

# Innate C–H Trifluoromethylation of Heterocycles

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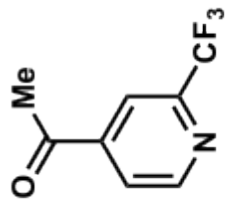
## SUPPORTING INFORMATION – SPECTRA

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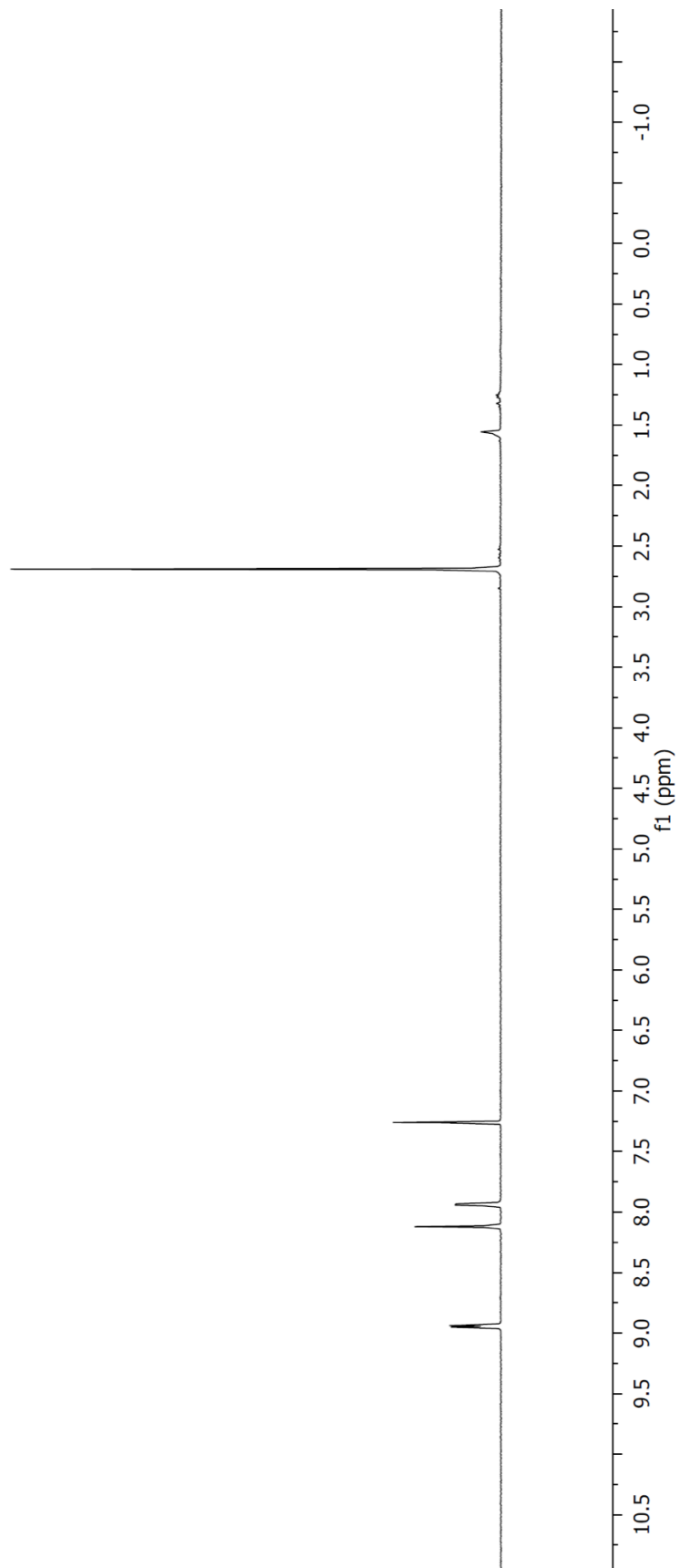
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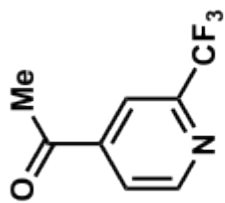
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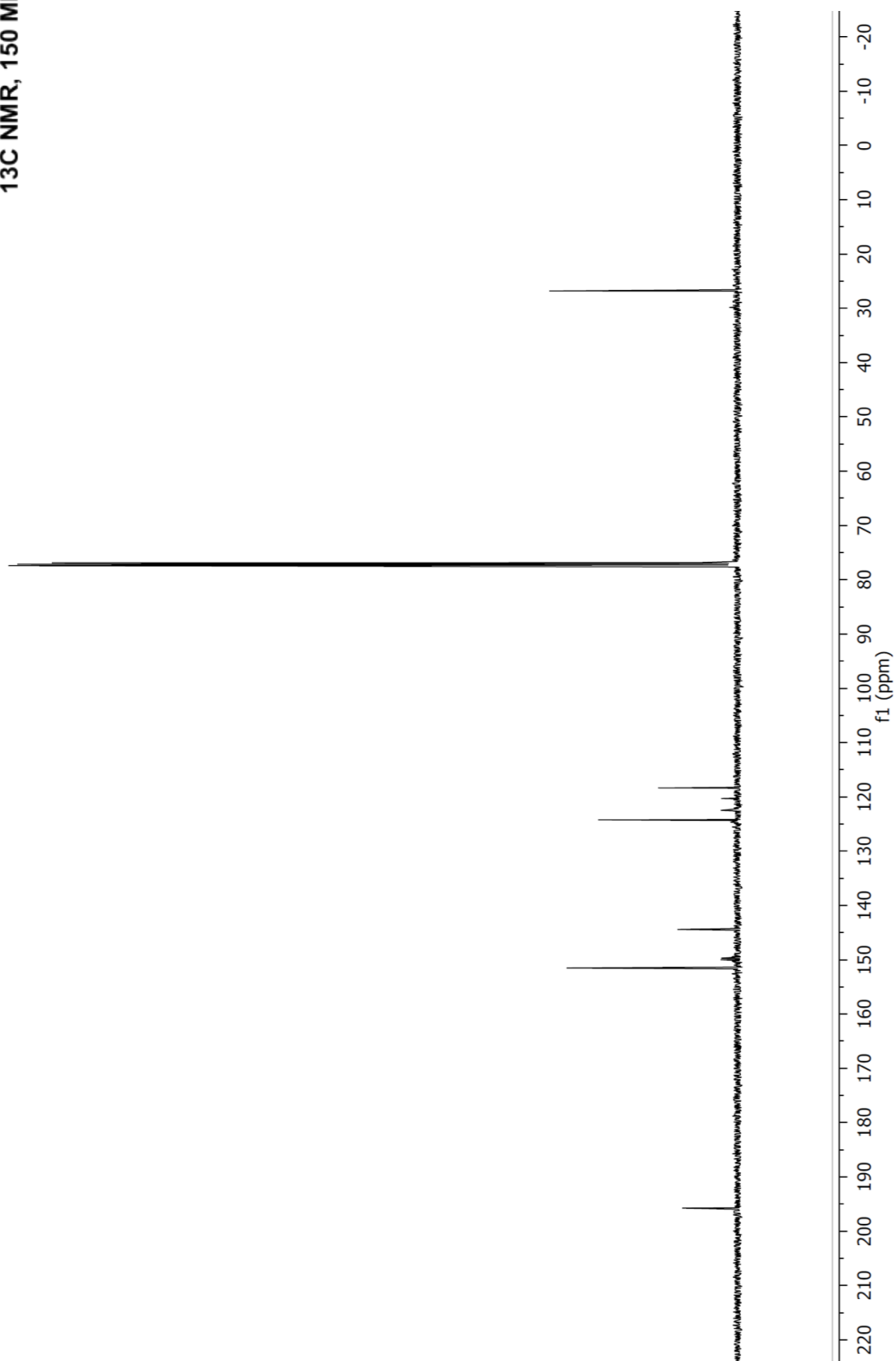


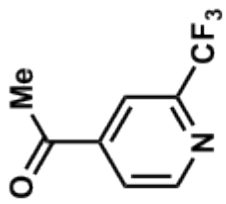
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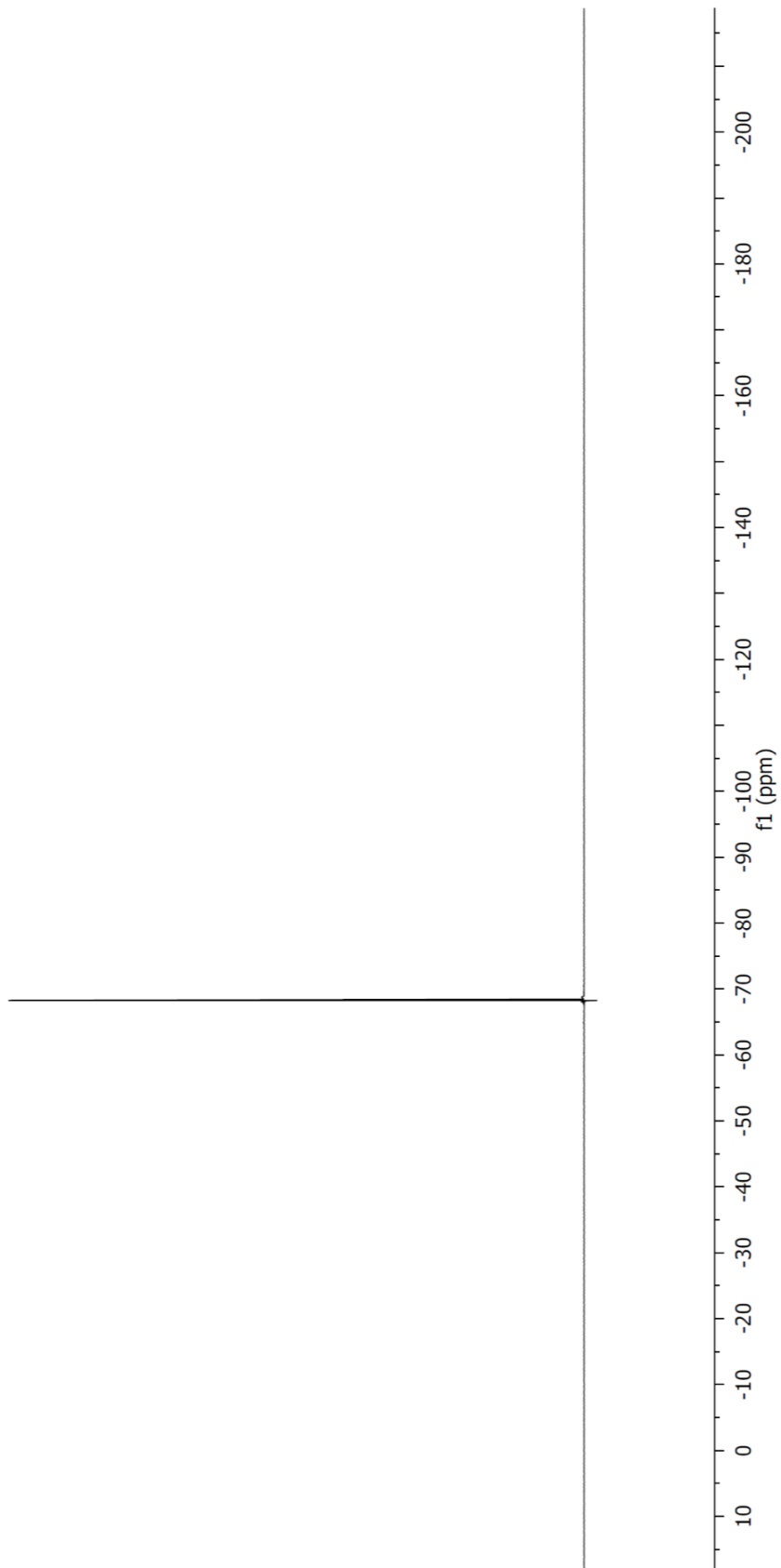


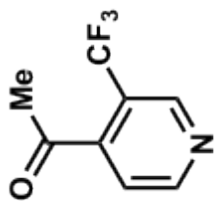
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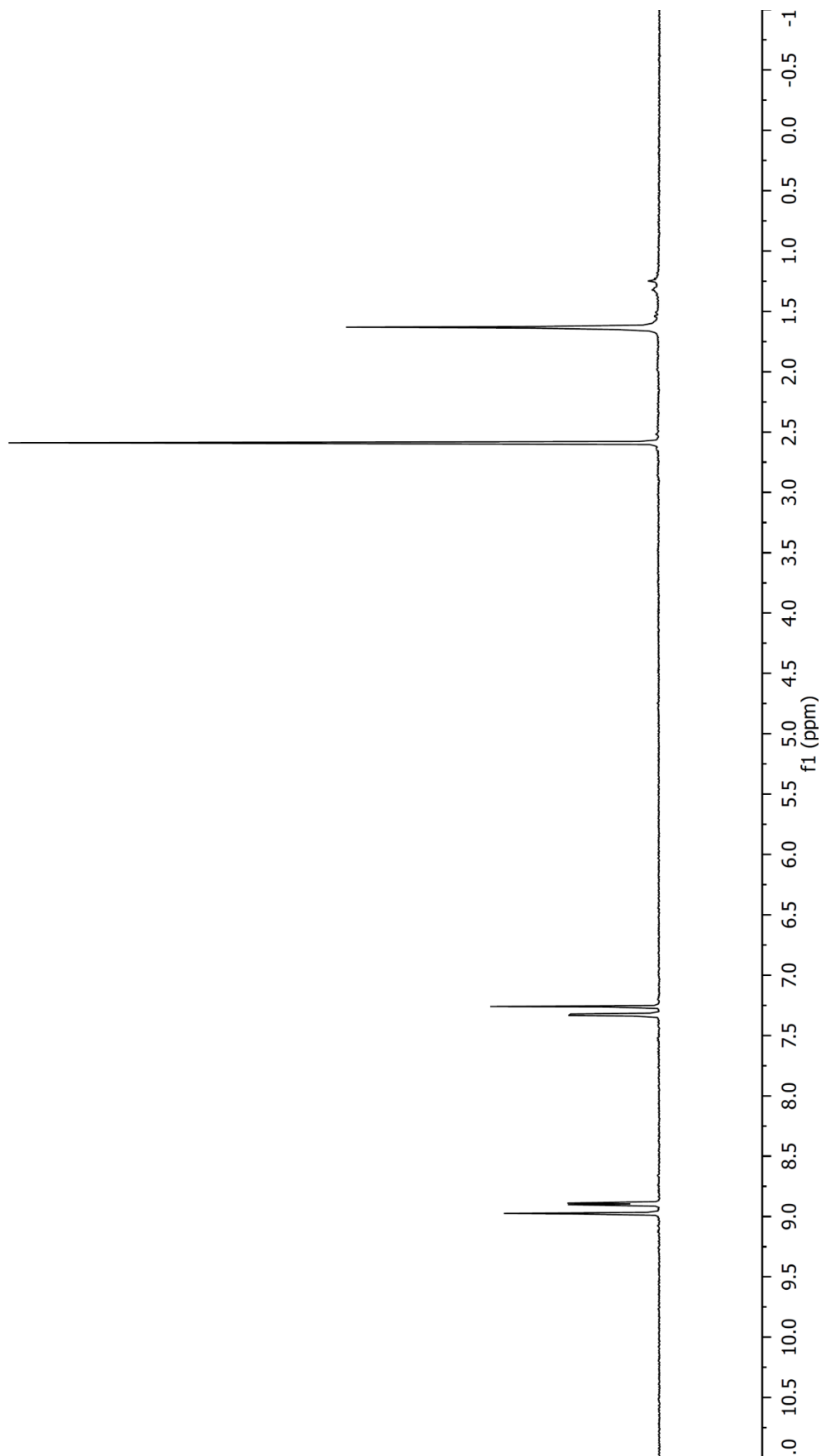


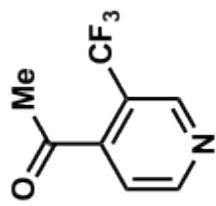
Compound 1-C2  
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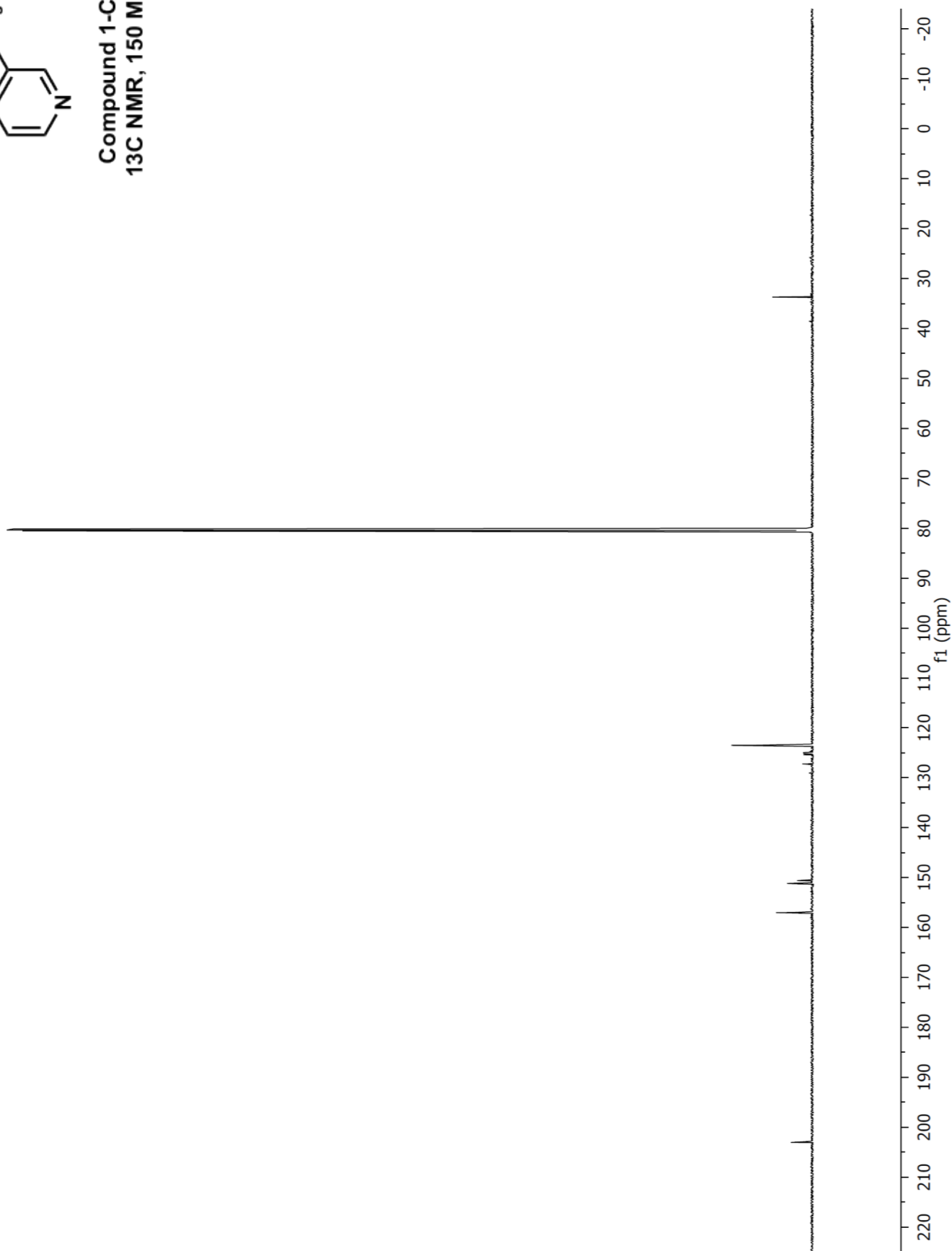


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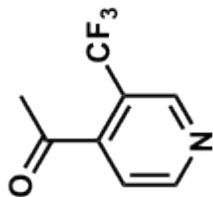




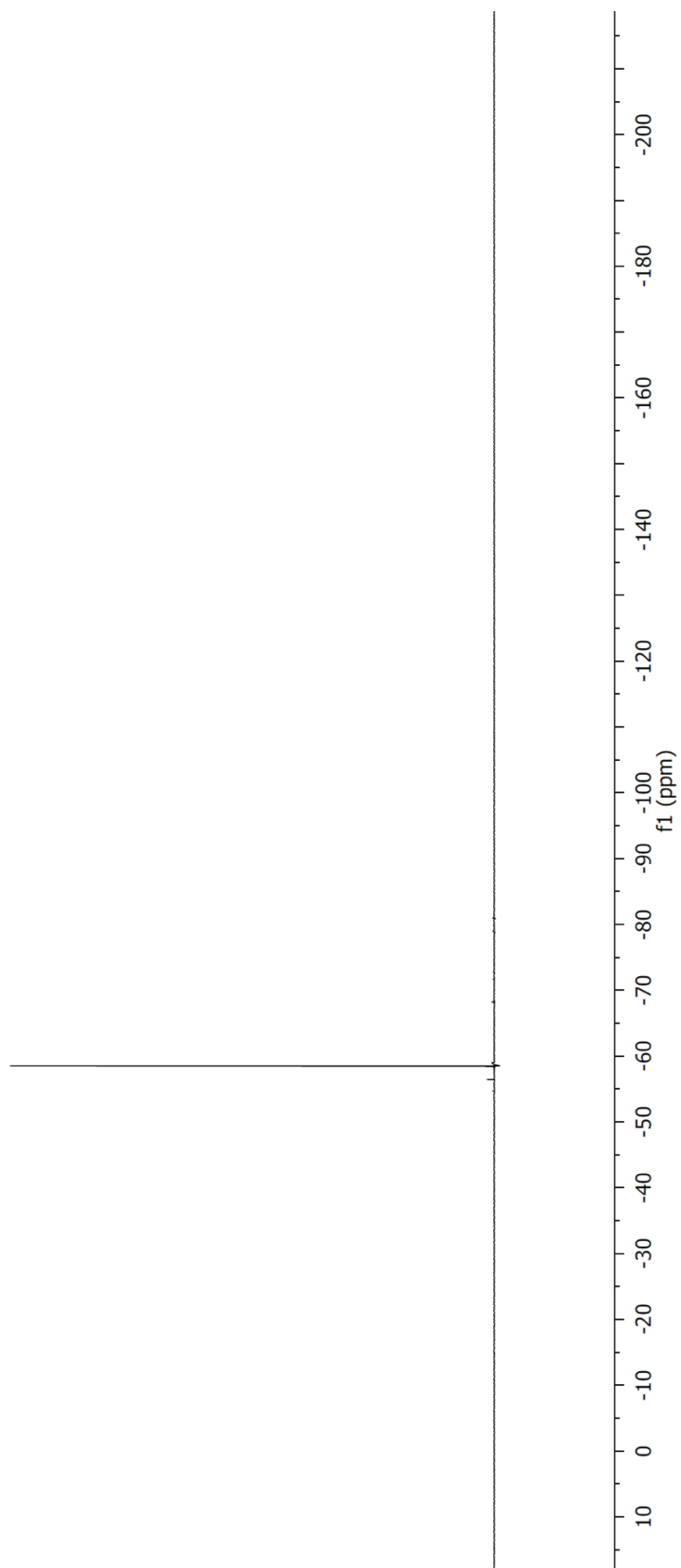
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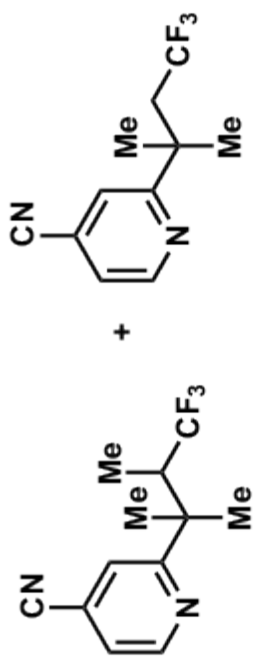




