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# Hypervalent iodine mediated para-selective fluorination of anilides

## Supporting information

*Tian Tian, Wen-He Zhong, Shuai Meng, Xiang-Bao Meng\*, Zhong-Jun Li\**

The State Key Laboratory of Natural and Biomimetic Drugs, School of Pharmaceutical Sciences,

Peking University, Beijing 100191, P R China

[xbmeng@bjmu.edu.cn](mailto:xbmeng@bjmu.edu.cn), [zjli@bjmu.edu.cn](mailto:zjli@bjmu.edu.cn)

## Supplementary Information

|                                                                                               |        |
|-----------------------------------------------------------------------------------------------|--------|
| Nonreactive substrates using $\text{PhI}(\text{OPiv})_2/\text{HF}\cdot\text{Py}$ system ..... | S1     |
| NMR spectra for all compounds .....                                                           | S2-S63 |
| HRMS spectra of hypervalent iodine activated fluorine reagent<br>intermediate .....           | S64    |

### Nonreactive substrates using $\text{PhI}(\text{OPiv})_2/\text{HF}\cdot\text{Py}$ system

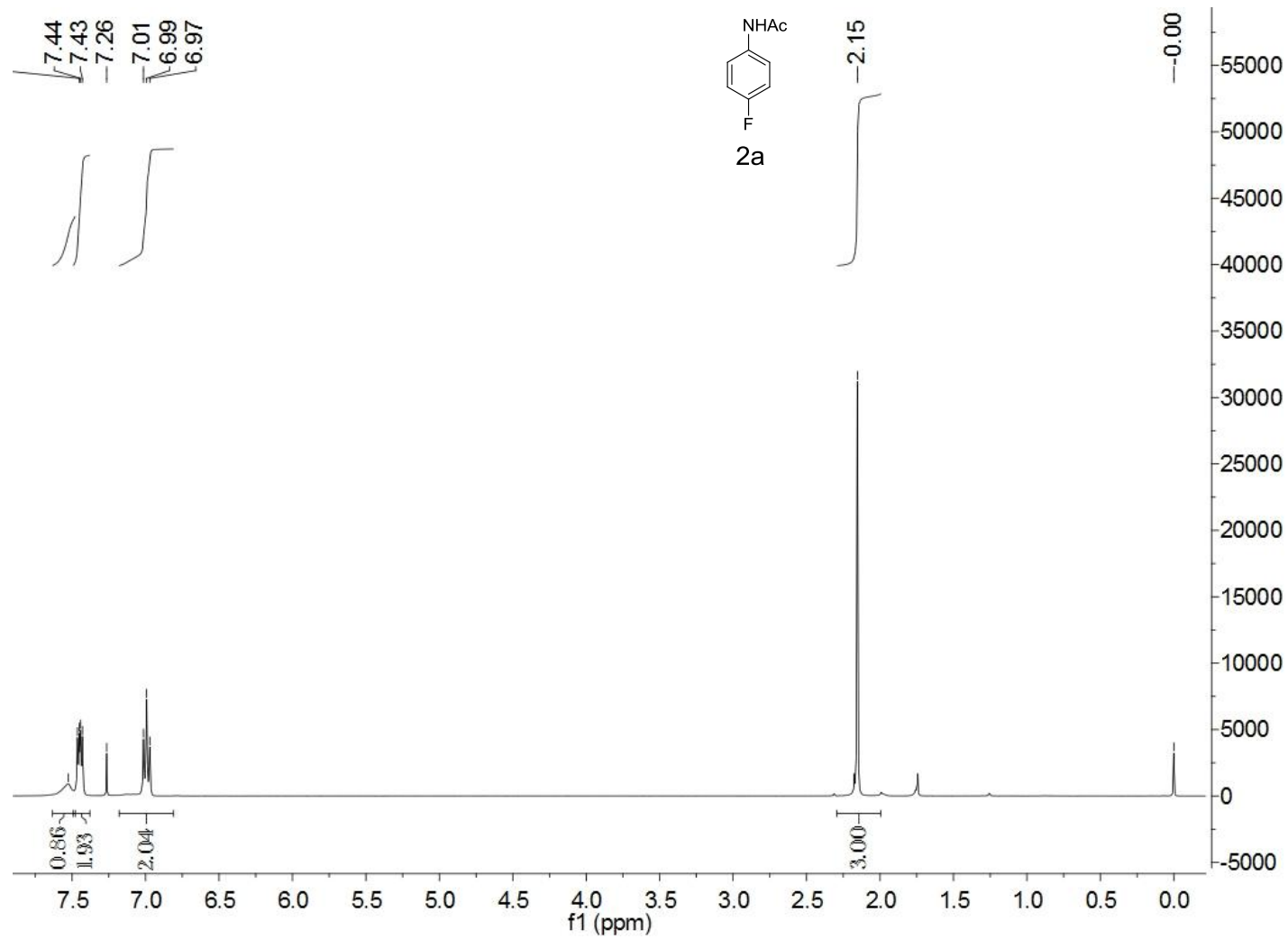
In the exploration of the substrate scope we attempted other anilides listed in Table 1 below; however, no desired products were detected.

**Table 1.** *p*-Fluorination of anilides using  $\text{PhI}(\text{OPiv})_2/\text{HF}\cdot\text{Py}$  system <sup>a</sup>

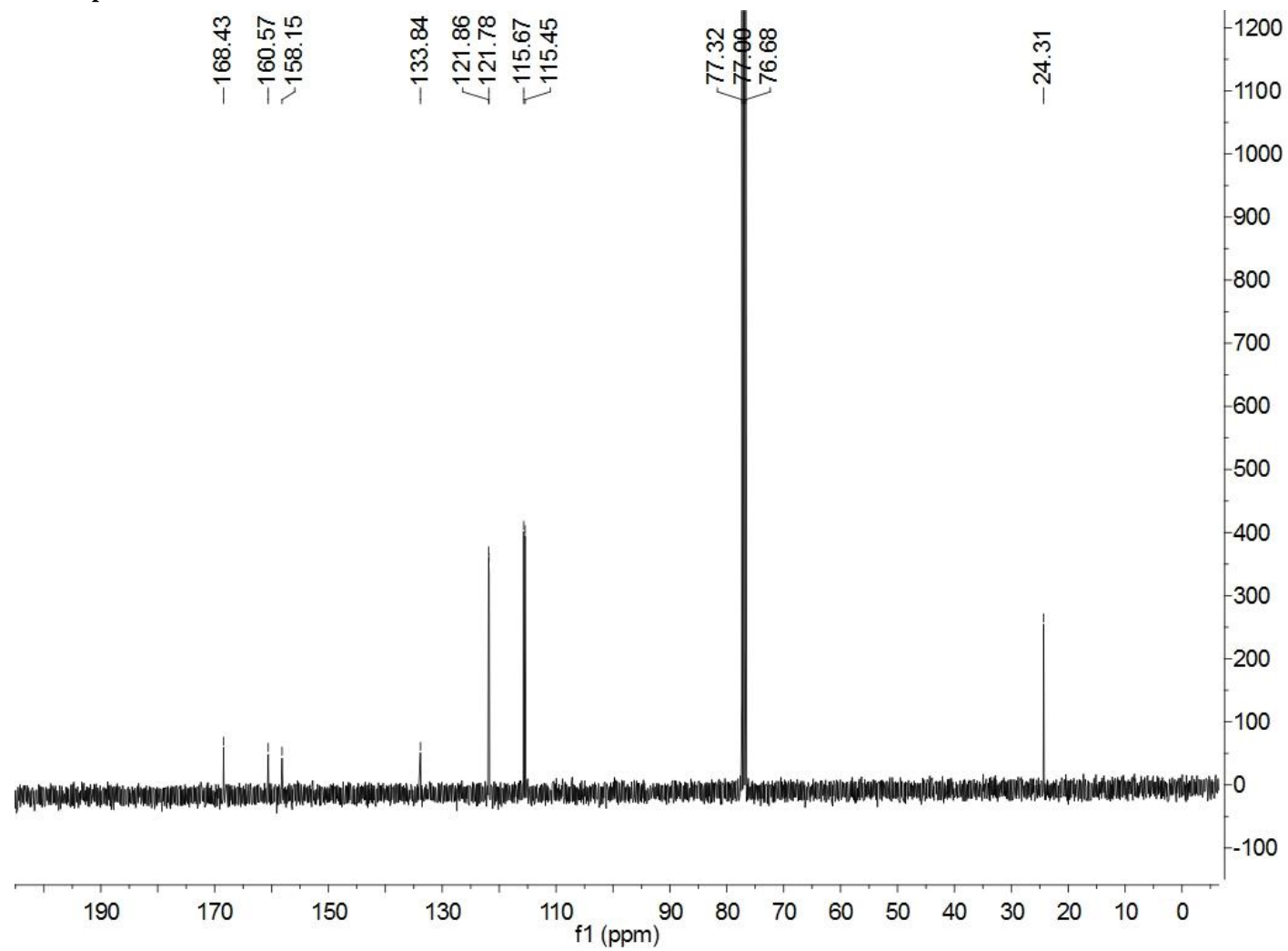
| Entry | Substrate | Product | Yield <sup>b</sup> (%) |
|-------|-----------|---------|------------------------|
| 1     | <br>1m    | <br>2m  | n.d. <sup>c</sup>      |
| 2     | <br>1n    | <br>2n  | n.d. <sup>c</sup>      |
| 3     | <br>3k    | <br>4k  | n.d. <sup>c</sup>      |
| 4     | <br>3l    | <br>4l  | n.d. <sup>c</sup>      |
| 5     | <br>3m    | <br>4m  | n.d. <sup>c</sup>      |

<sup>a</sup> Reaction conditions: **1m, 1n, 3l-n** (0.5 mmol),  $\text{PhI}(\text{OPiv})_2$  (1.5 equiv),  $\text{HF}\cdot\text{Py}$  (6 equiv) and  $\text{CH}_2\text{Cl}_2$  (5 mL) at room temperature. <sup>b</sup> Isolated yields. <sup>c</sup> No desired product was detected by NMR analysis

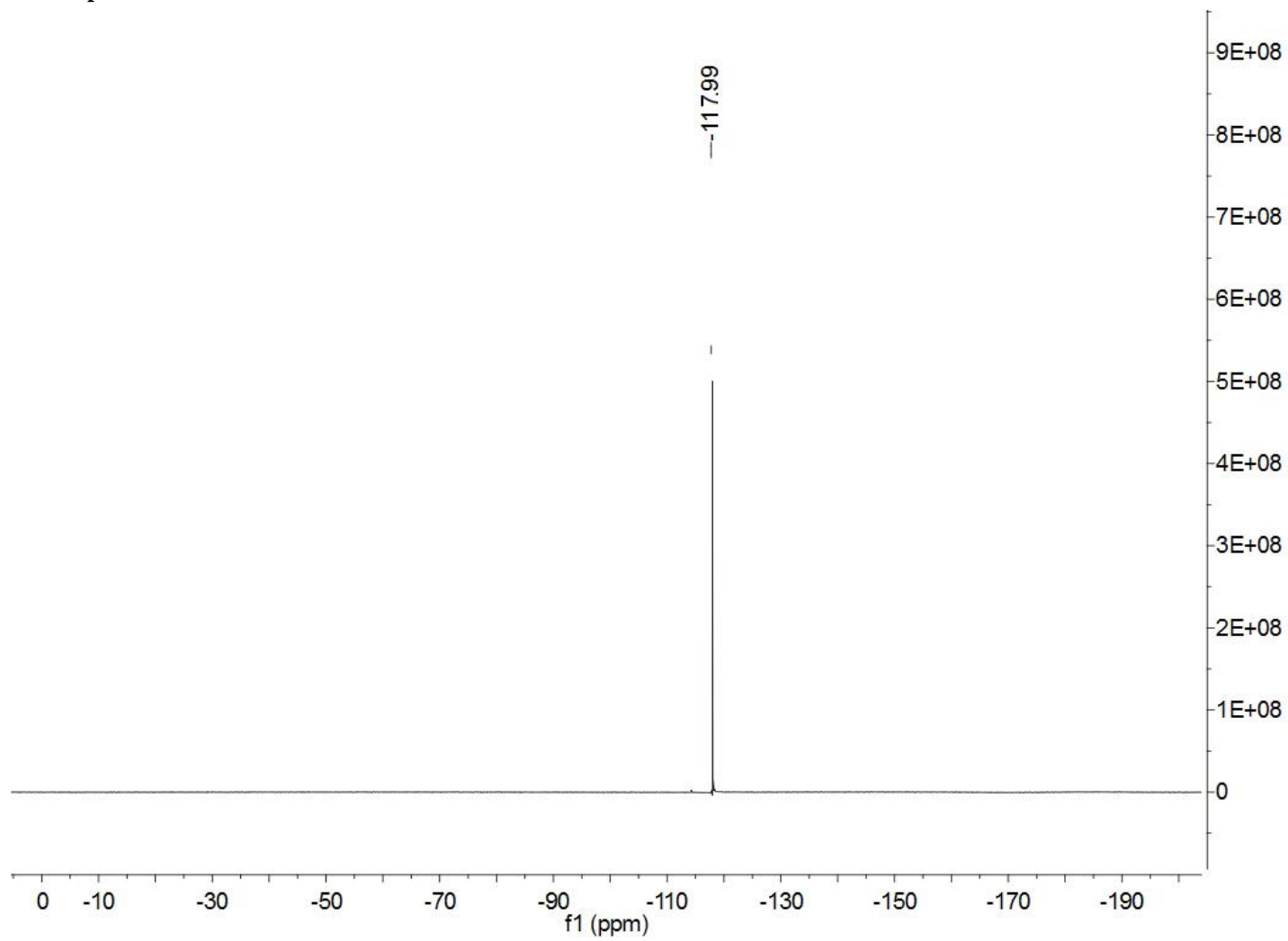
NMR spectra for 2a  $^1\text{H}$  NMR



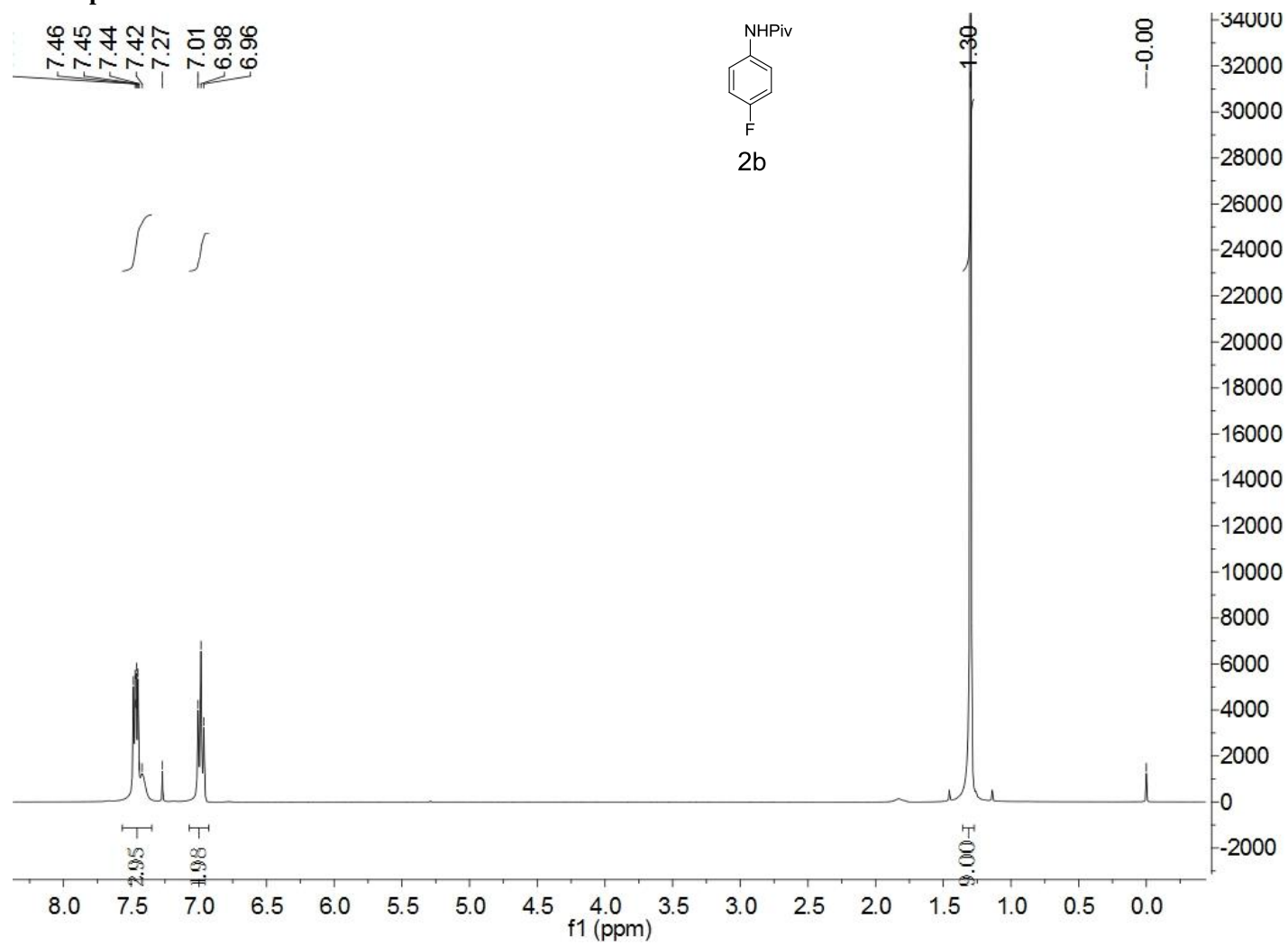
NMR spectra for 2a <sup>13</sup>C NMR



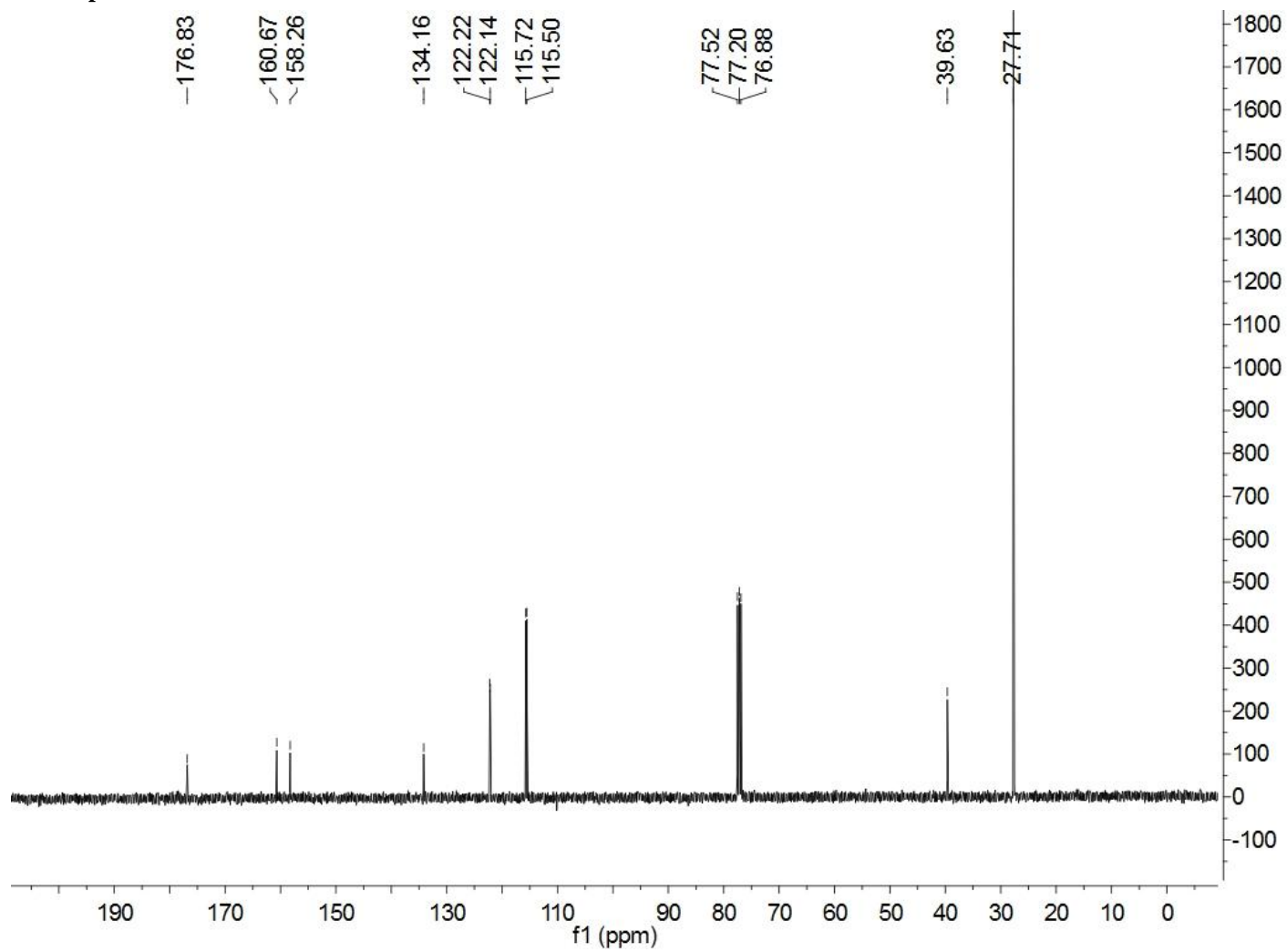
NMR spectra for 2a  $^{19}\text{F}$  NMR



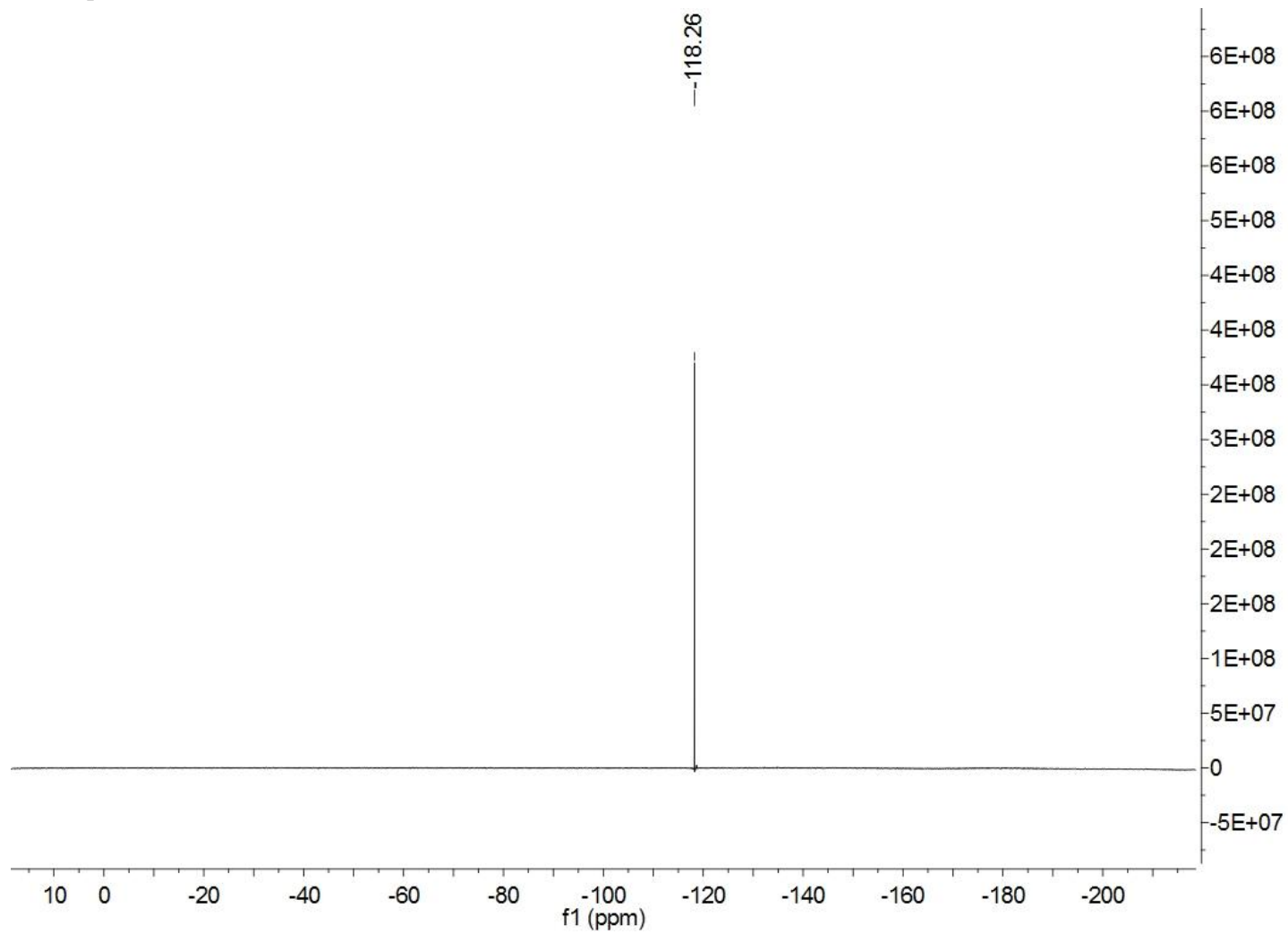
NMR spectra for 2b <sup>1</sup>H NMR



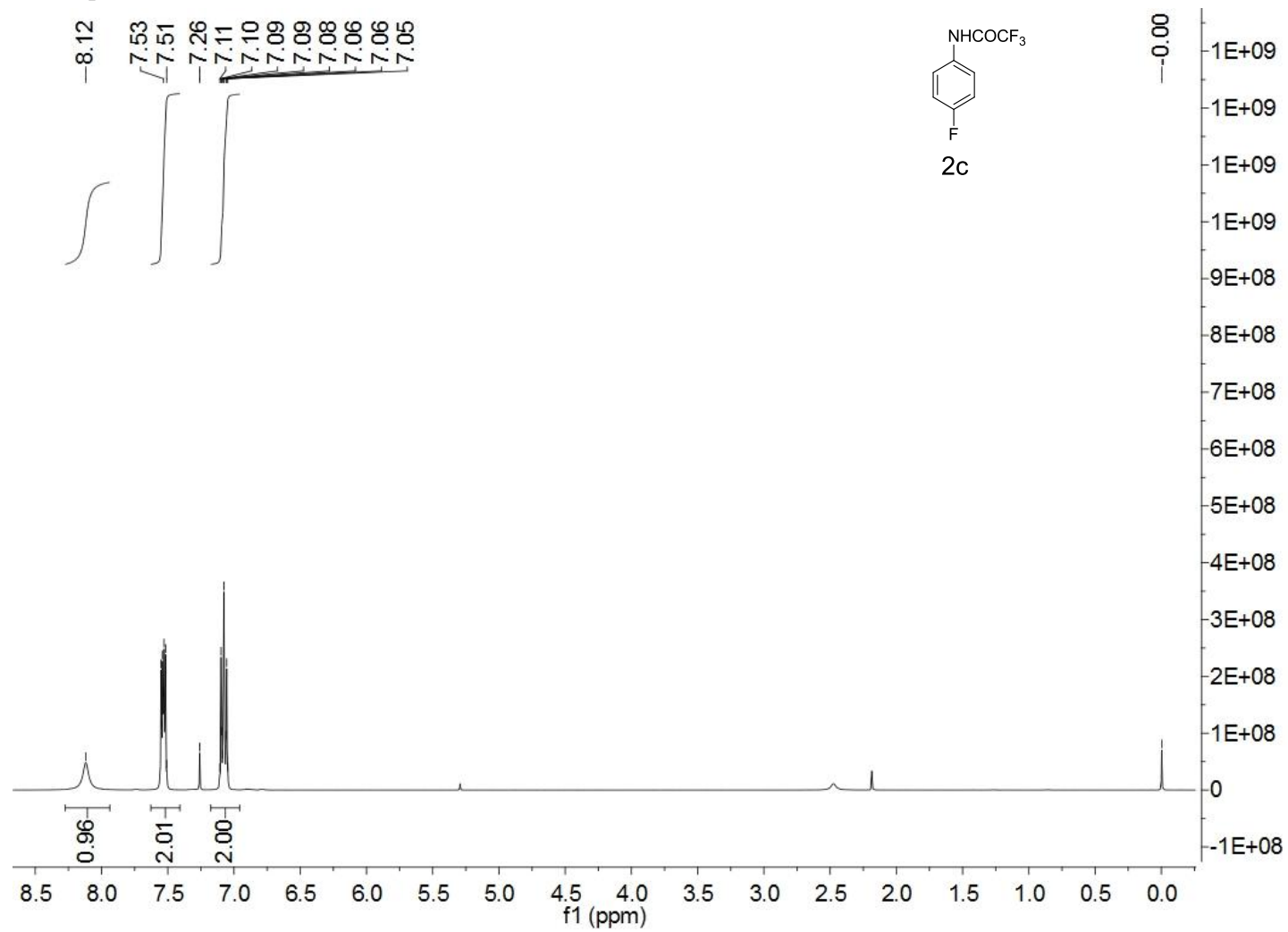
NMR spectra for 2b  $^{13}\text{C}$  NMR



