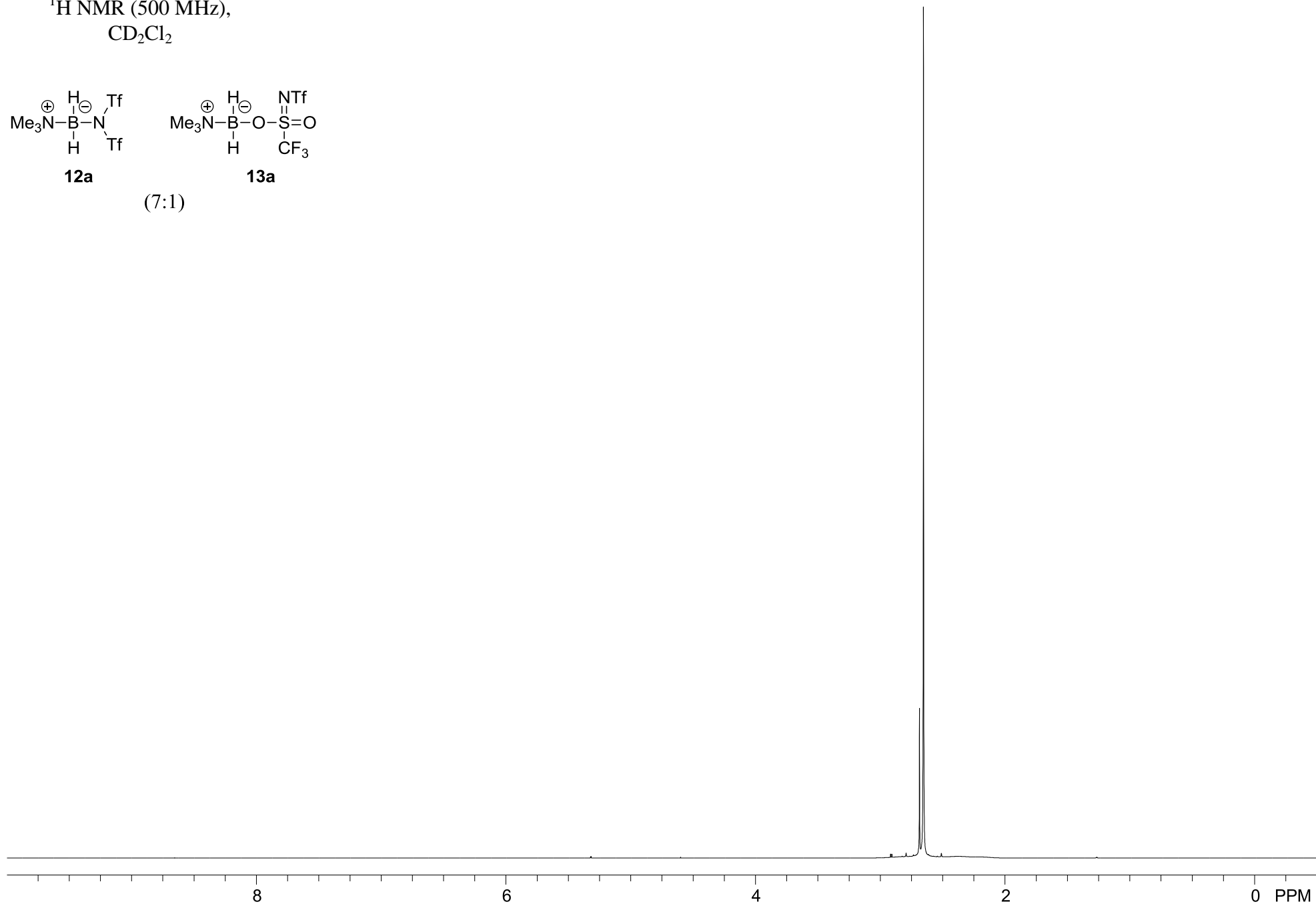


12a

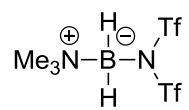


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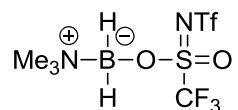
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^{11}B NMR (160 MHz),
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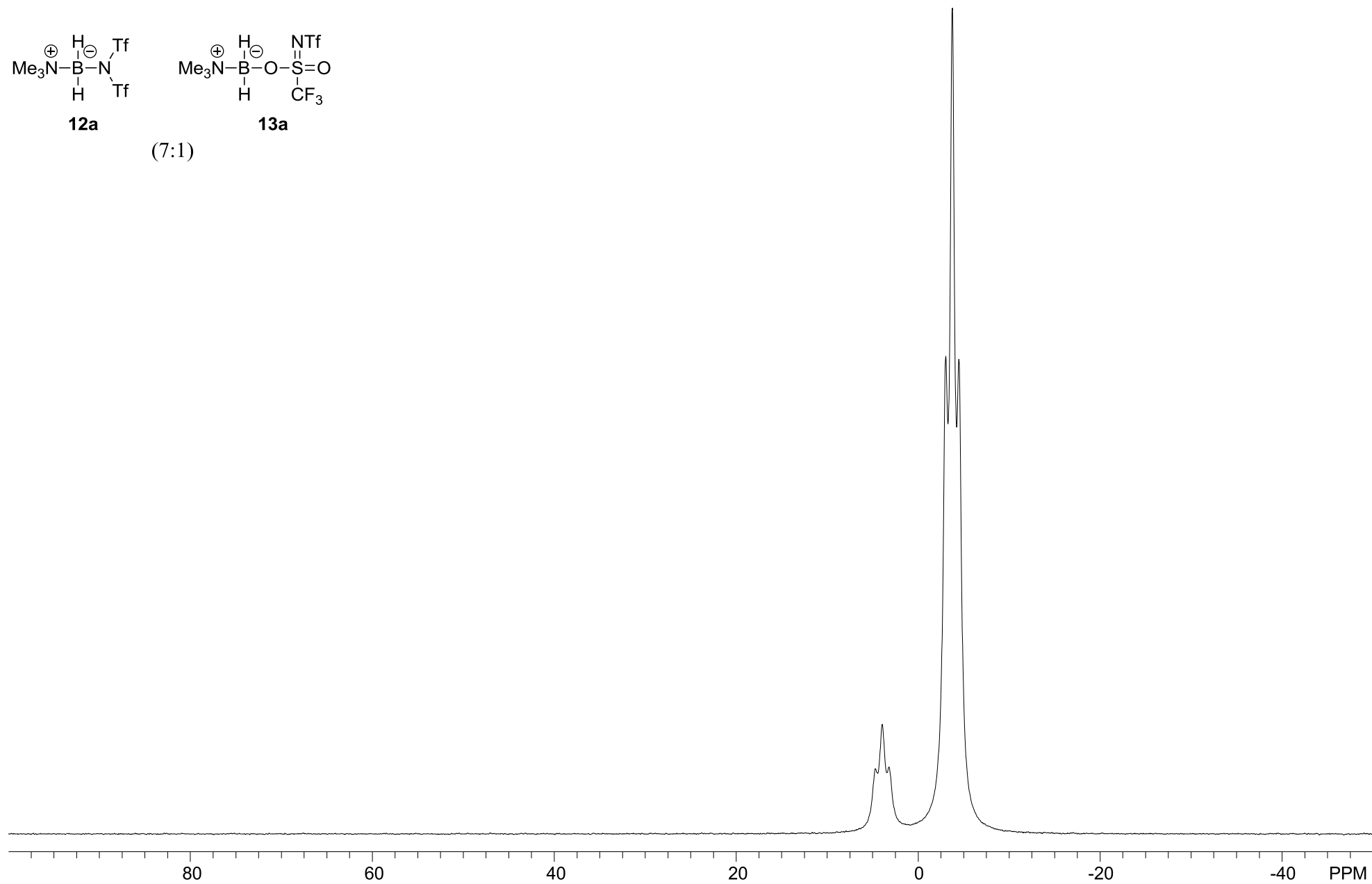


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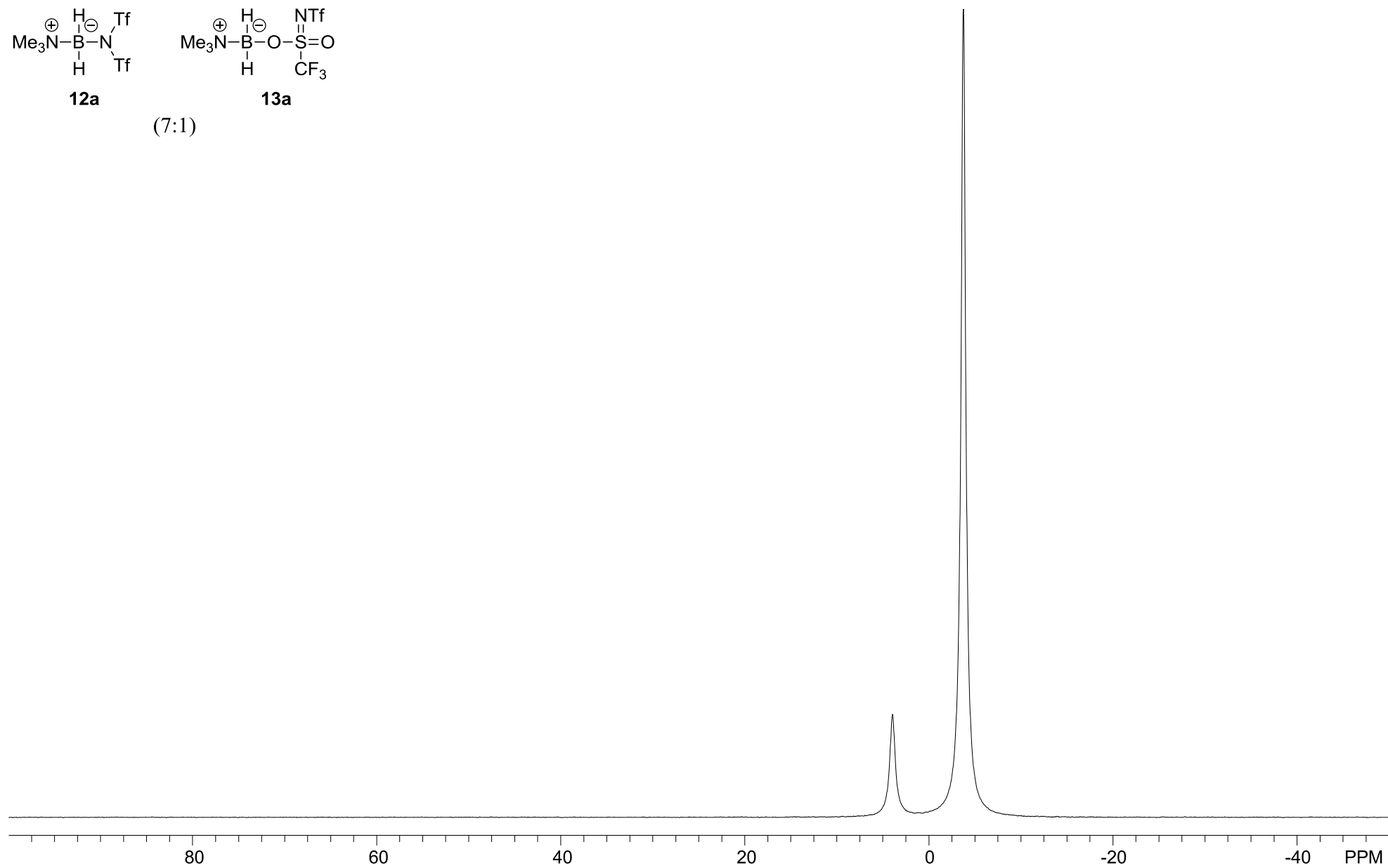
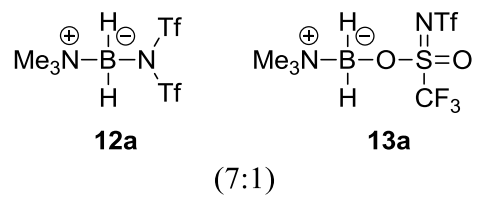


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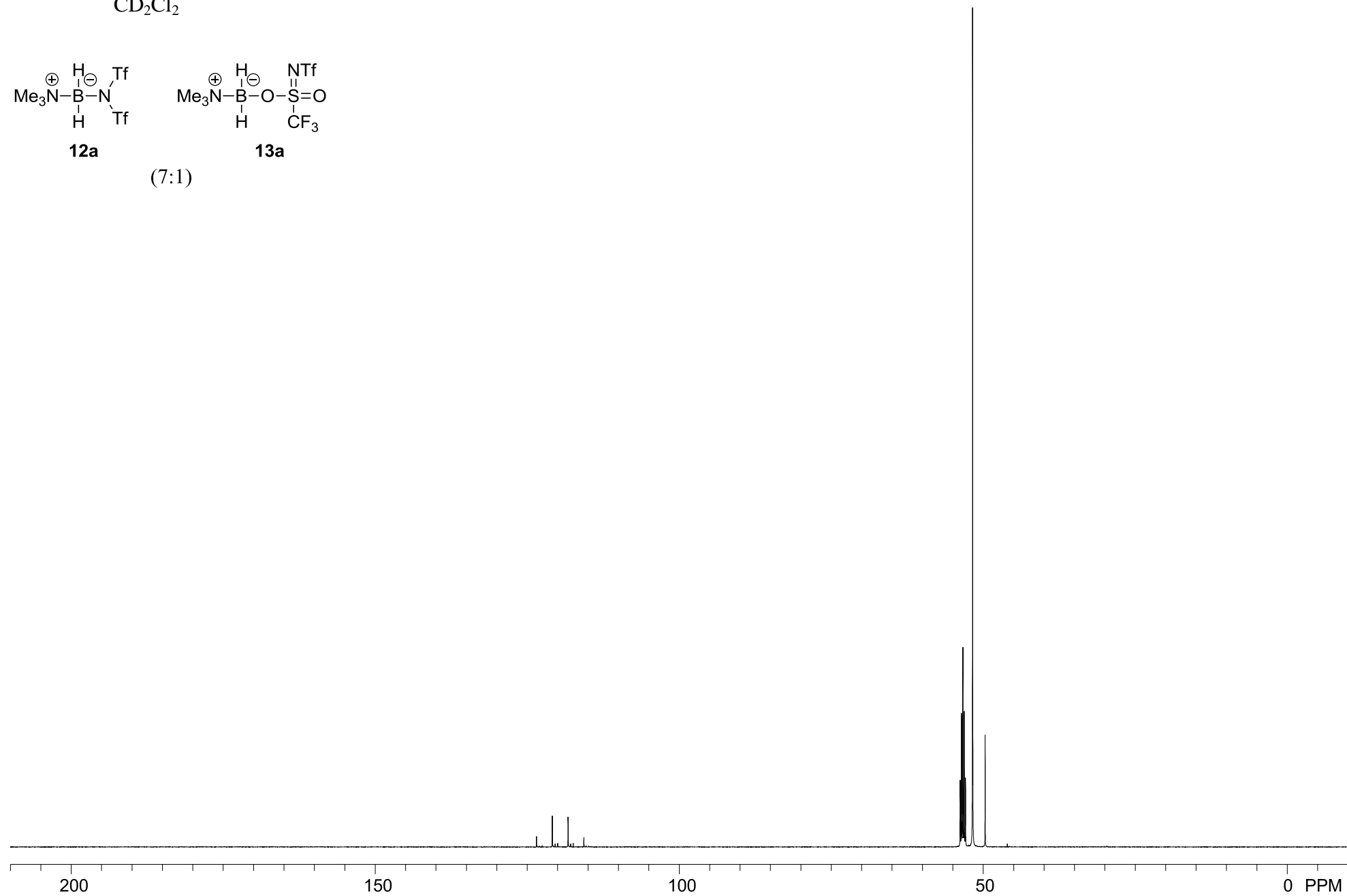
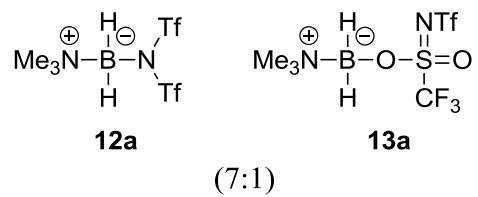
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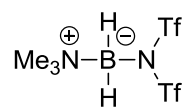
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 CD_2Cl_2



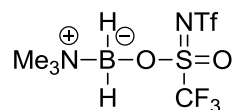
$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CD_2Cl_2



^{19}F NMR (471 MHz),
 CD_2Cl_2

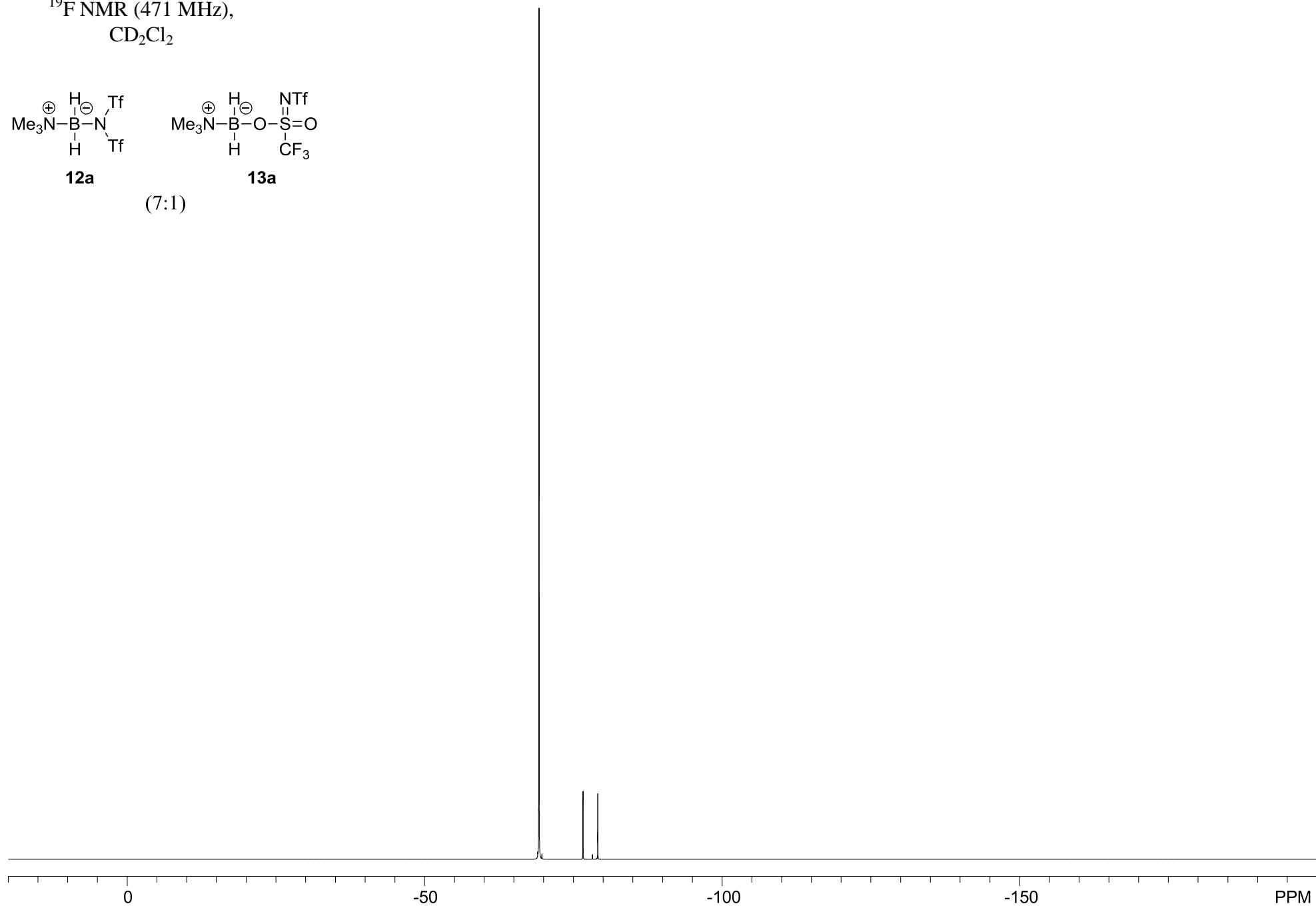


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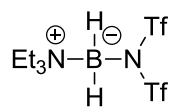


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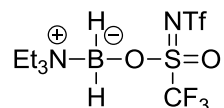
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^1H NMR (500 MHz),
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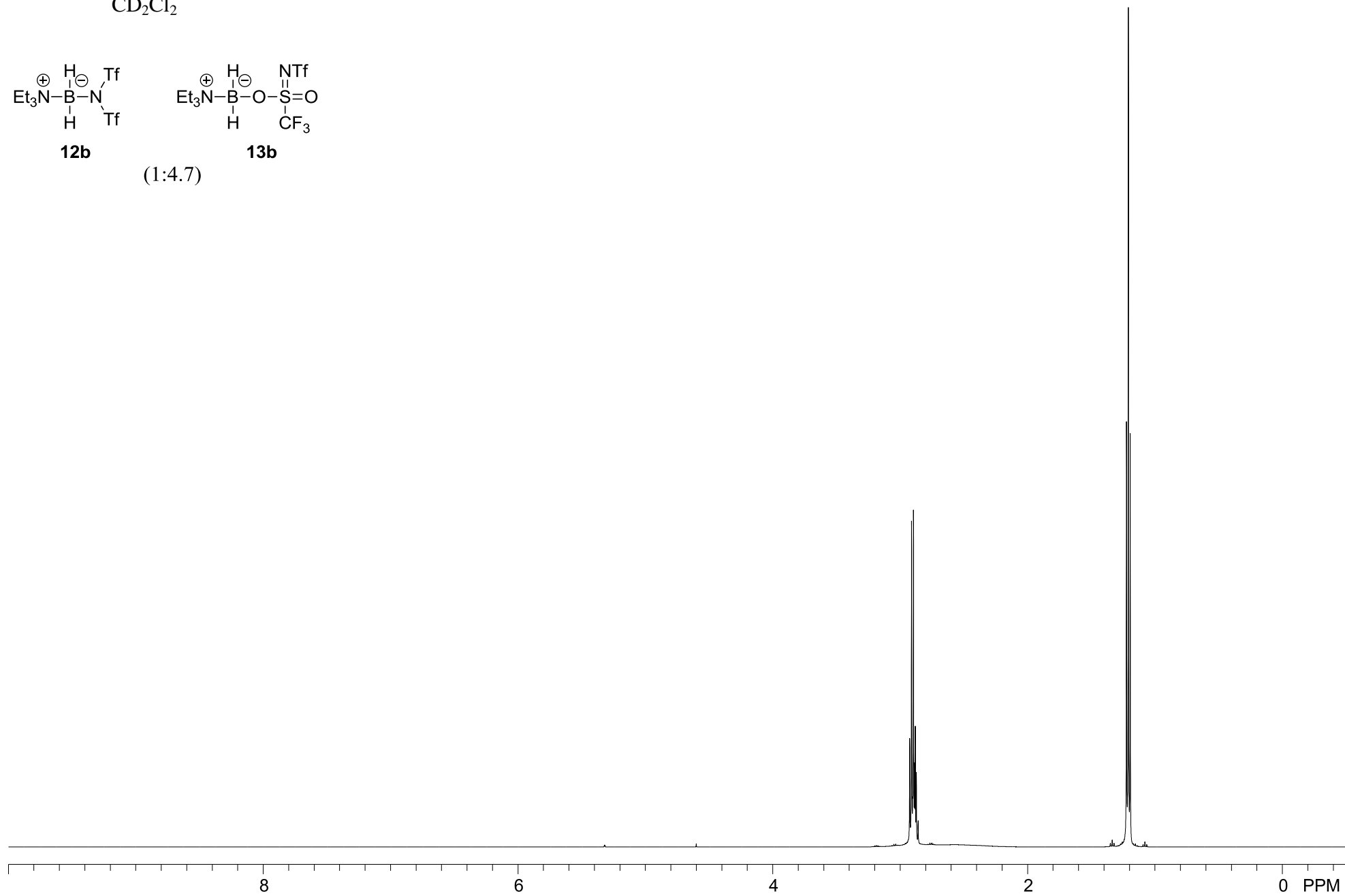


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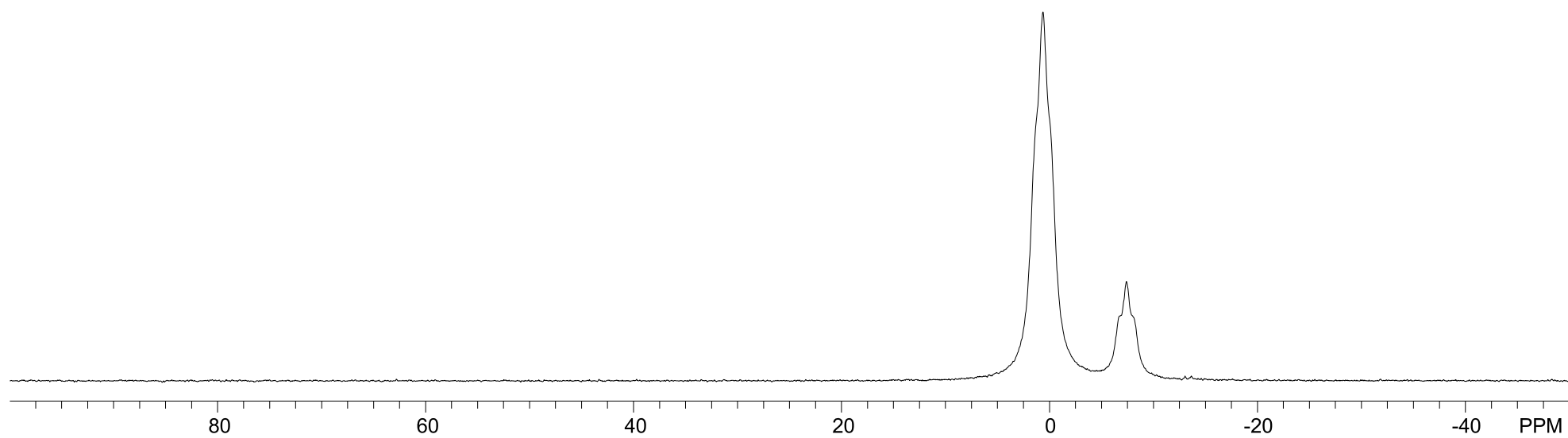
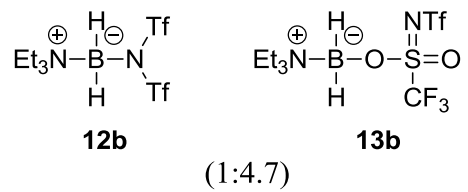


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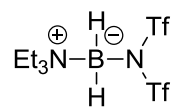
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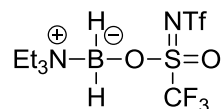
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 CD_2Cl_2



$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz),
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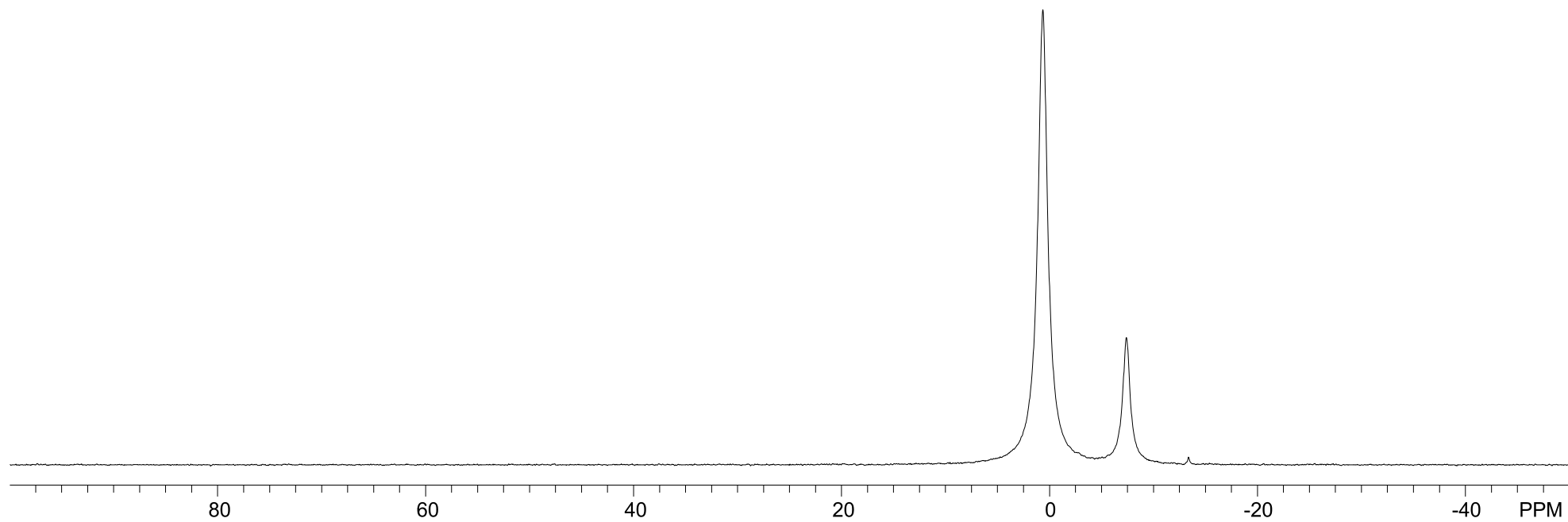


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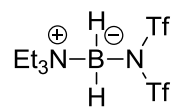


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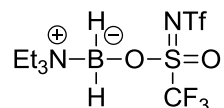
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$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CD_2Cl_2

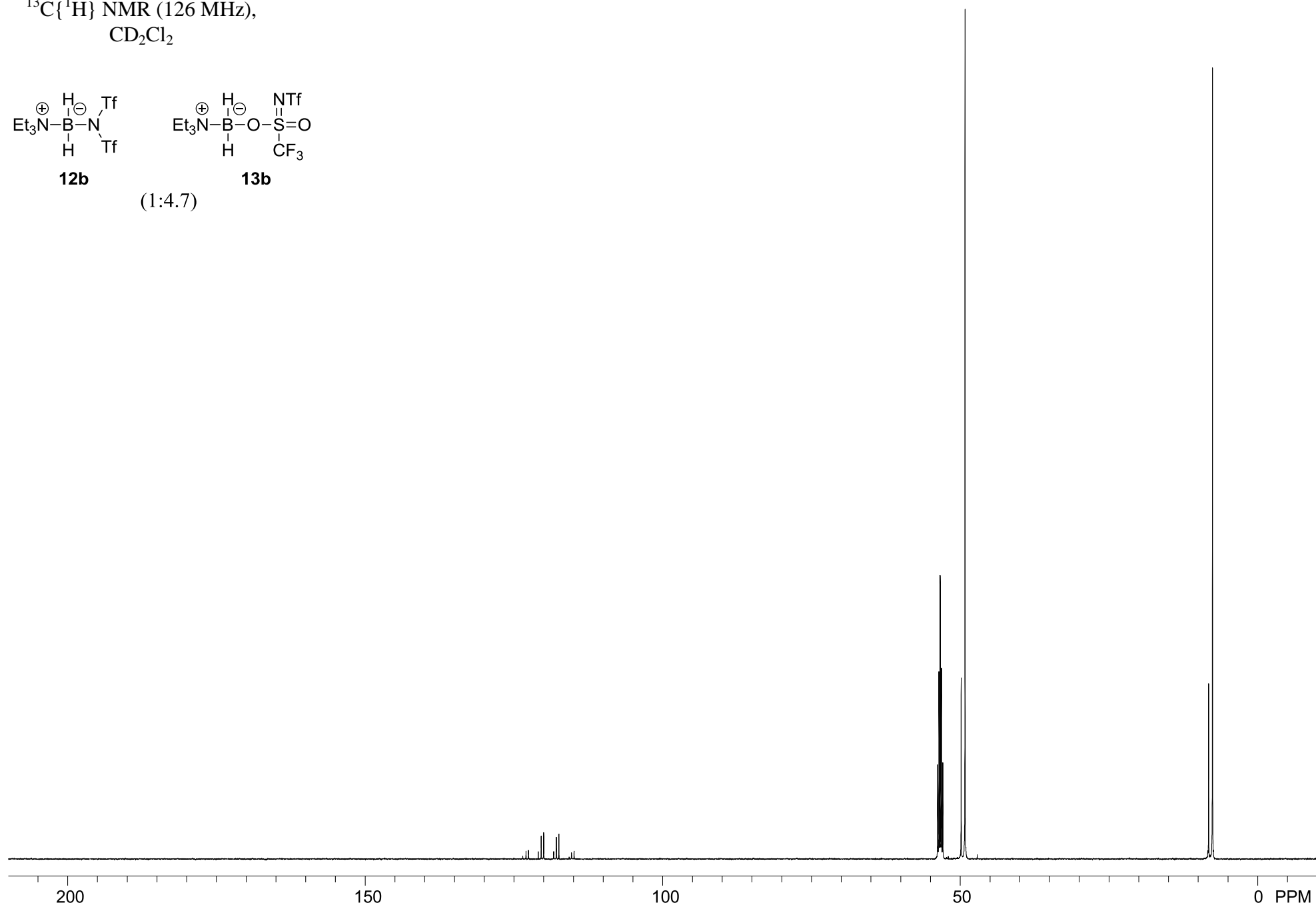


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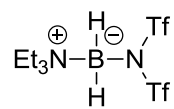


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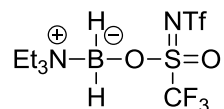
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^{19}F NMR (471 MHz),
 CD_2Cl_2

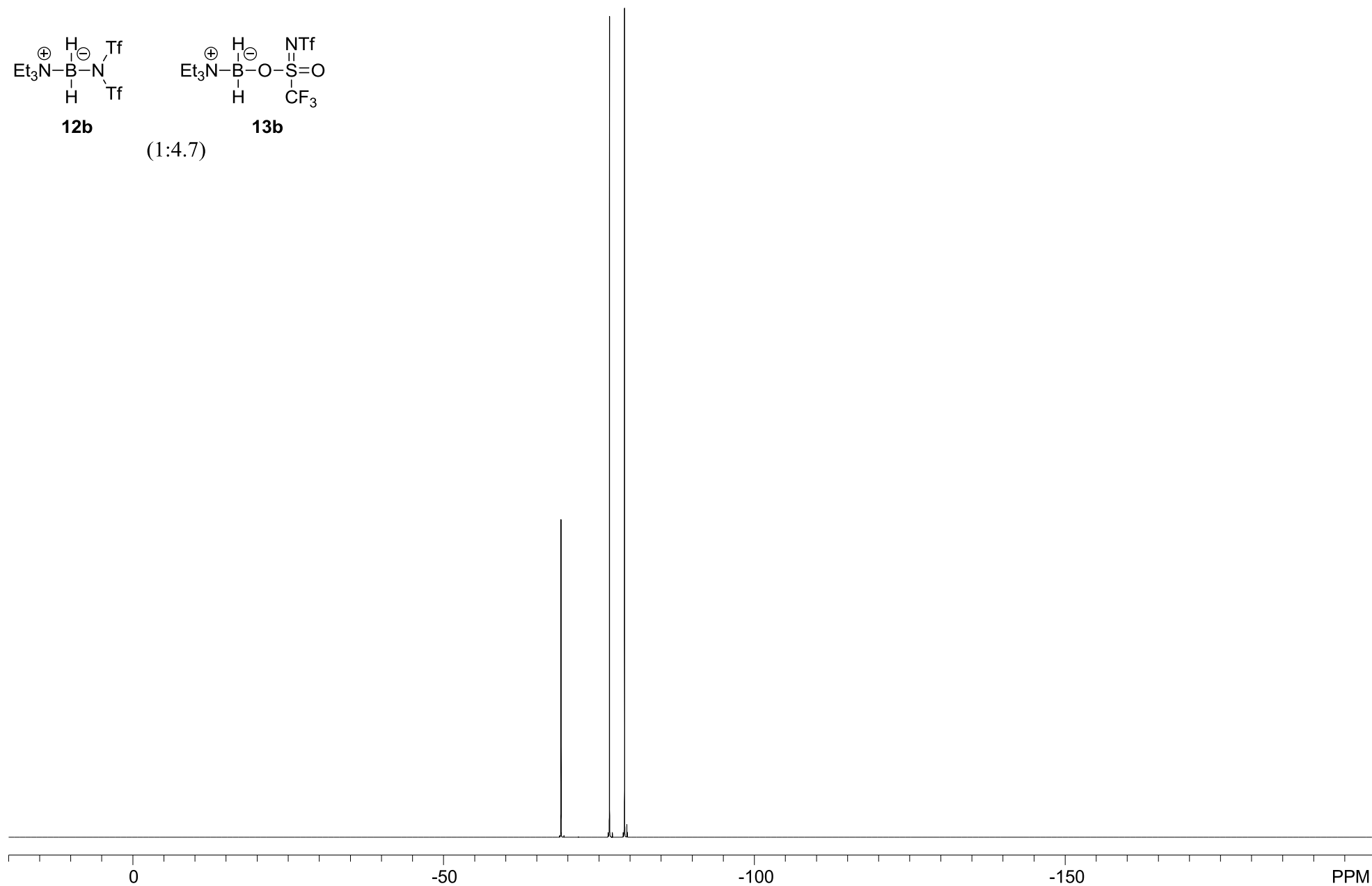


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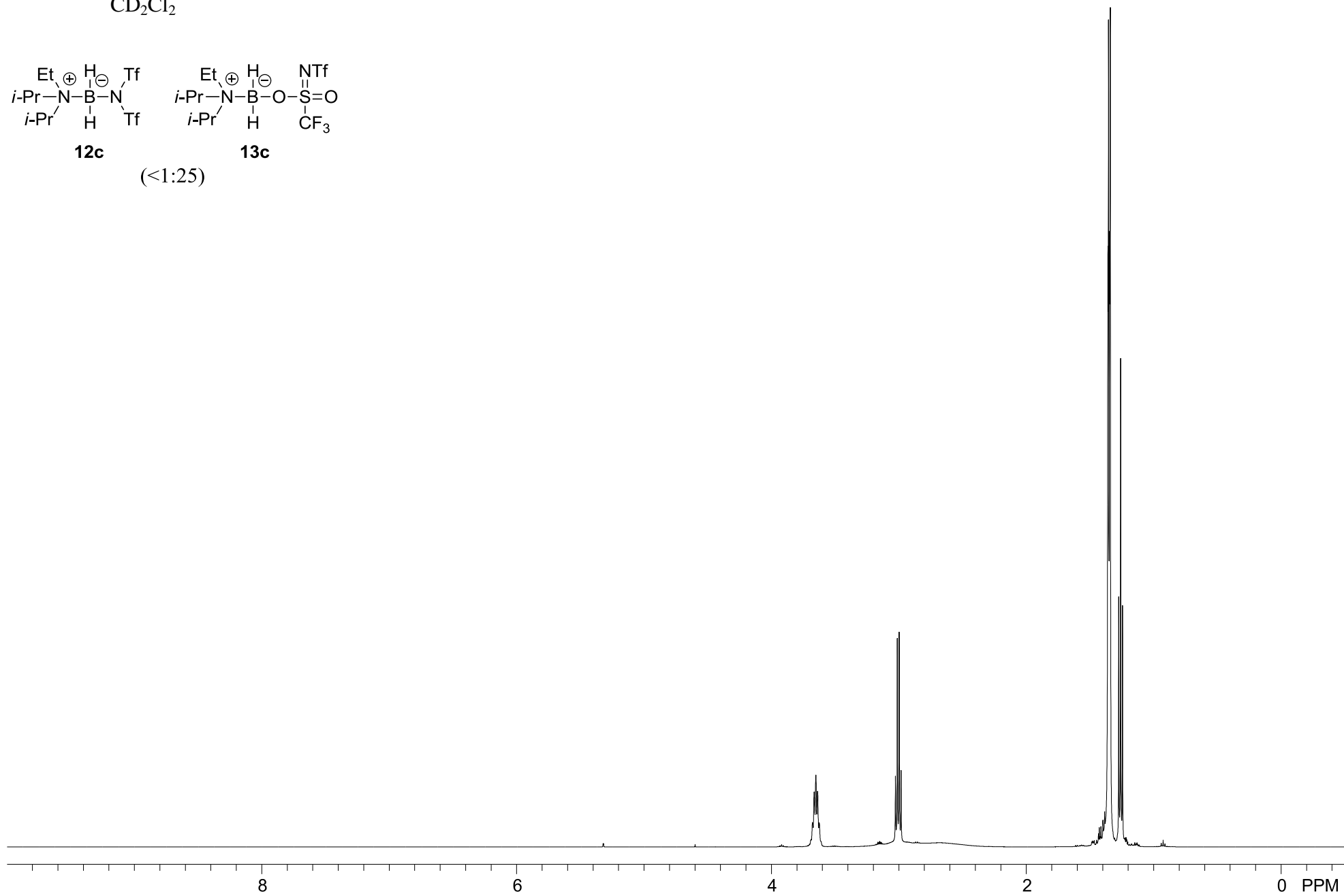
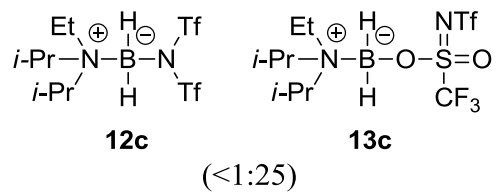


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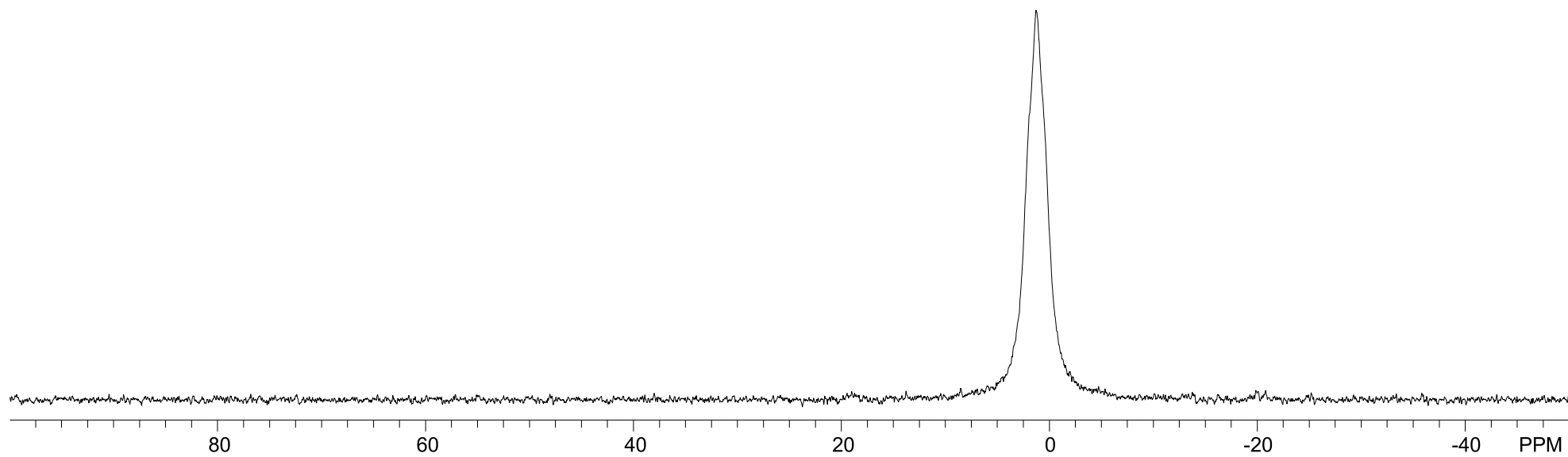
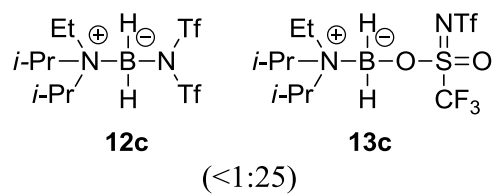
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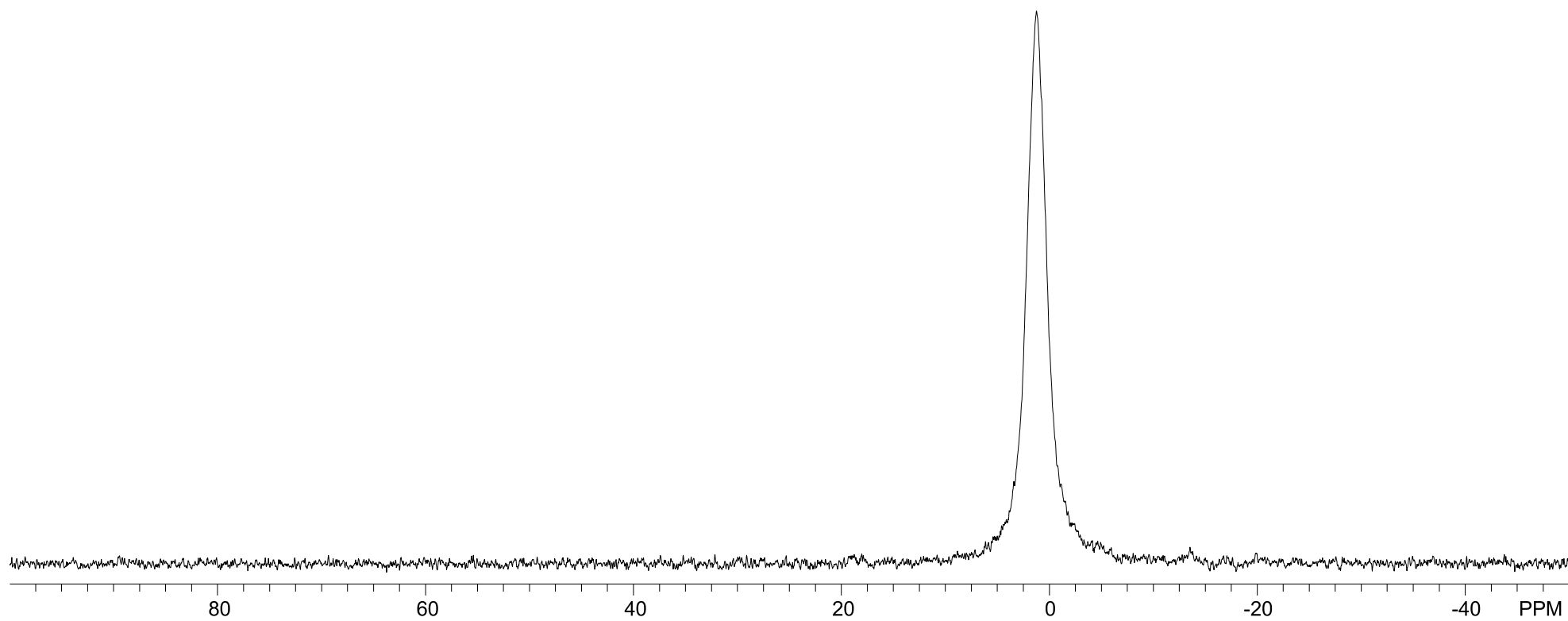
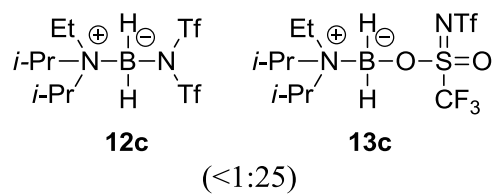
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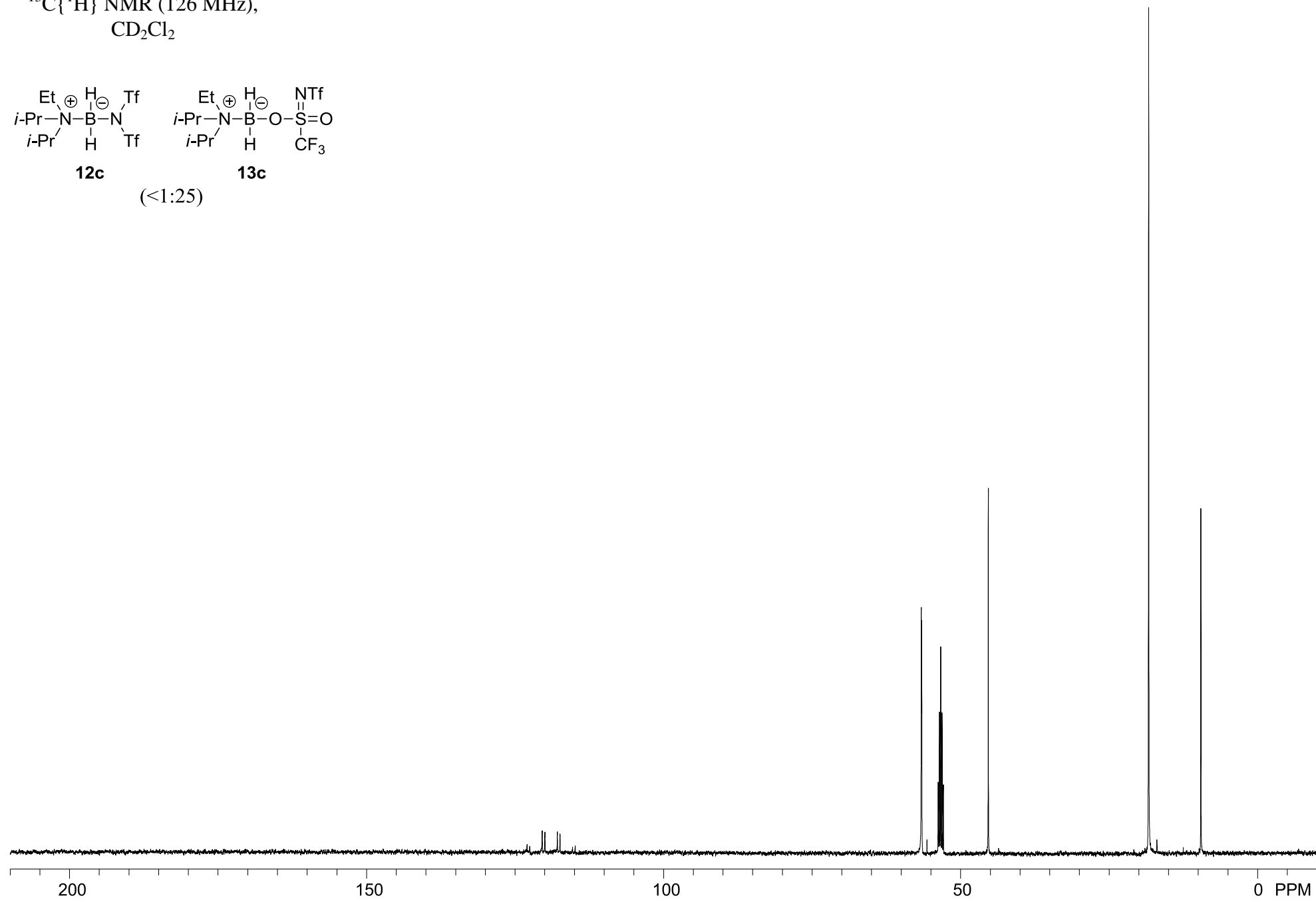
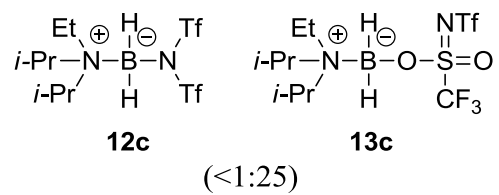
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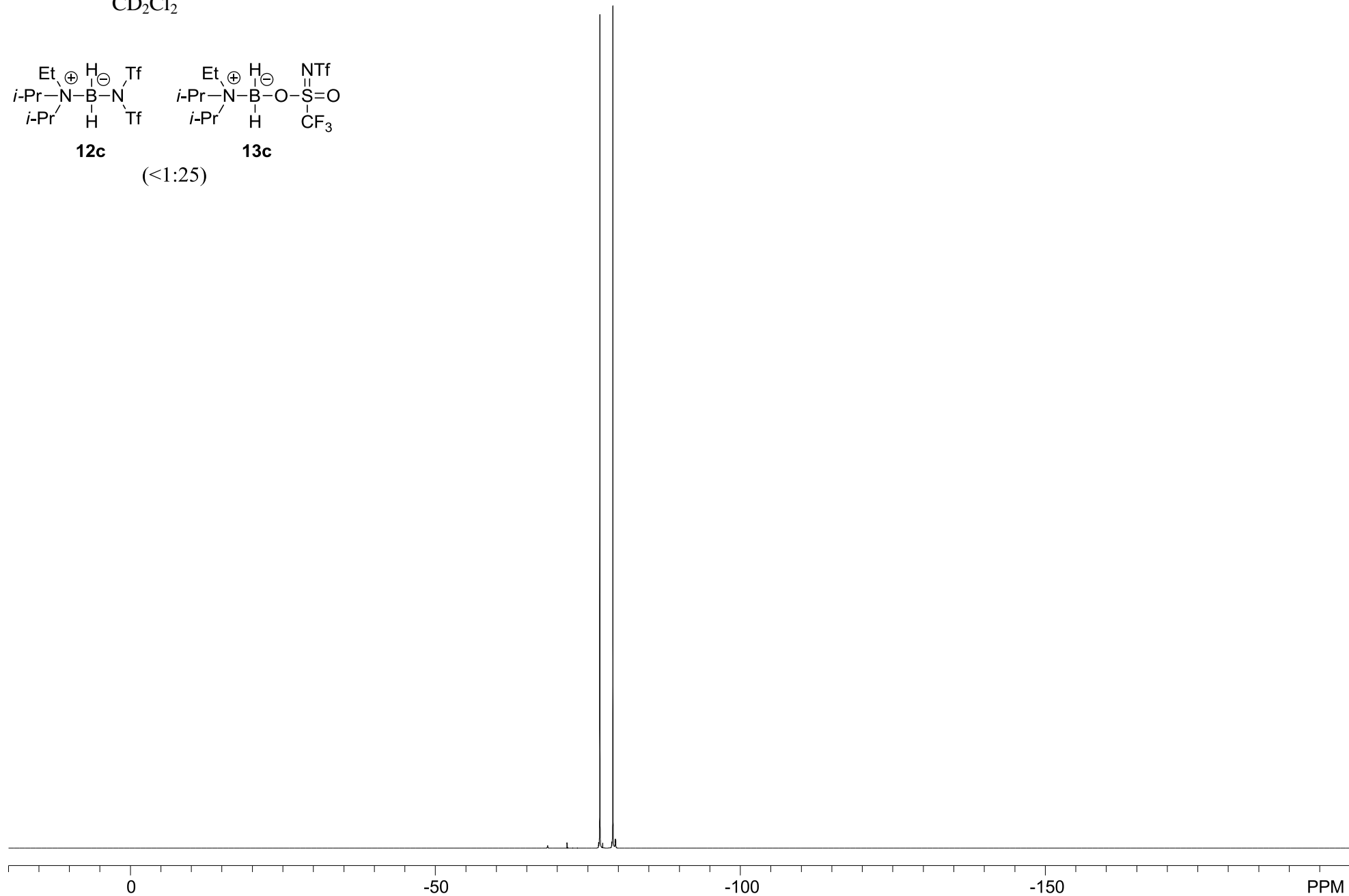
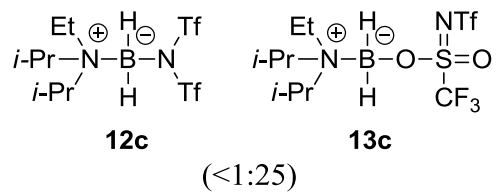
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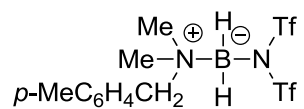
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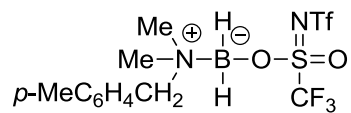
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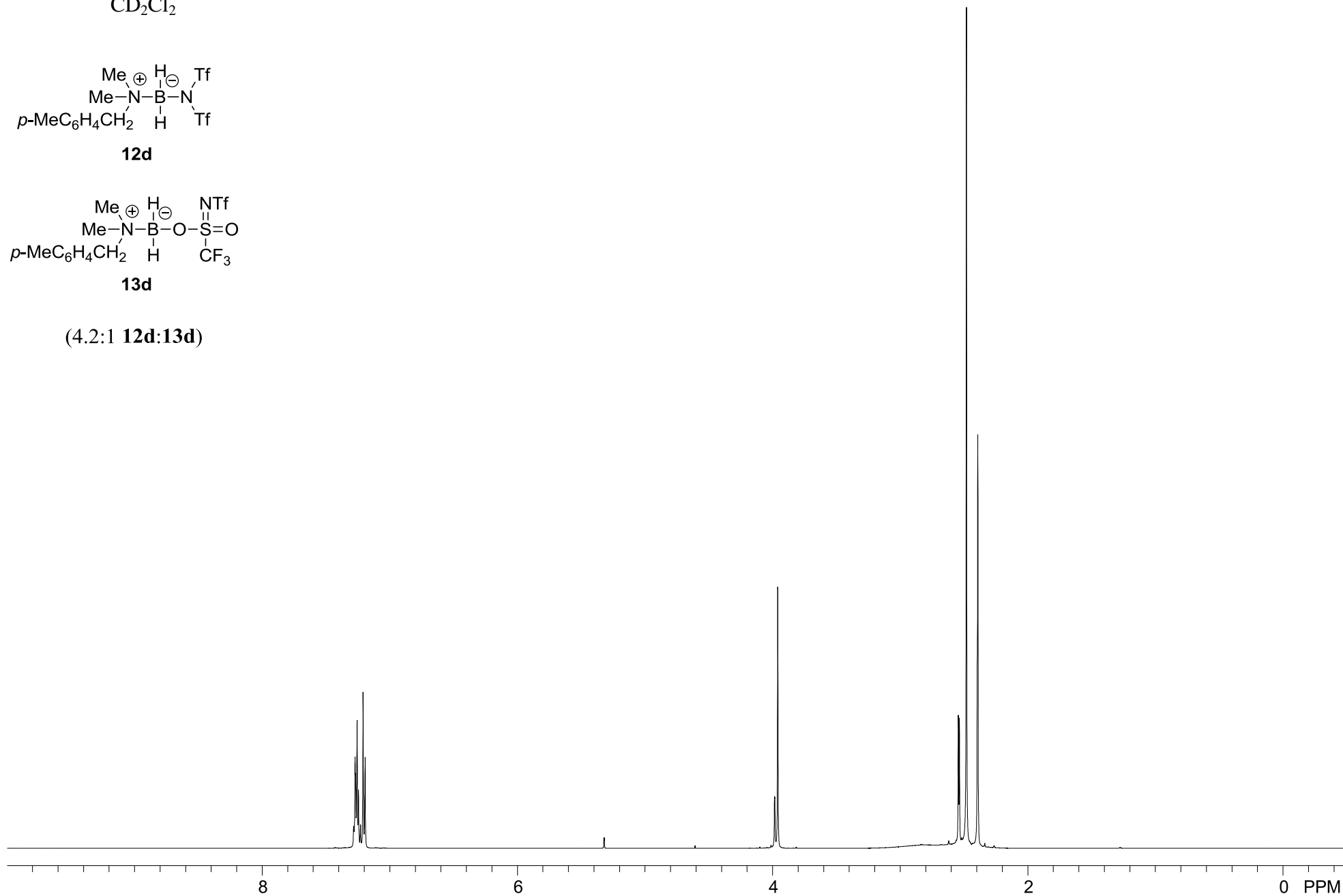