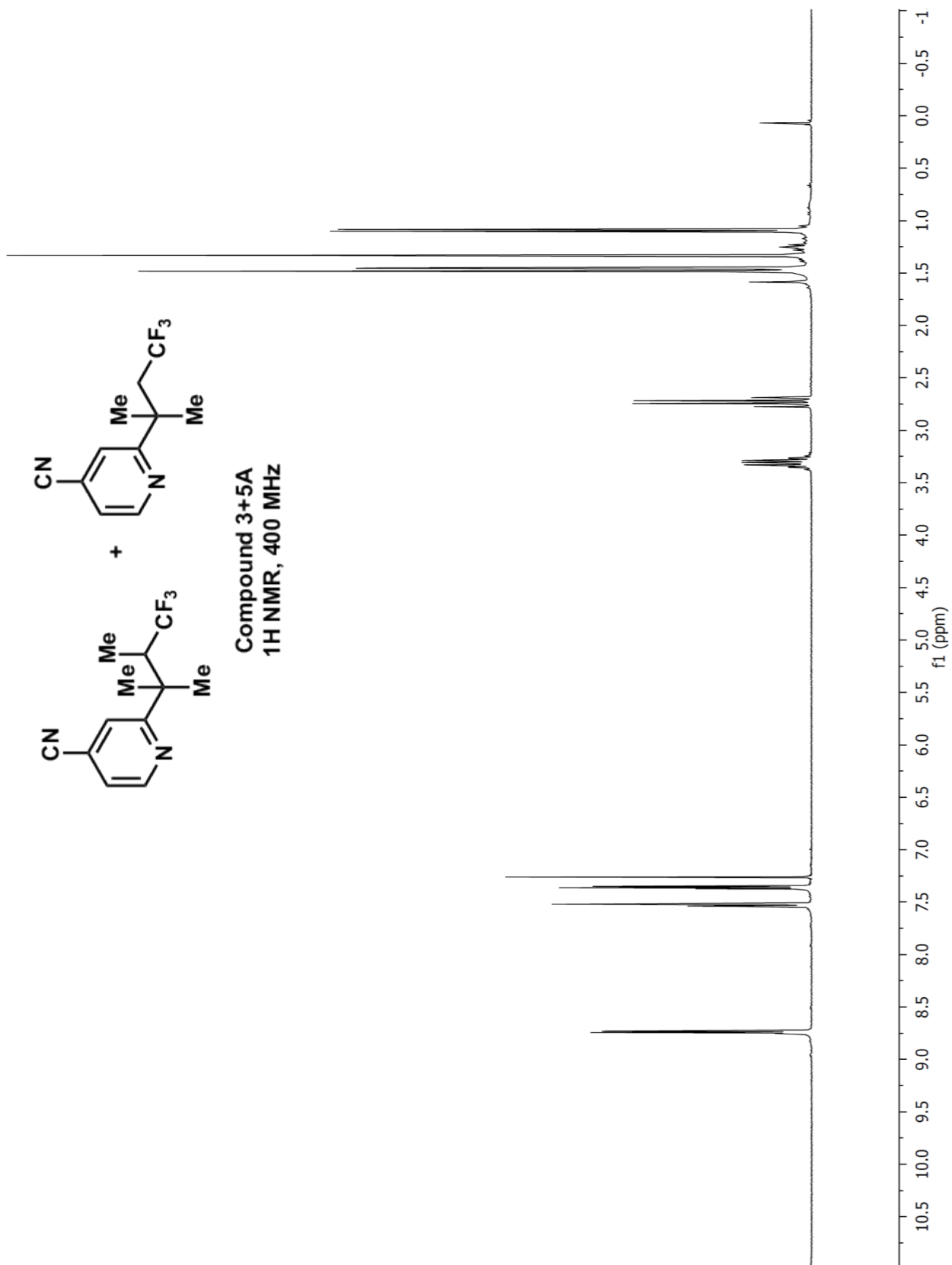


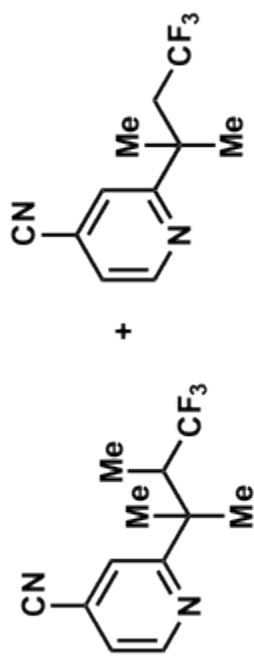
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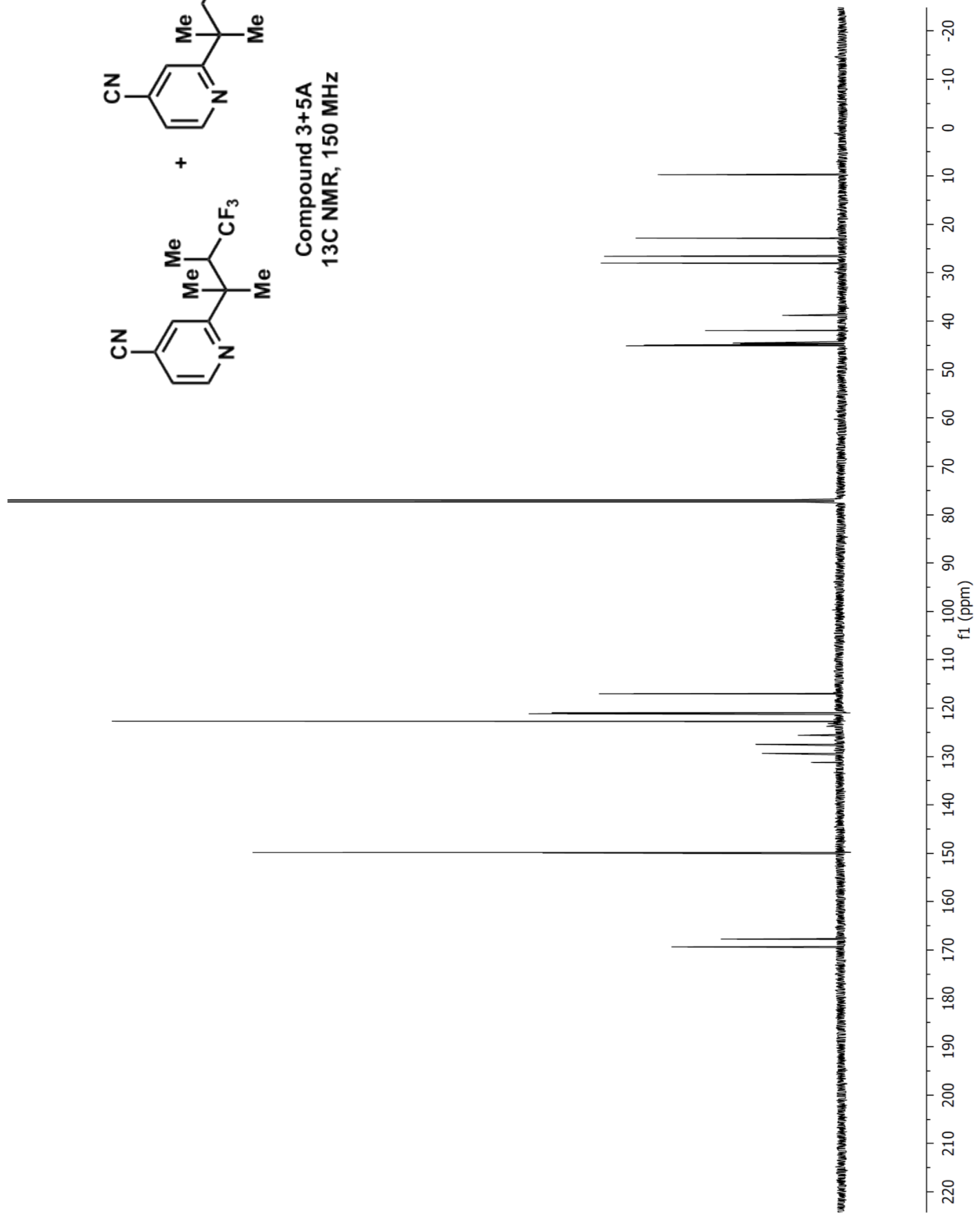


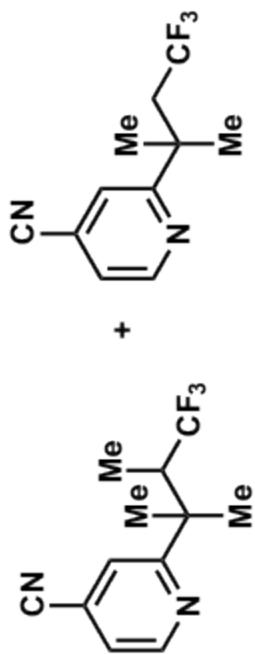
Compound 3+5A  
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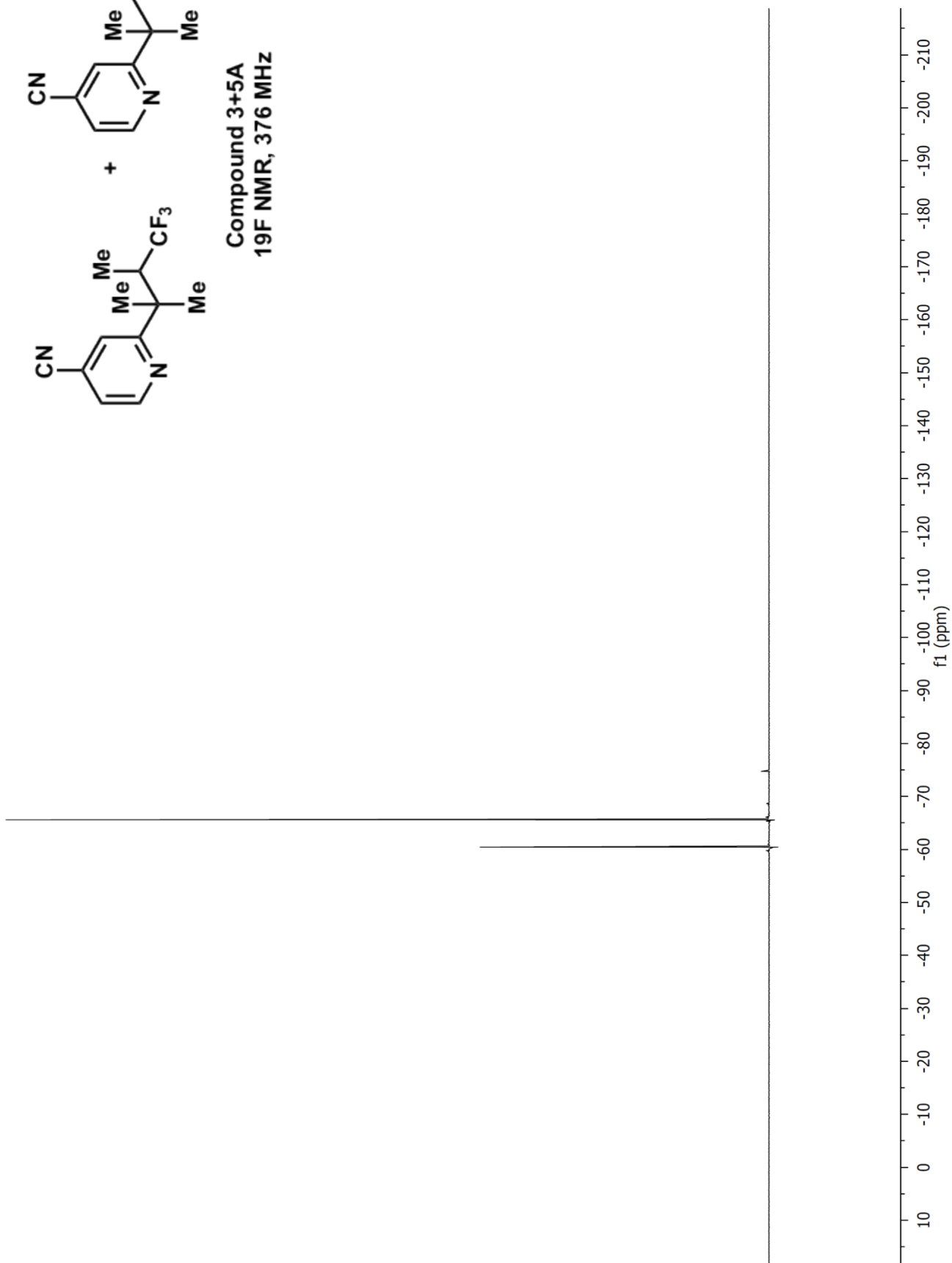


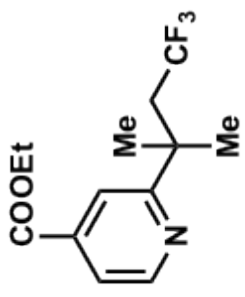
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<sup>13</sup>C NMR, 150 MHz



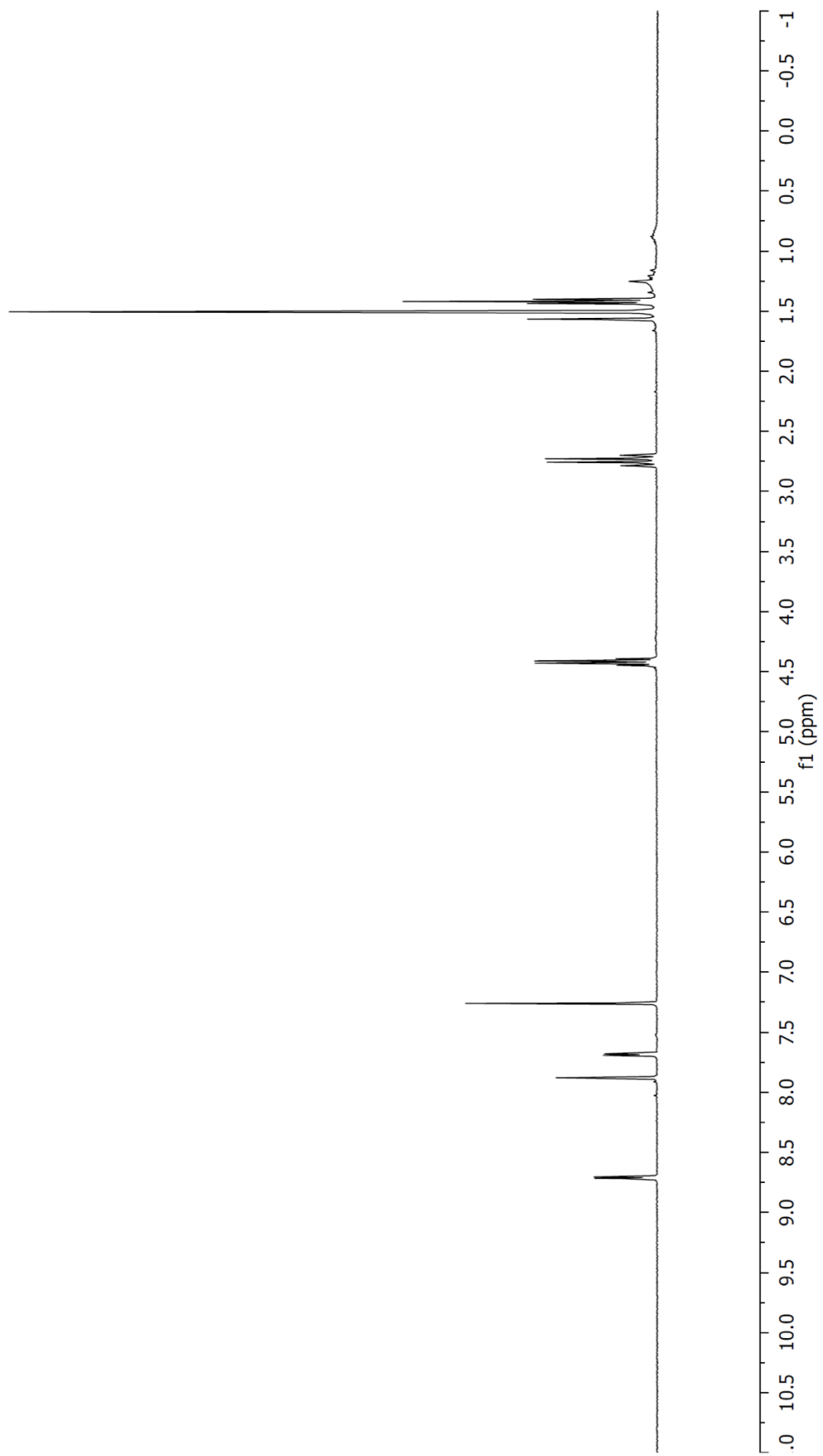


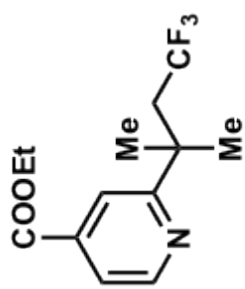
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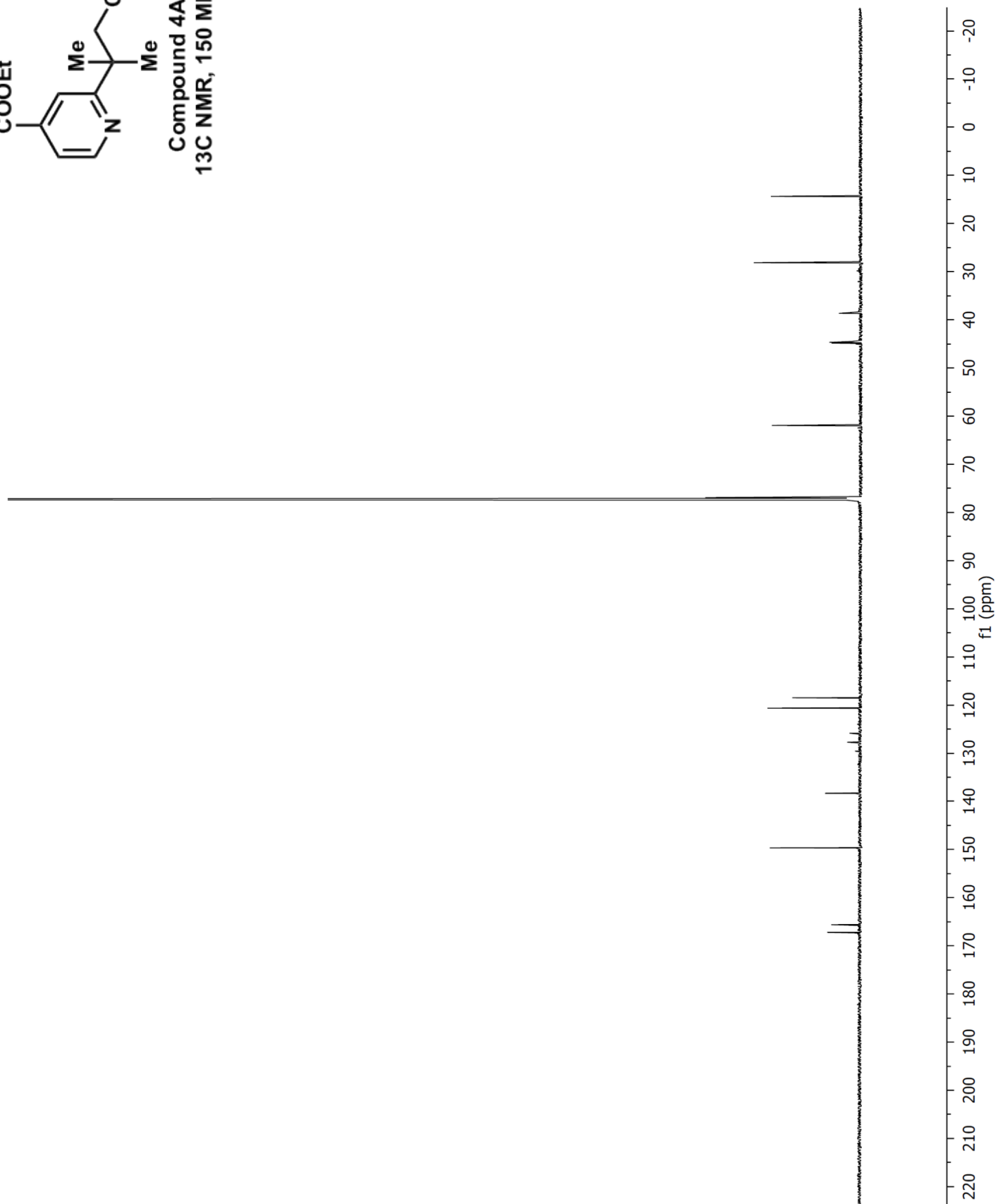


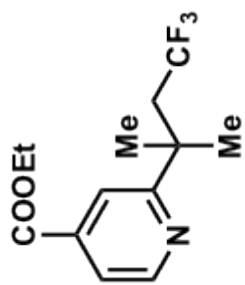
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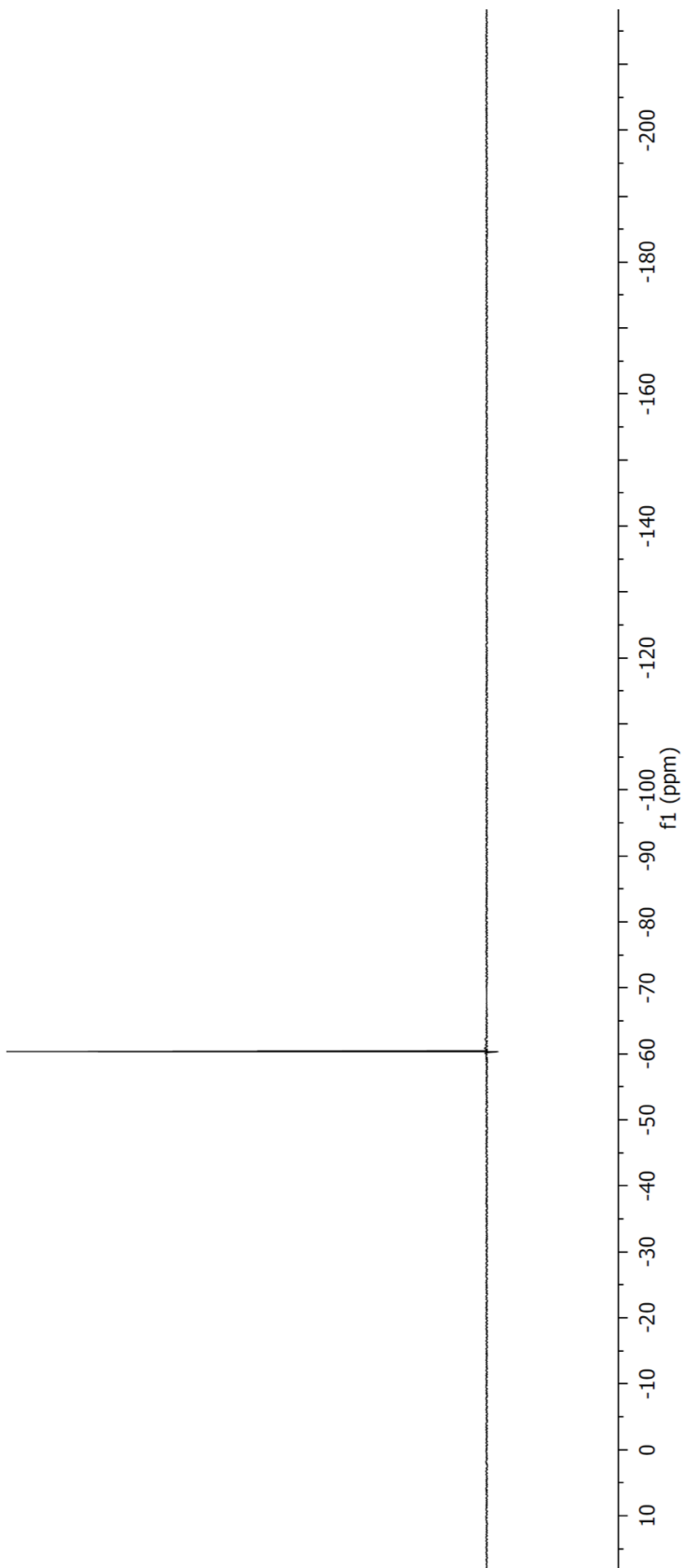


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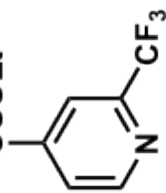




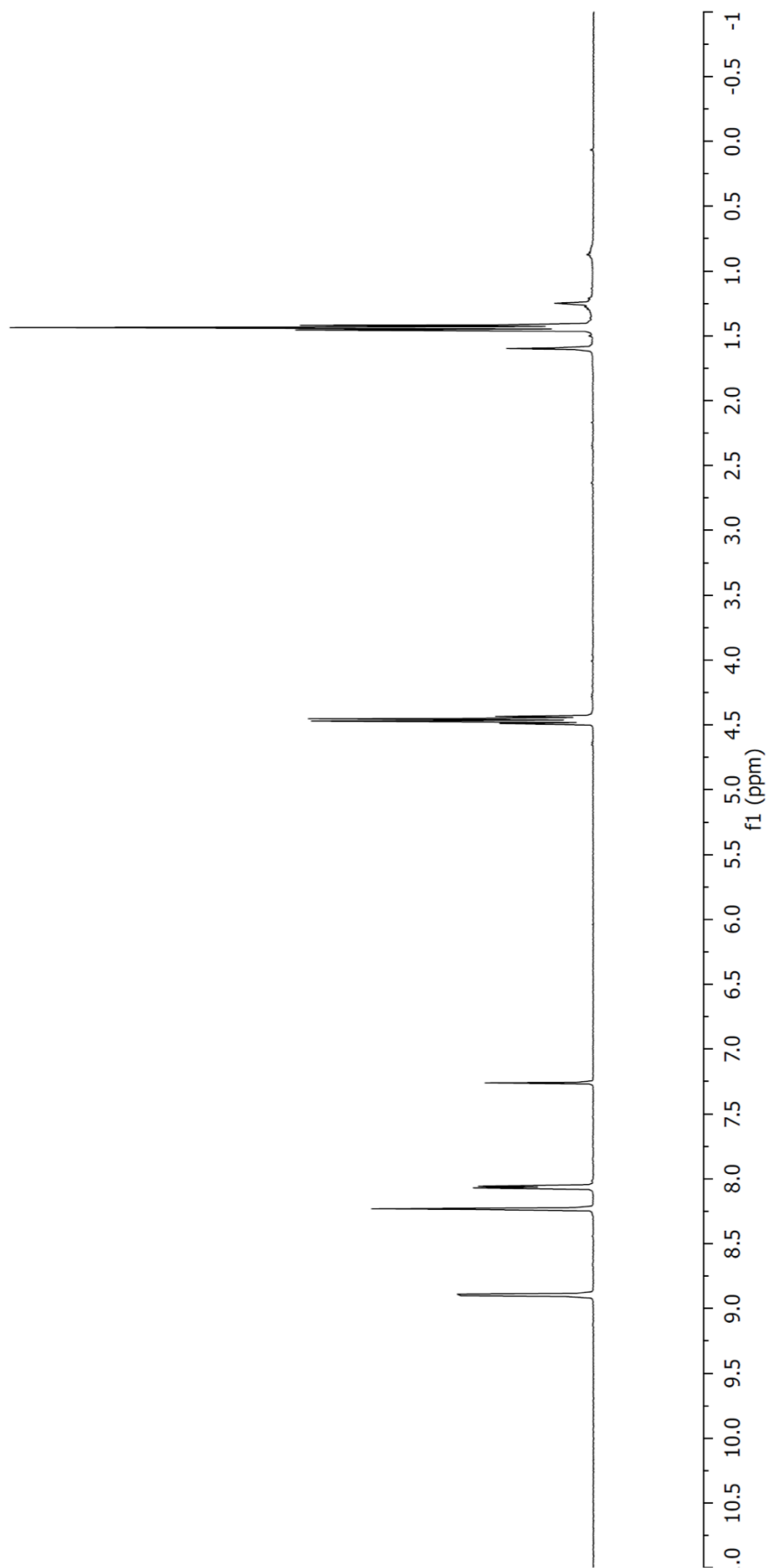
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COOEt