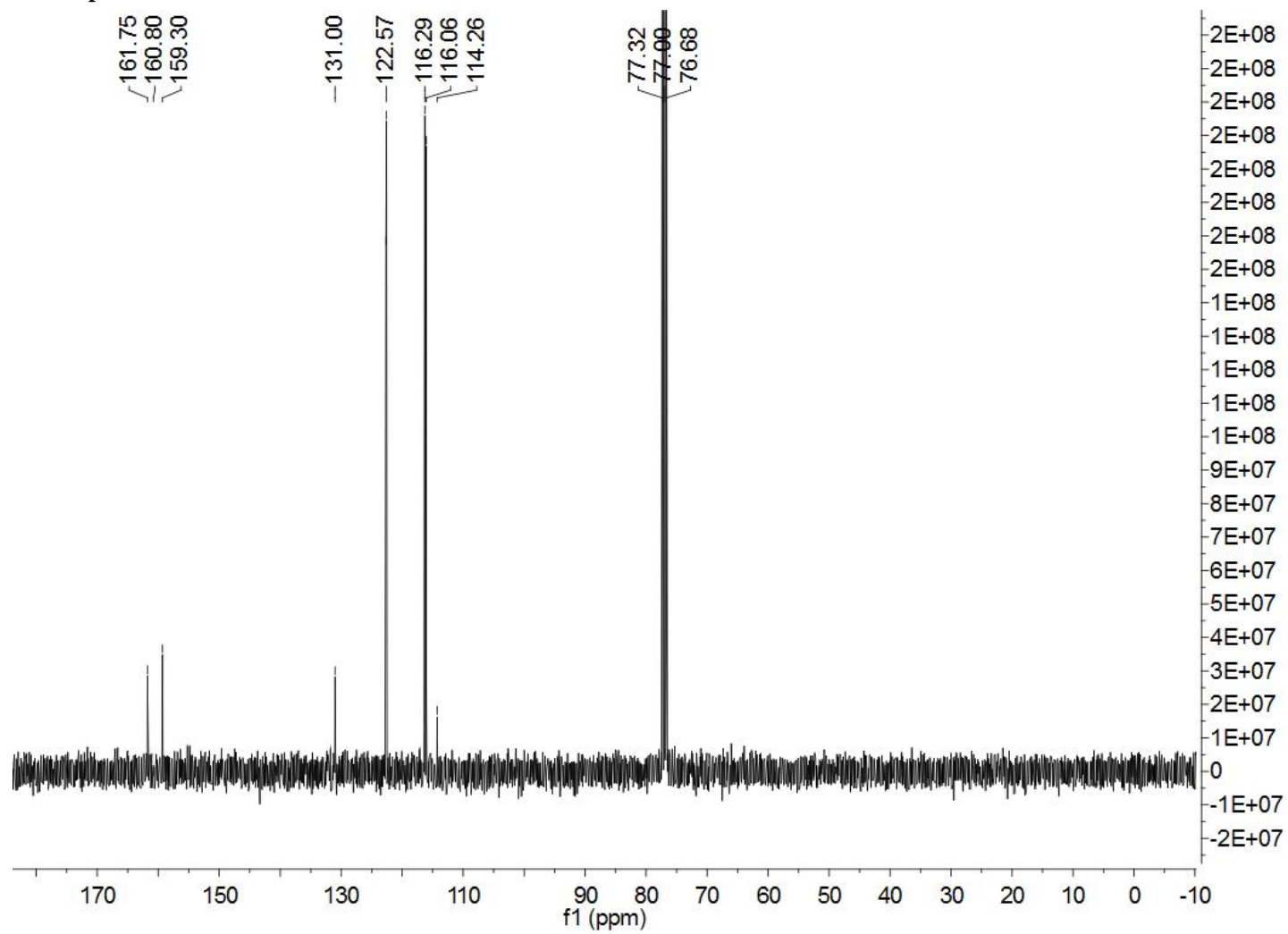
NMR spectra for 2b  $^{19}\text{F}$  NMR



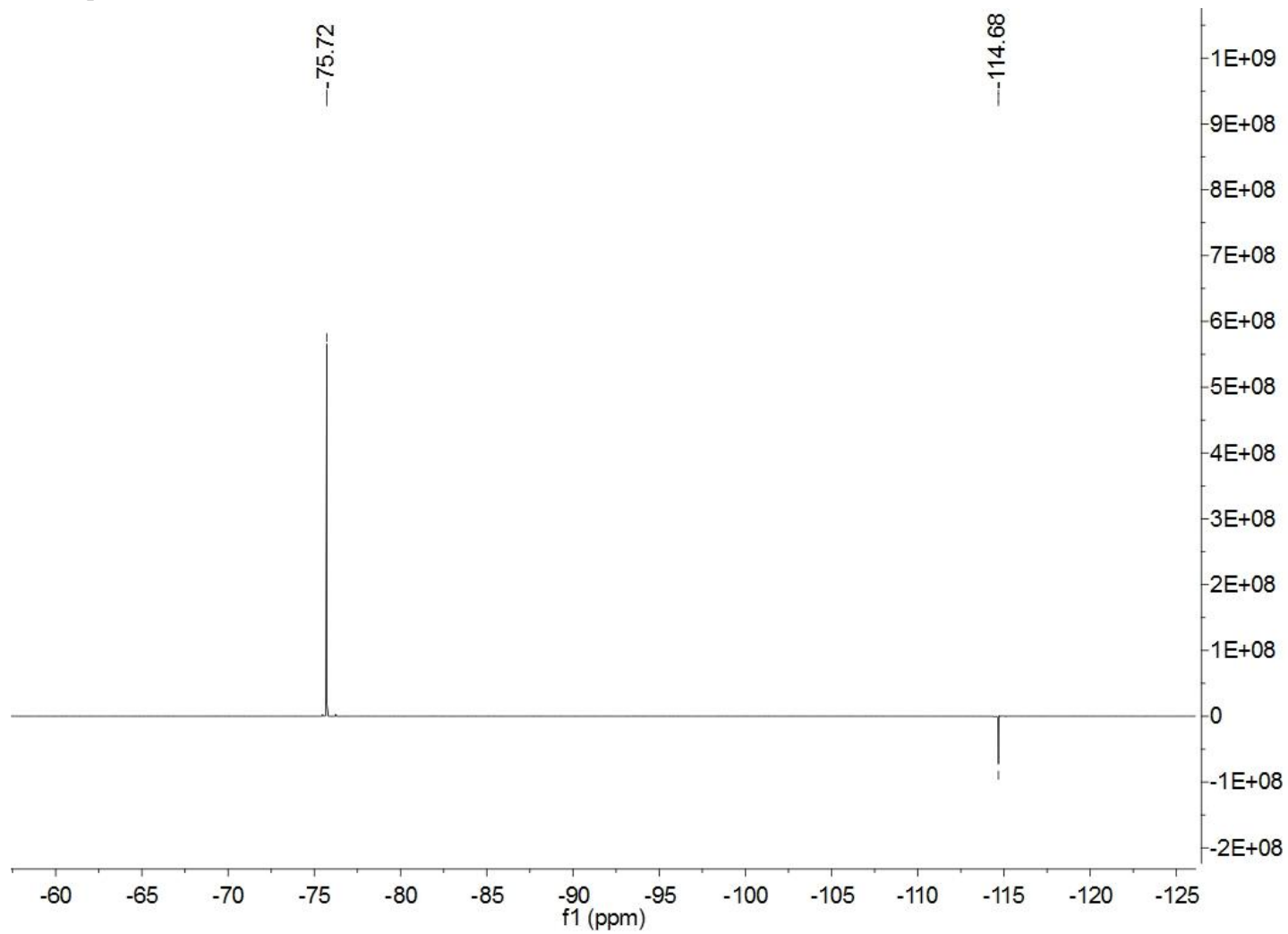
NMR spectra for 2c <sup>1</sup>H NMR



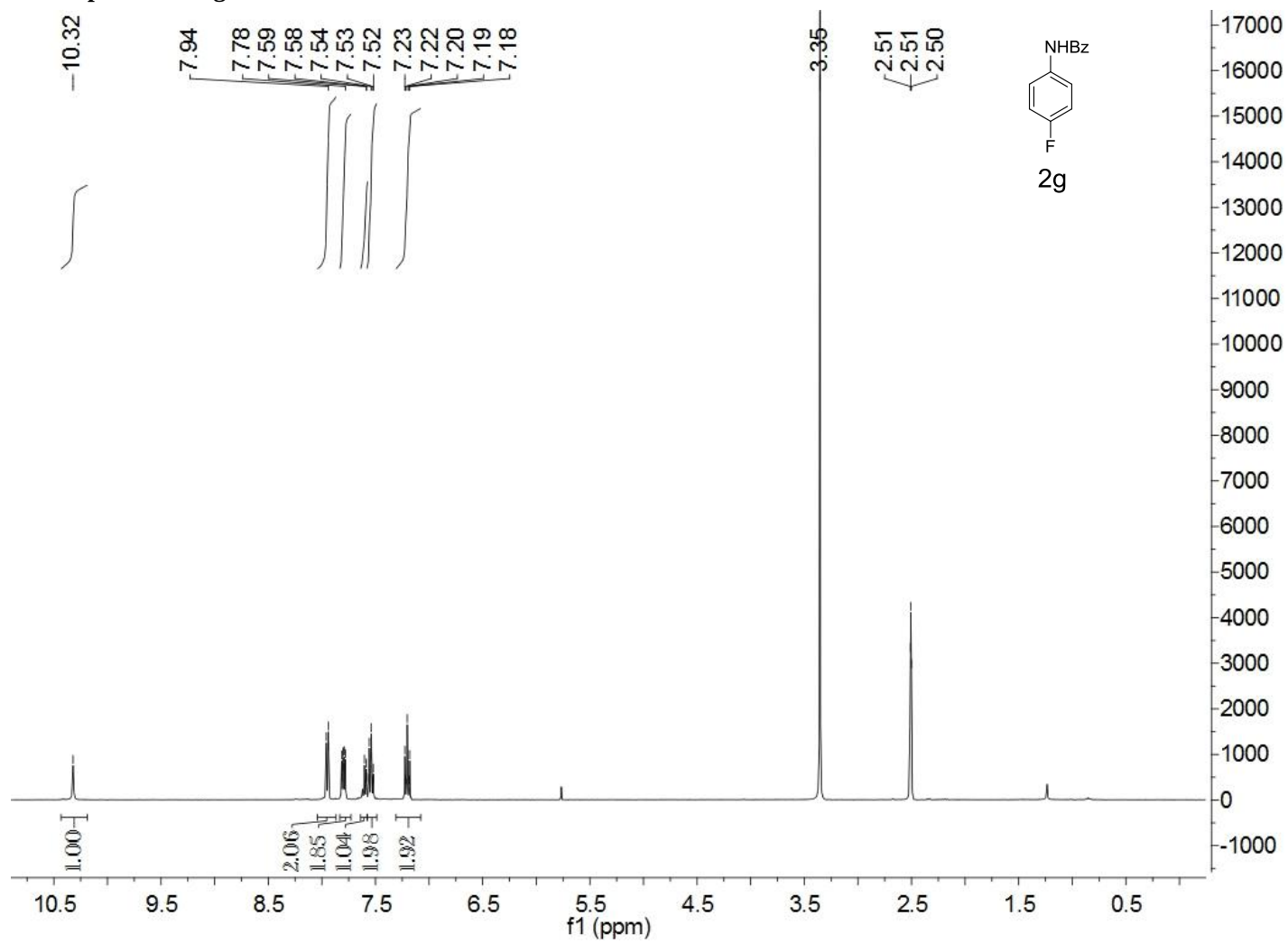
NMR spectra for 2c  $^{13}\text{C}$  NMR



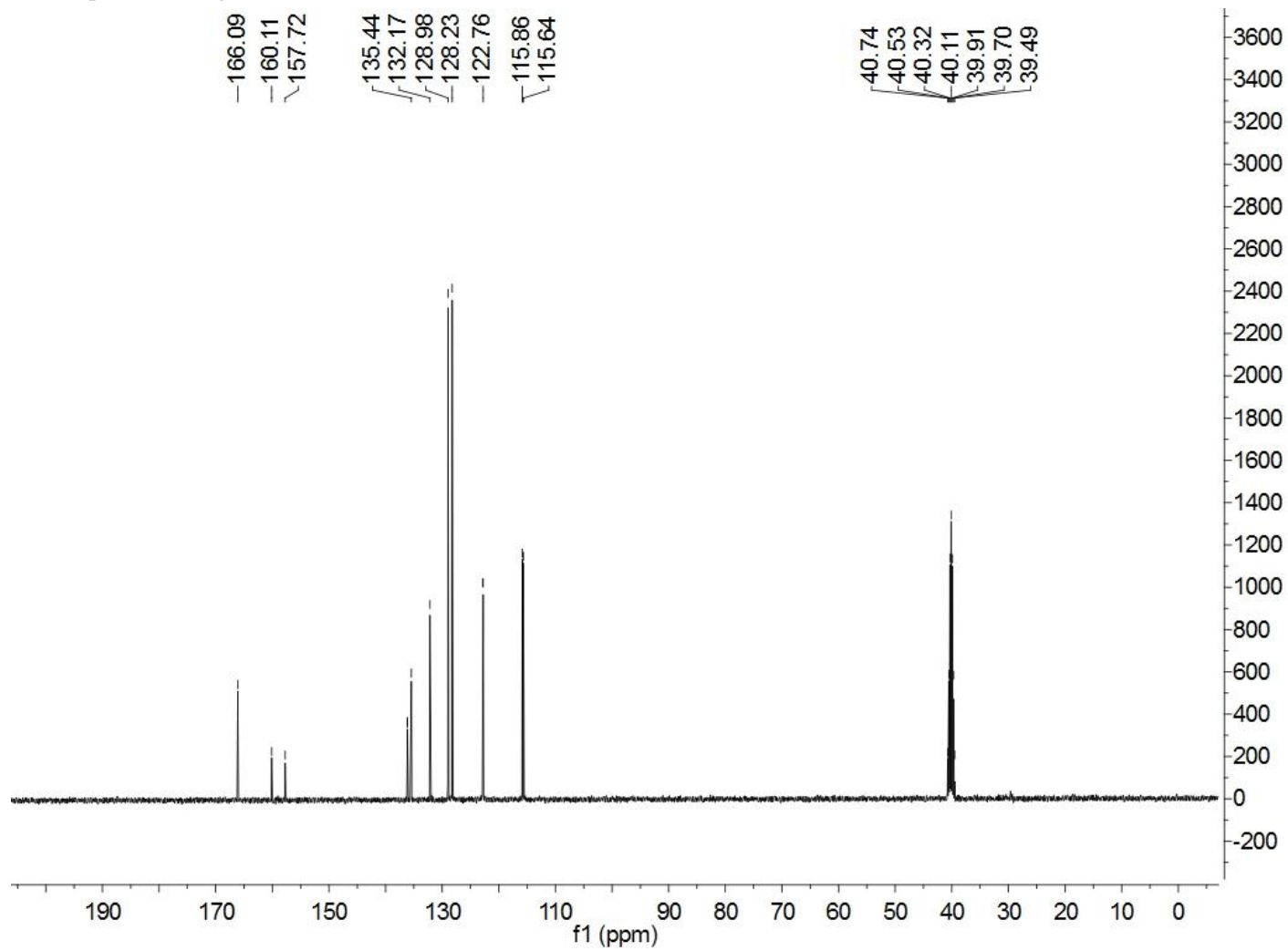
NMR spectra for 2c  $^{19}\text{F}$  NMR



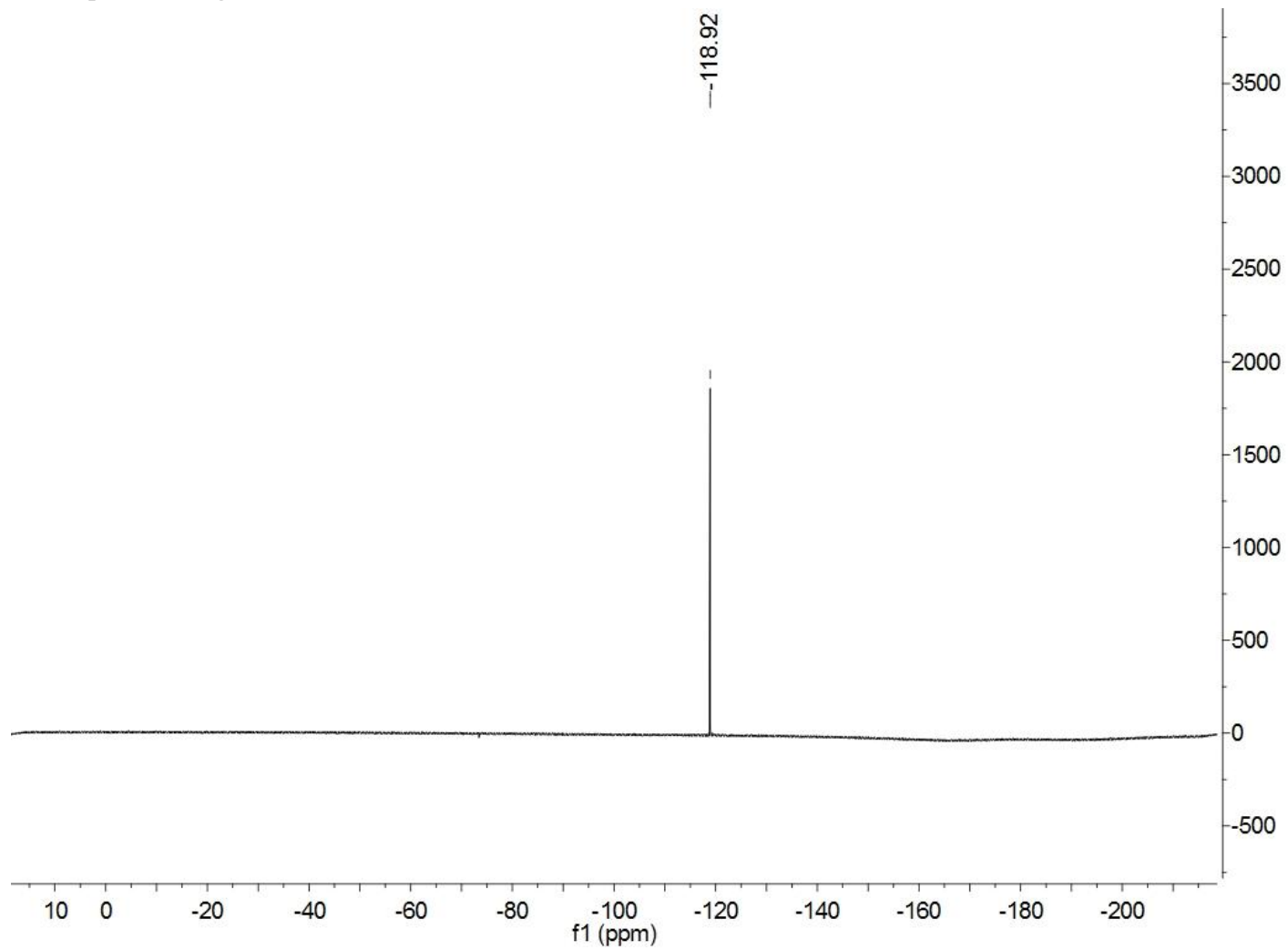
NMR spectra for 2g  $^1\text{H}$  NMR



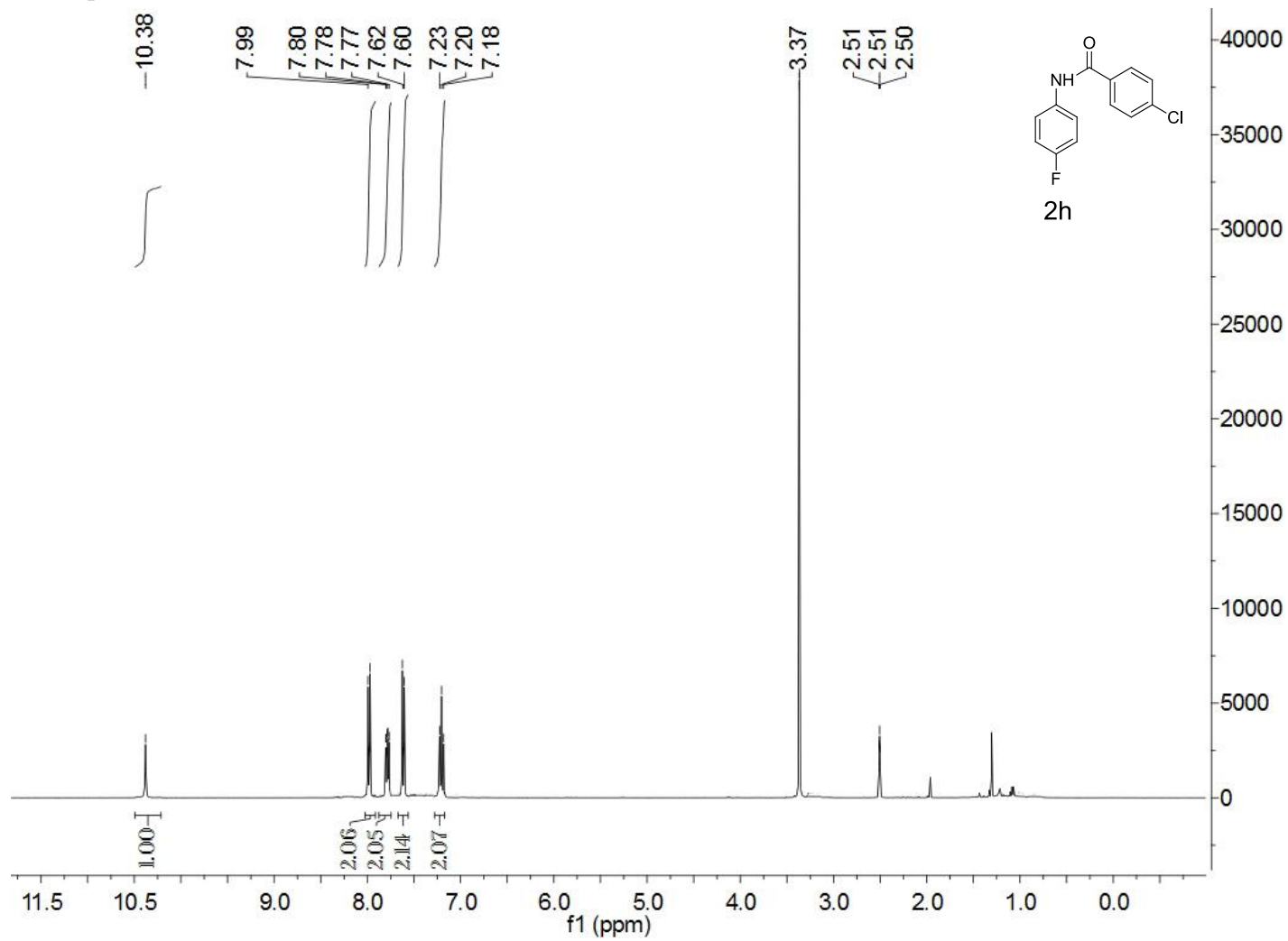
NMR spectra for 2g  $^{13}\text{C}$  NMR



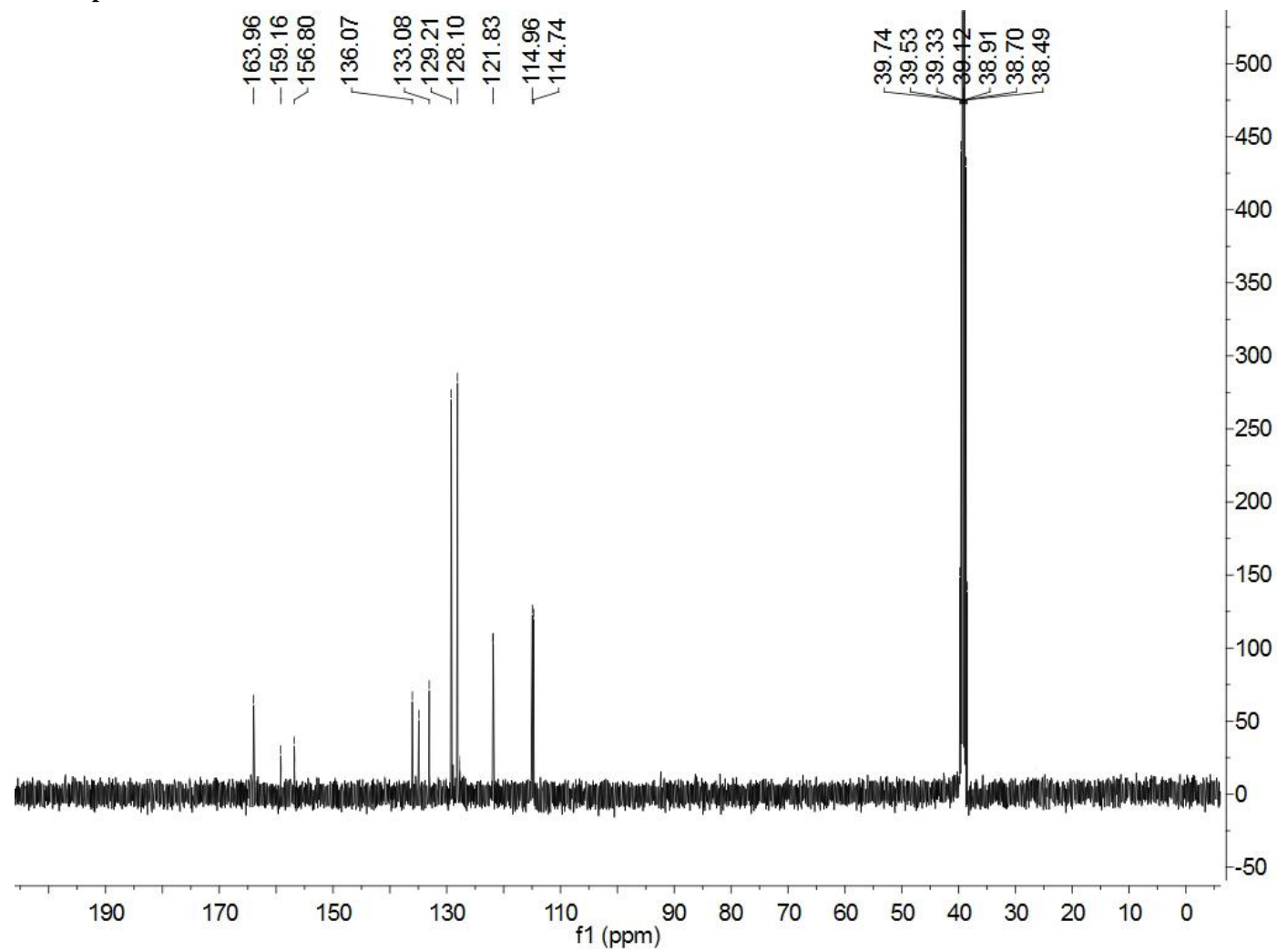
NMR spectra for 2g  $^{19}\text{F}$  NMR



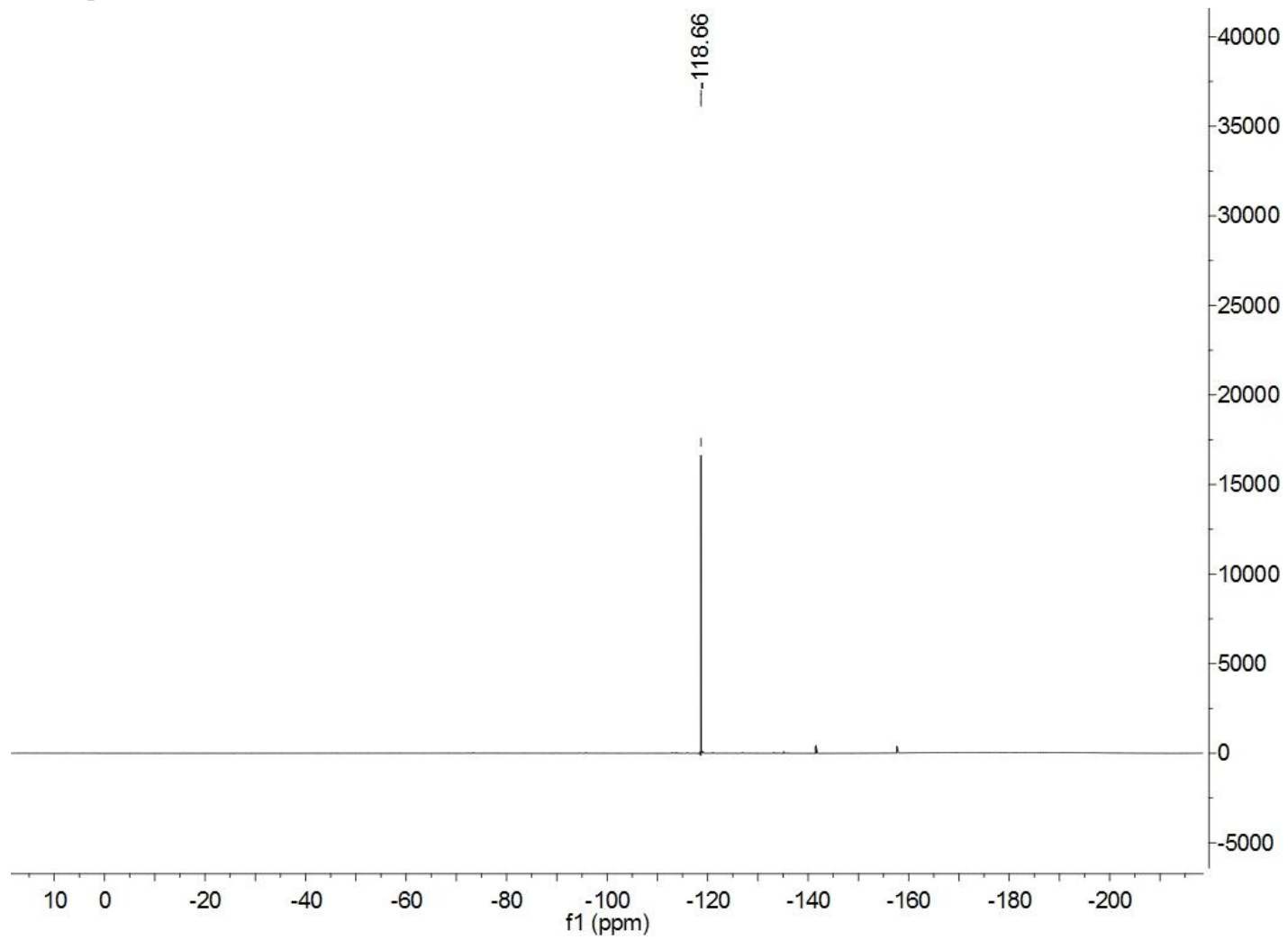
NMR spectra for 2h  $^1\text{H}$  NMR



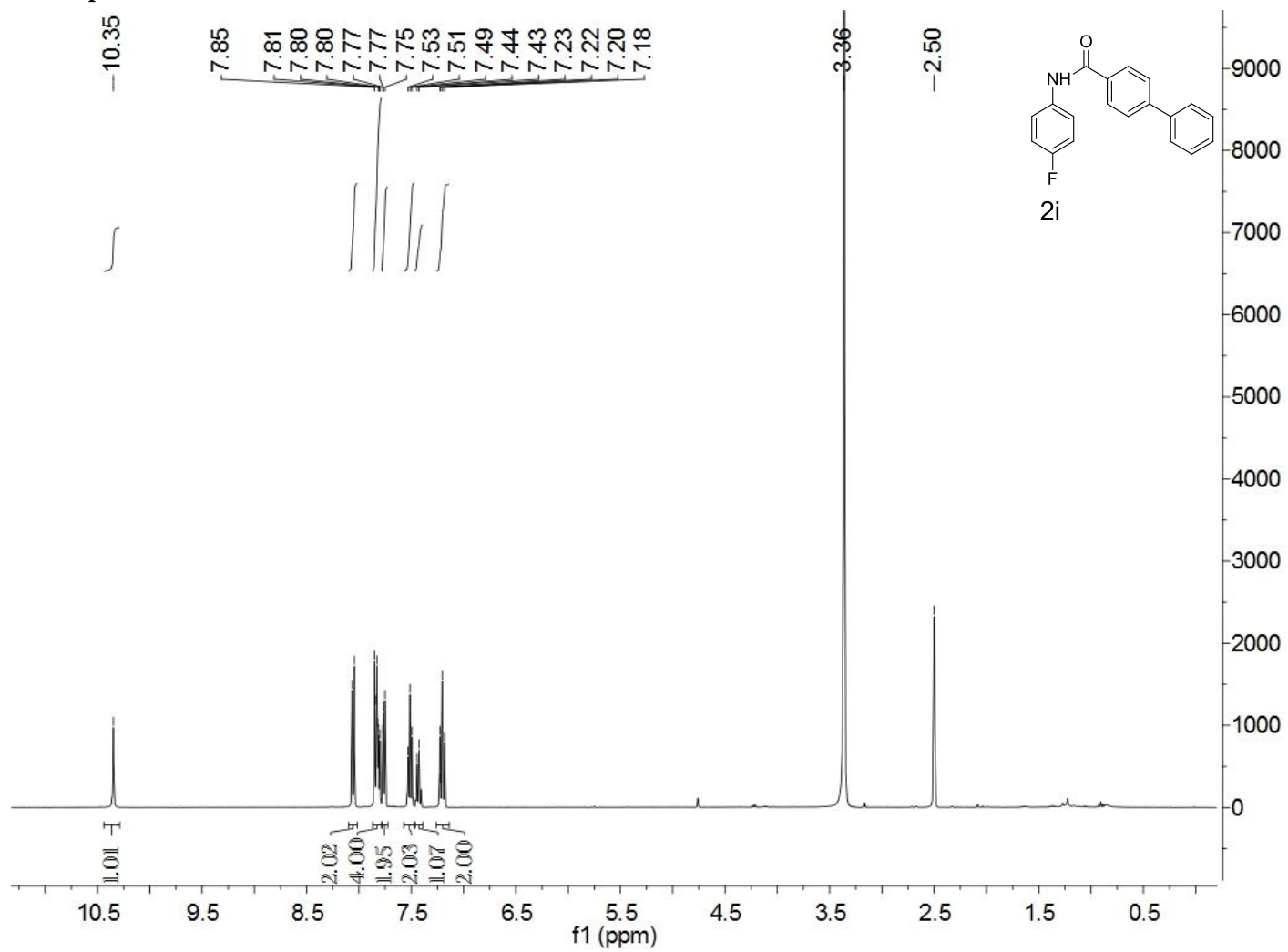
NMR spectra for 2h  $^{13}\text{C}$  NMR