12d

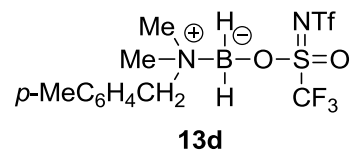
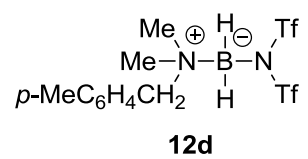


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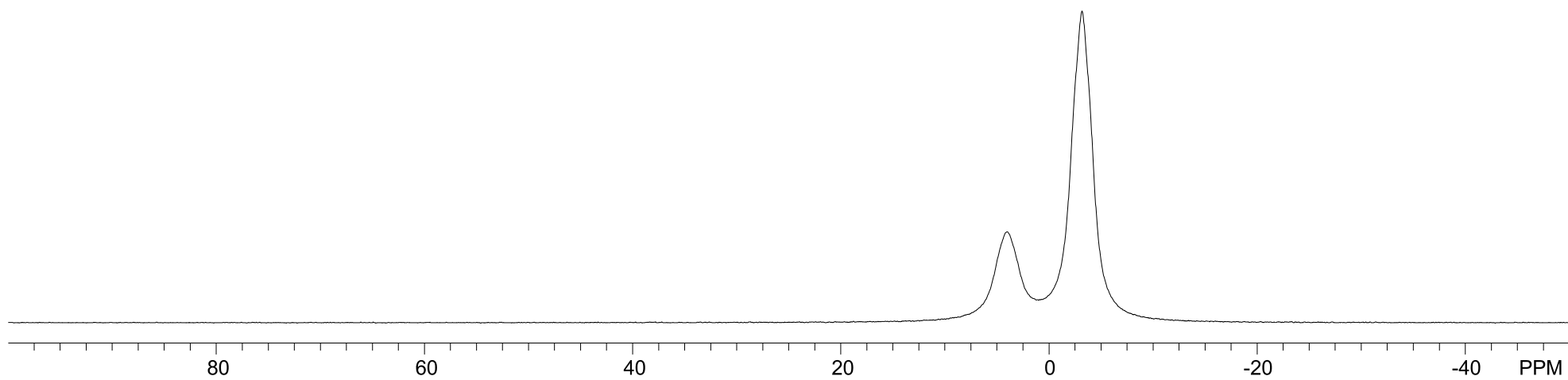
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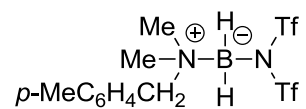
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 CD_2Cl_2



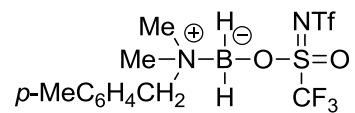
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$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz),
 CD_2Cl_2

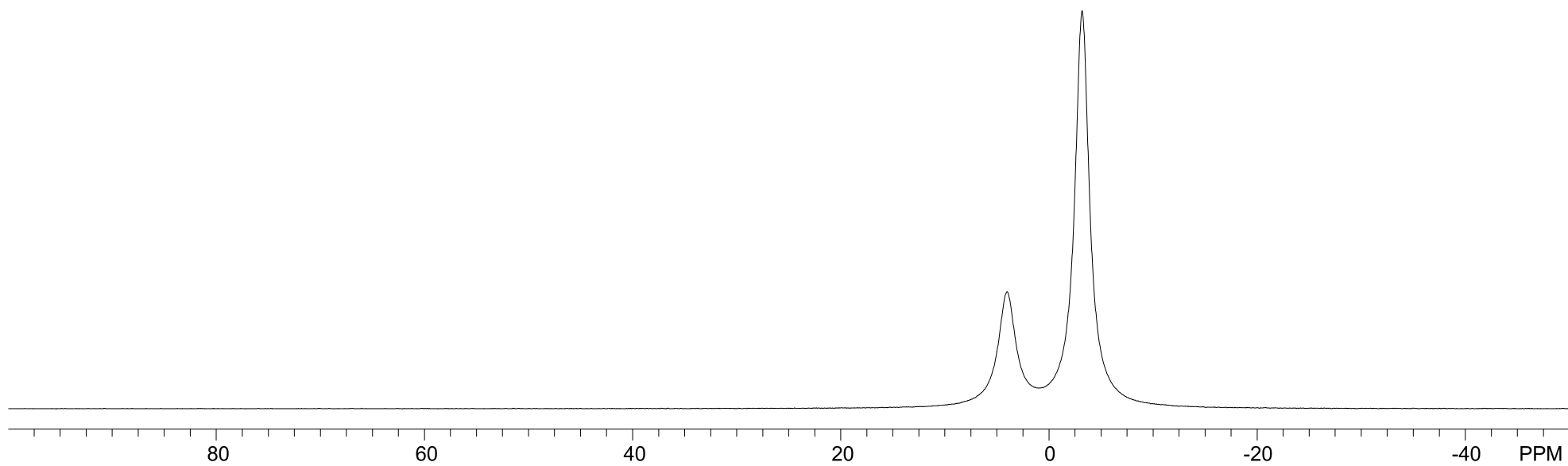


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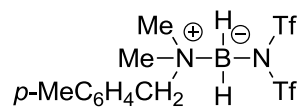


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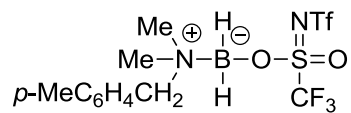
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 CD_2Cl_2

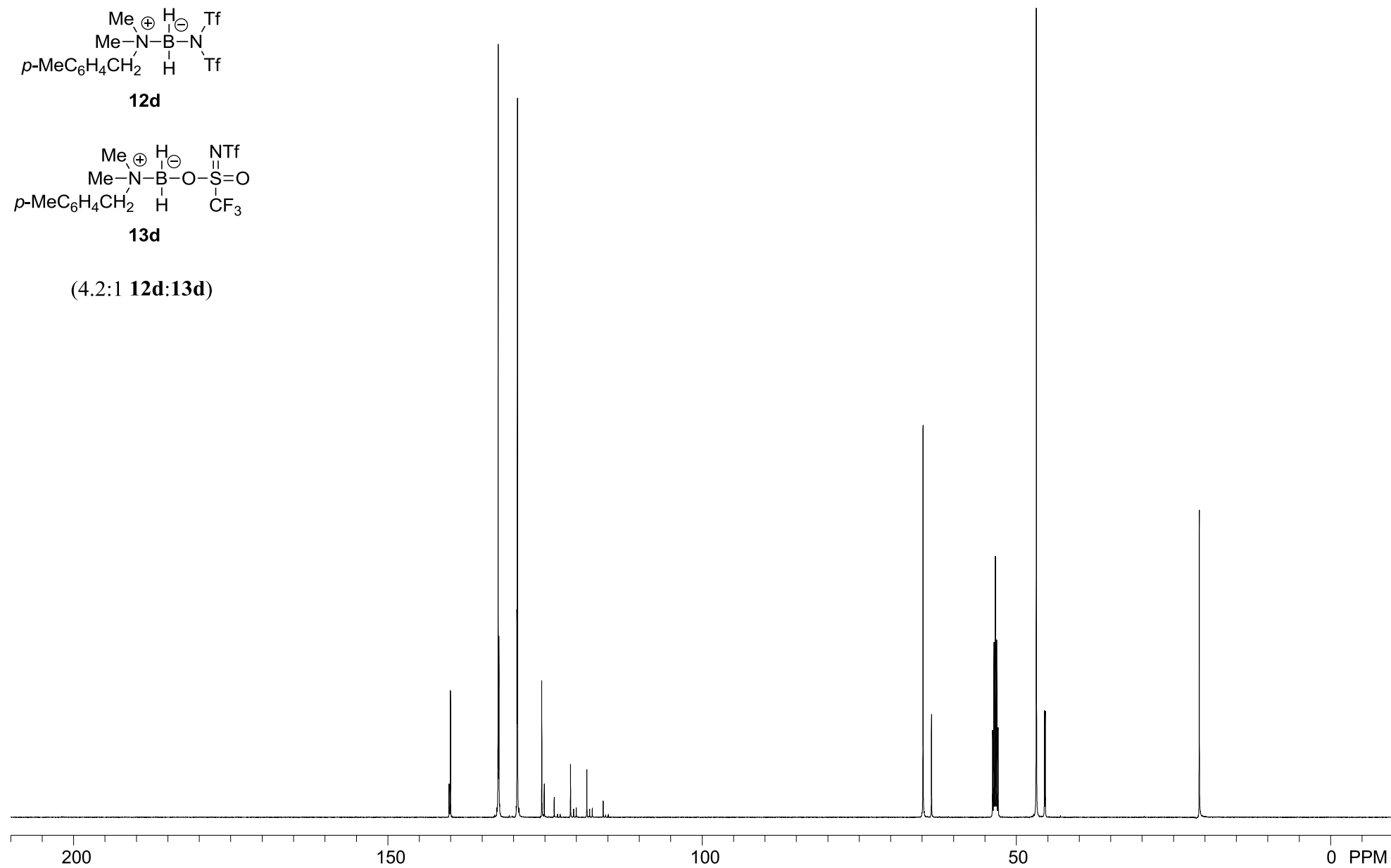


12d

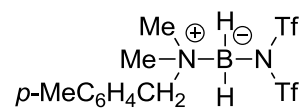


13d

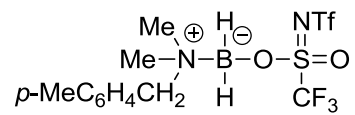
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 CD_2Cl_2

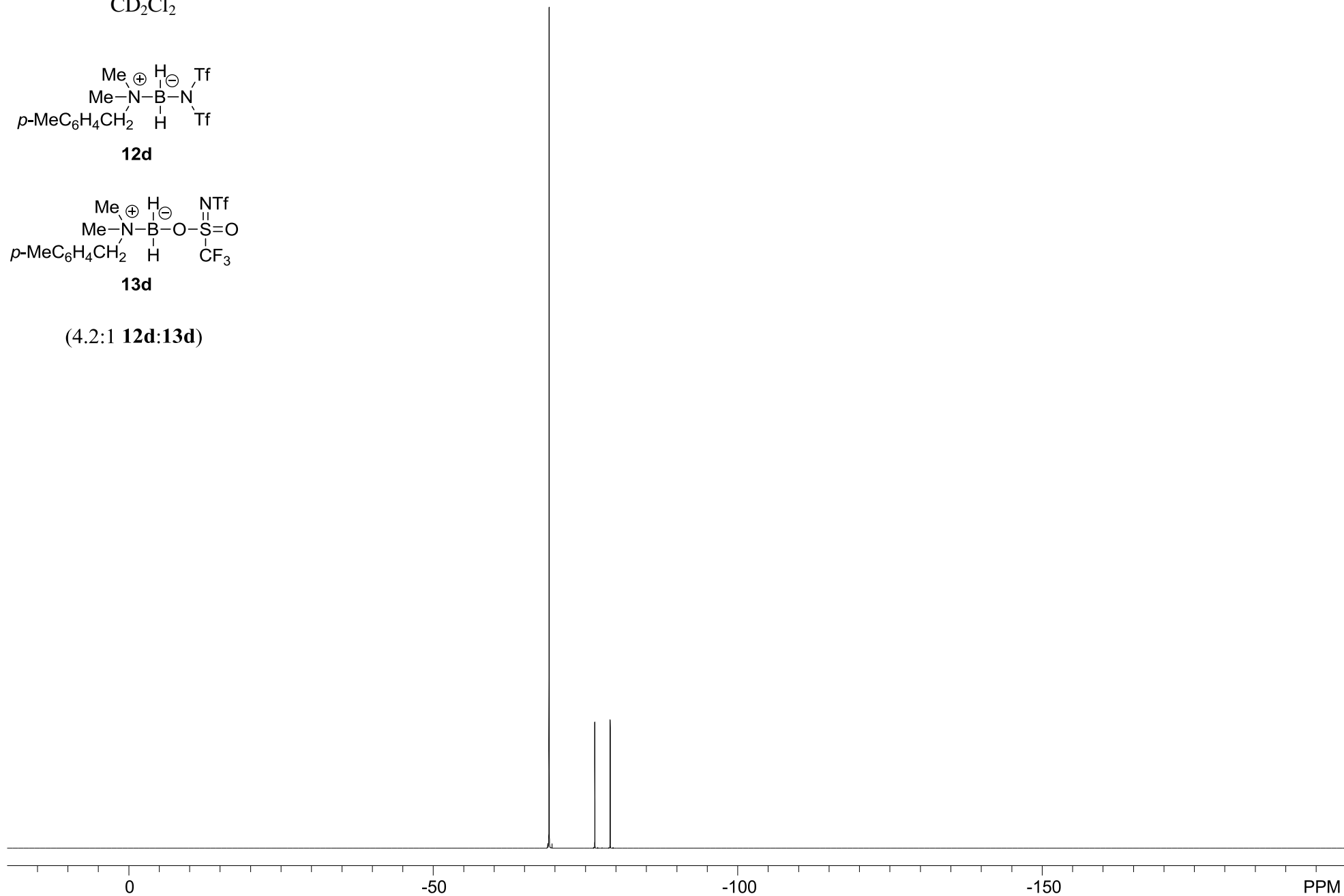


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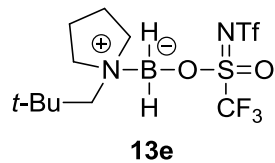
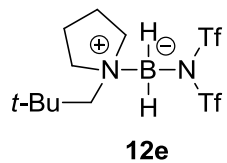


13d

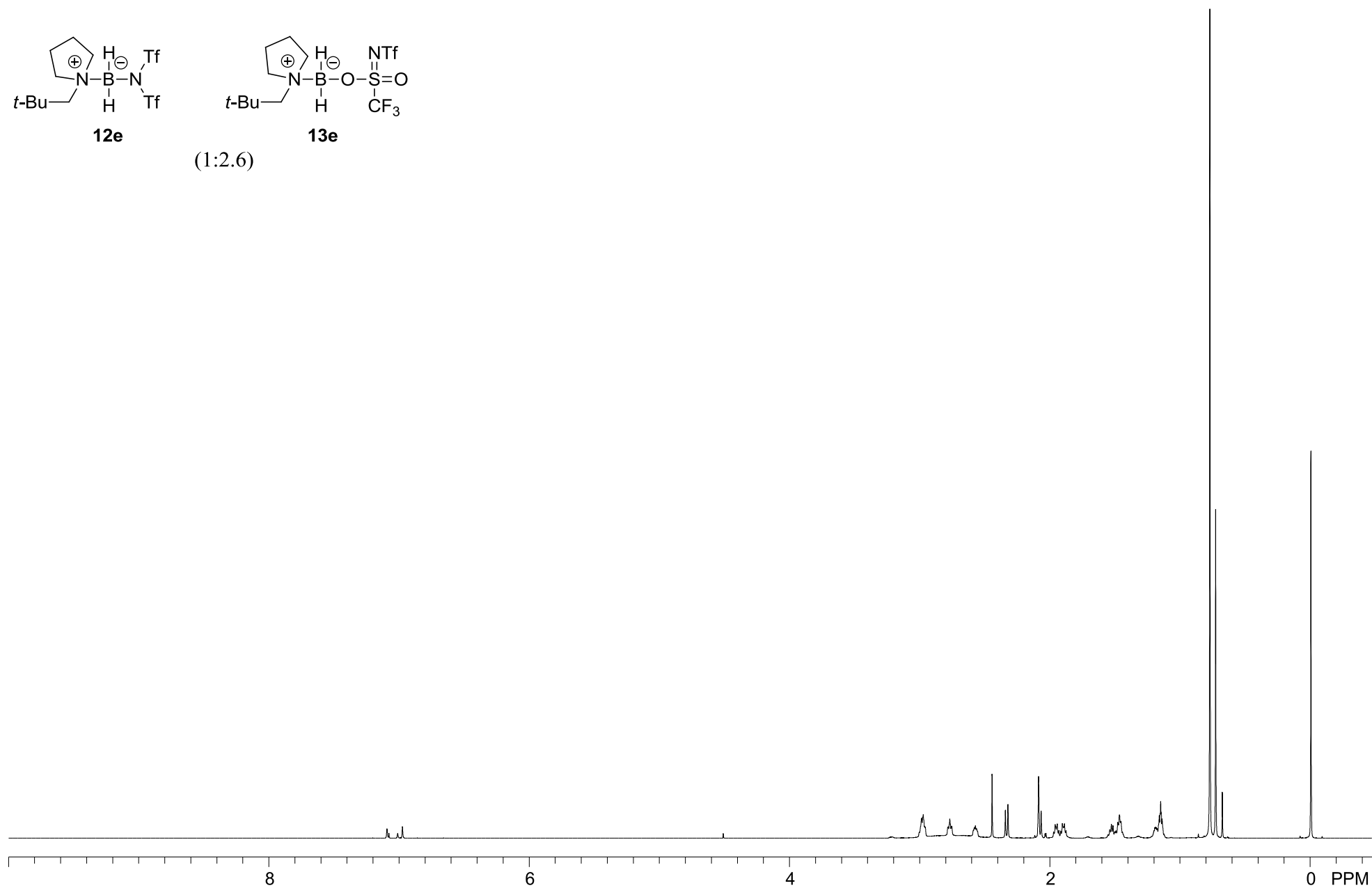
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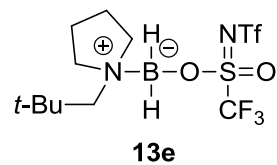
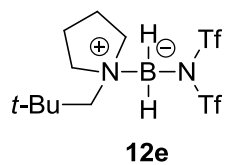
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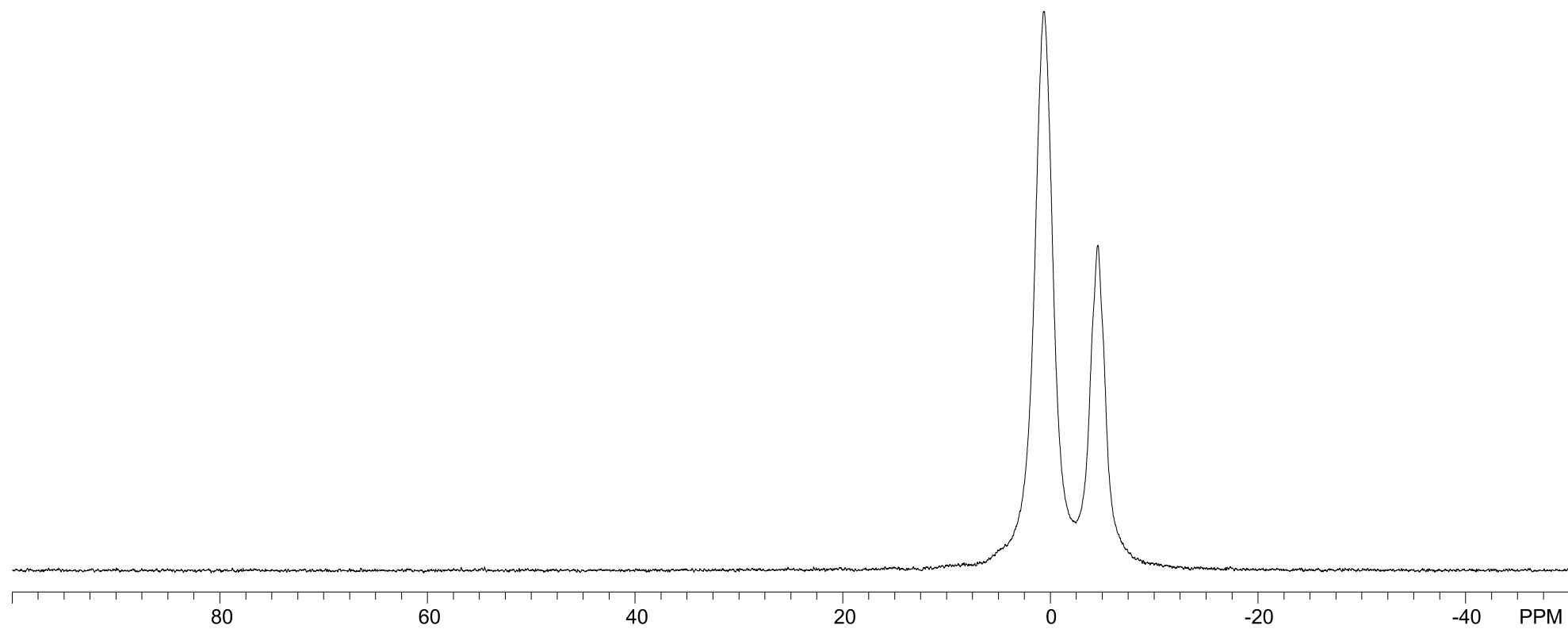
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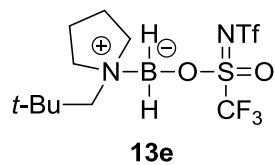
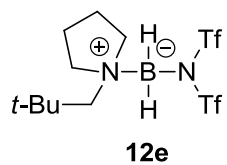
^{11}B NMR (225 MHz),
 $d_8\text{-PhMe}$



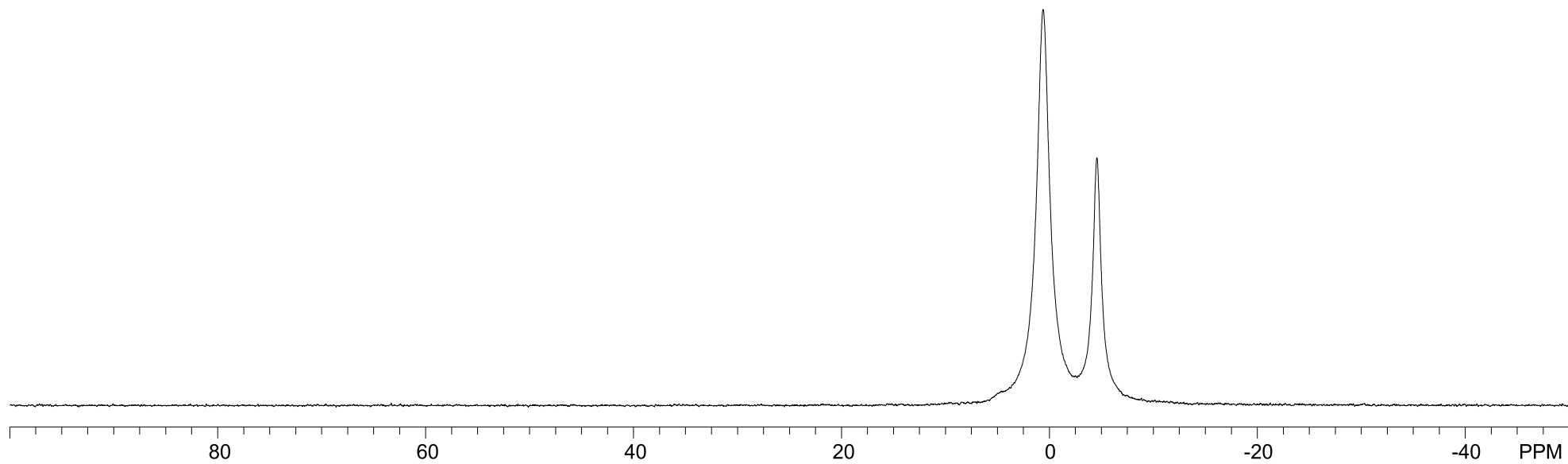
(1:2.6)



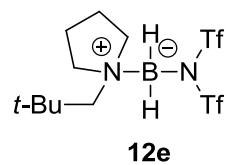
$^{11}\text{B}\{^1\text{H}\}$ NMR (225 MHz),
 $d_8\text{-PhMe}$



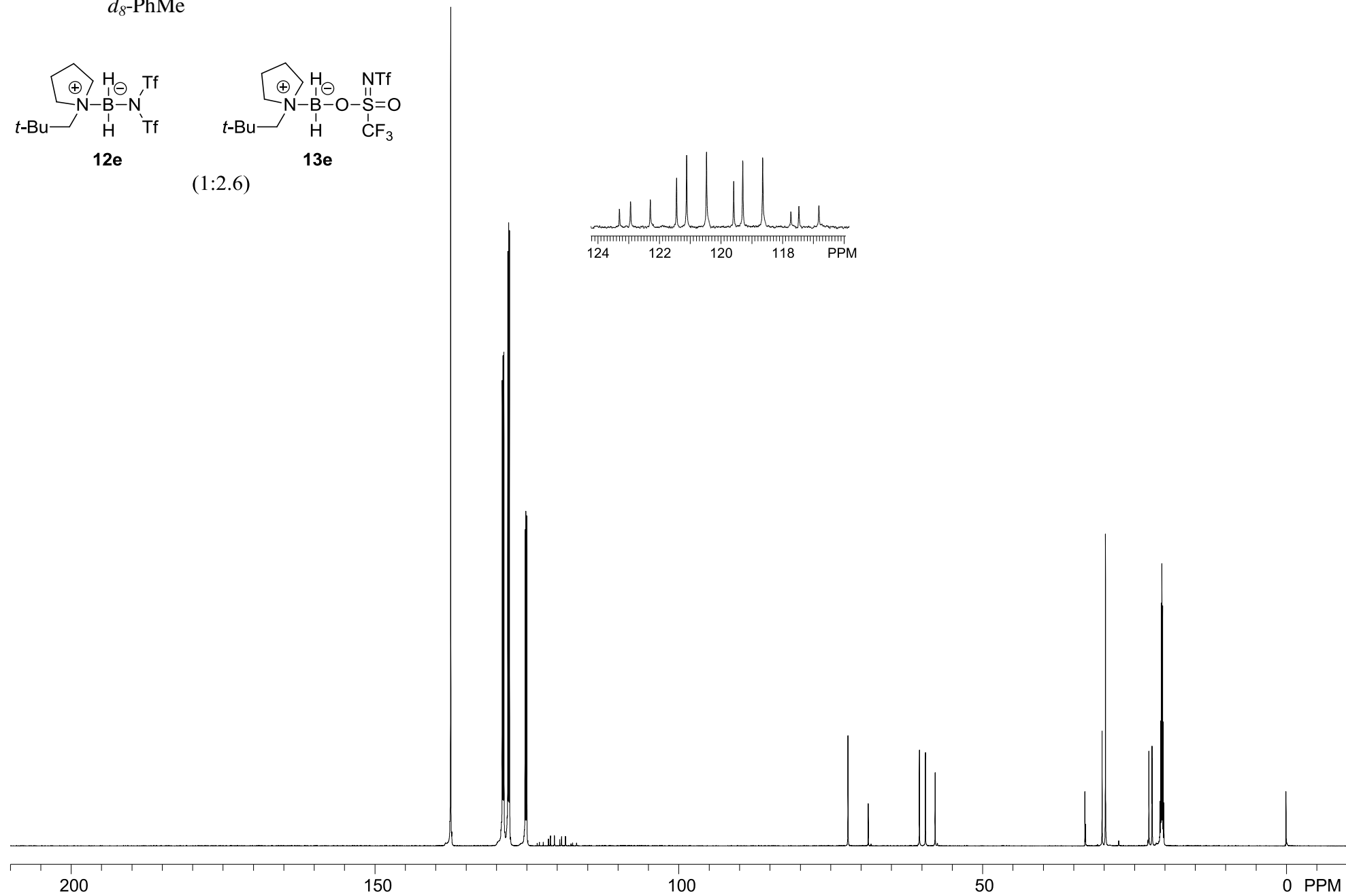
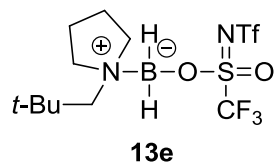
(1:2.6)



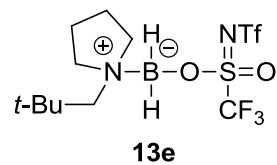
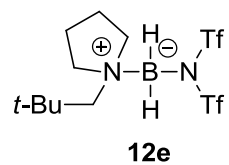
$^{13}\text{C}\{^1\text{H}\}$ NMR (176 MHz),
 $d_8\text{-PhMe}$



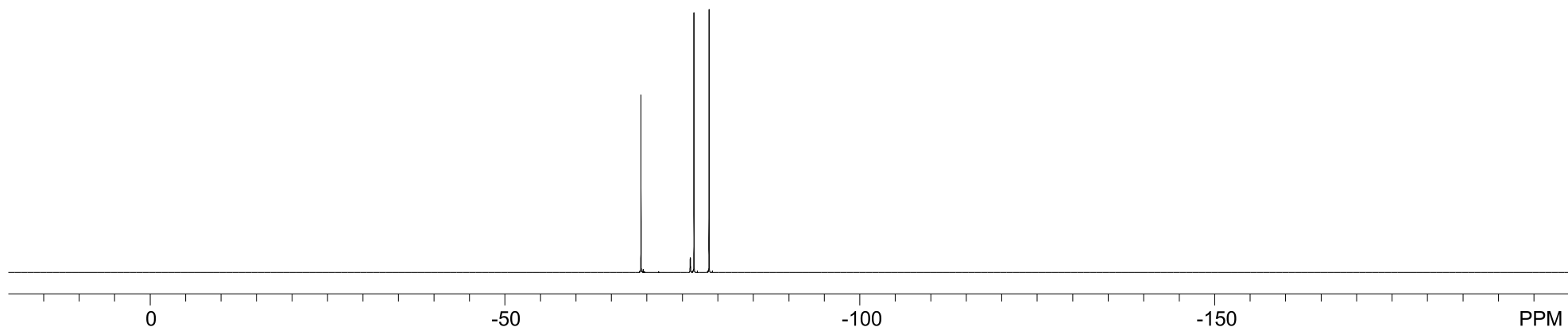
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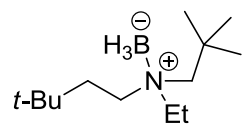
^{19}F NMR (471 MHz),
 d_8 -PhMe



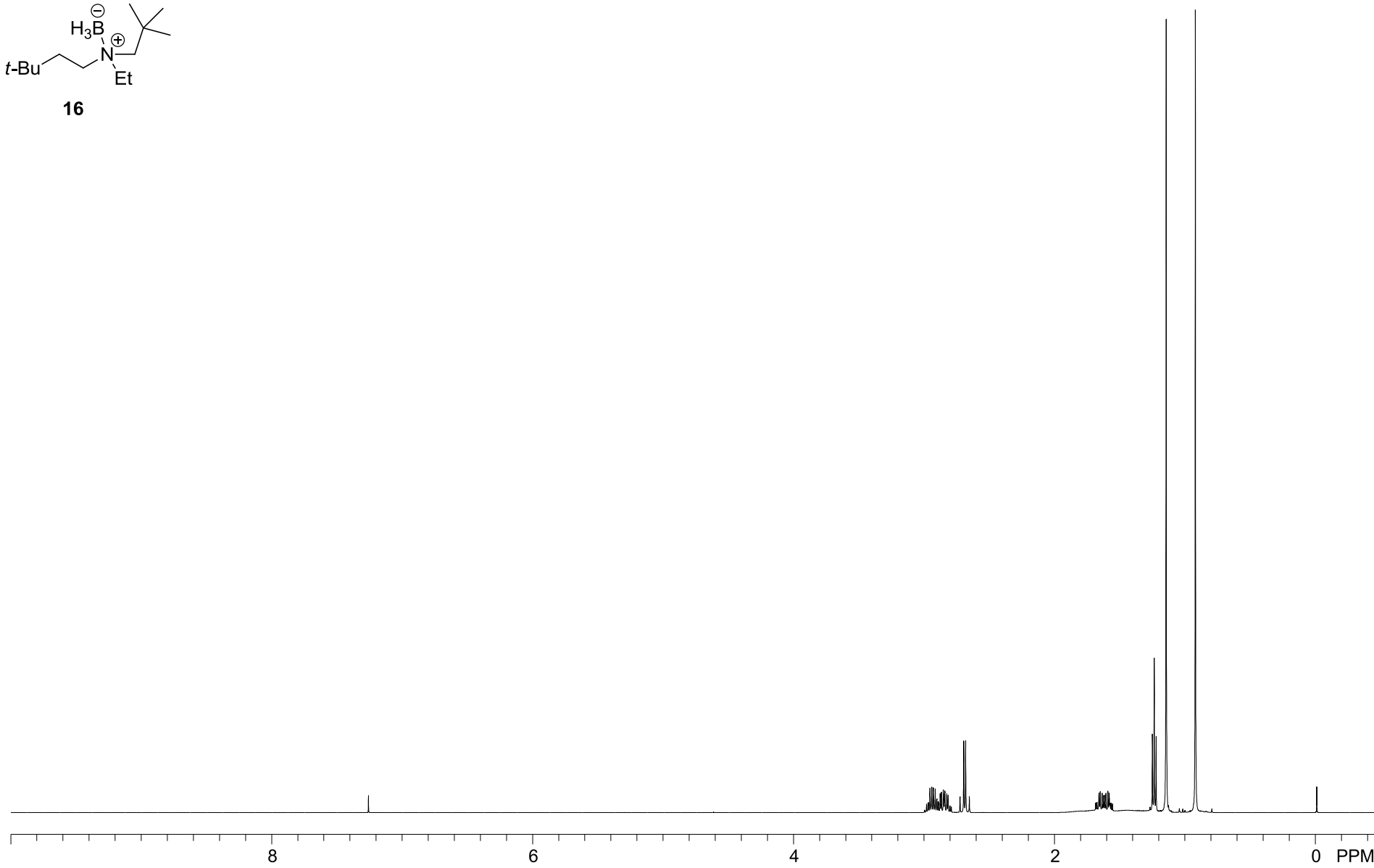
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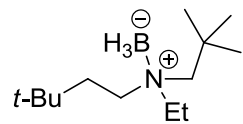
^1H NMR (500 MHz),
 CDCl_3



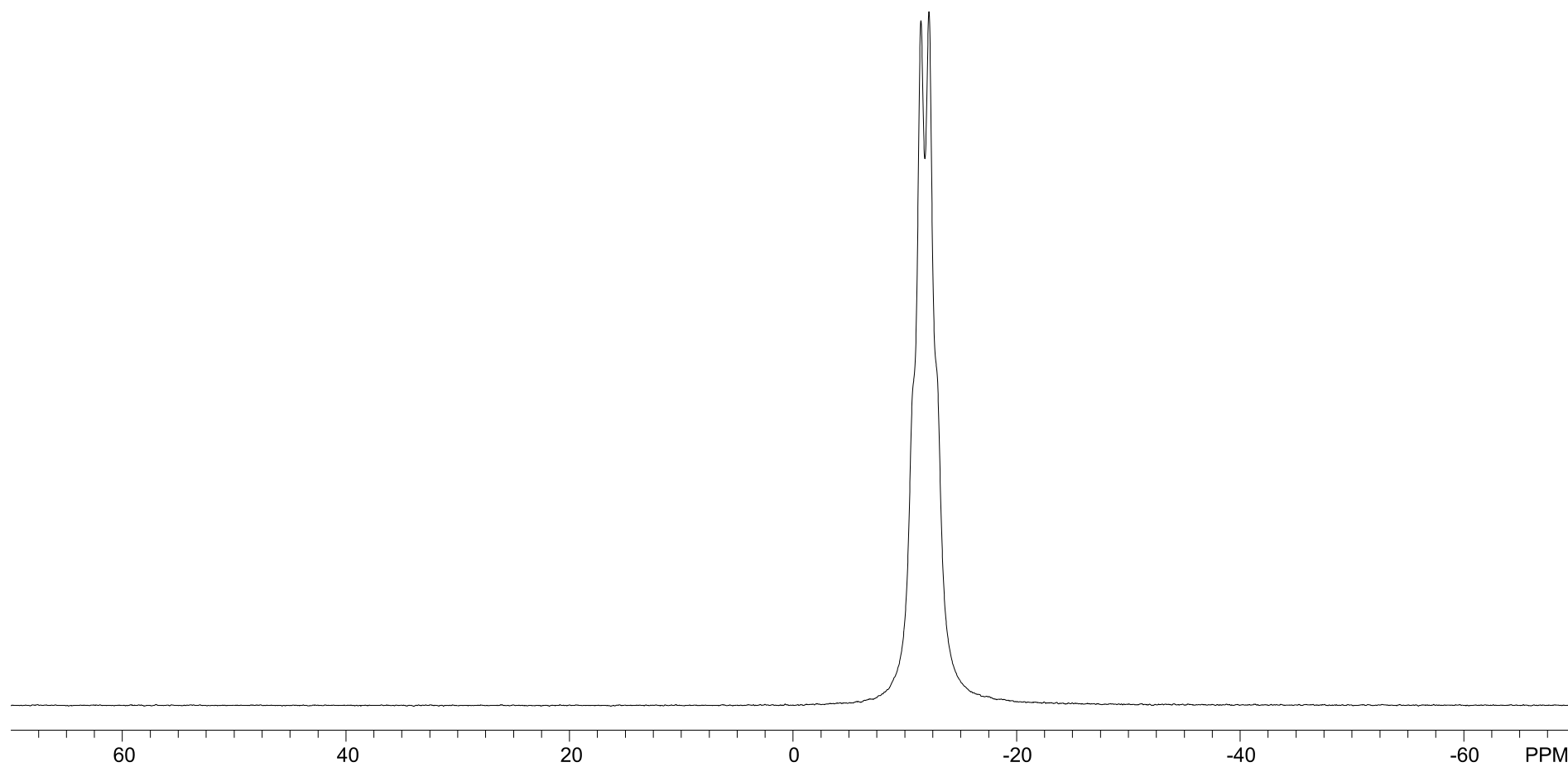
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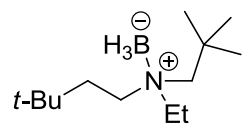
^{11}B NMR (128 MHz),
 CDCl_3



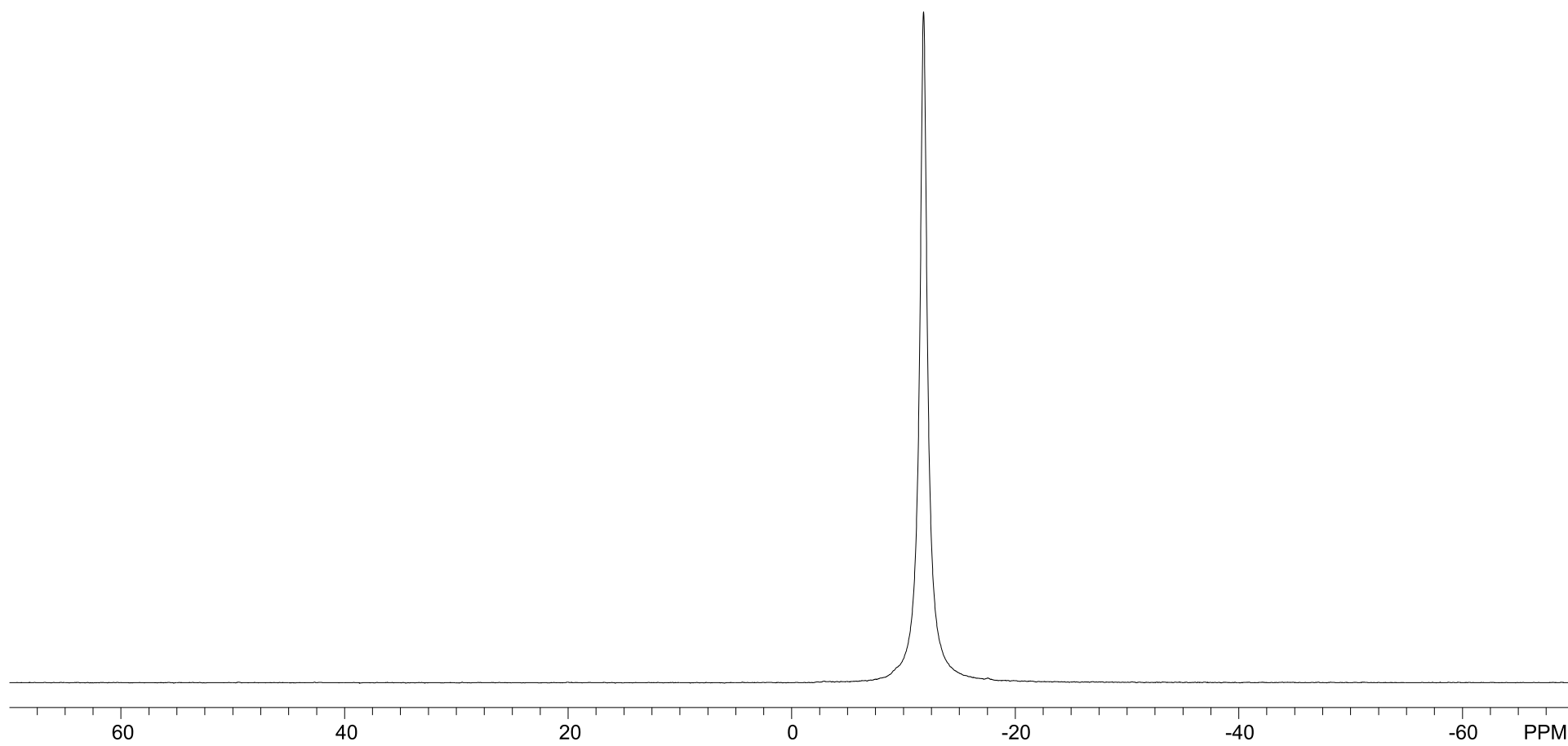
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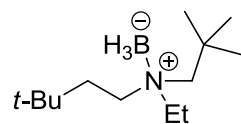
$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3



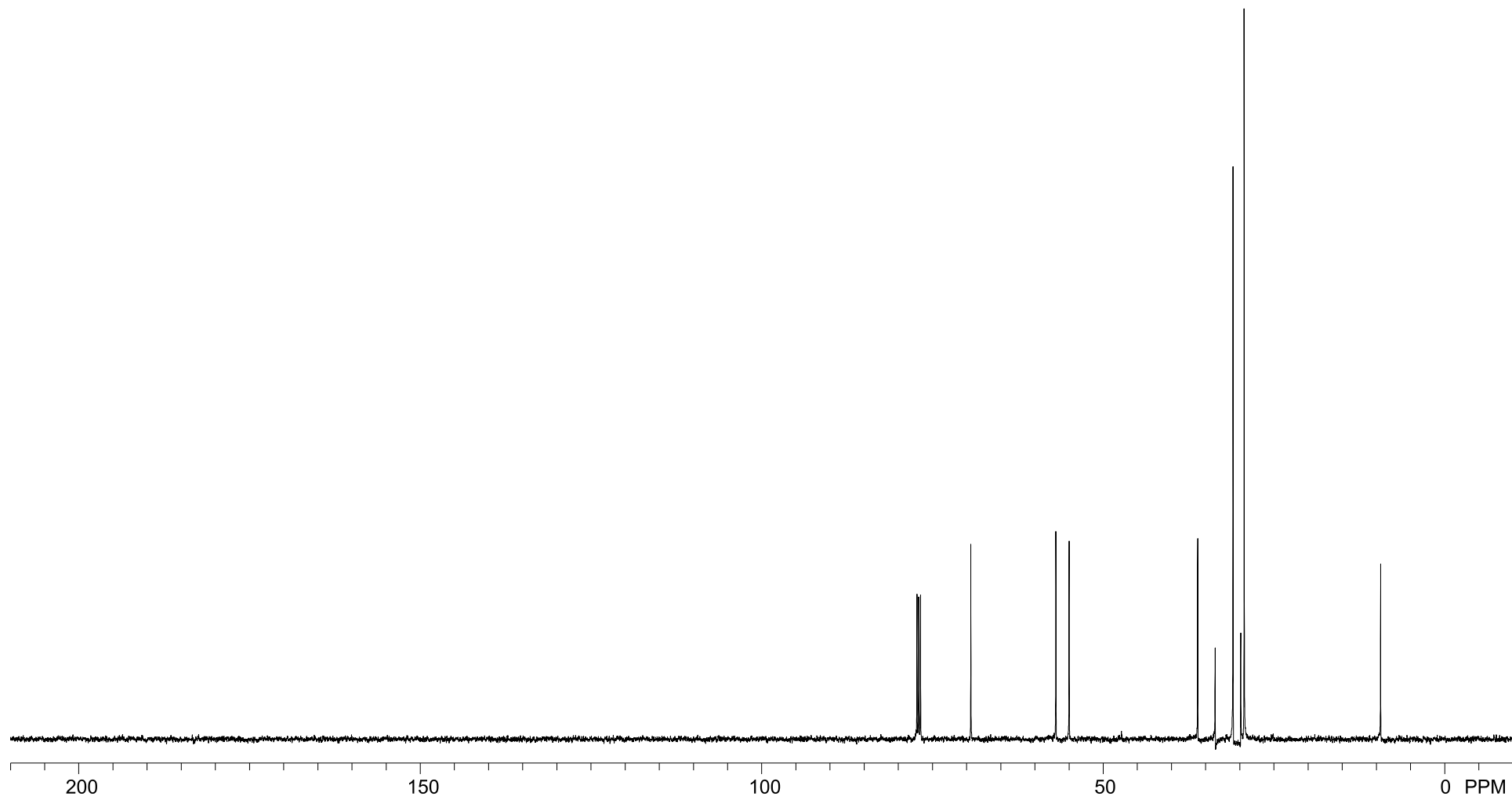
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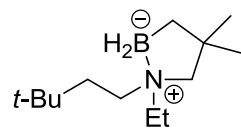
$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CDCl_3



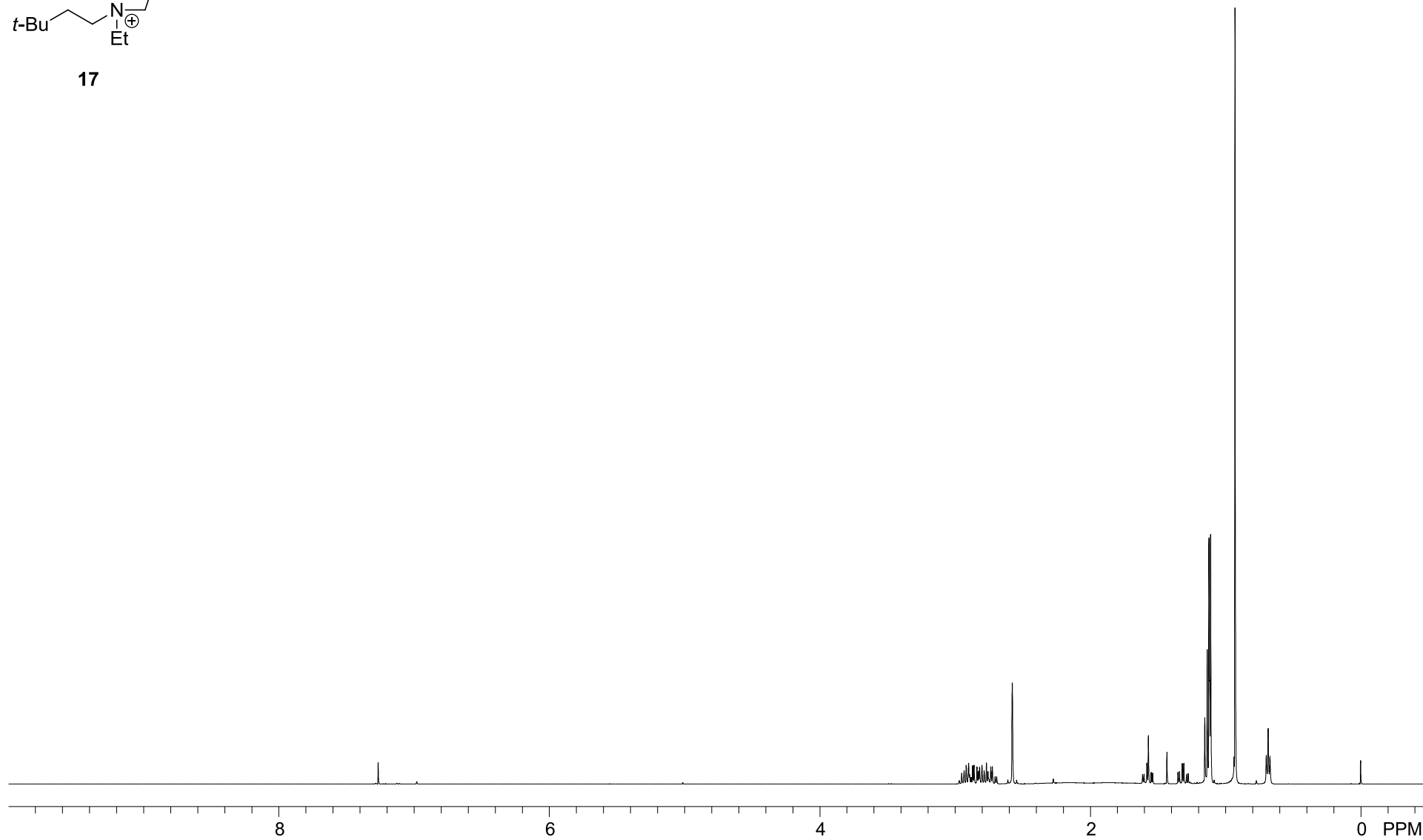
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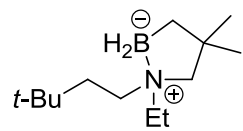
^1H NMR (500 MHz),
 CDCl_3