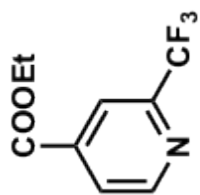


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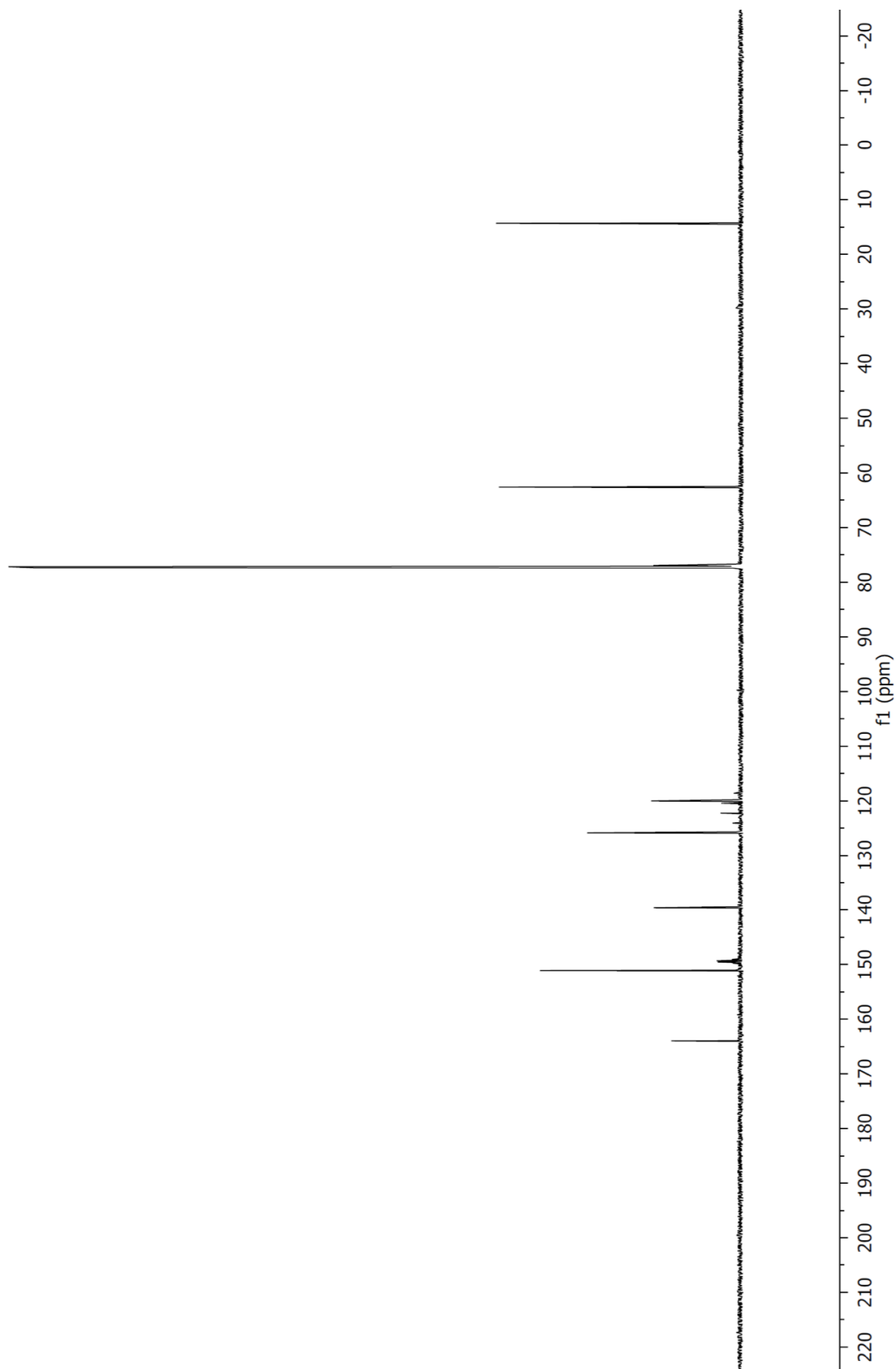




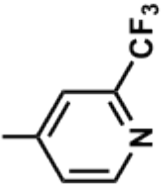
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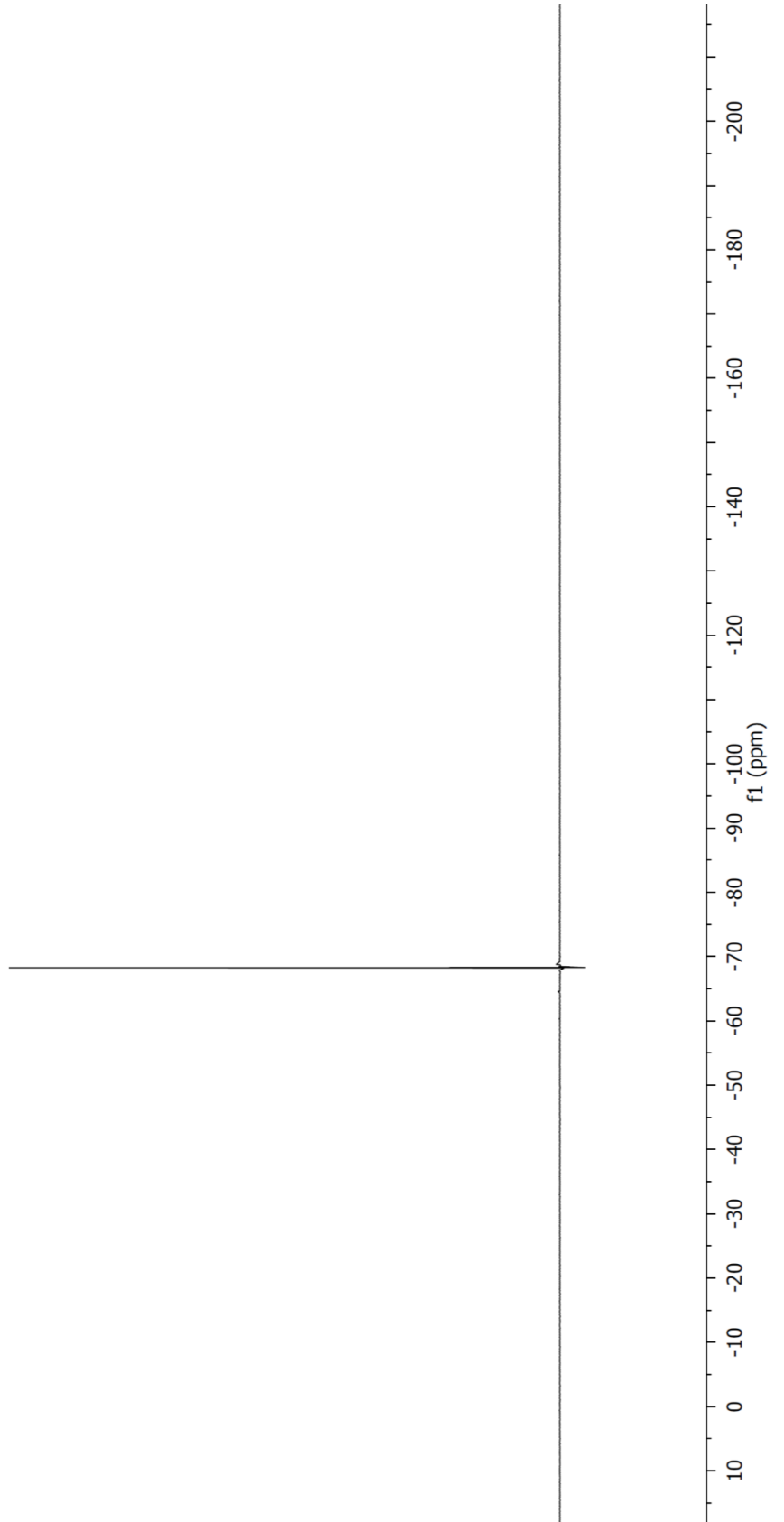
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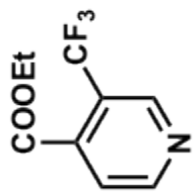


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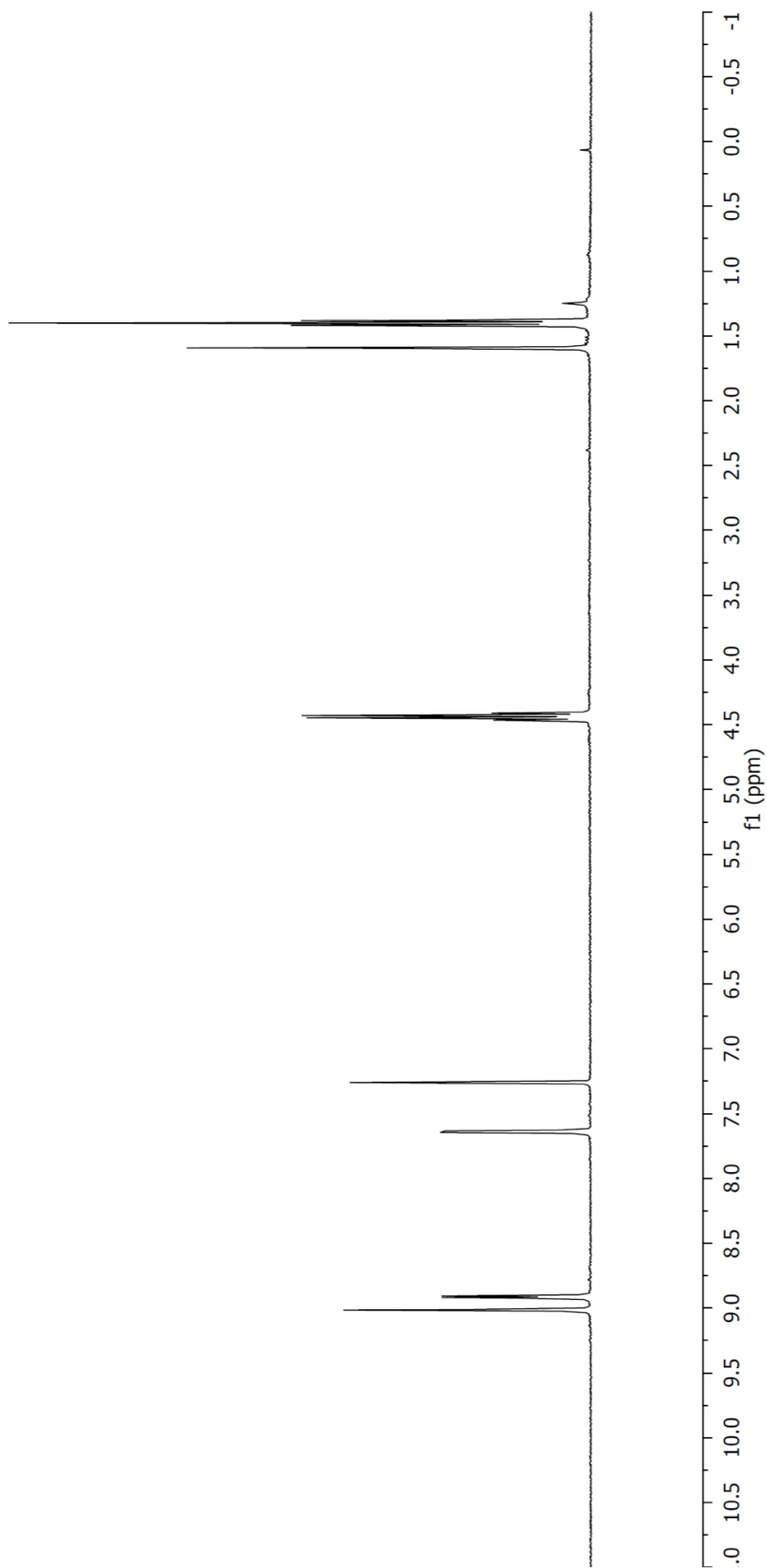


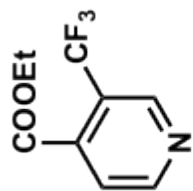
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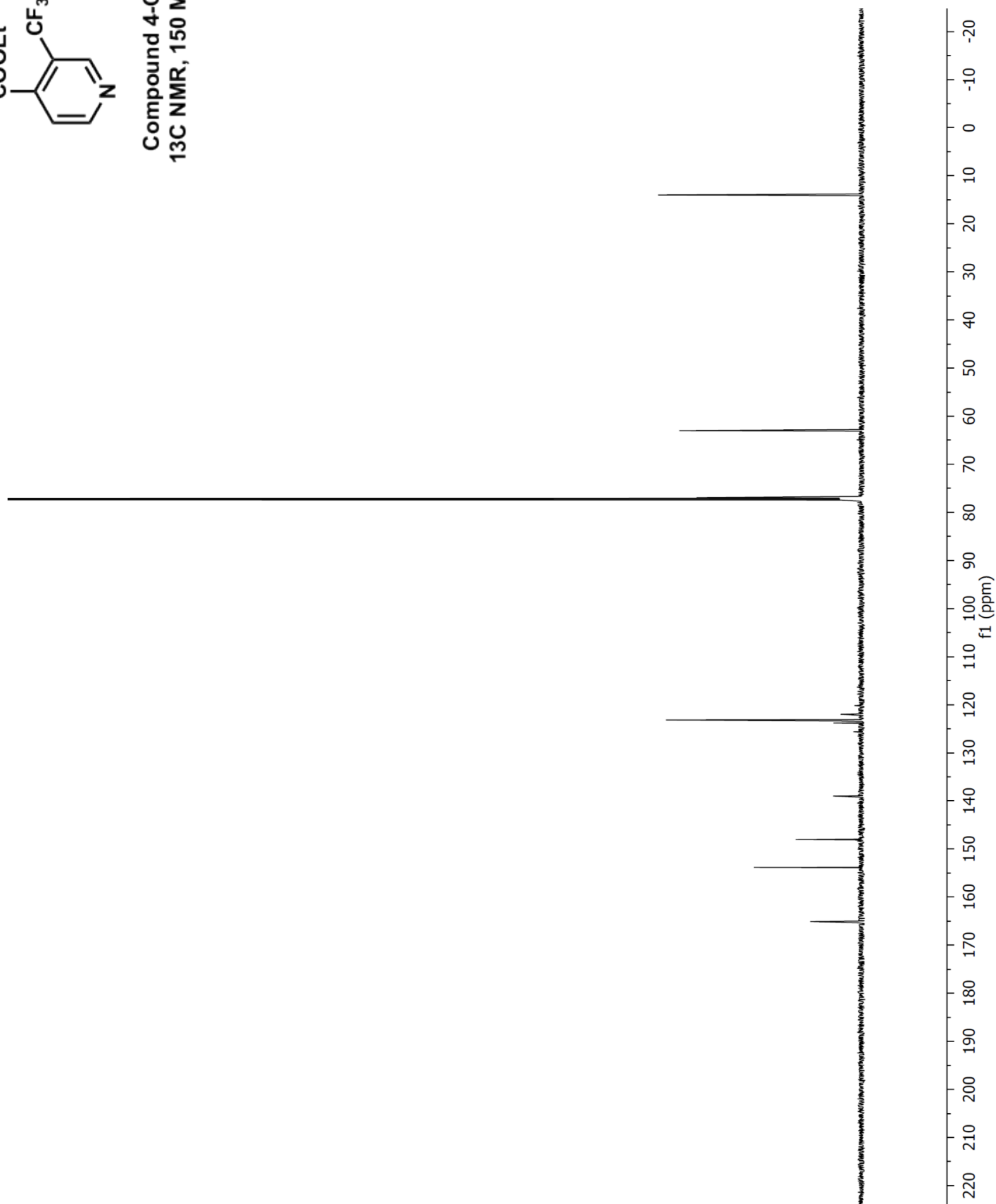


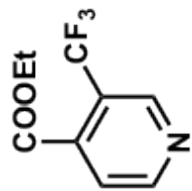
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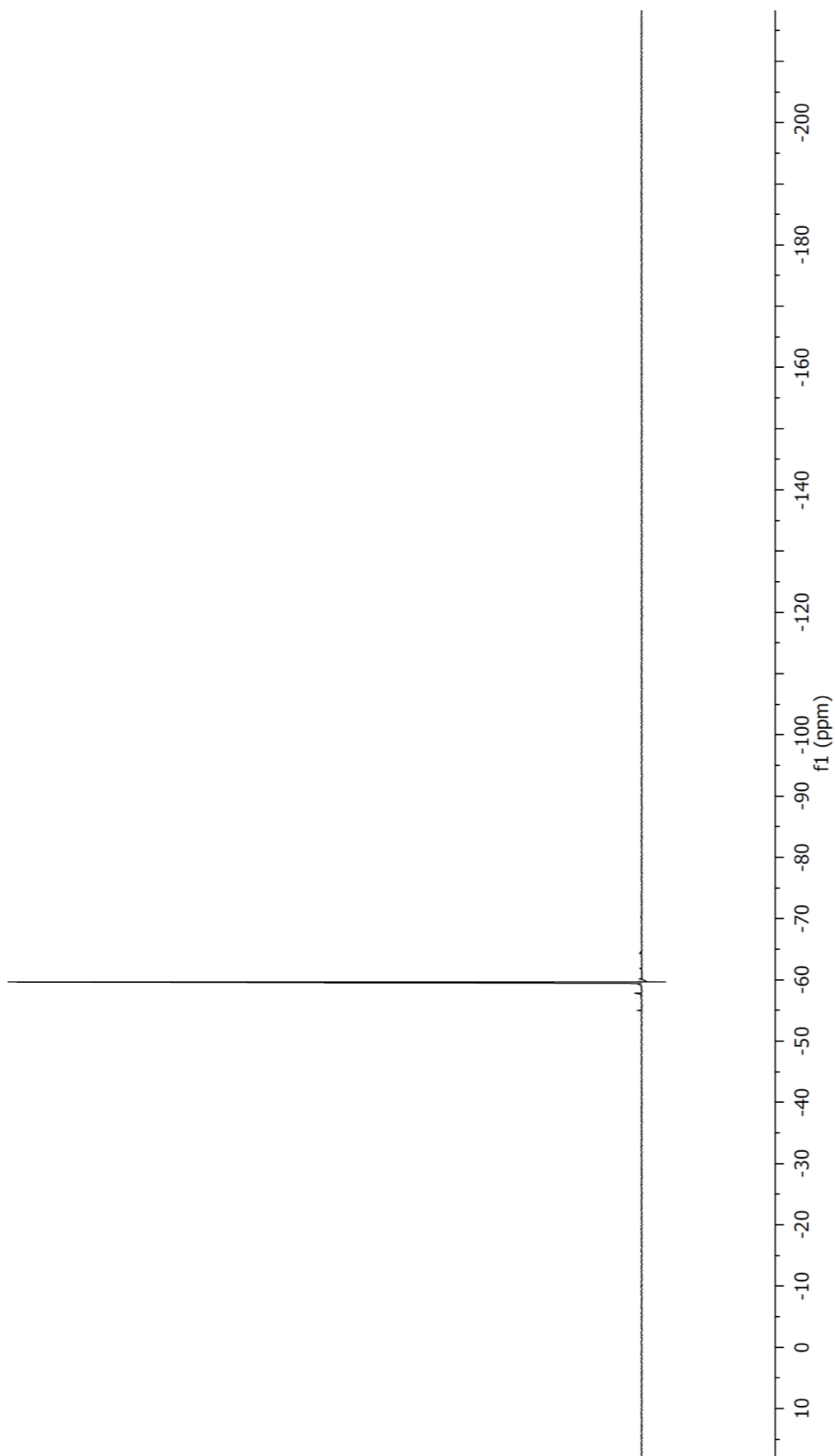


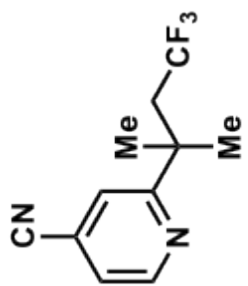
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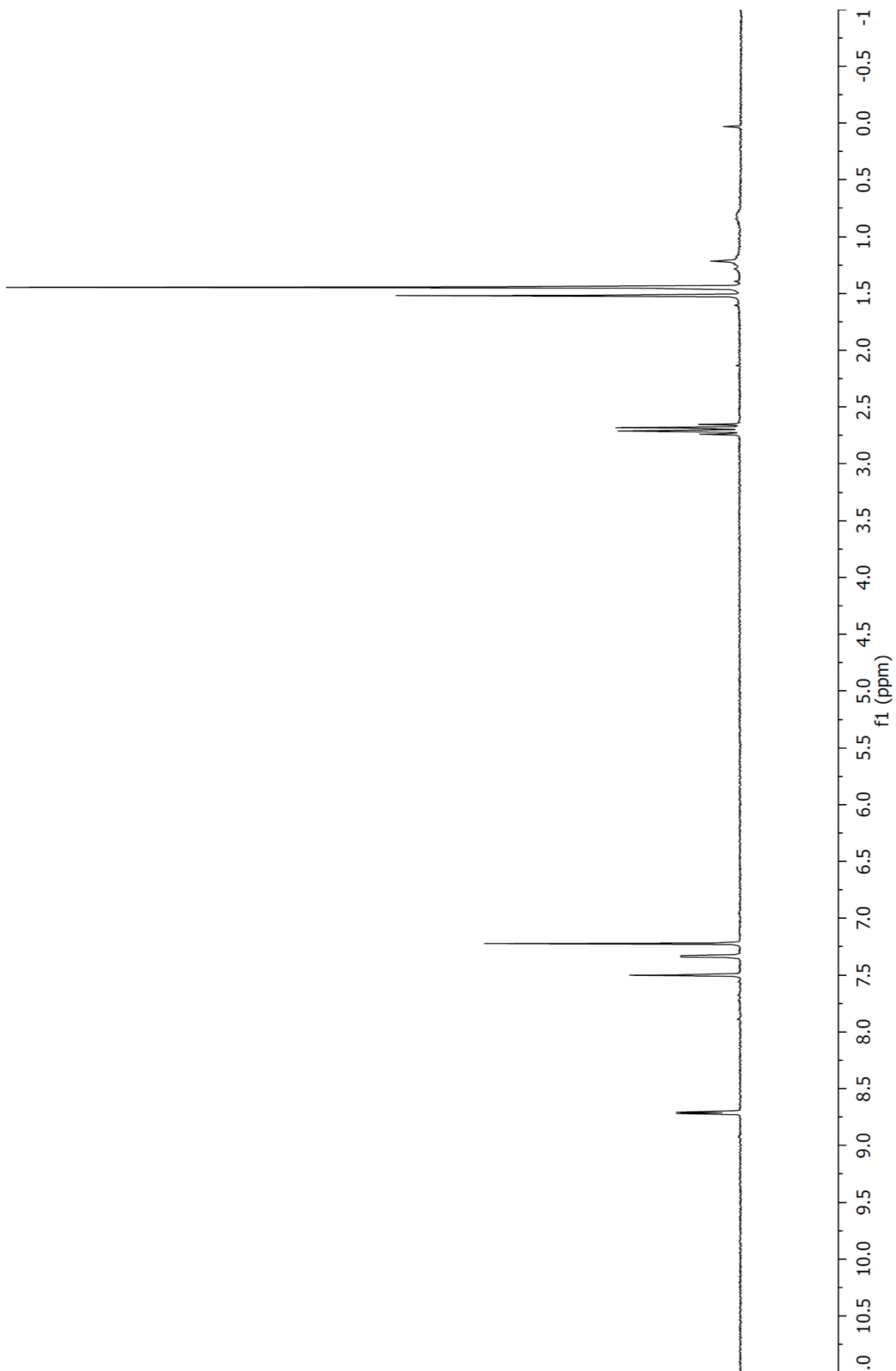