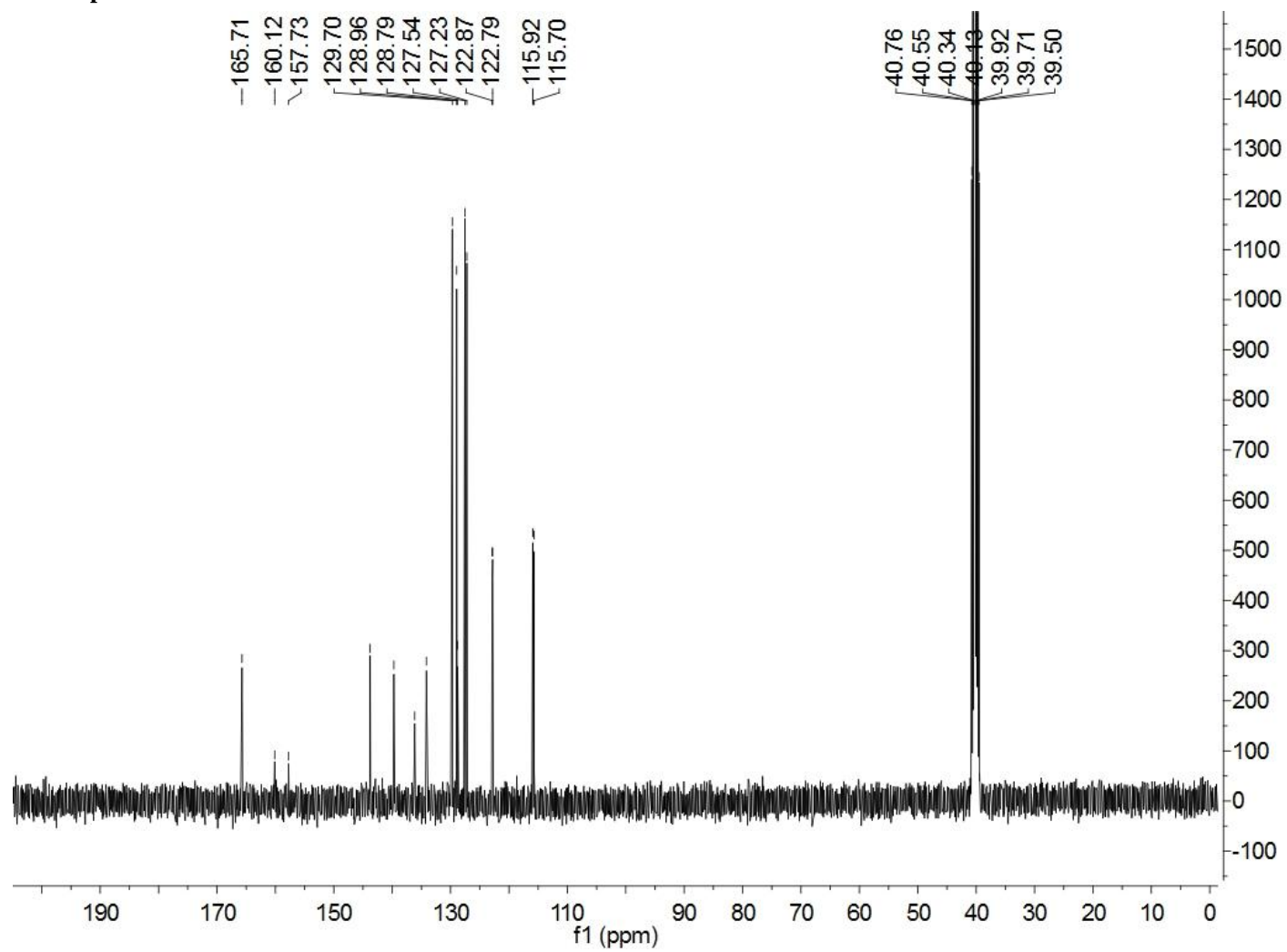
NMR spectra for 2h  $^{19}\text{F}$  NMR



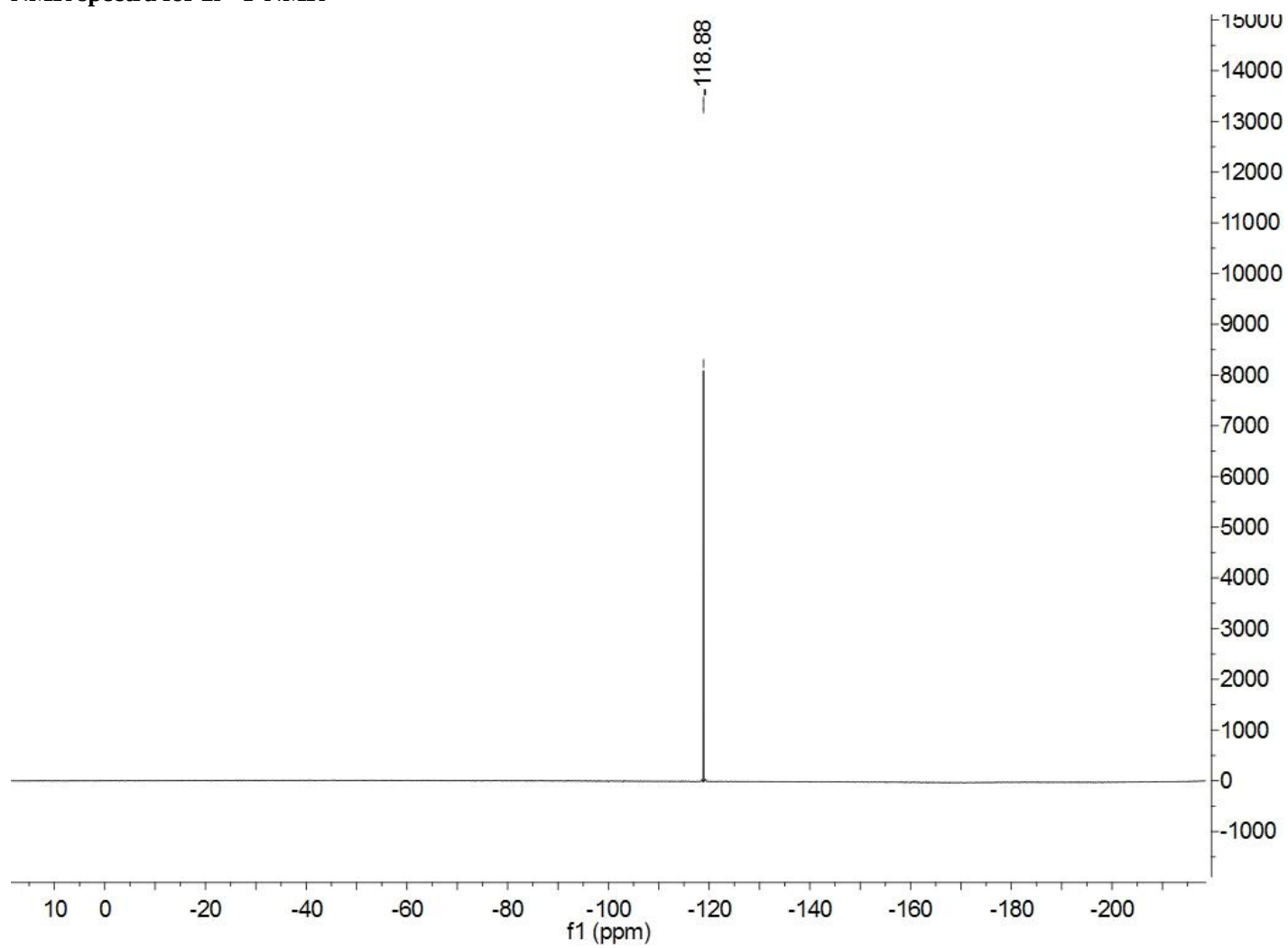
NMR spectra for 2i  $^1\text{H}$  NMR



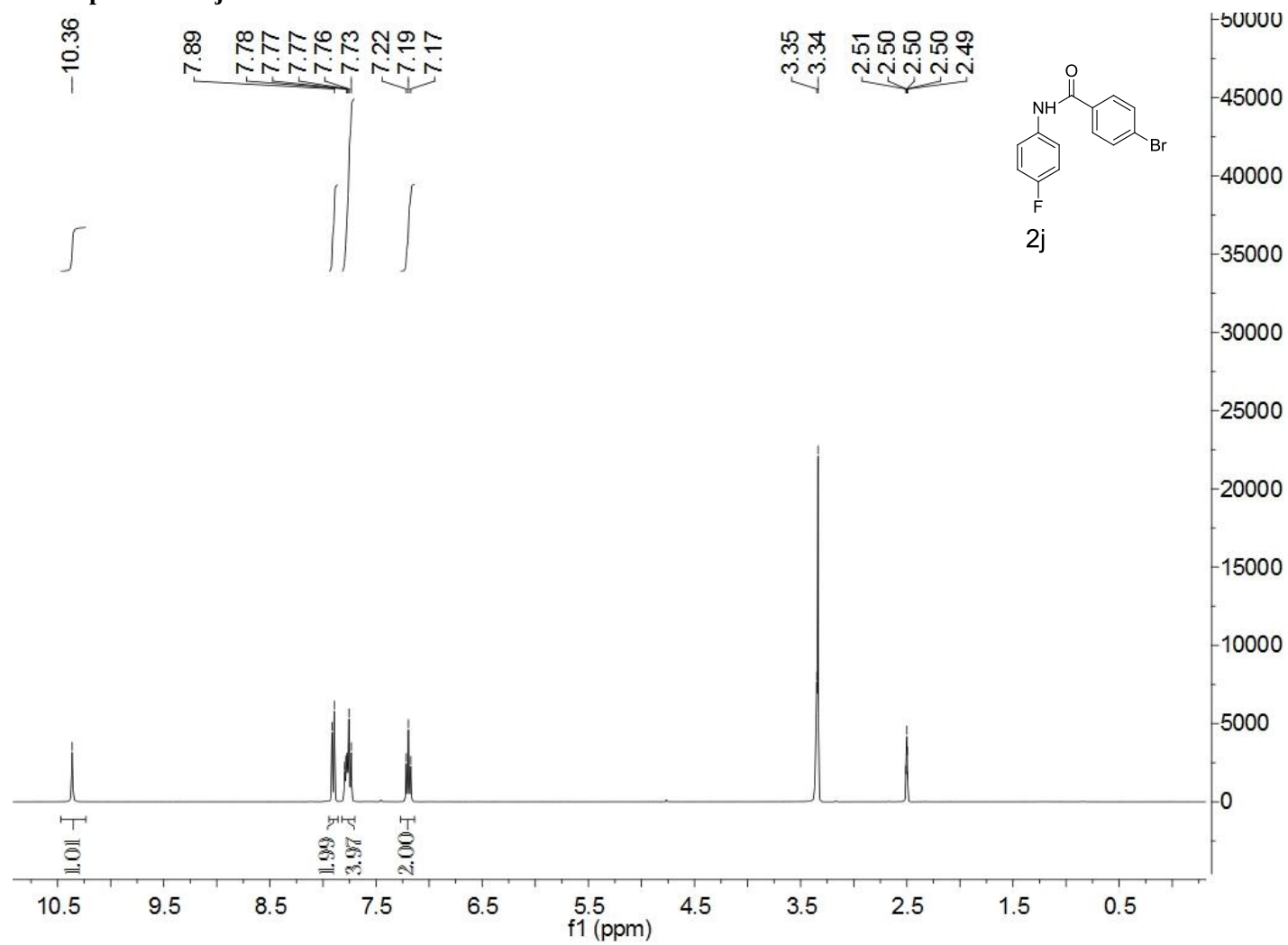
NMR spectra for 2i <sup>13</sup>C NMR



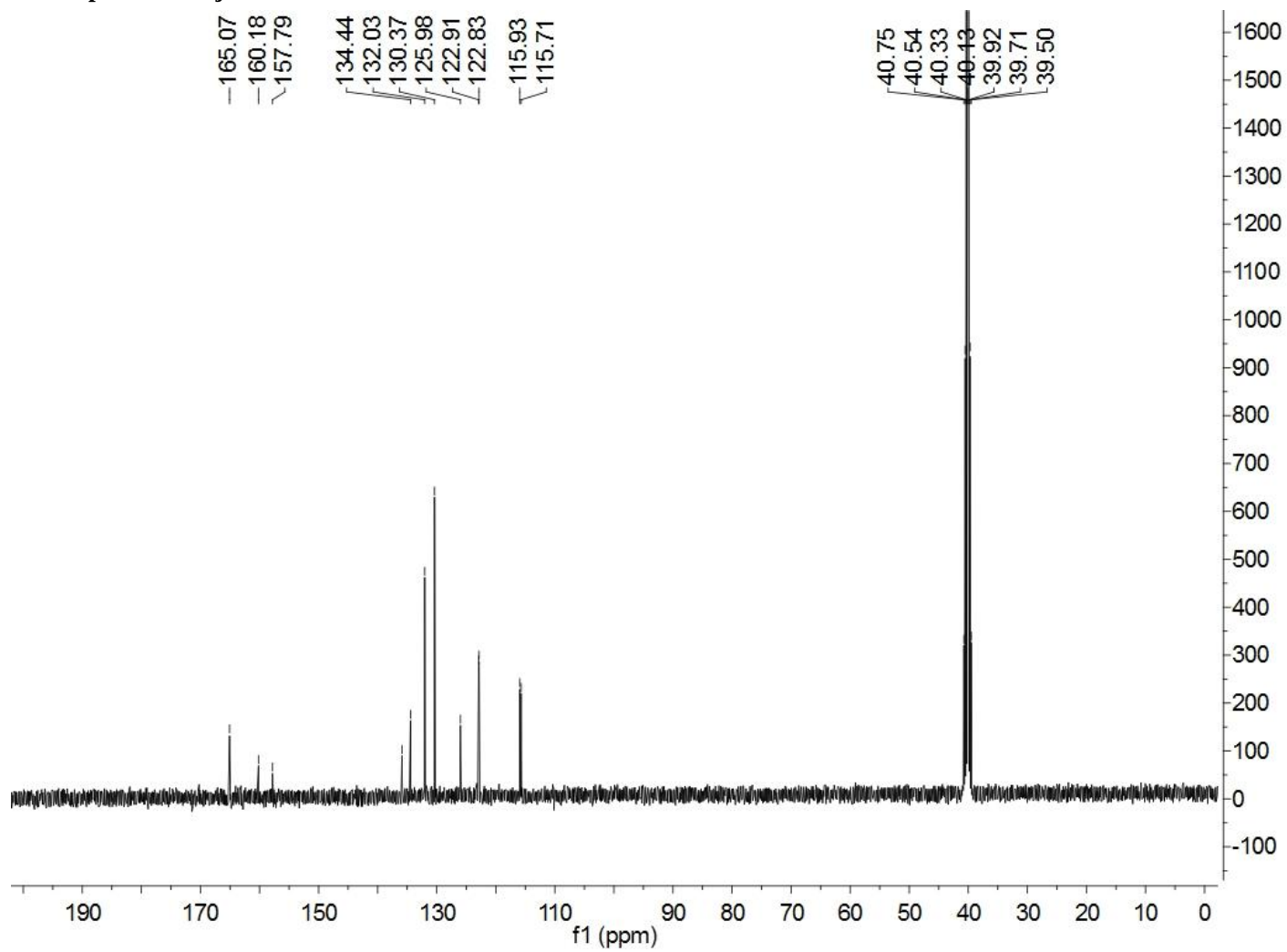
NMR spectra for 2i <sup>19</sup>F NMR



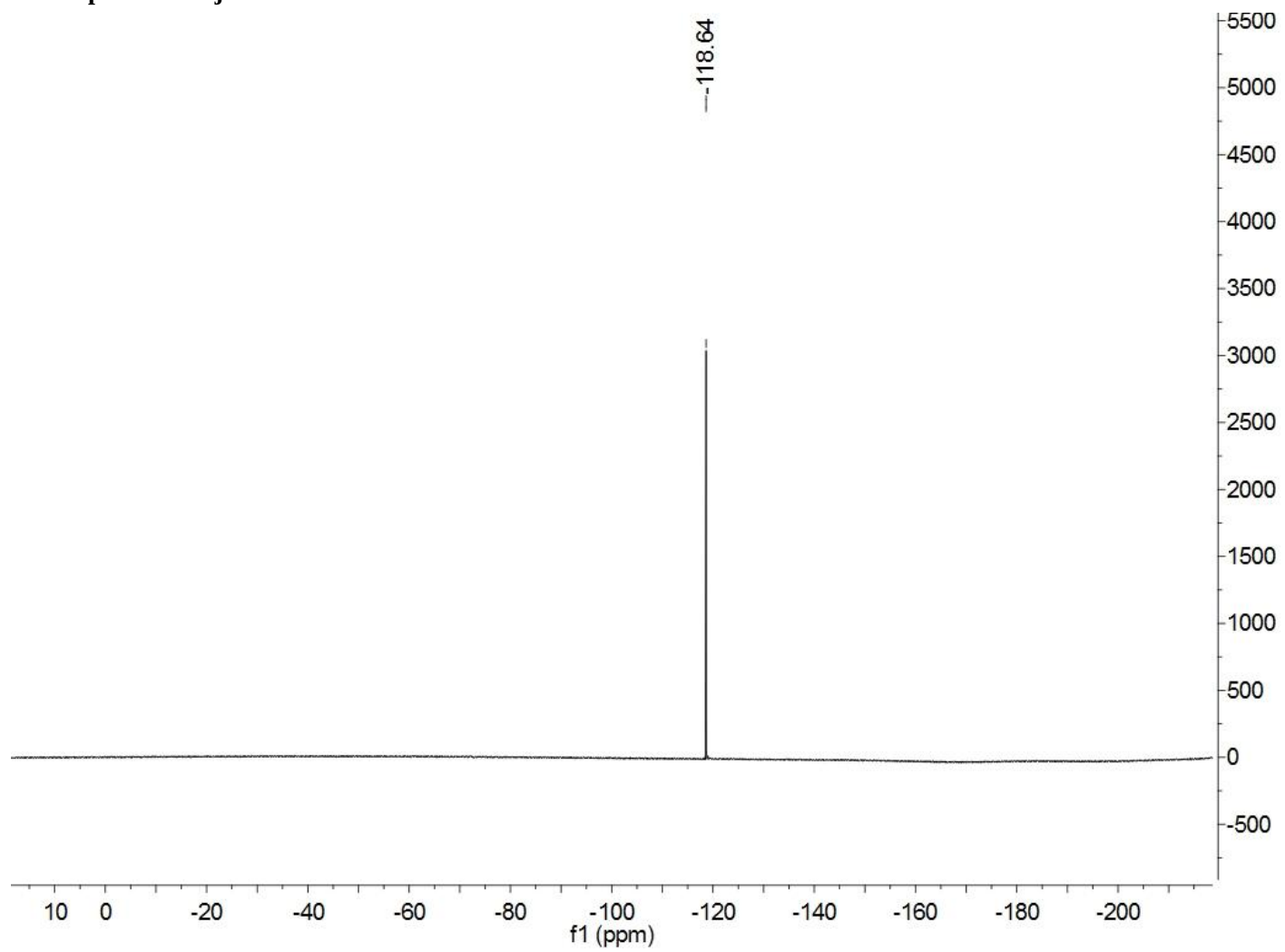
NMR spectra for 2j <sup>1</sup>H NMR



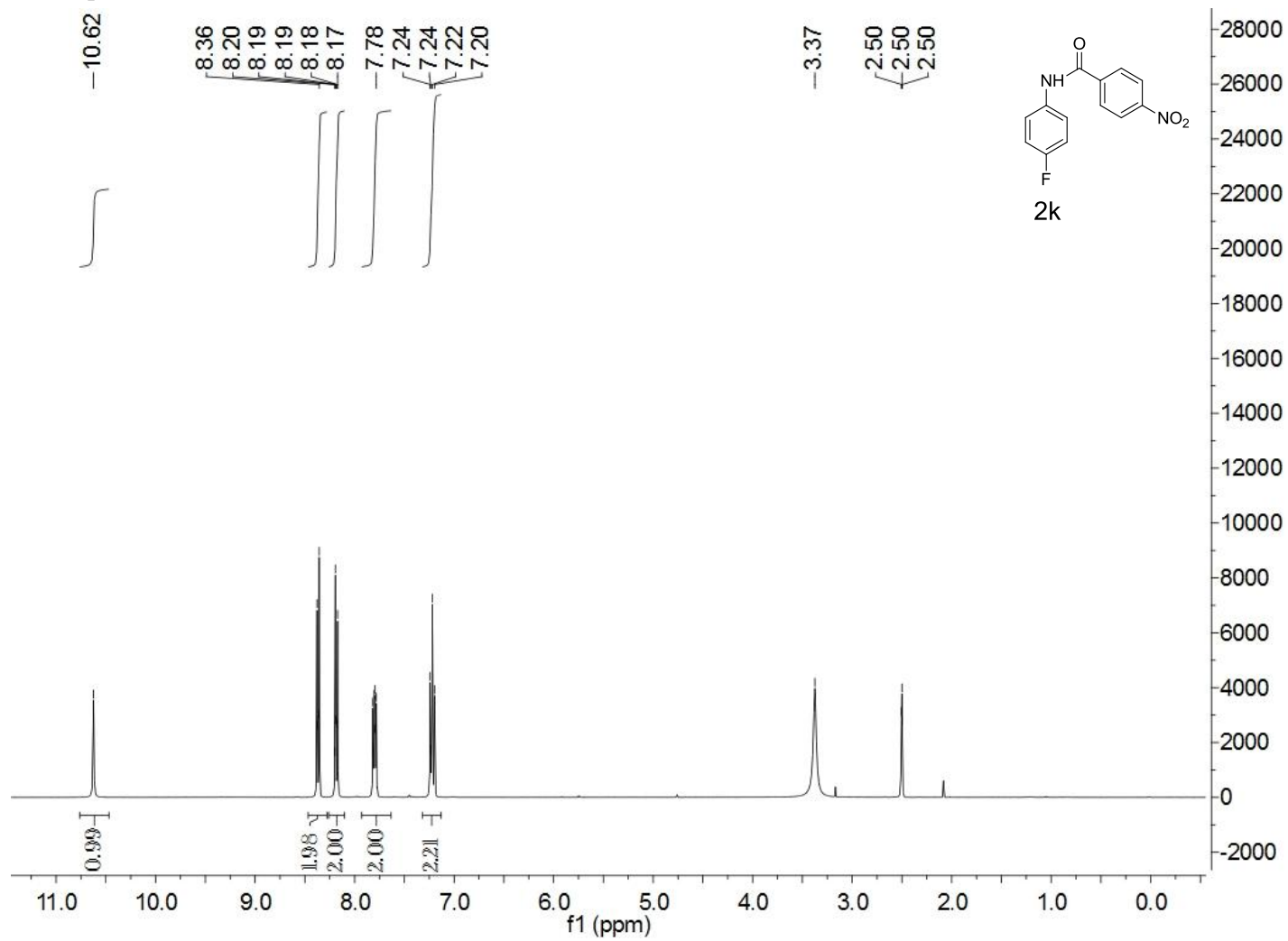
NMR spectra for 2j  $^{13}\text{C}$  NMR



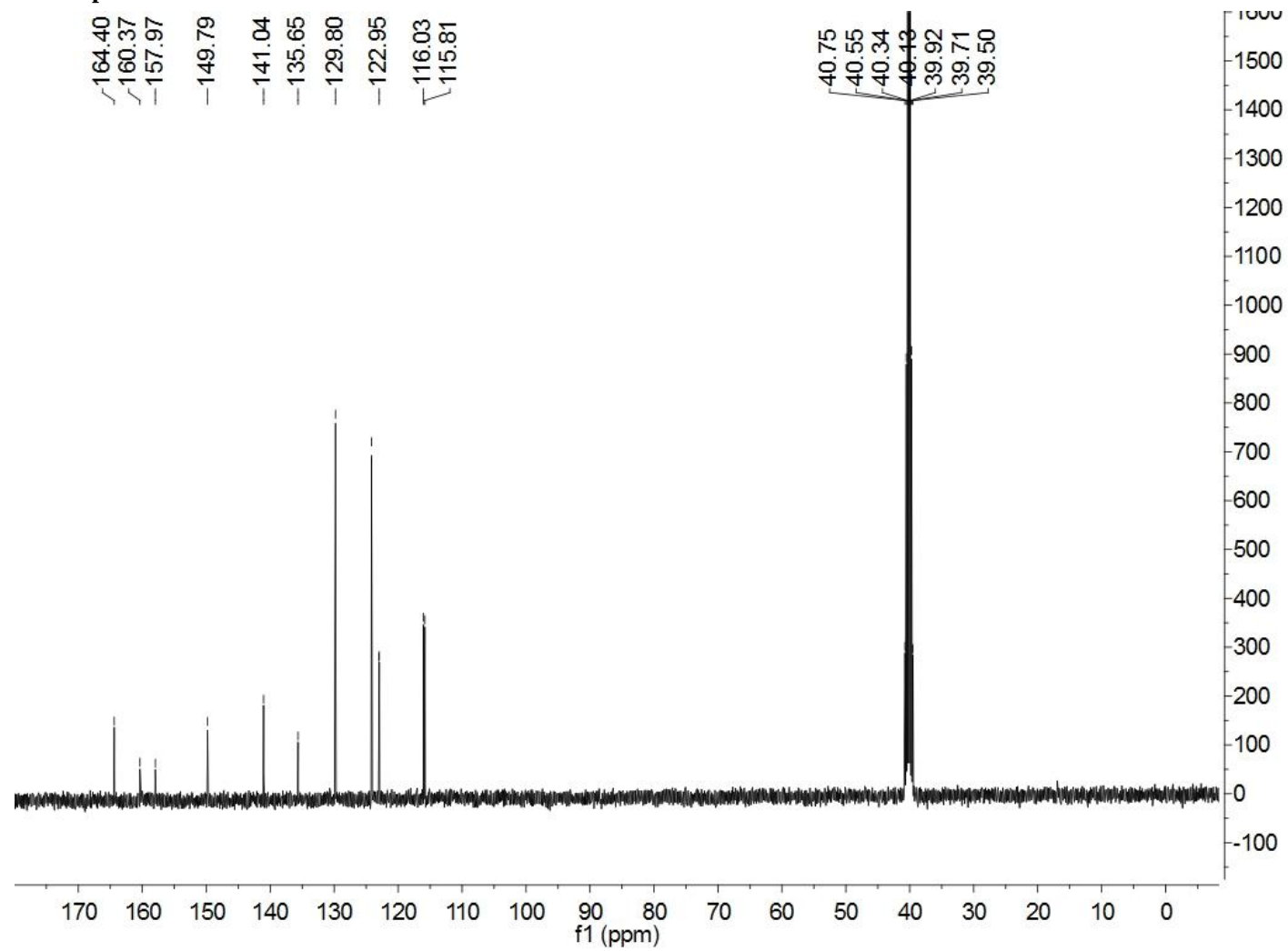
NMR spectra for 2j  $^{19}\text{F}$  NMR