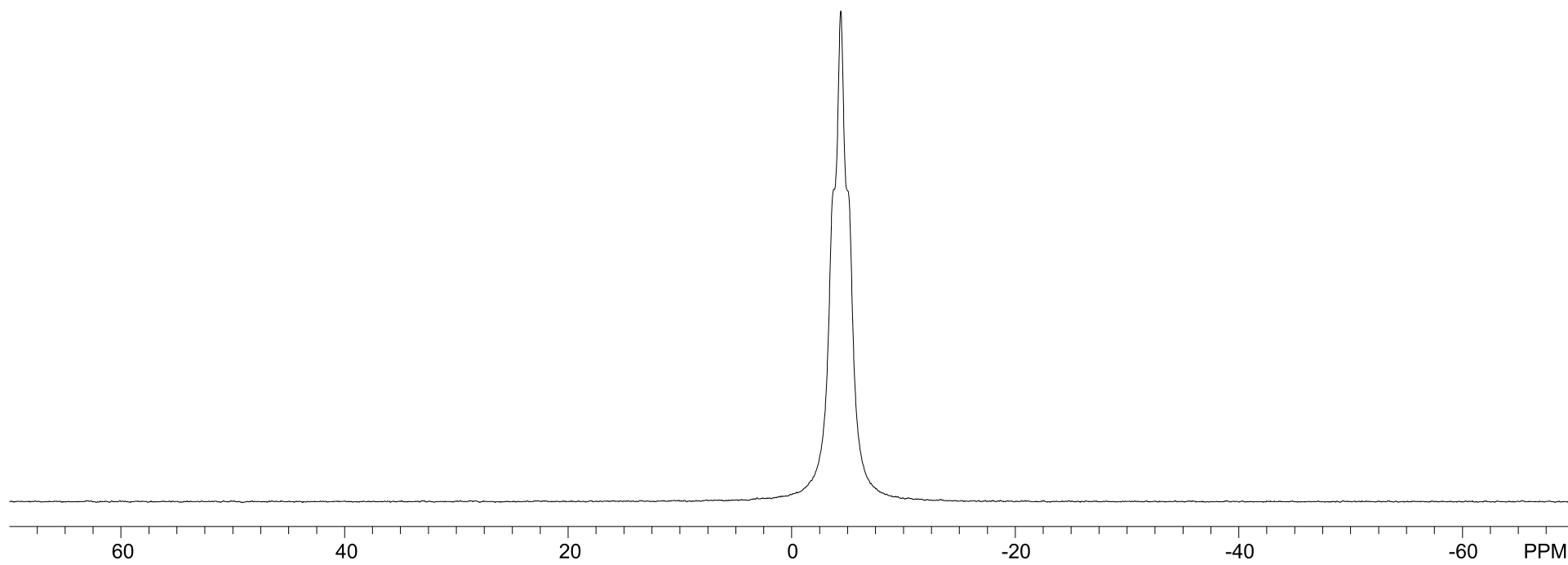
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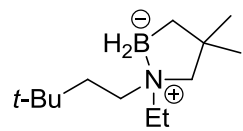
^{11}B NMR (128 MHz),
 CDCl_3



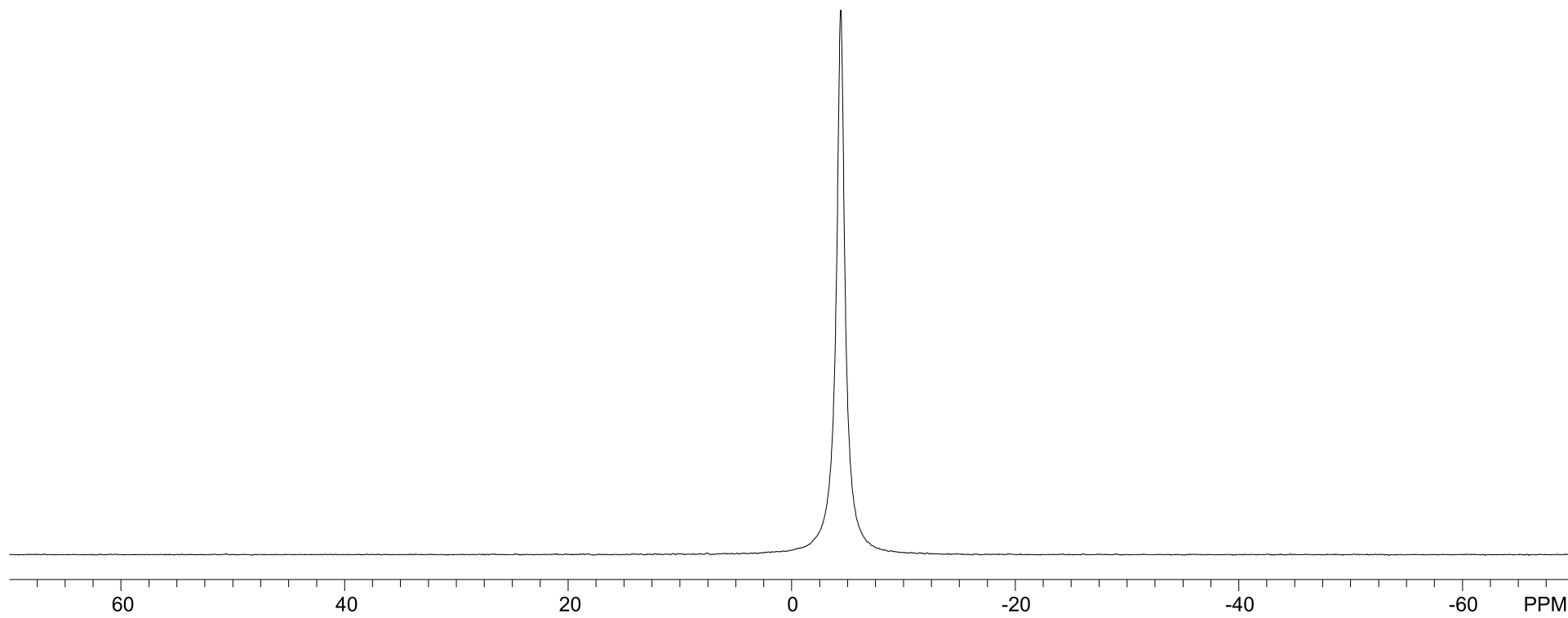
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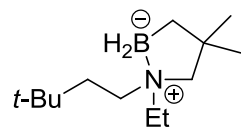
$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3



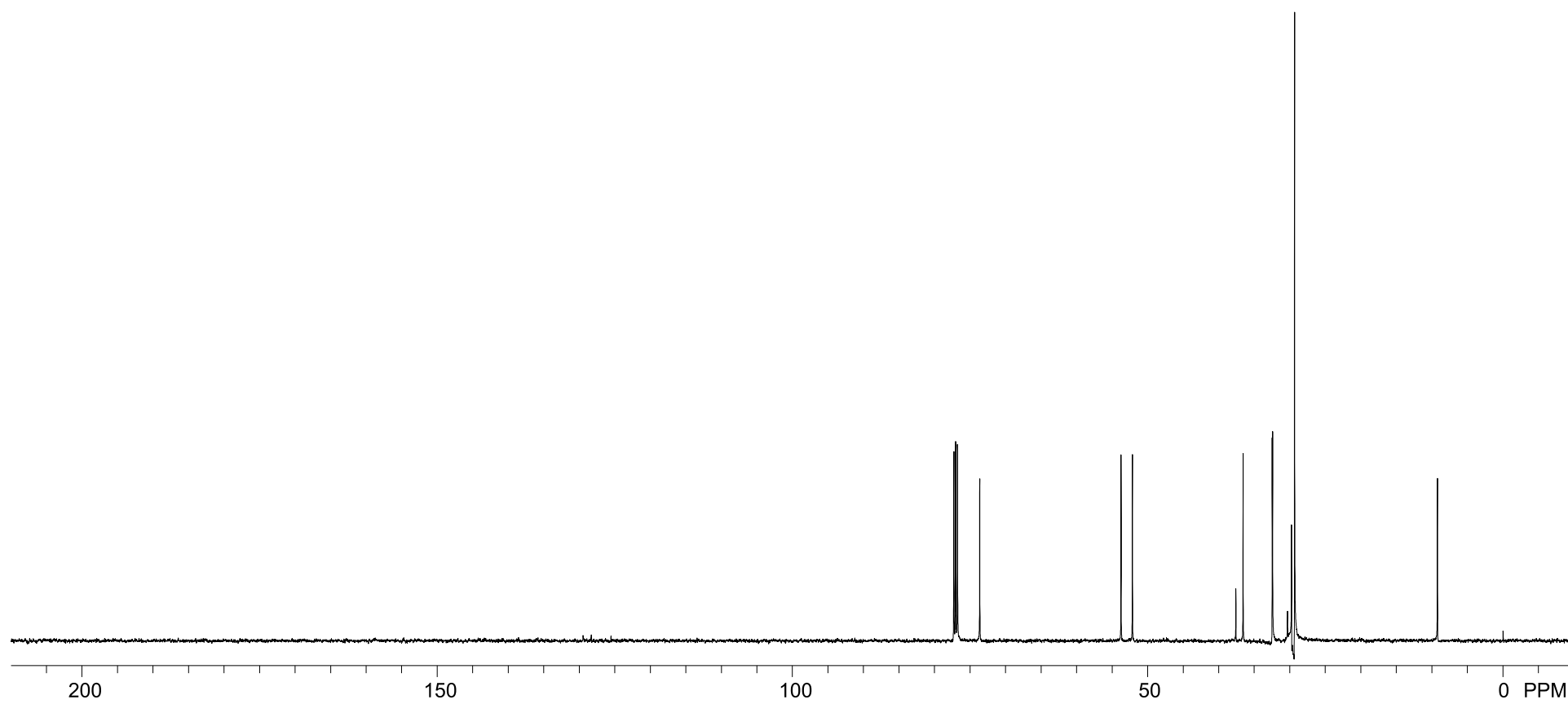
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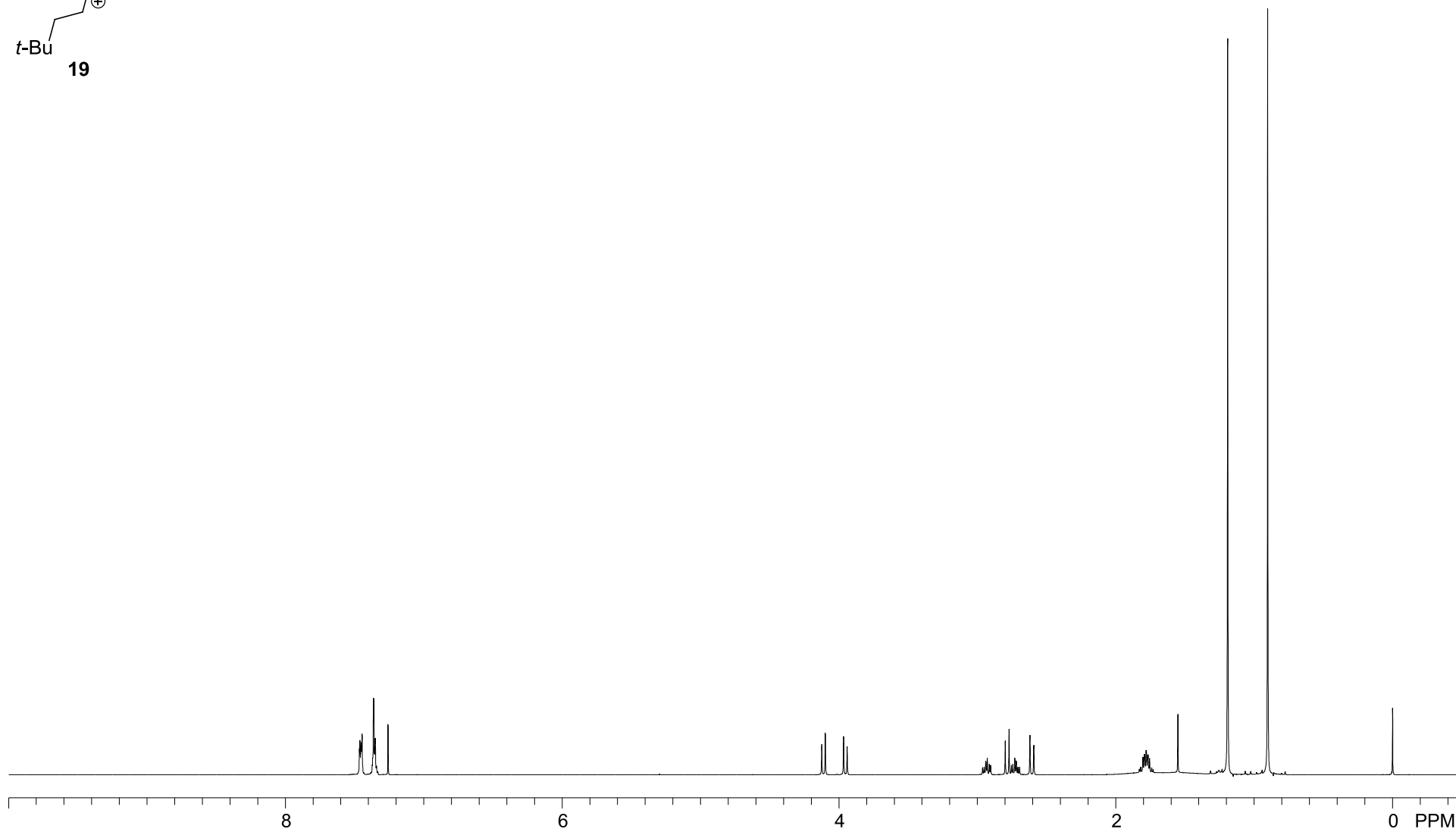
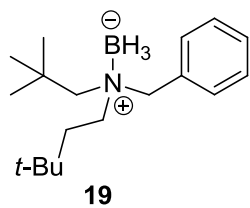
$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CDCl_3



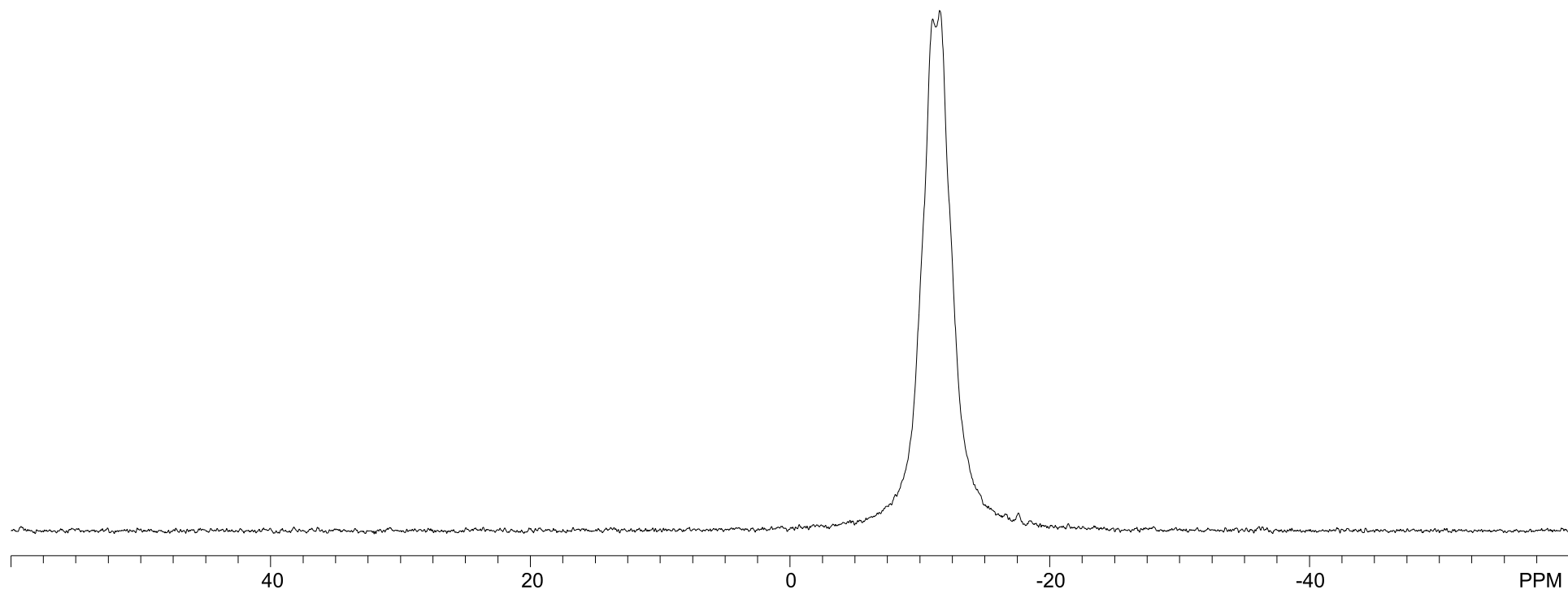
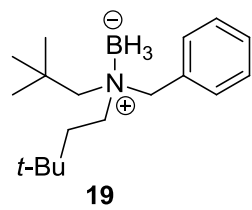
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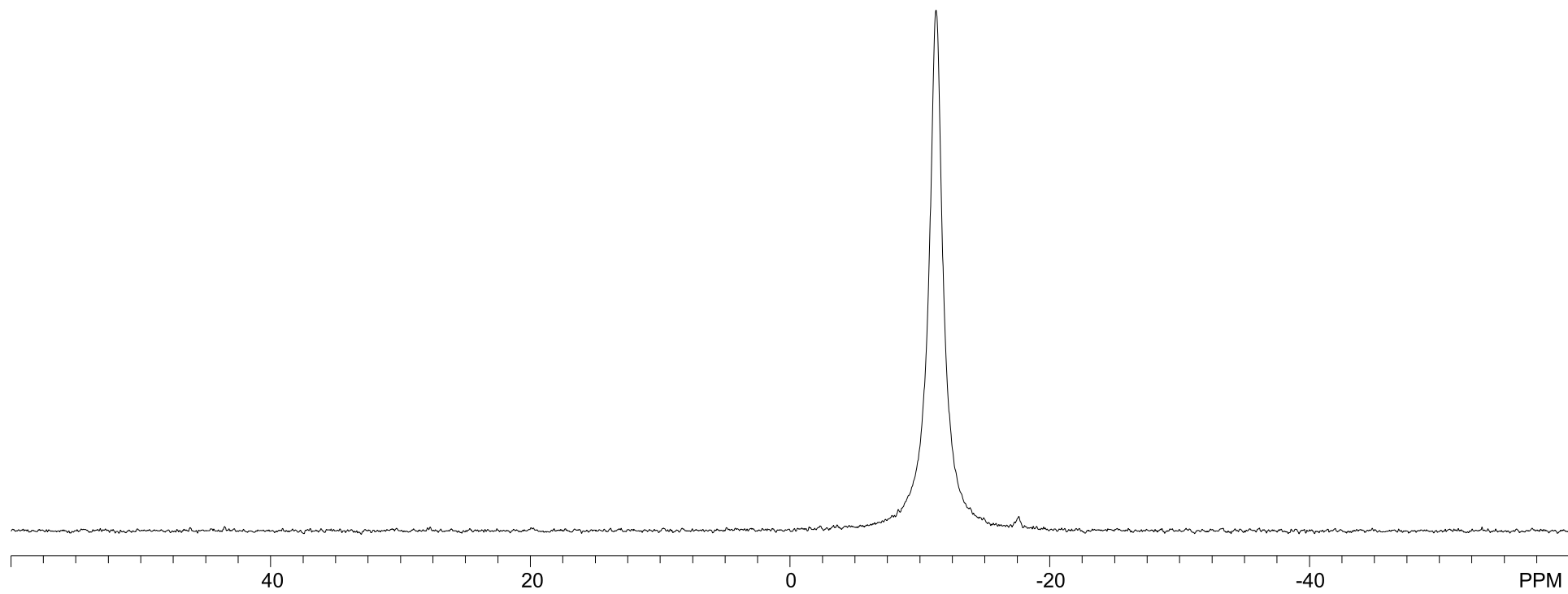
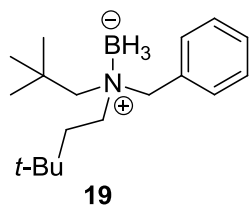
^1H NMR (500 MHz),
 CDCl_3



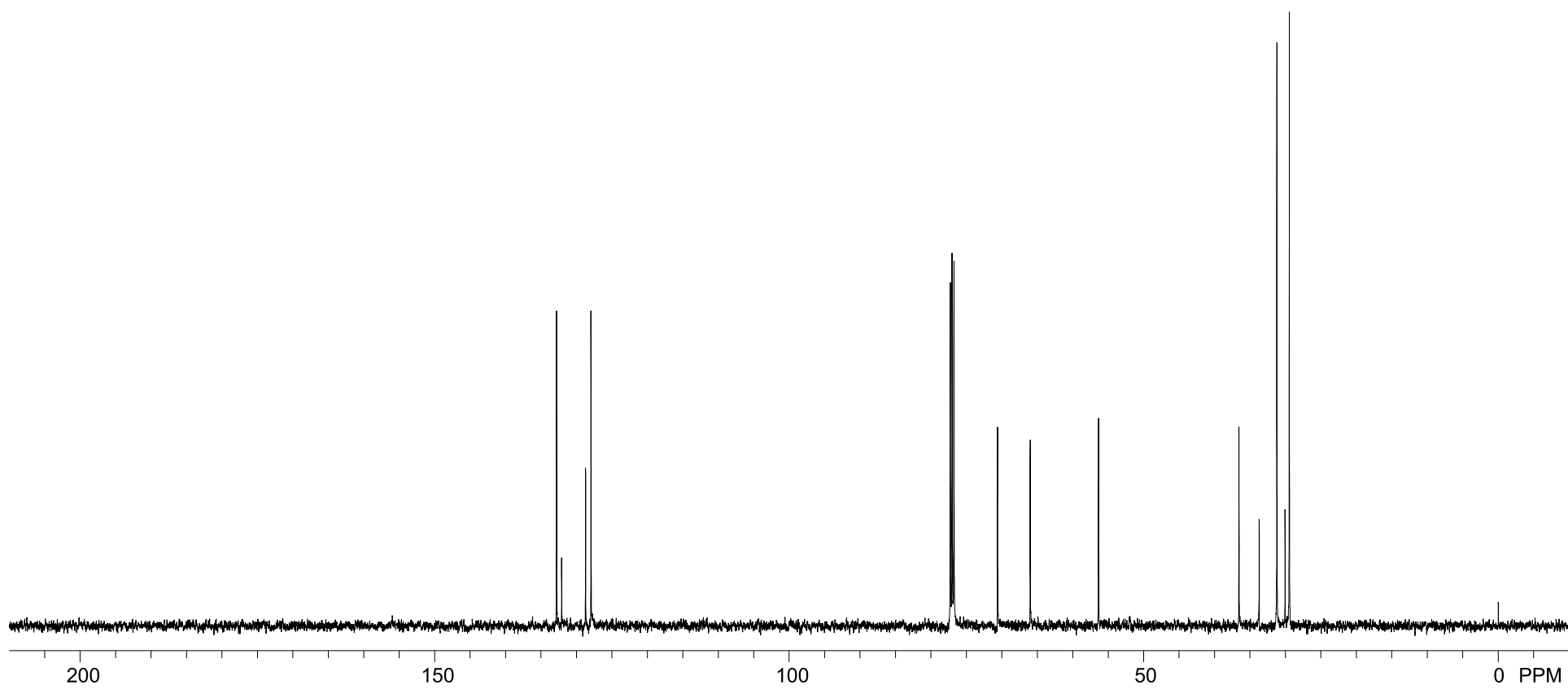
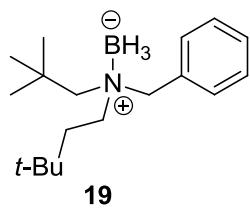
^{11}B NMR (128 MHz),
 CDCl_3



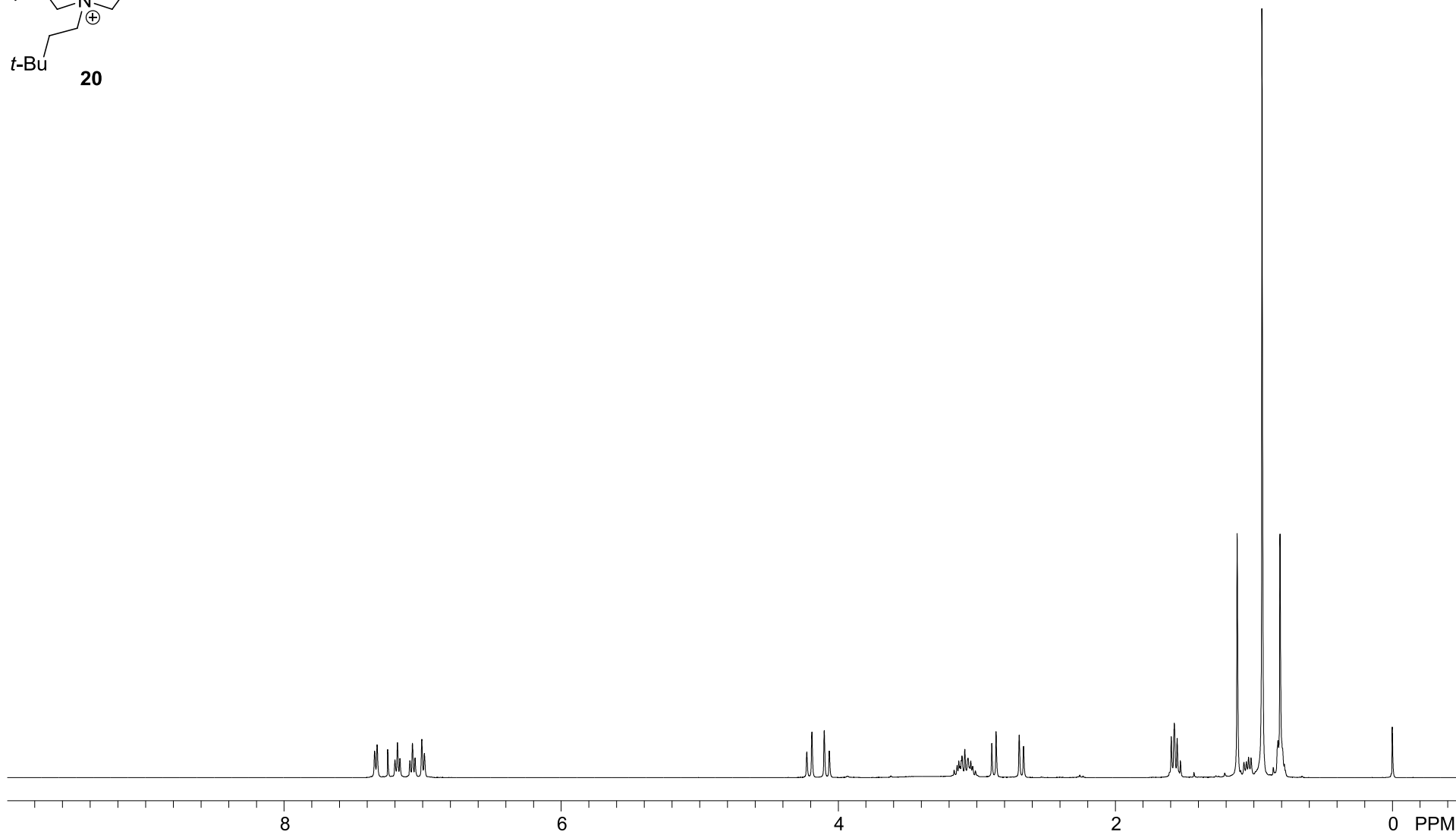
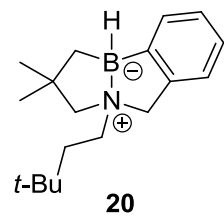
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 CDCl_3



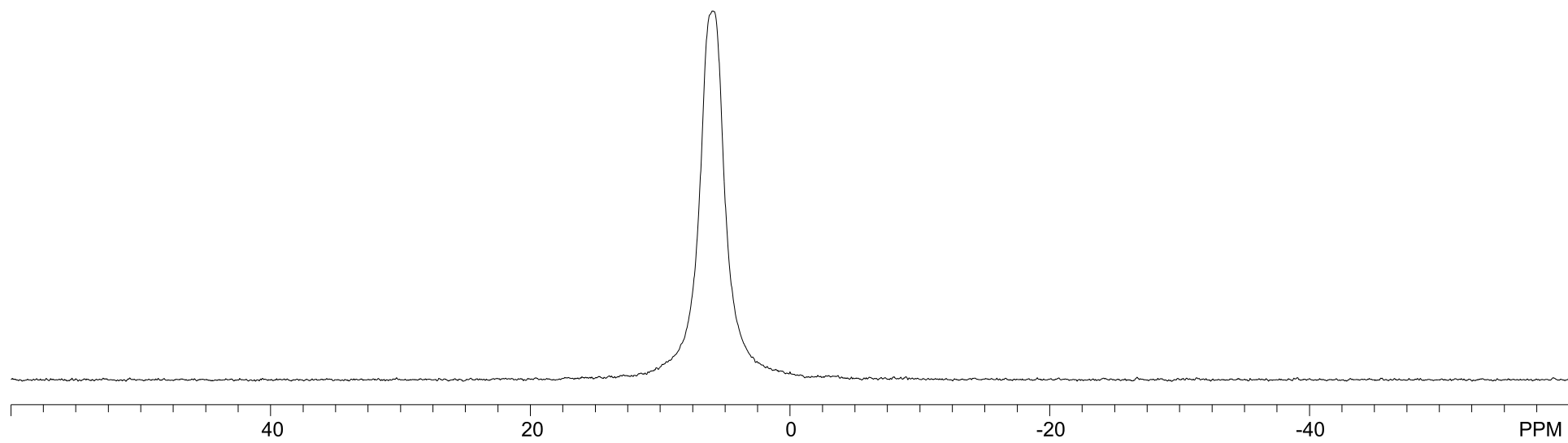
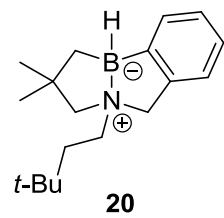
$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CDCl_3



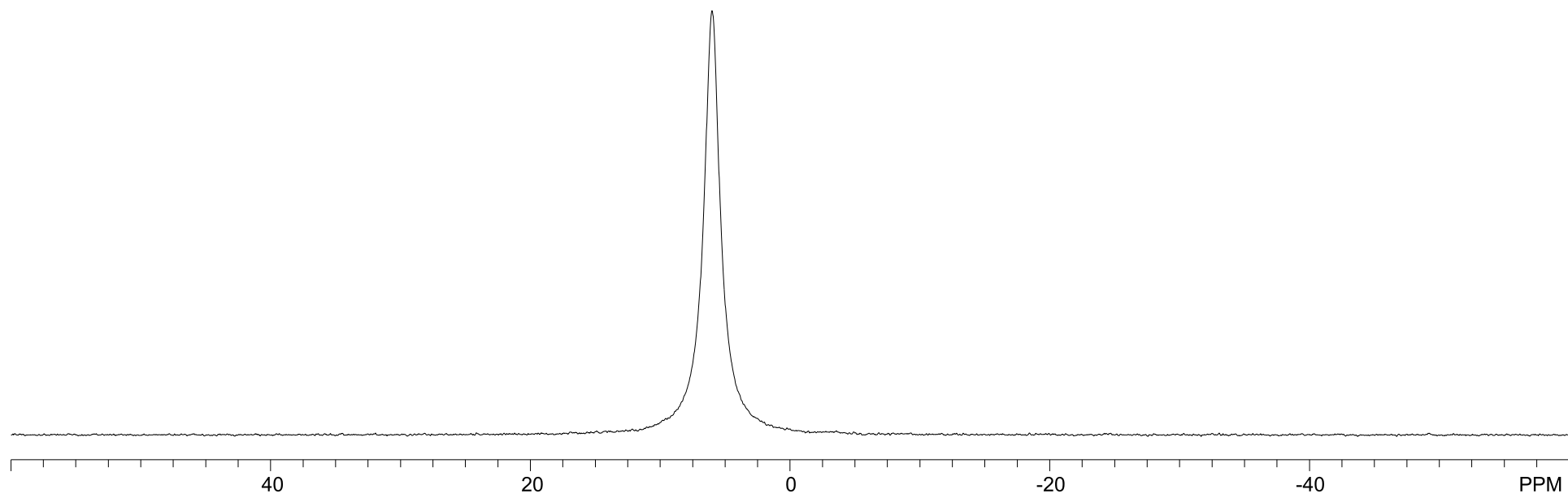
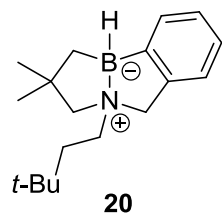
^1H NMR (400 MHz),
 CDCl_3



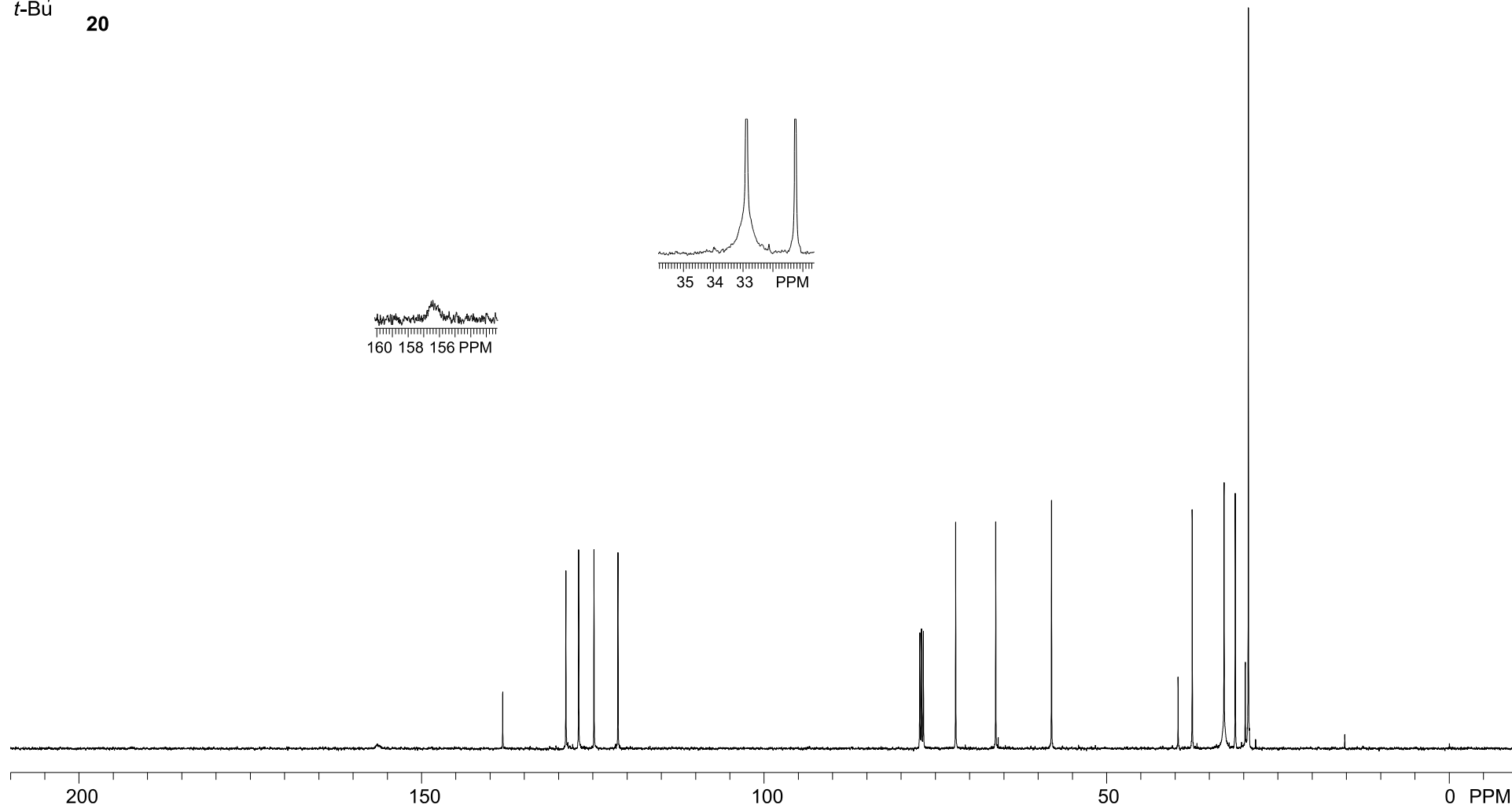
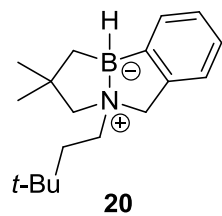
^{11}B NMR (128 MHz),
 CDCl_3



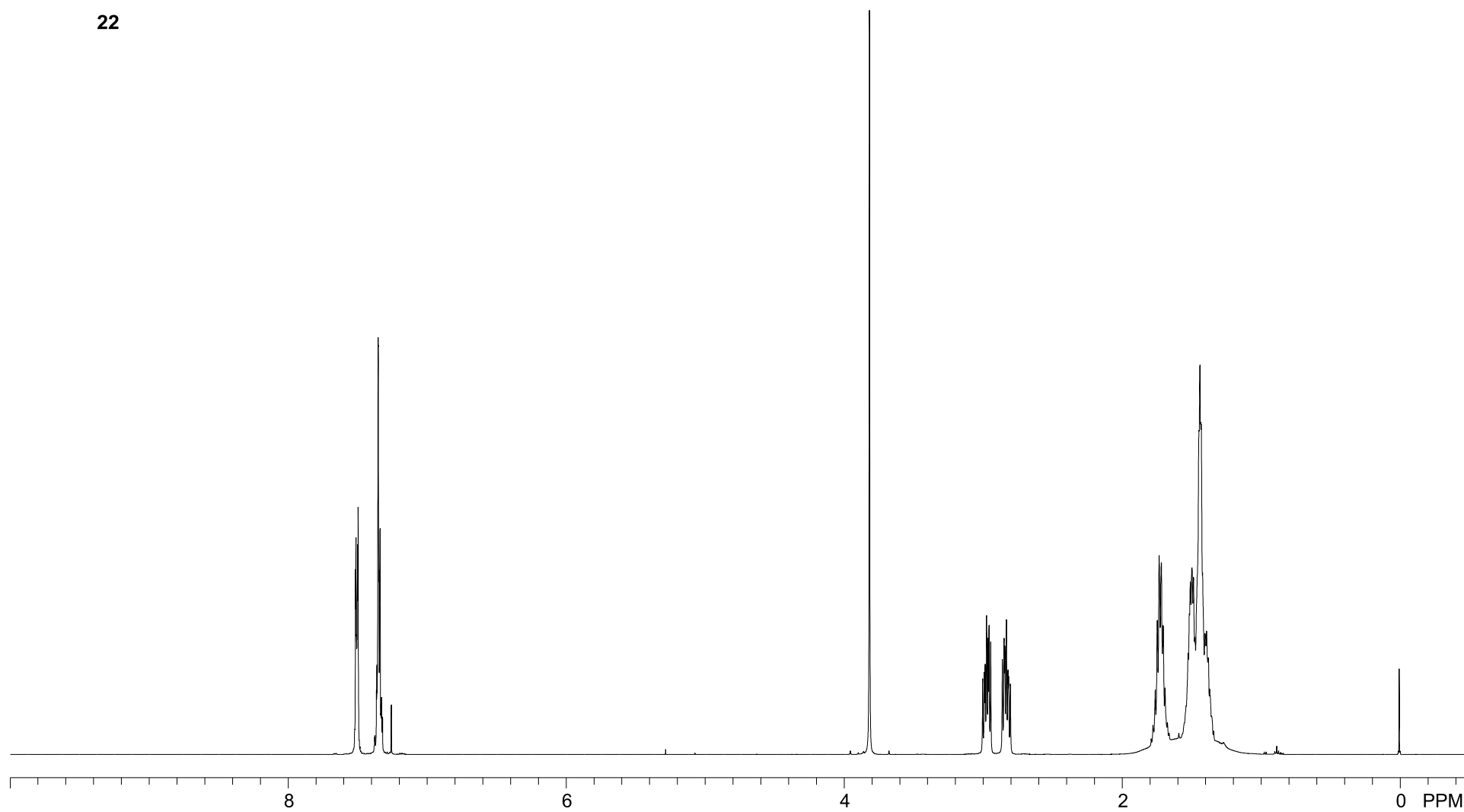
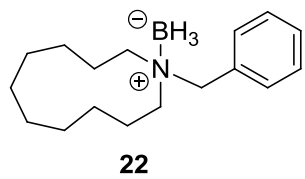
$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3



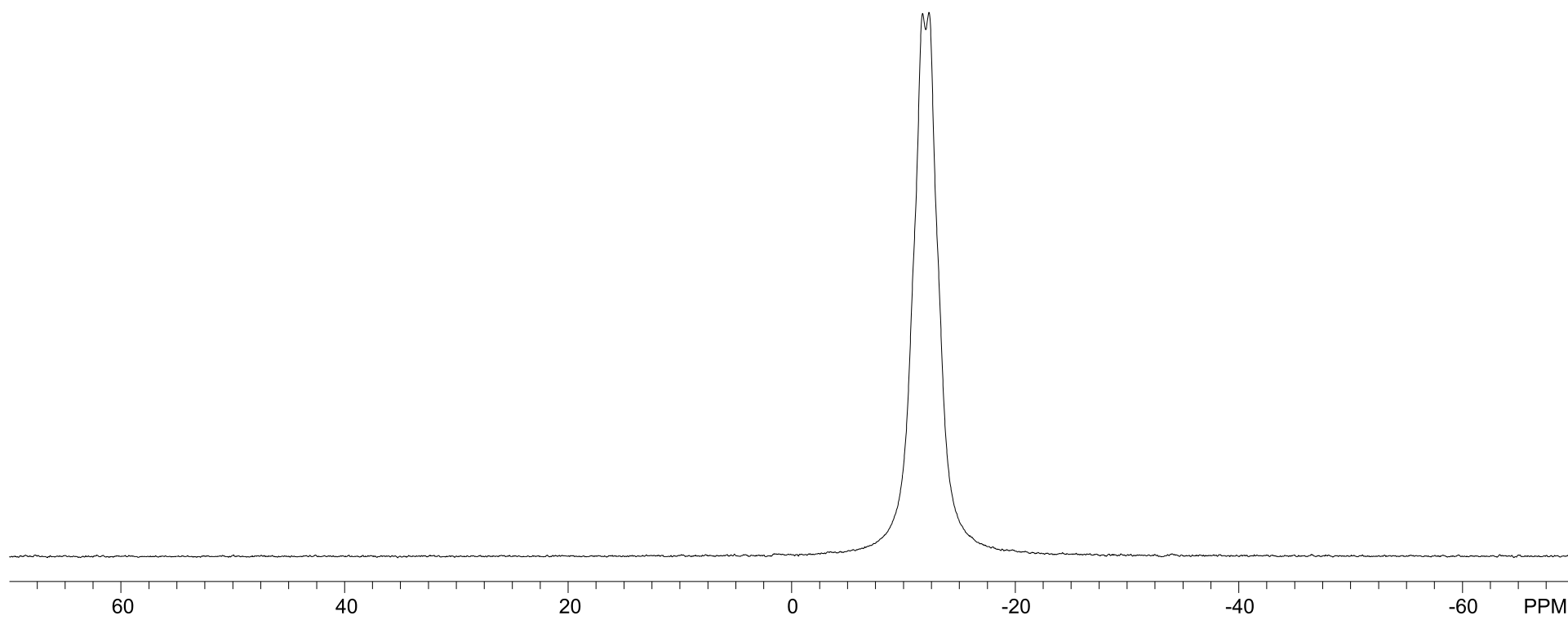
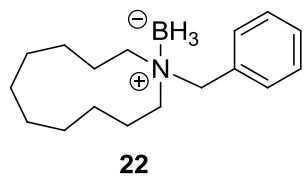
$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CDCl_3



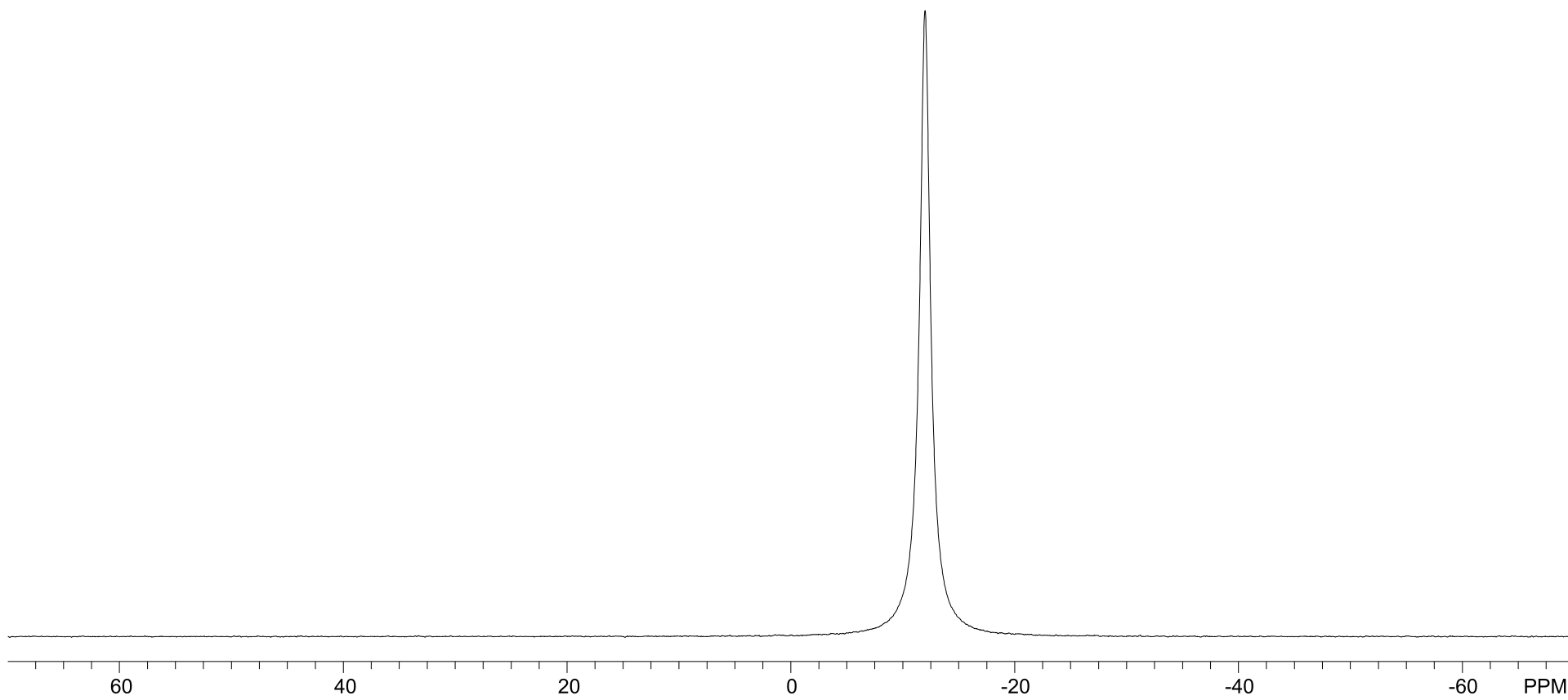
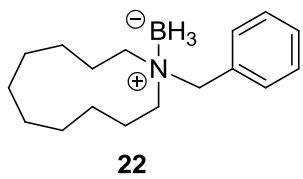
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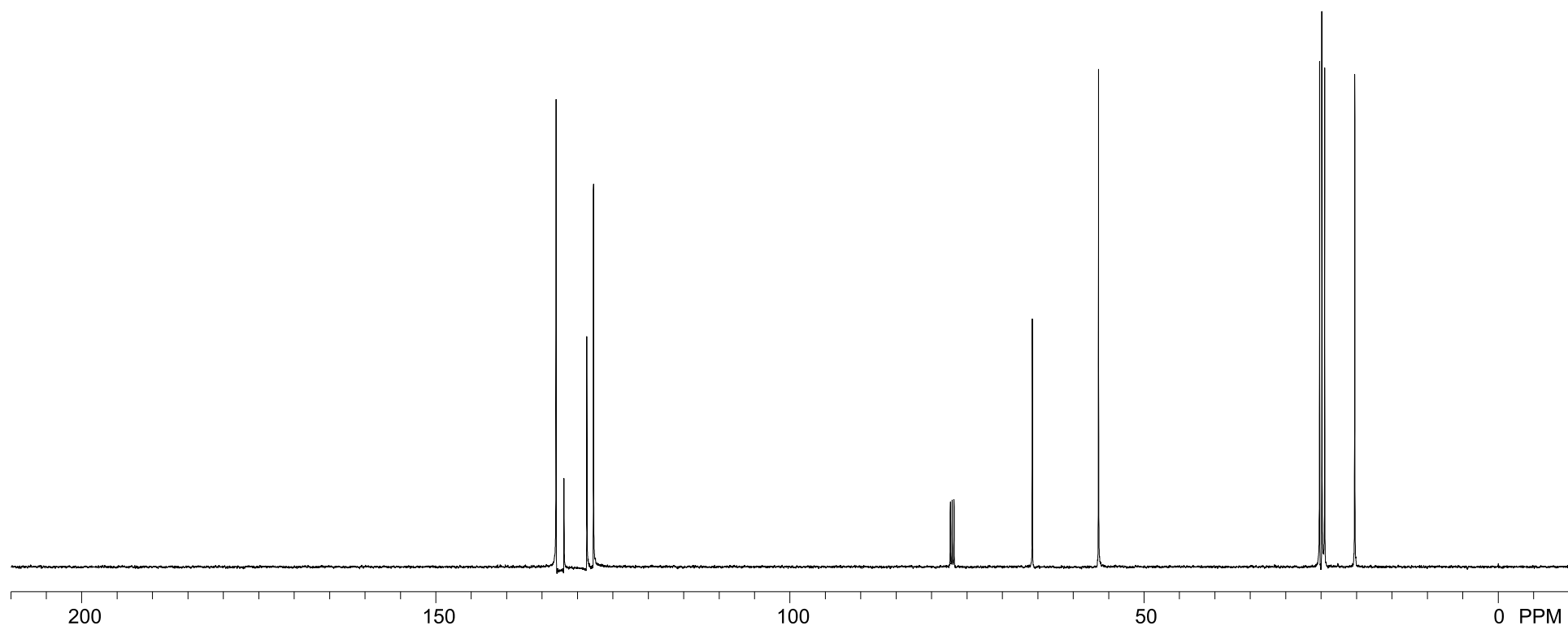
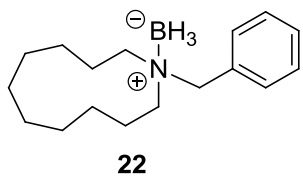
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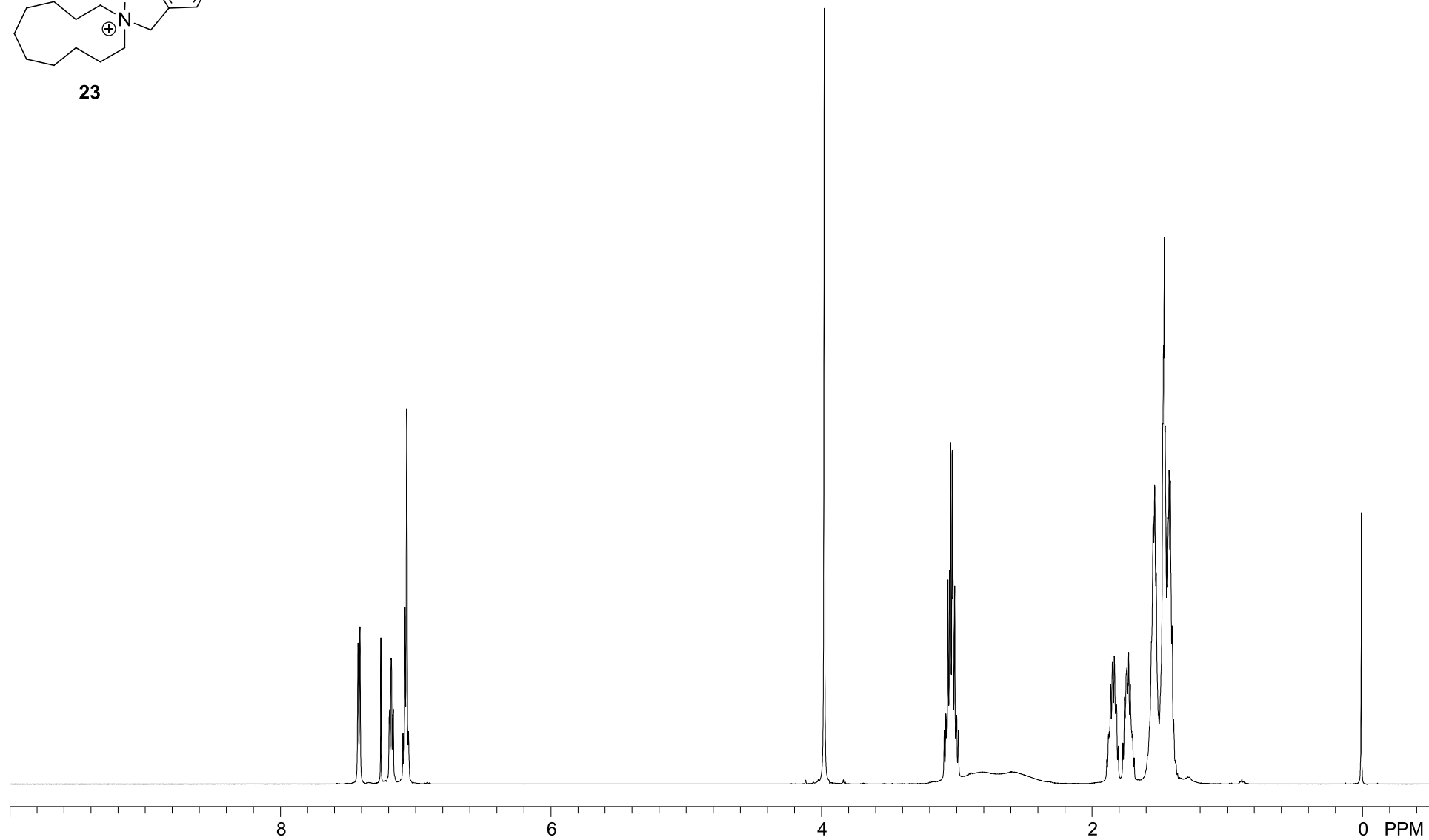
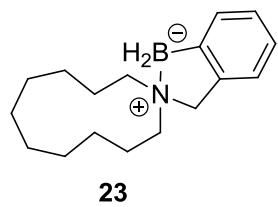
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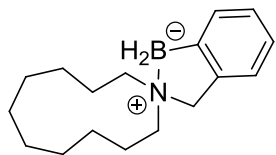
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 CDCl_3