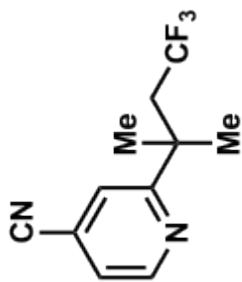
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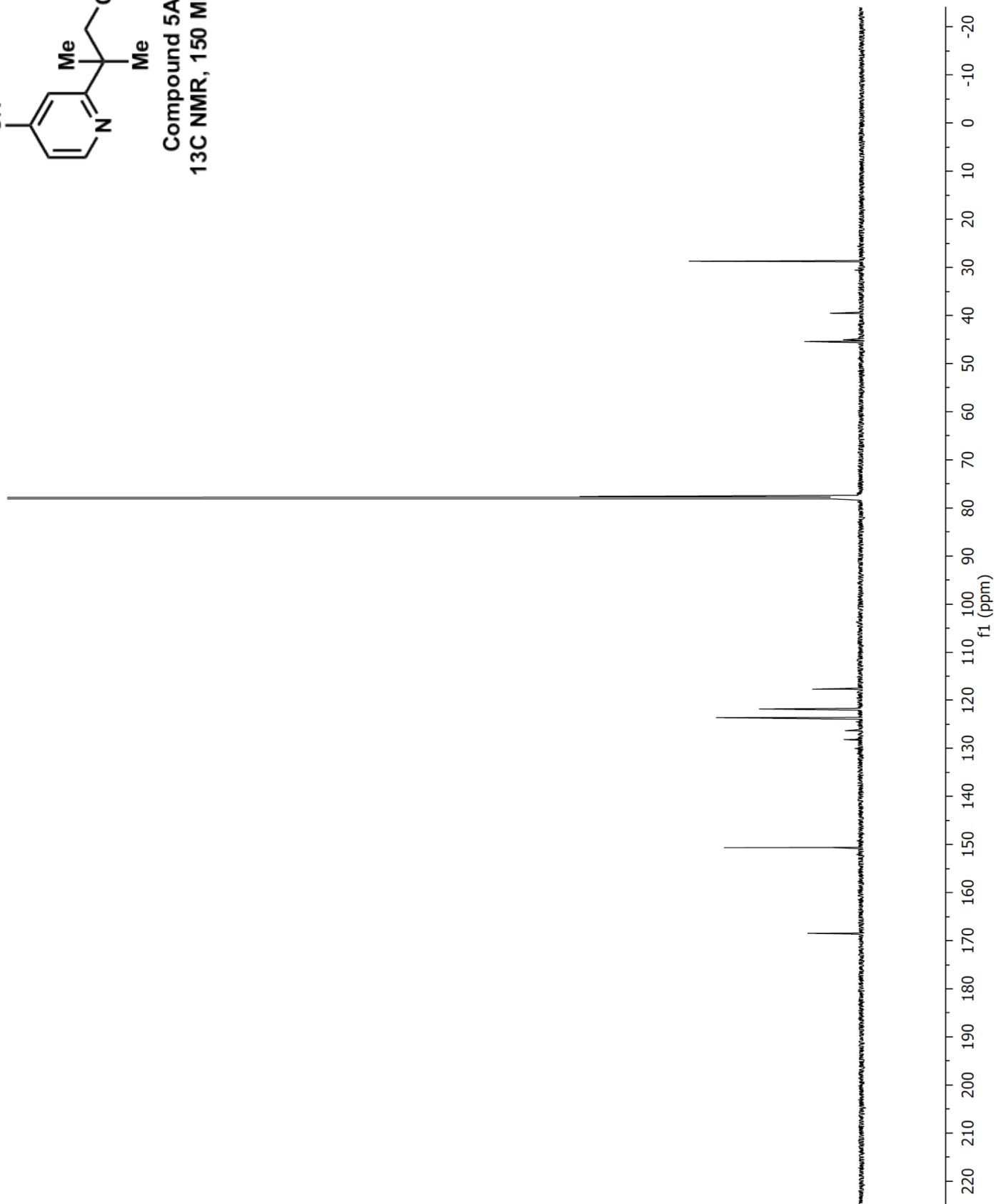


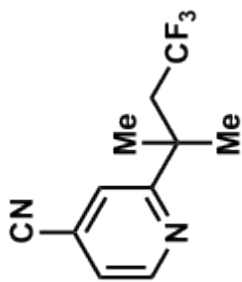
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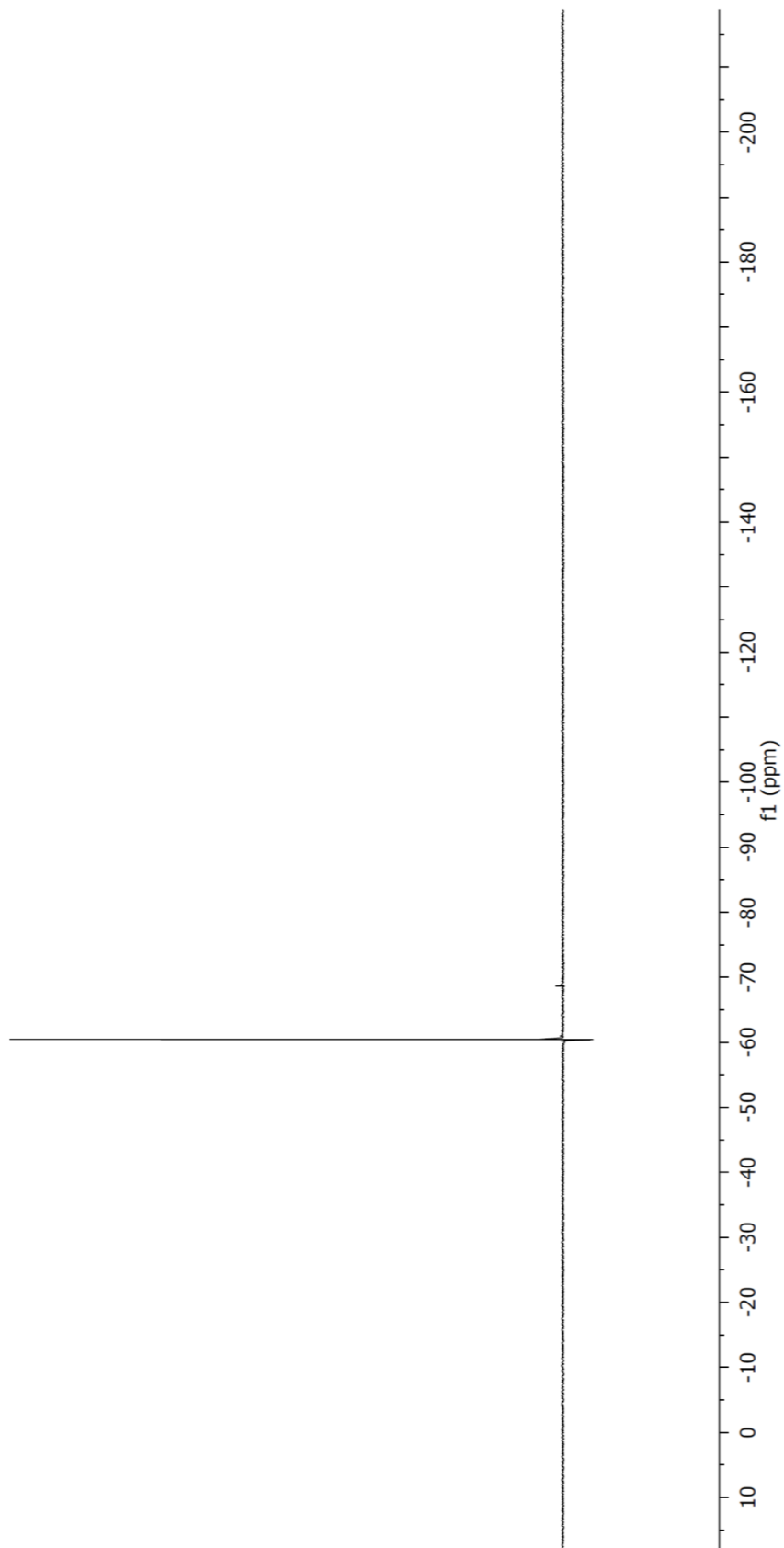


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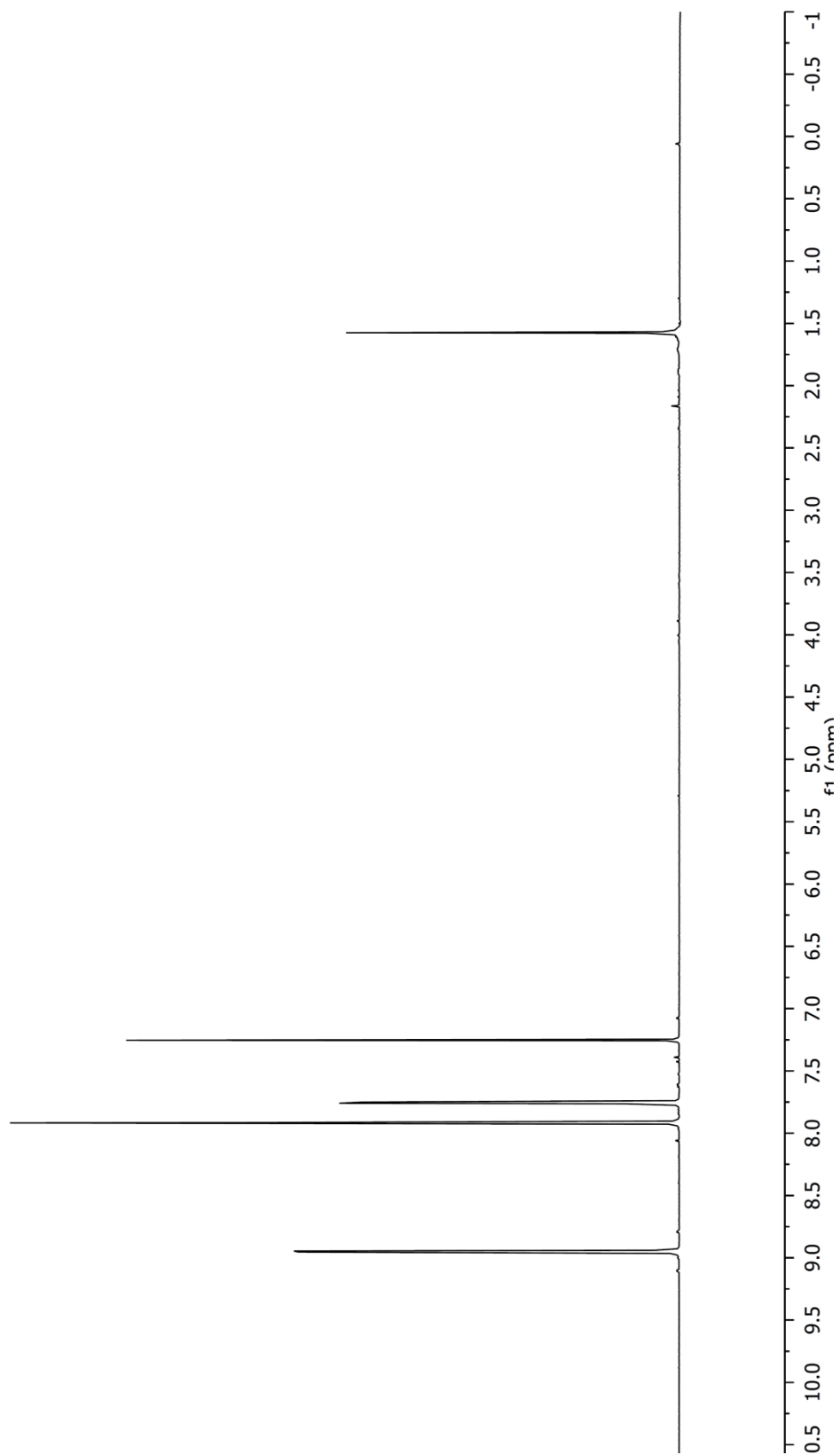
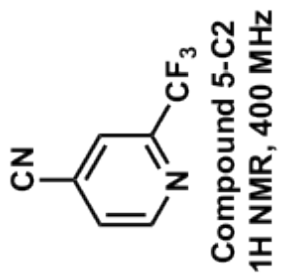


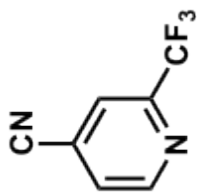


Compound 5A  
19F NMR, 376 MHz

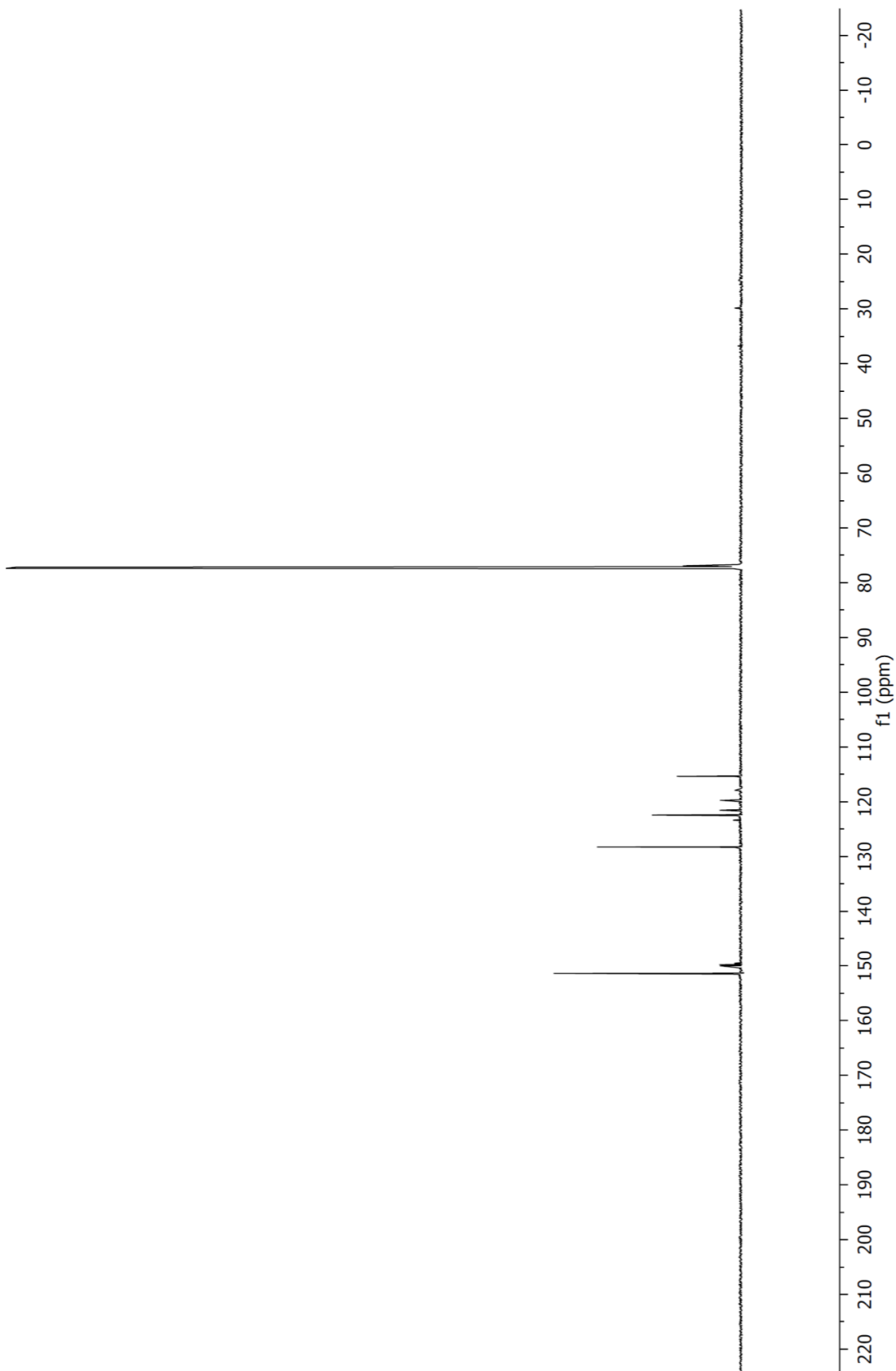


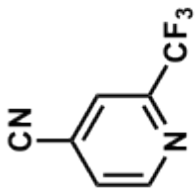




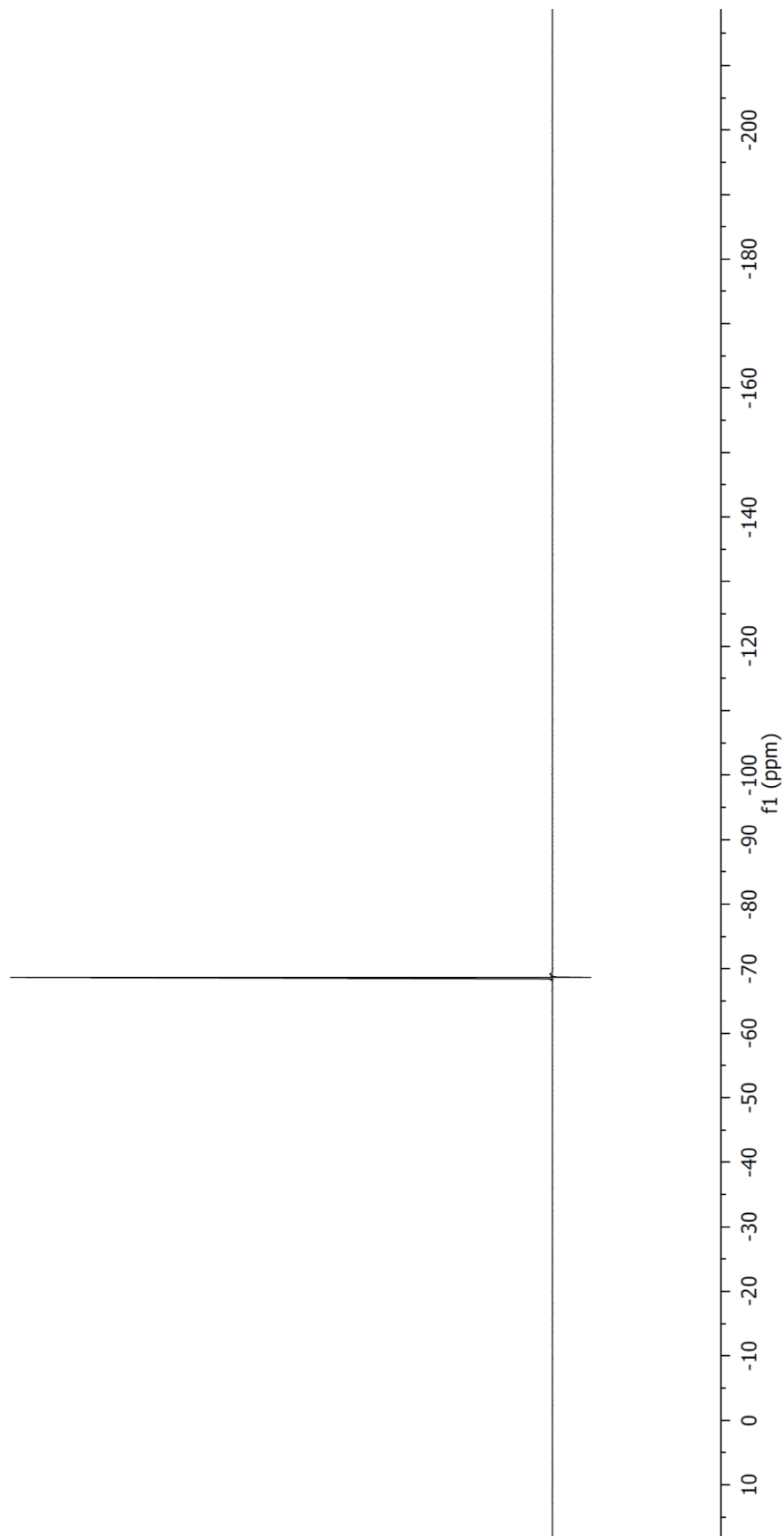


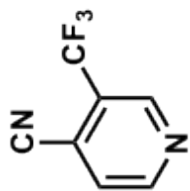
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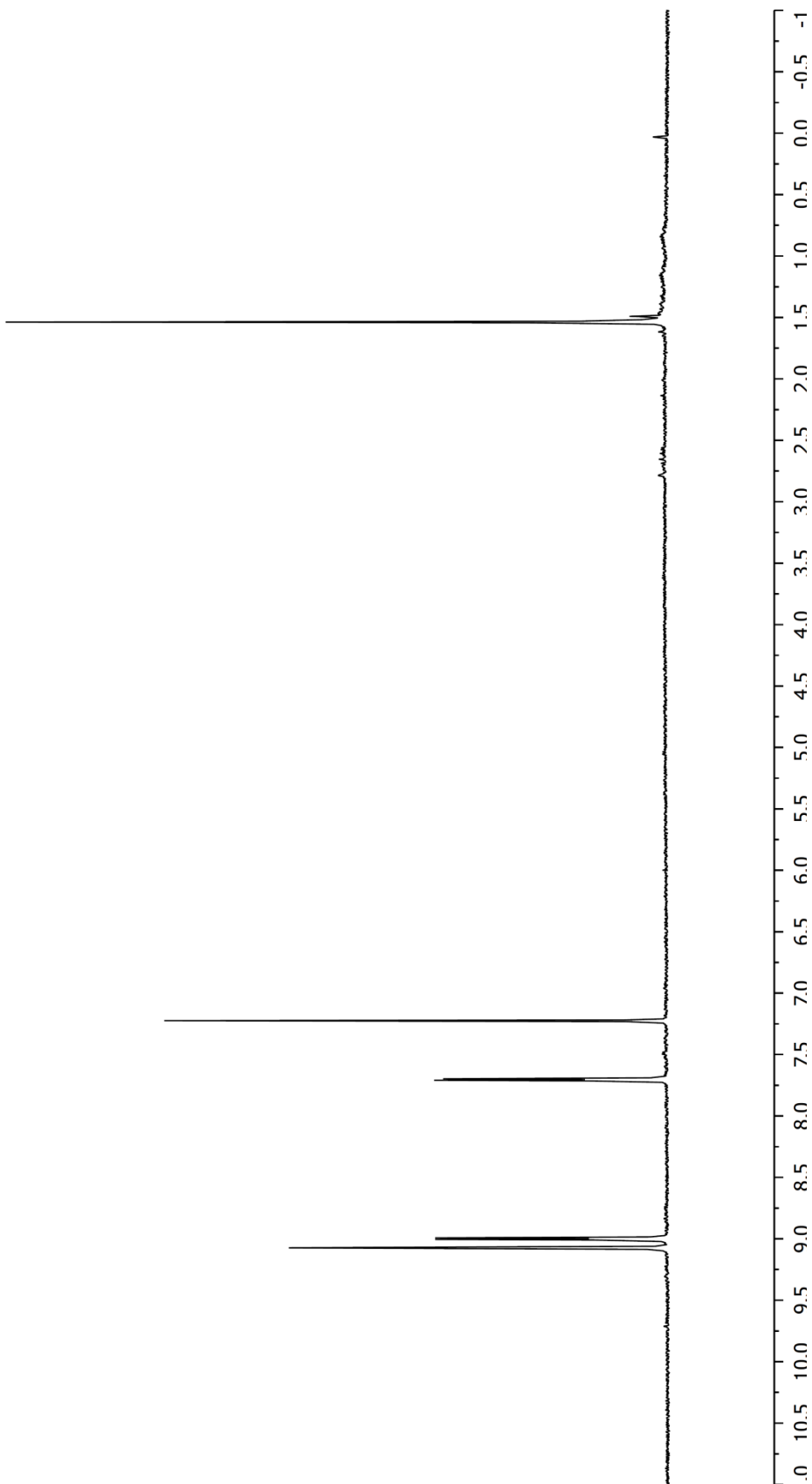