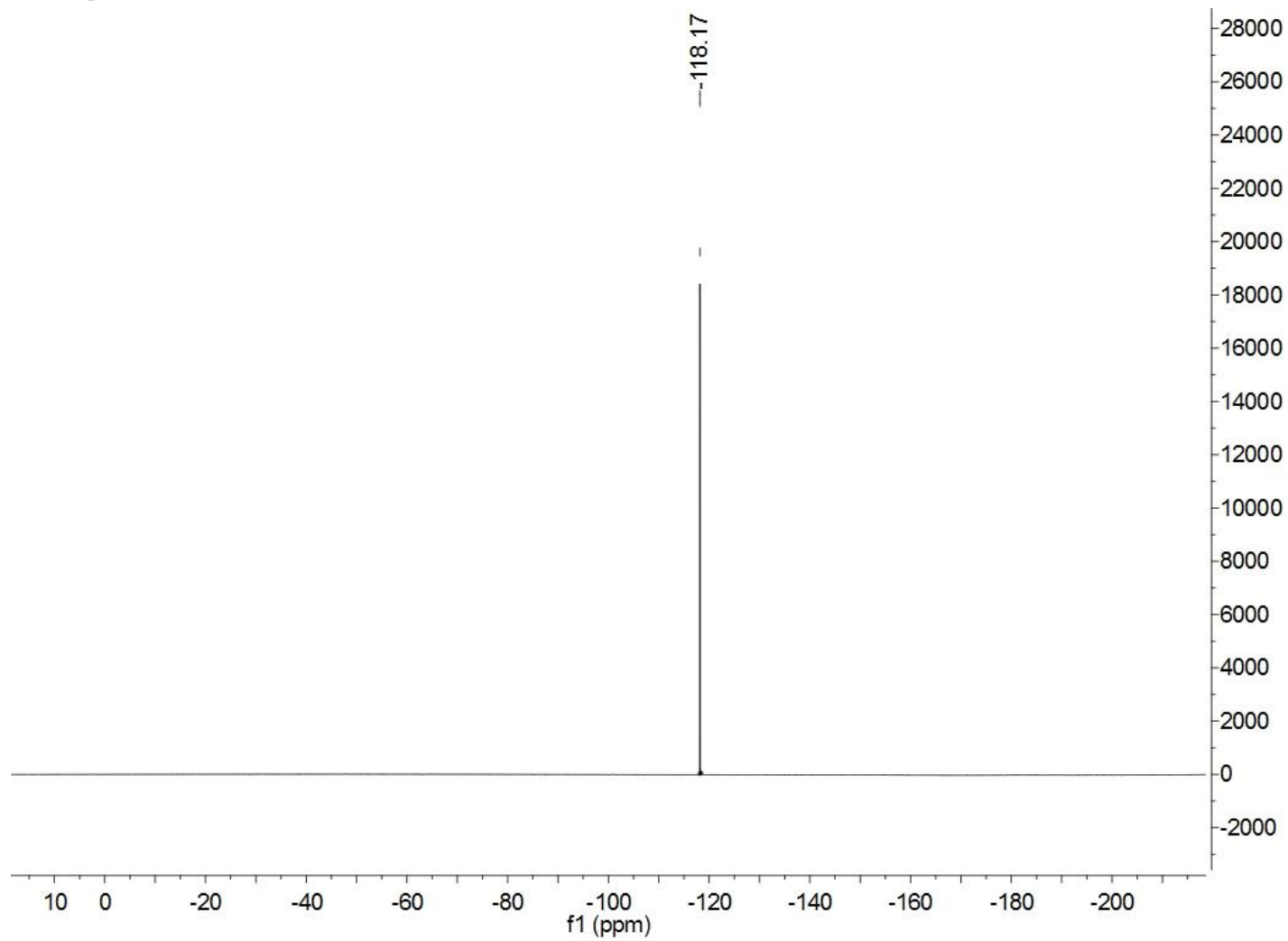
NMR spectra for 2k  $^1\text{H}$  NMR



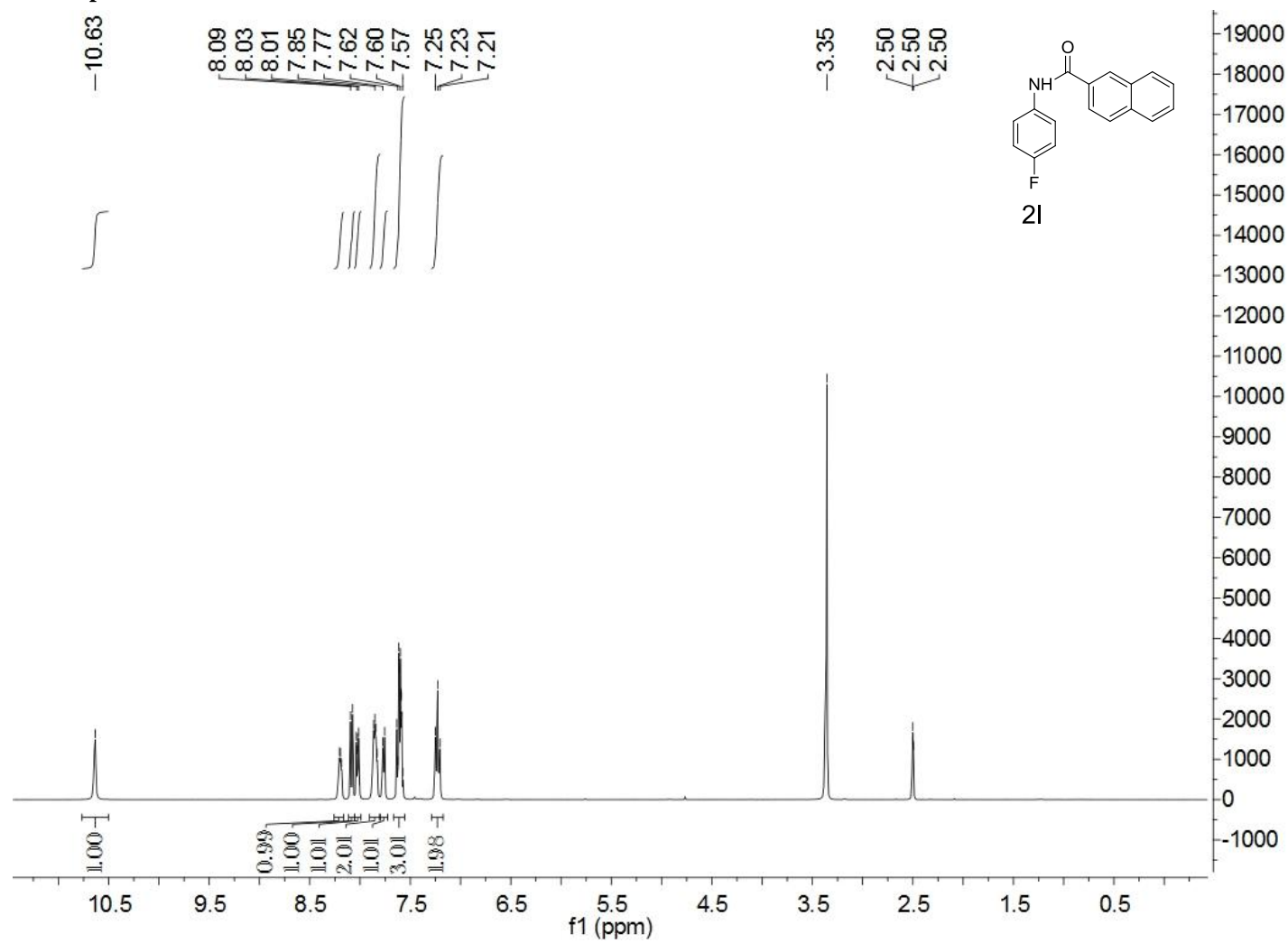
NMR spectra for 2k  $^{13}\text{C}$  NMR



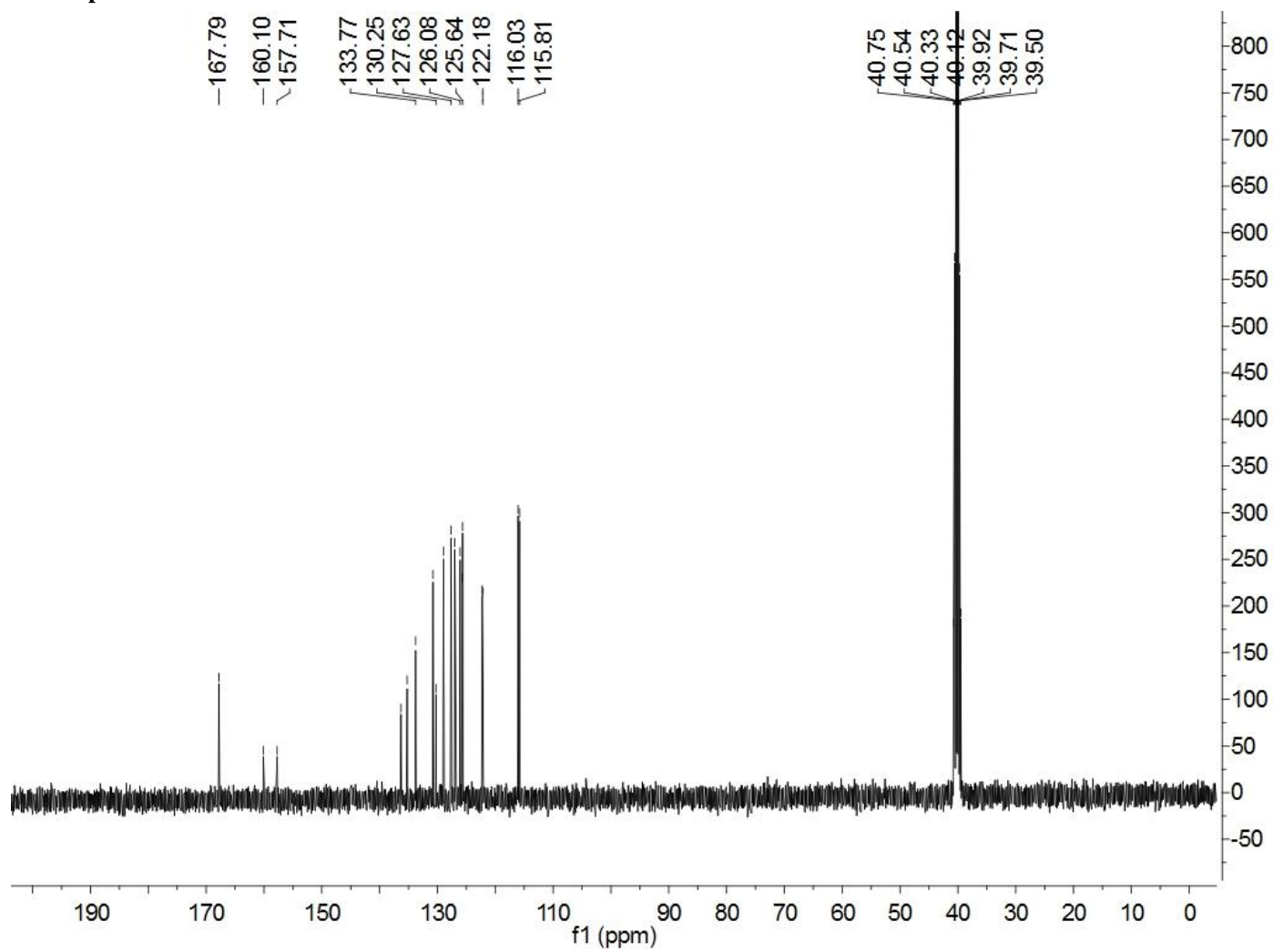
NMR spectra for 2k  $^{19}\text{F}$  NMR



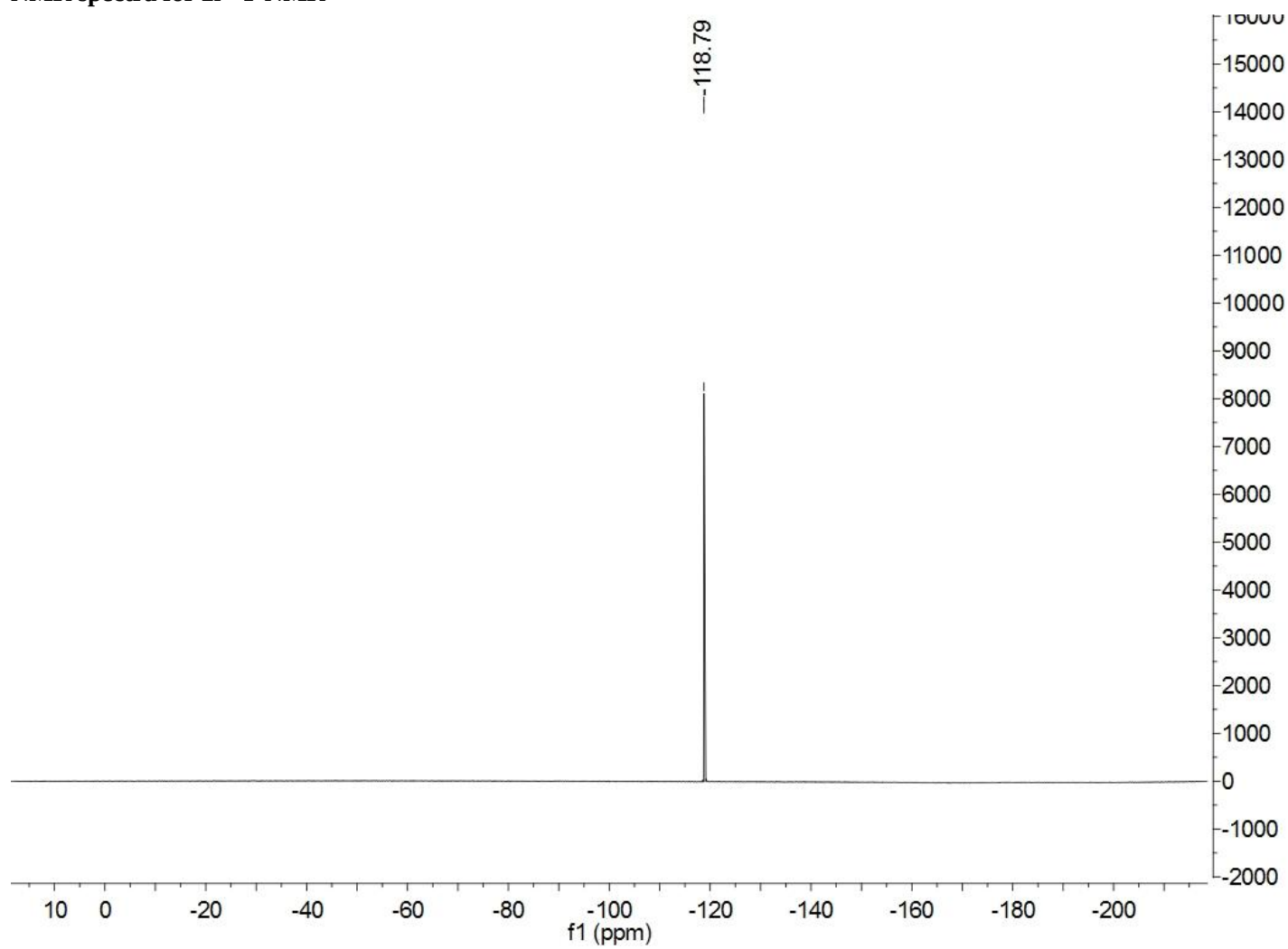
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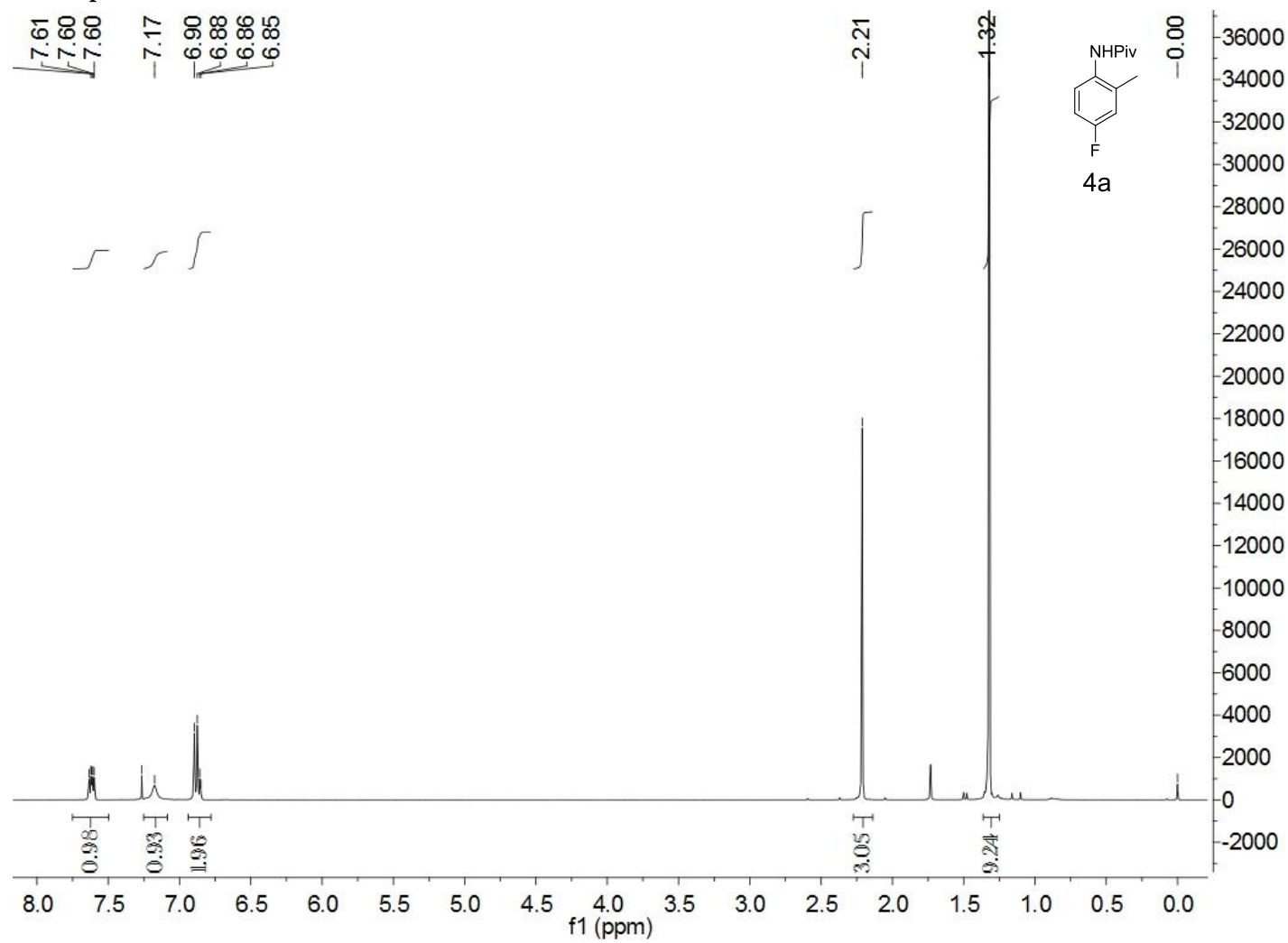
NMR spectra for 2l  $^{13}\text{C}$  NMR



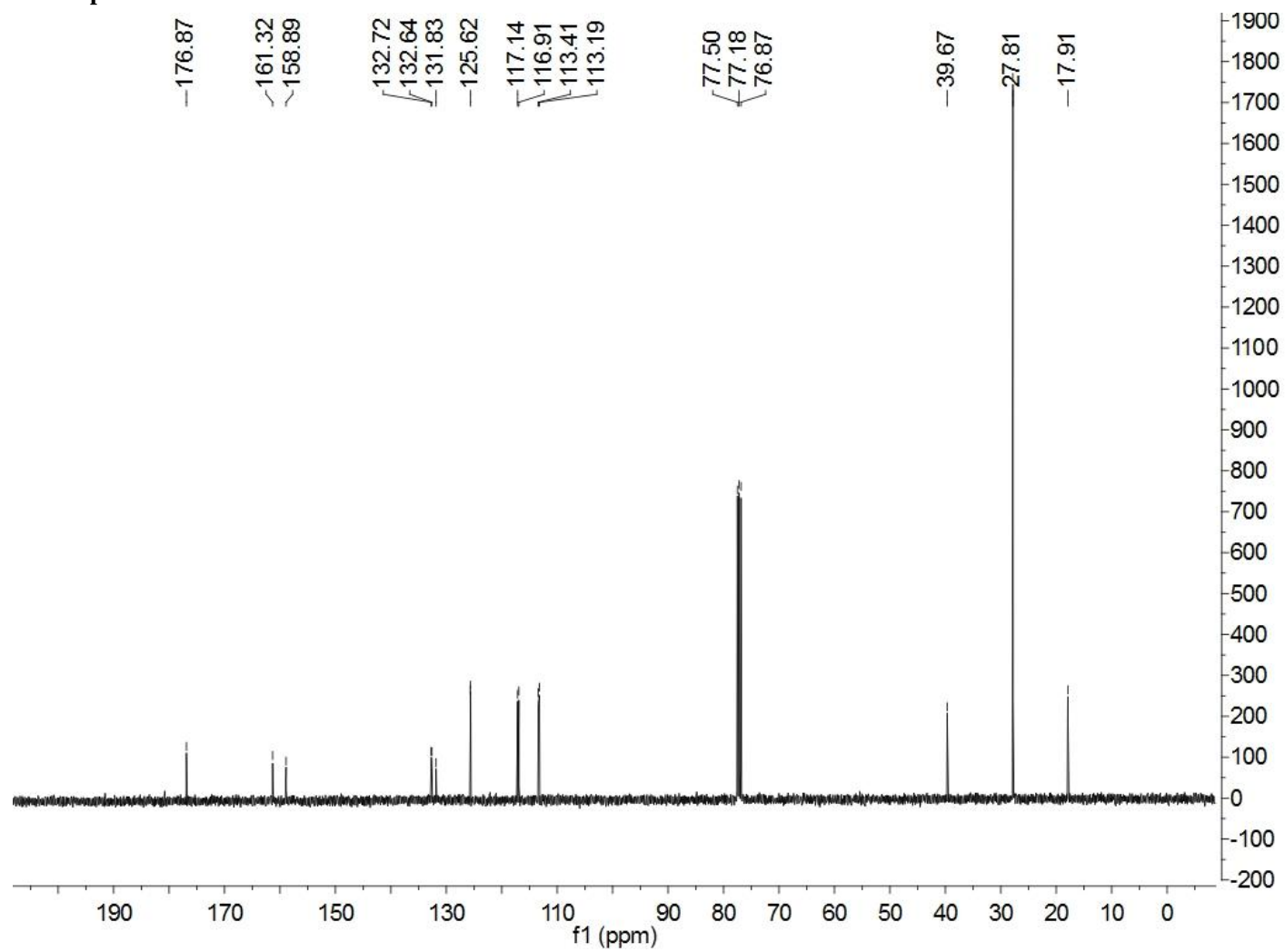
NMR spectra for 2l  $^{19}\text{F}$  NMR