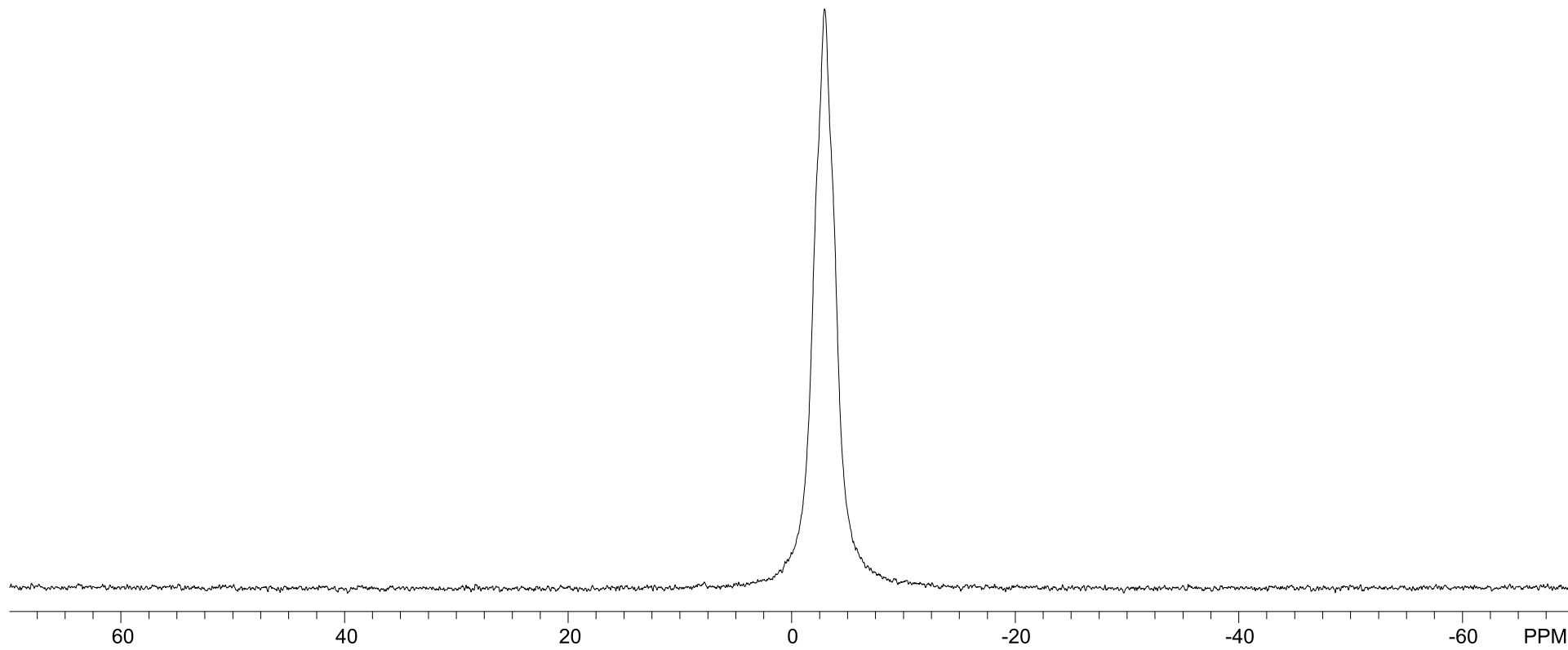
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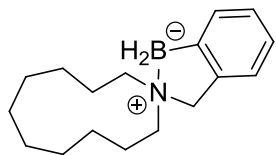
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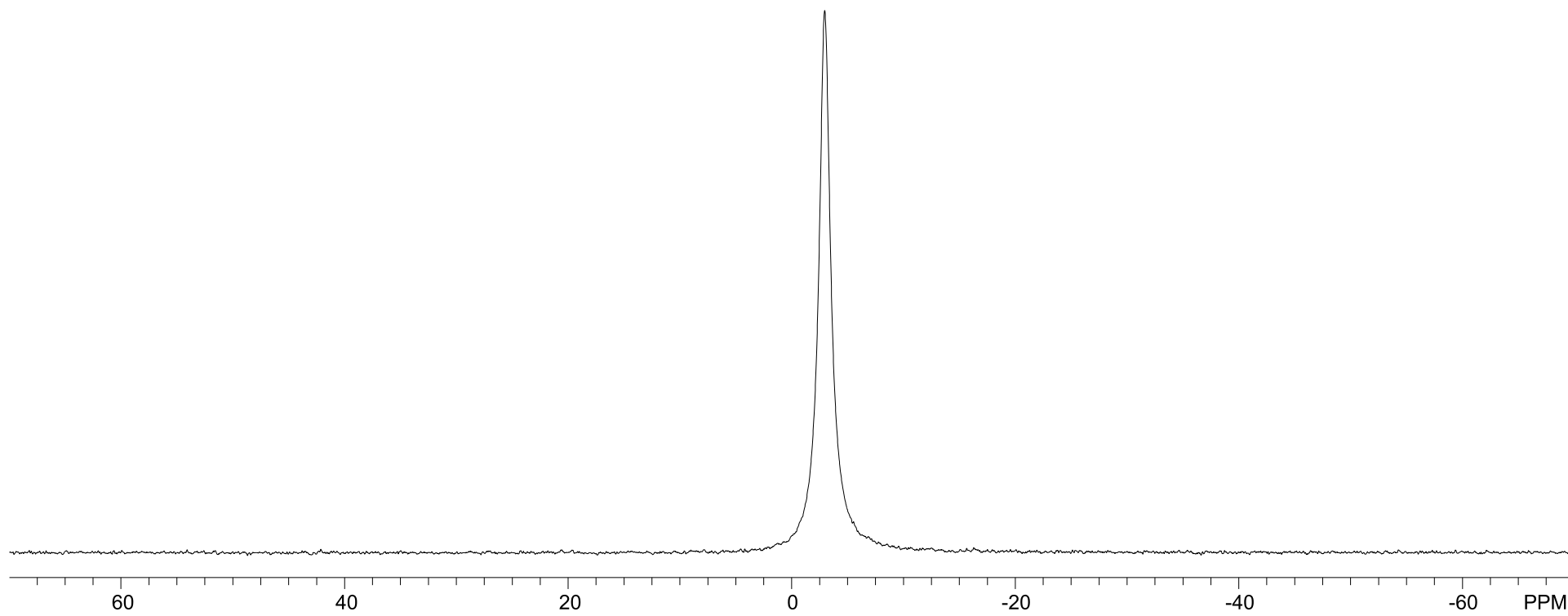
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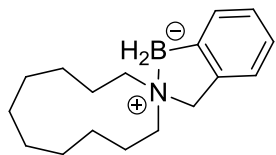
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 CDCl_3



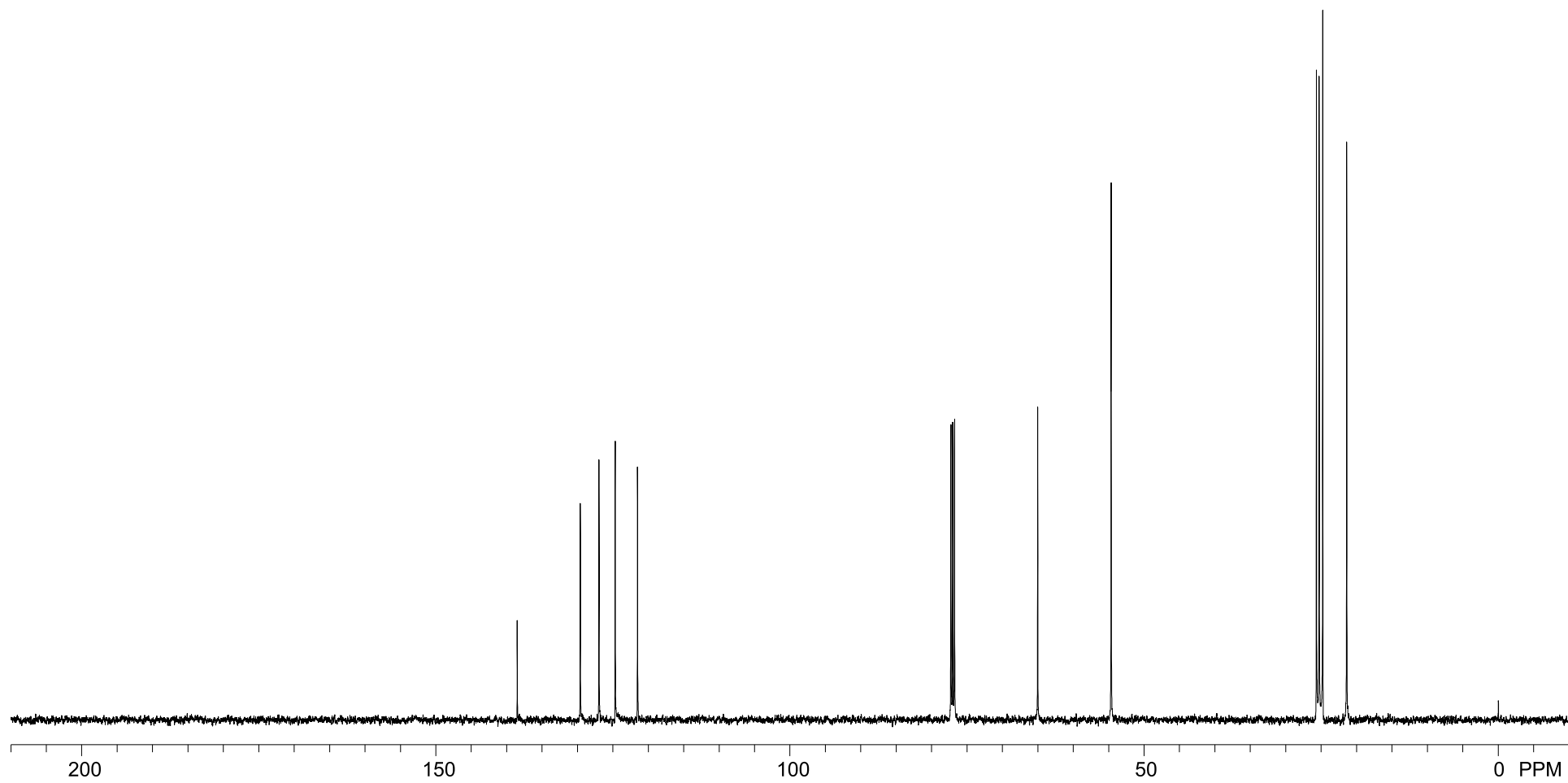
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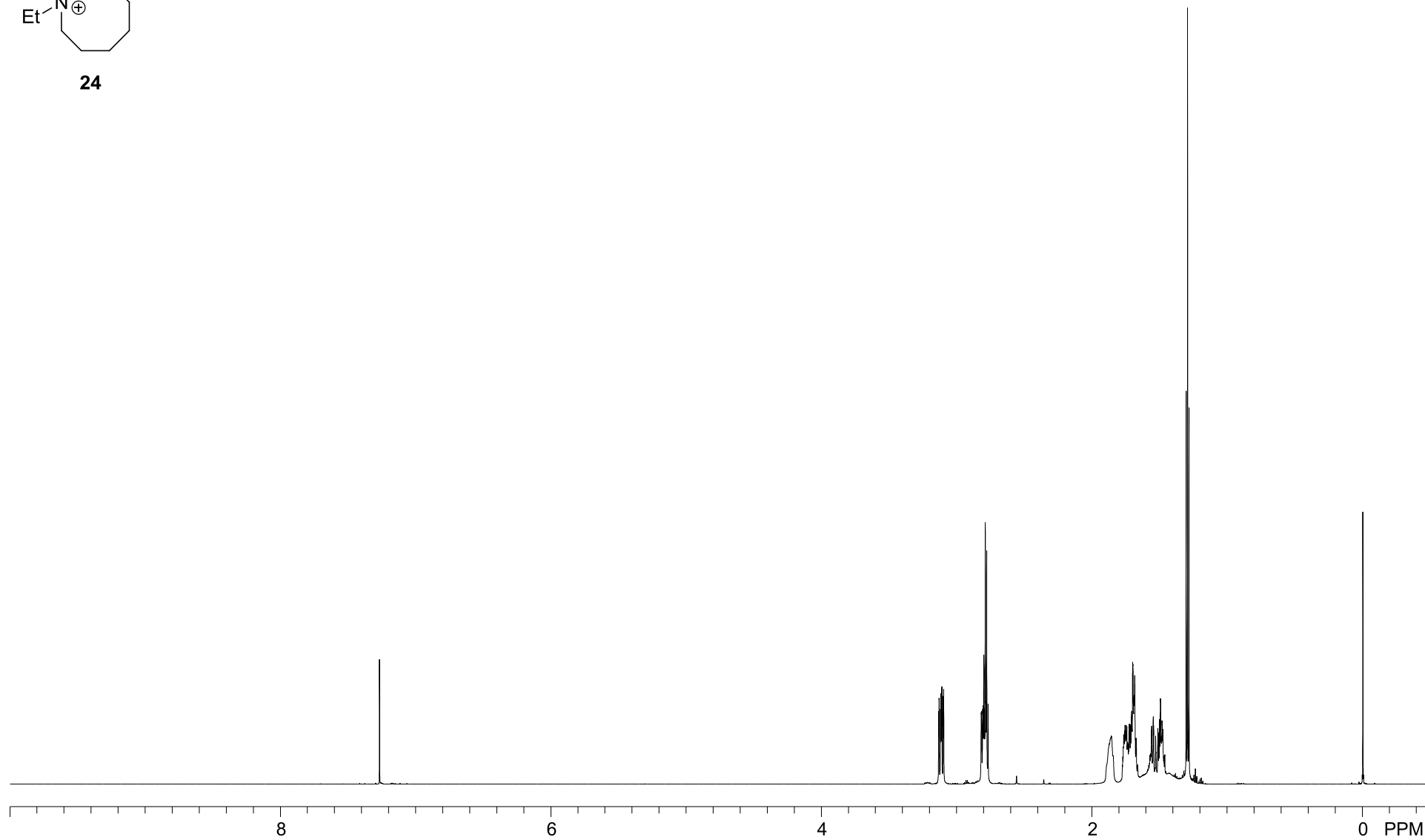
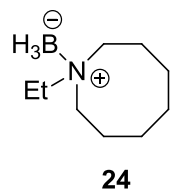
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 CDCl_3



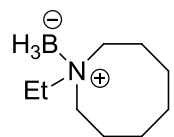
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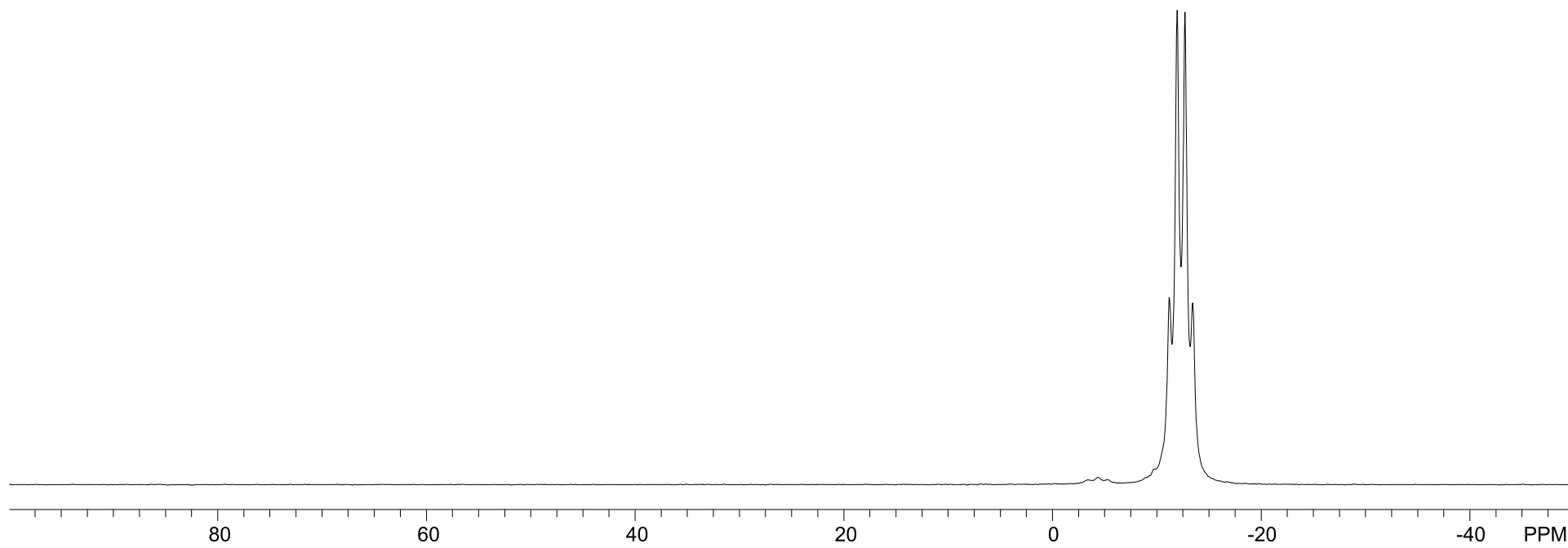
^1H NMR (700 MHz),
 CDCl_3



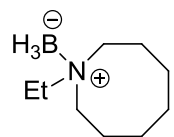
^{11}B NMR (128 MHz),
 CDCl_3



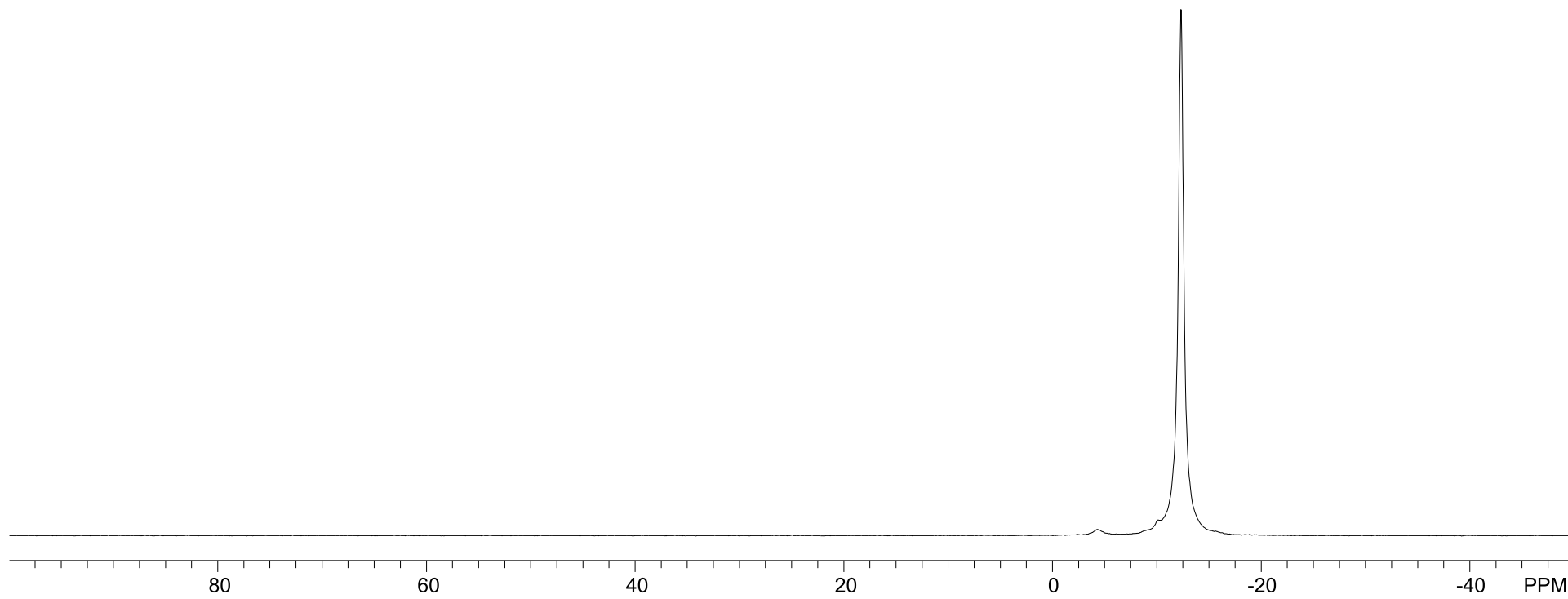
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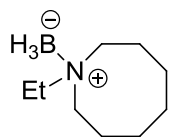
$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3



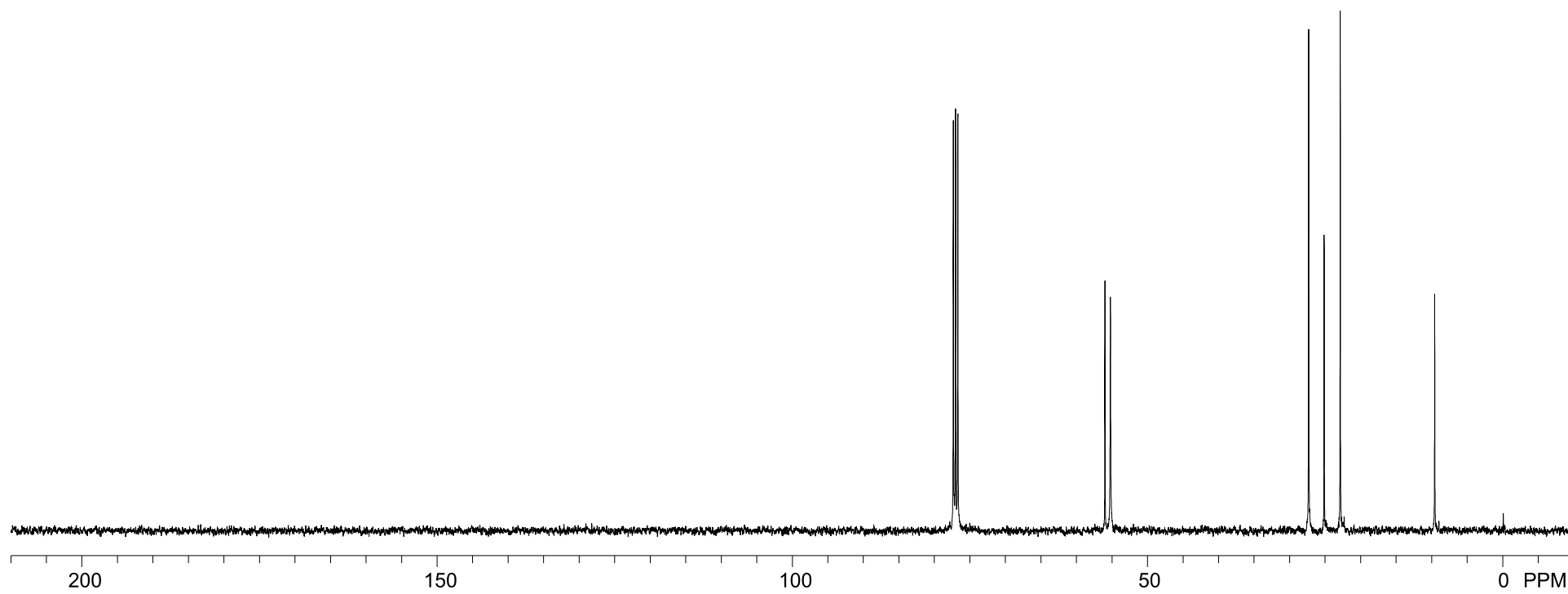
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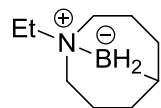
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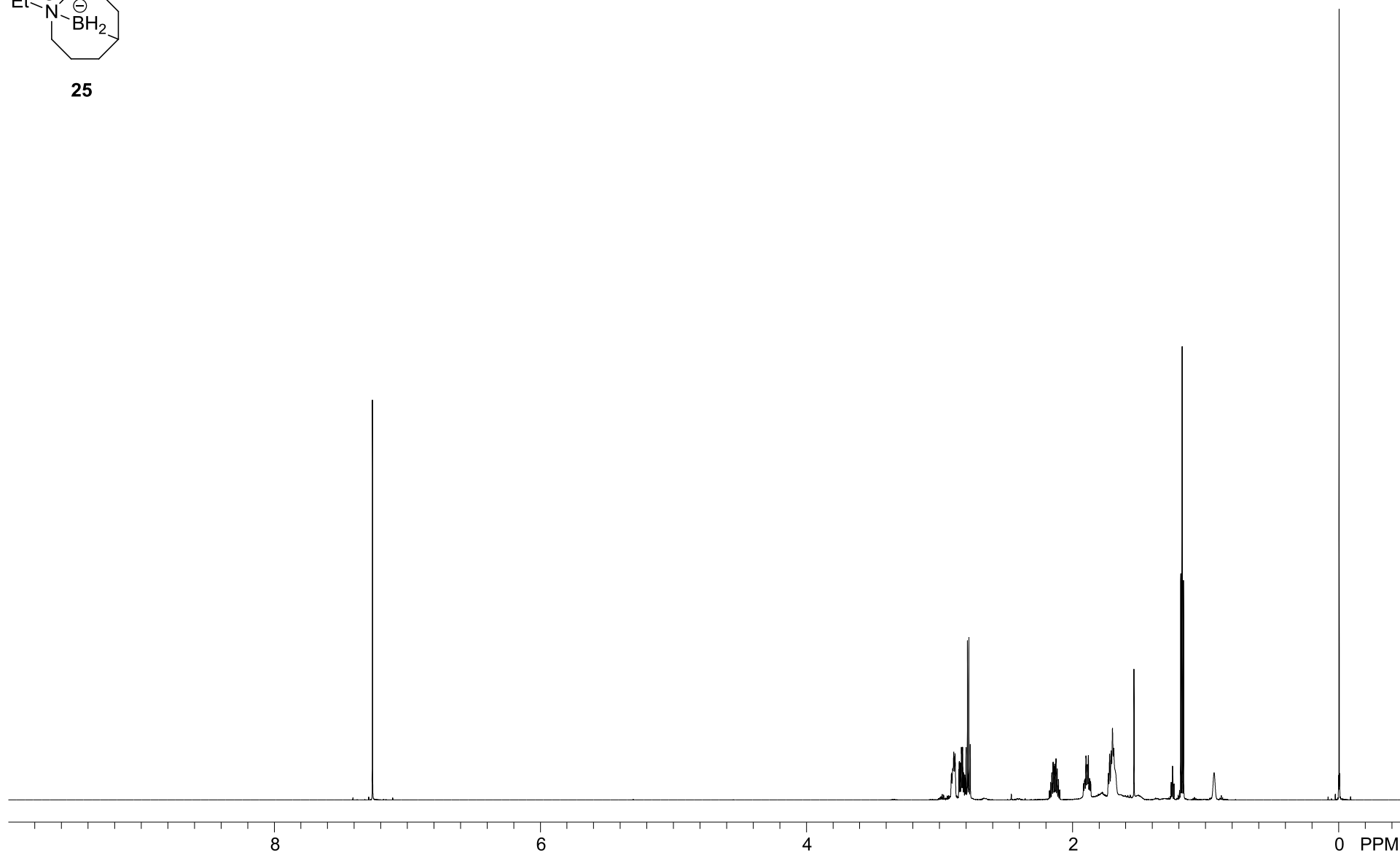
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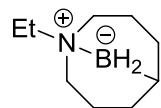
^1H NMR (700 MHz),
 CDCl_3



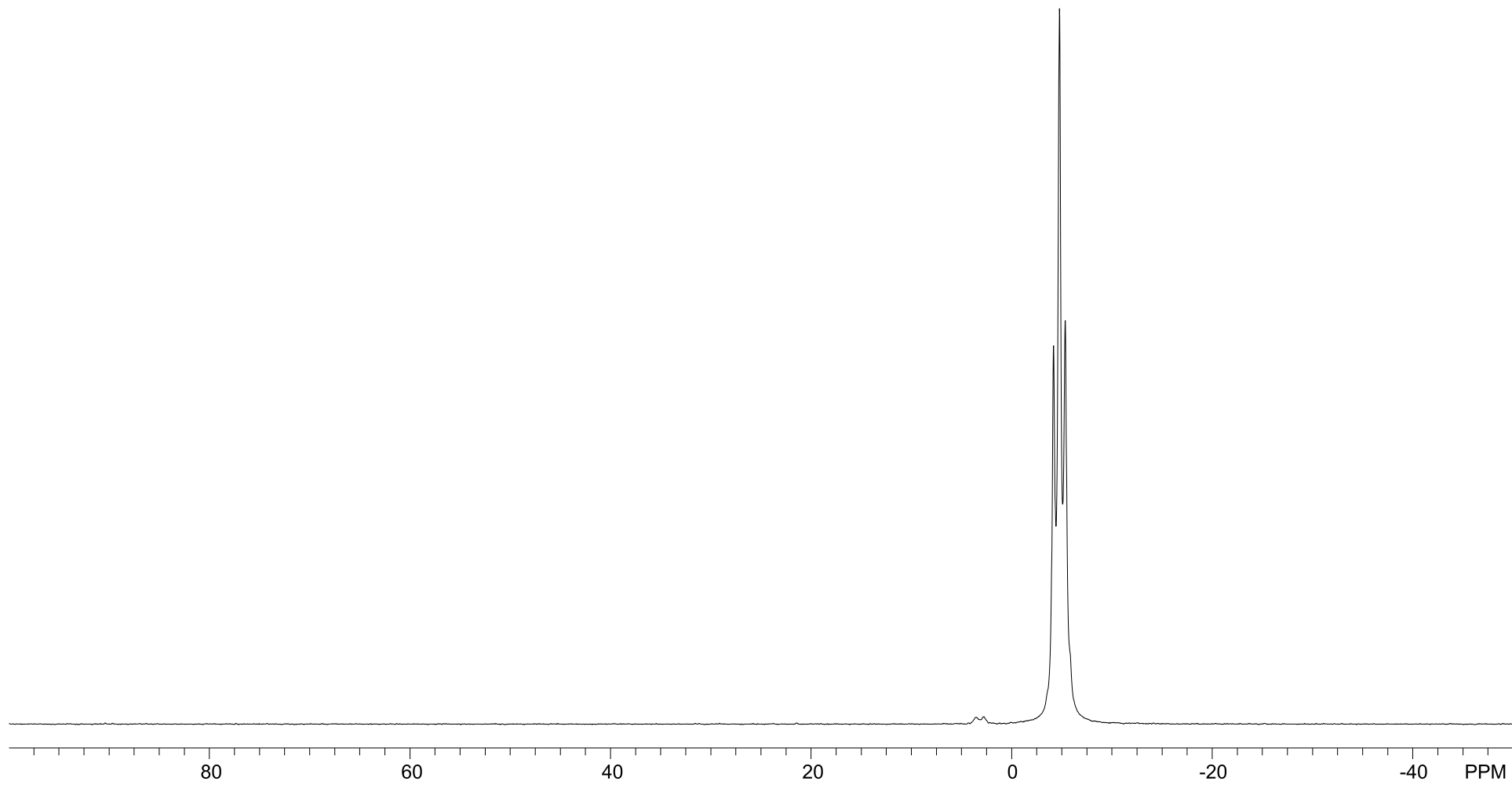
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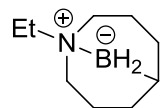
^{11}B NMR (160 MHz),
 CDCl_3



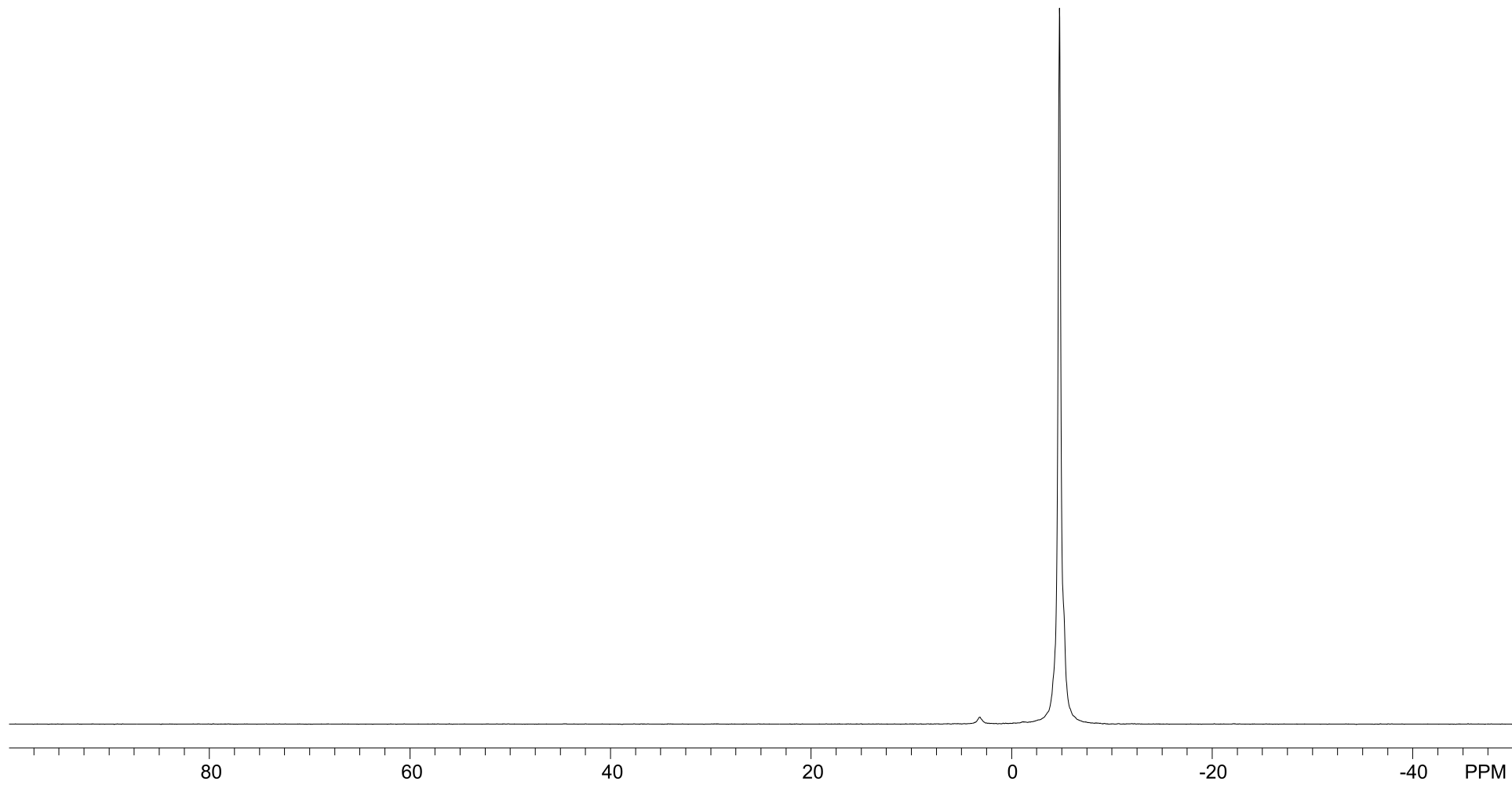
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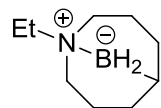
$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz),
 CDCl_3



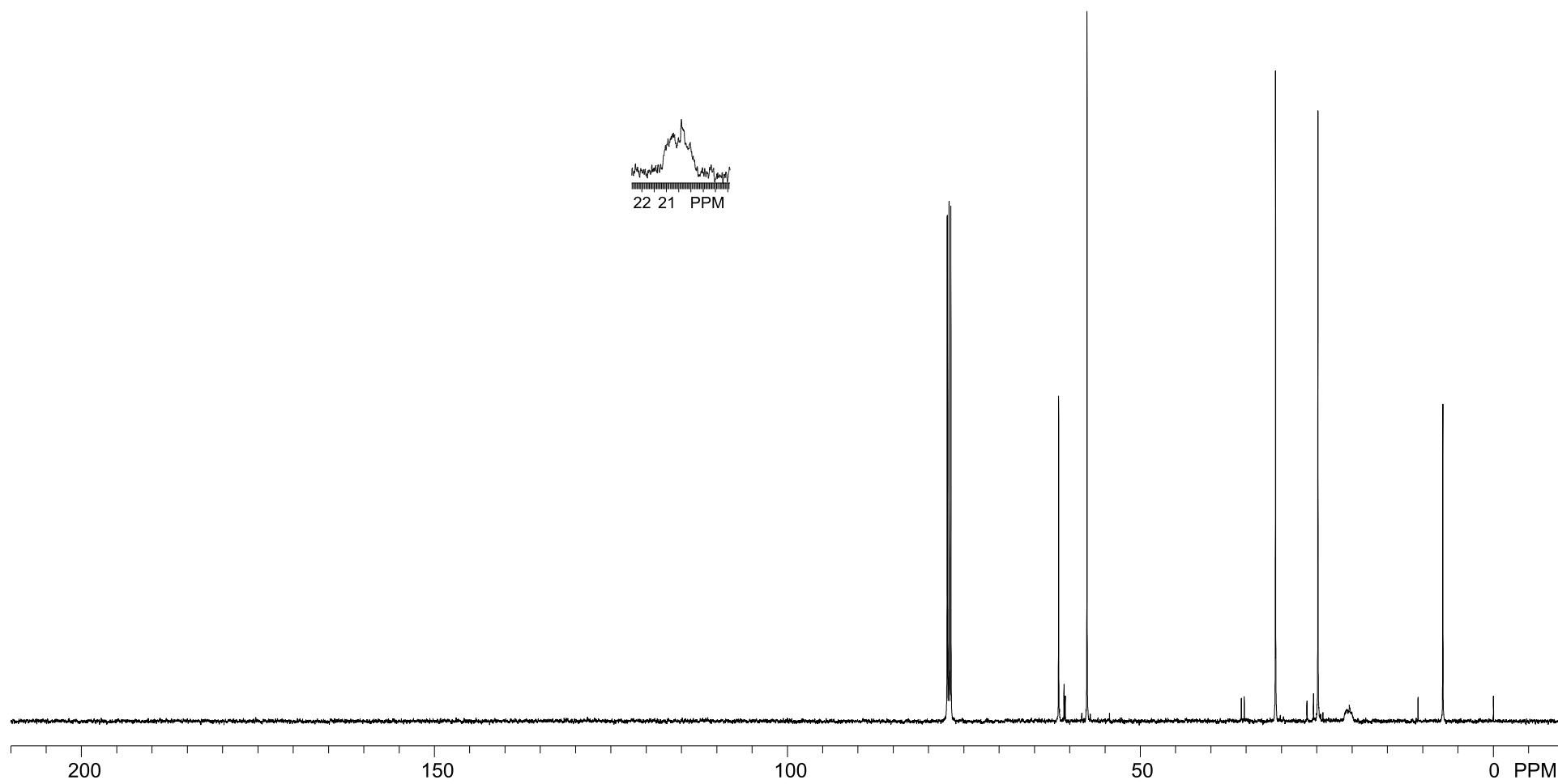
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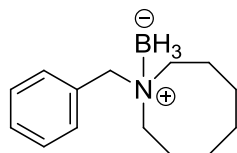
$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CDCl_3



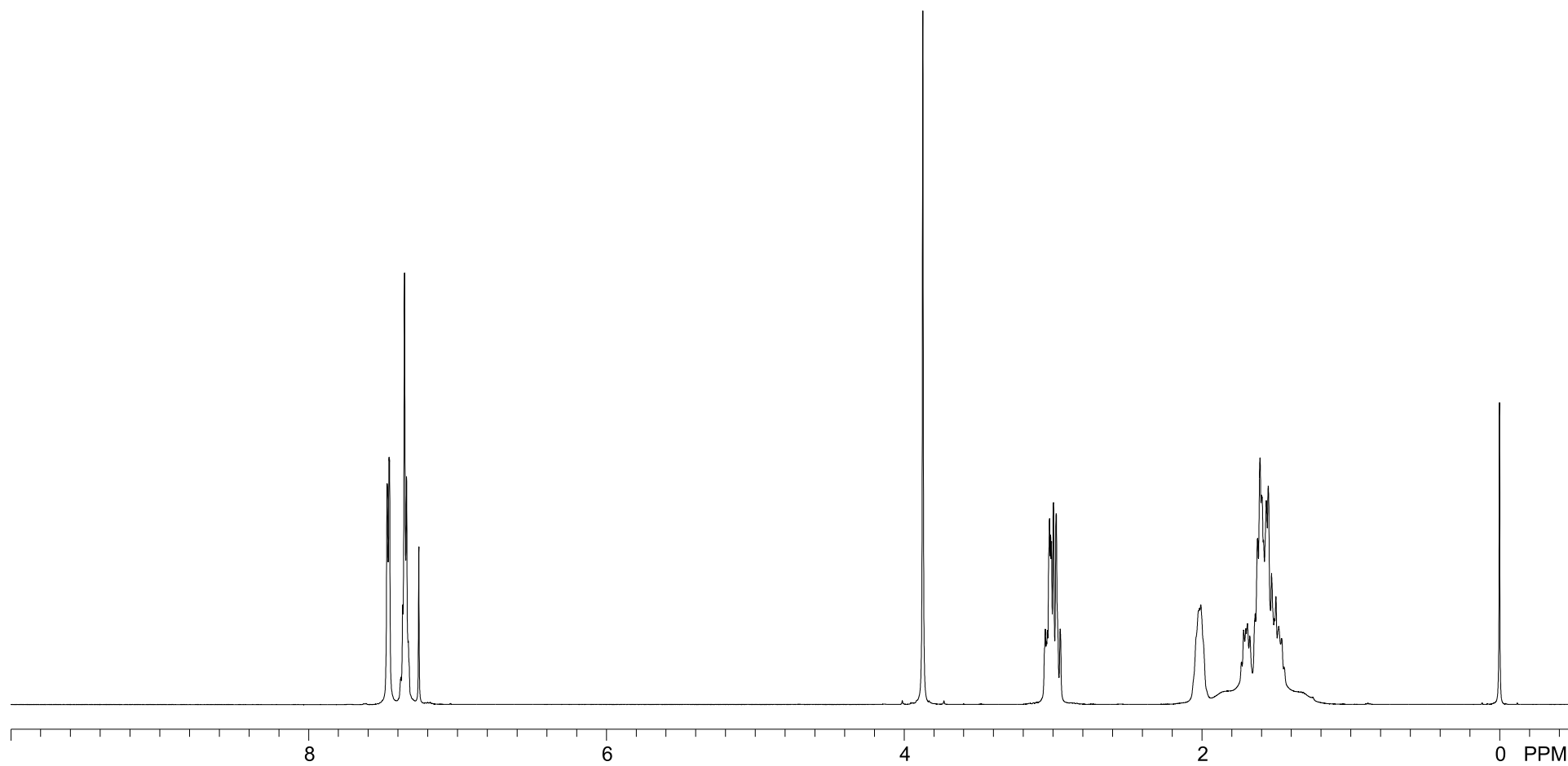
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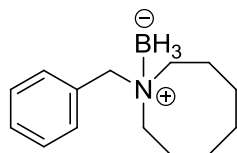
^1H NMR (500 MHz),
 CDCl_3



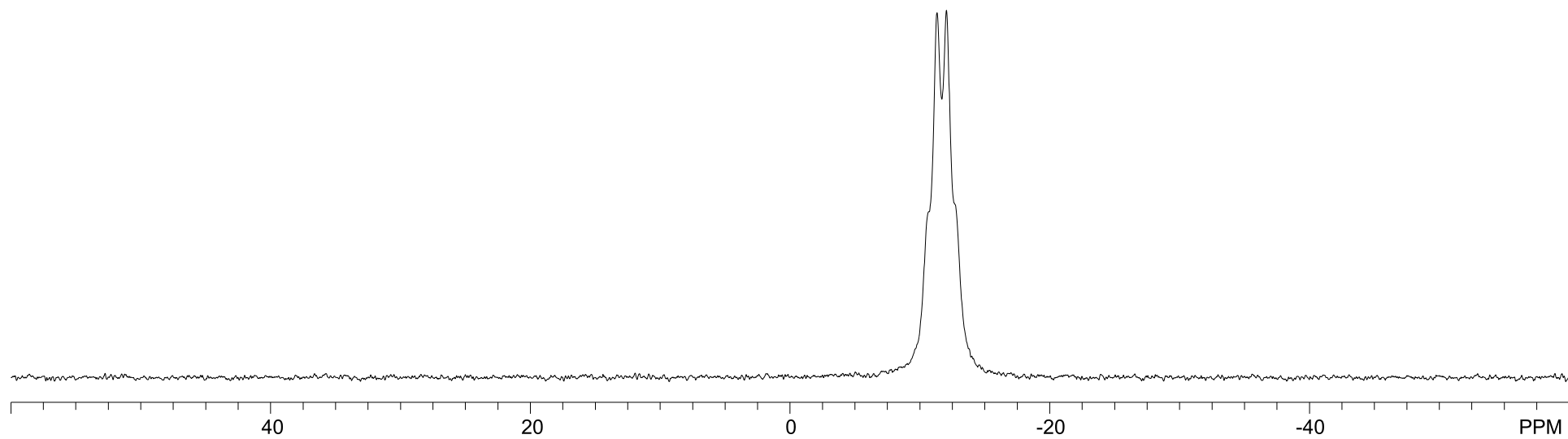
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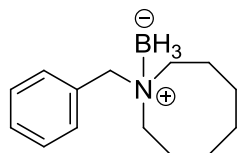
^{11}B NMR (128 MHz),
 CDCl_3



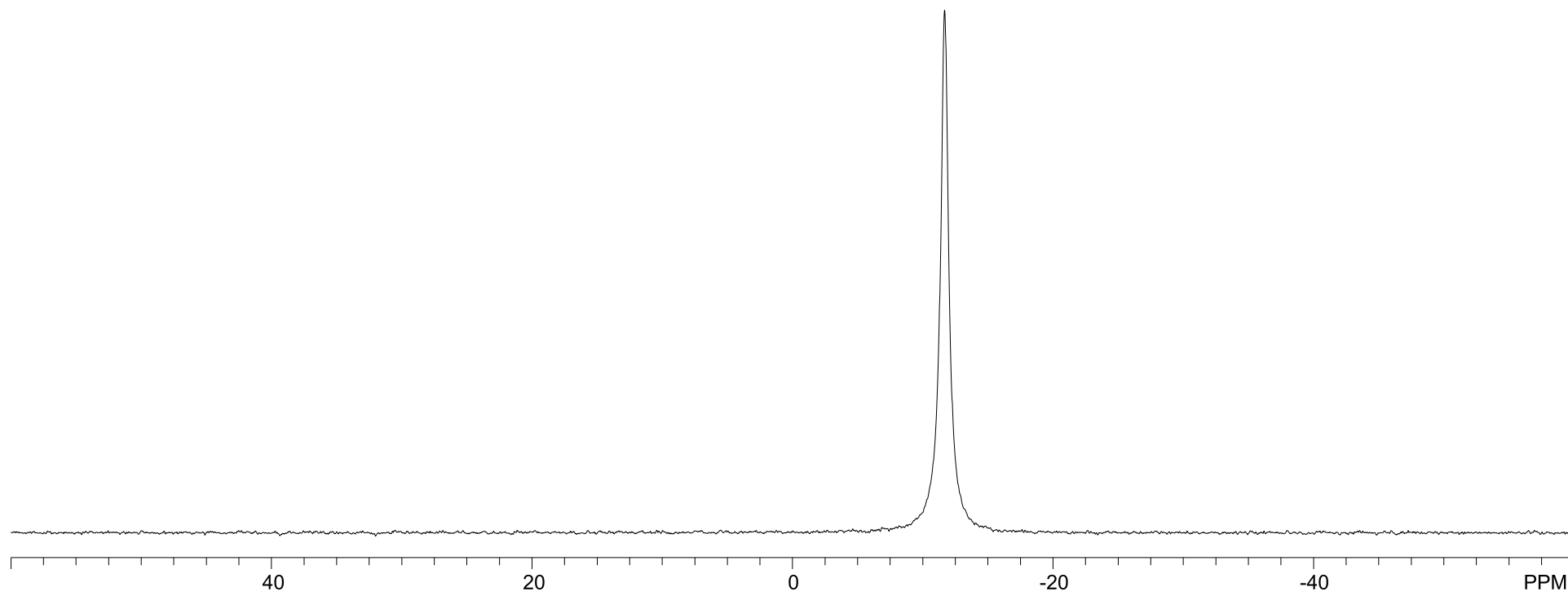
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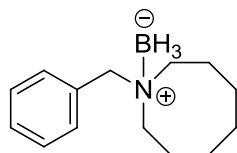
$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3