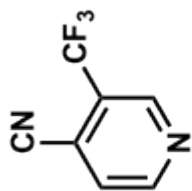
Compound 5-C2  
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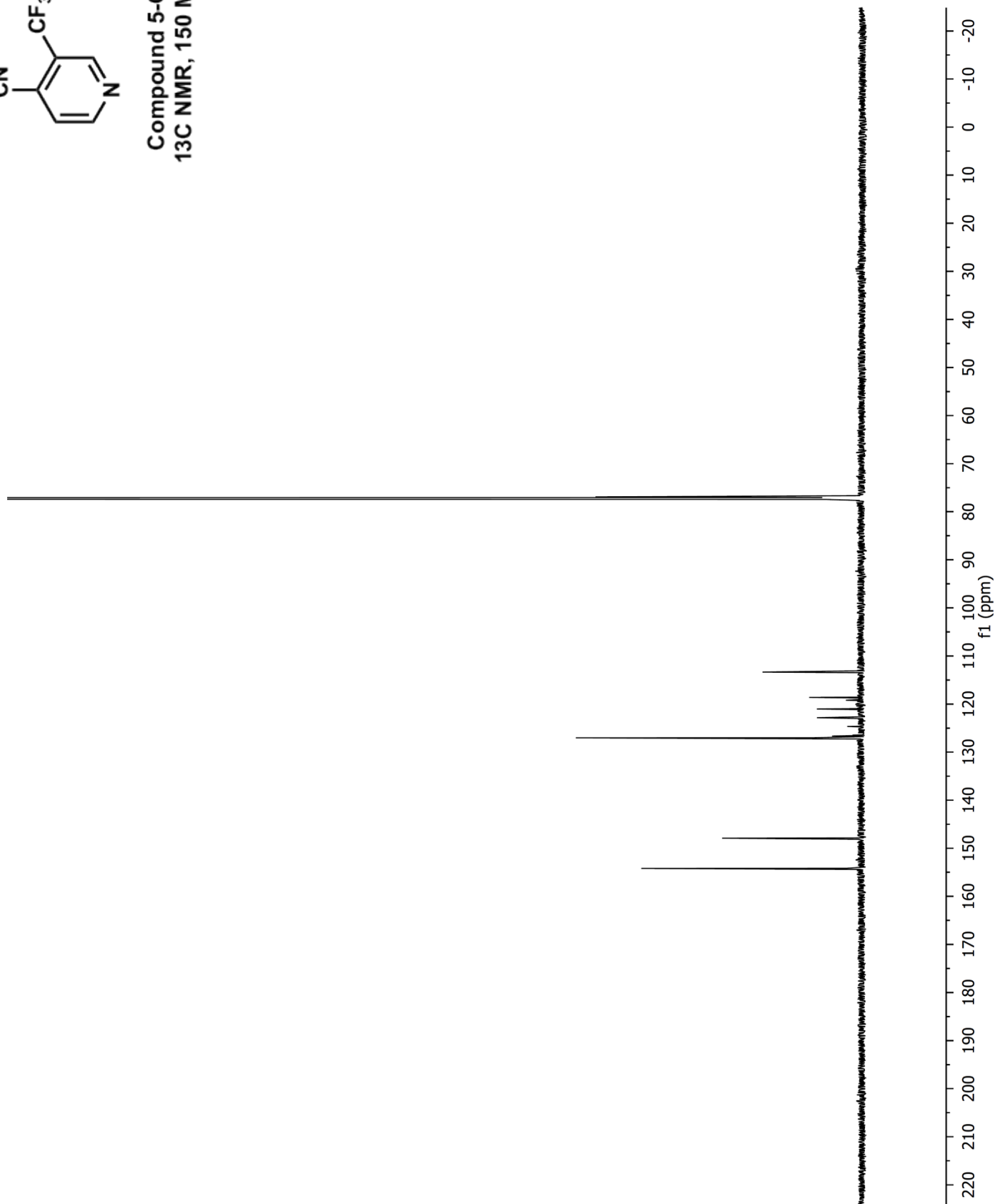