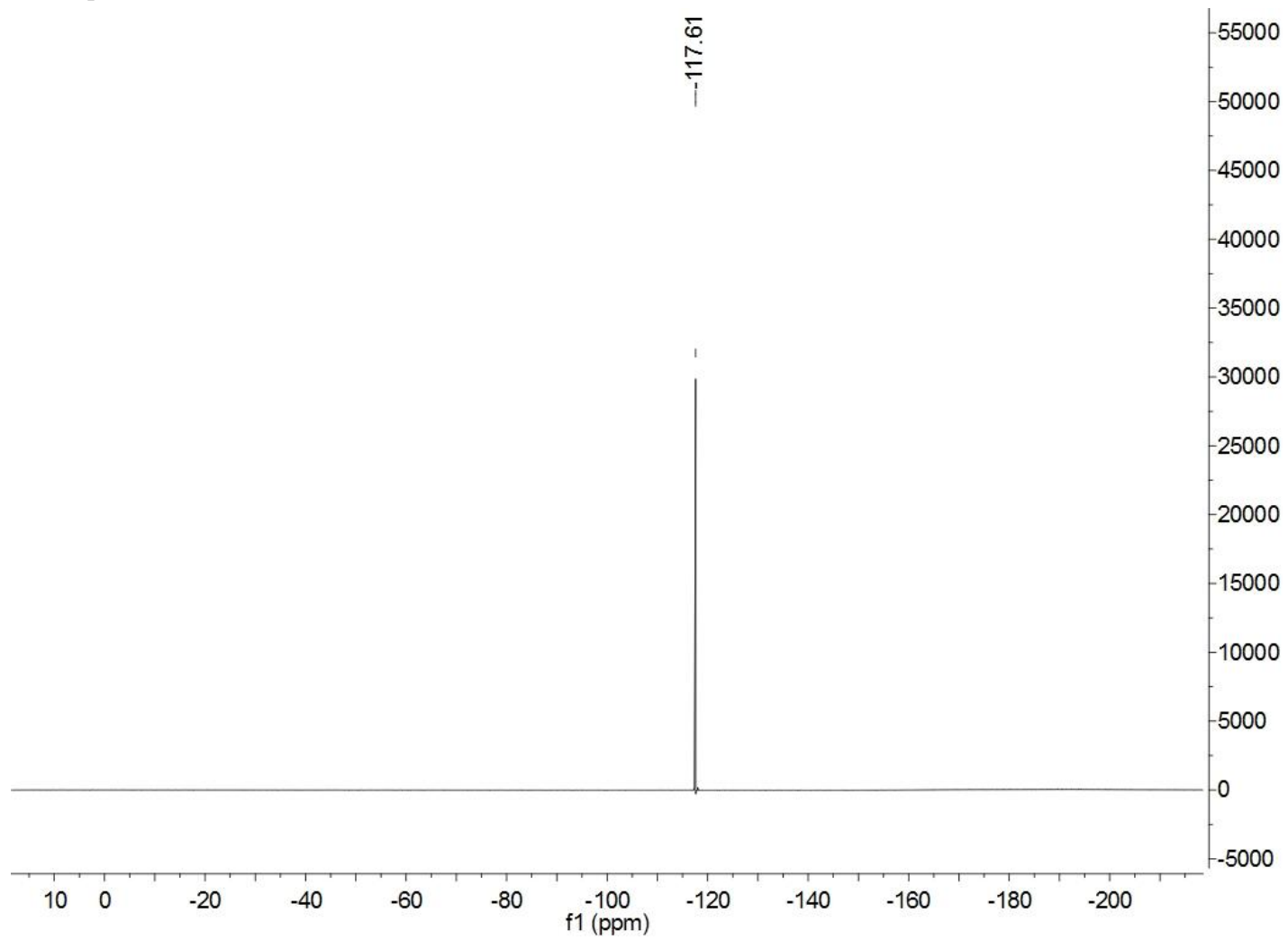
NMR spectra for 4a <sup>1</sup>H NMR

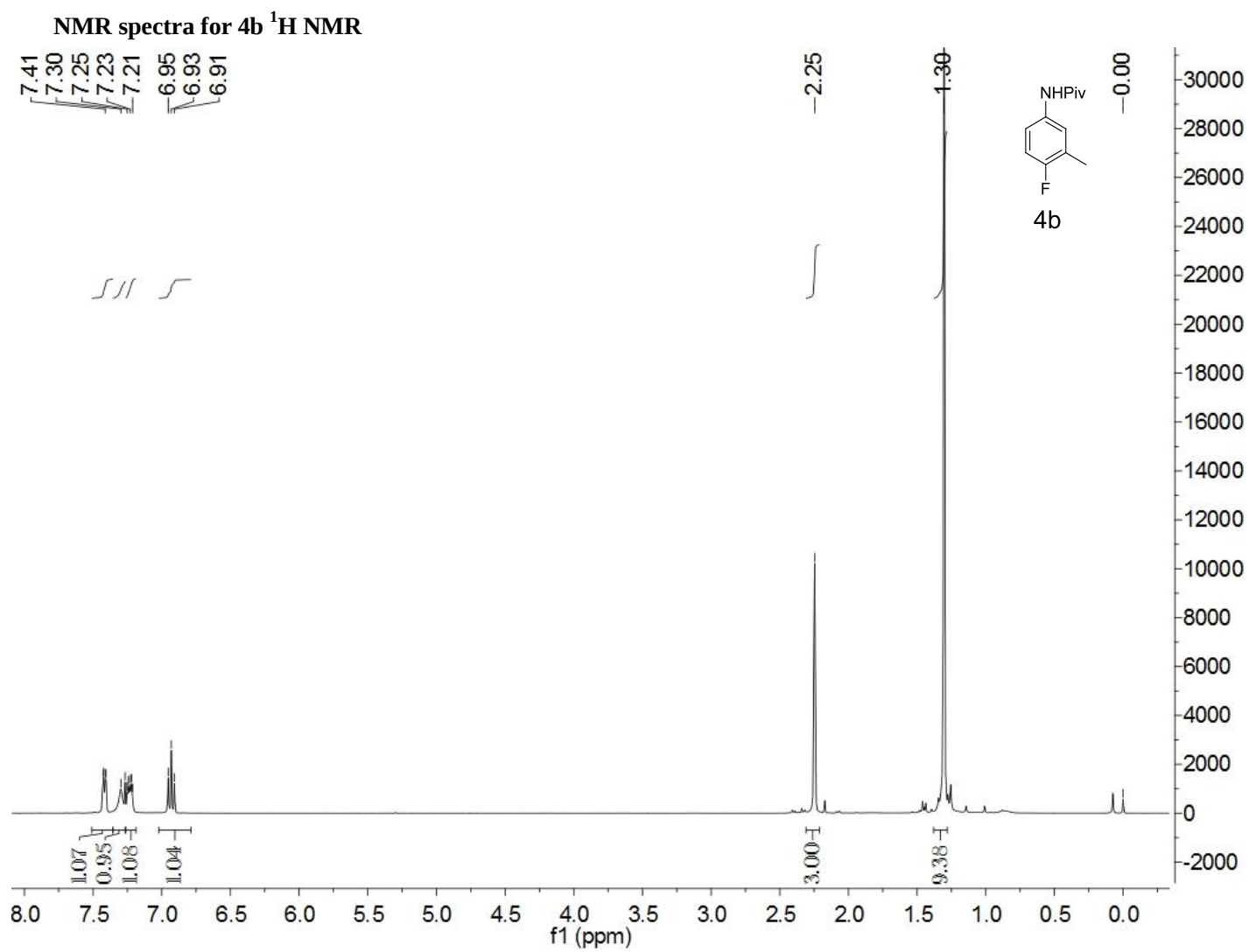


NMR spectra for 4a  $^{13}\text{C}$  NMR

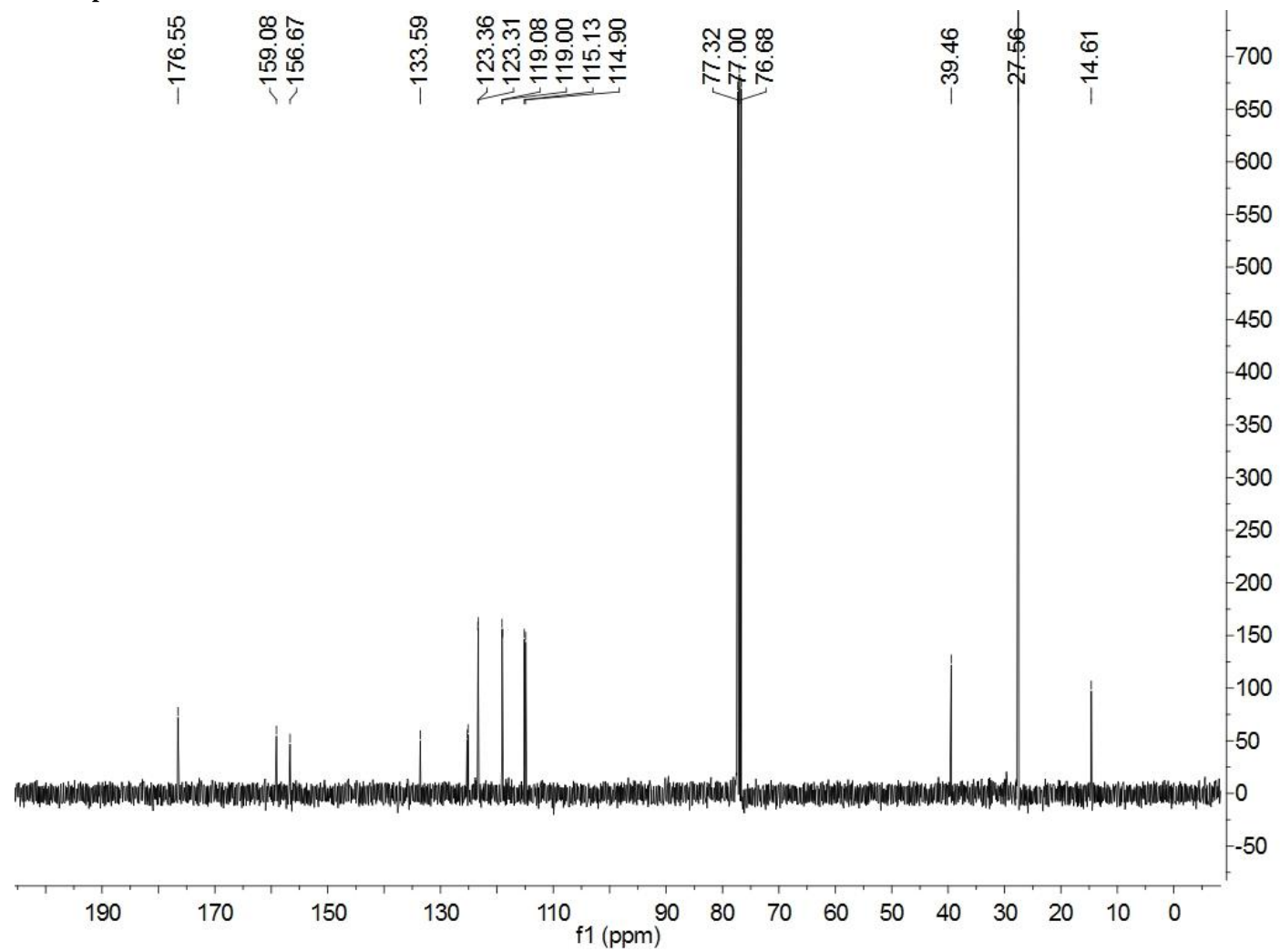


NMR spectra for 4a  $^{19}\text{F}$  NMR

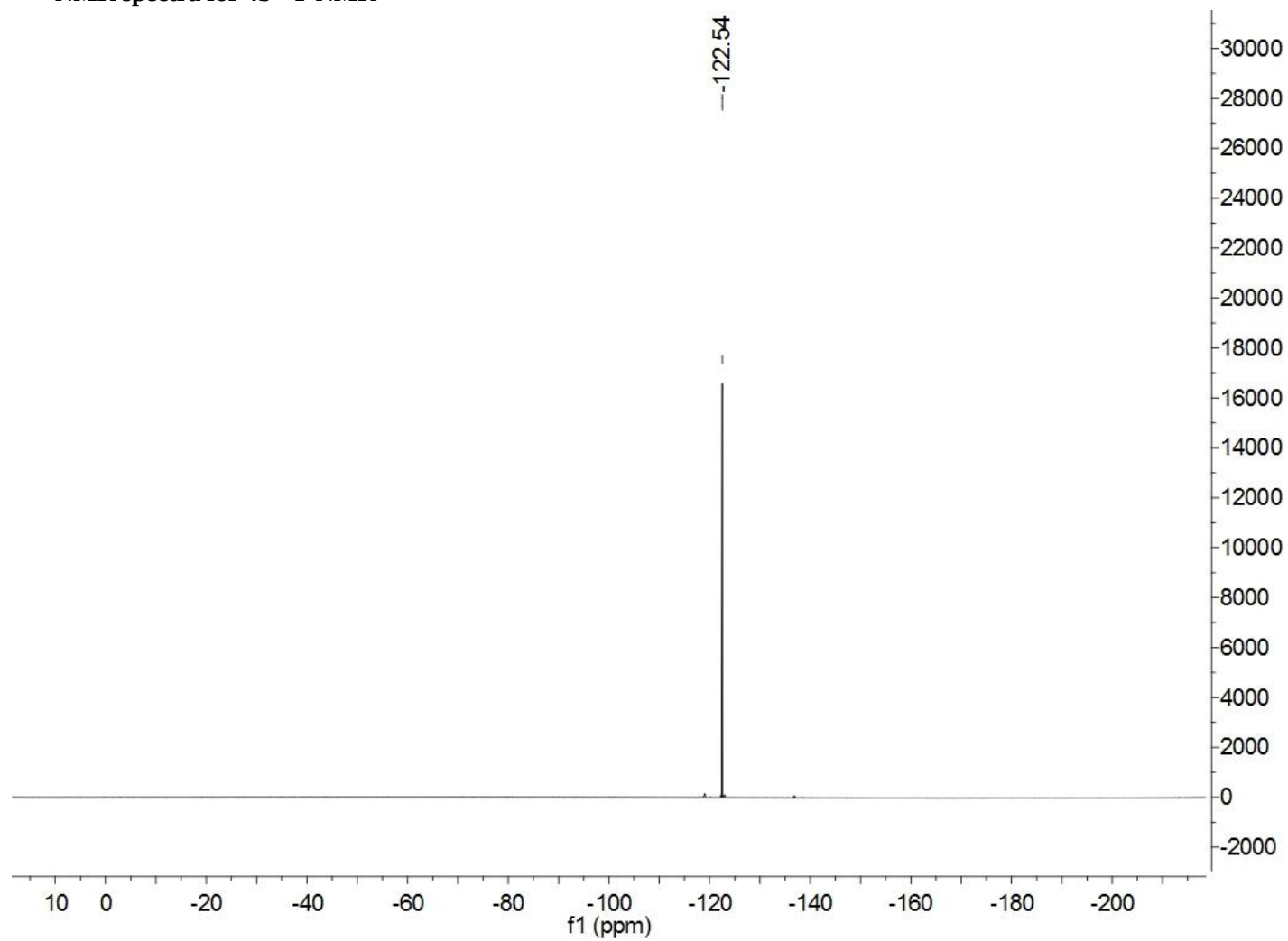




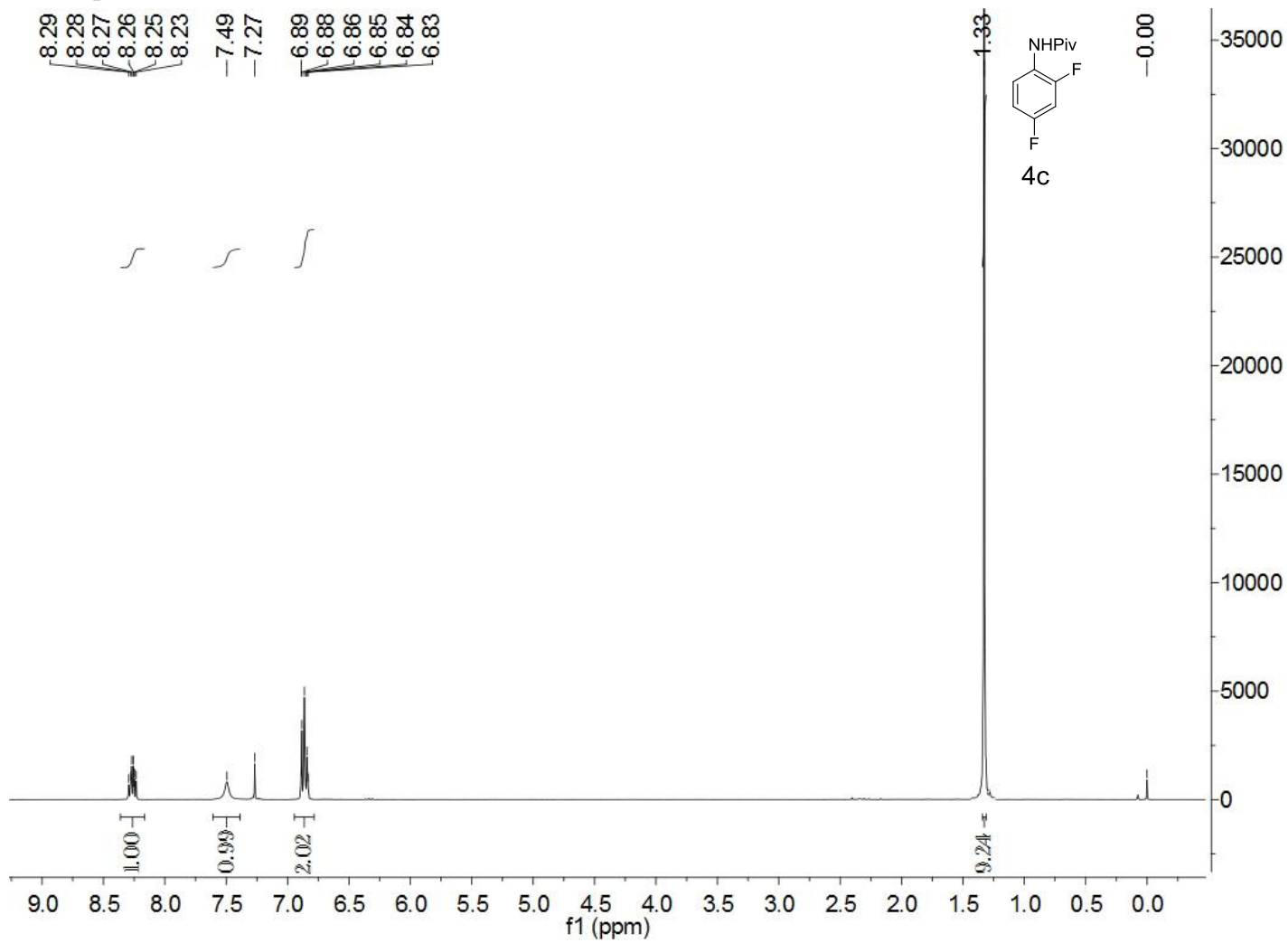
NMR spectra for 4b  $^{13}\text{C}$  NMR