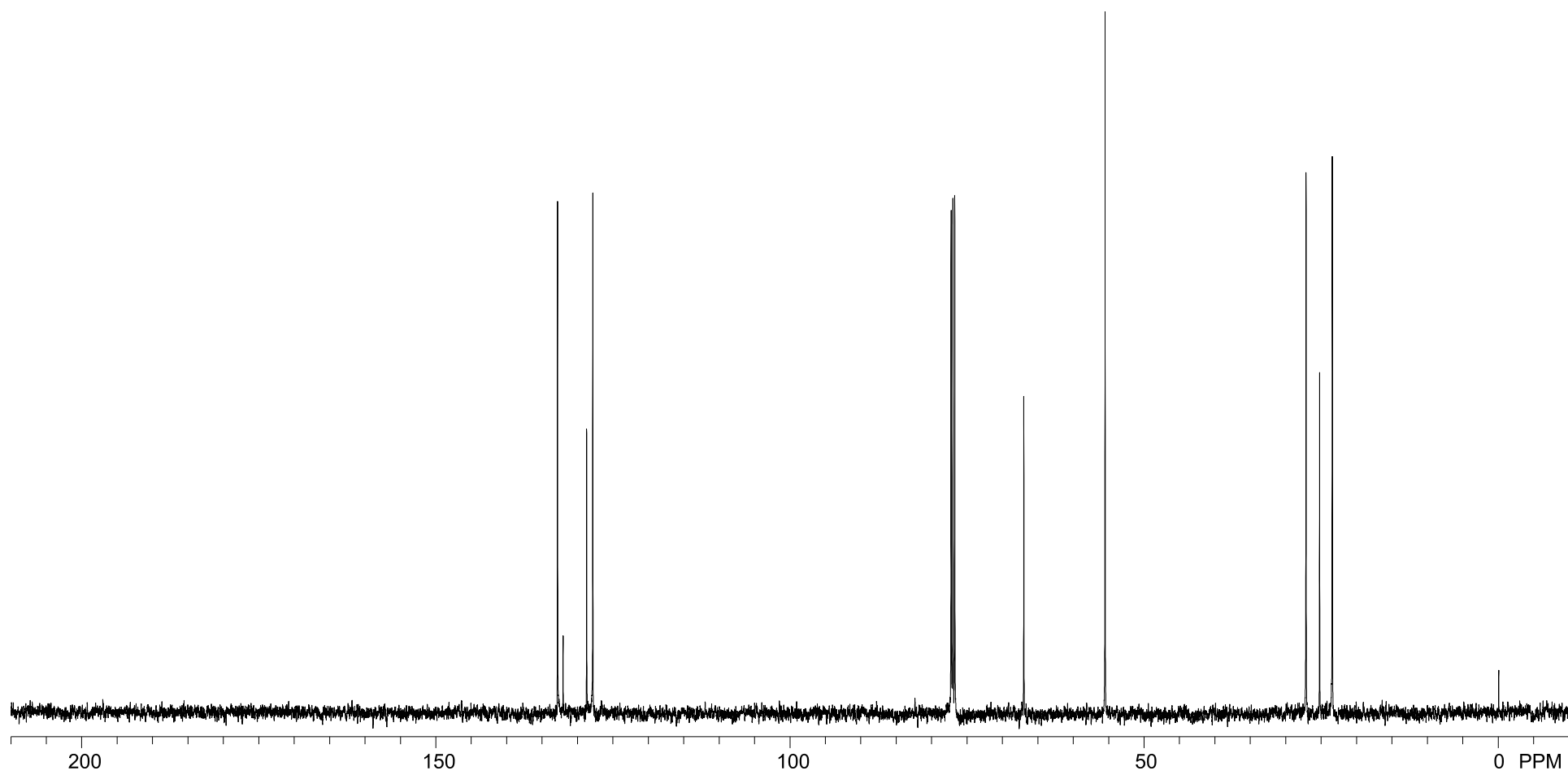
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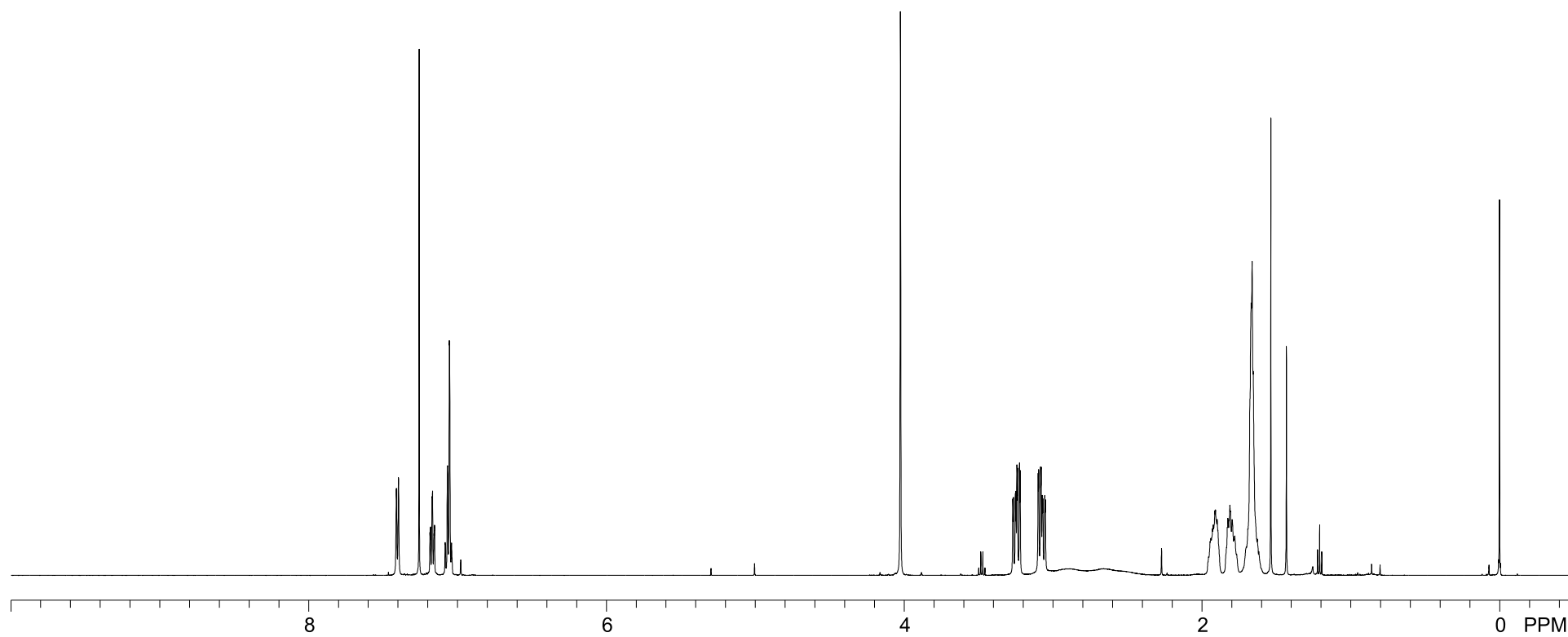
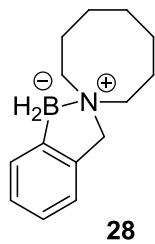
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 CDCl_3



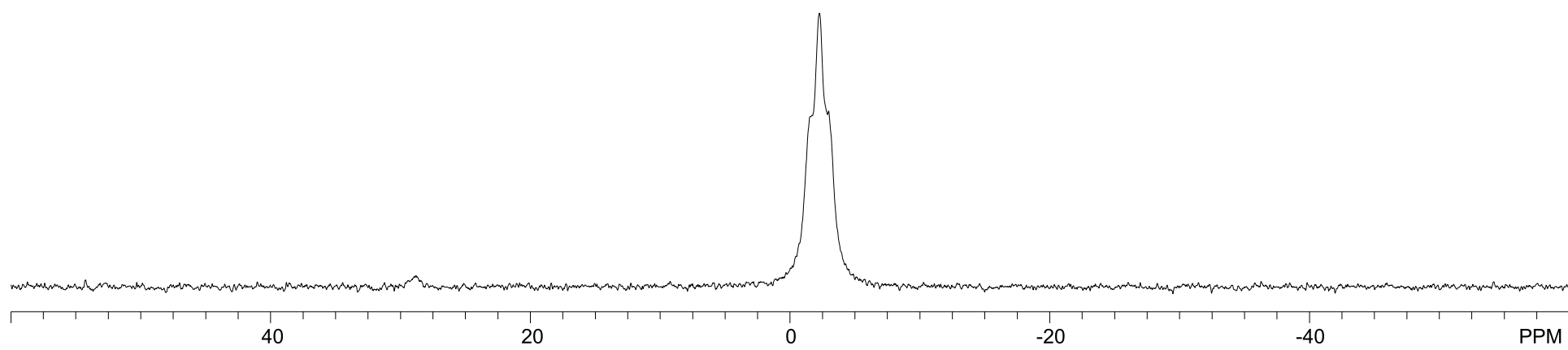
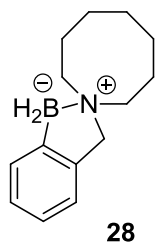
27



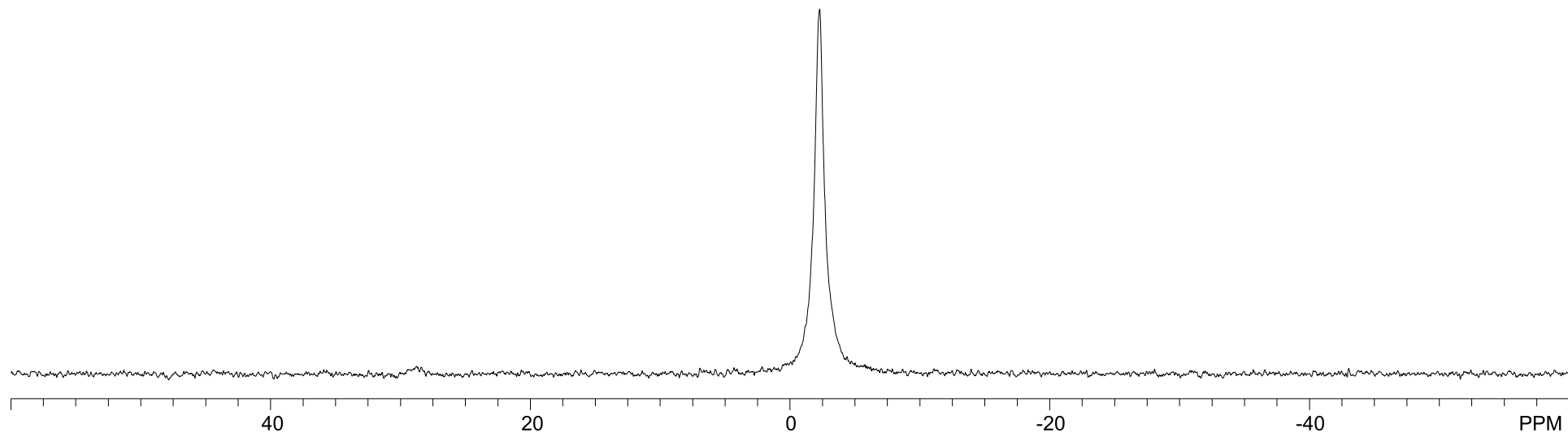
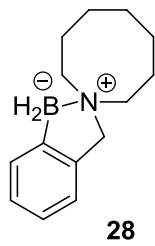
^1H NMR (500 MHz),
 CDCl_3



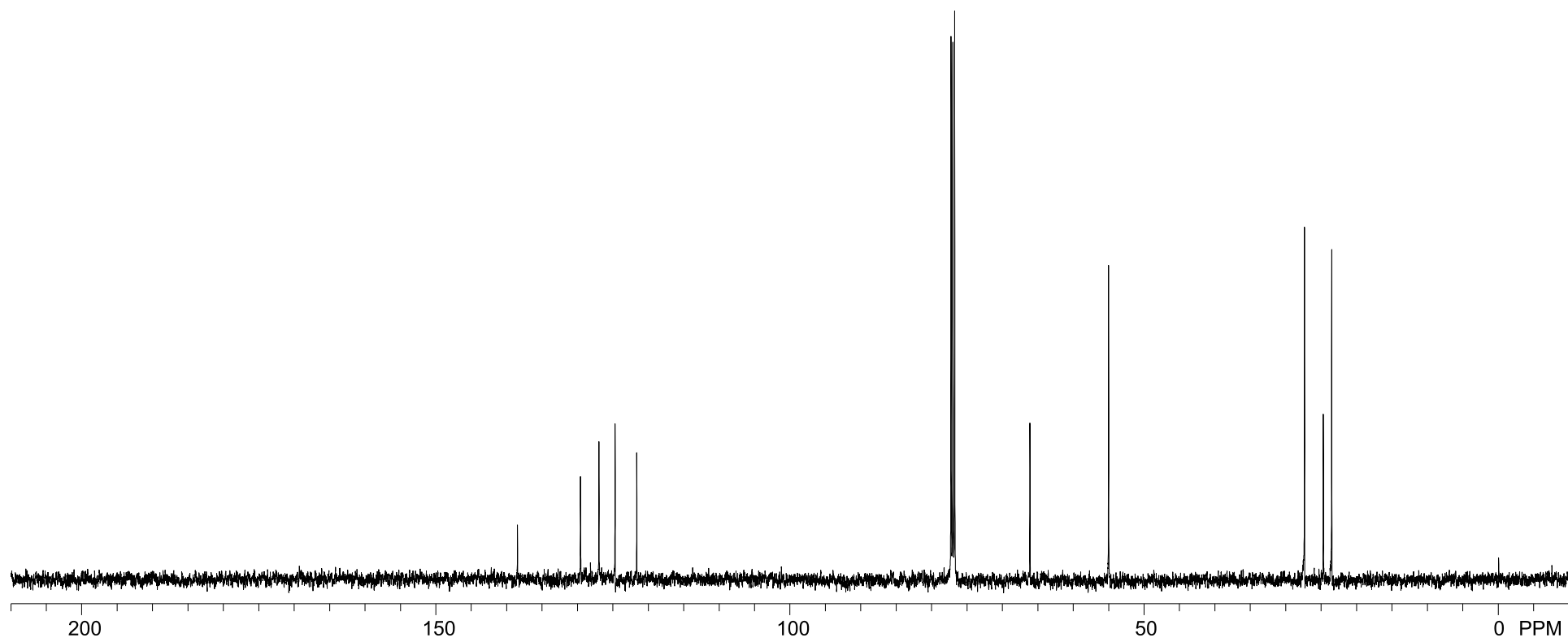
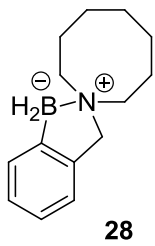
^{11}B NMR (128 MHz),
 CDCl_3



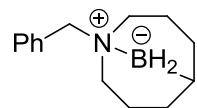
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 CDCl_3



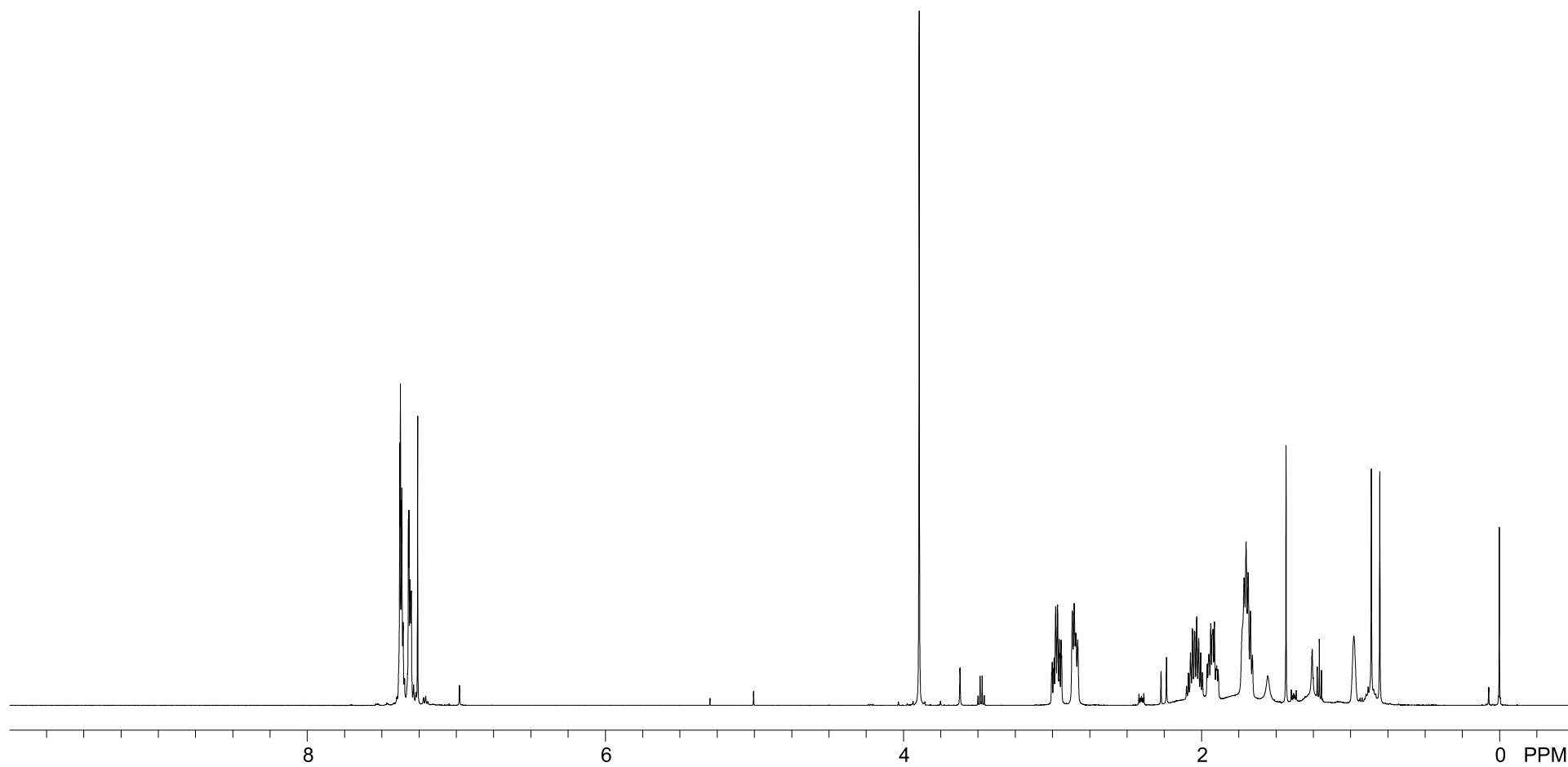
$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CDCl_3



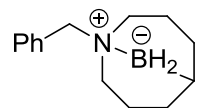
^1H NMR (500 MHz),
 CDCl_3



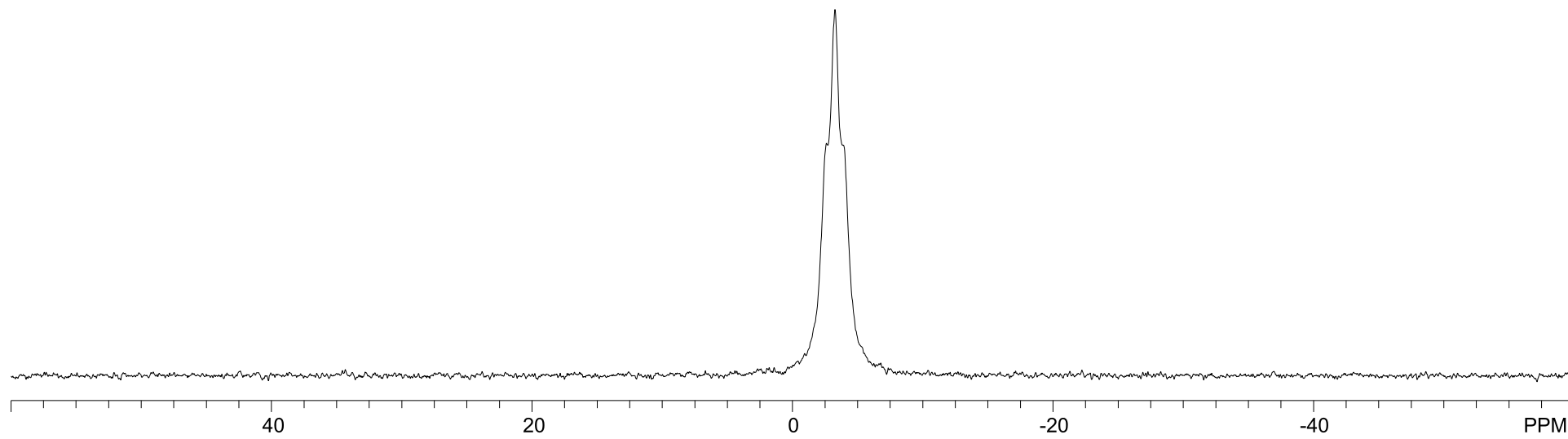
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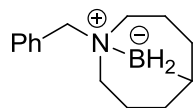
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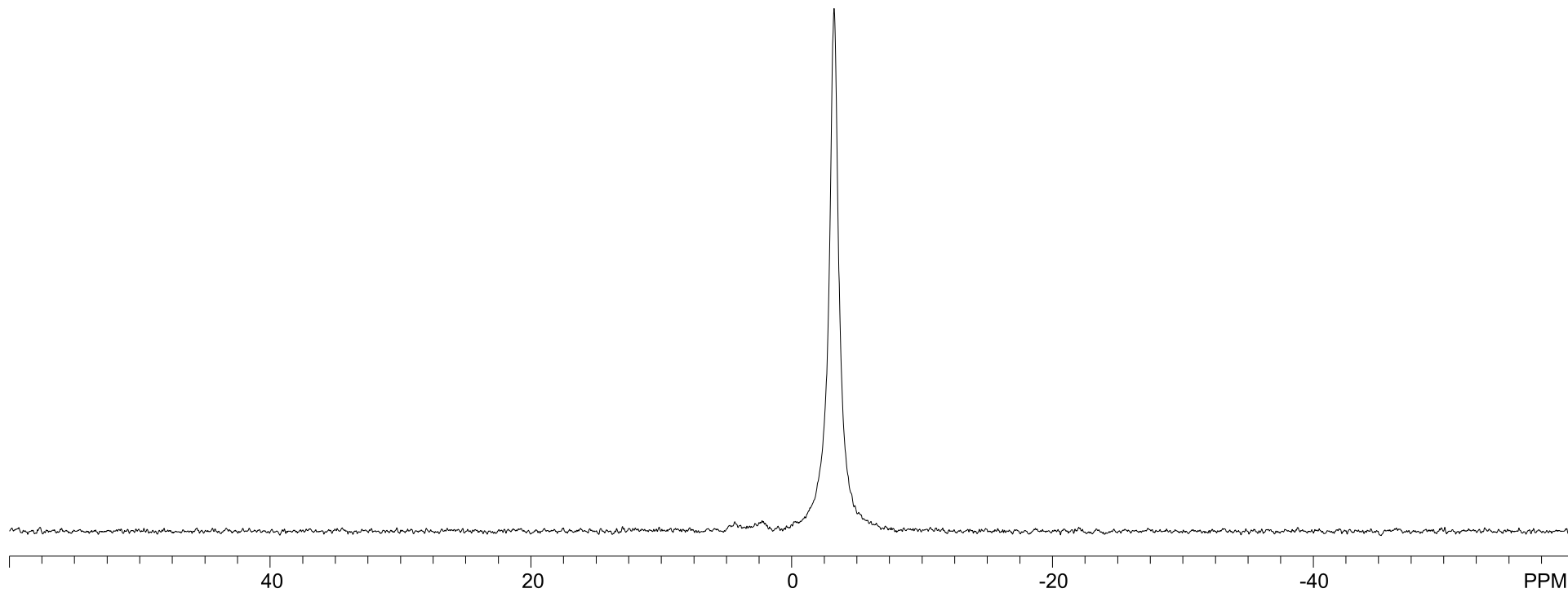
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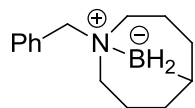
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 CDCl_3



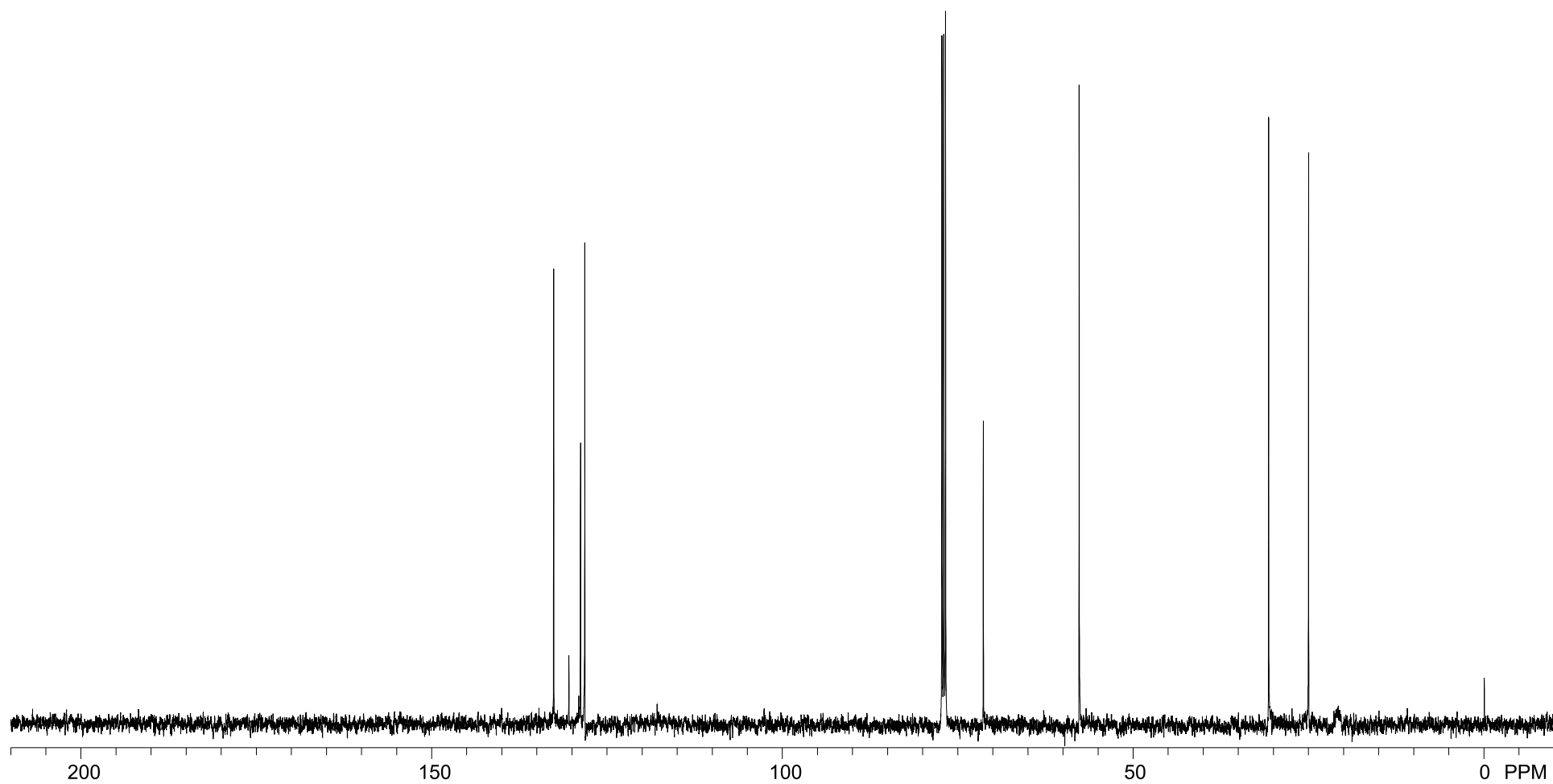
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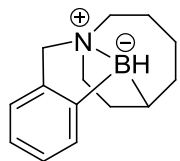
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 CDCl_3



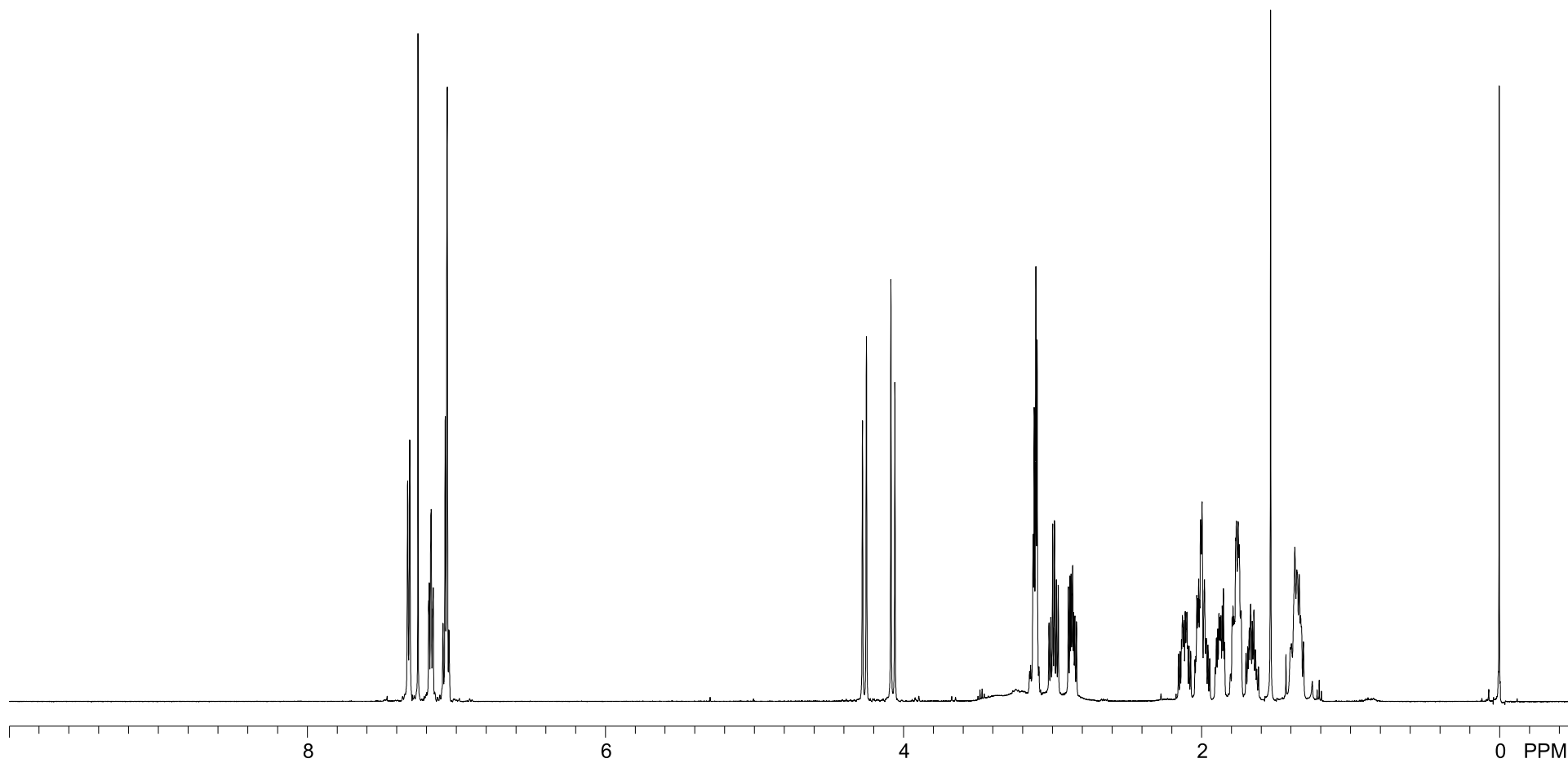
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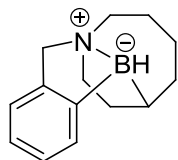
$^1\text{H NMR}$ (500 MHz),
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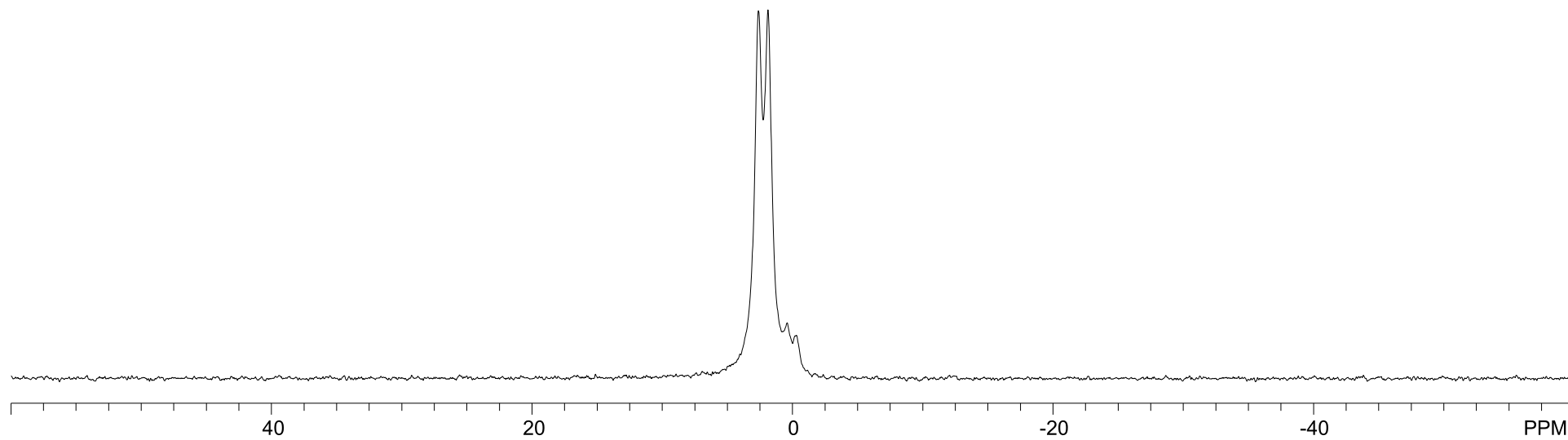
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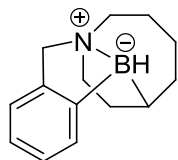
^{11}B NMR (128 MHz),
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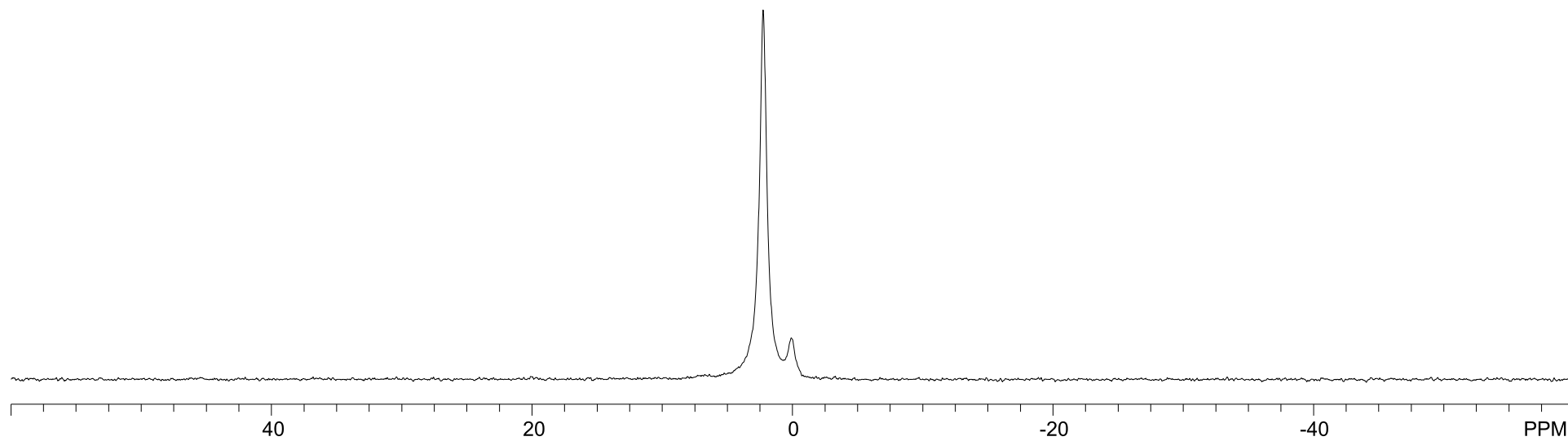
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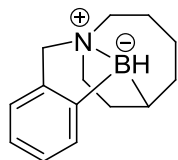
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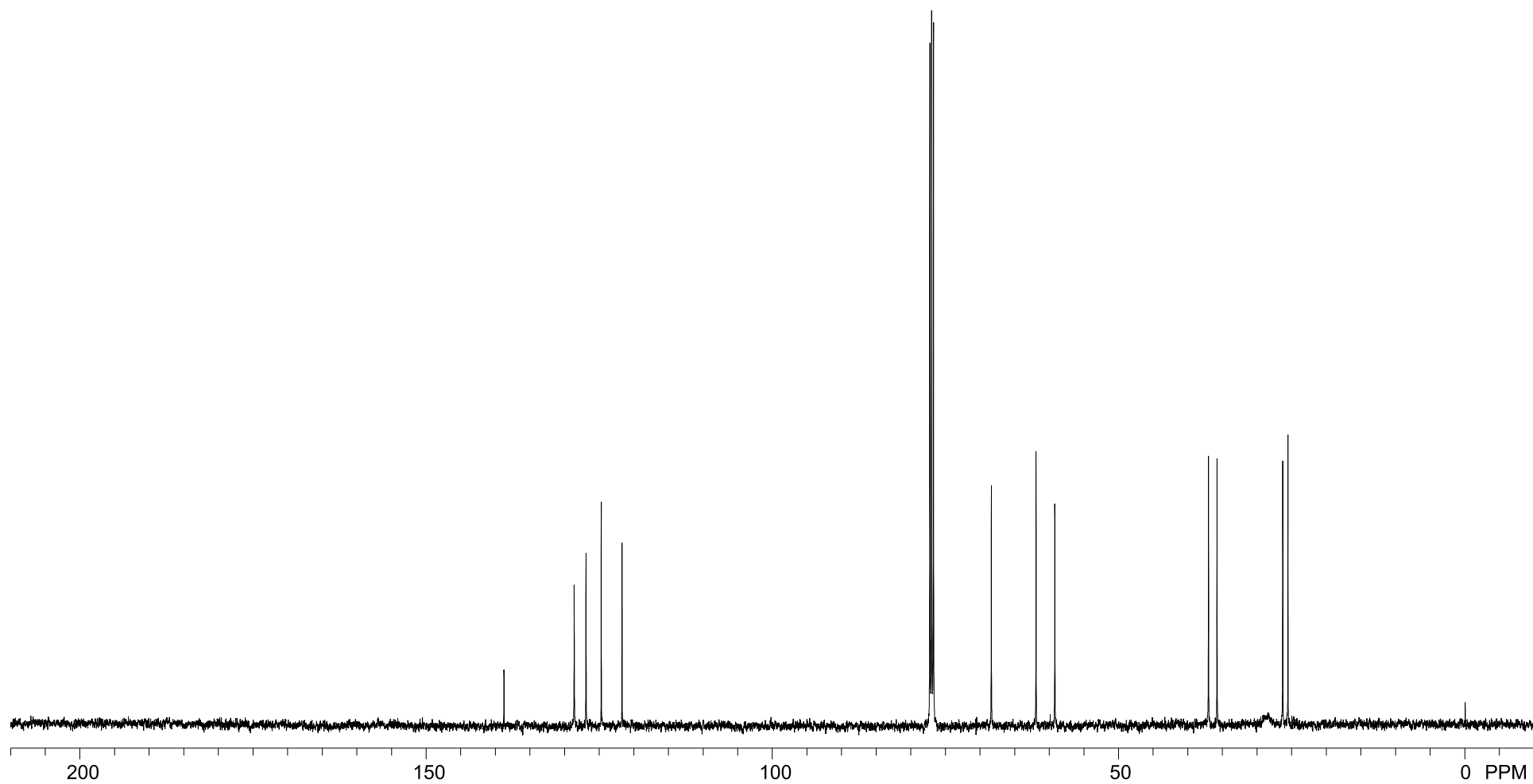
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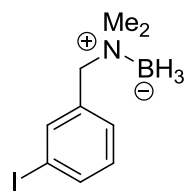
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 CDCl_3



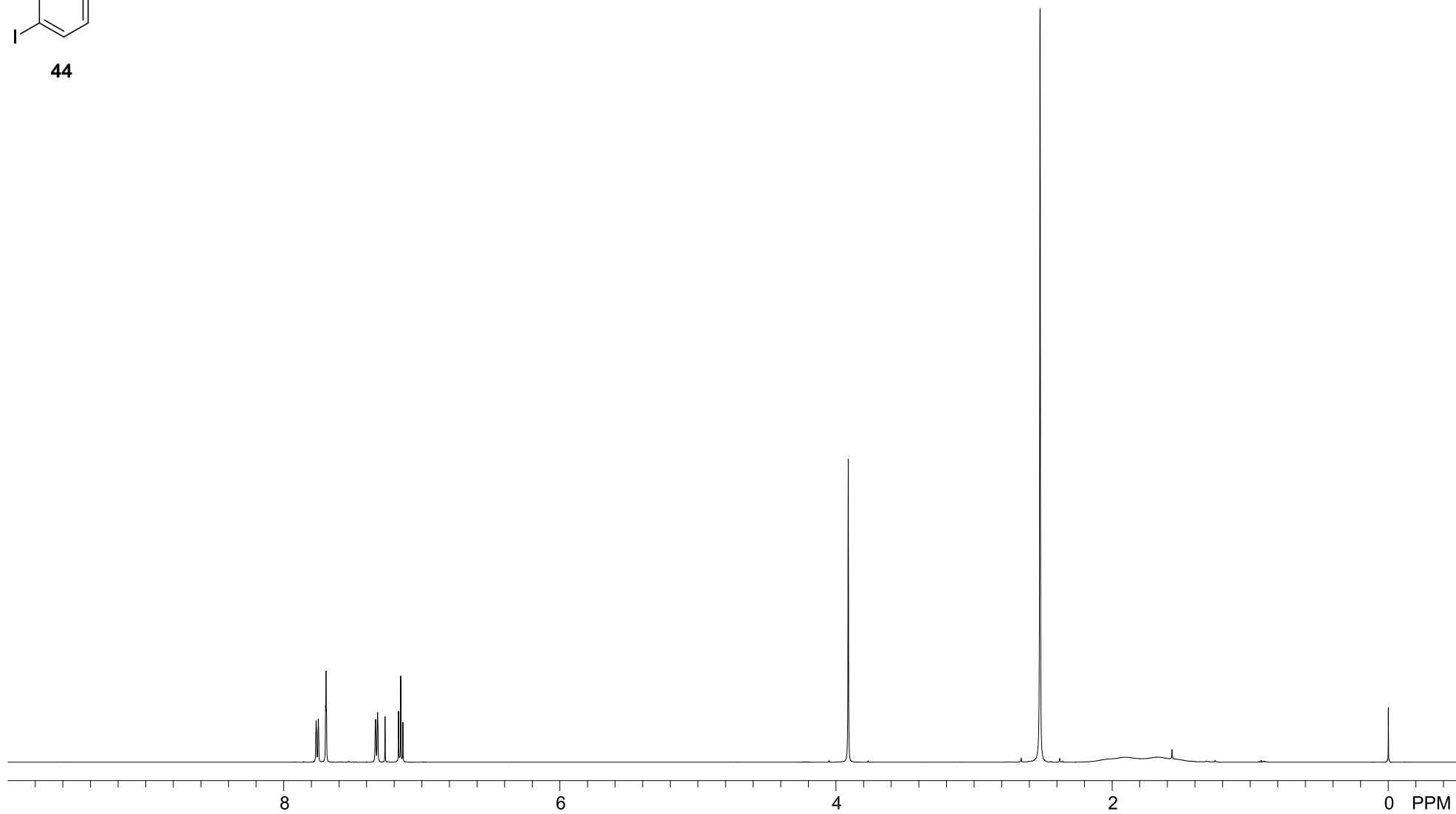
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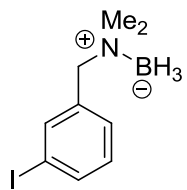
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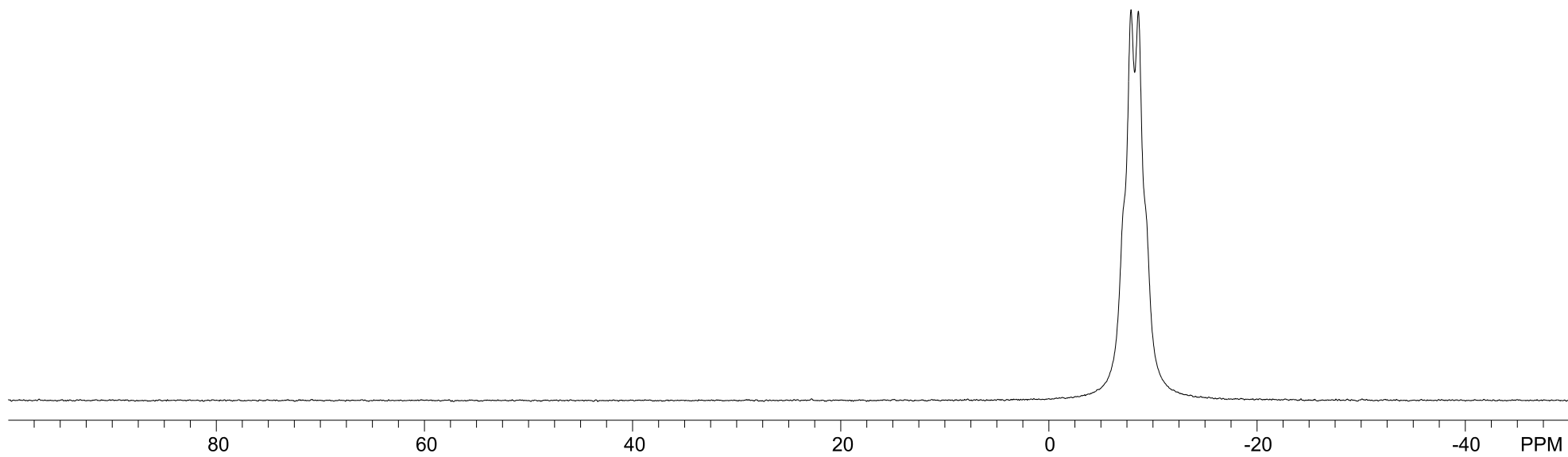
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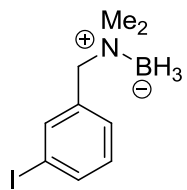
^{11}B NMR (128 MHz),
 CDCl_3



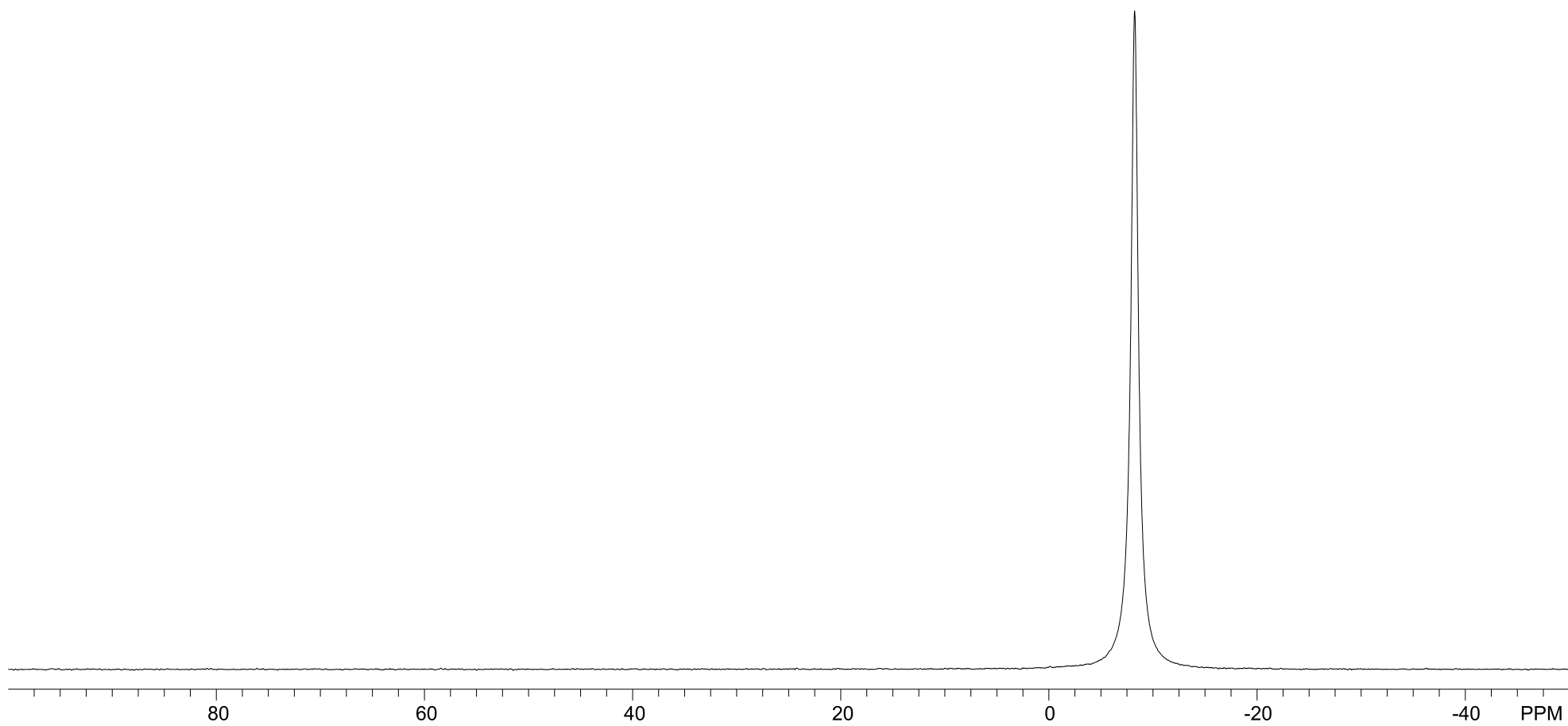
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$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3

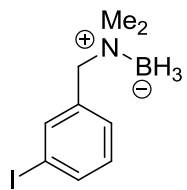


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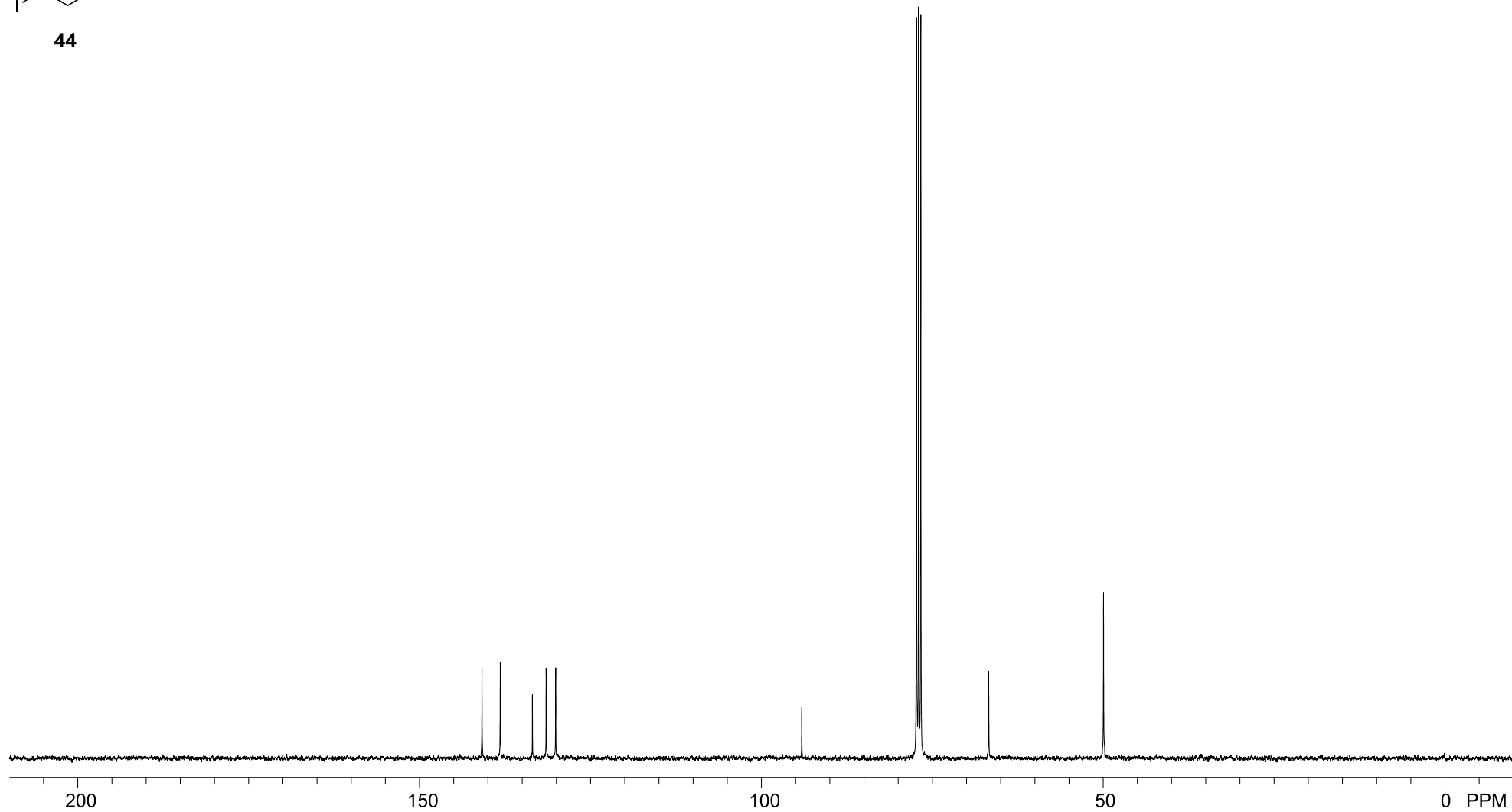