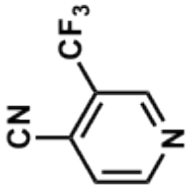
Compound 5-C3  
1H NMR, 400 MHz



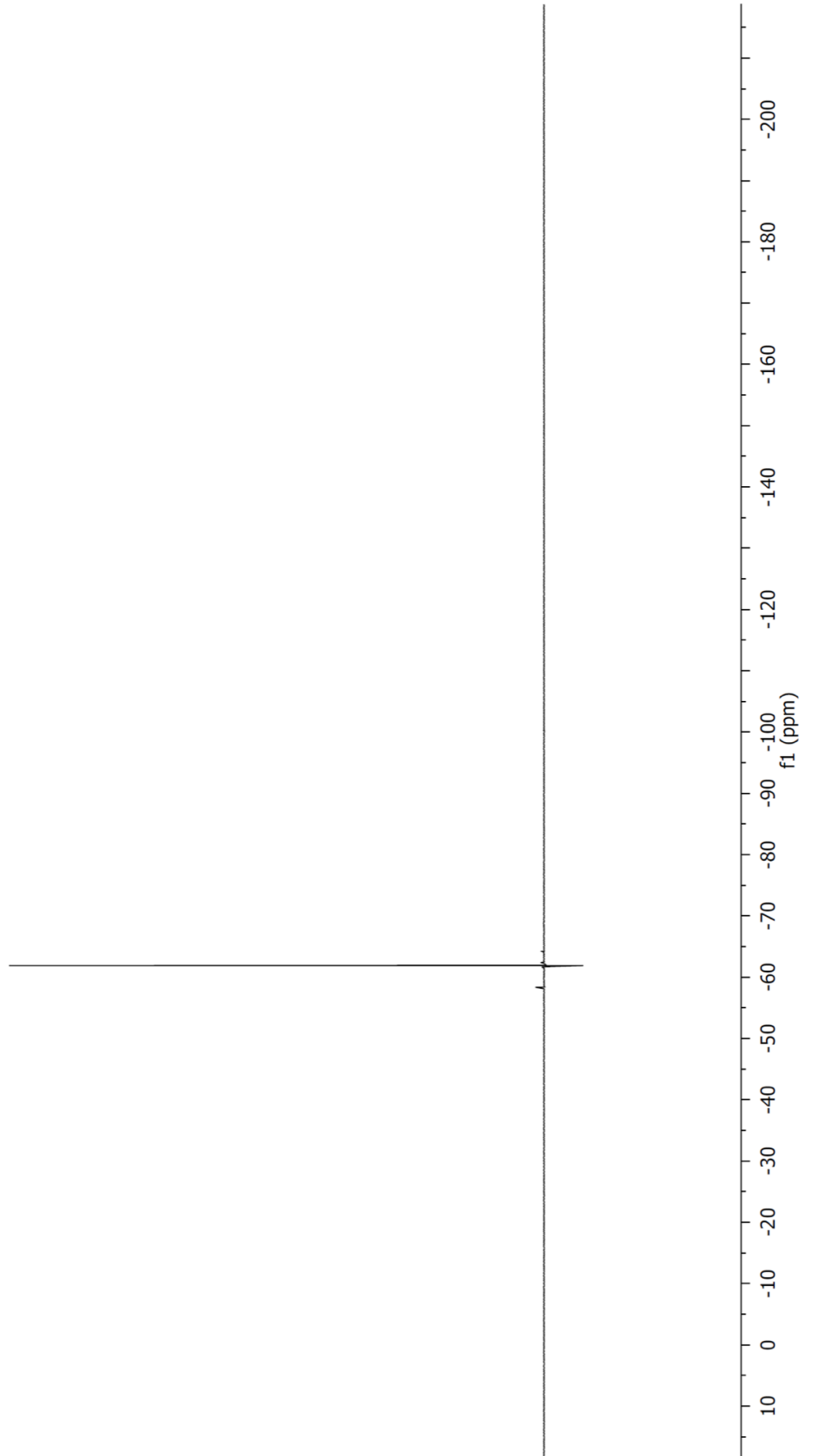


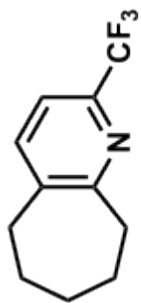
Compound 5-C3  
13C NMR, 150 MHz



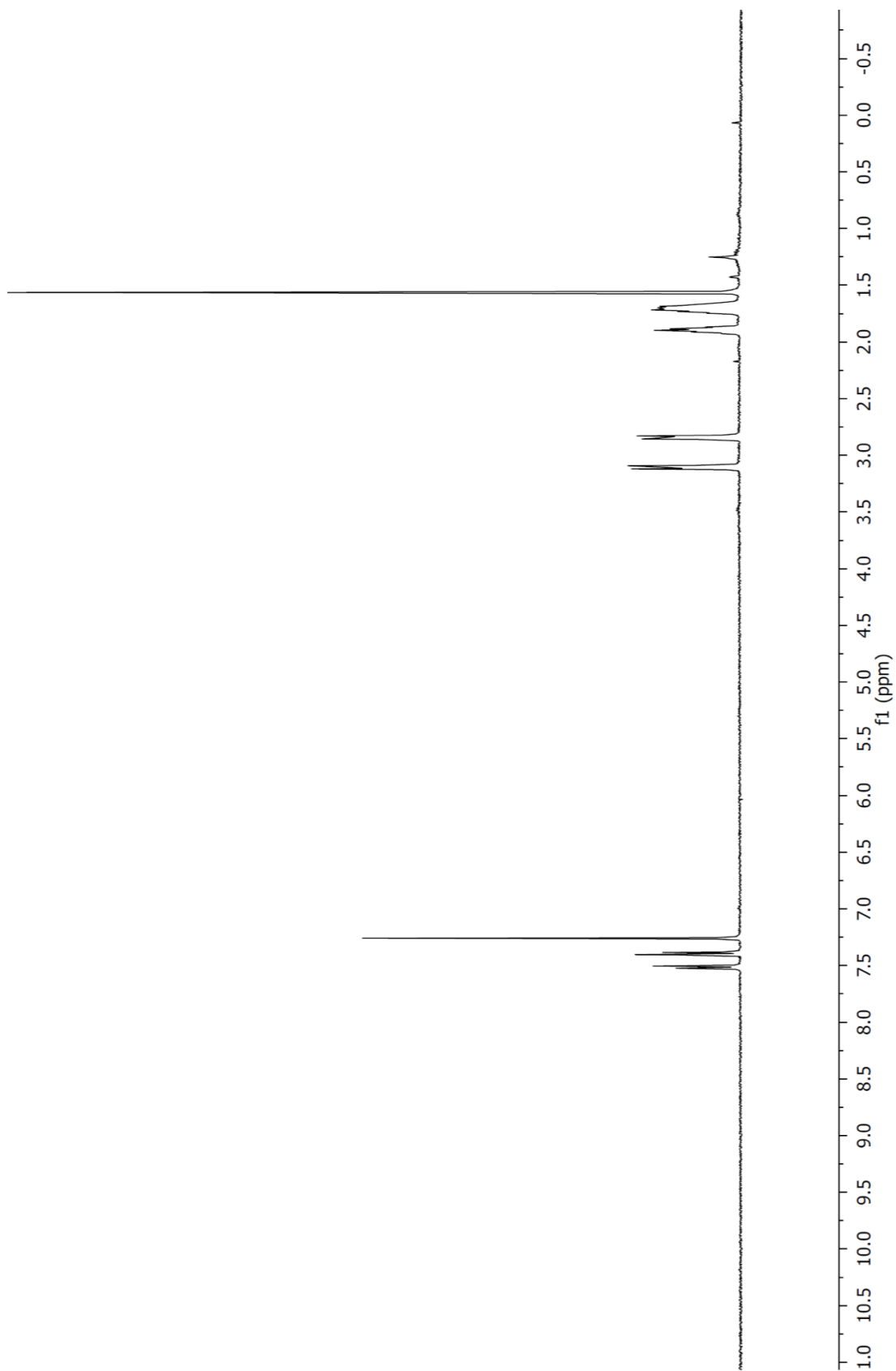


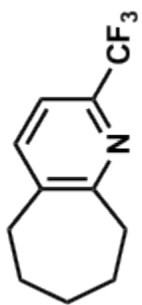
Compound 5-C3  
19F NMR, 376 MHz



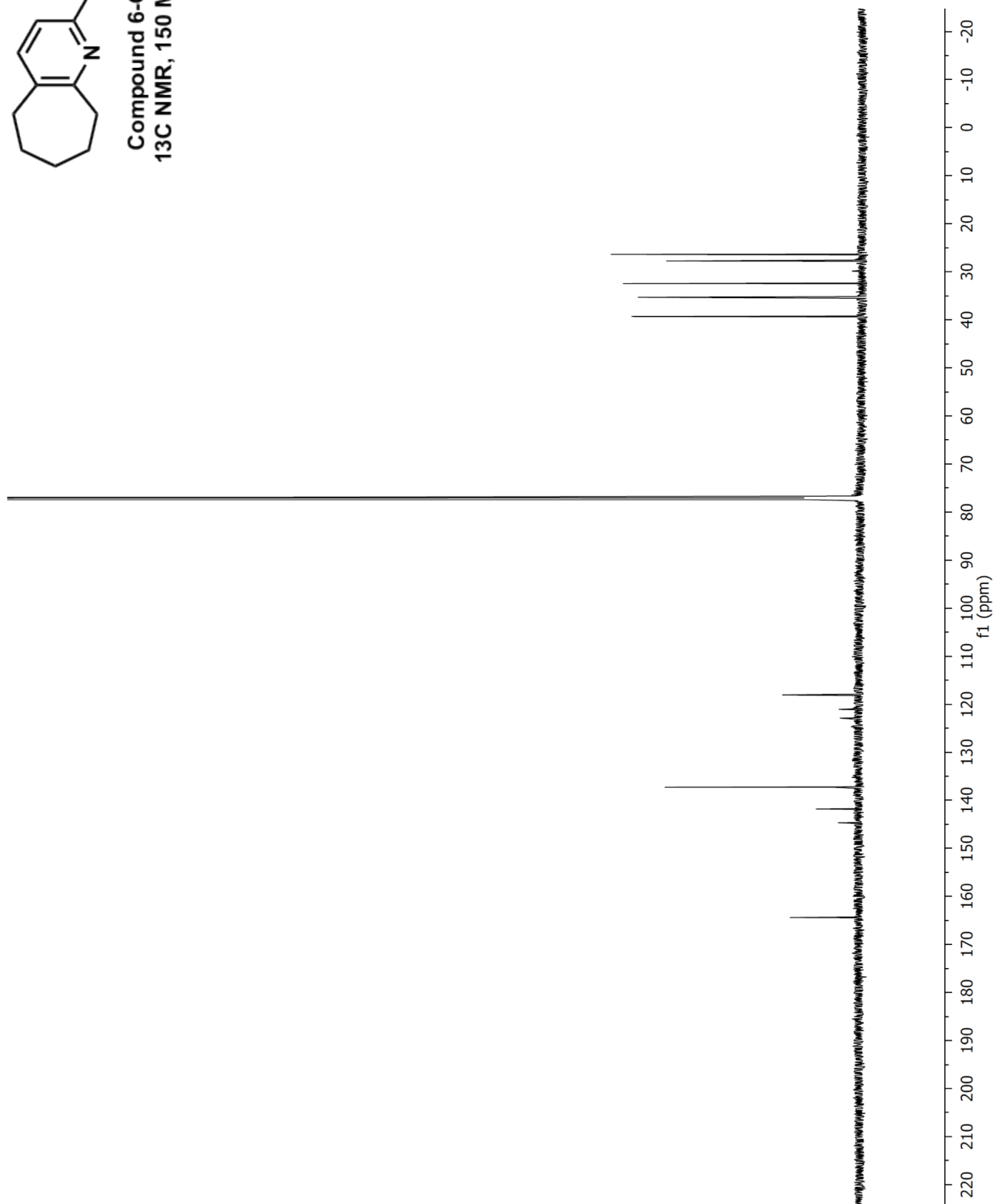


Compound 6-C2  
1H NMR, 400 MHz

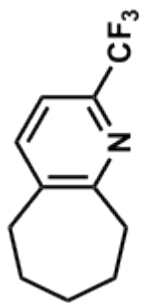




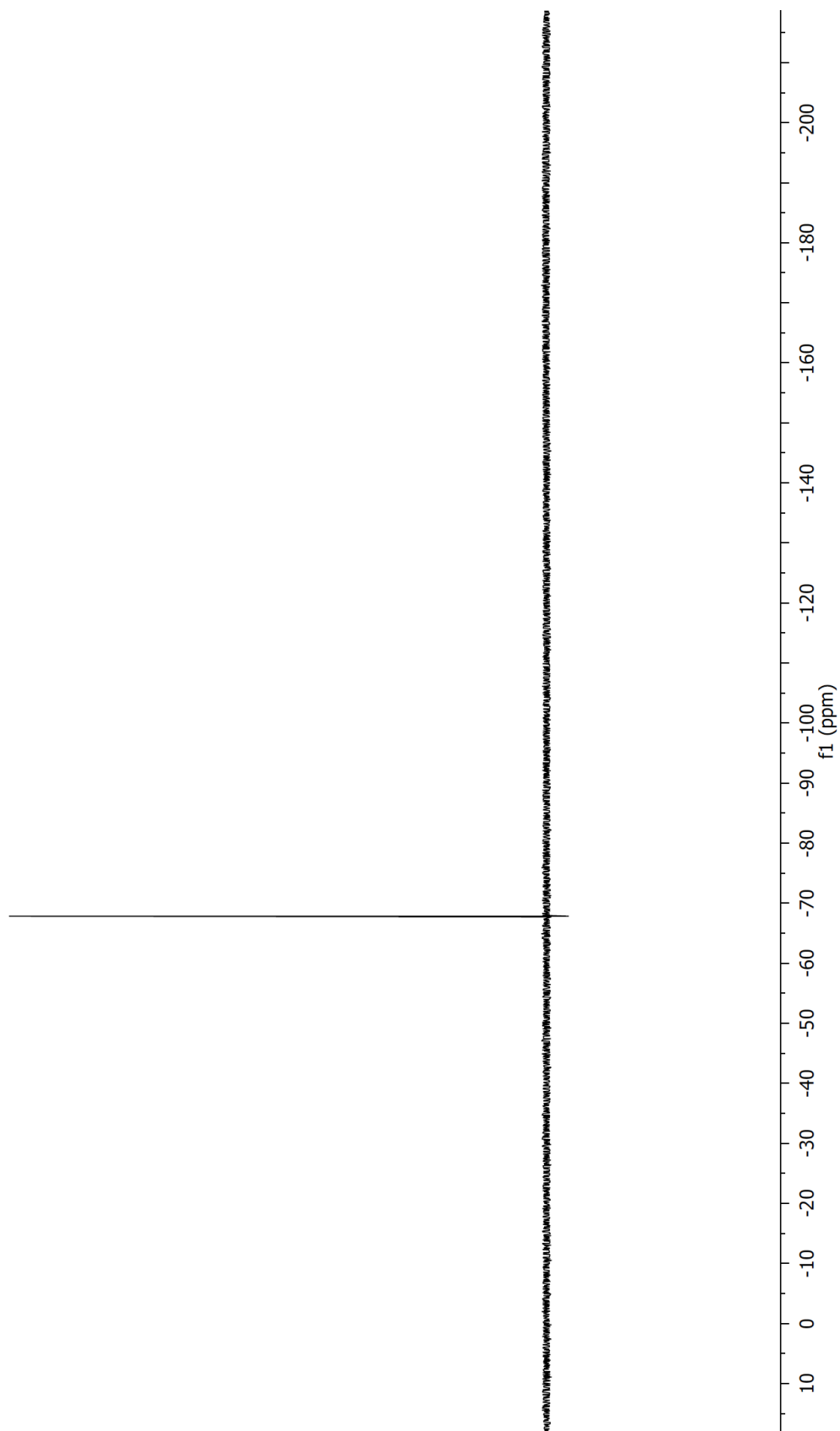
Compound 6-C2  
13C NMR, 150 MHz

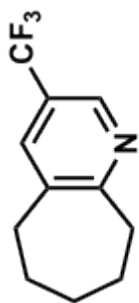




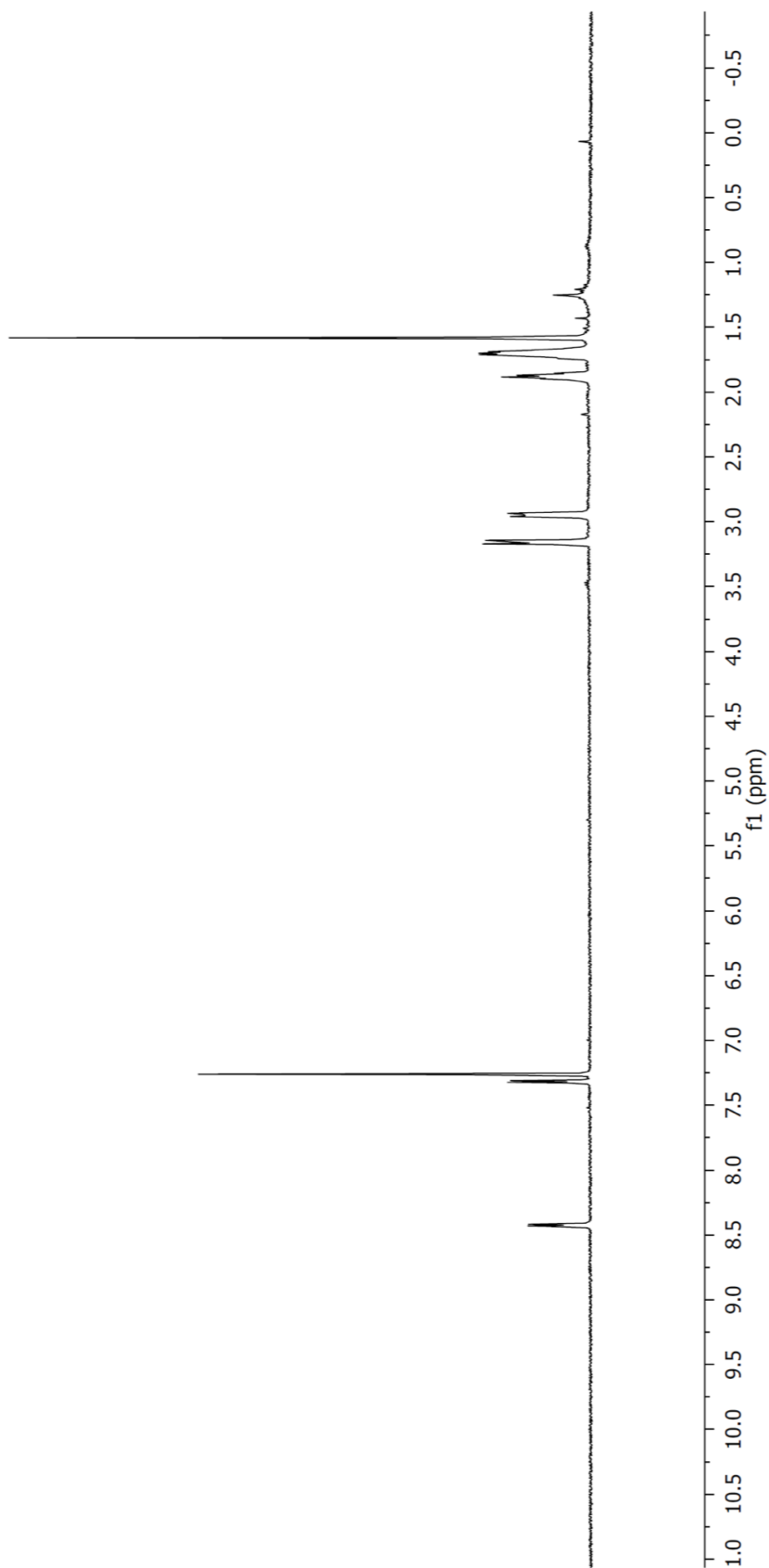


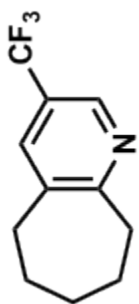
Compound 6-C2  
19F NMR, 376 MHz



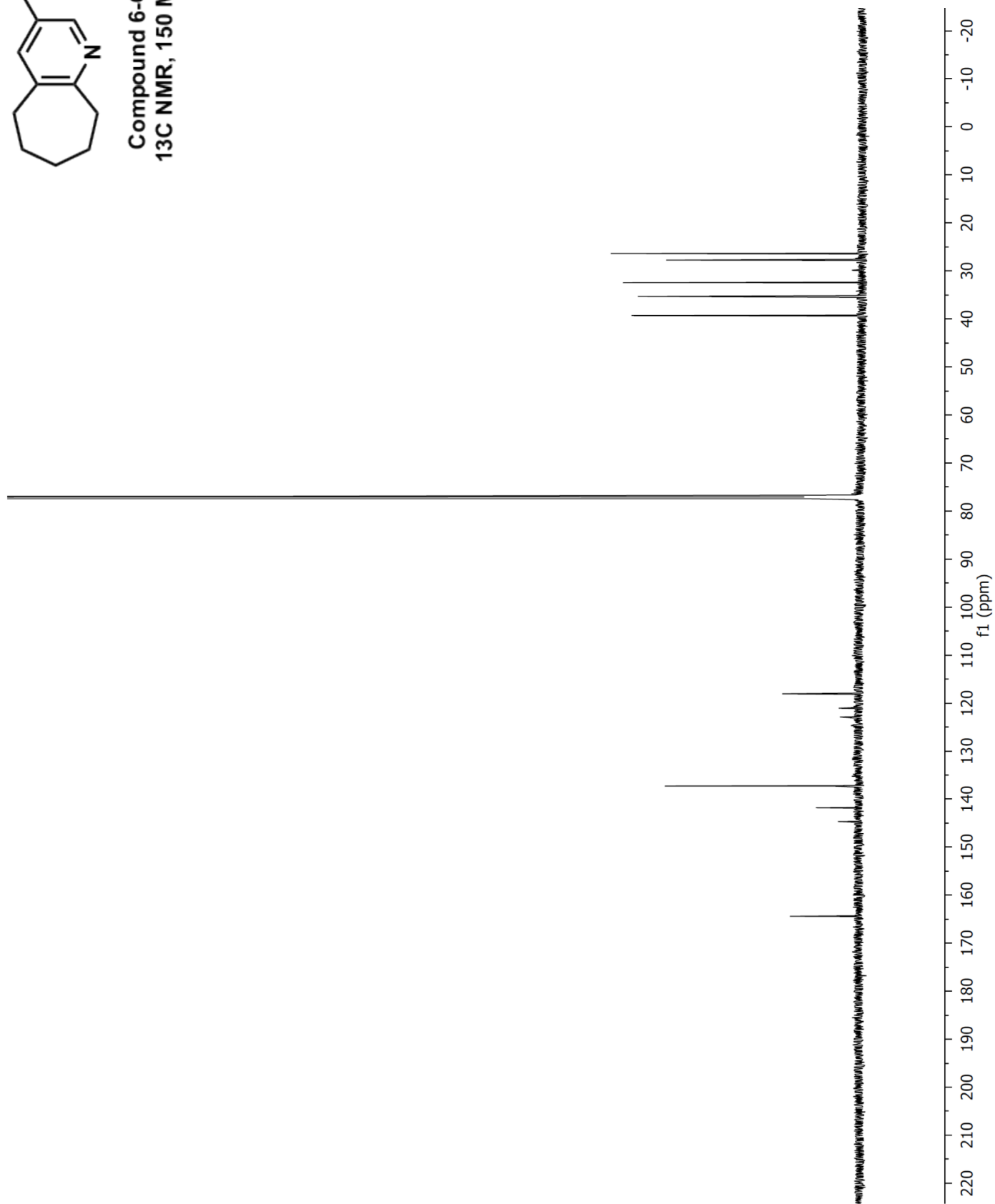


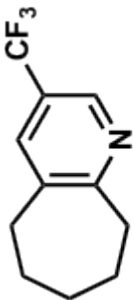
Compound 6-C3  
1H NMR, 400 MHz



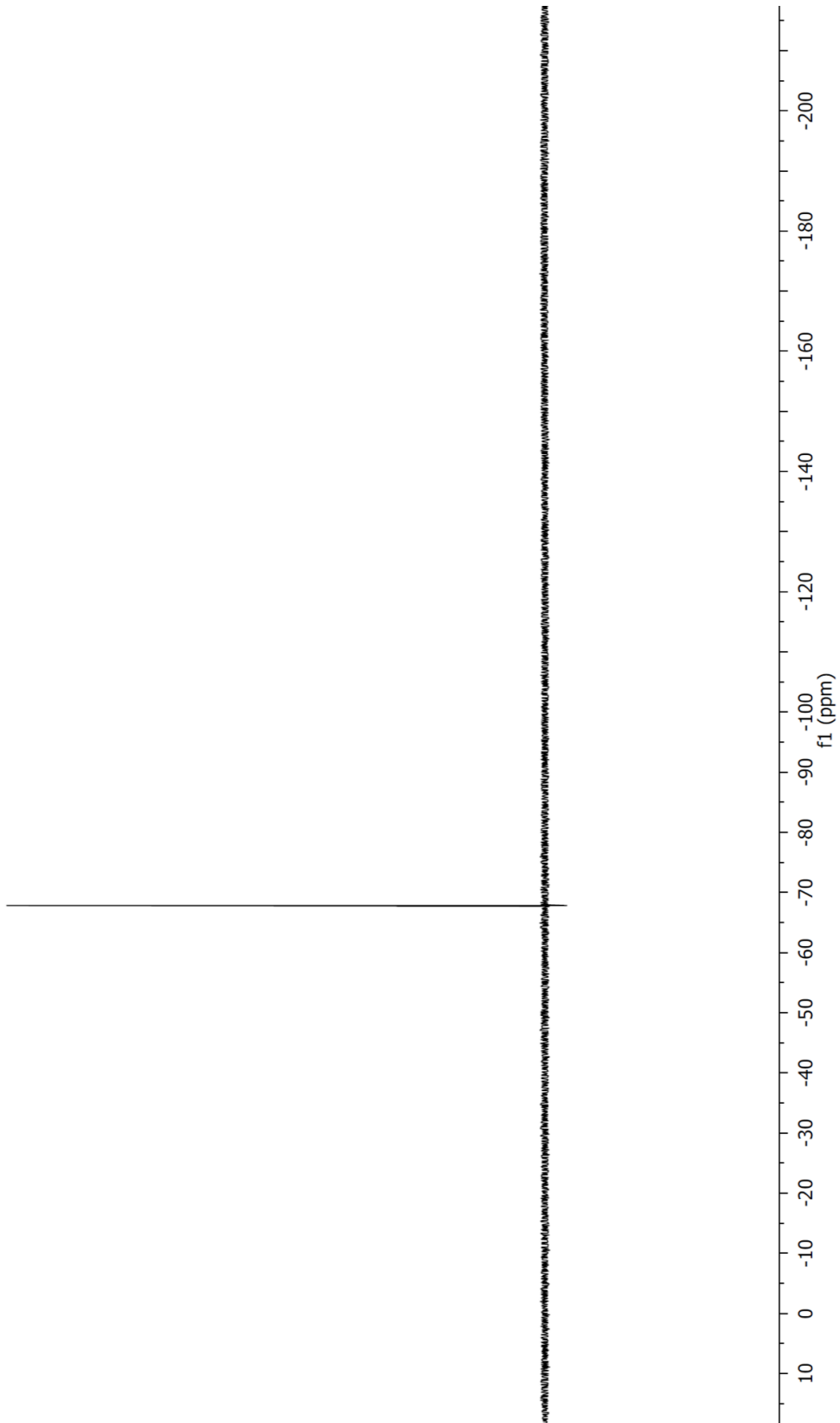


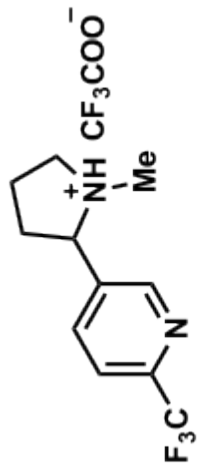
Compound 6-C3  
13C NMR, 150 MHz



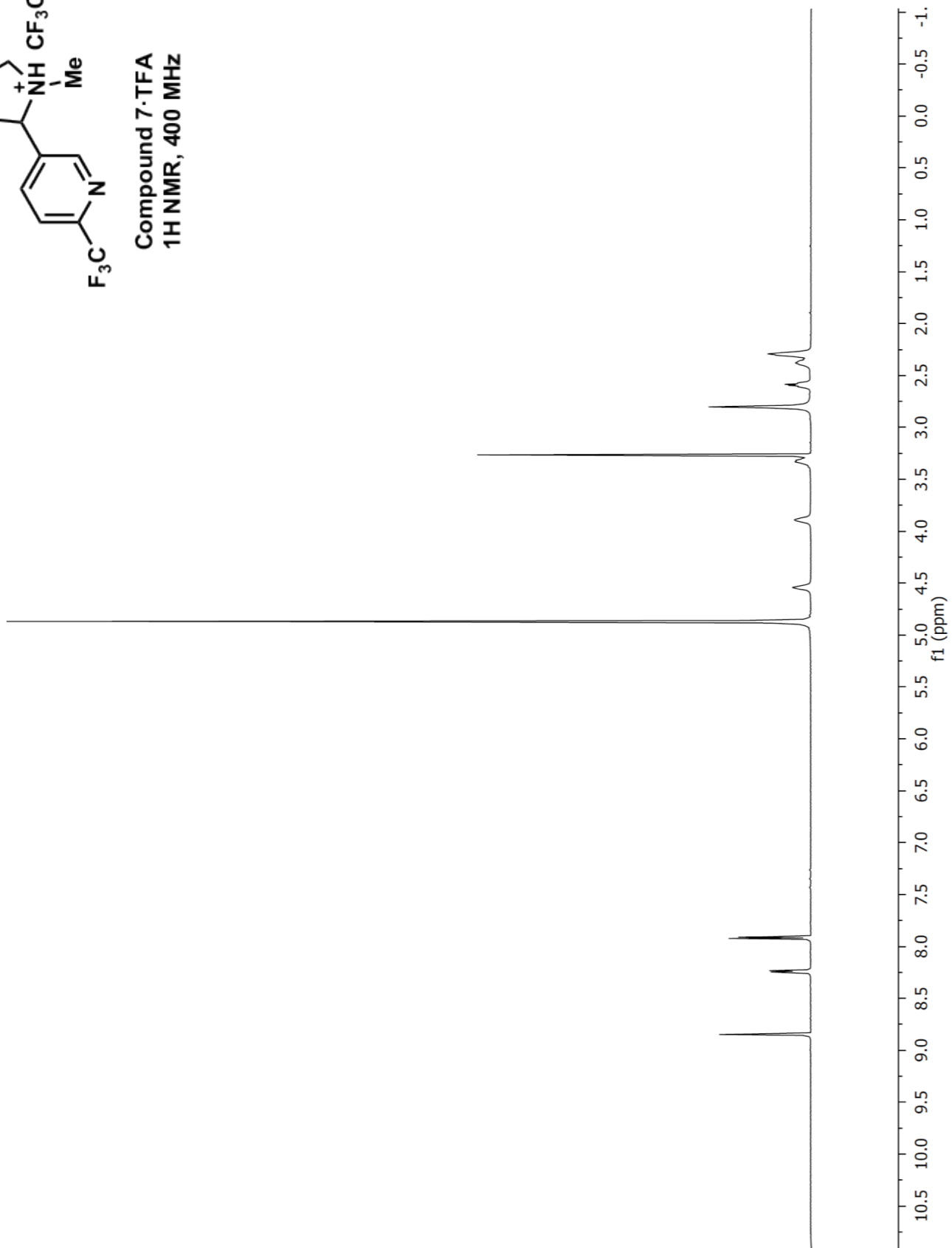