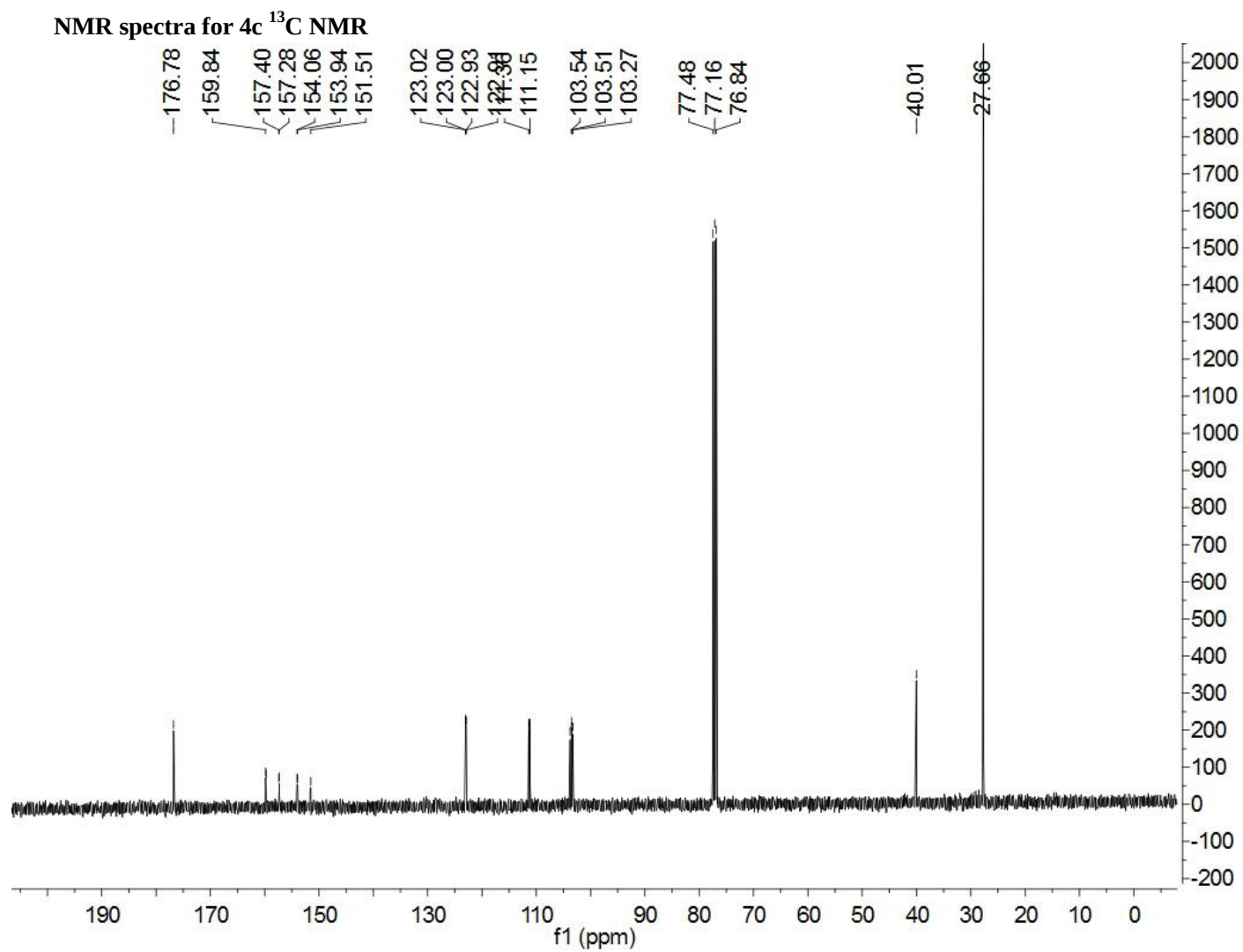


NMR spectra for 4b  $^{19}\text{F}$  NMR

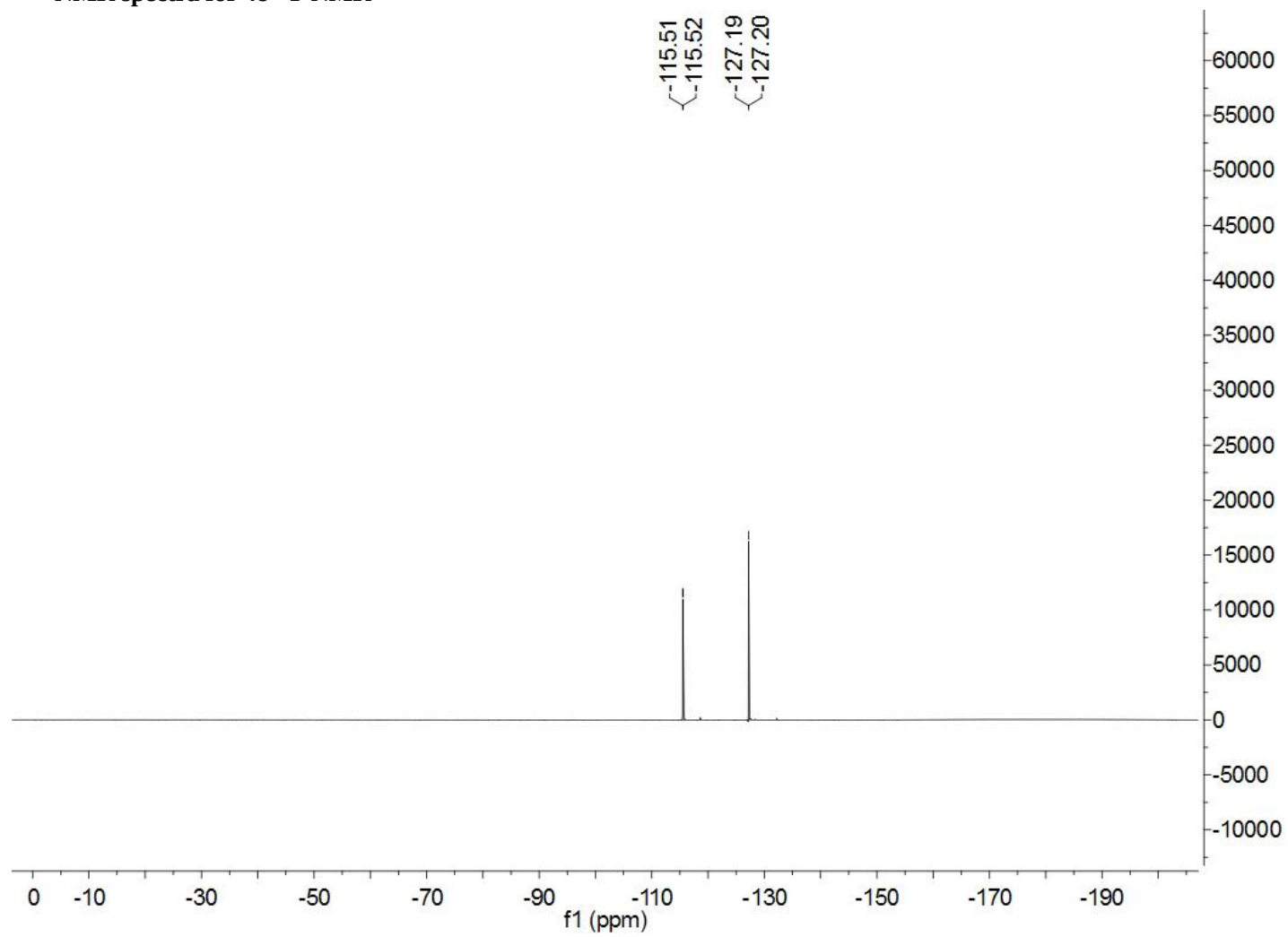


NMR spectra for 4c  $^1\text{H}$  NMR

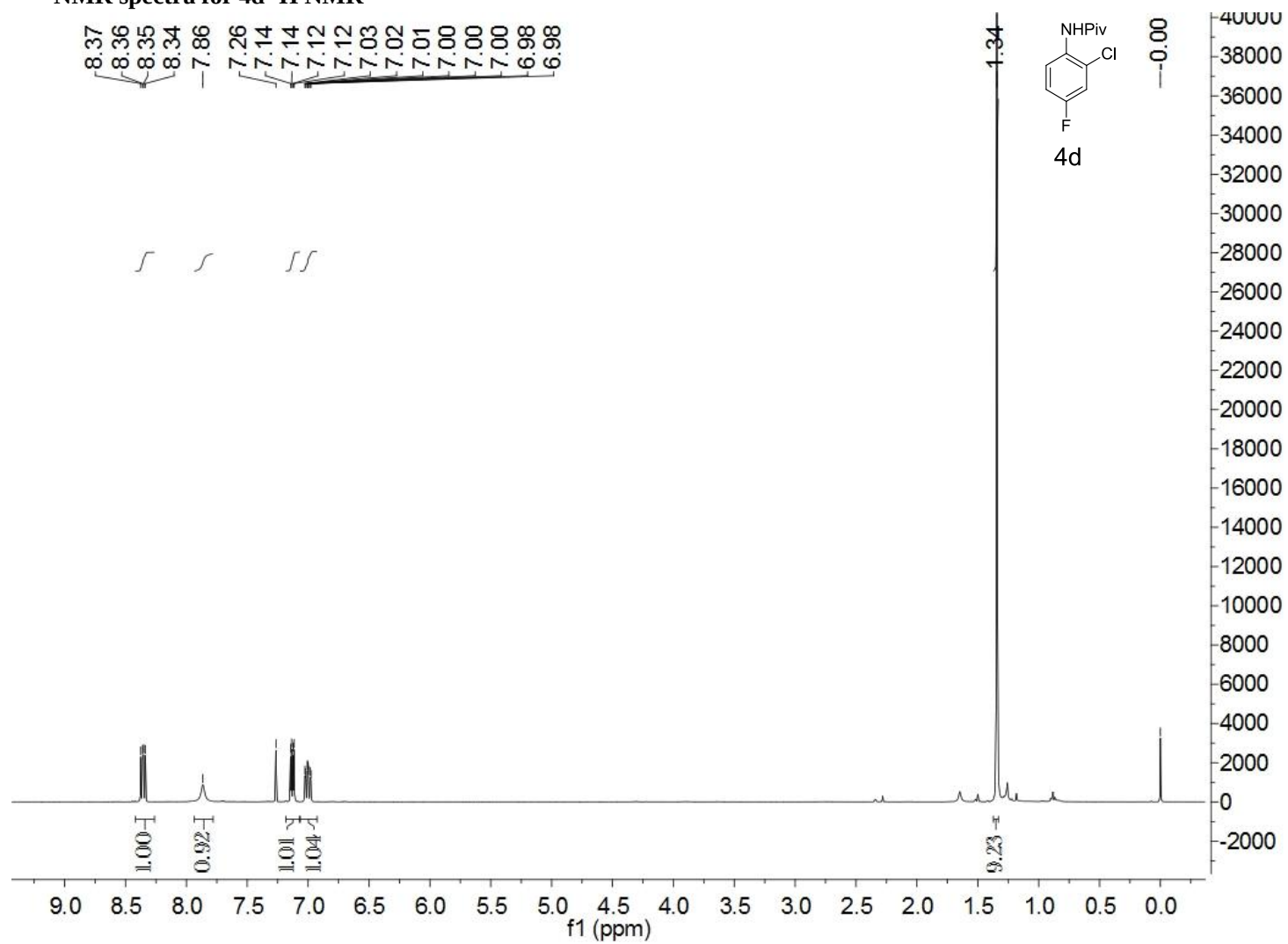


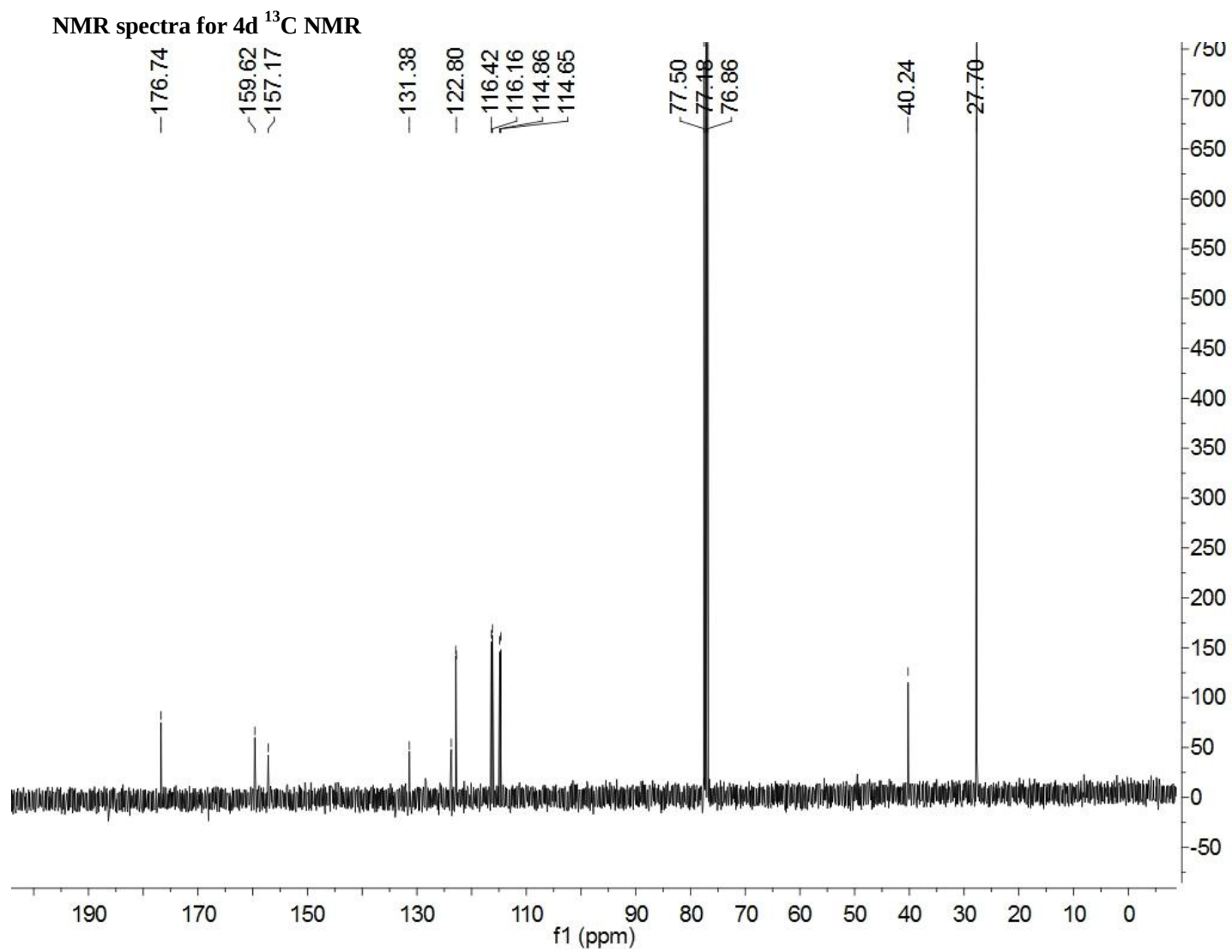


NMR spectra for 4c  $^{19}\text{F}$  NMR

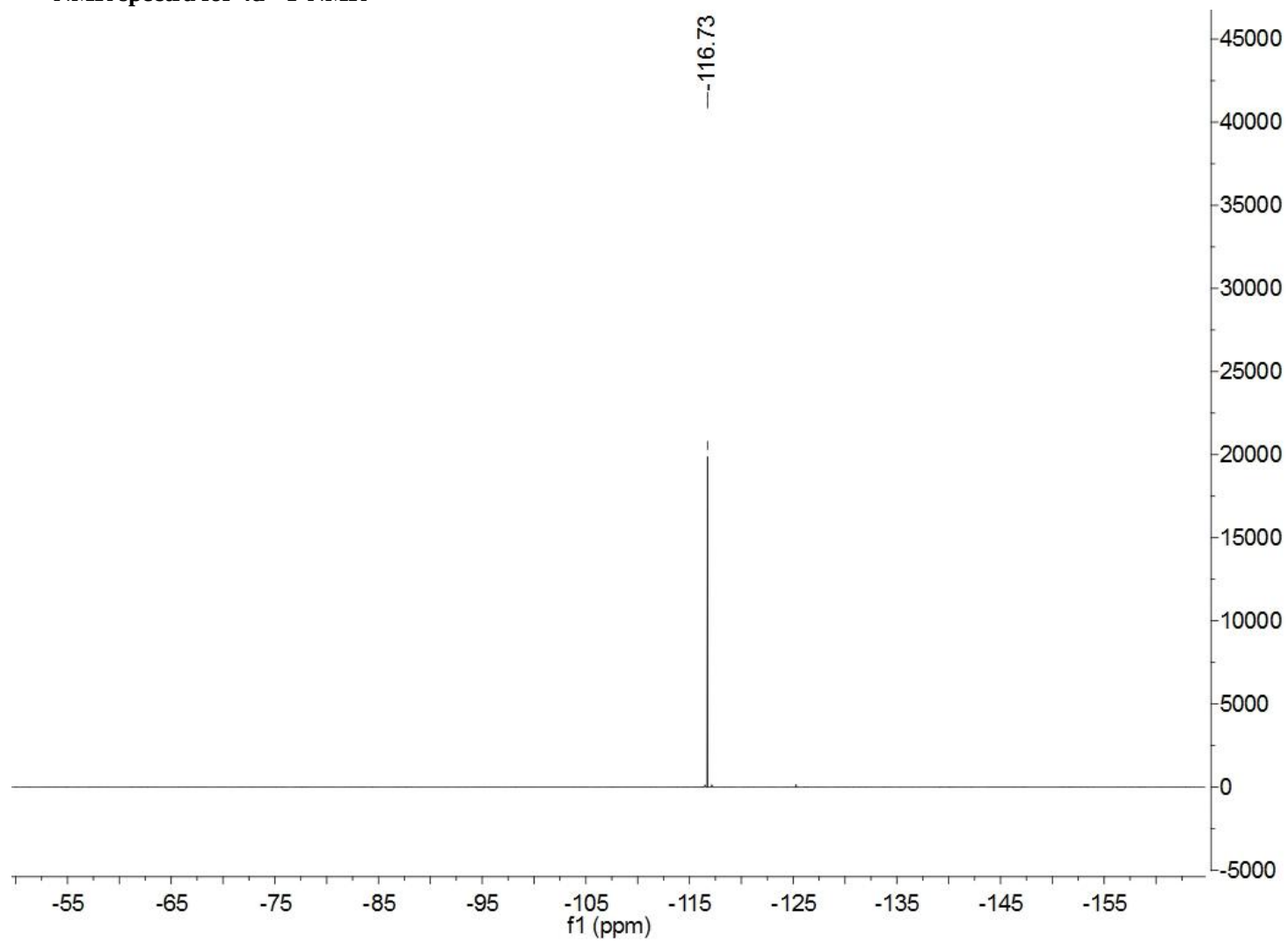


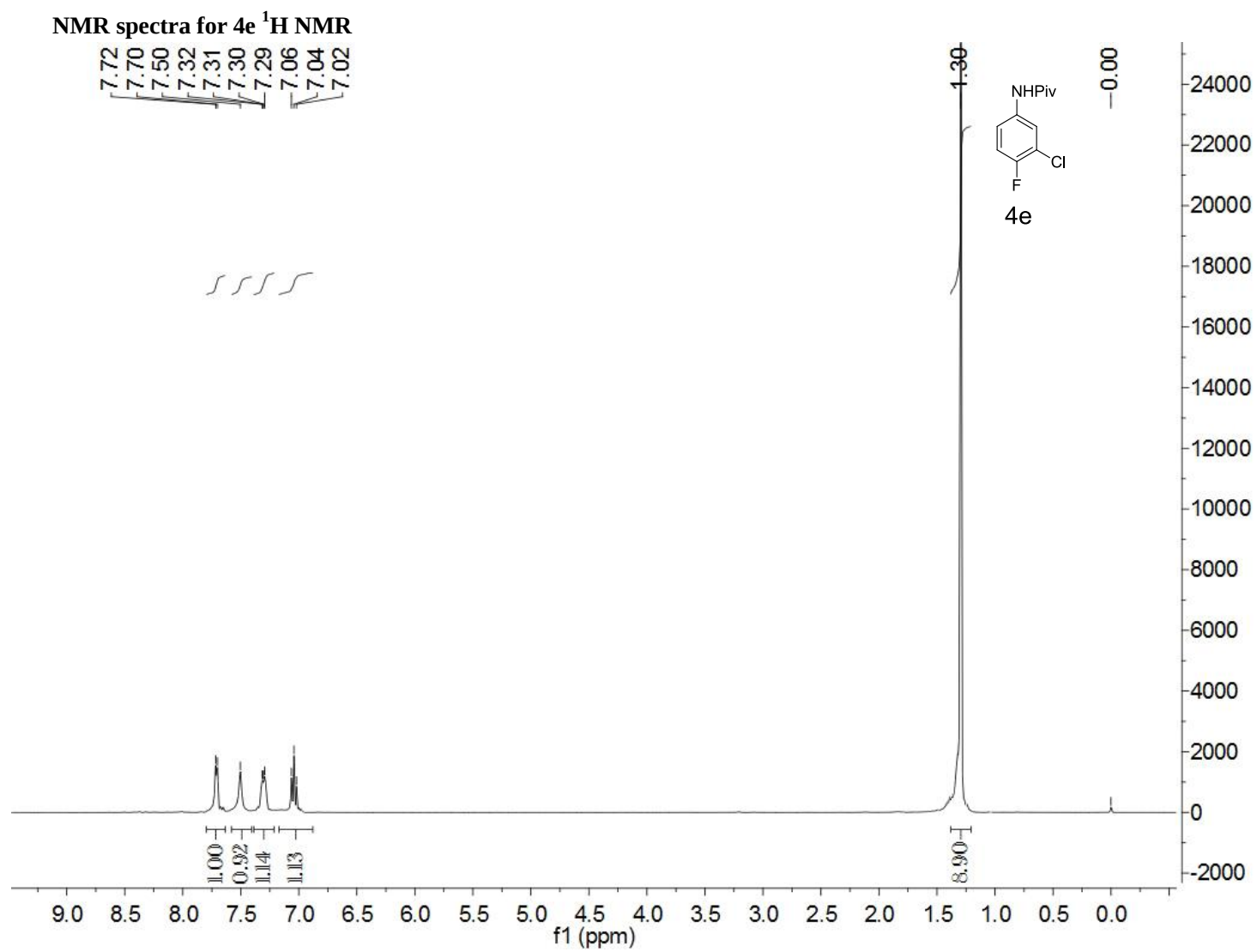
NMR spectra for 4d  $^1\text{H}$  NMR



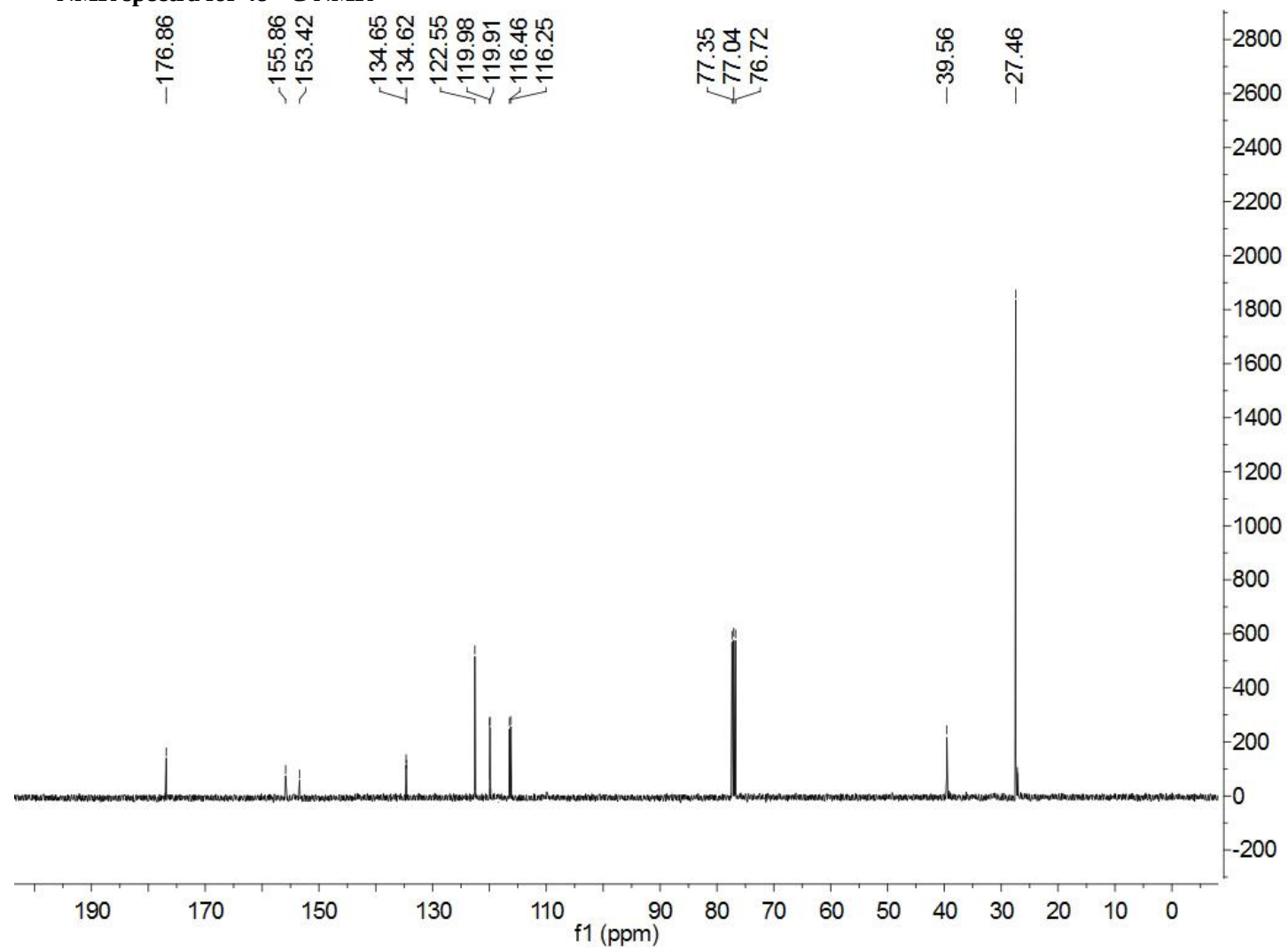


NMR spectra for 4d  $^{19}\text{F}$  NMR

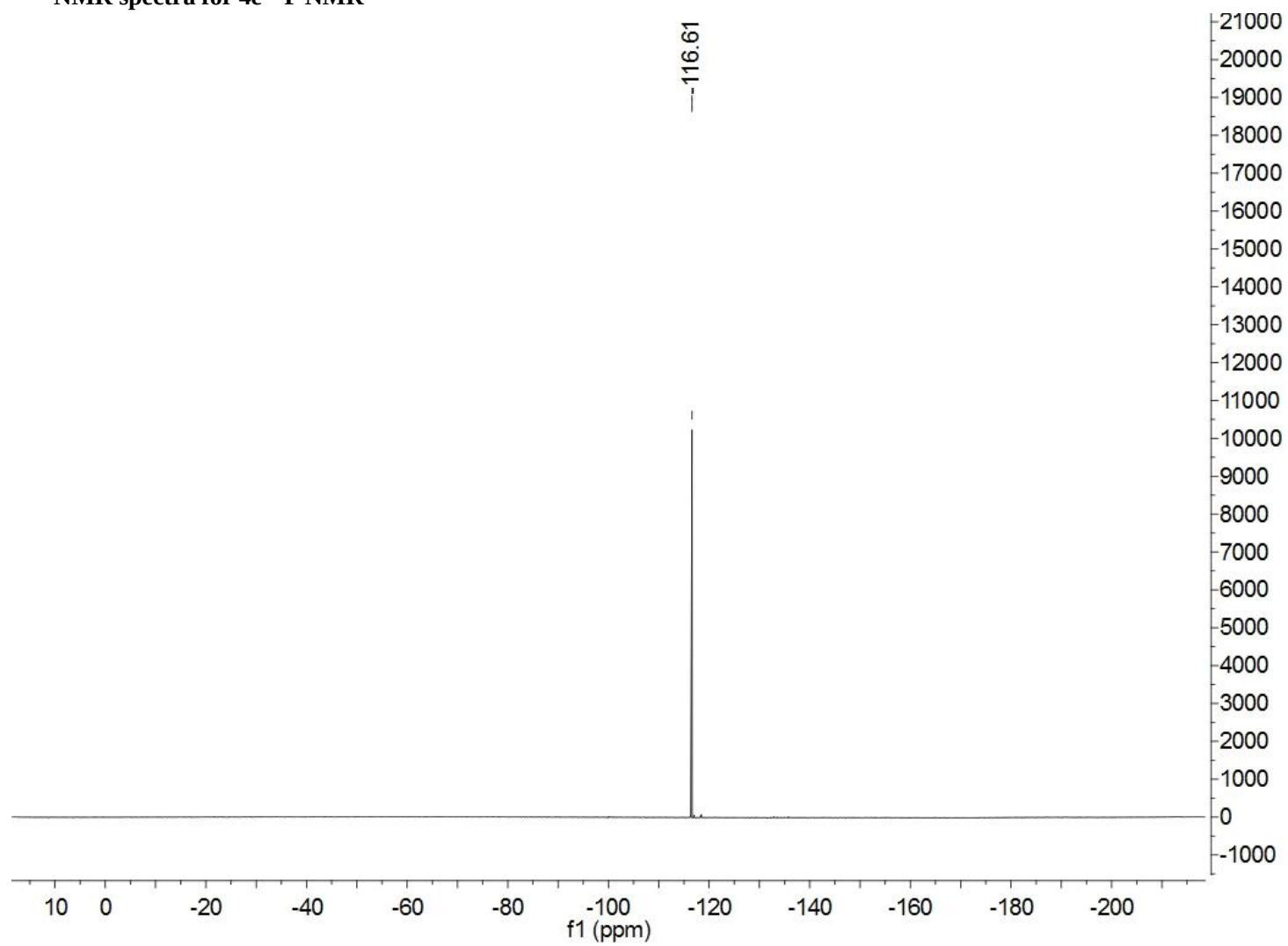




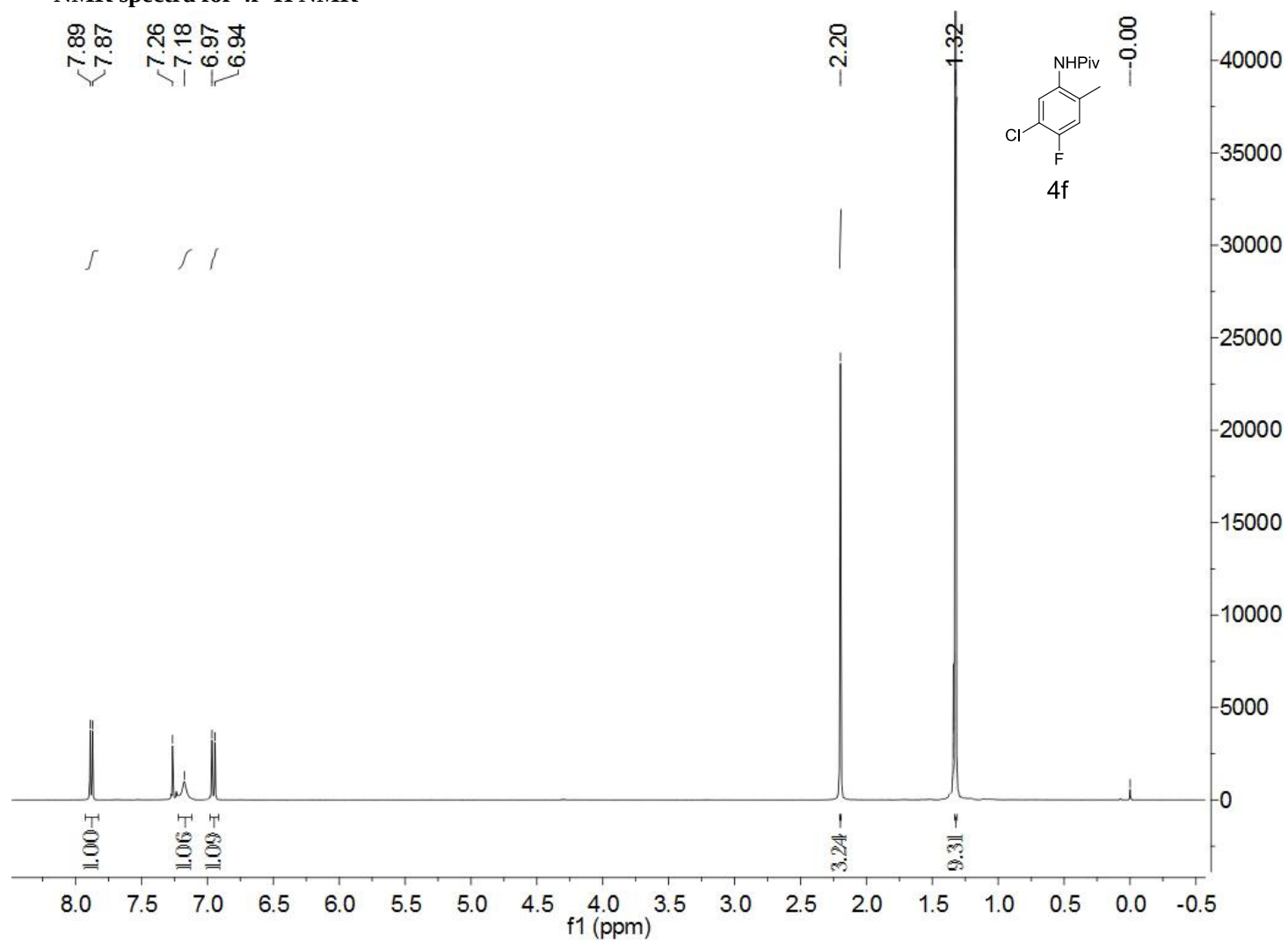
NMR spectra for 4e  $^{13}\text{C}$  NMR



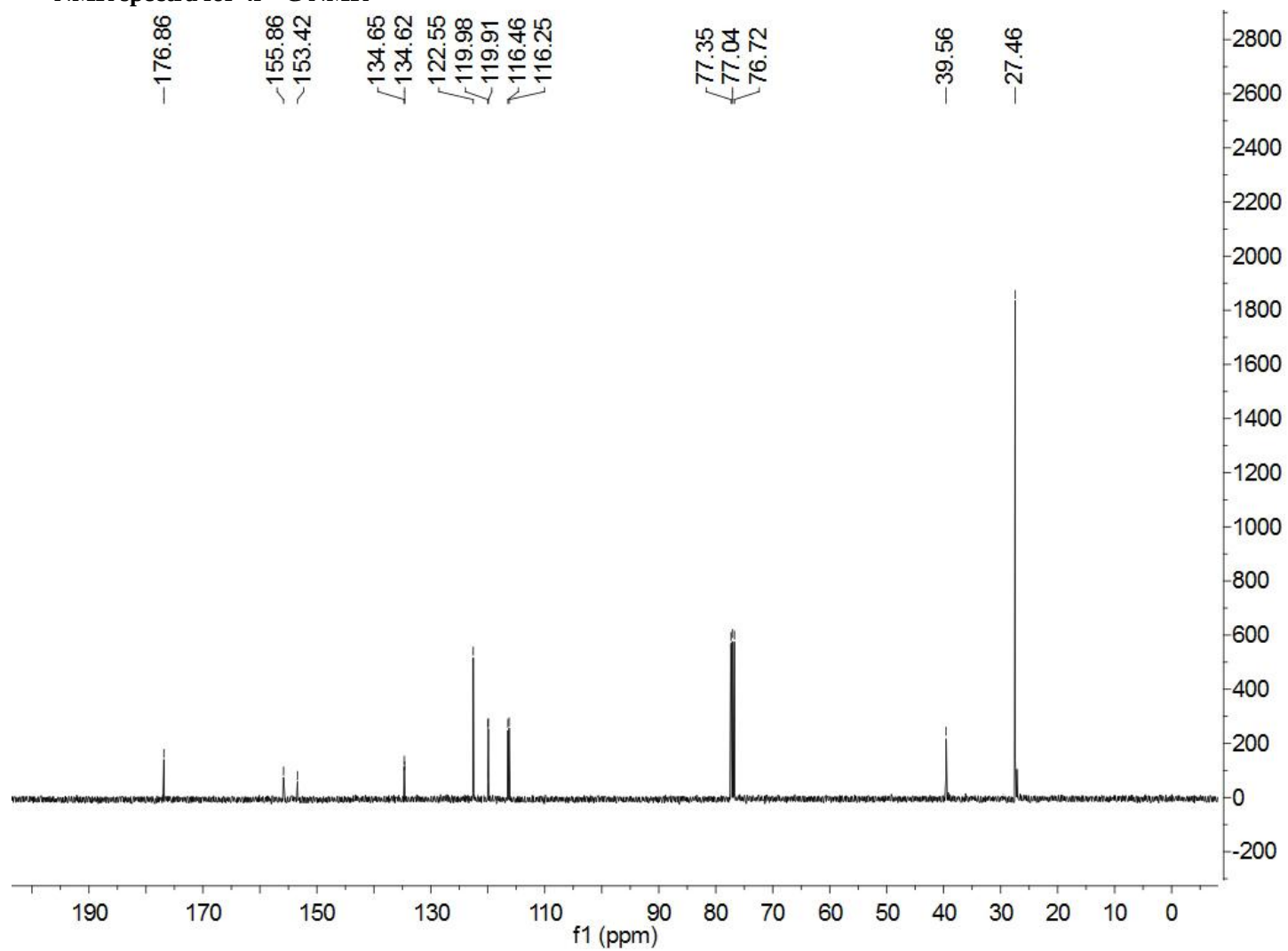
NMR spectra for 4e  $^{19}\text{F}$  NMR



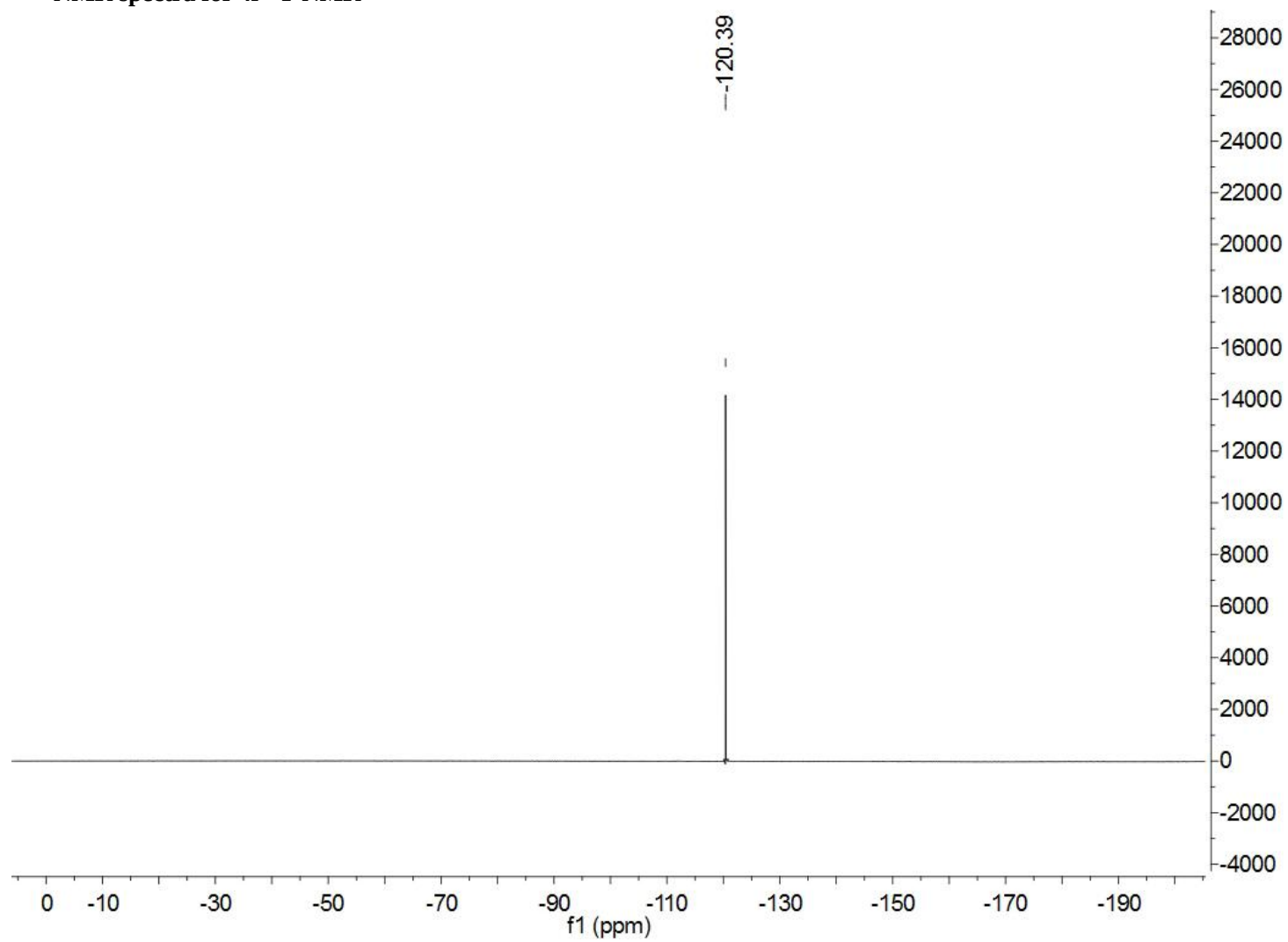
NMR spectra for 4f  $^1\text{H}$  NMR



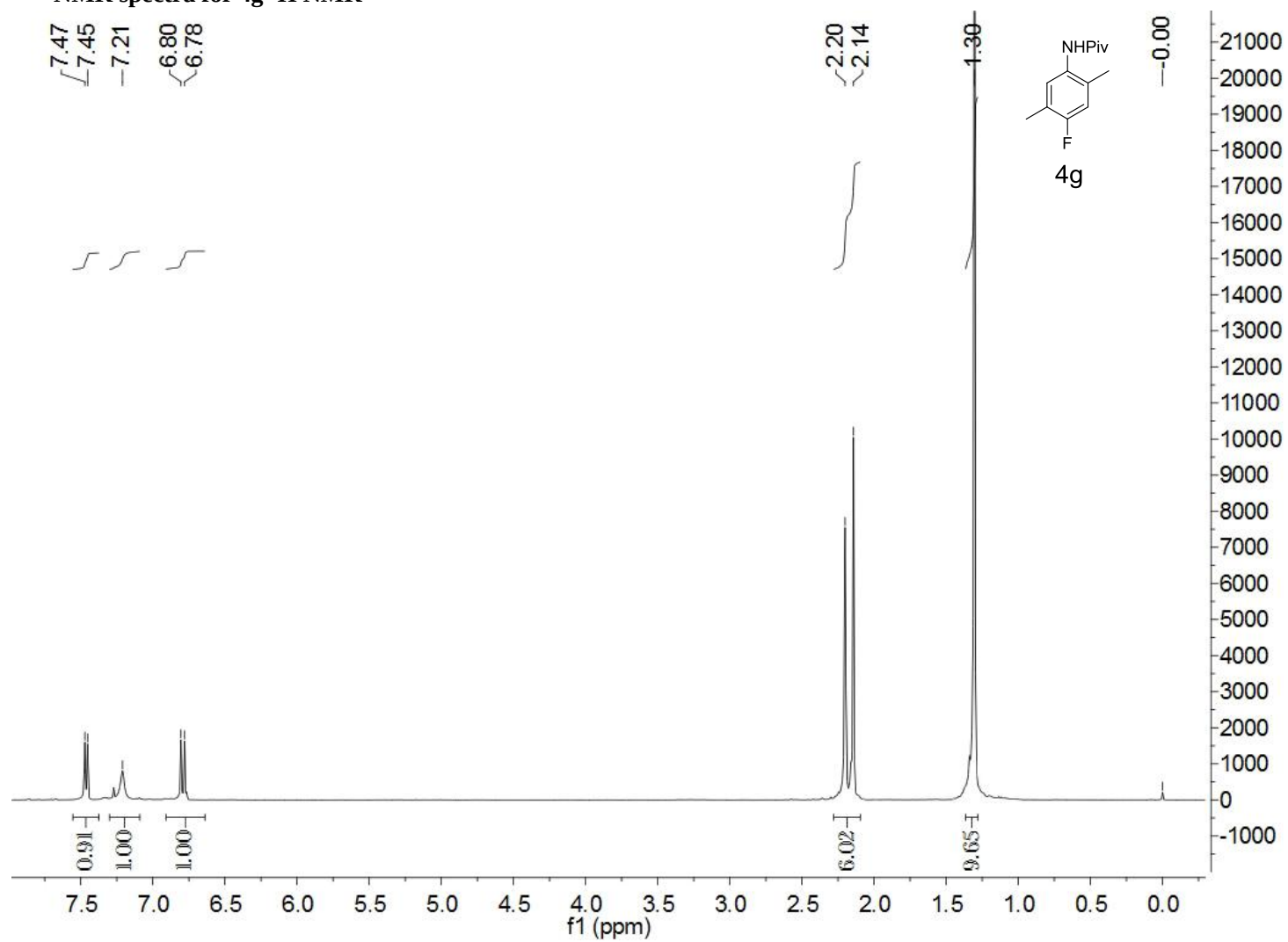
NMR spectra for 4f  $^{13}\text{C}$  NMR