S83

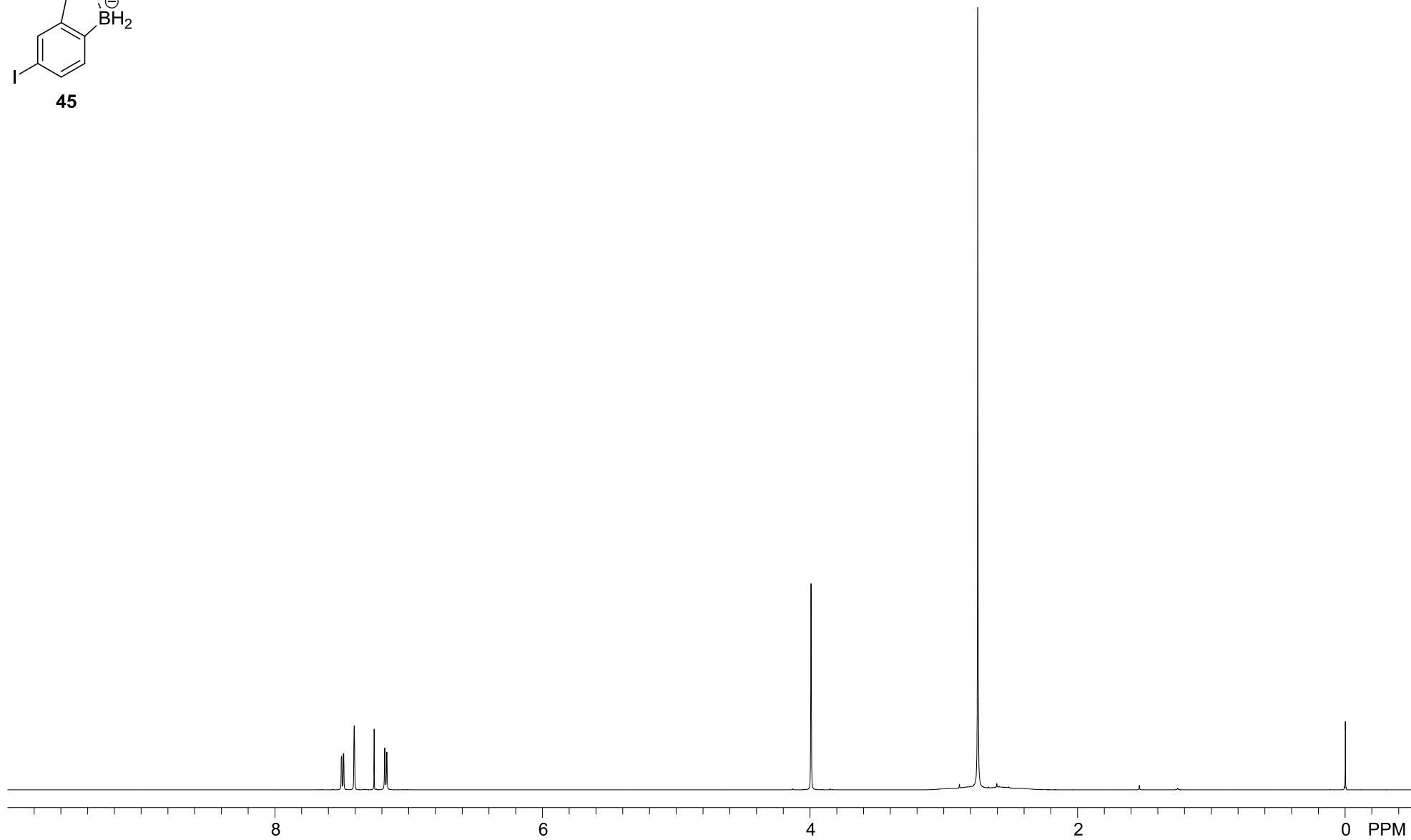
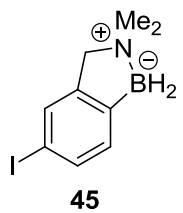
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 CDCl_3



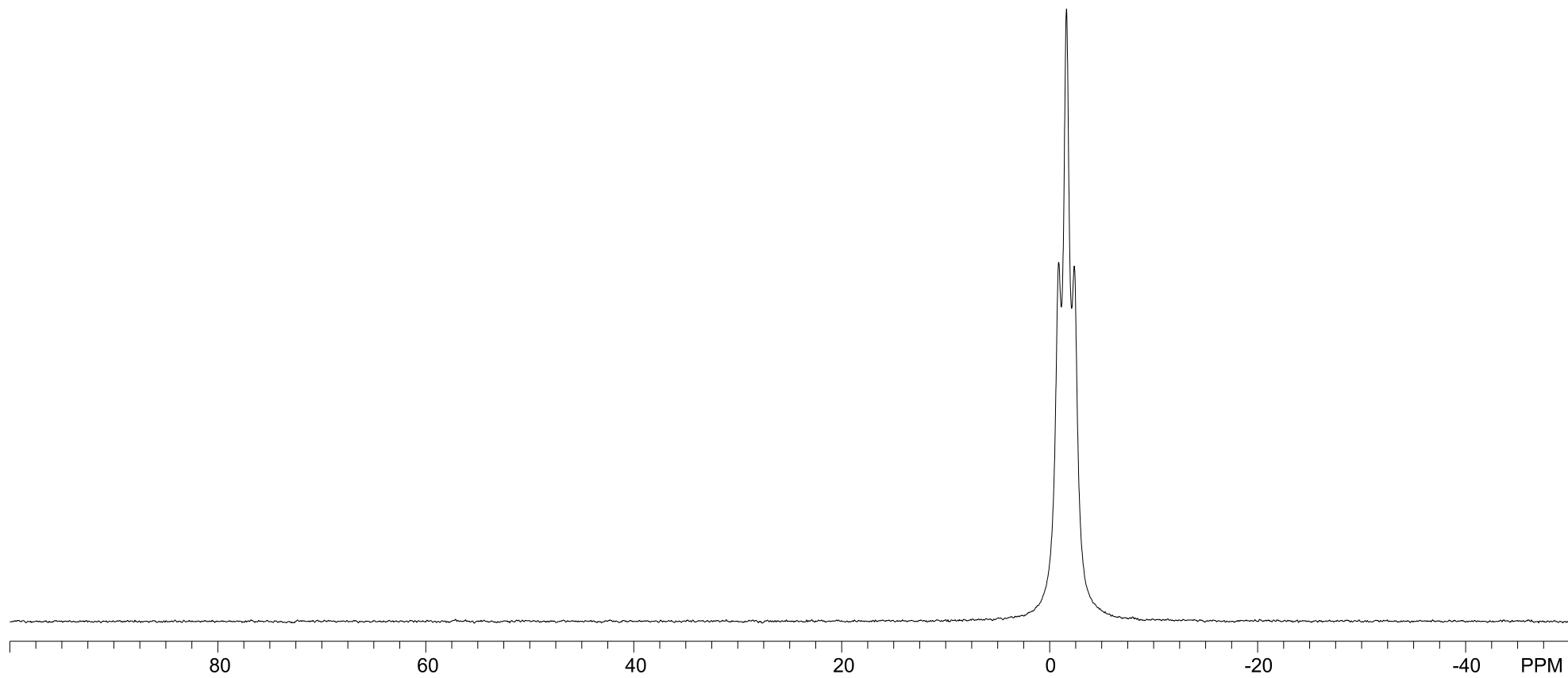
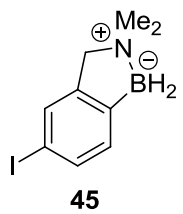
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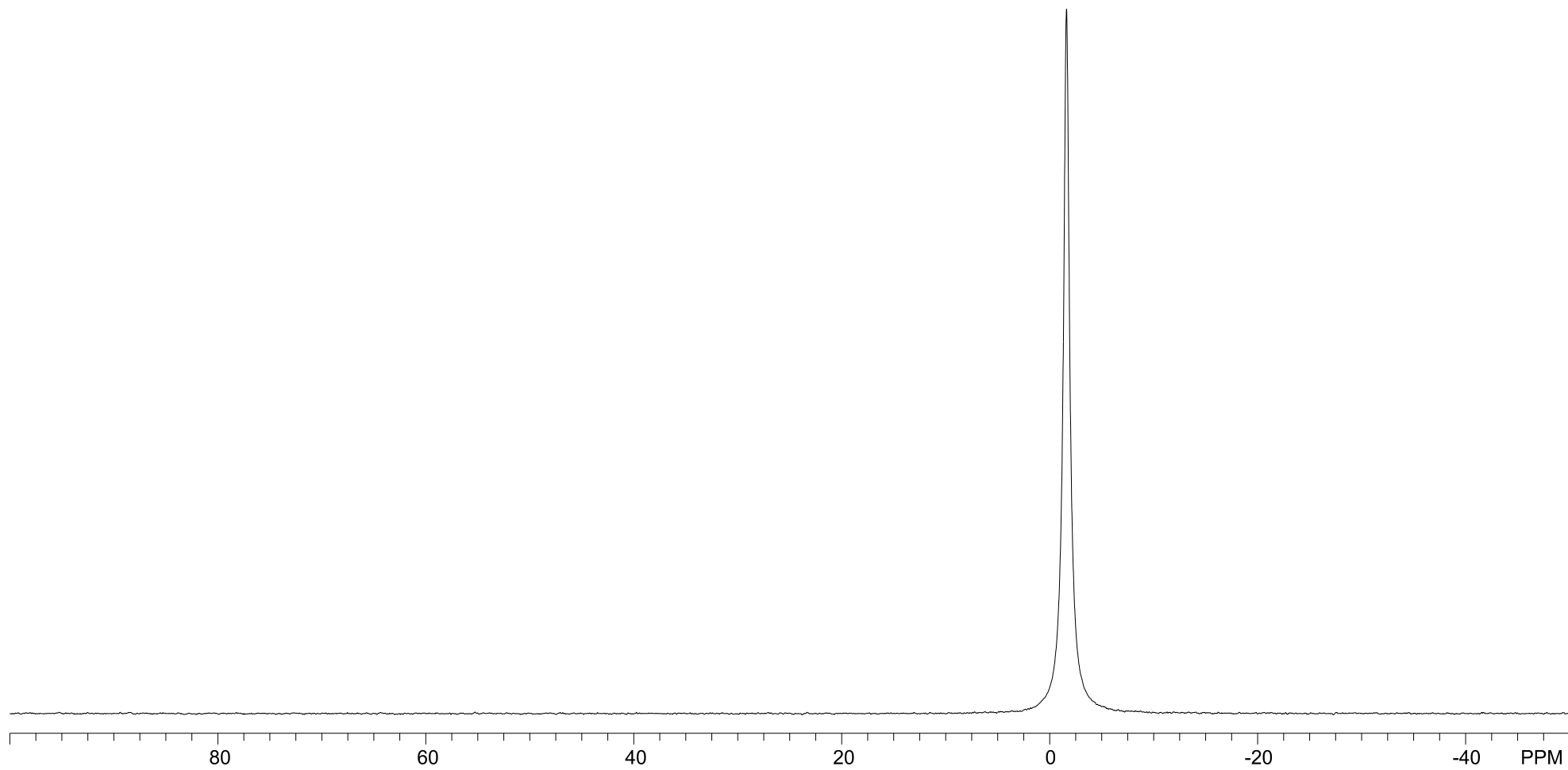
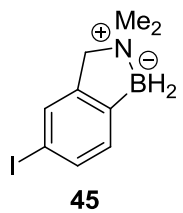
^1H NMR (500 MHz),
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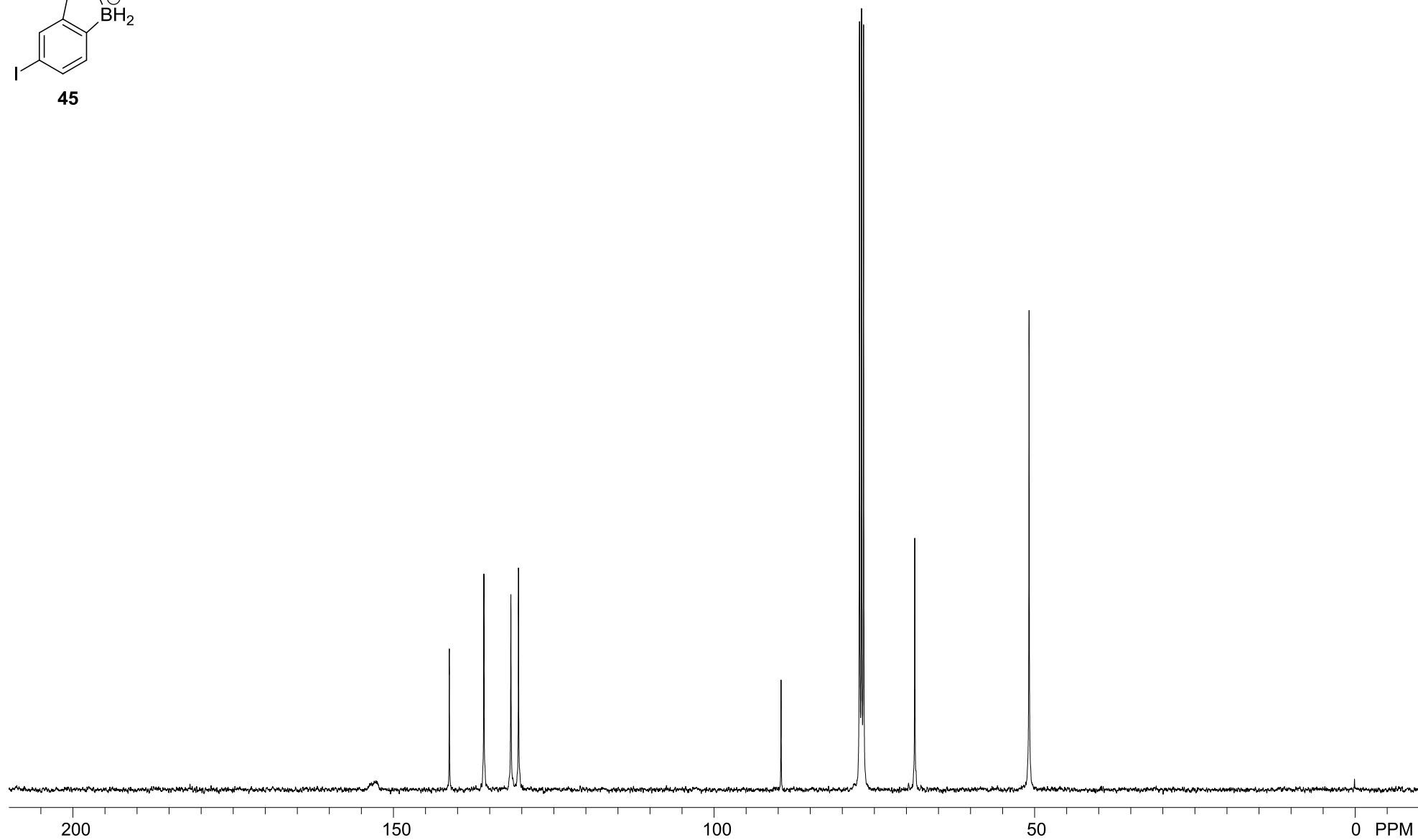
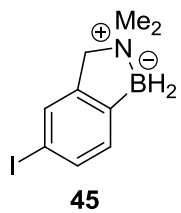
^{11}B NMR (128 MHz),
 CDCl_3



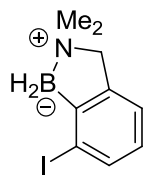
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 CDCl_3



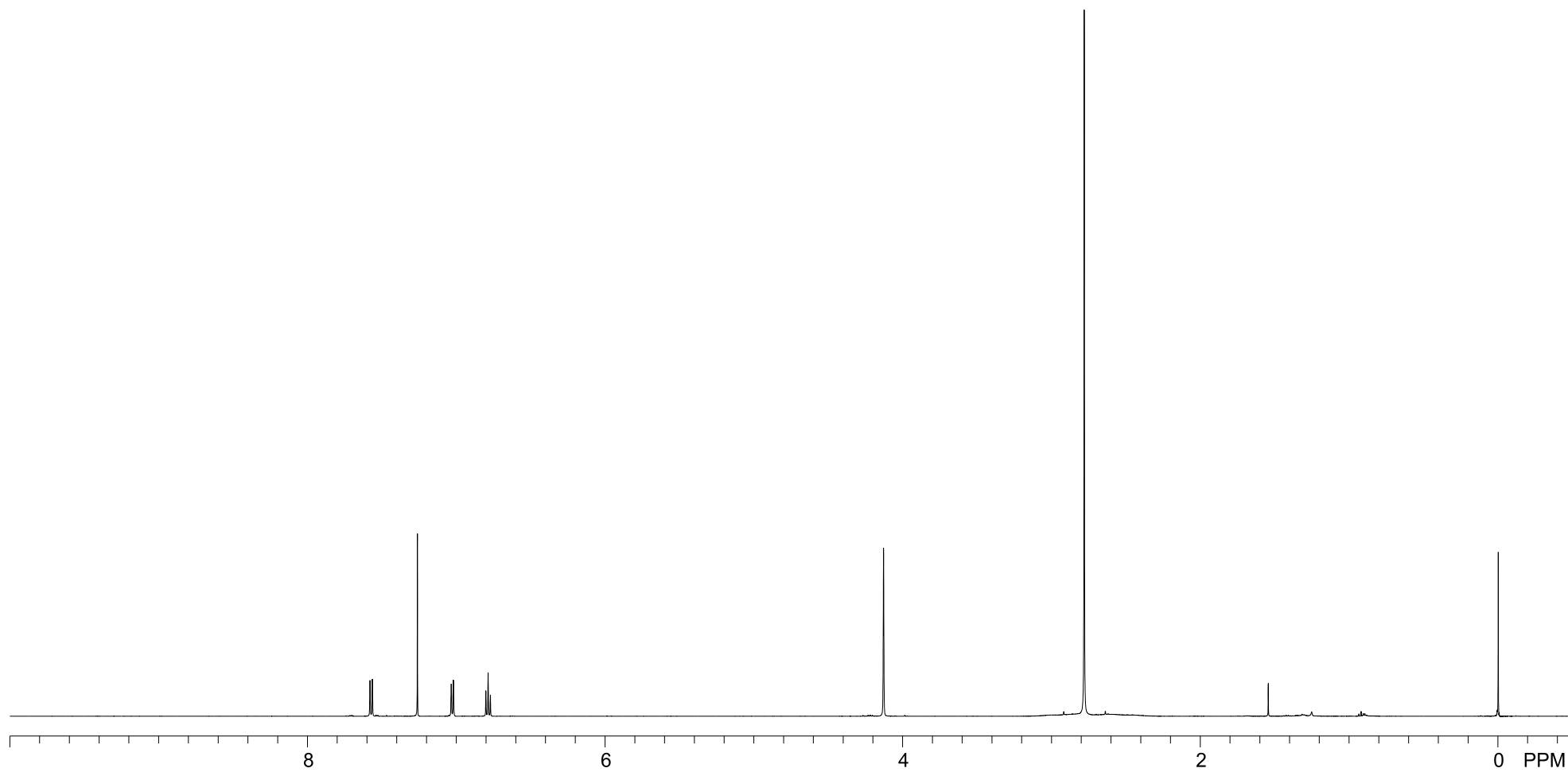
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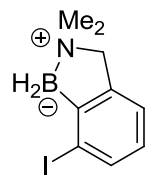
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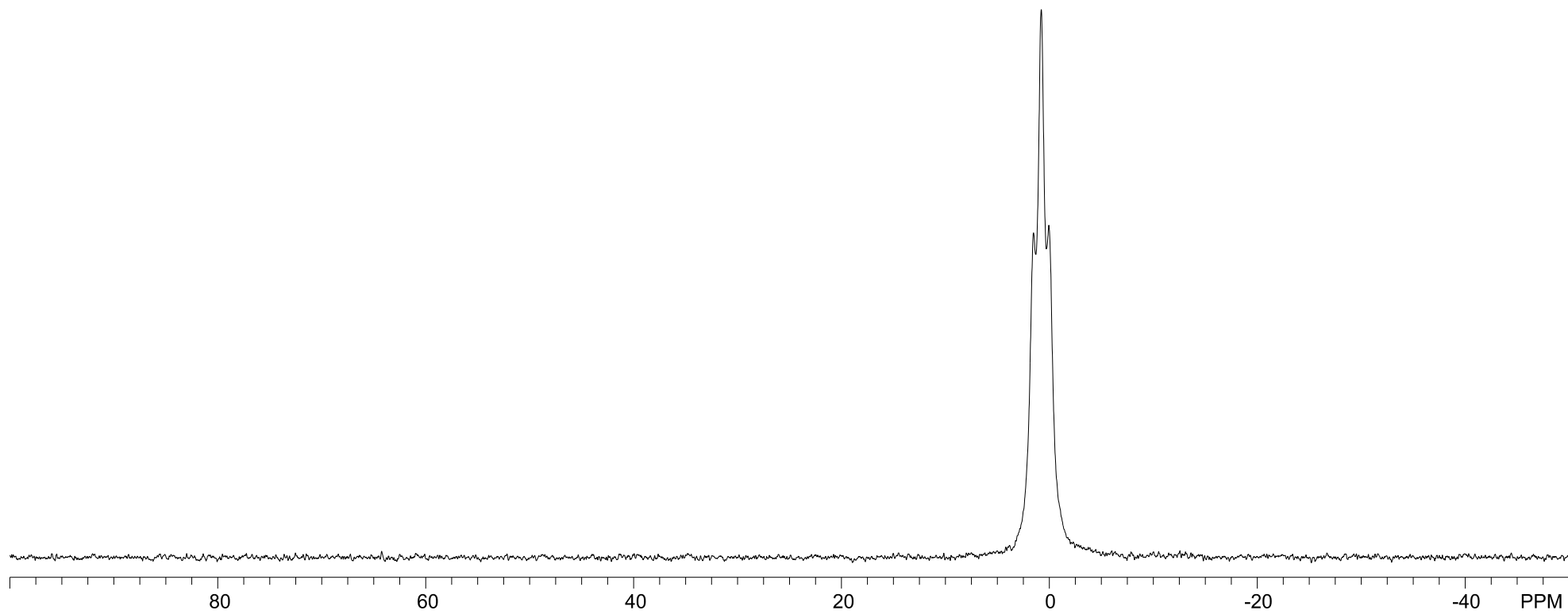
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^{11}B NMR (128 MHz),
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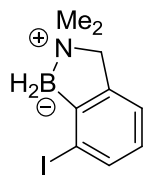


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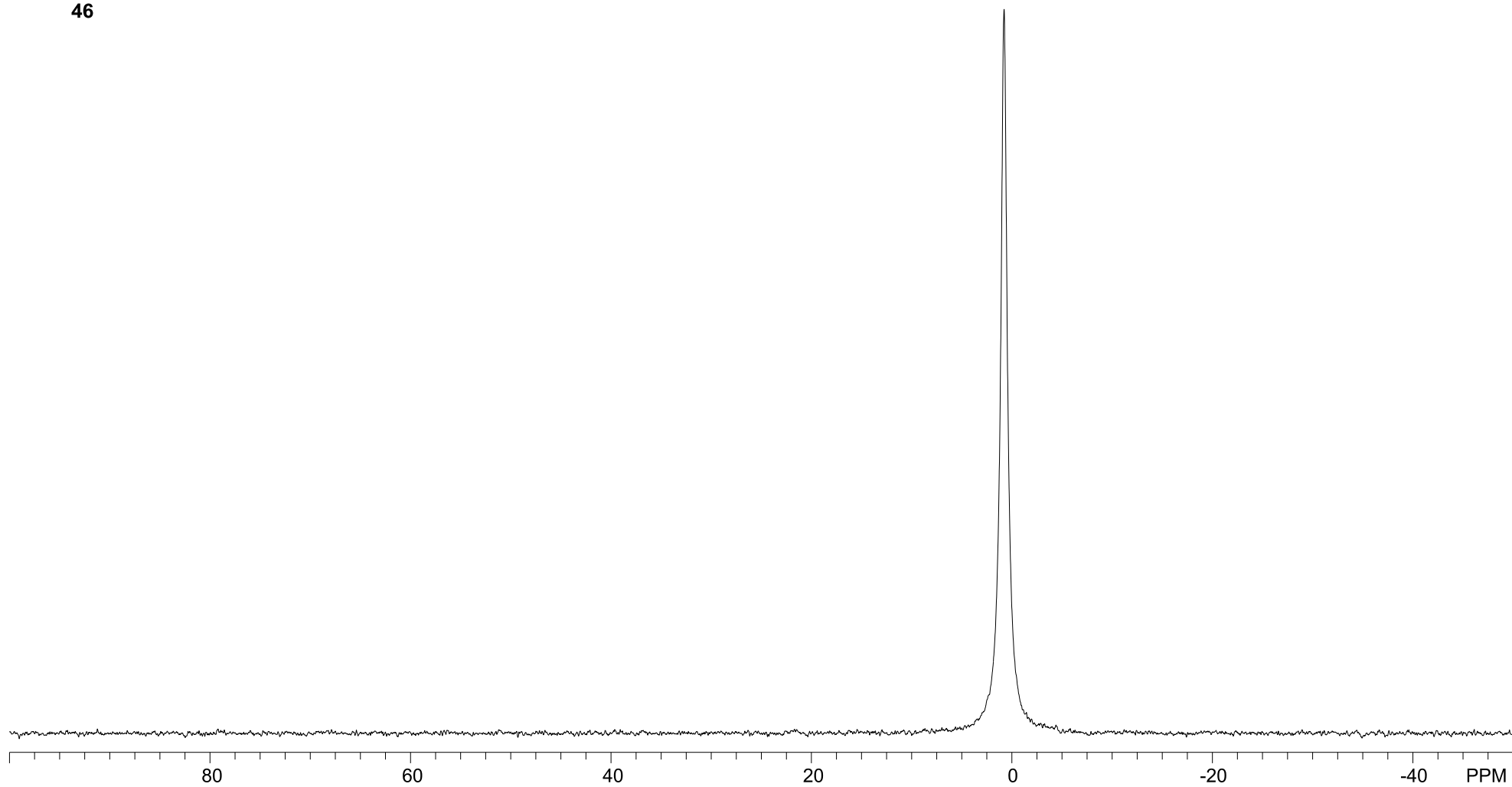


S90

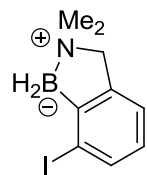
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 CDCl_3