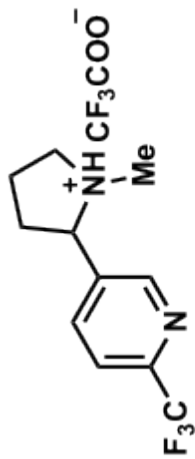
Compound 6-C3  
19F NMR, 376 MHz



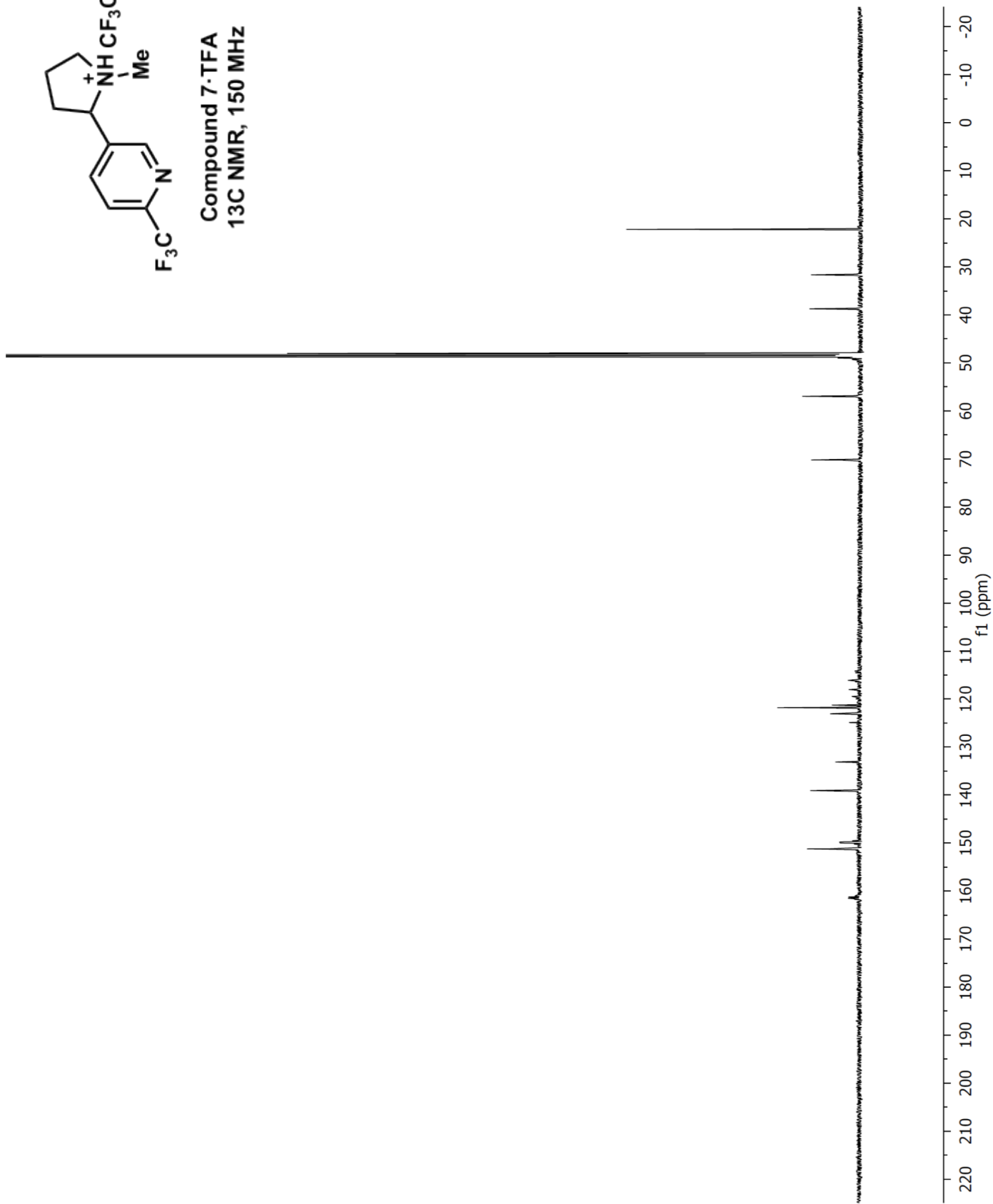


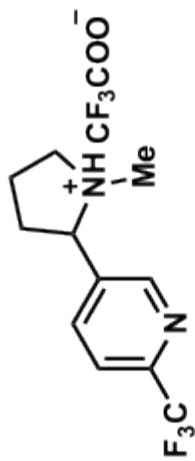
Compound 7·TFA  
1H NMR, 400 MHz



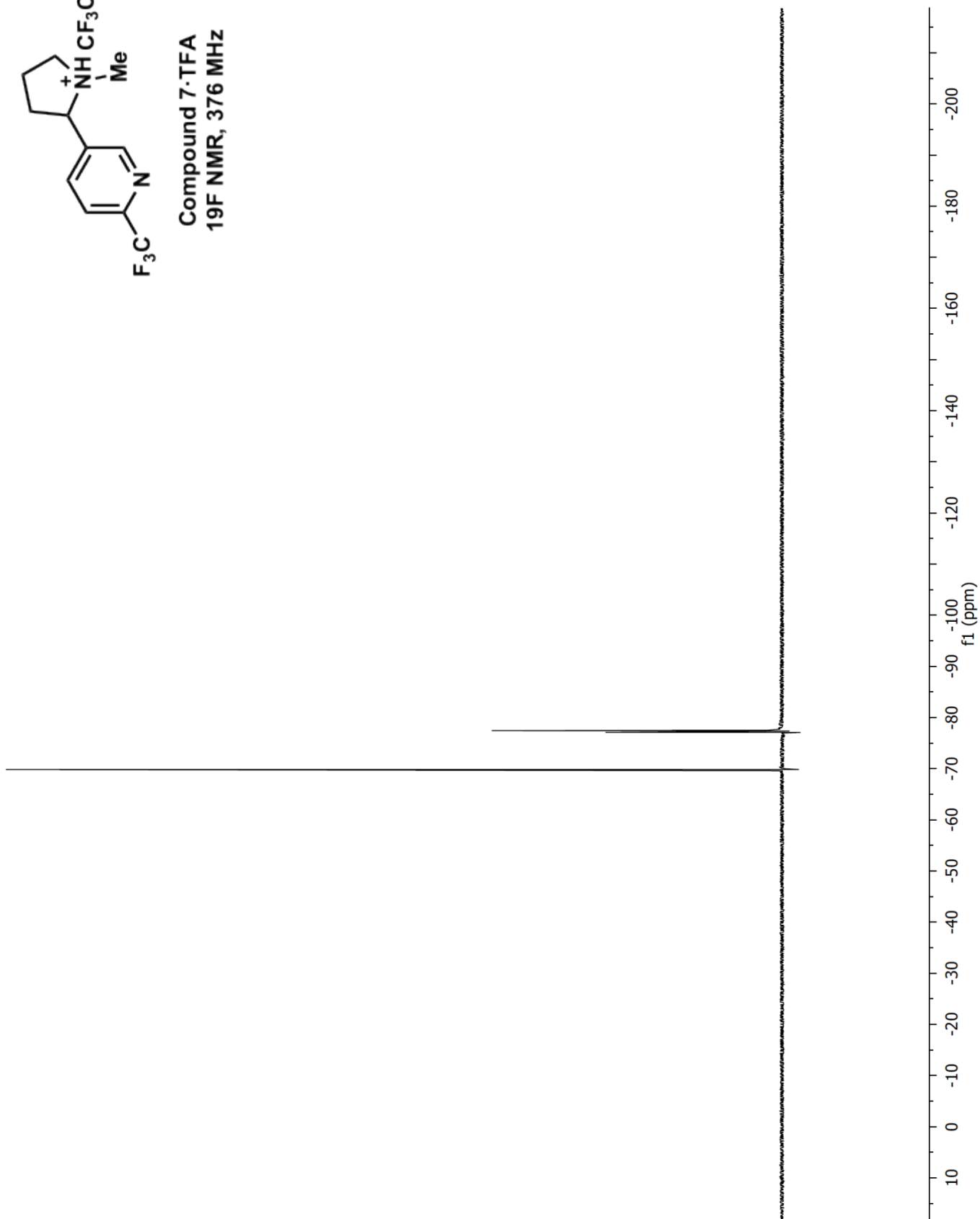


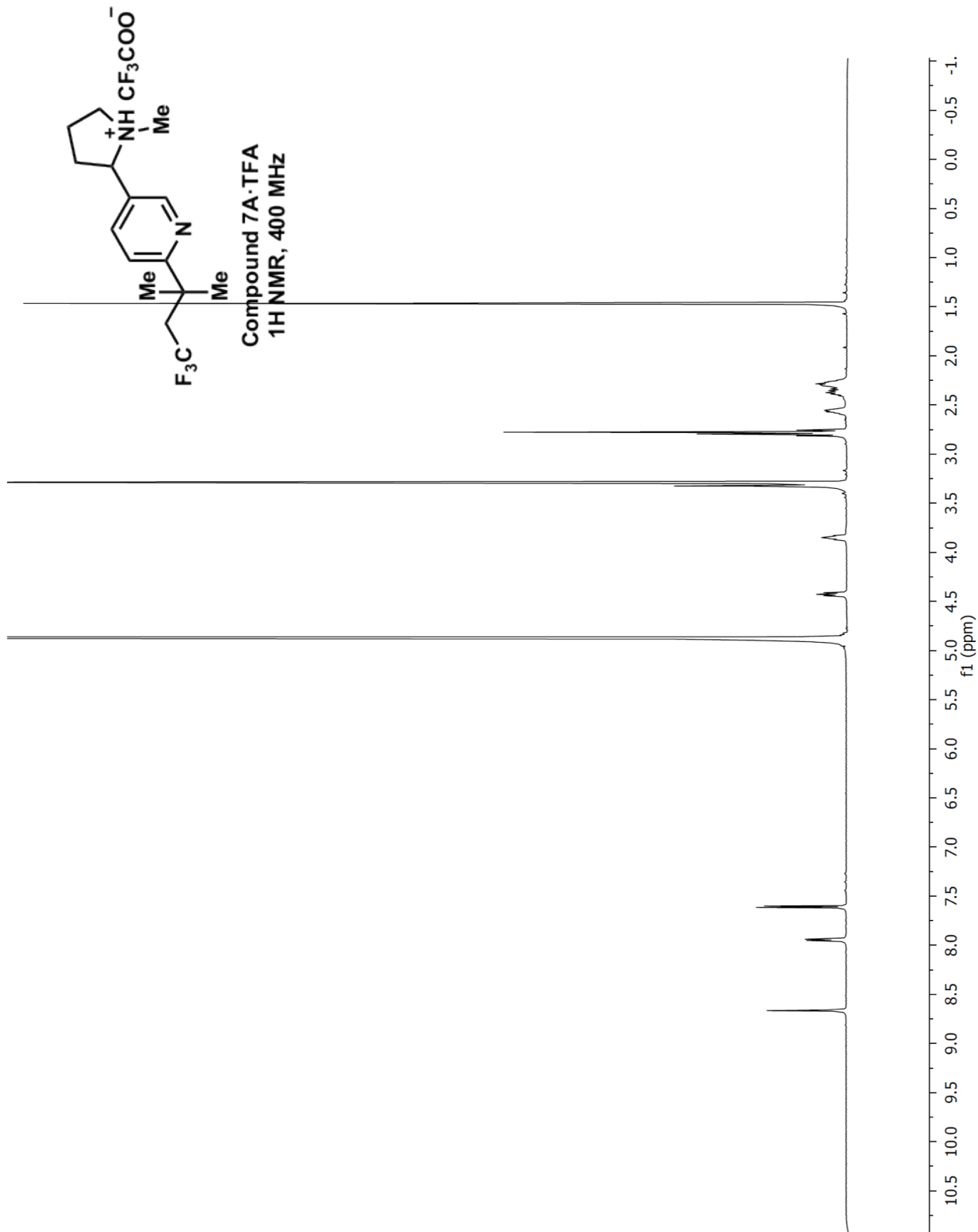
Compound 7·TFA  
13C NMR, 150 MHz



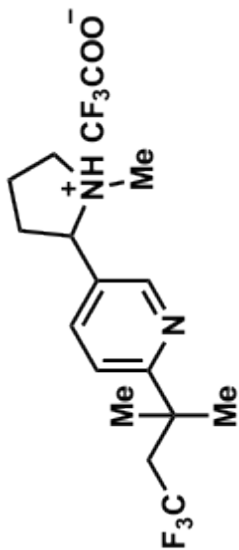


Compound 7·TFA  
19F NMR, 376 MHz

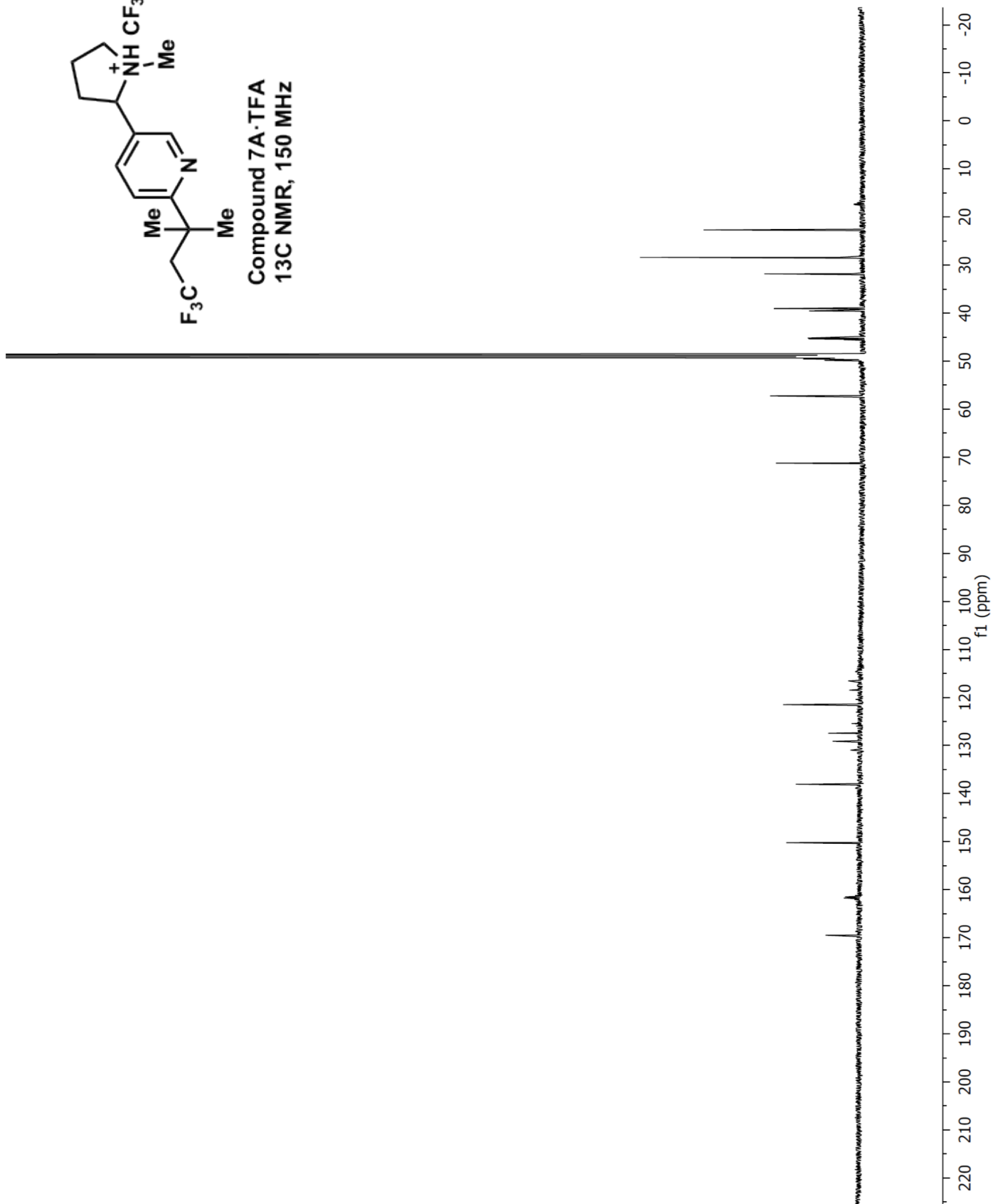


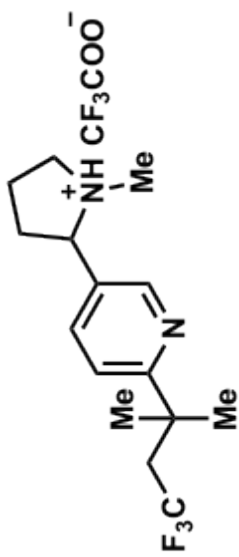




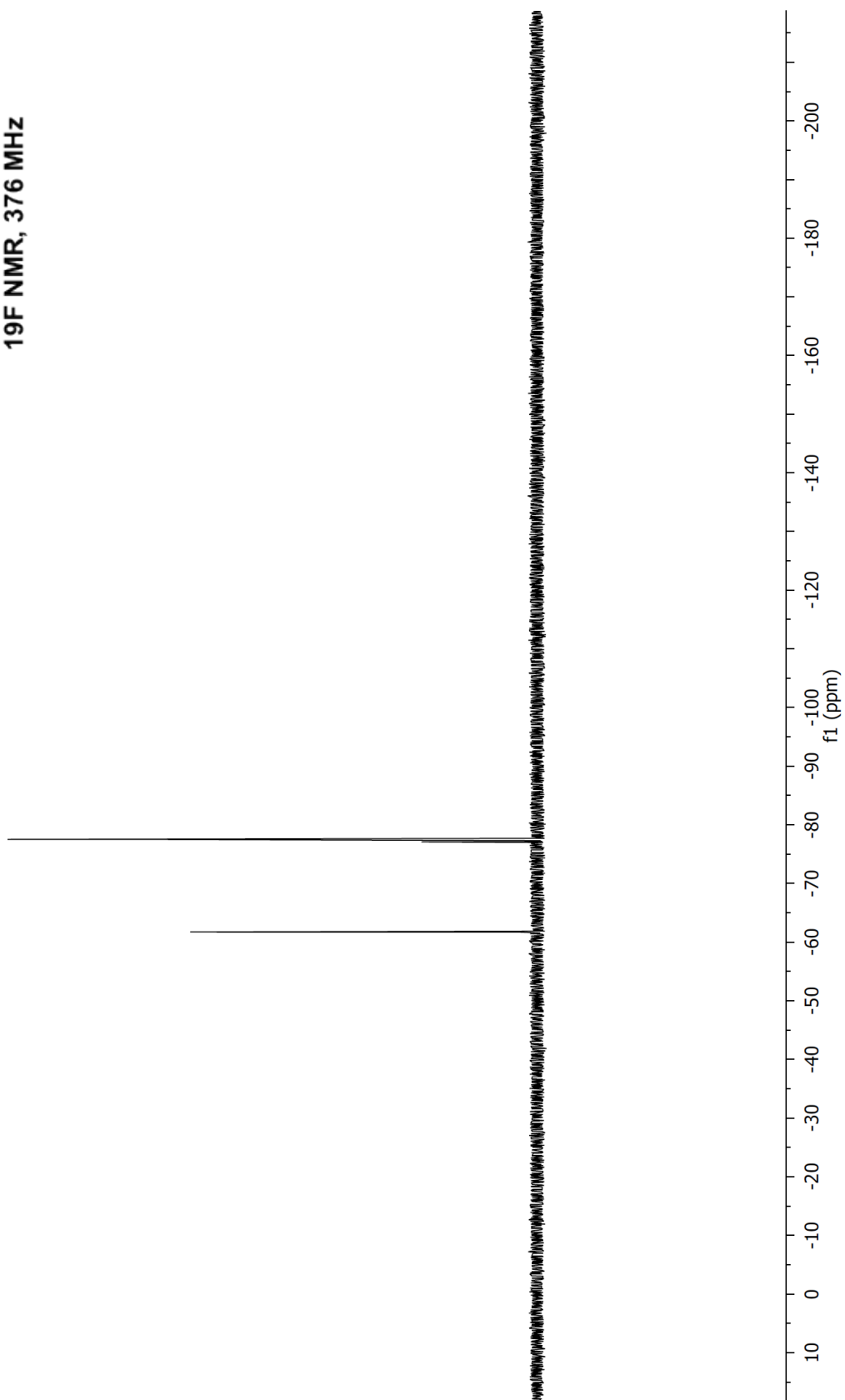


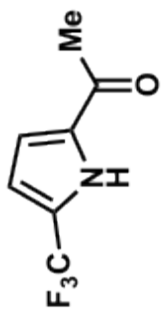
Compound 7A·TFA  
13C NMR, 150 MHz



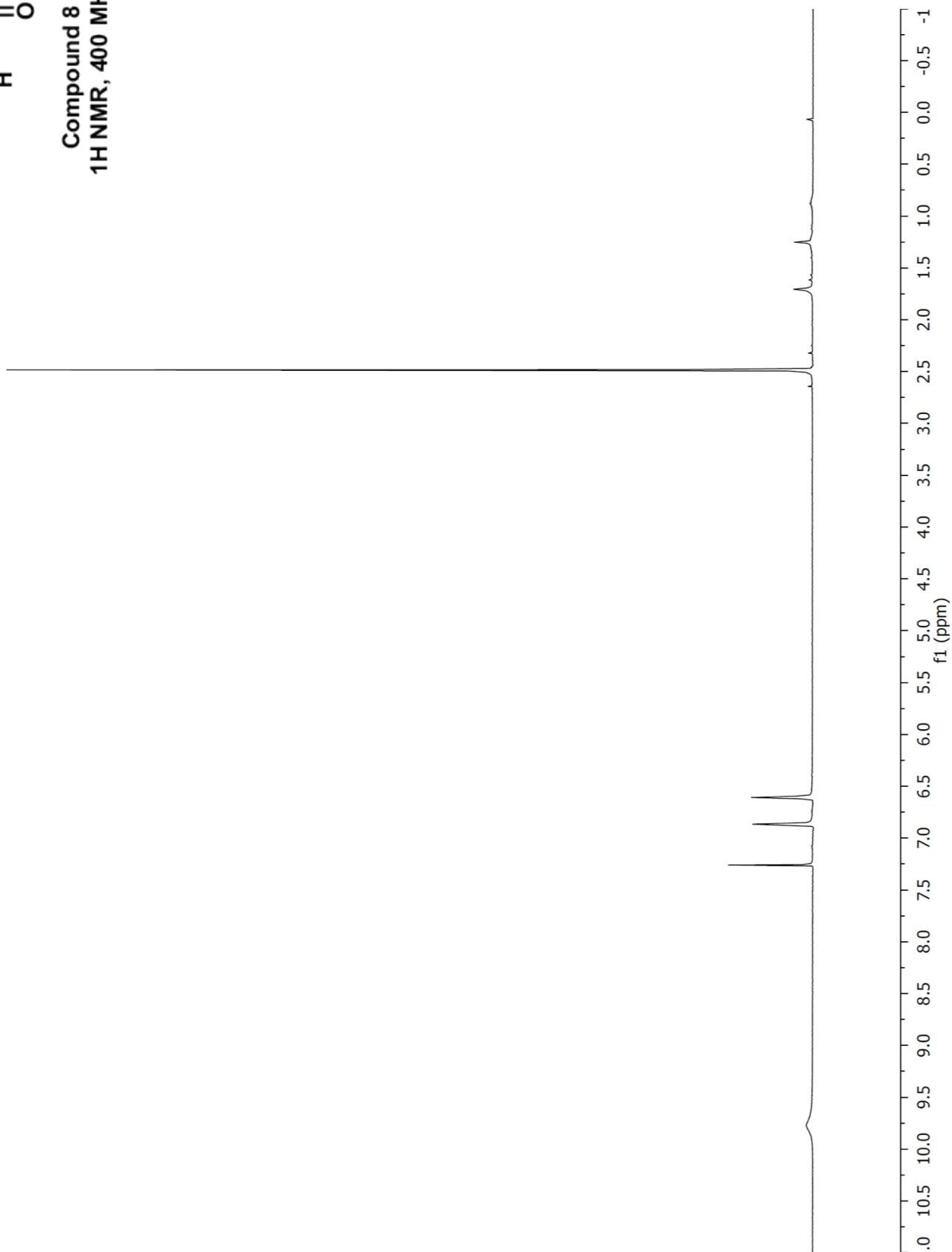


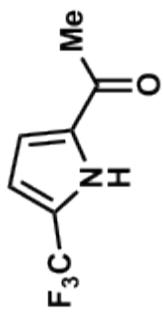
Compound 7A·TFA  
19F NMR, 376 MHz



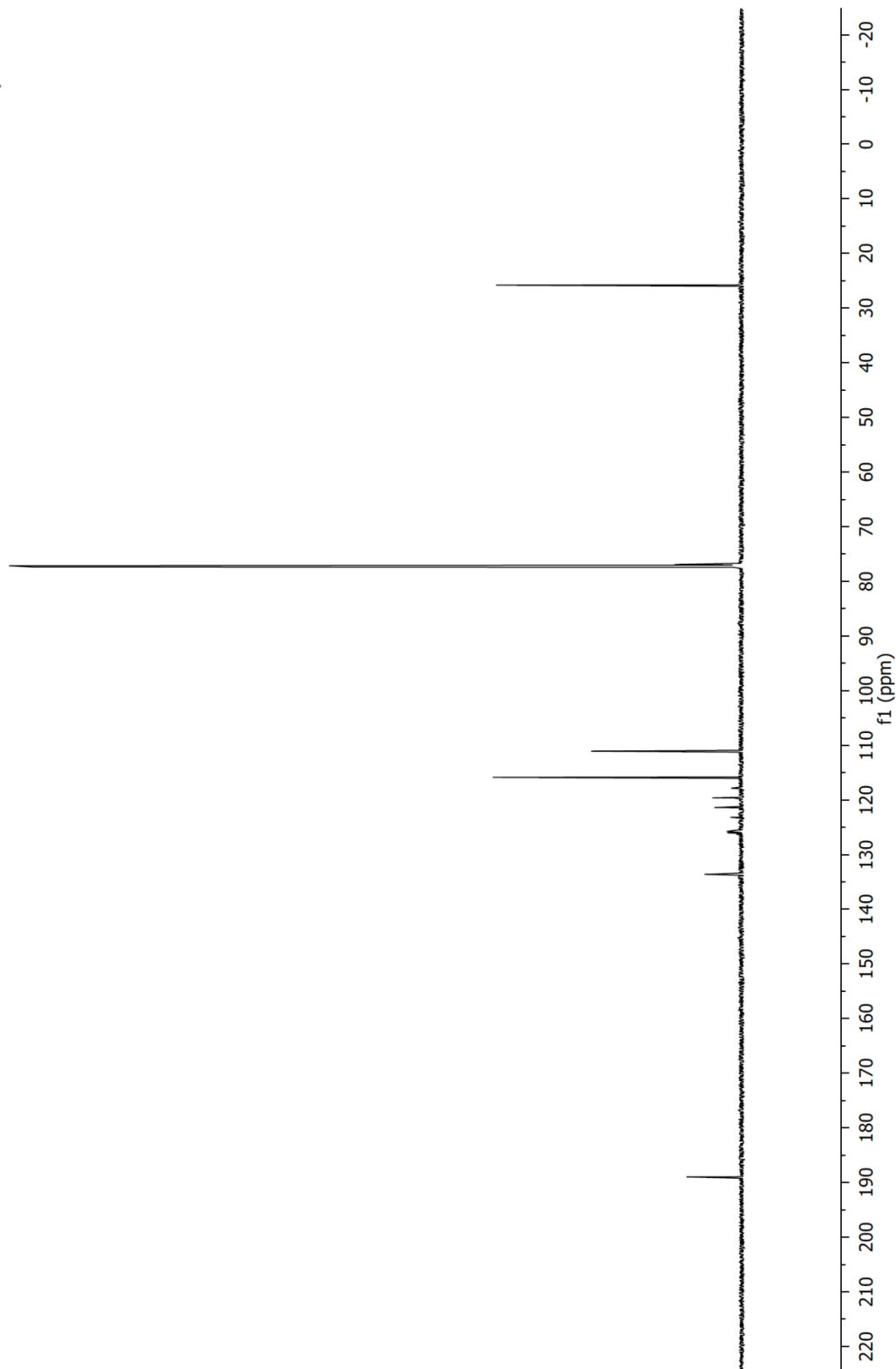


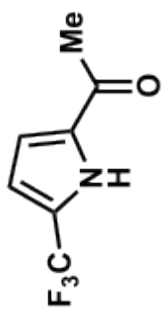
Compound 8  
1H NMR, 400 MHz



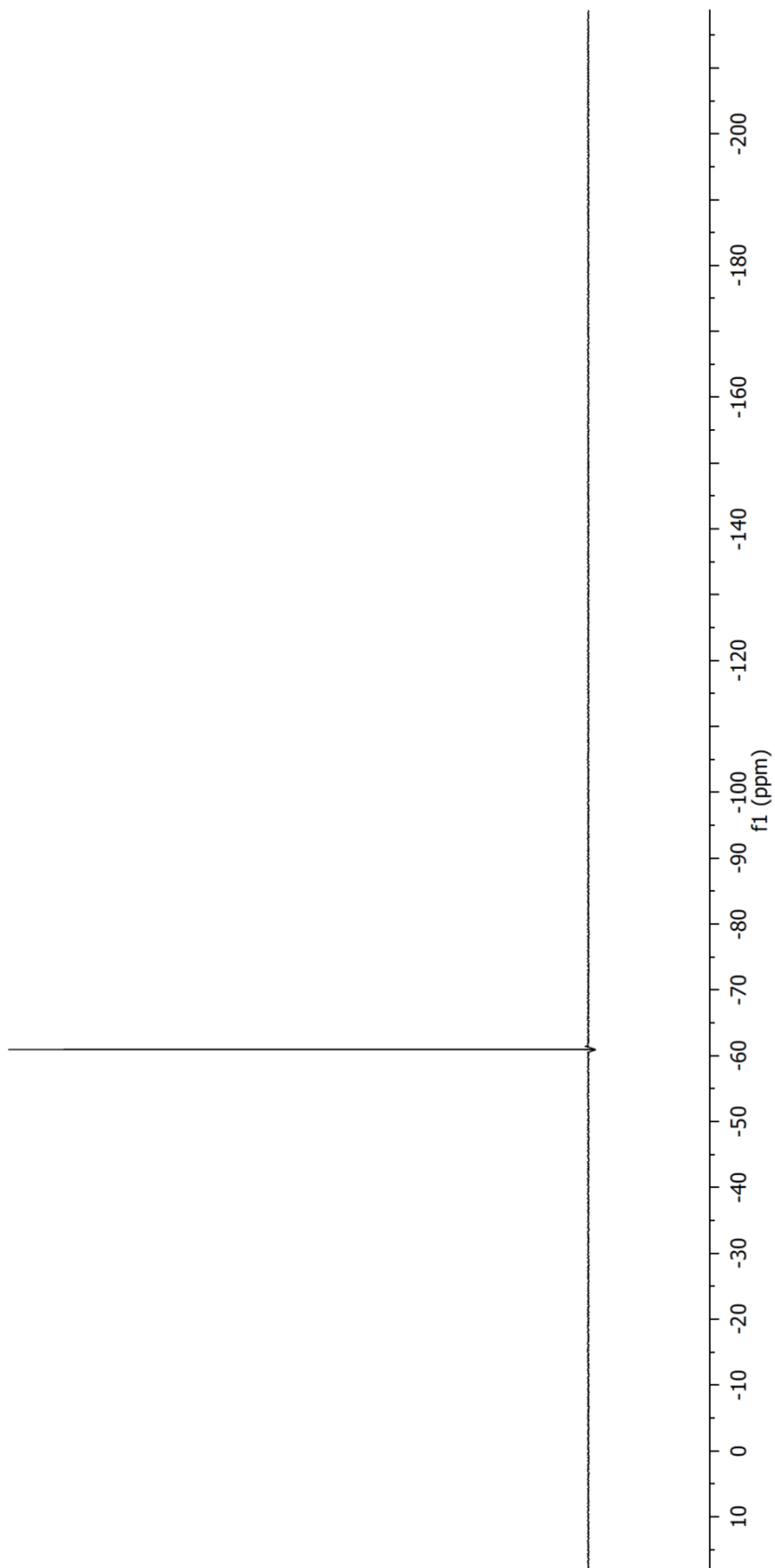


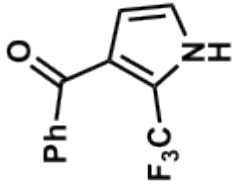
Compound 8  