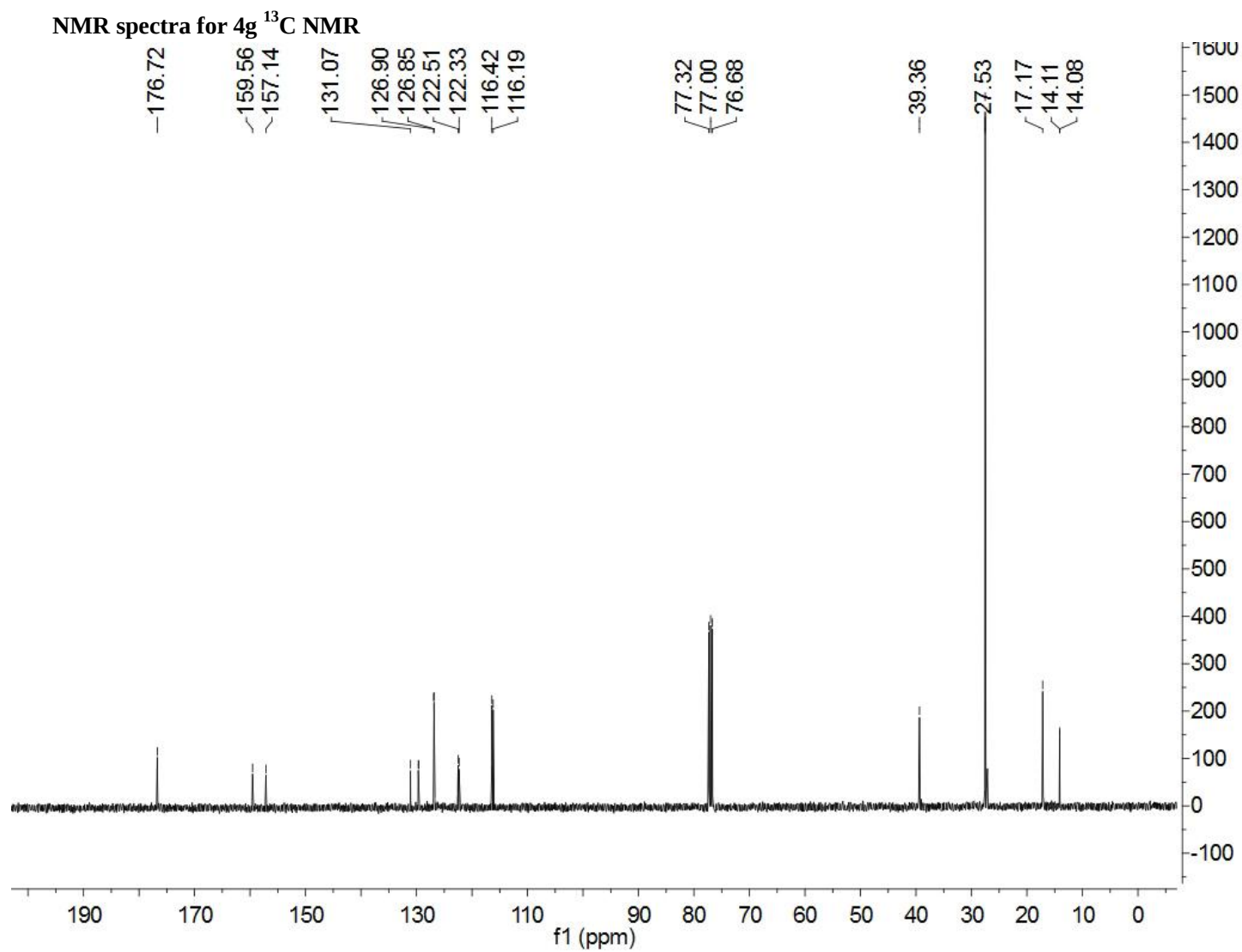


NMR spectra for 4f  $^{19}\text{F}$  NMR

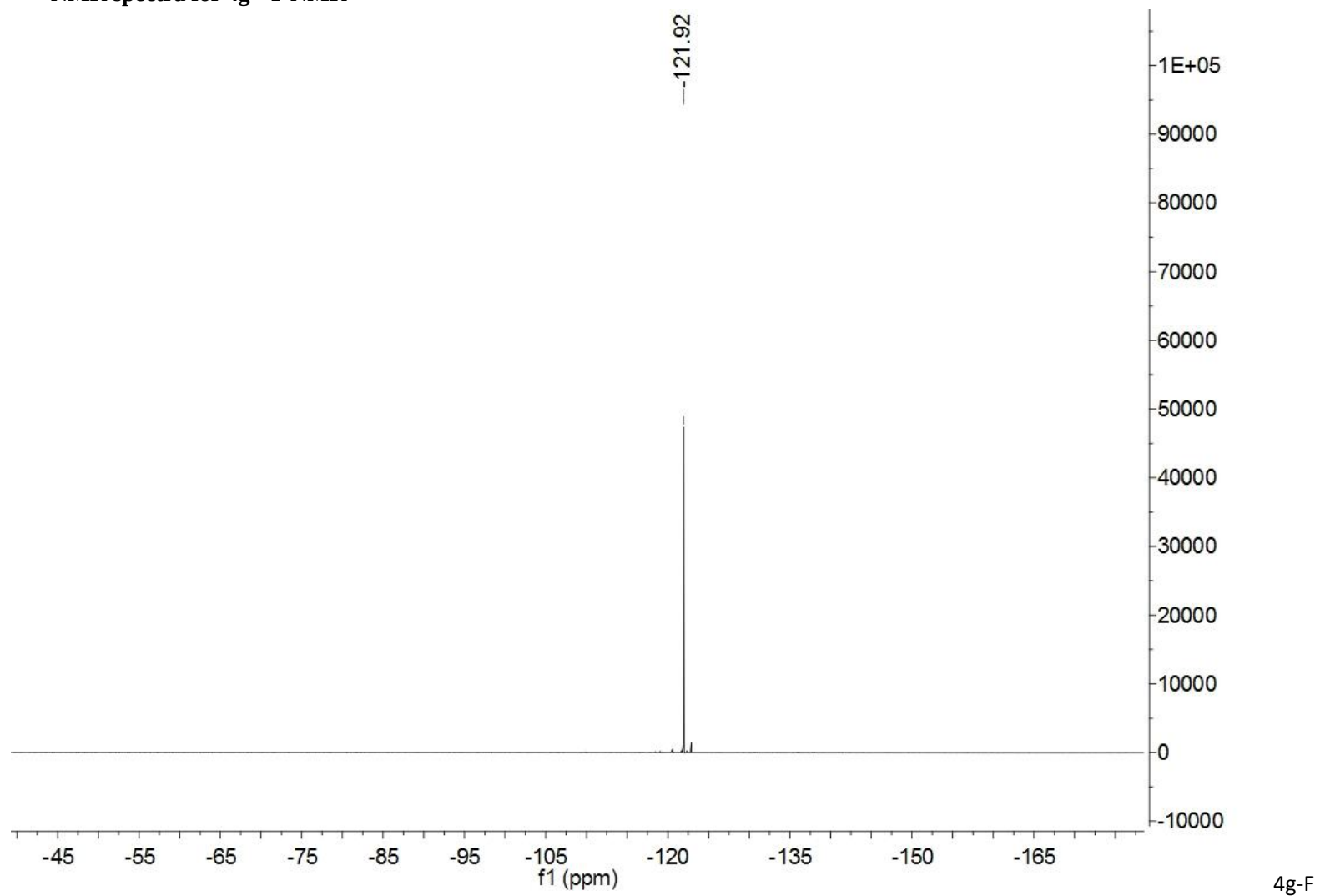


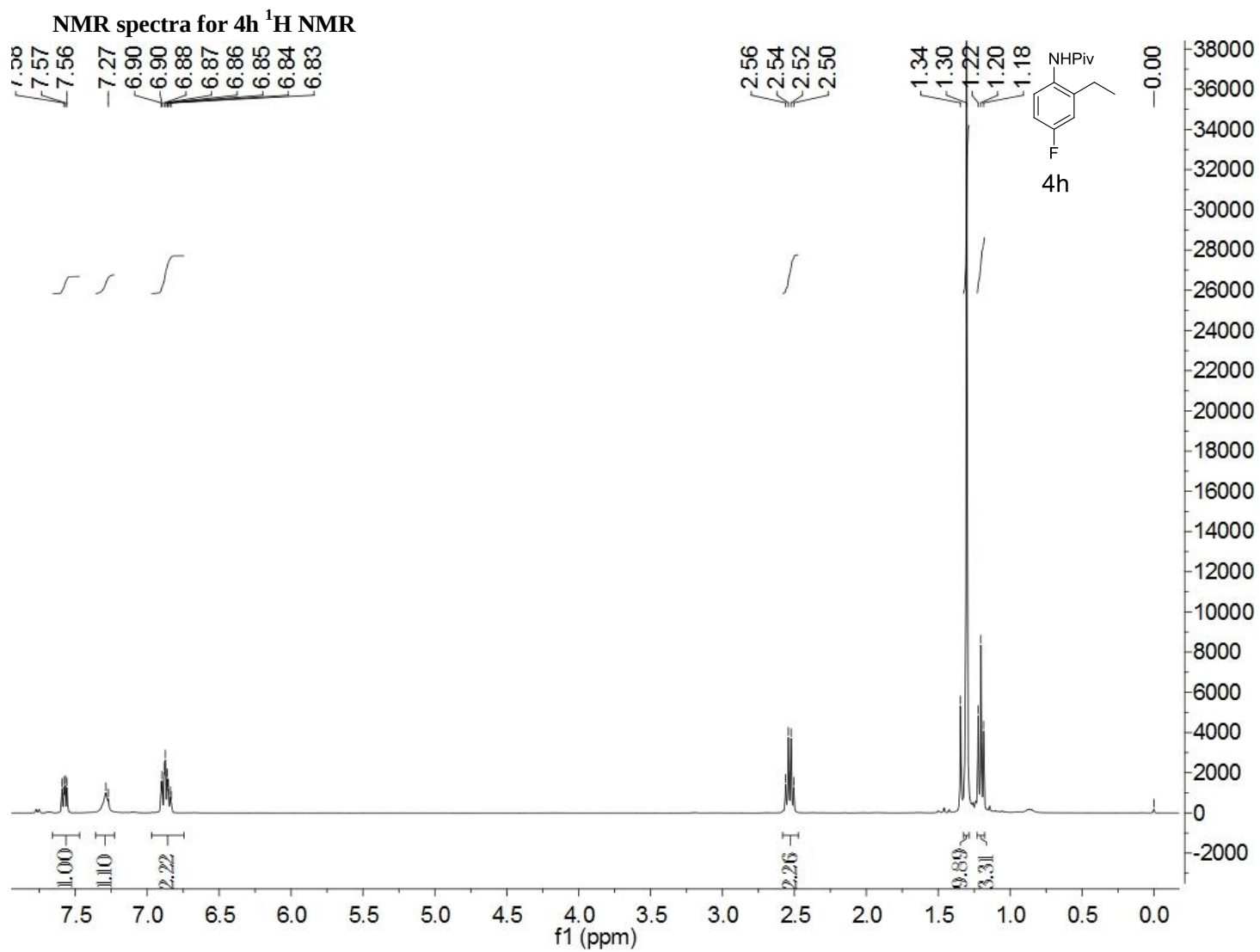
NMR spectra for 4g  $^1\text{H}$  NMR



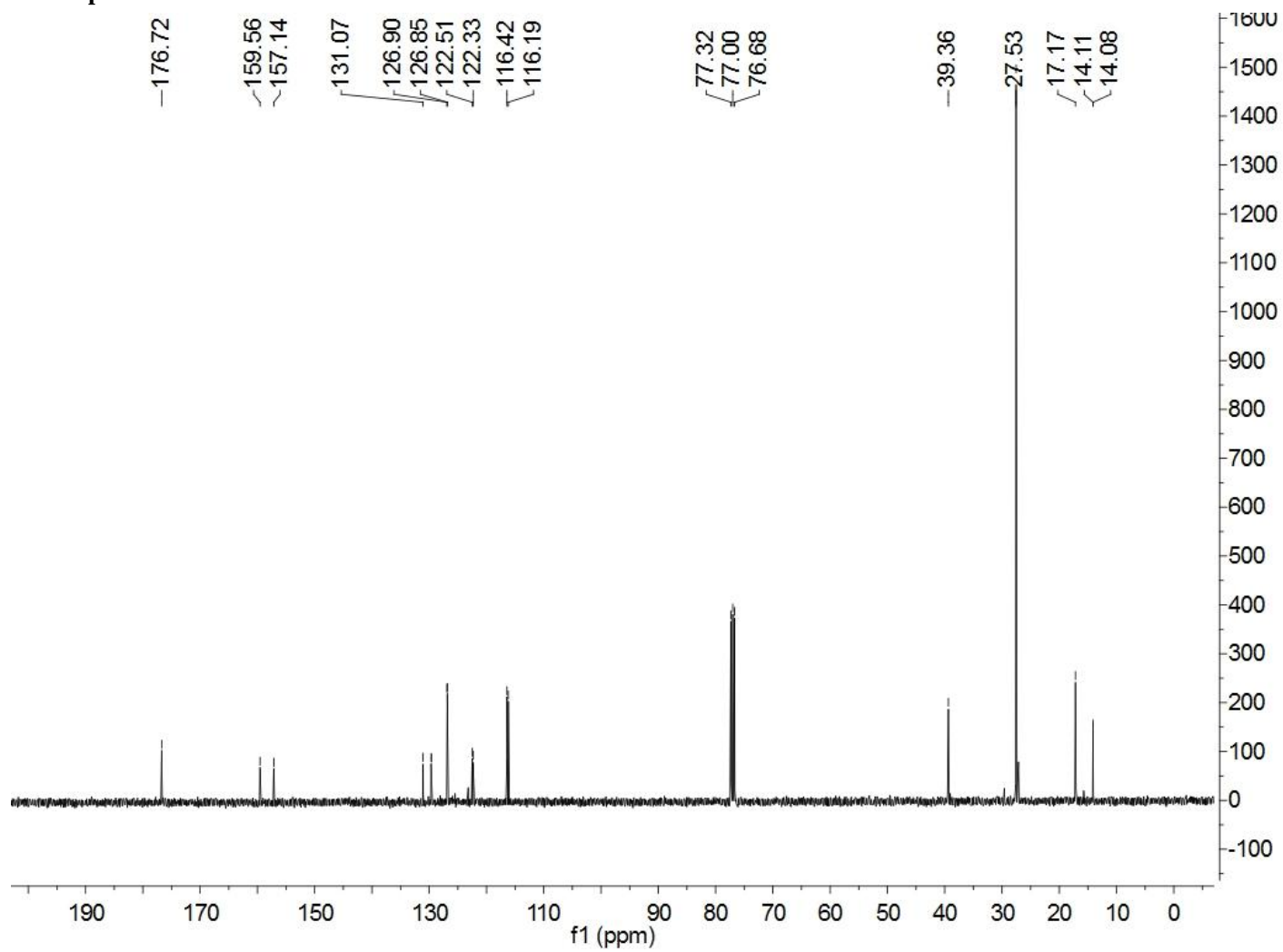


NMR spectra for 4g  $^{19}\text{F}$  NMR

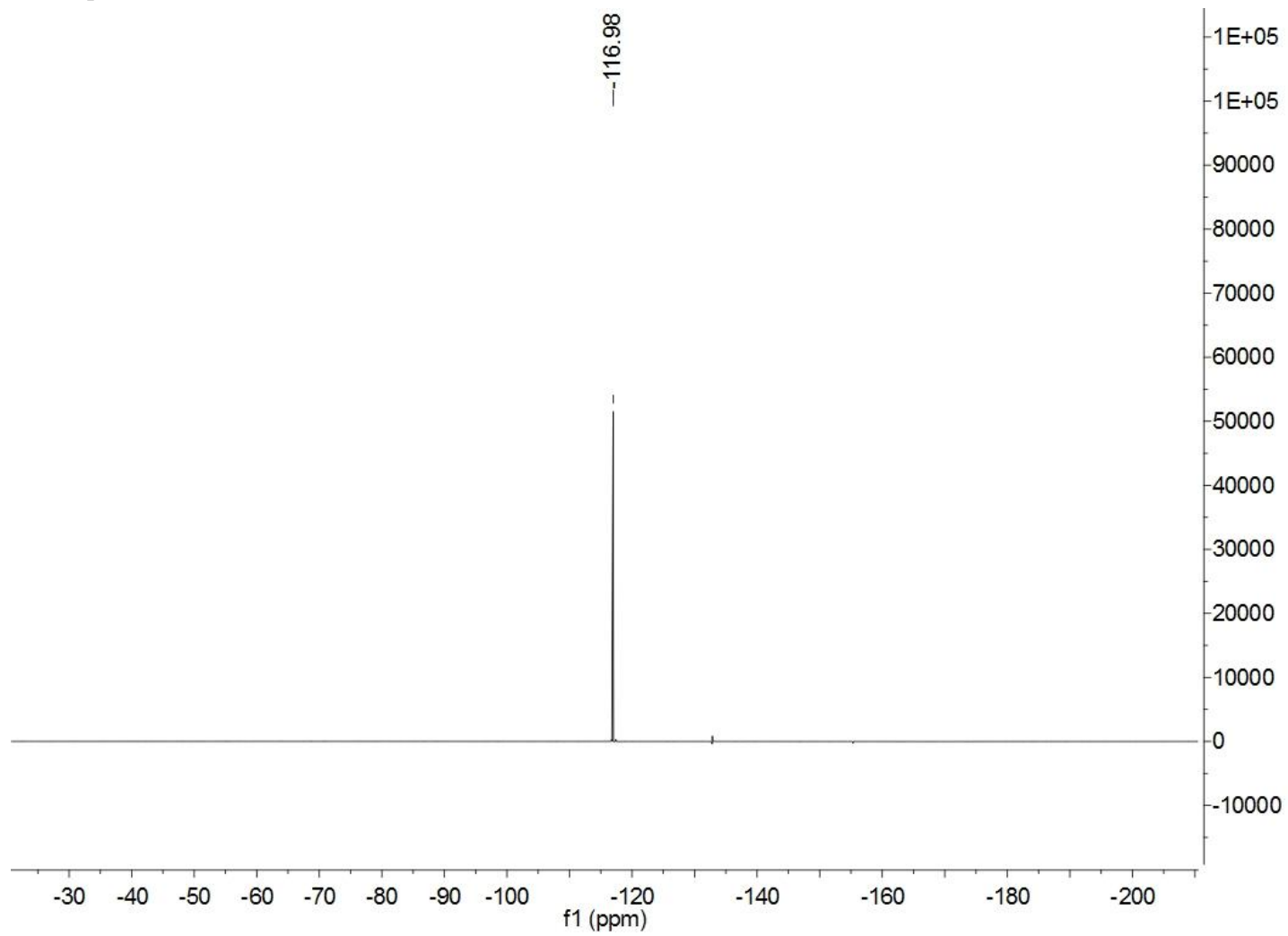


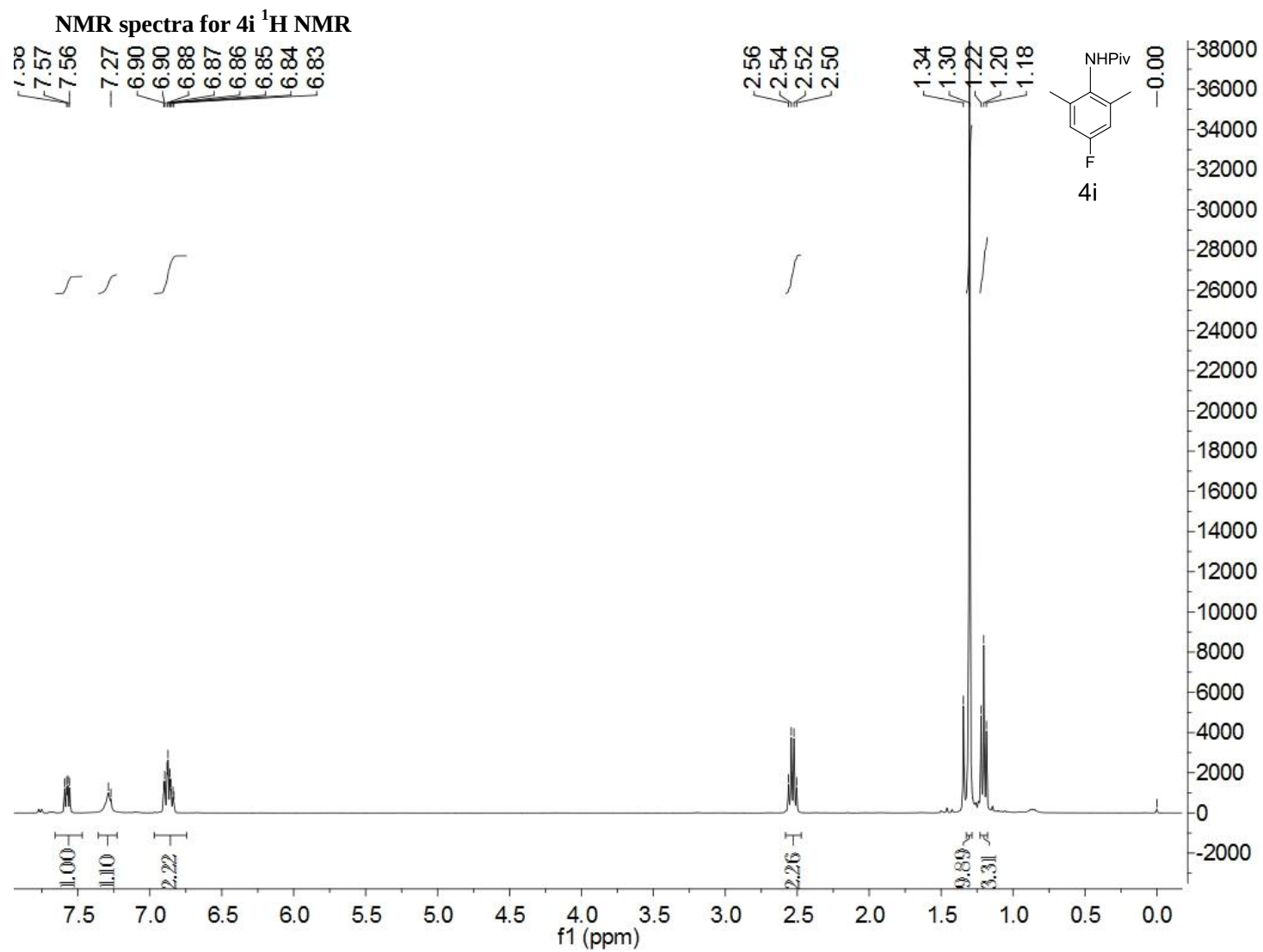


NMR spectra for 4h  $^{13}\text{C}$  NMR

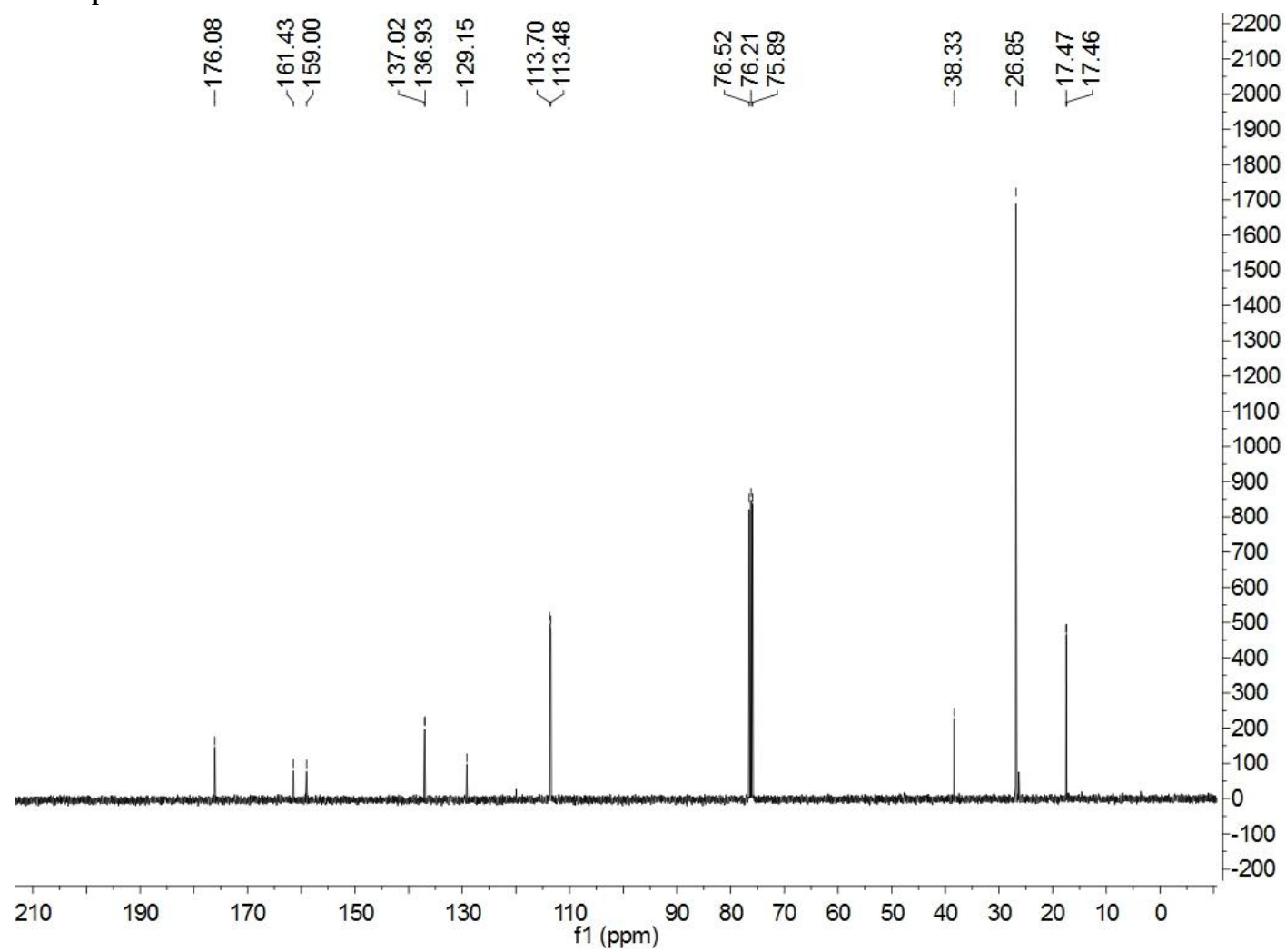


NMR spectra for 4h  $^{19}\text{F}$  NMR

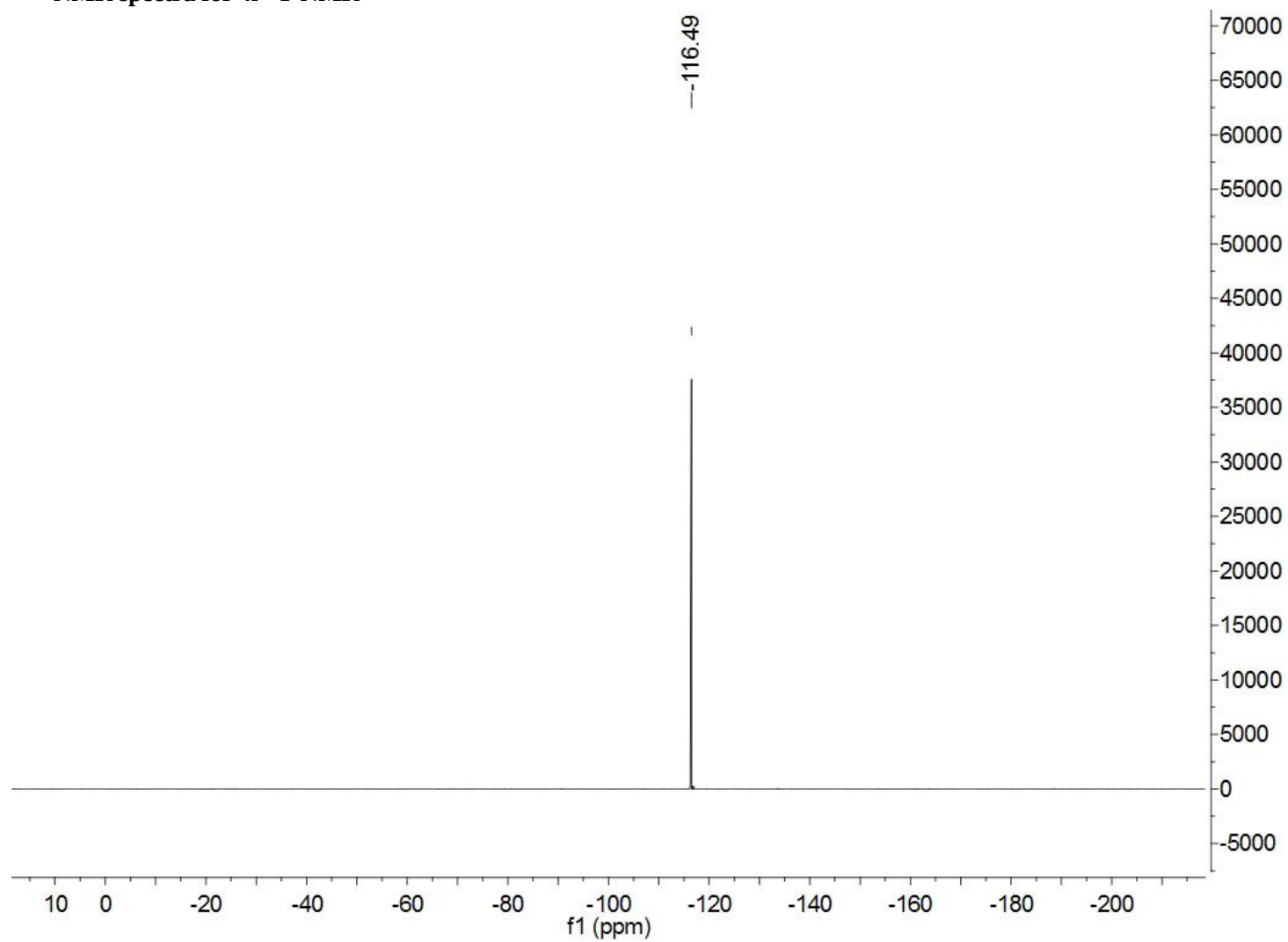


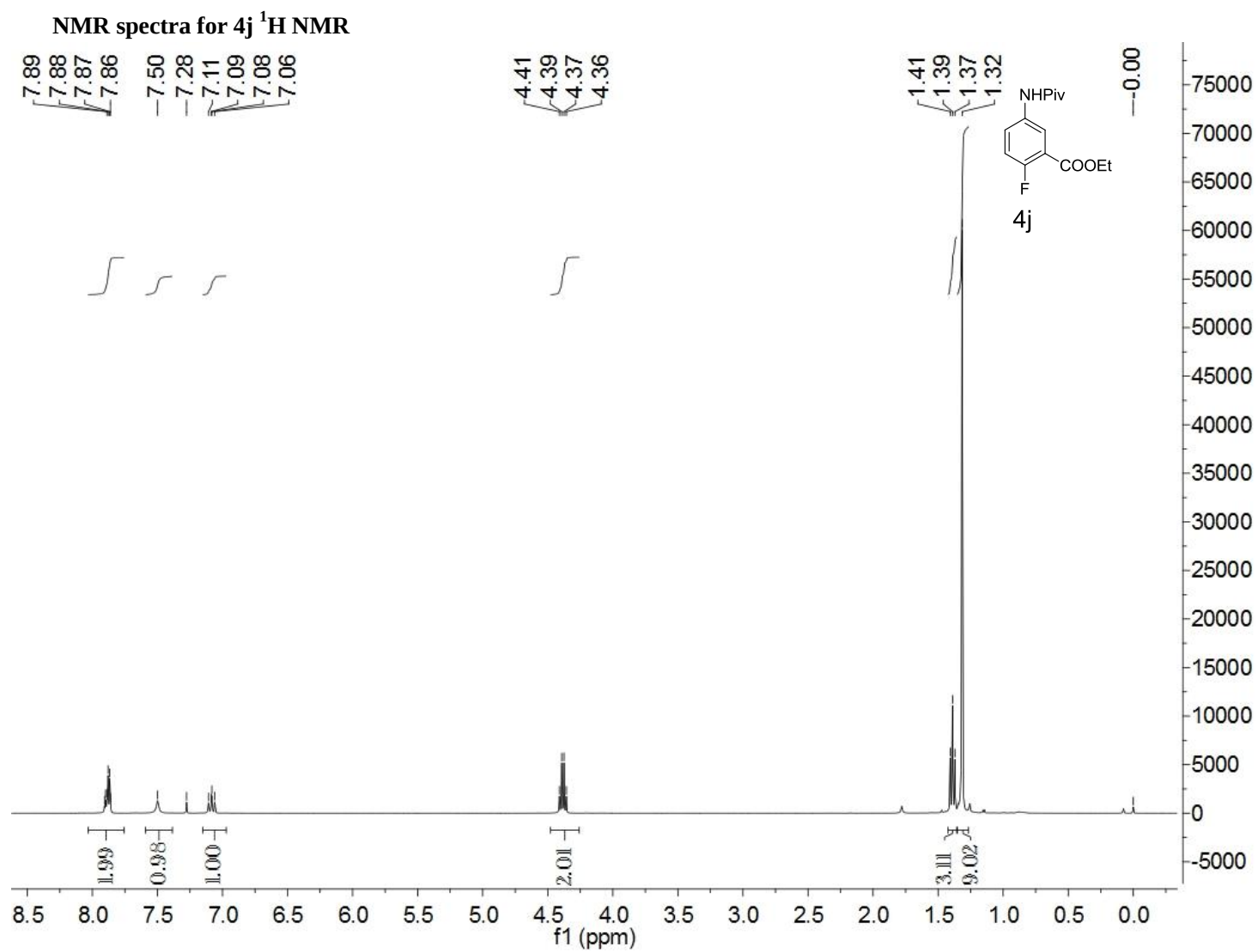


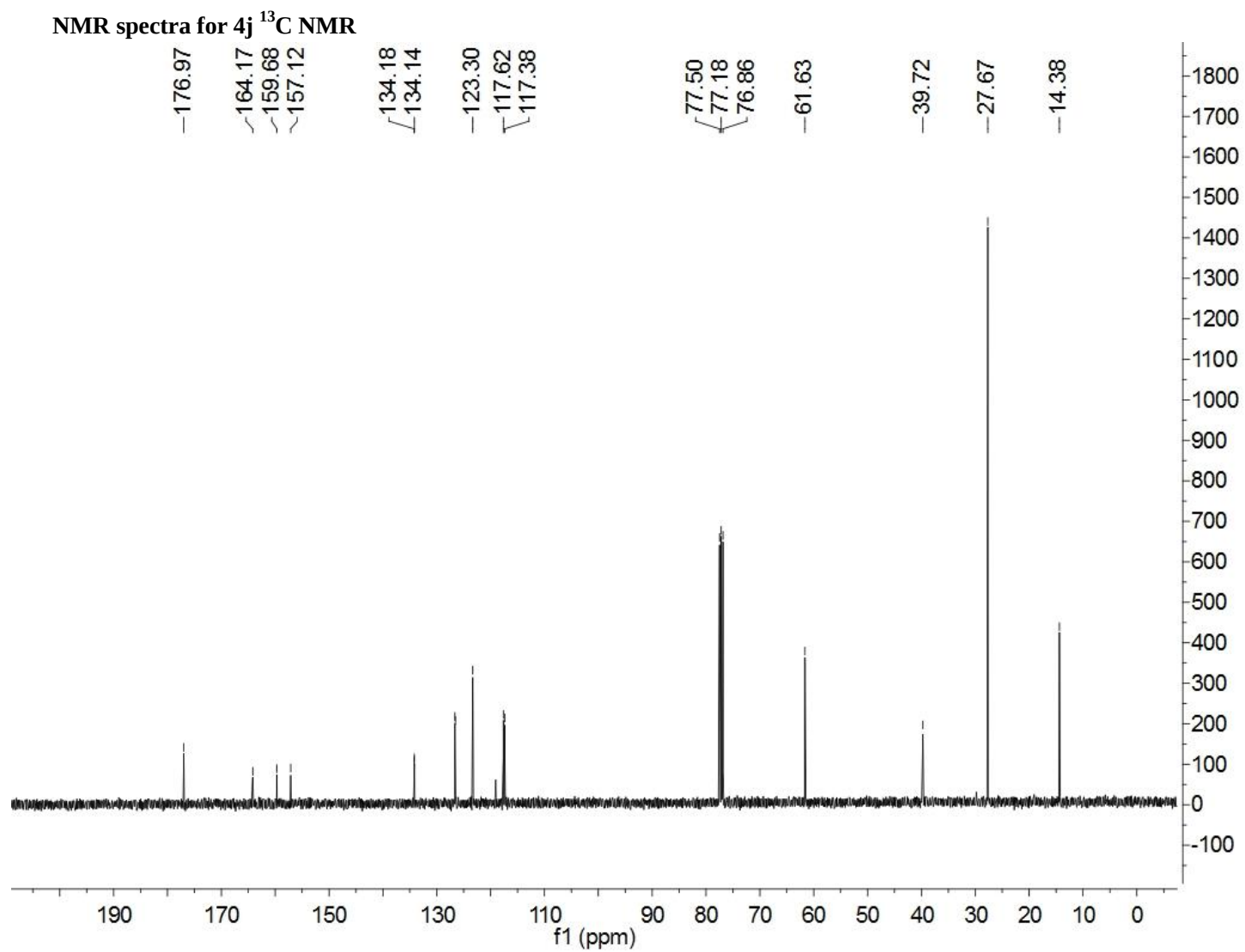
NMR spectra for 4i <sup>13</sup>C NMR



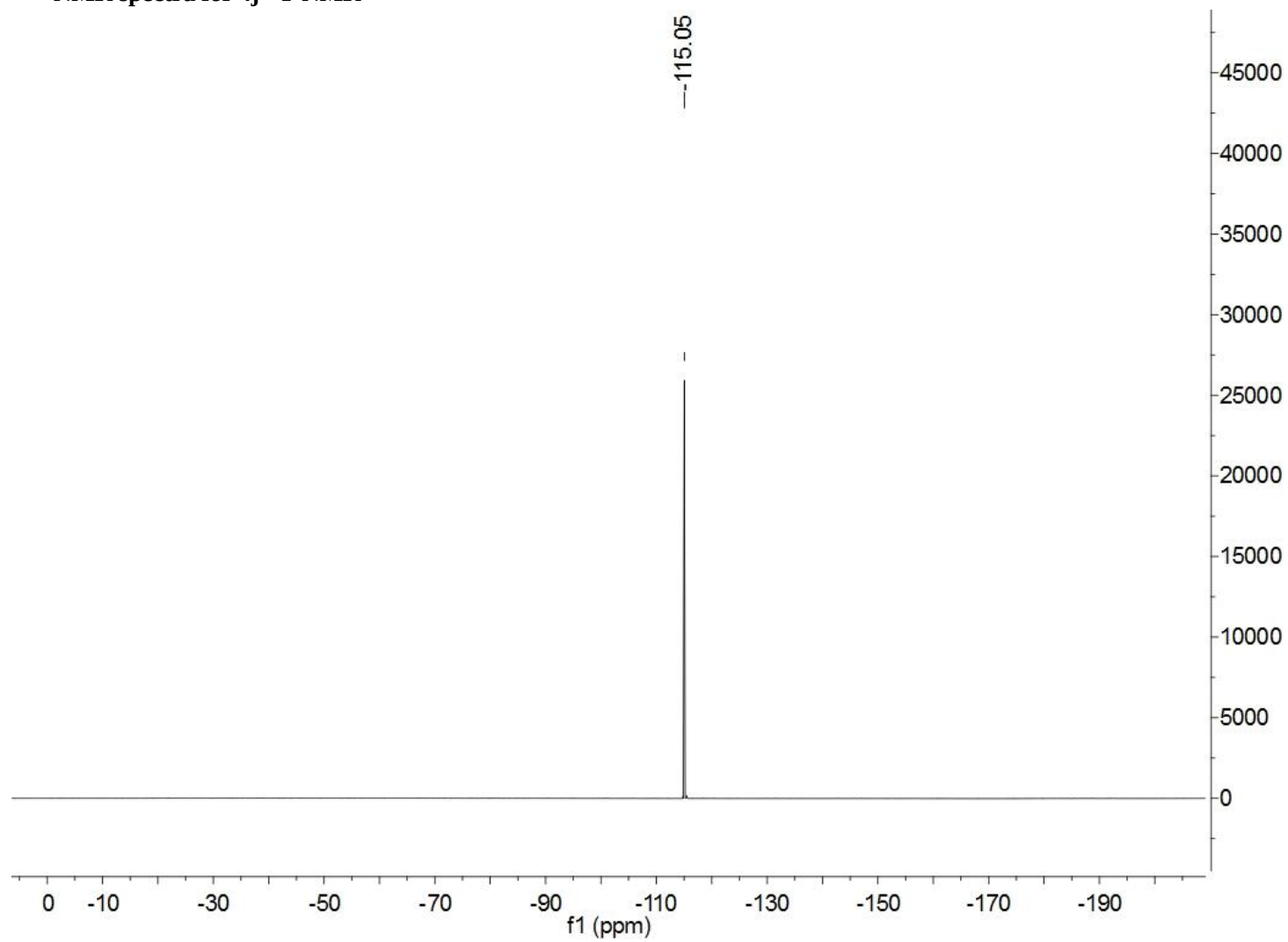
NMR spectra for 4i  $^{19}\text{F}$  NMR



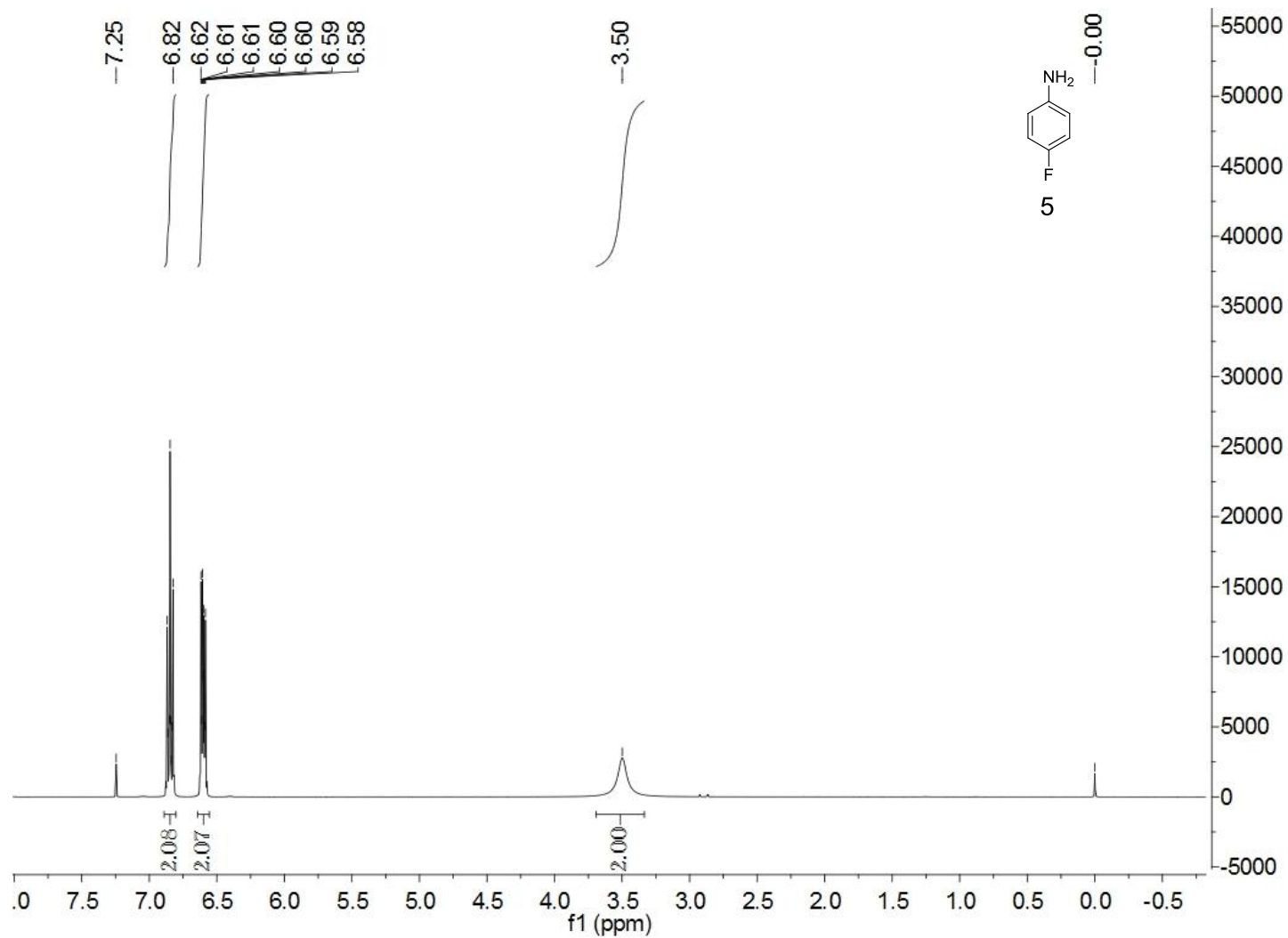




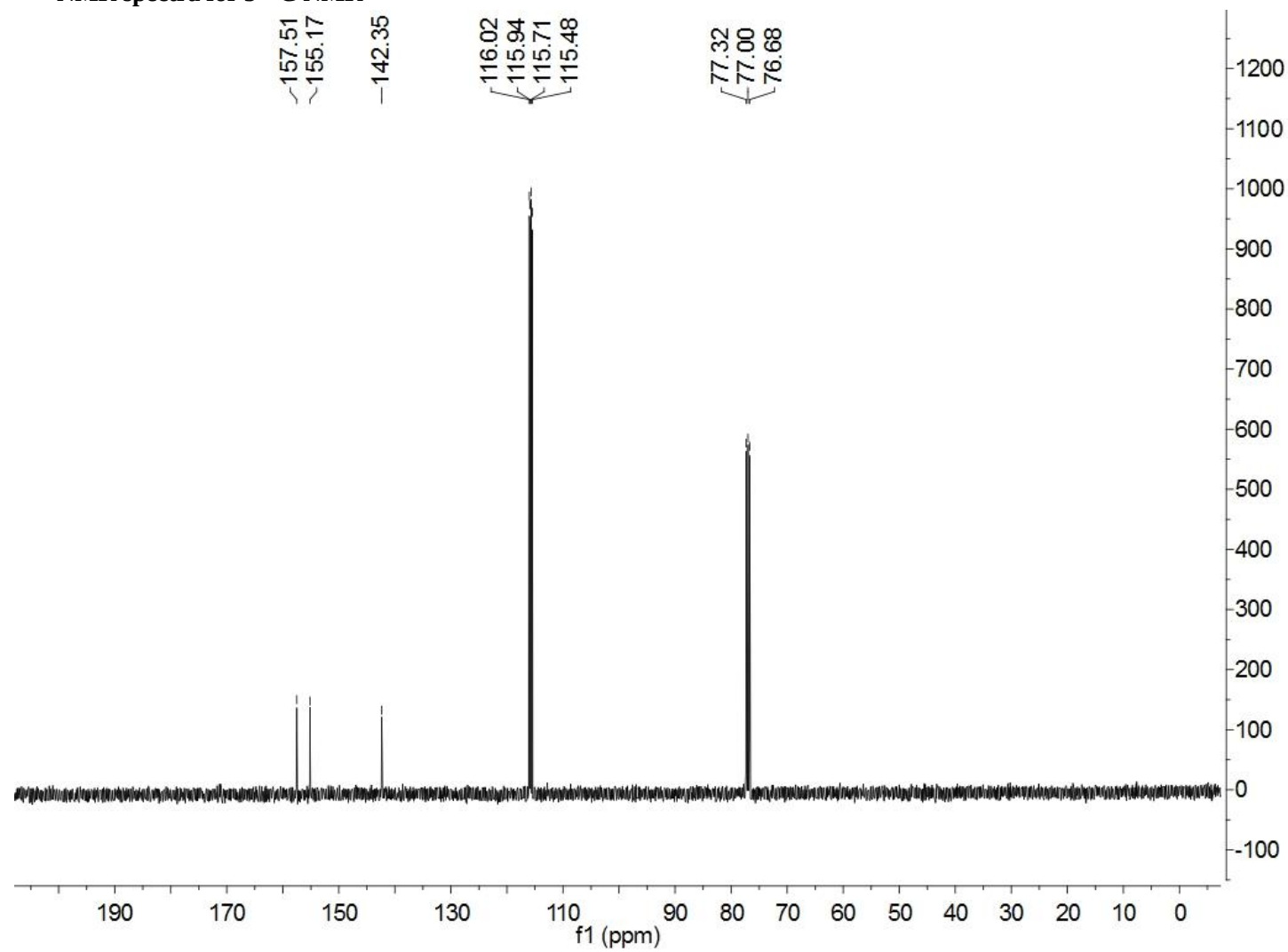
NMR spectra for 4j  $^{19}\text{F}$  NMR



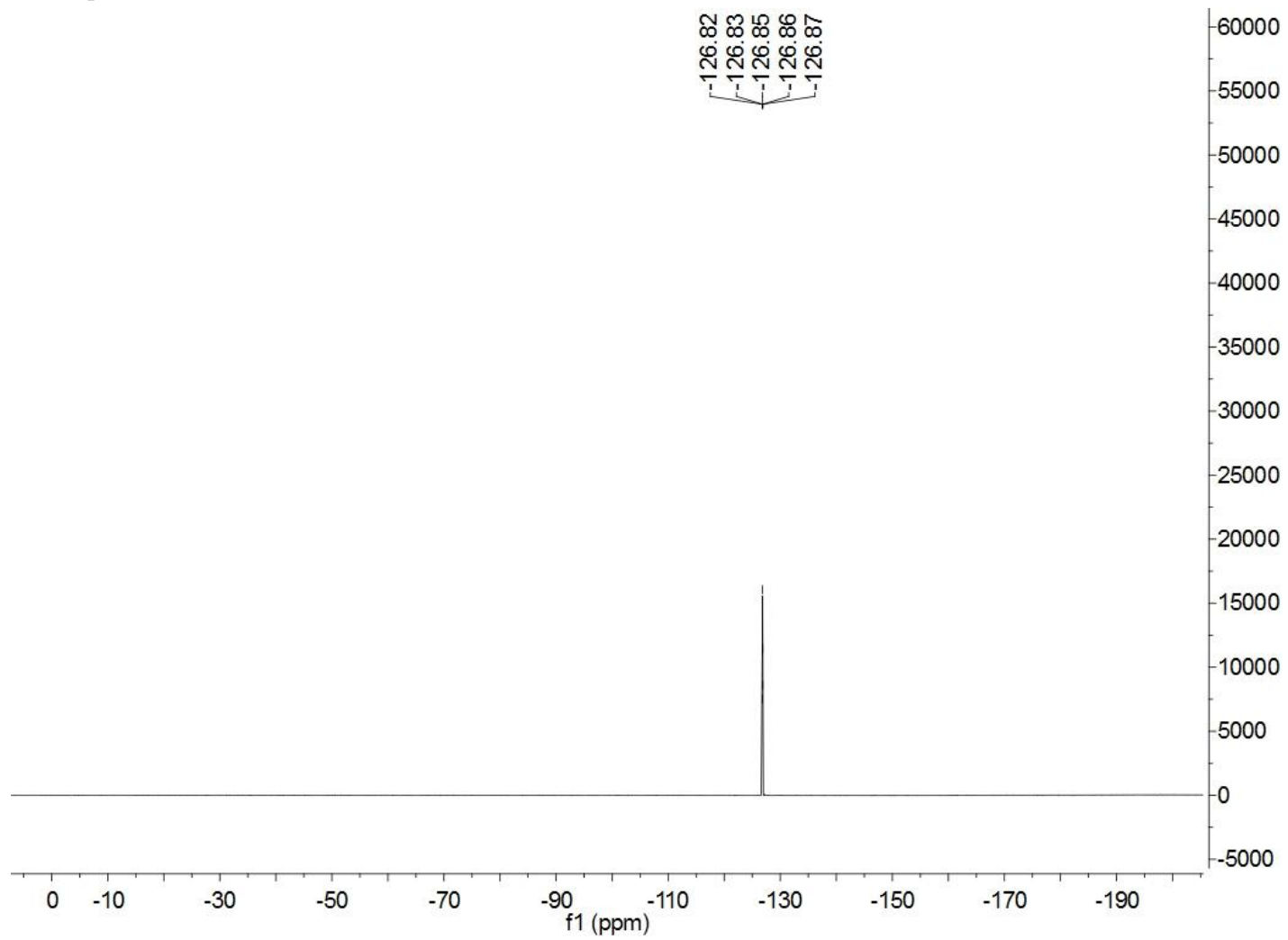
NMR spectra for 5  $^1\text{H}$  NMR



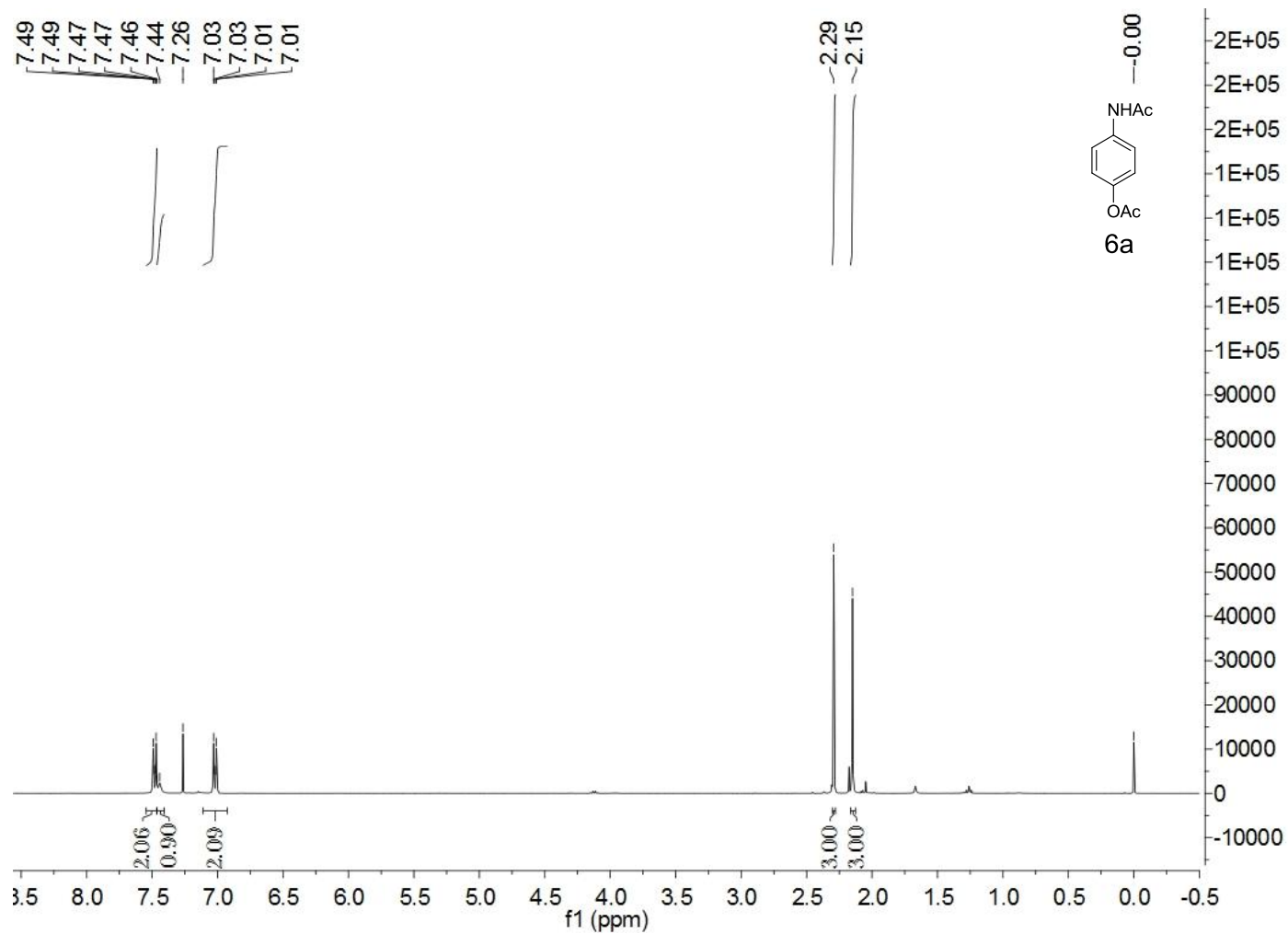