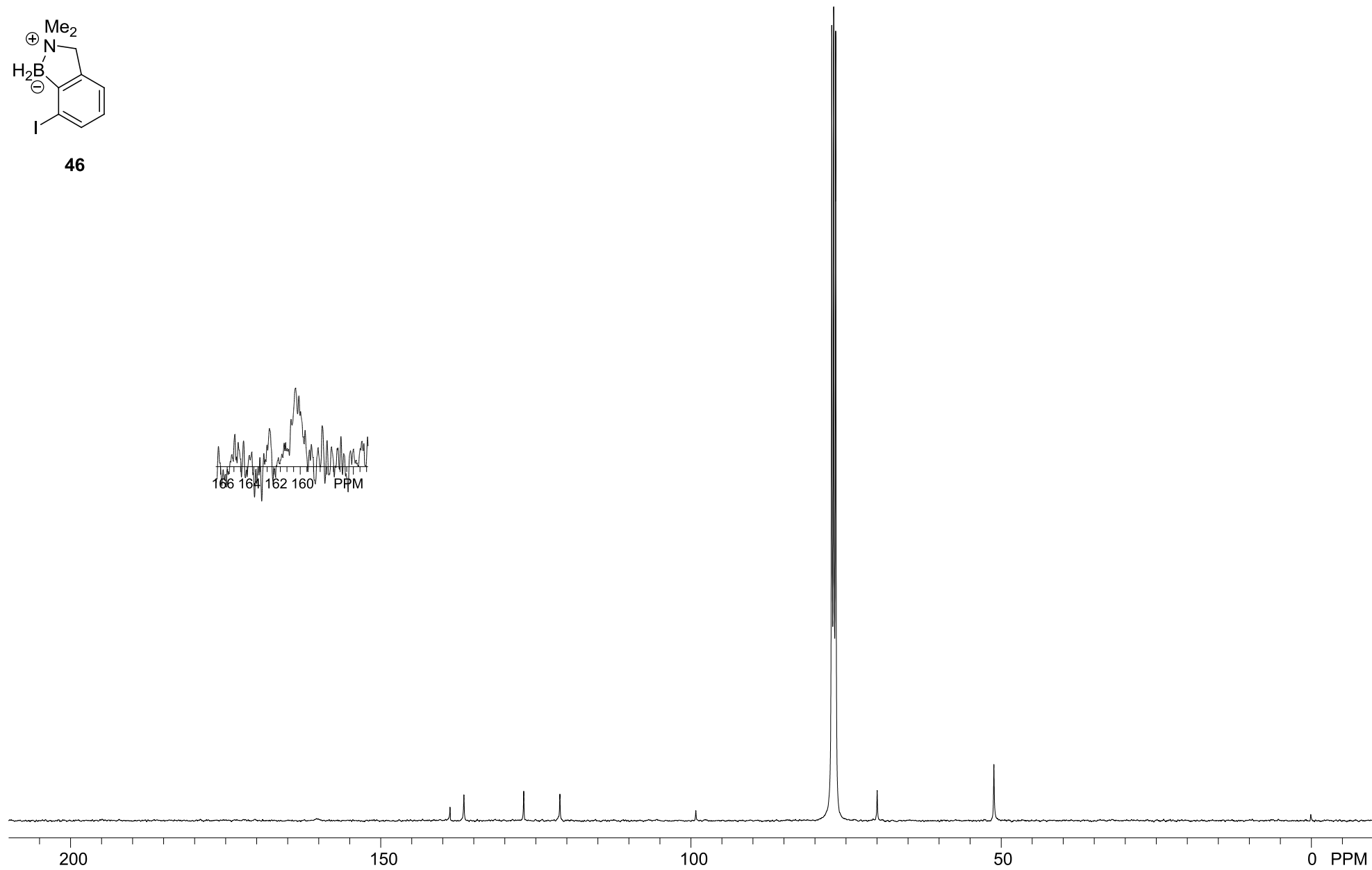
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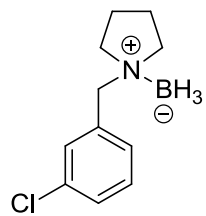
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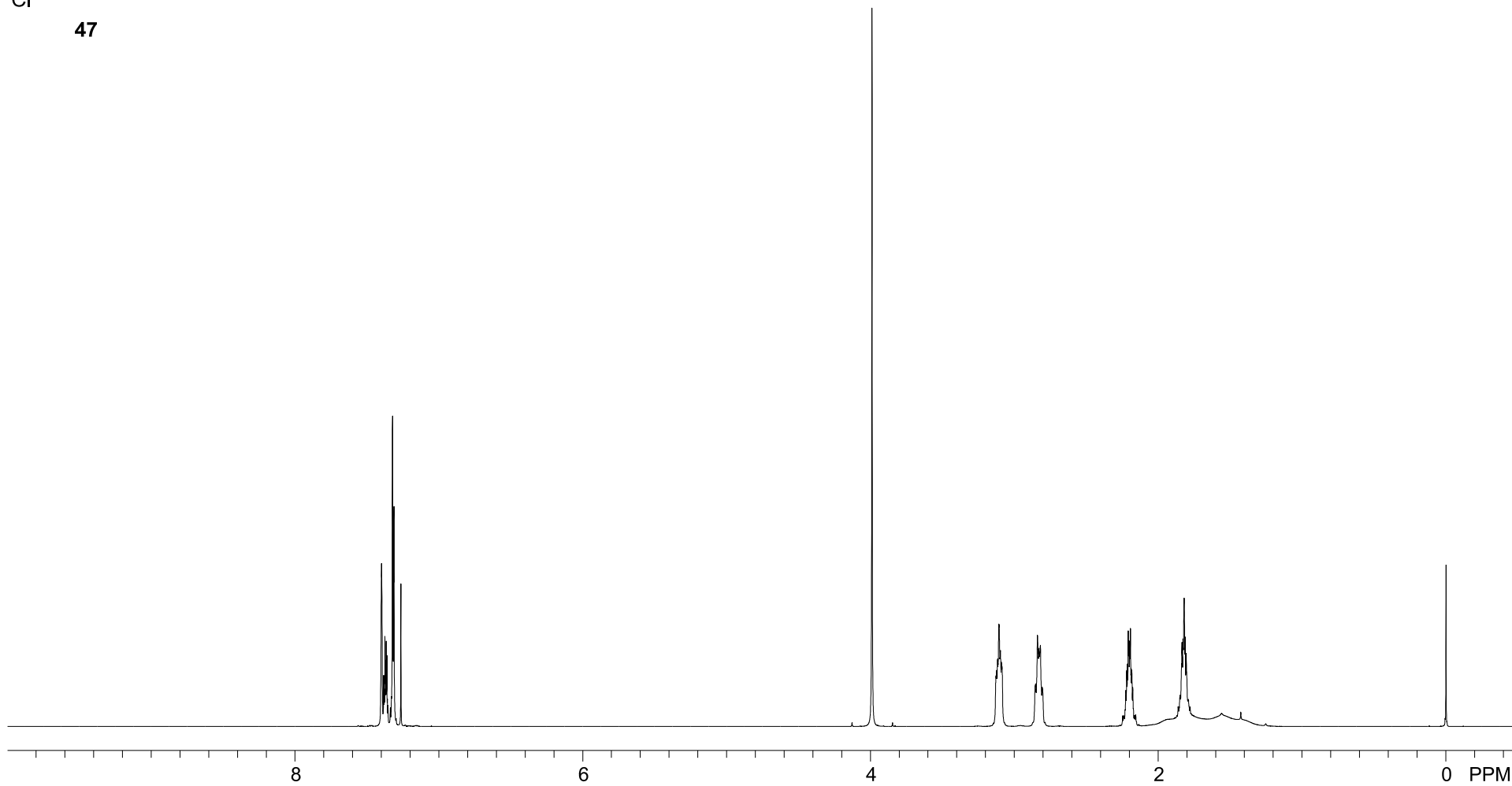
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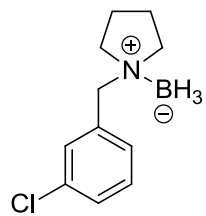
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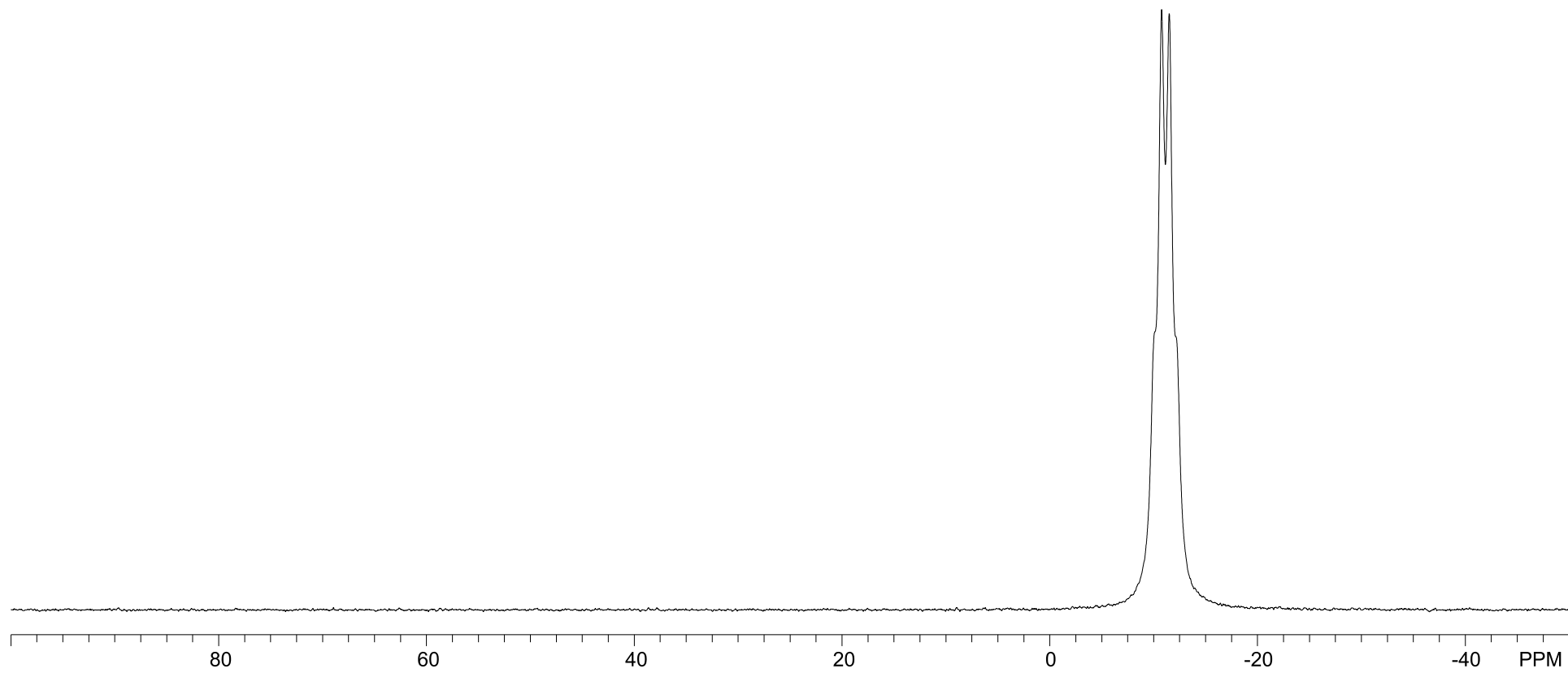
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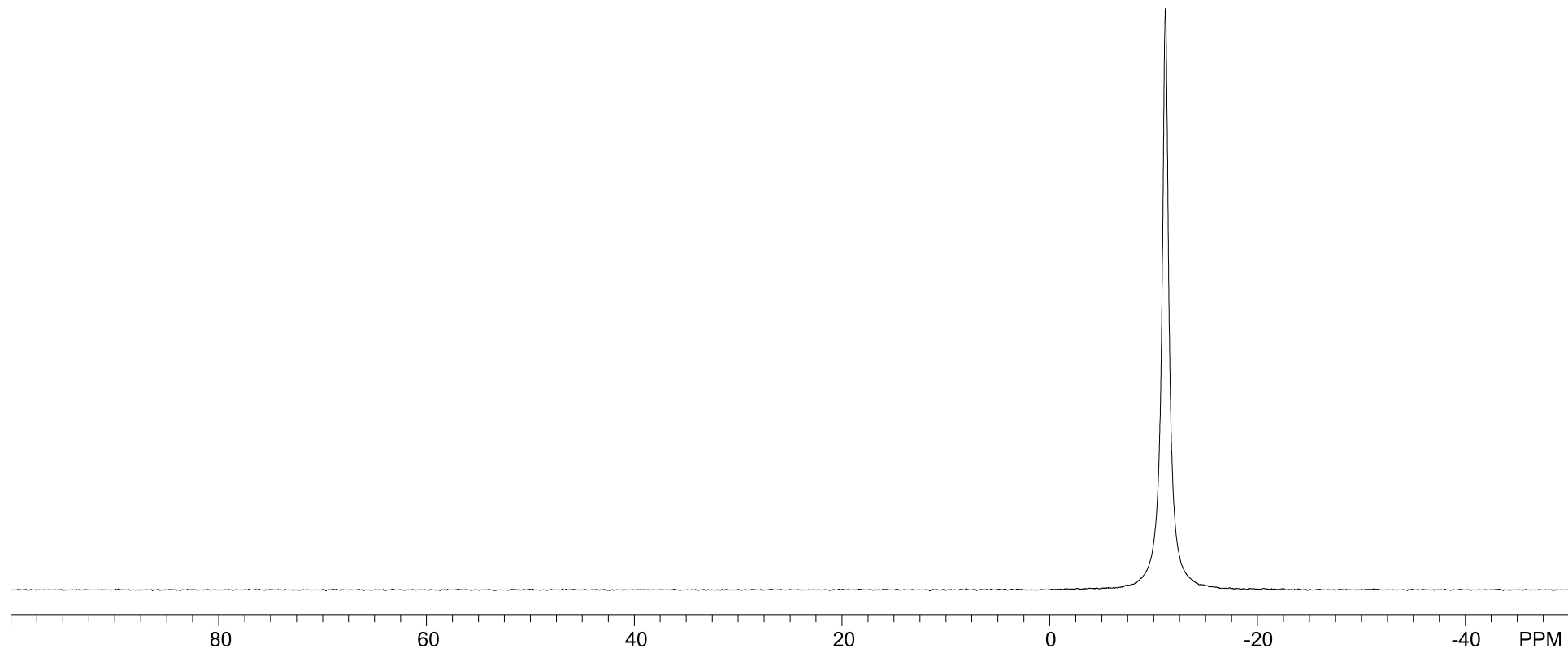
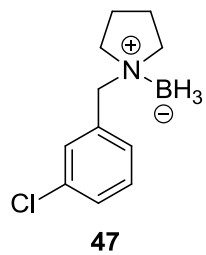
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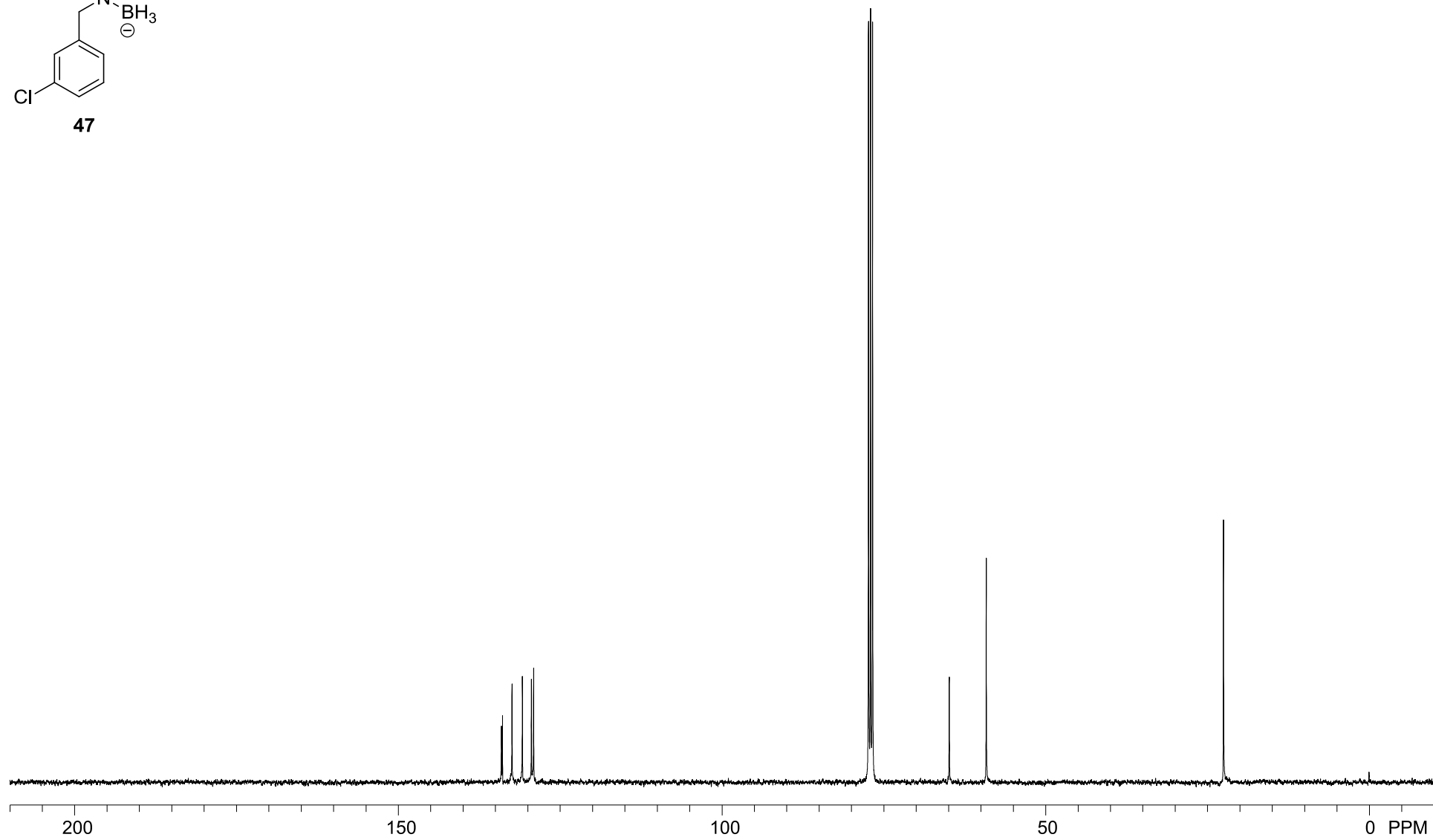
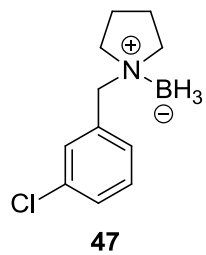
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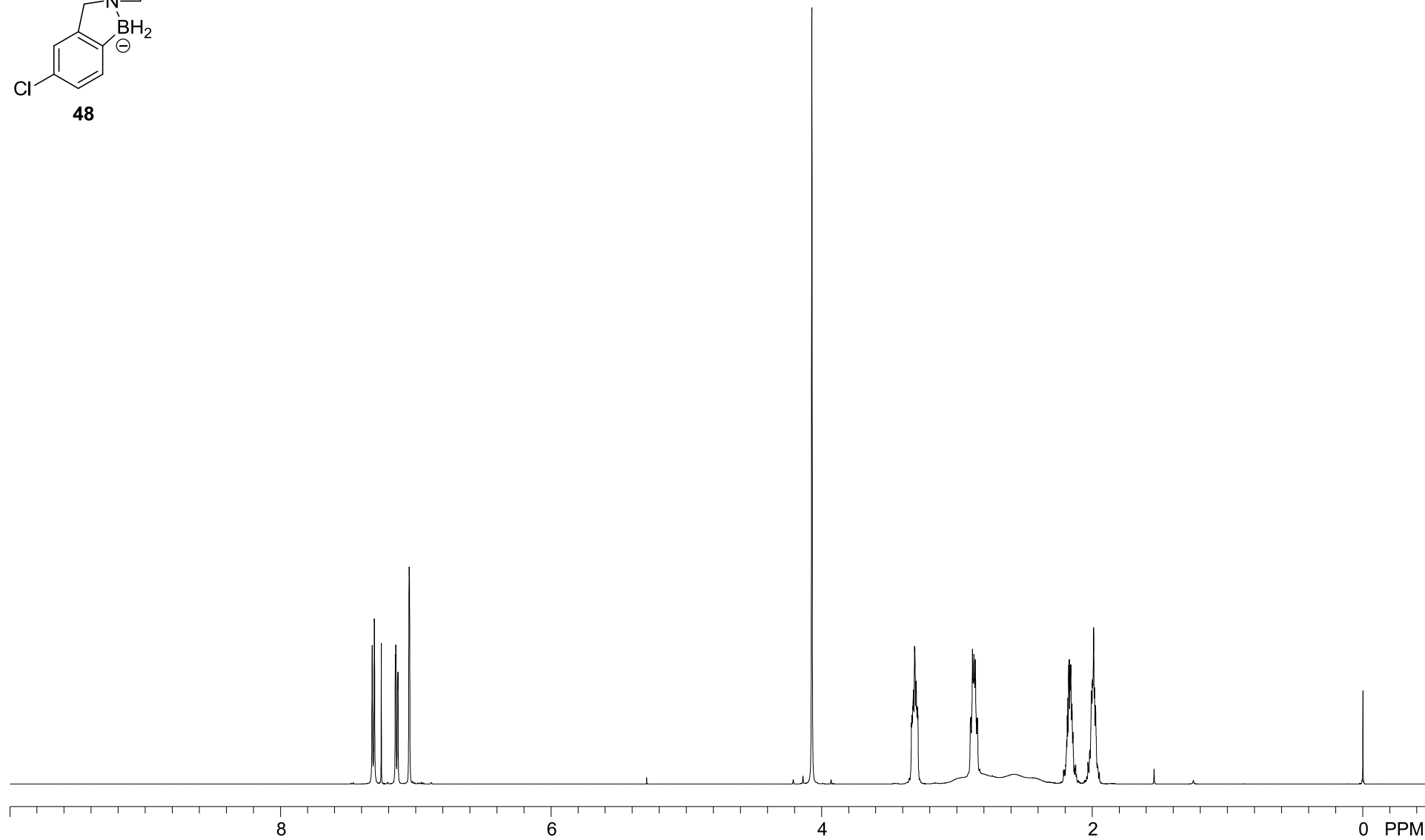
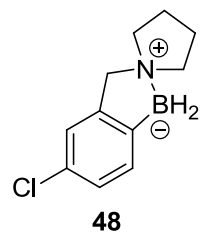
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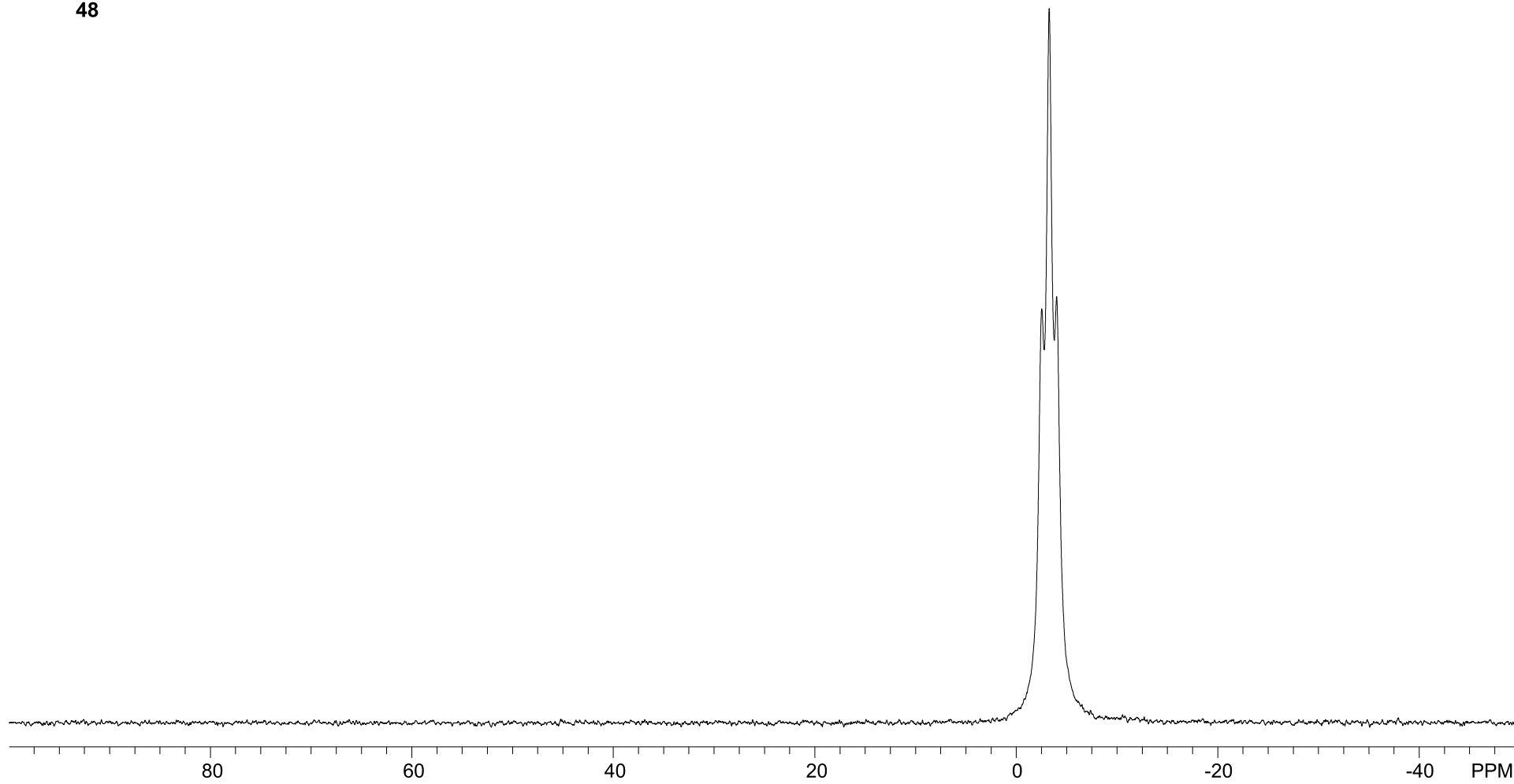
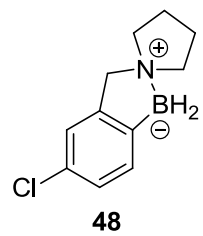
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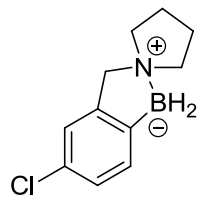
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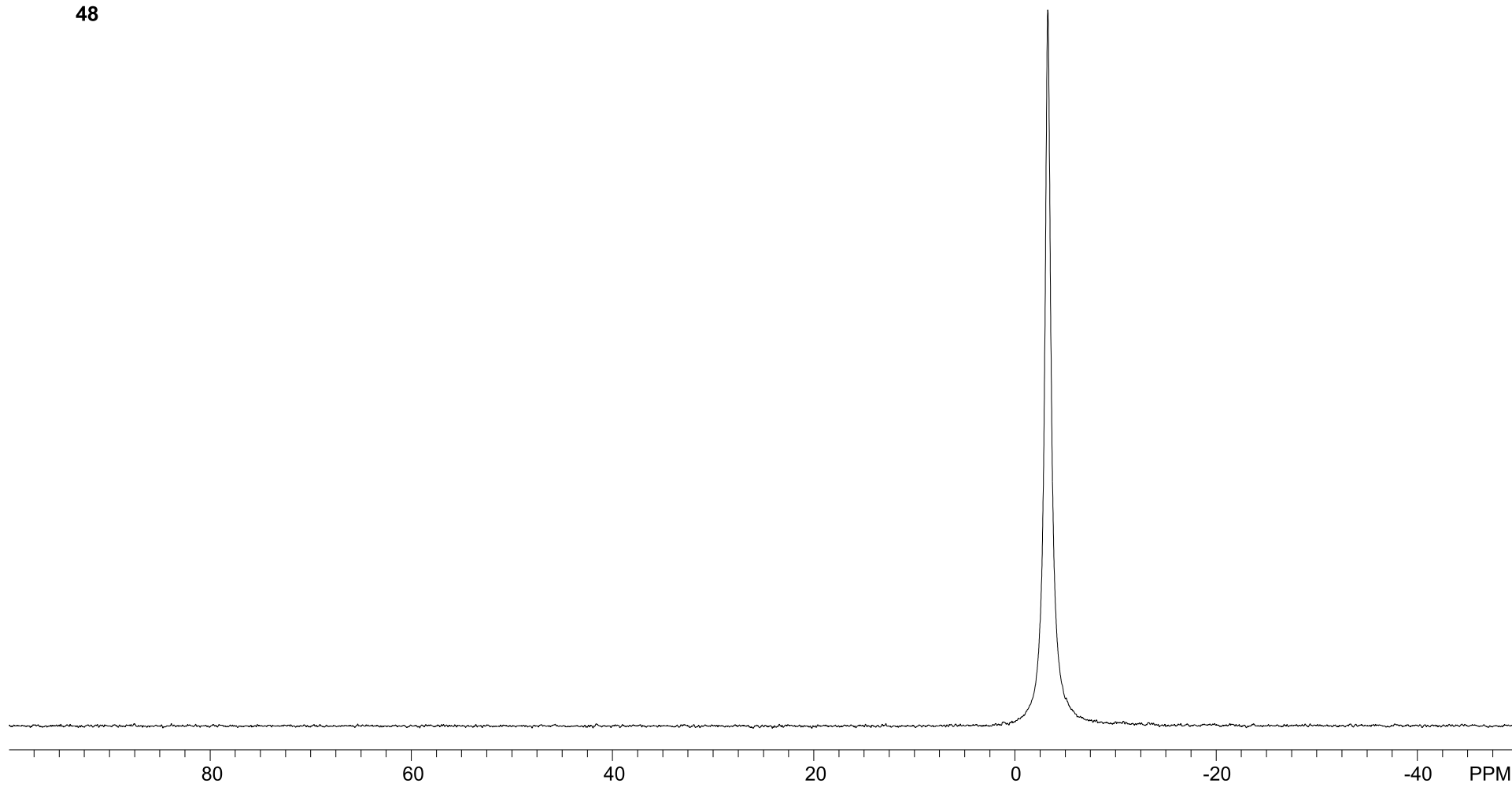
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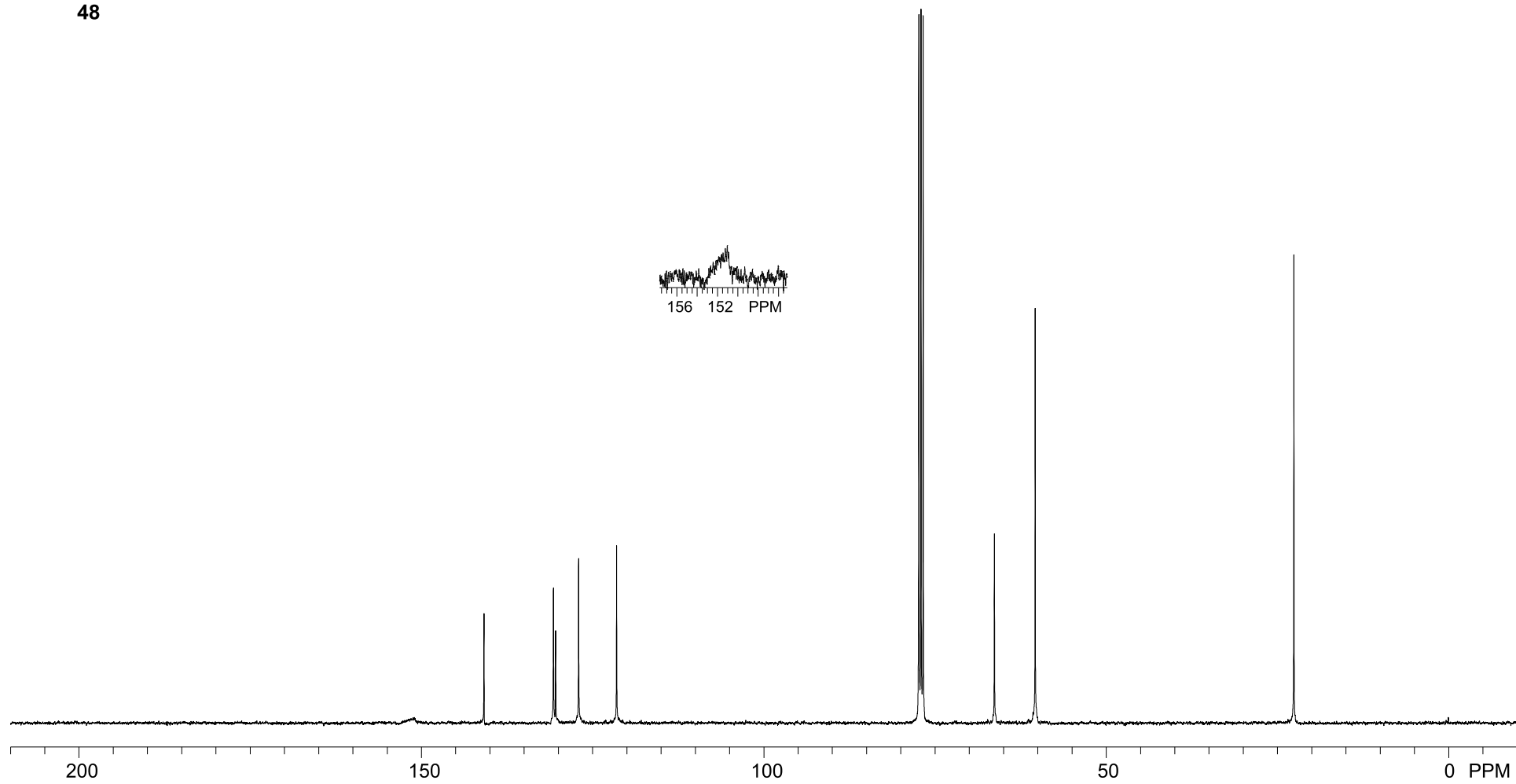
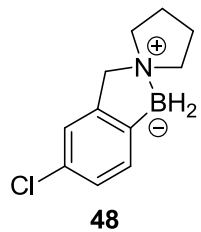
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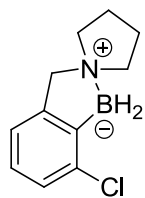
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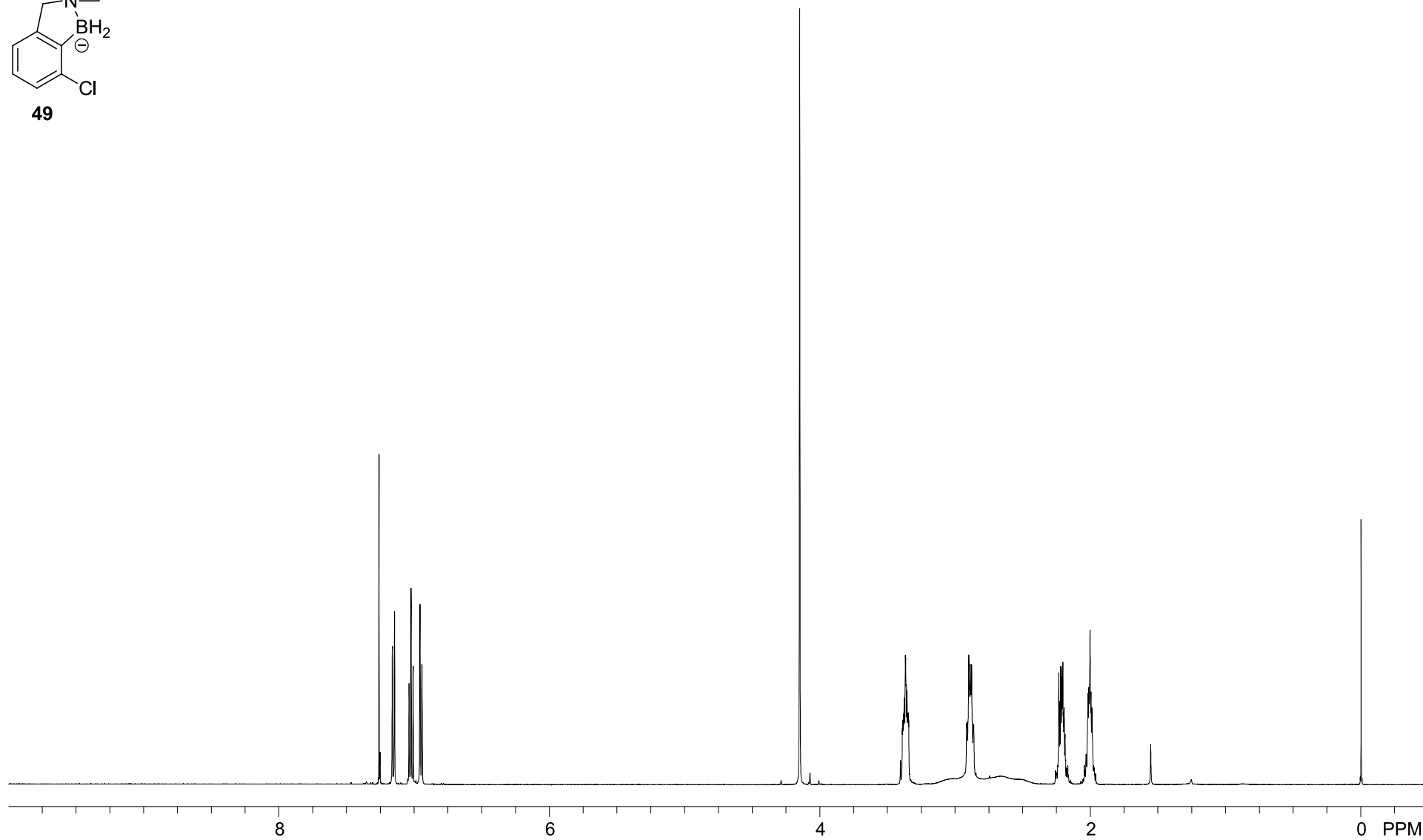
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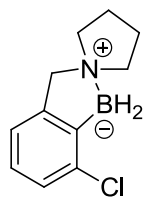
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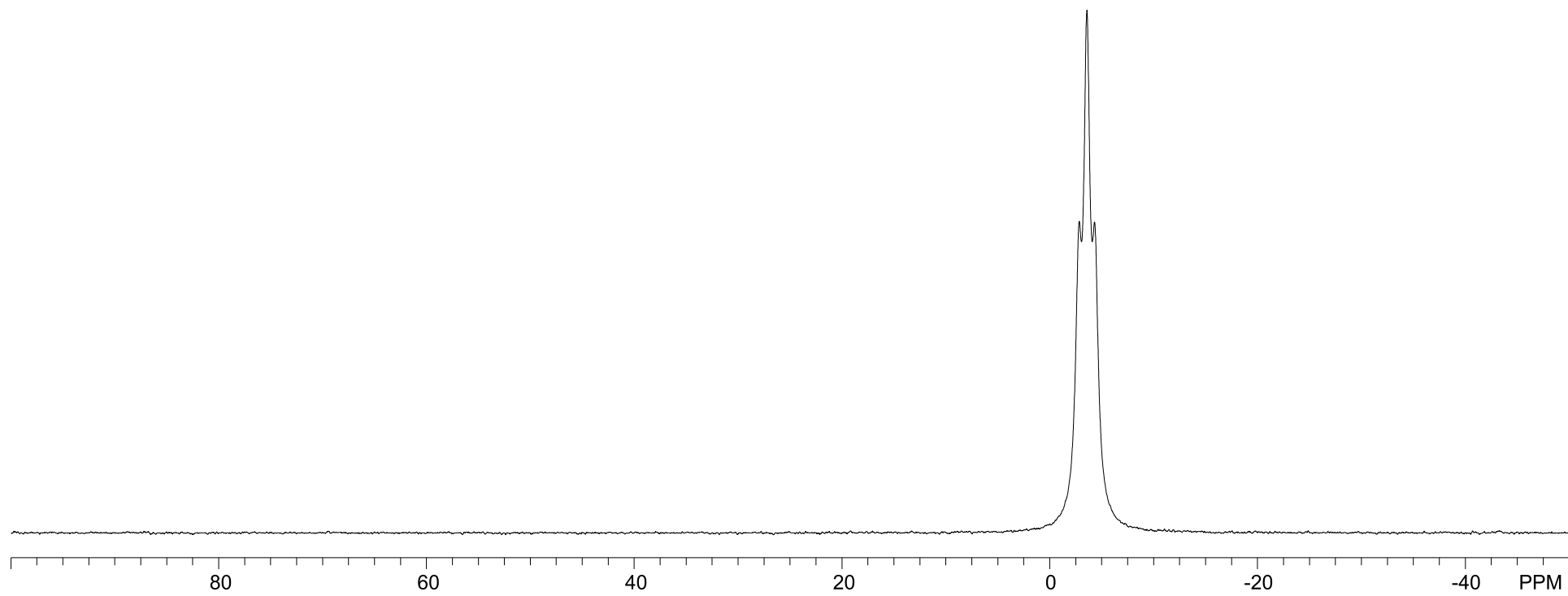
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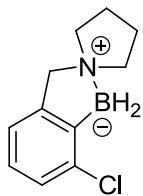
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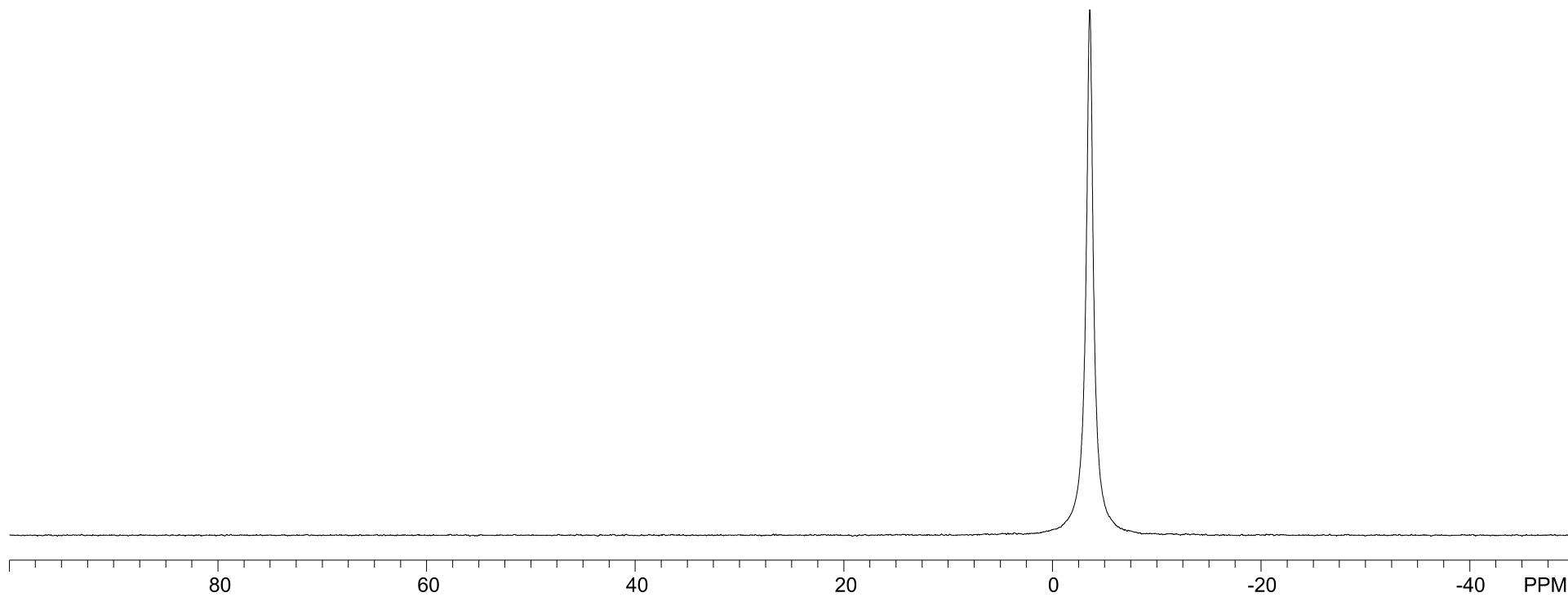
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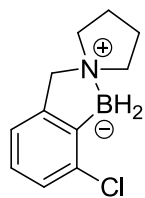
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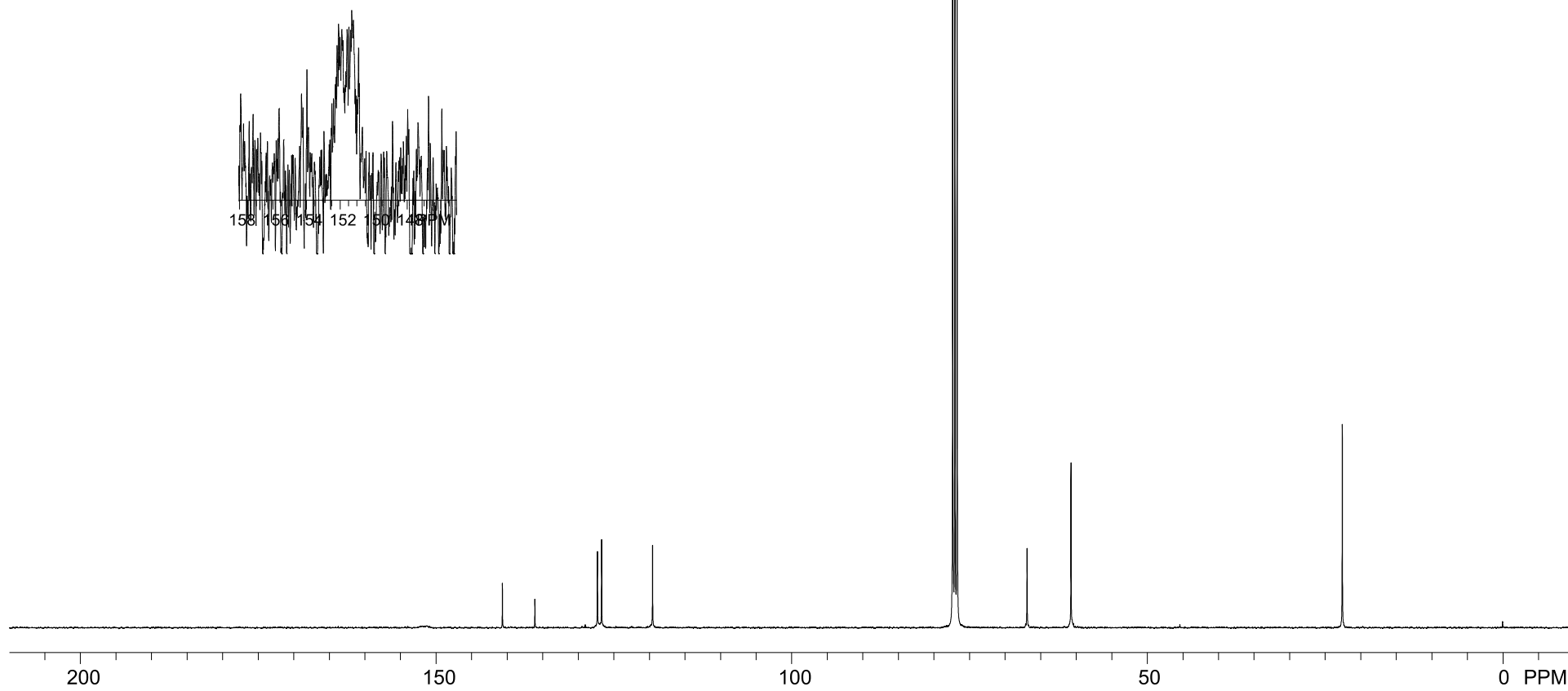
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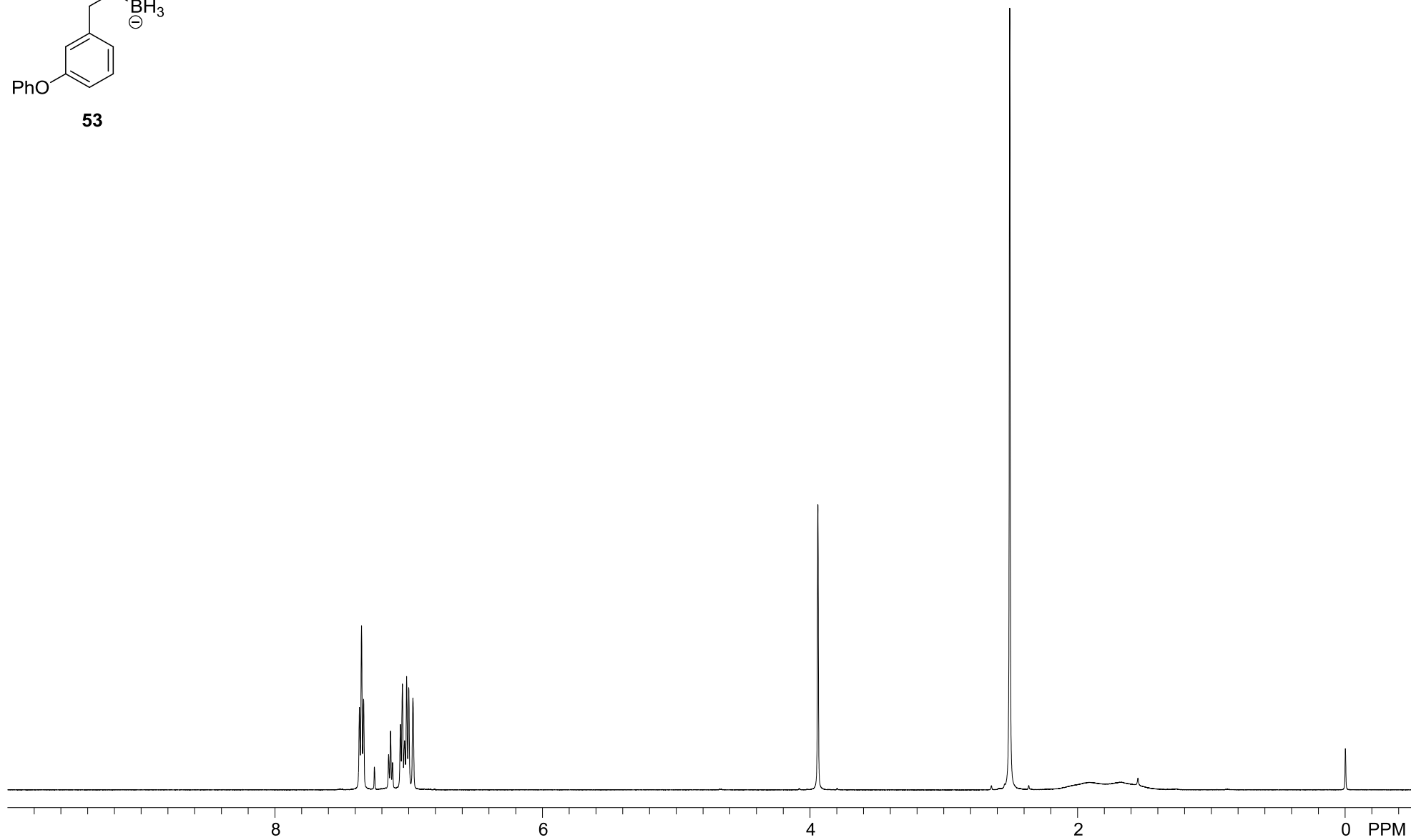
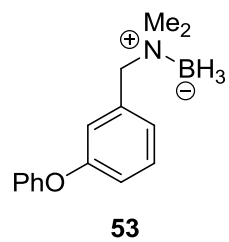
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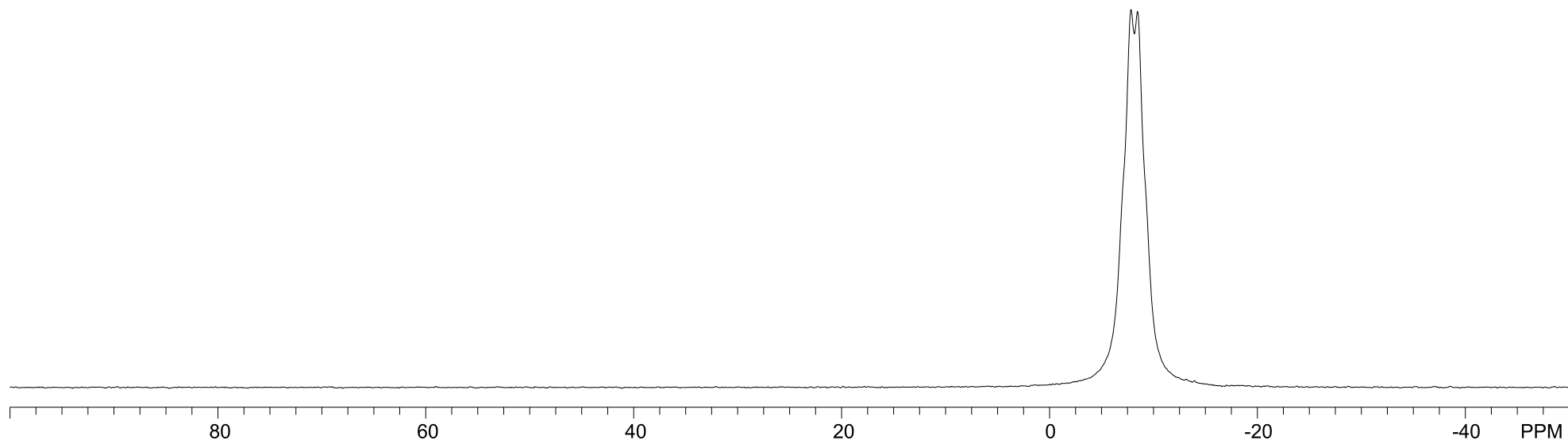
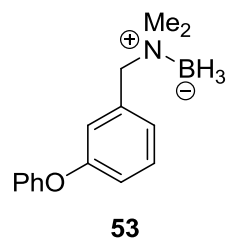
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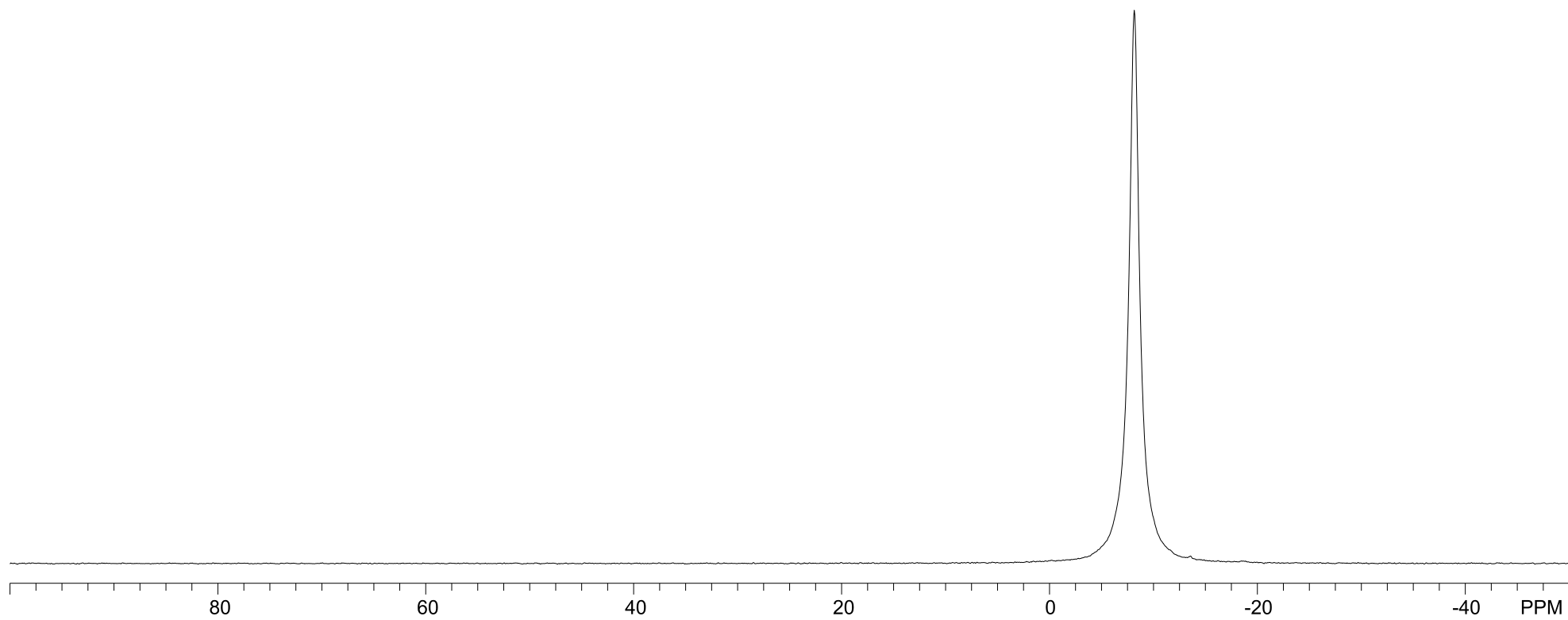
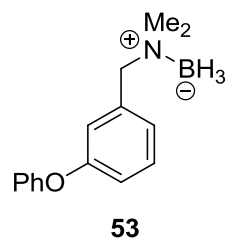
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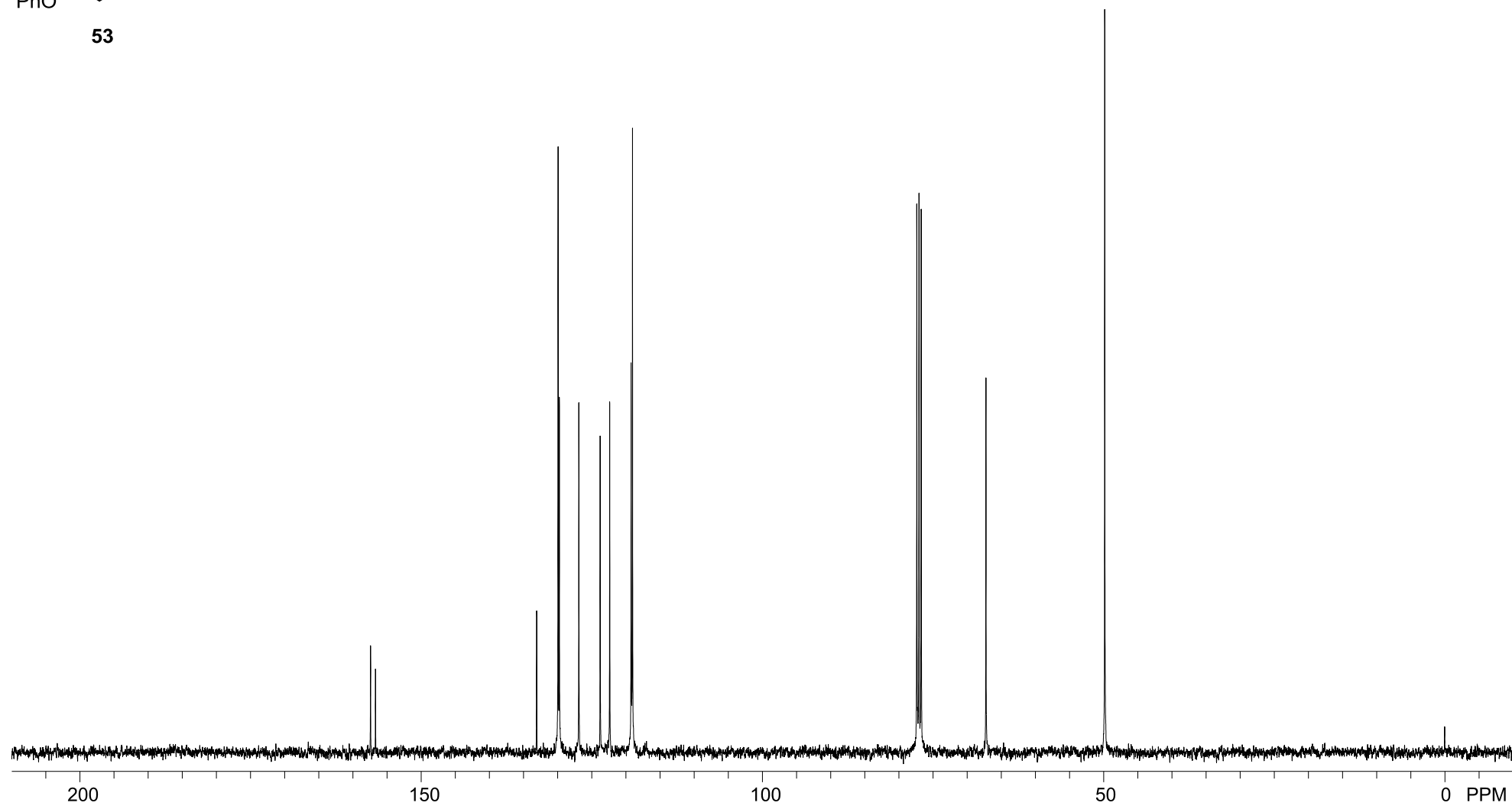
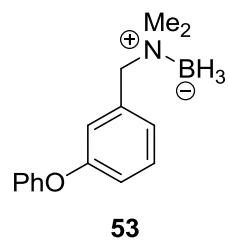
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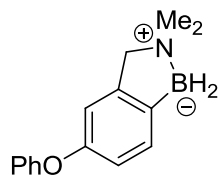
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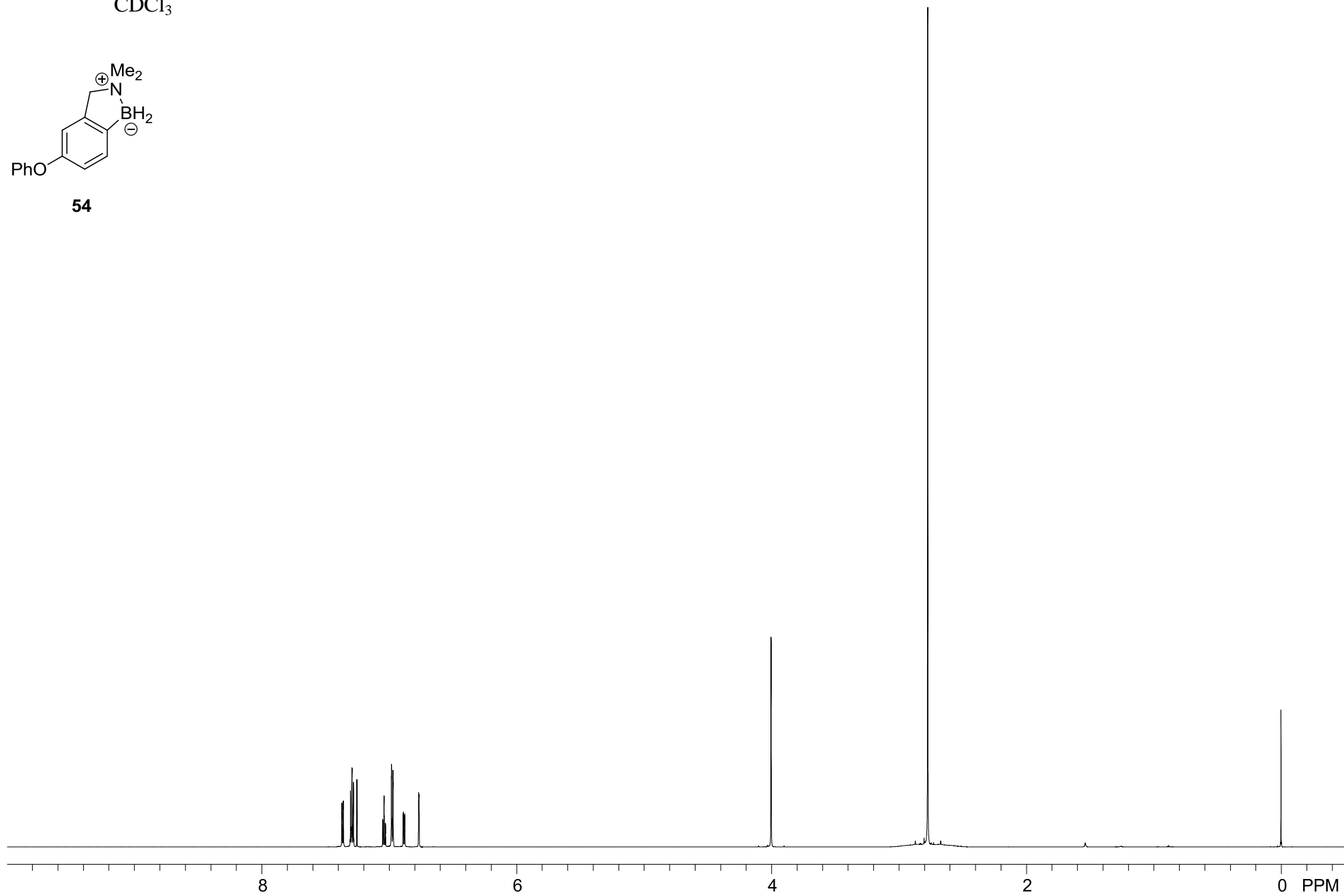
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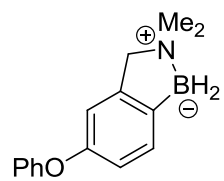
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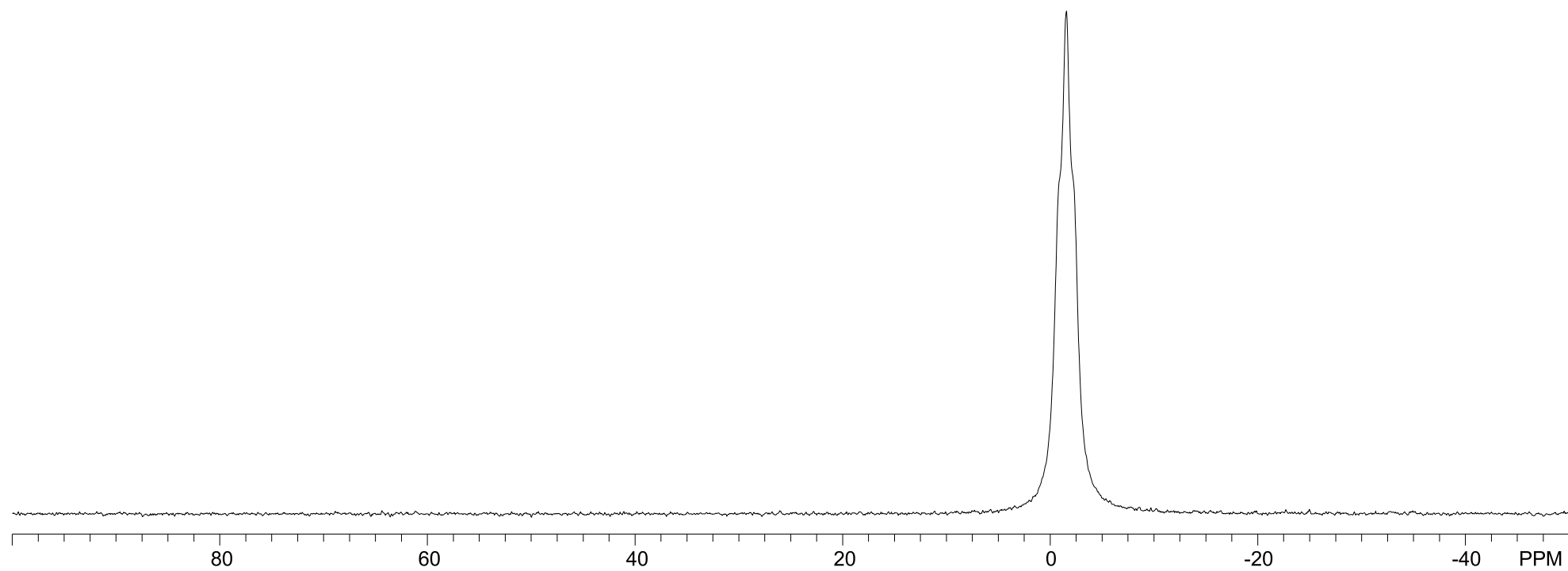
54



^{11}B NMR (128 MHz),
 CDCl_3

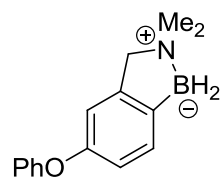


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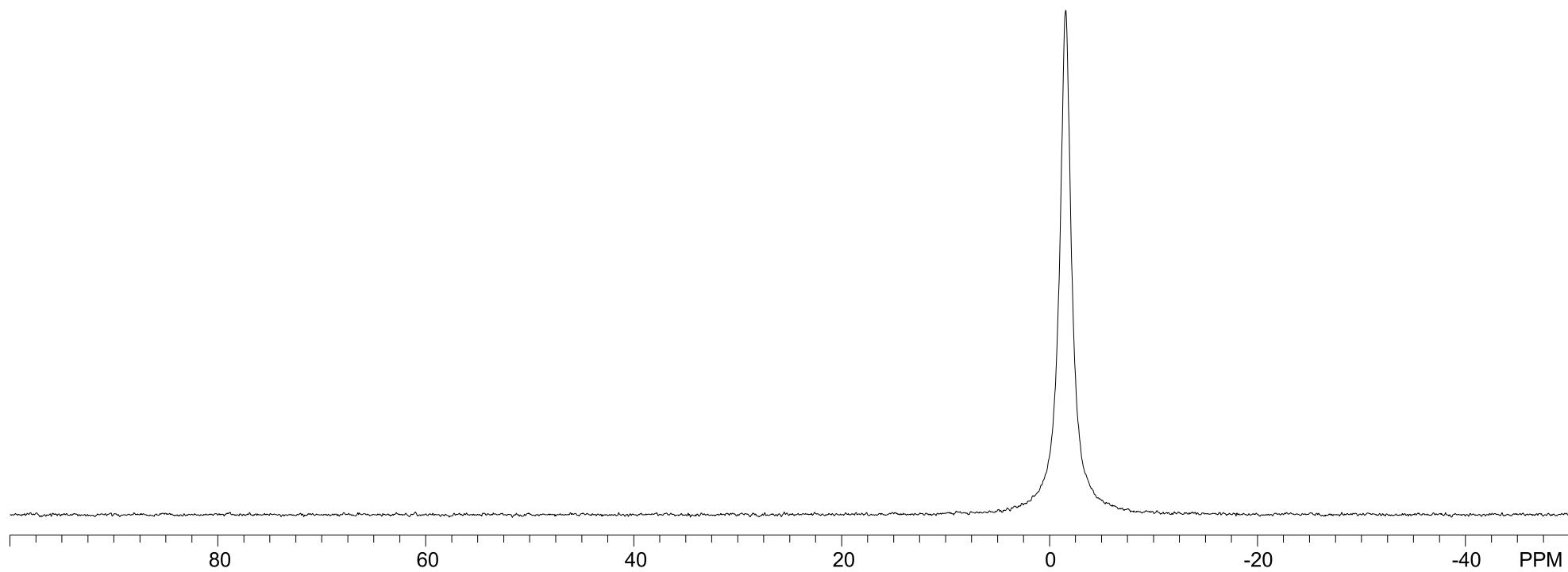


S110

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3

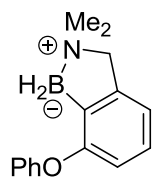


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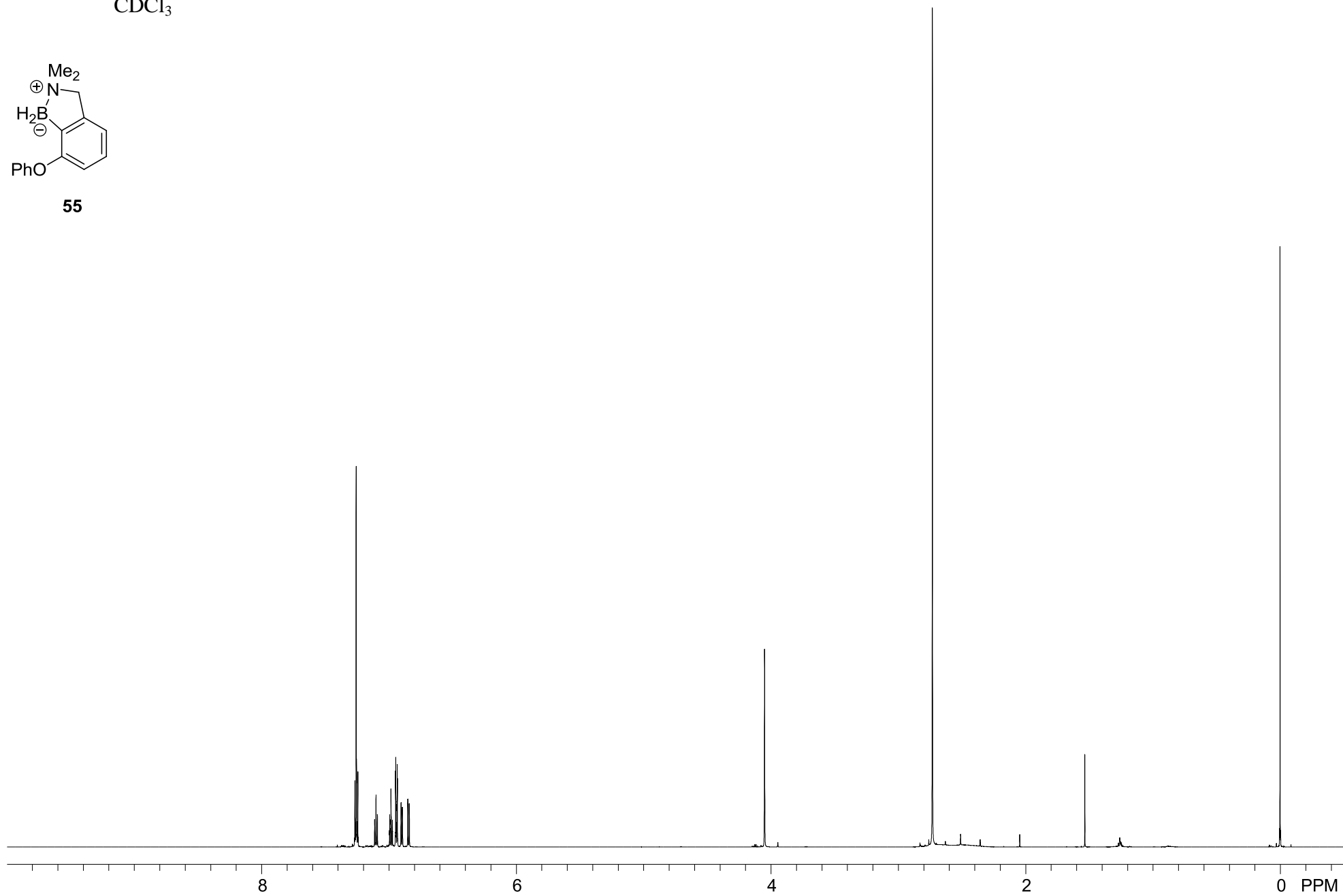


S111

^1H NMR (700 MHz),
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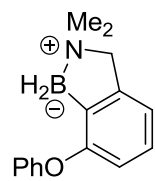


55

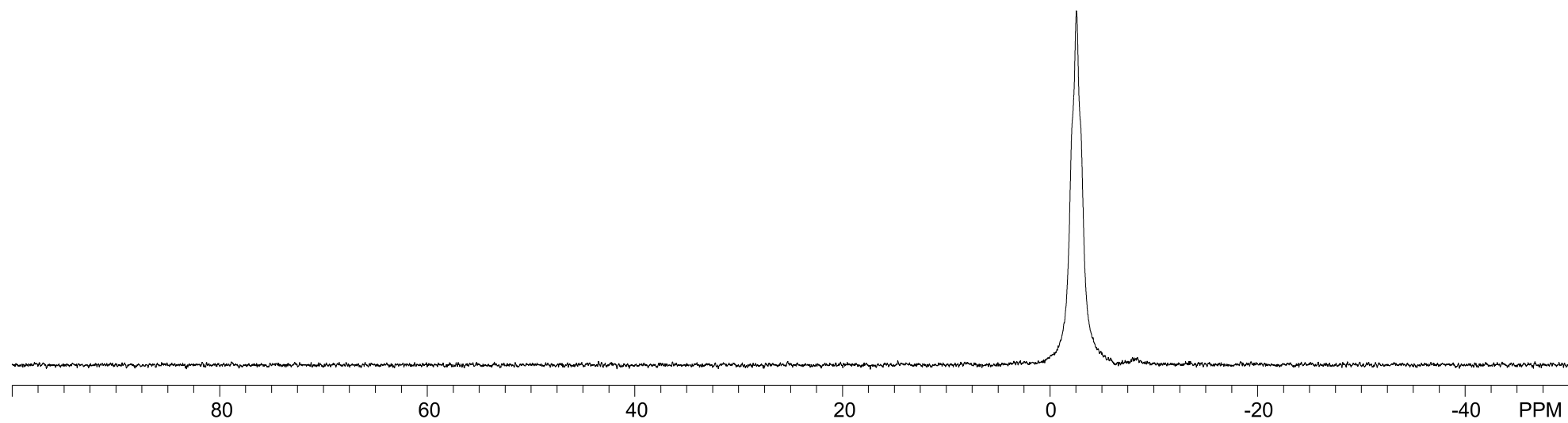


S113

^{11}B NMR (225 MHz),
 CDCl_3

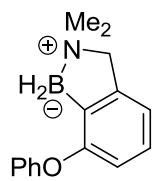


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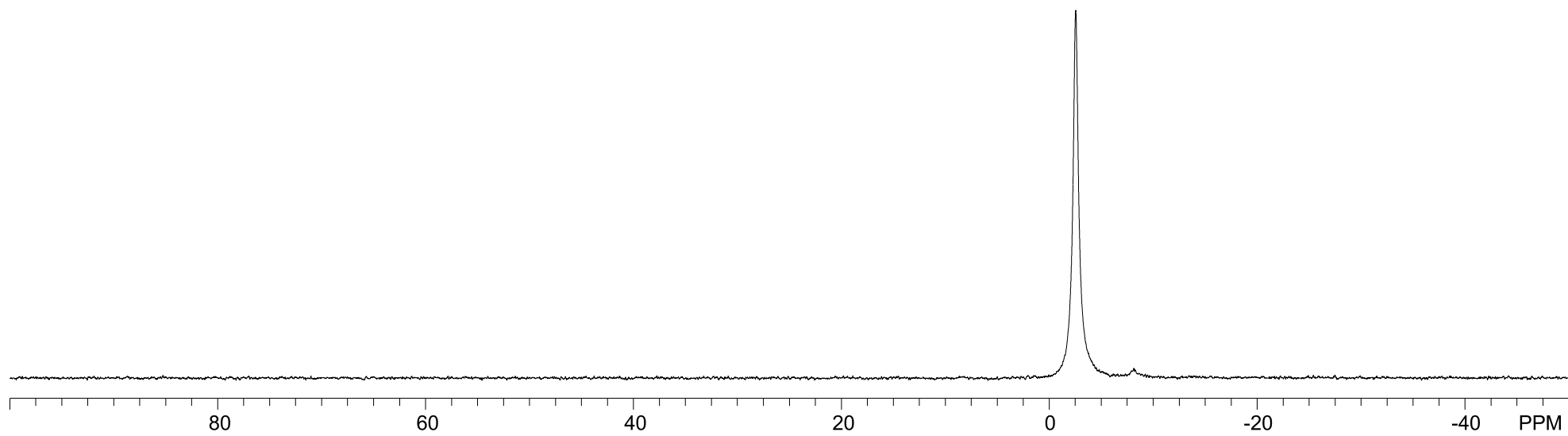


S114

$^{11}\text{B}\{^1\text{H}\}$ NMR (225 MHz),
 CDCl_3

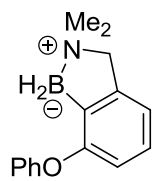


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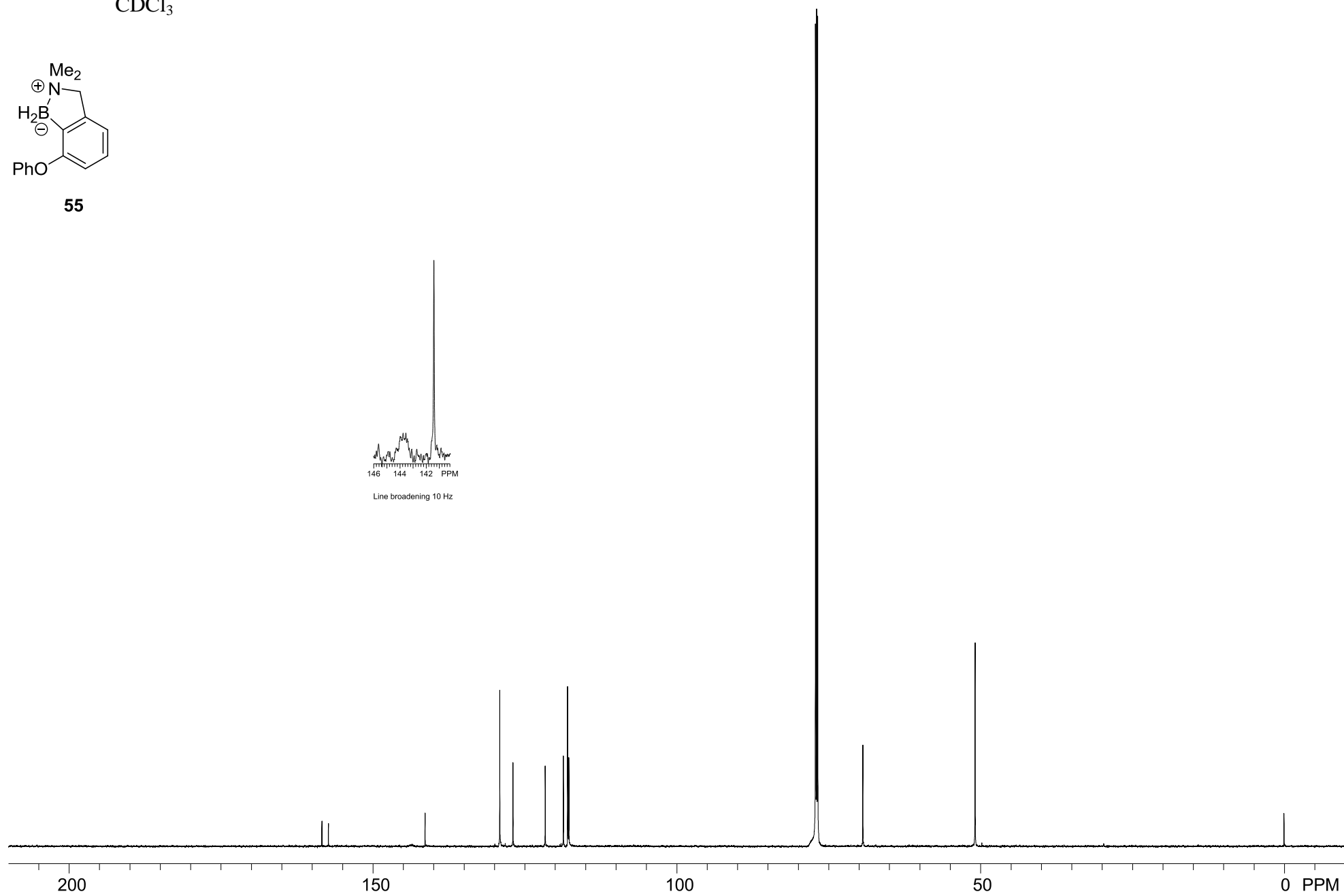


S115

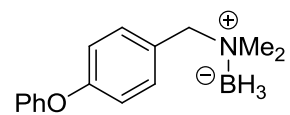
$^{13}\text{C}\{^1\text{H}\}$ NMR (176 MHz),
 CDCl_3



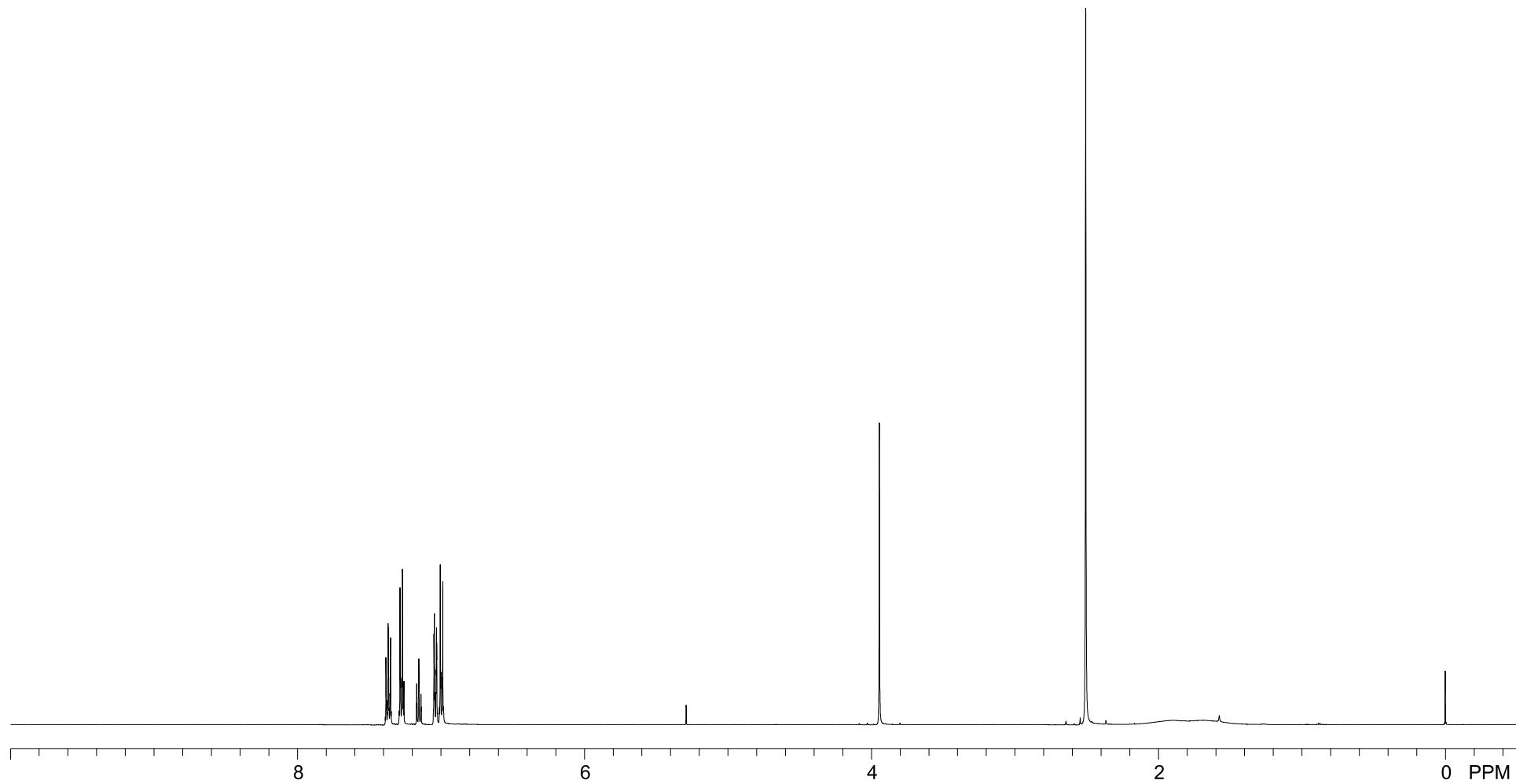
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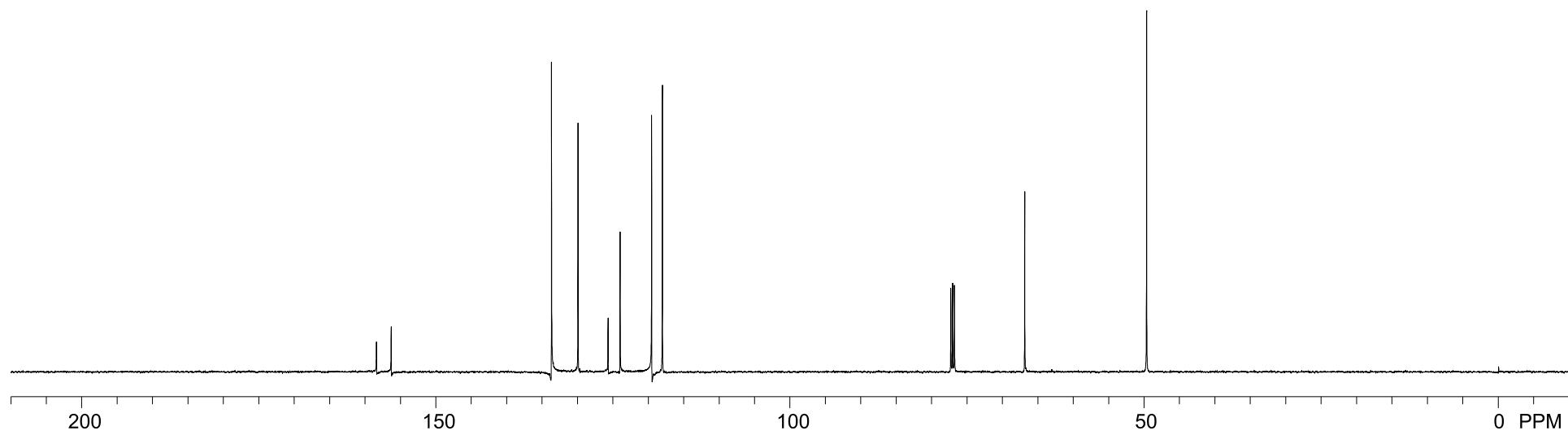
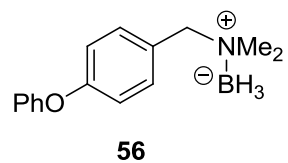
^1H NMR (500 MHz),
 CDCl_3



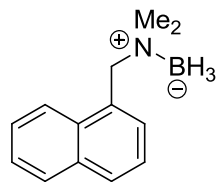
56



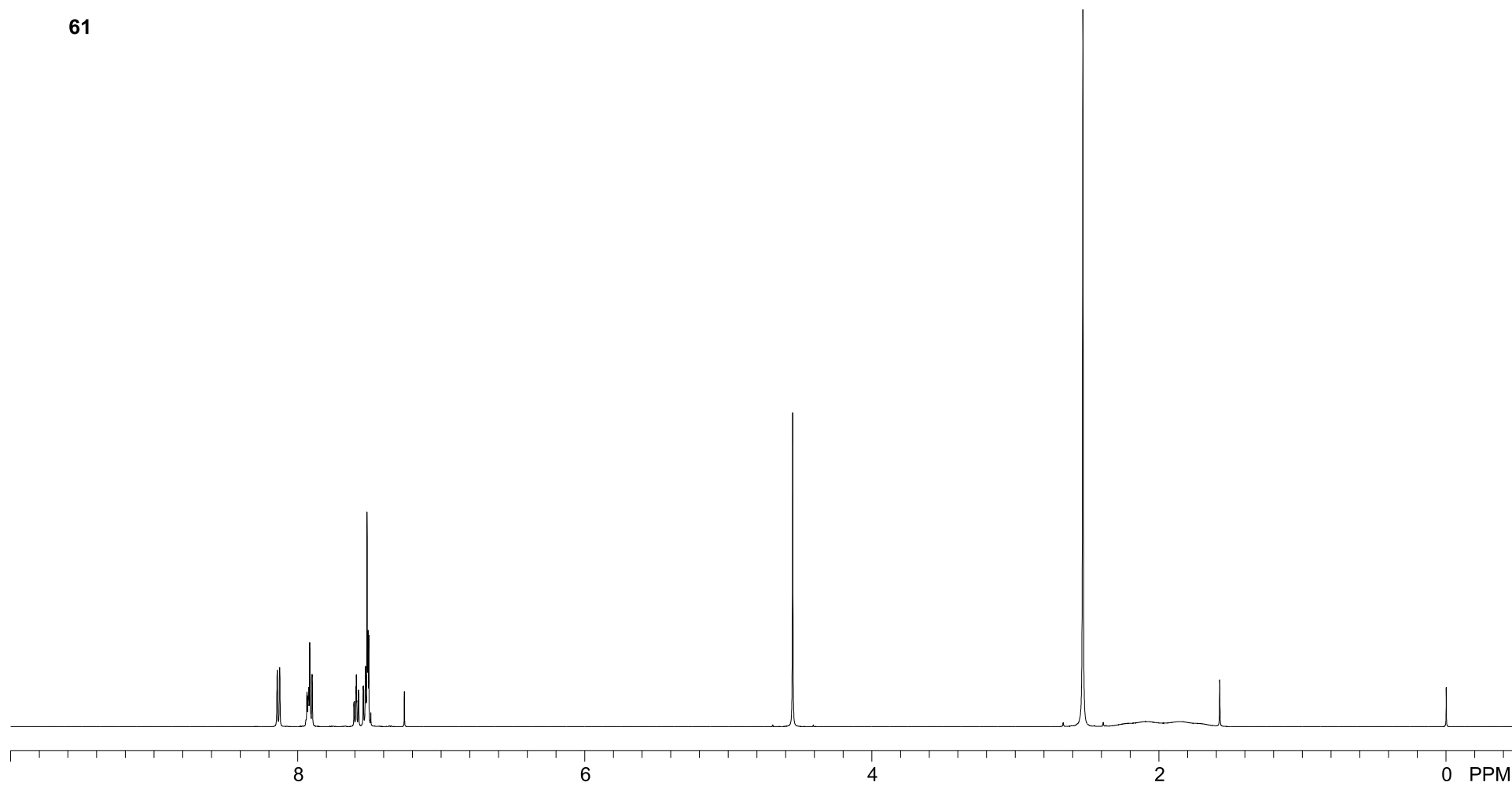
$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CDCl_3



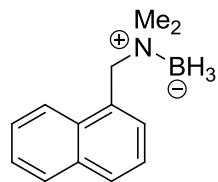
^1H NMR (500 MHz),
 CDCl_3



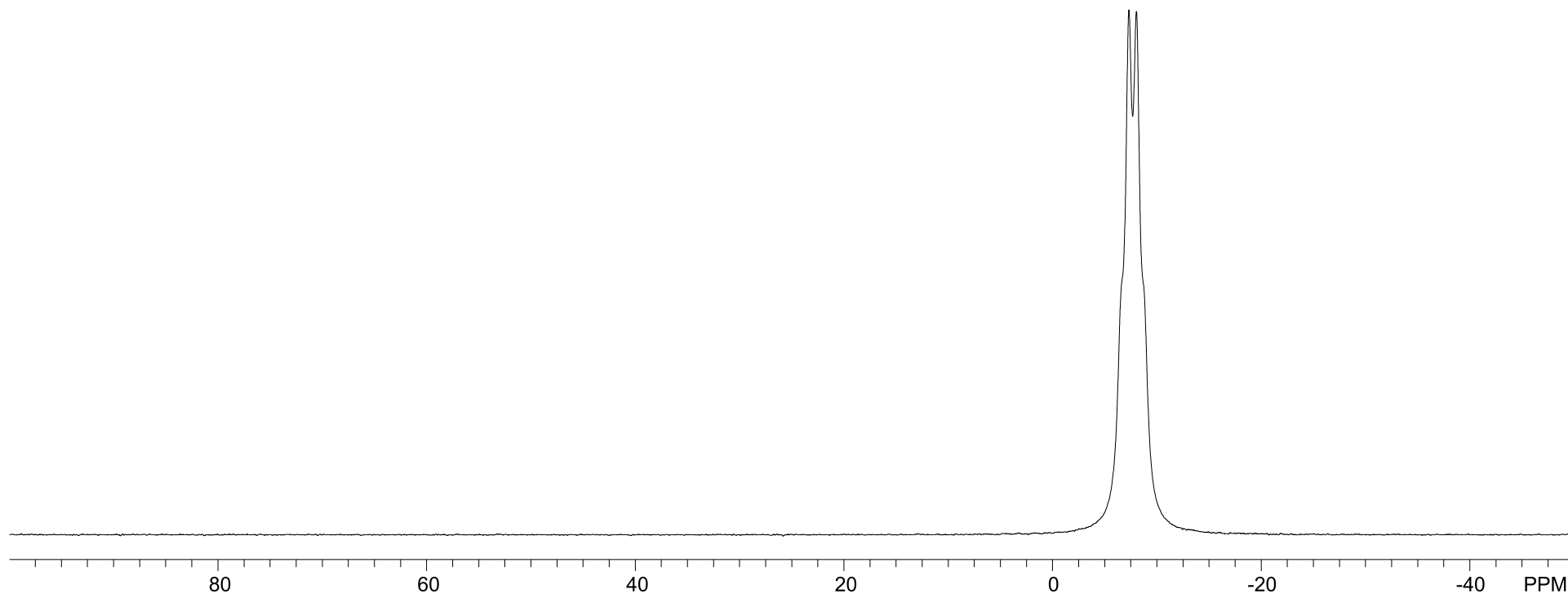
61



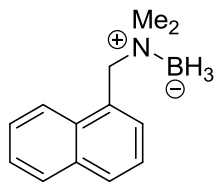
^{11}B NMR (128 MHz),
 CDCl_3



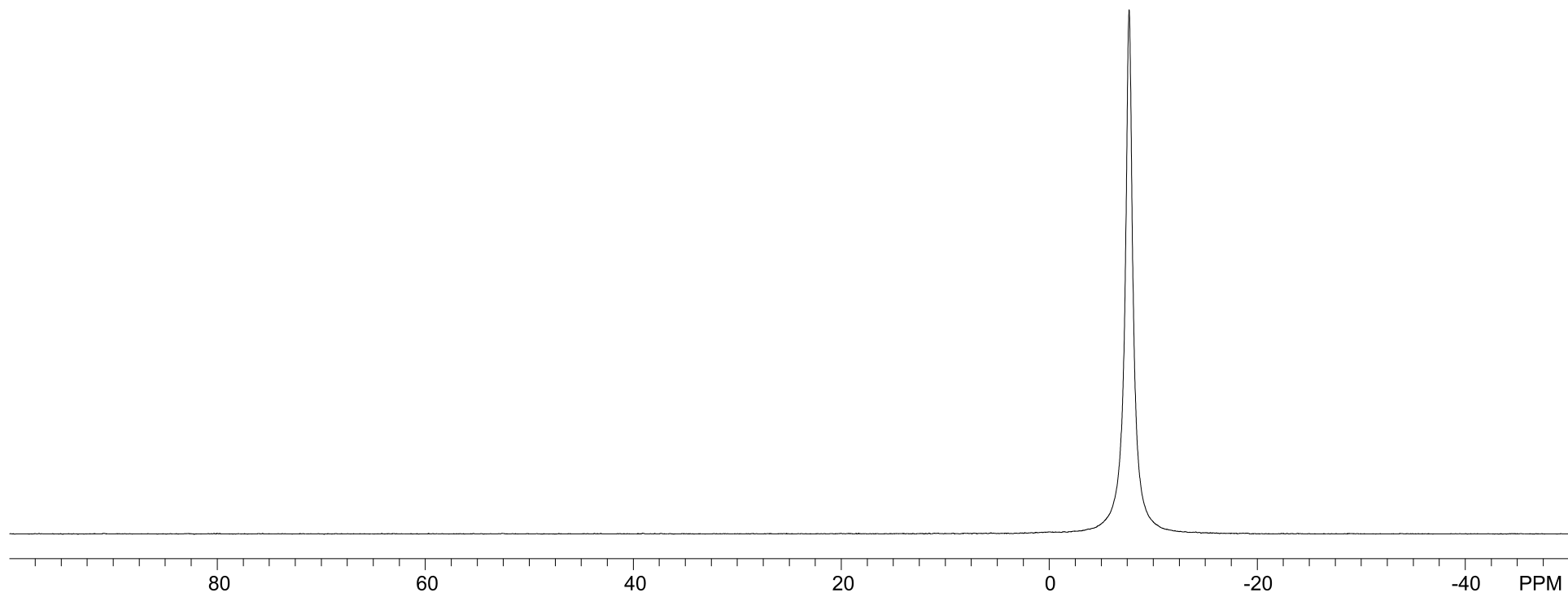
61



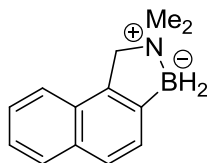
$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3



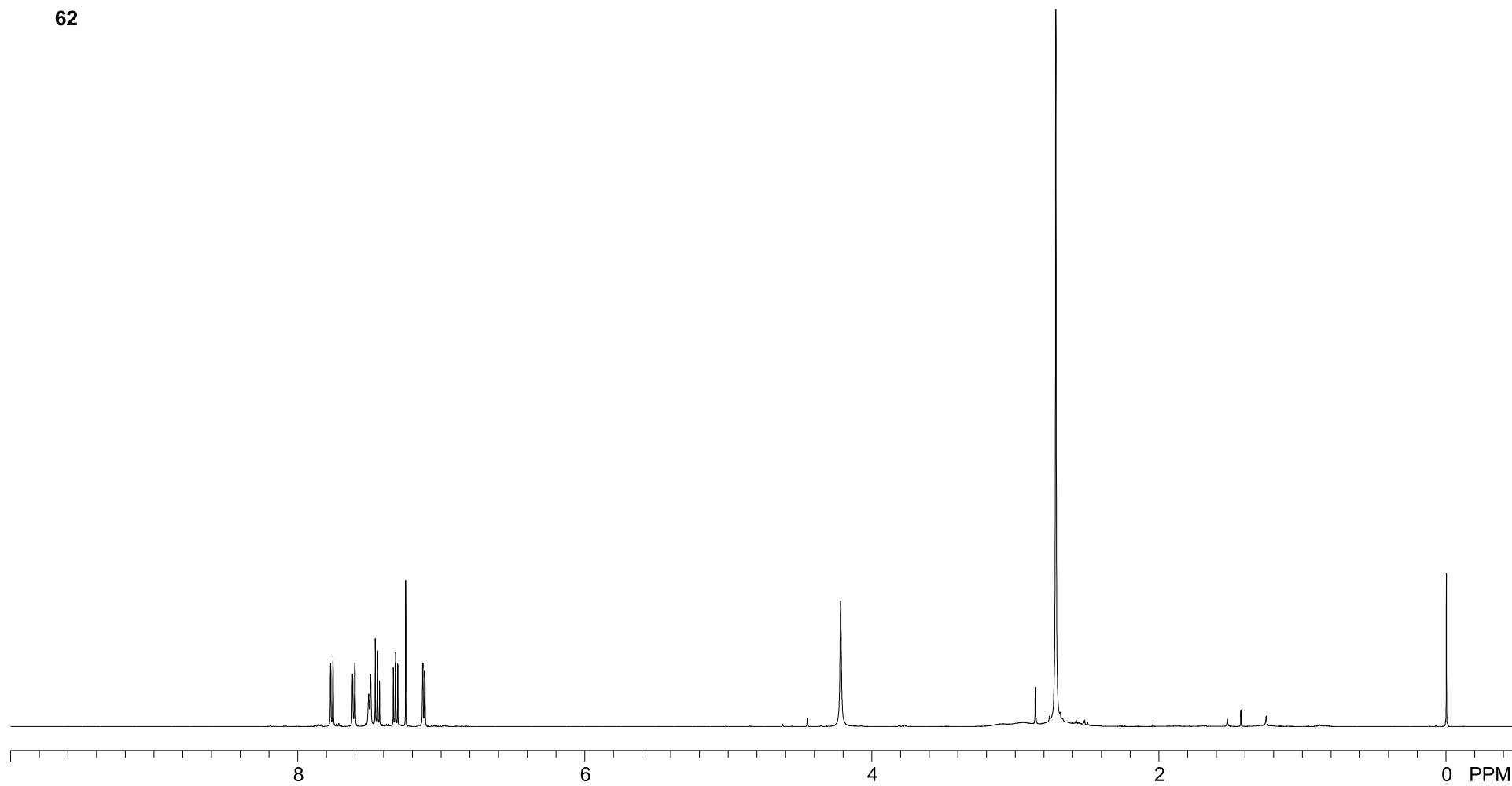
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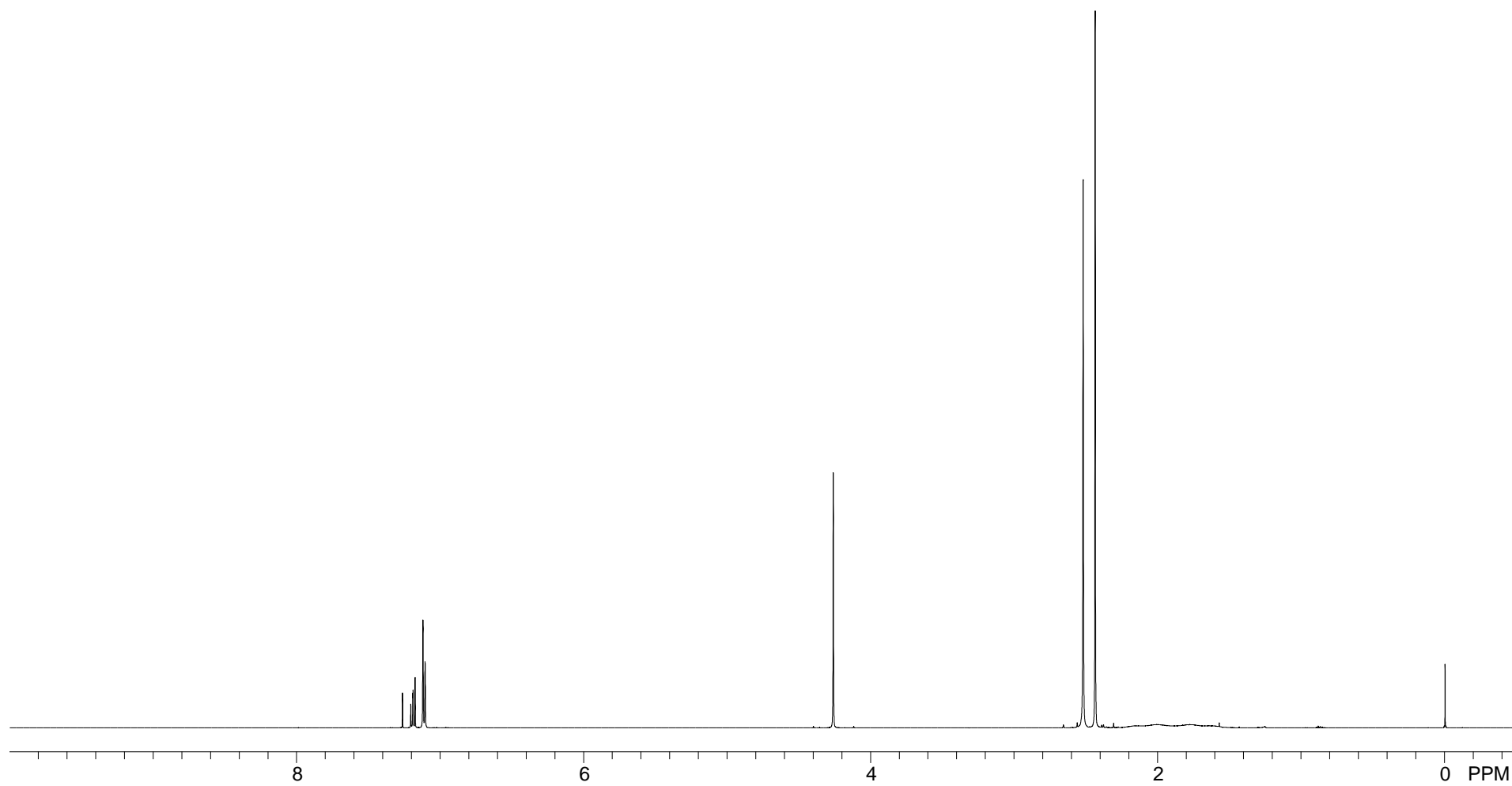
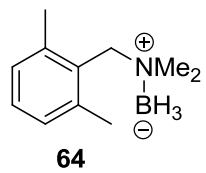
^1H NMR (500 MHz),
 CDCl_3



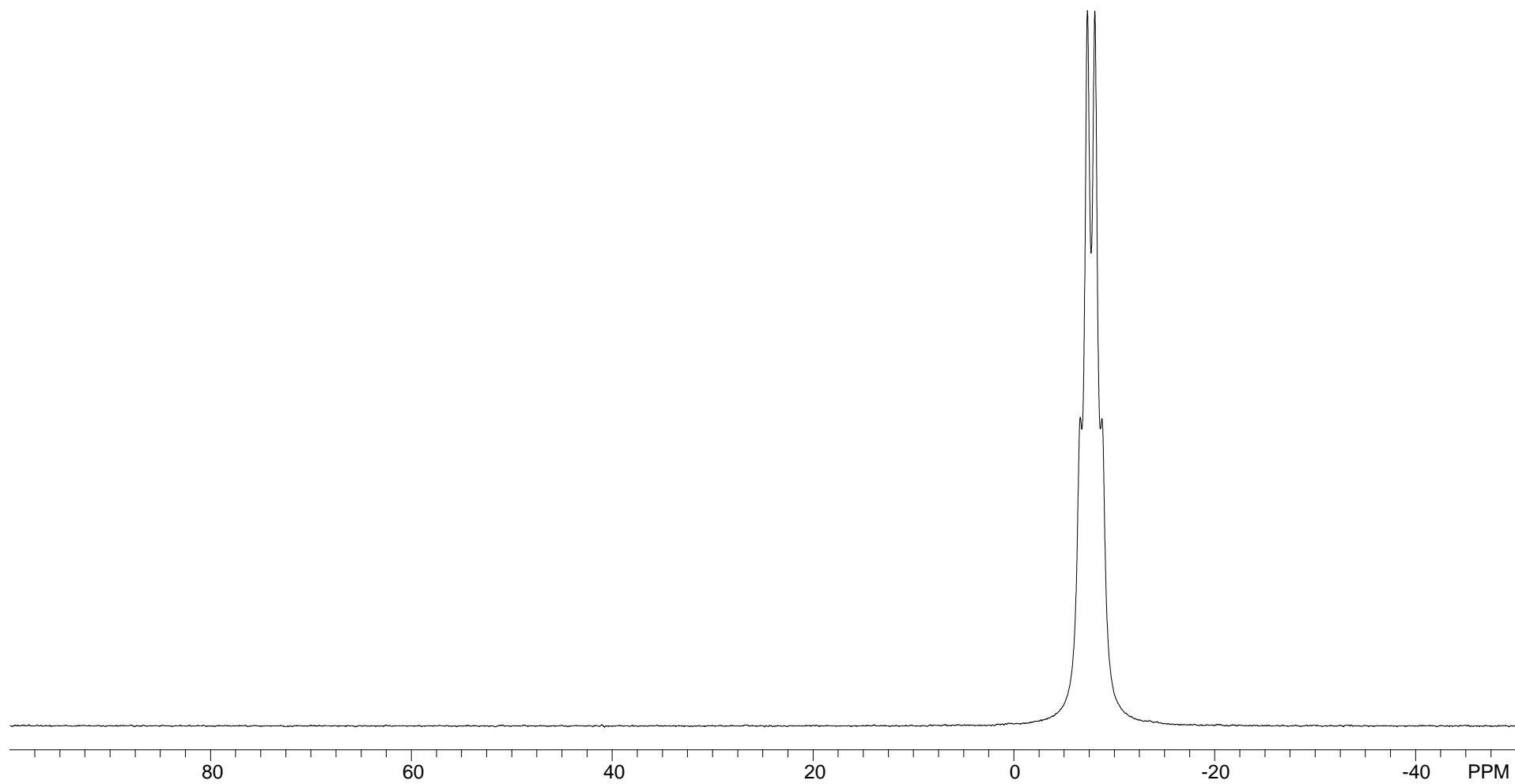
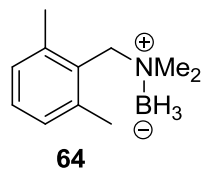
62



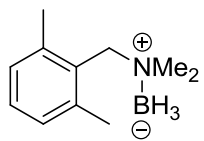
^1H NMR (500 MHz),
 CDCl_3



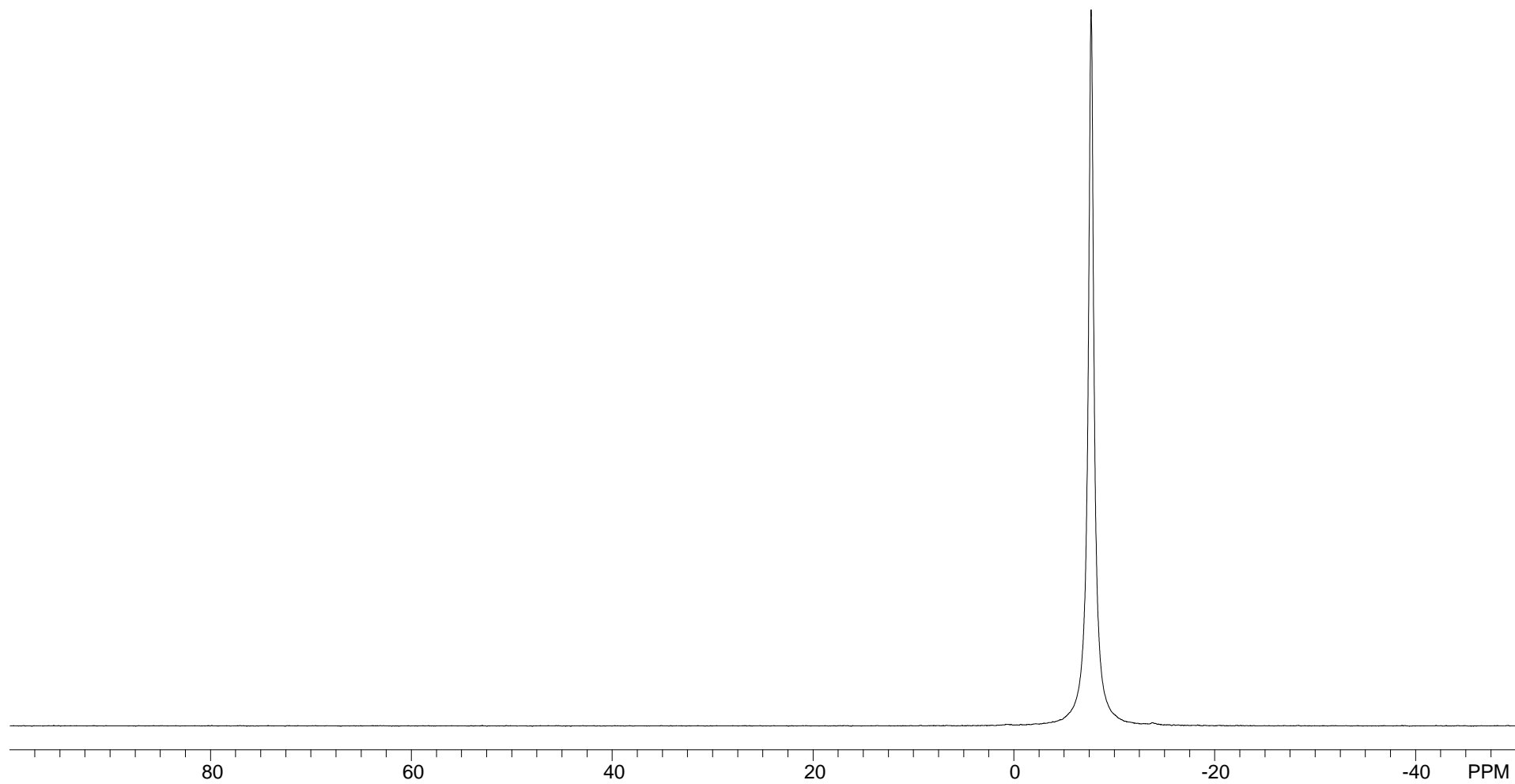
^{11}B NMR (128 MHz),
 CDCl_3



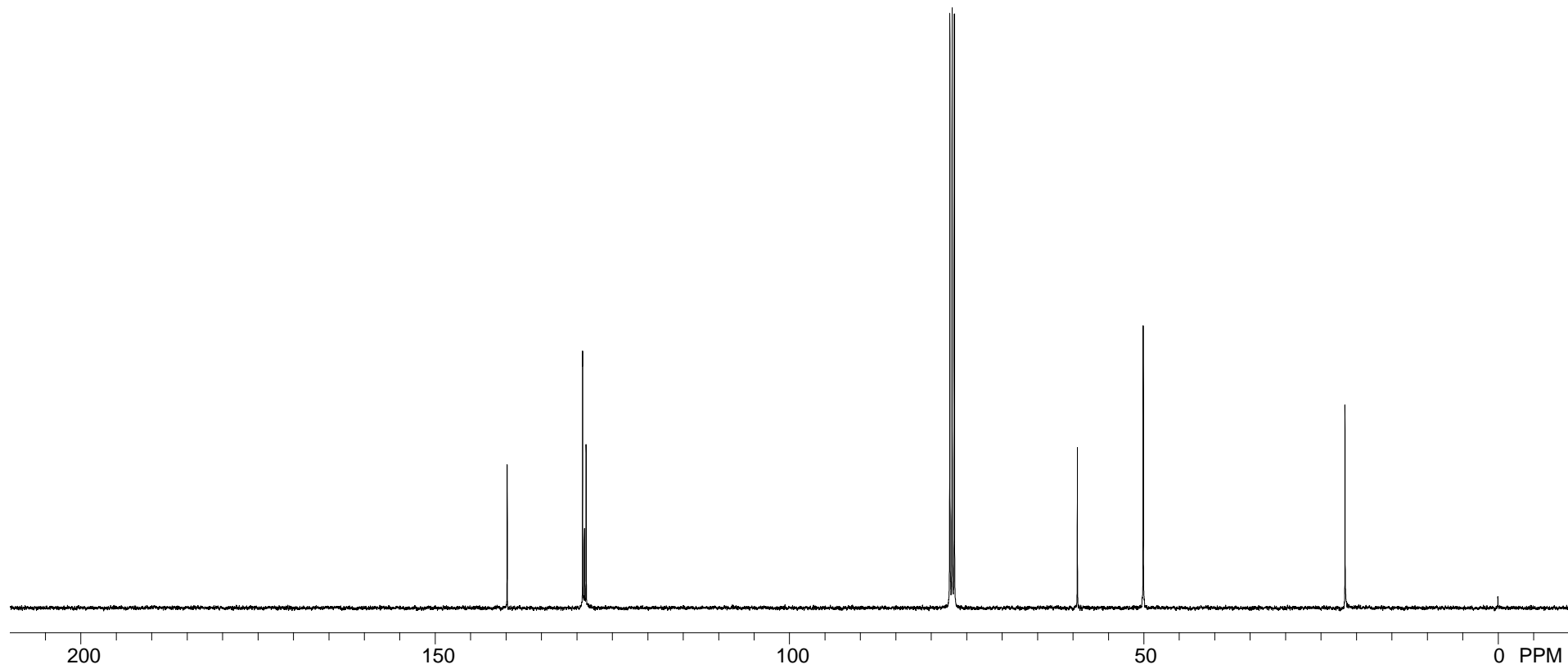
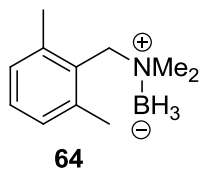
$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3



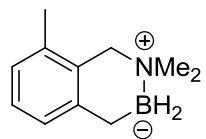
64



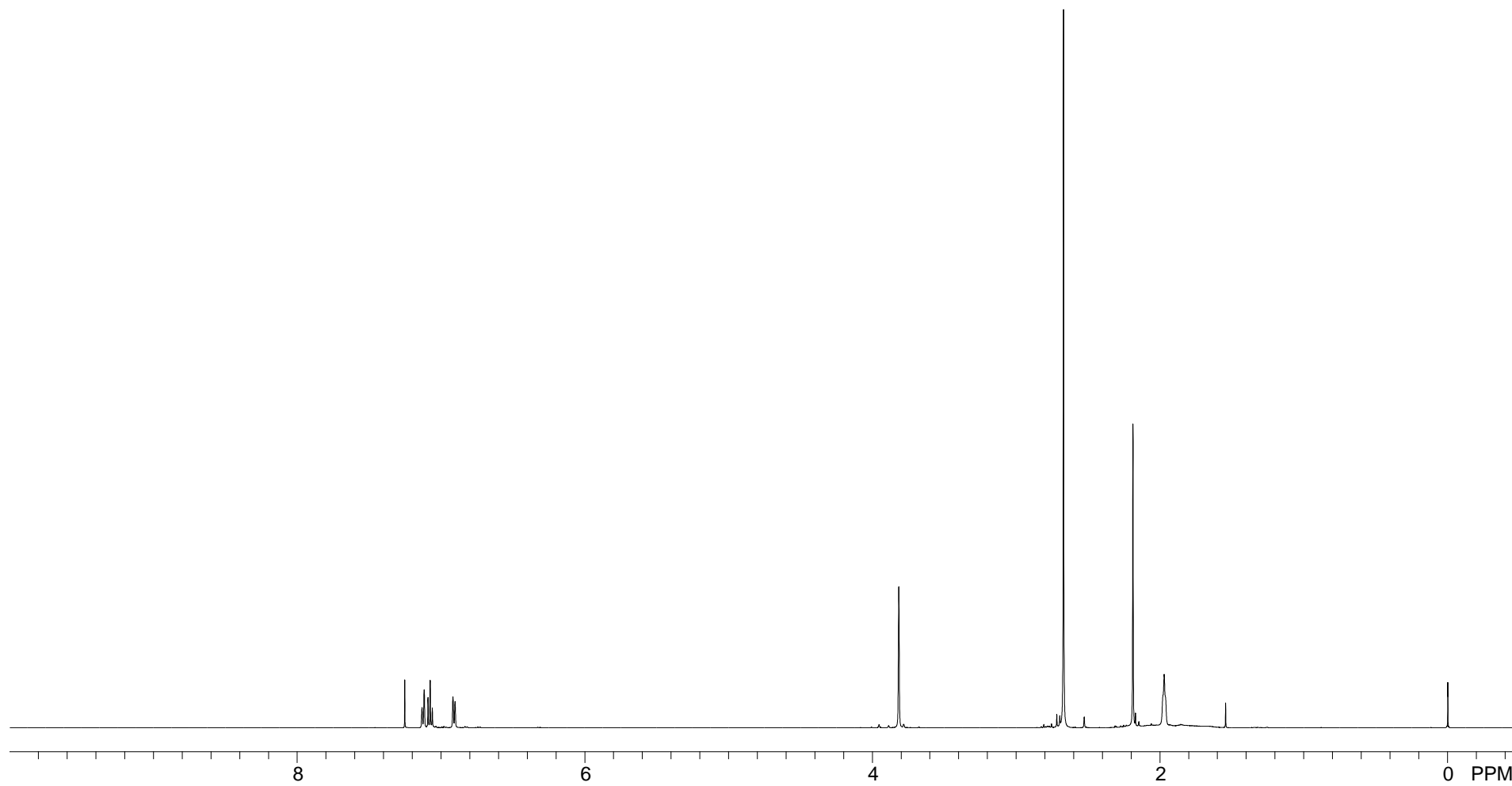
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz),
 CDCl_3



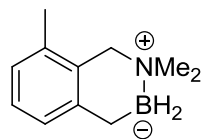
^1H NMR (500 MHz),
 CDCl_3



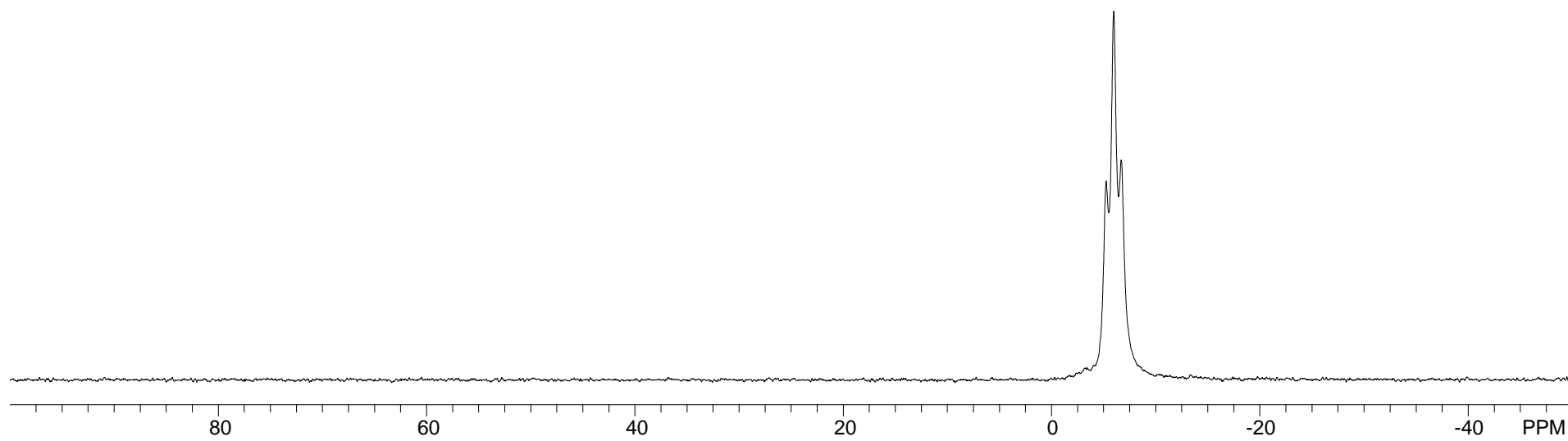
65



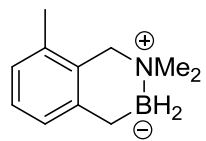
^{11}B NMR (128 MHz),
 CDCl_3



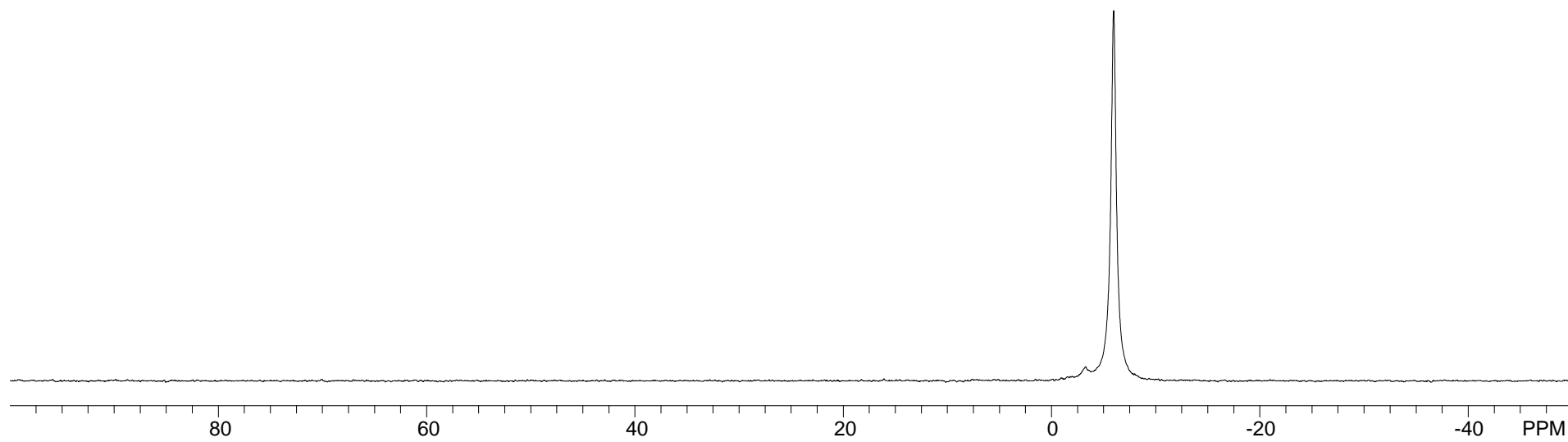
65



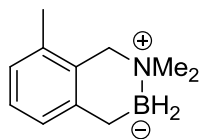
$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz),
 CDCl_3



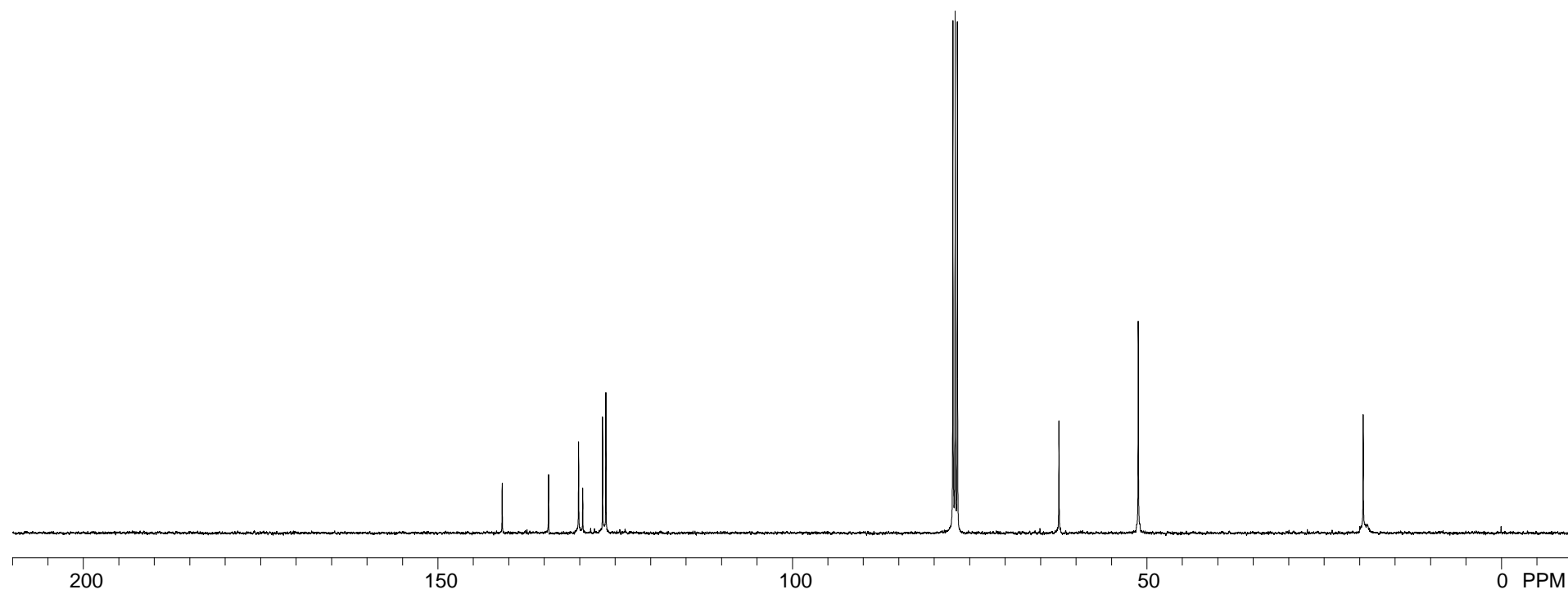
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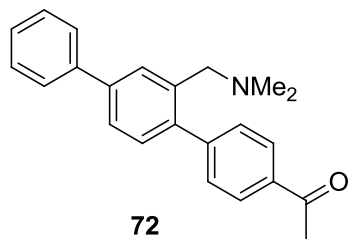
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz),
 CDCl_3



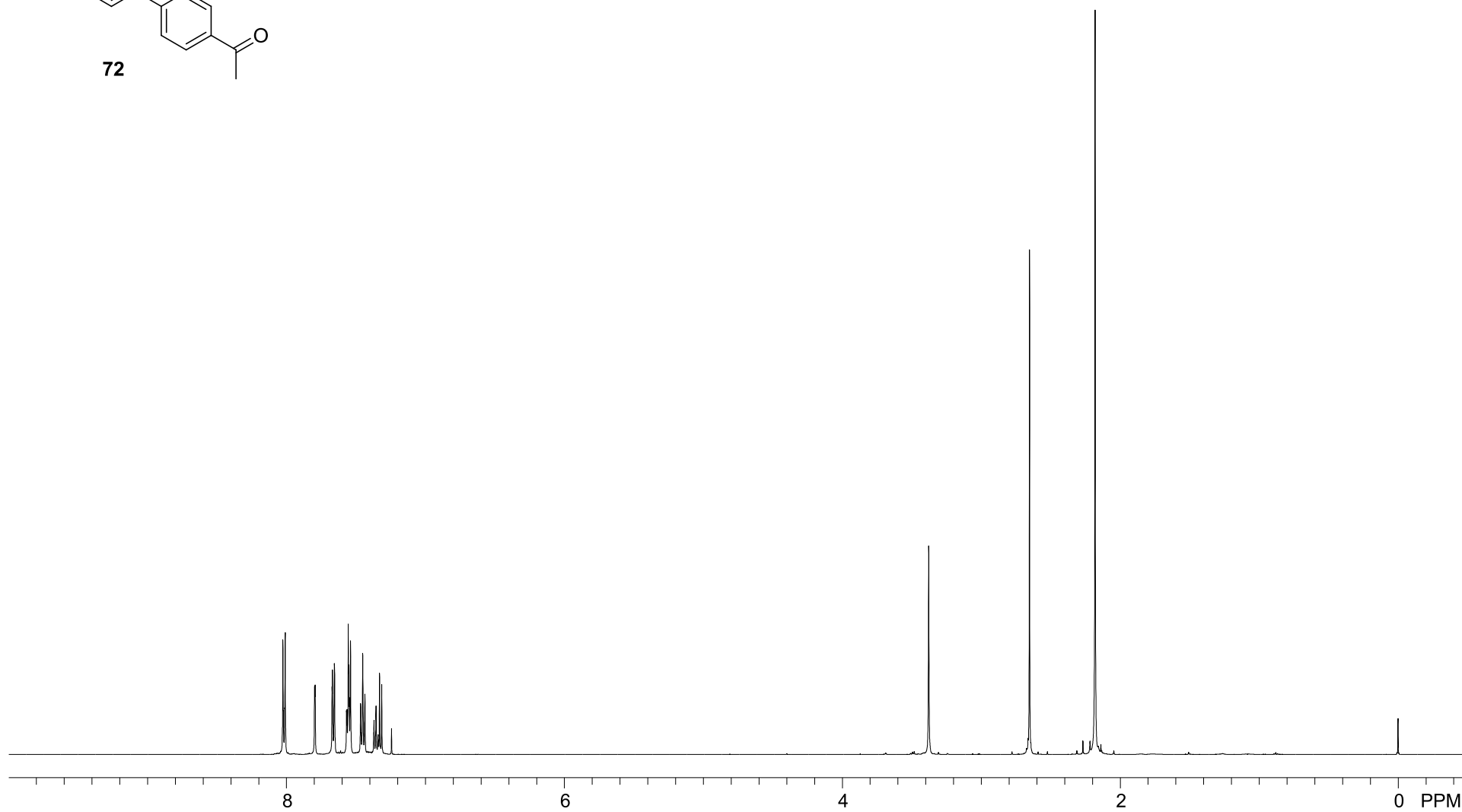
65



^1H NMR (500 MHz),
 CDCl_3



72



$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz),
 CDCl_3