NMR spectra for 5  $^{13}\text{C}$  NMR



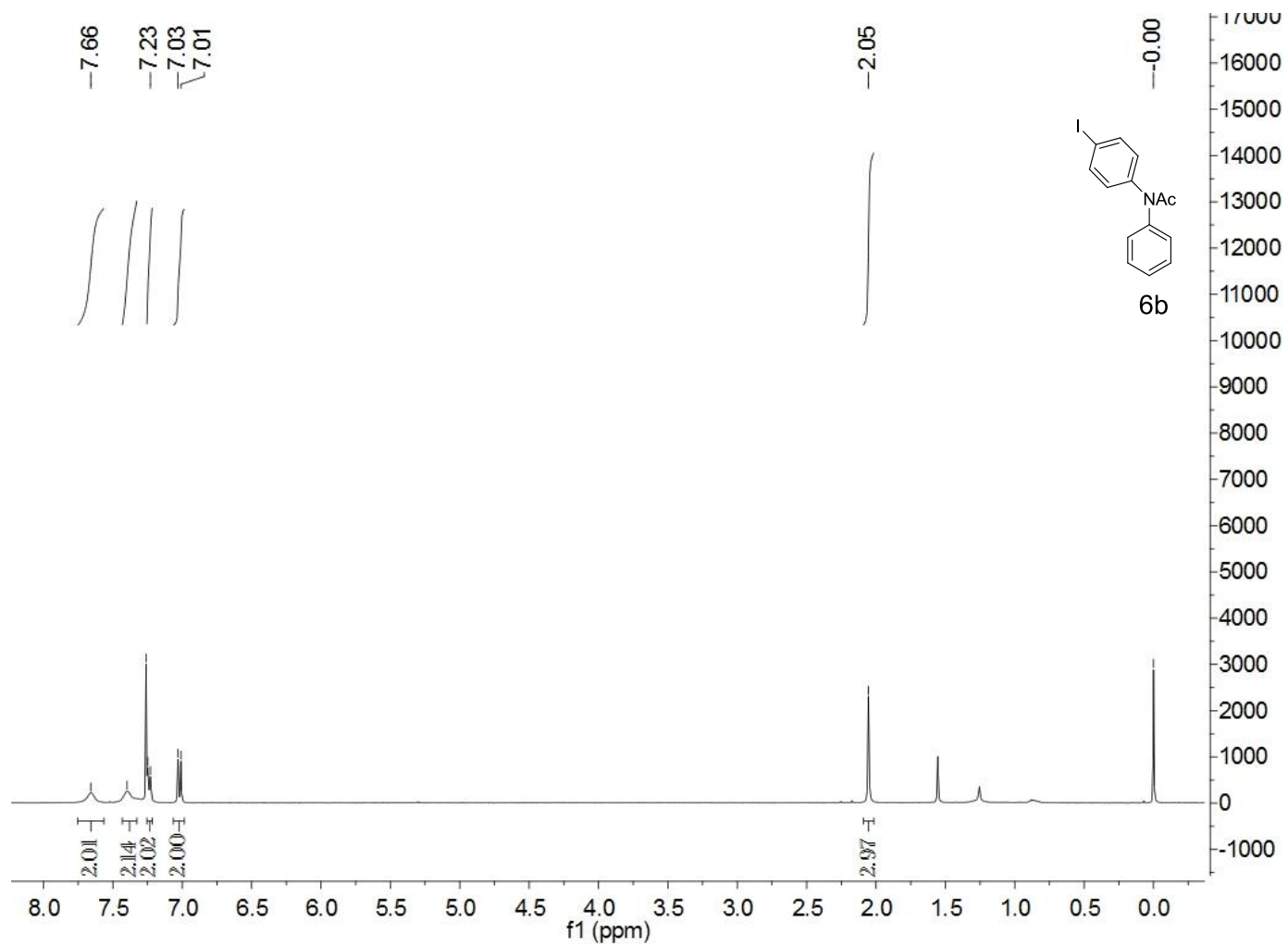
NMR spectra for 5  $^{19}\text{F}$  NMR



NMR spectra for 6a  $^1\text{H}$  NMR



NMR spectra for 6b  $^1\text{H}$  NMR



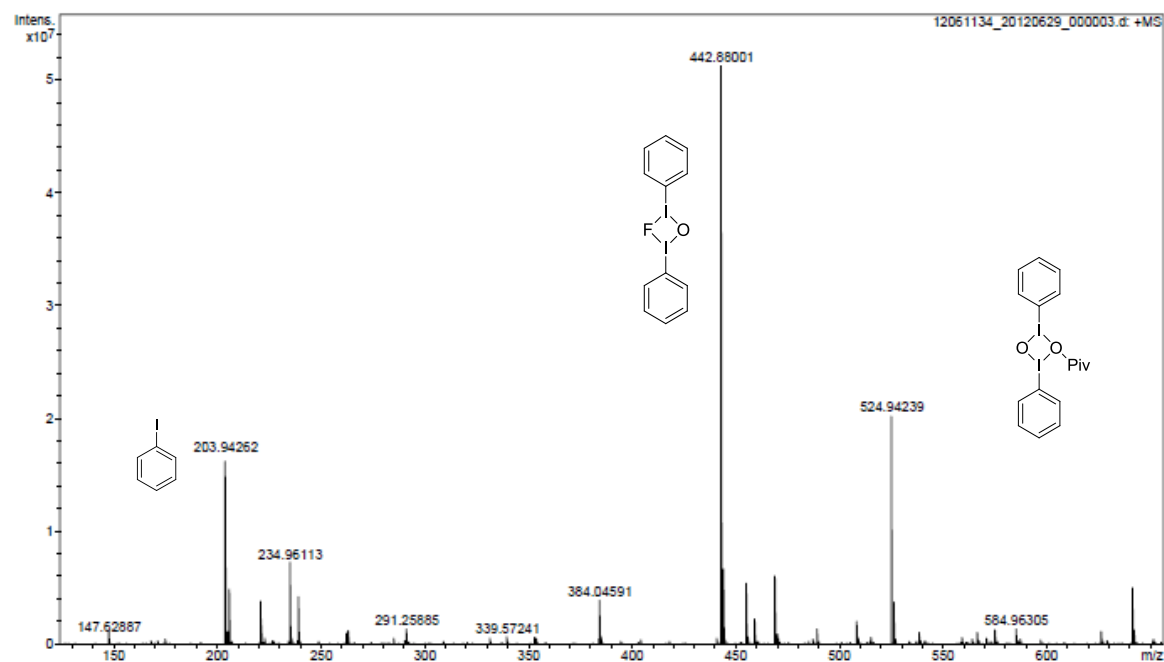
### HRMS spectra of hypervalent iodine activated fluorine reagent intermediate

## Peking University Mass Spectrometry Analysis Report

### Analysis Info

|               |                            |
|---------------|----------------------------|
| Analysis Name | 12061134_20120629_000003.d |
| Sample        | tt-pidp                    |
| Comment       | ESI Positive               |

|                  |                      |
|------------------|----------------------|
| Acquisition Date | 6/29/2012 2:17:40 PM |
| Instrument       | Bruker Apex IV FTMS  |
| Operator         | Peking University    |



Bruker Compass DataAnalysis 4.0

printed: 6/29/2012 2:26:07 PM

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