 $^{13}C$  NMR, 150 MHz



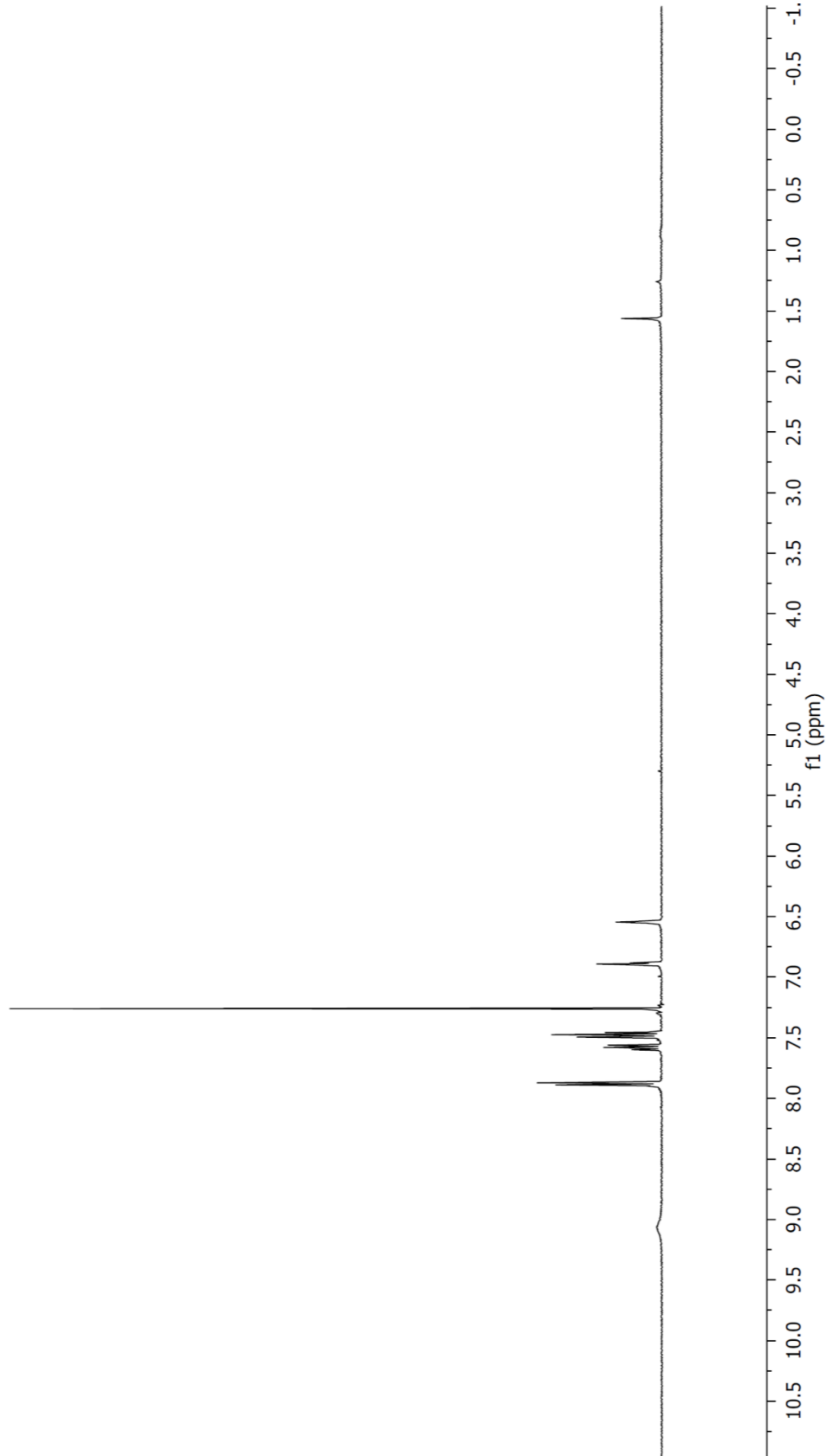


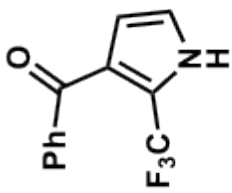
Compound 8  
19F NMR, 376 MHz



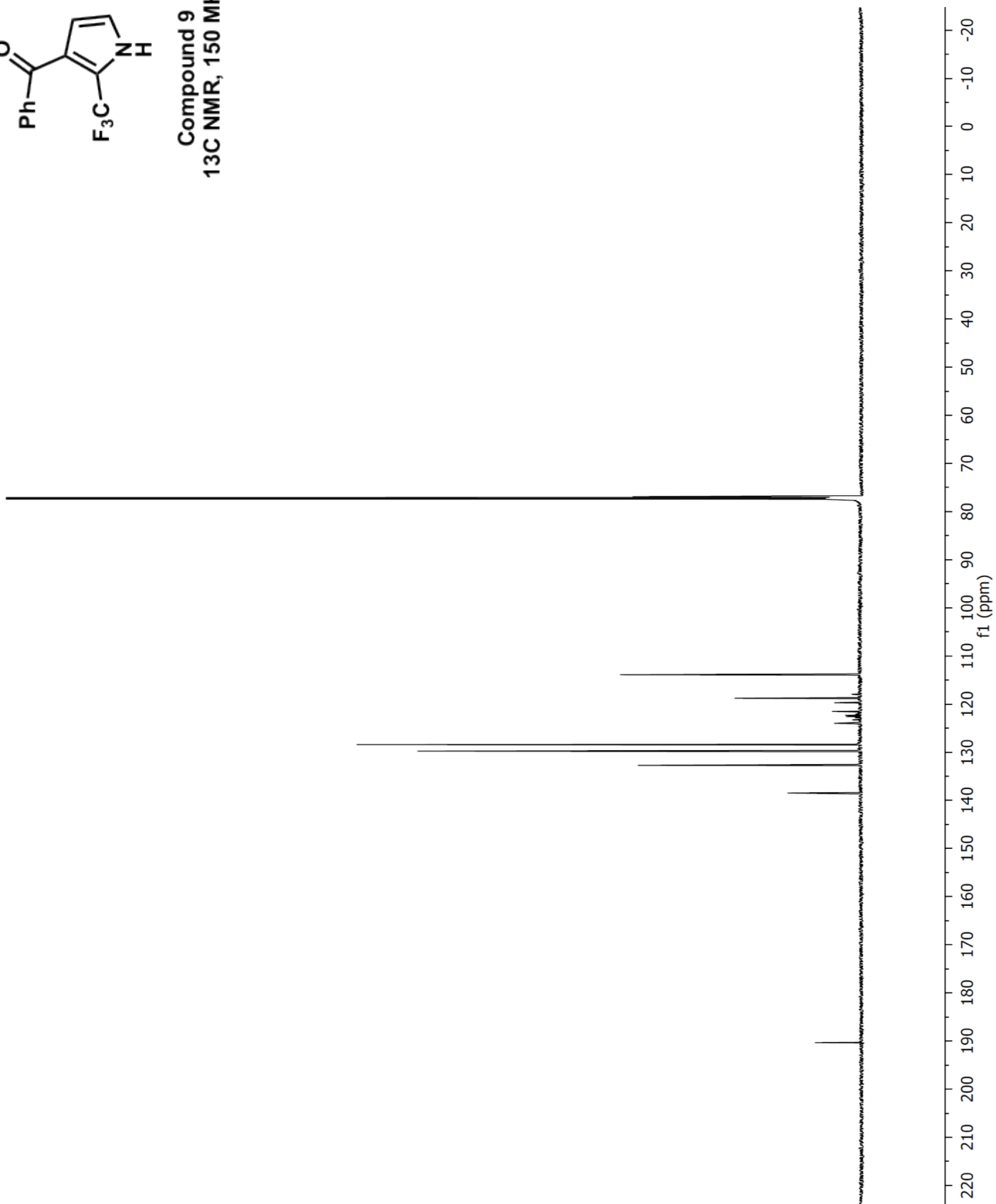


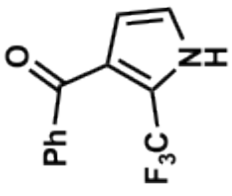
Compound 9  
1H NMR, 400 MHz



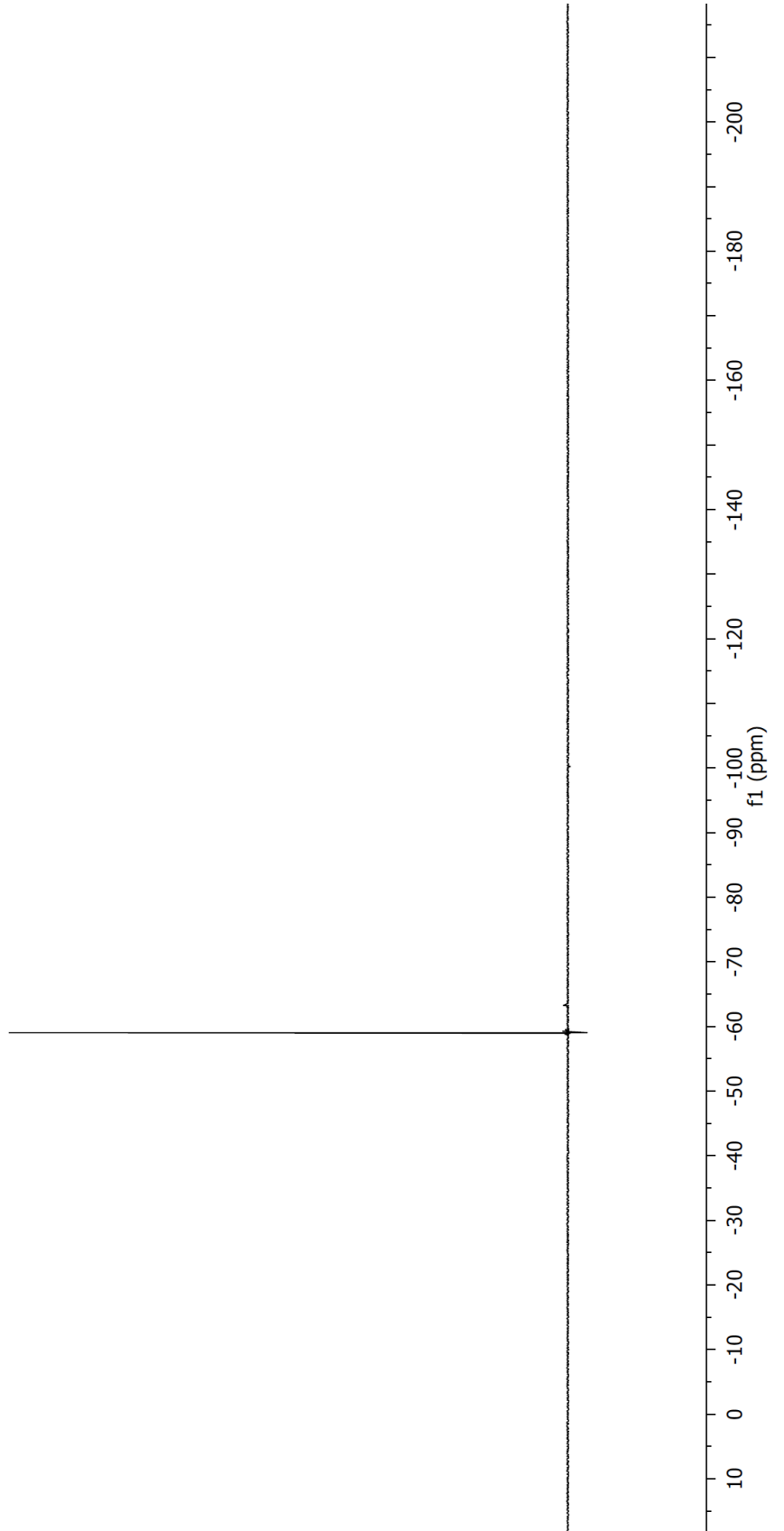


Compound 9  
13C NMR, 150 MHz

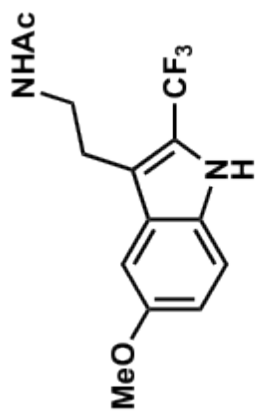




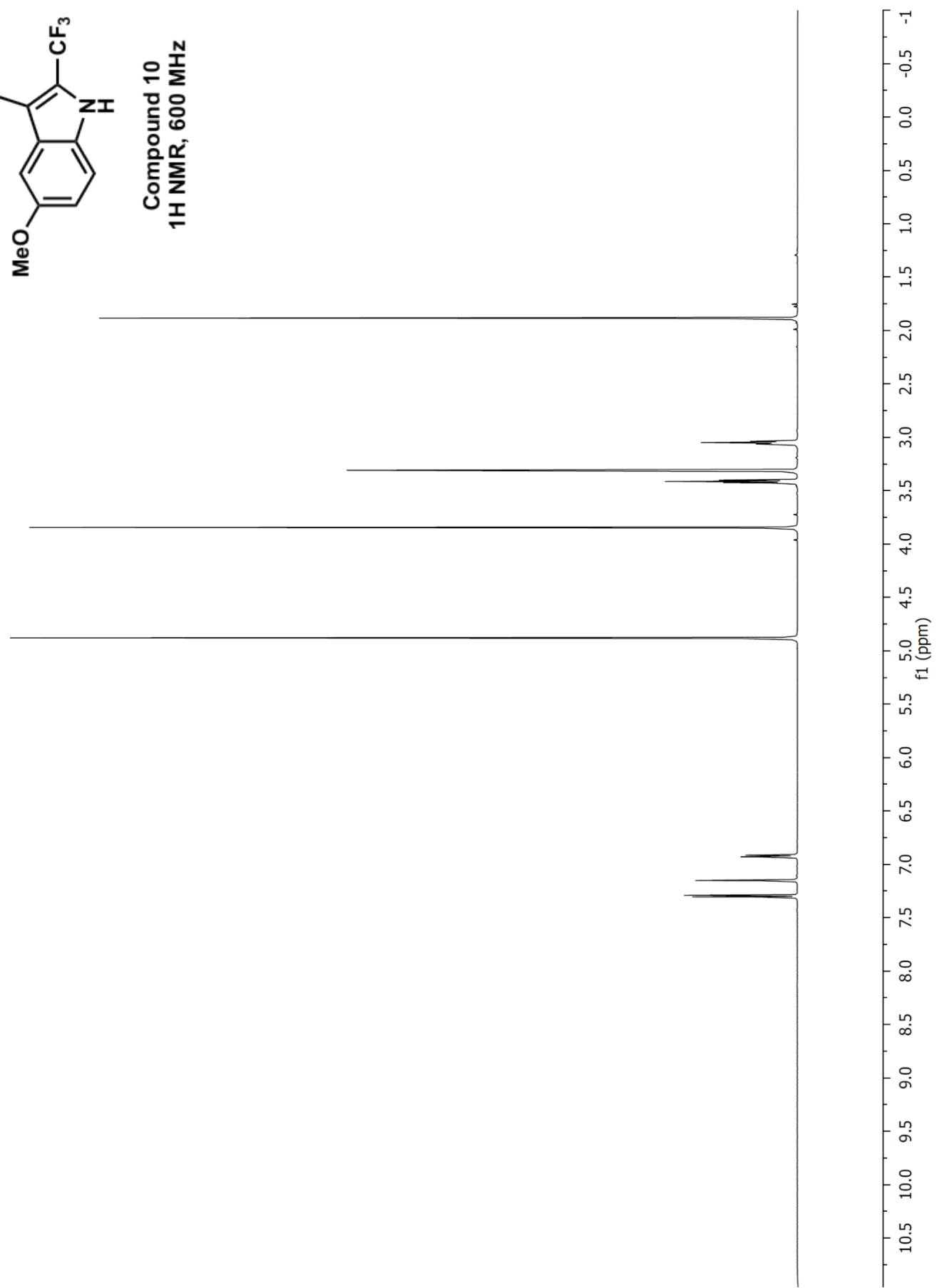
Compound 9  
19F NMR, 376 MHz

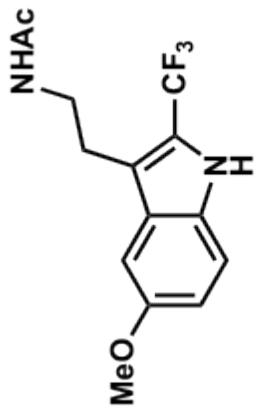




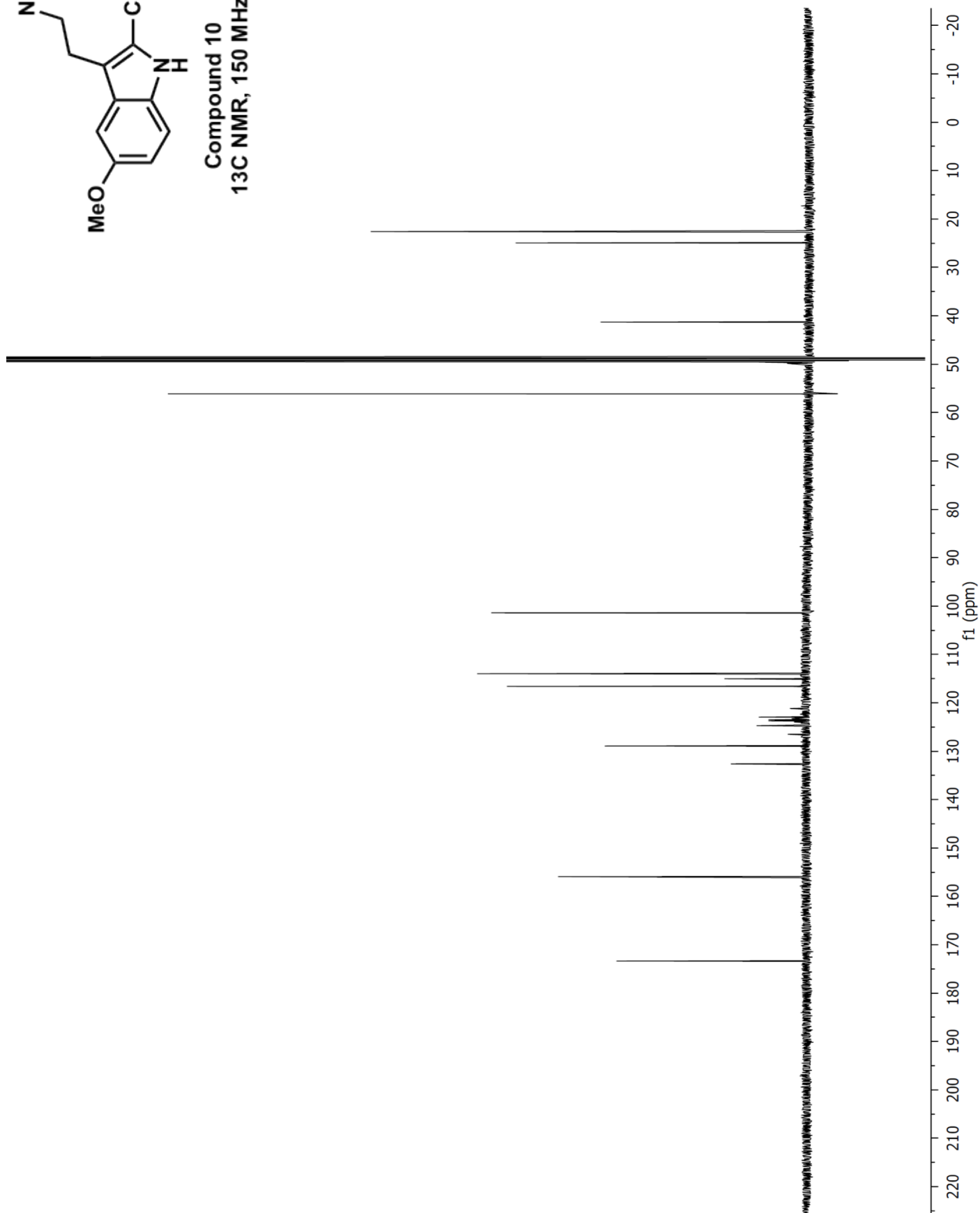


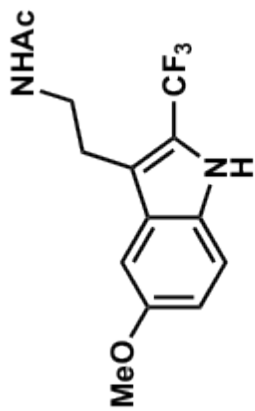
Compound 10  
1H NMR, 600 MHz



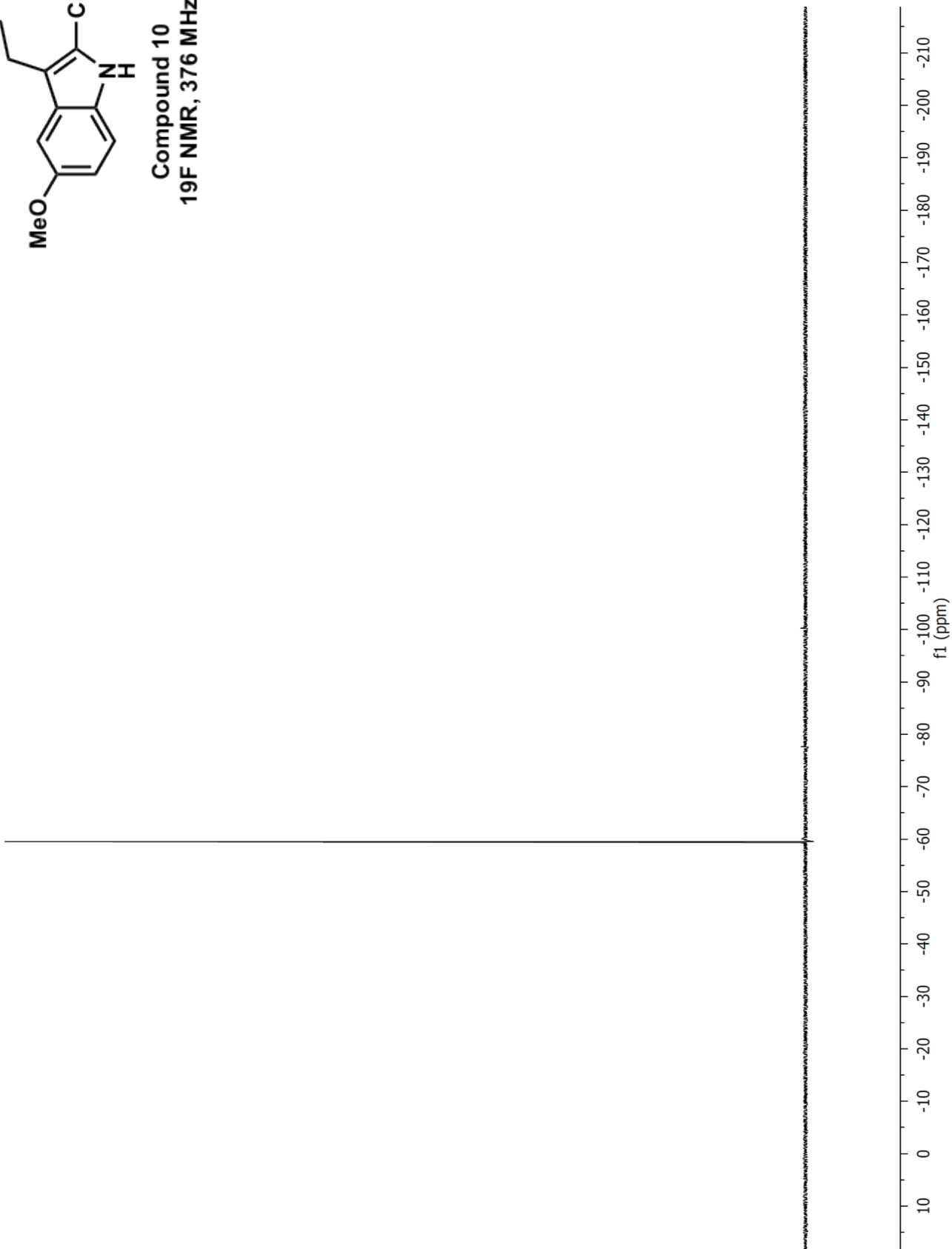


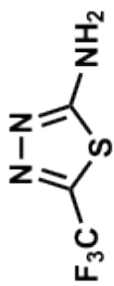
Compound 10  
13C NMR, 150 MHz



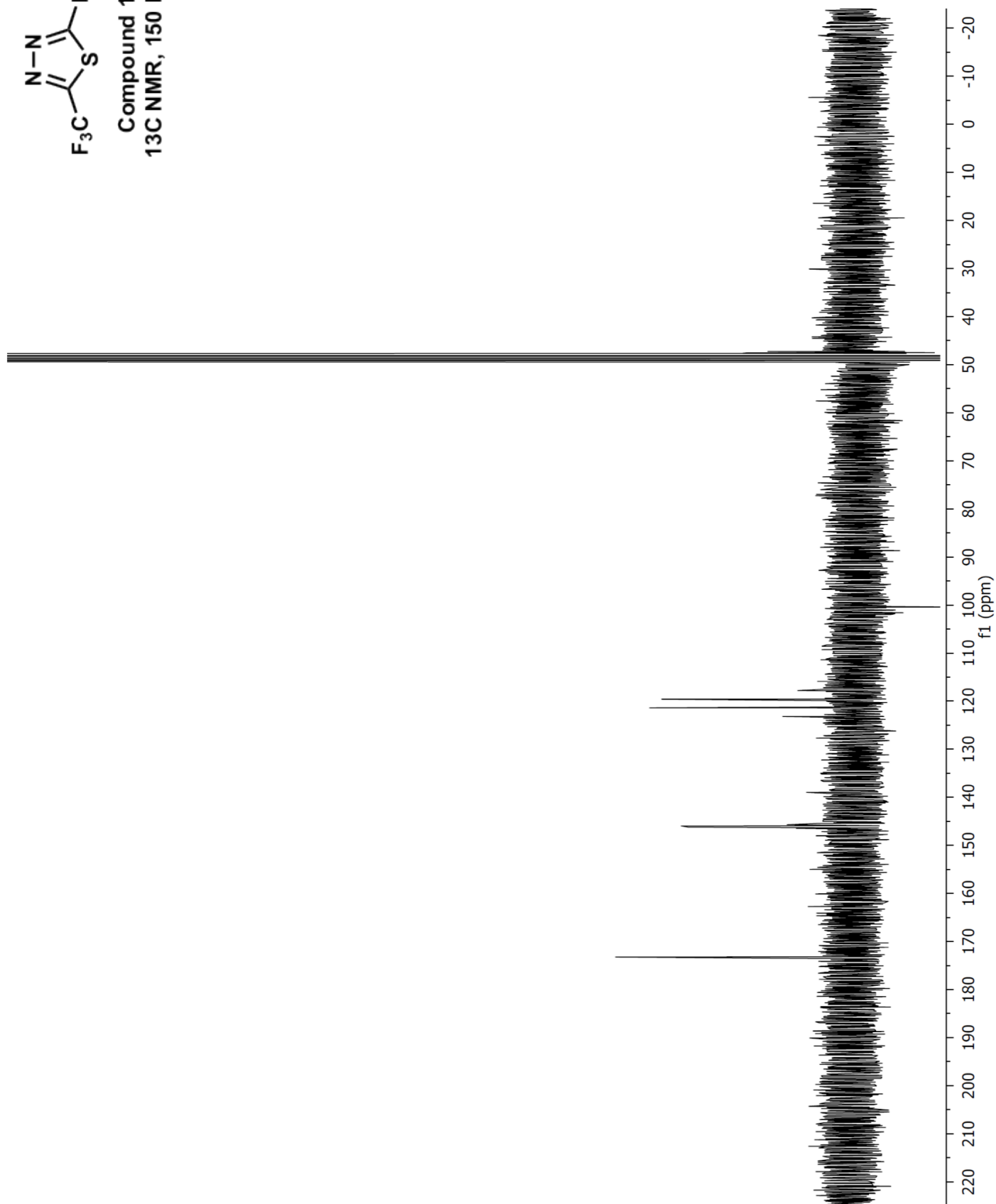


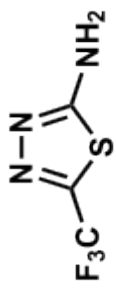
Compound 10  
19F NMR, 376 MHz



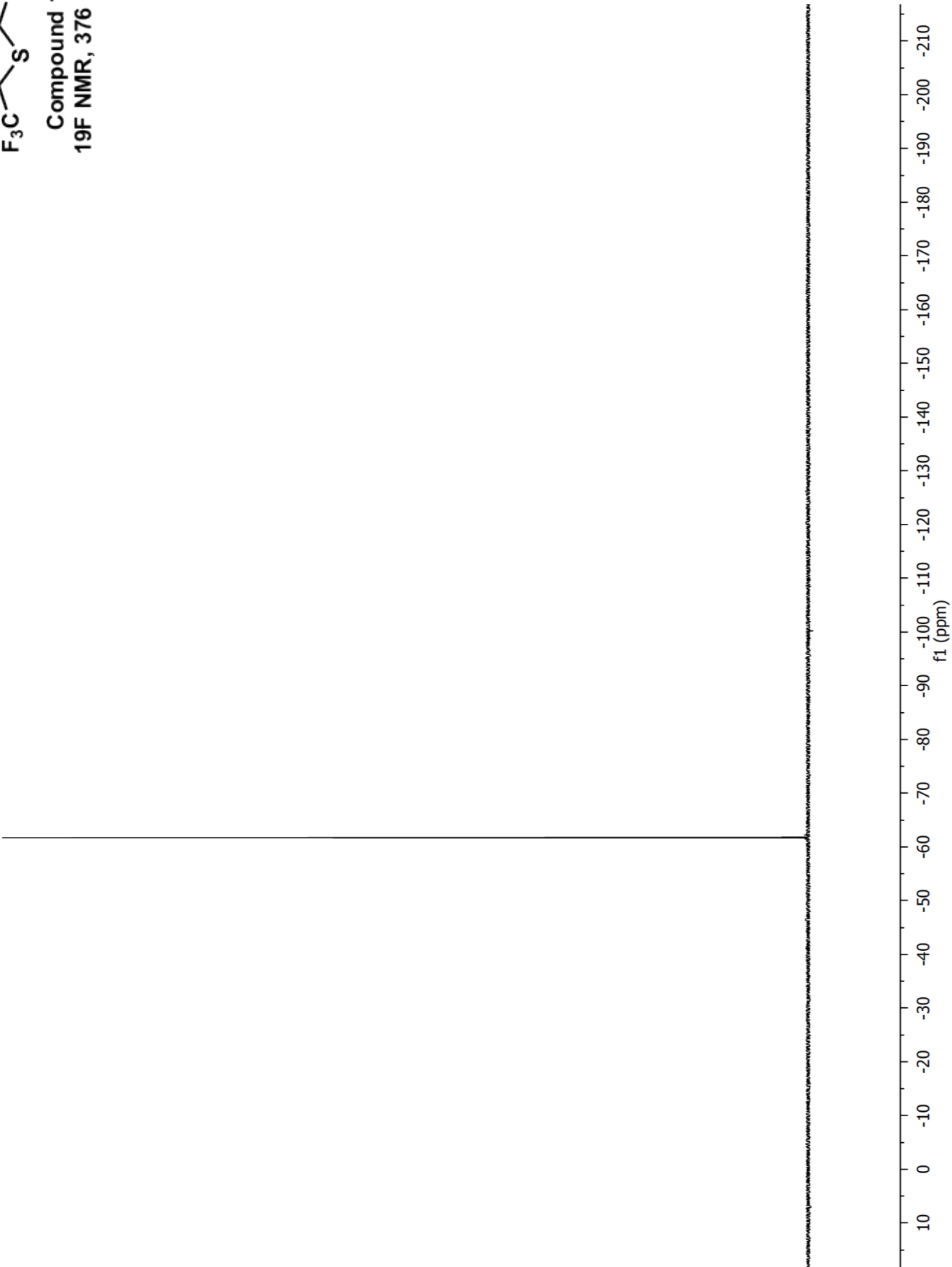


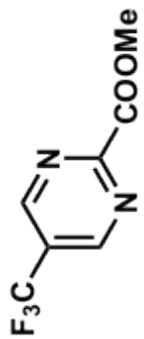
Compound 11  
13C NMR, 150 MHz



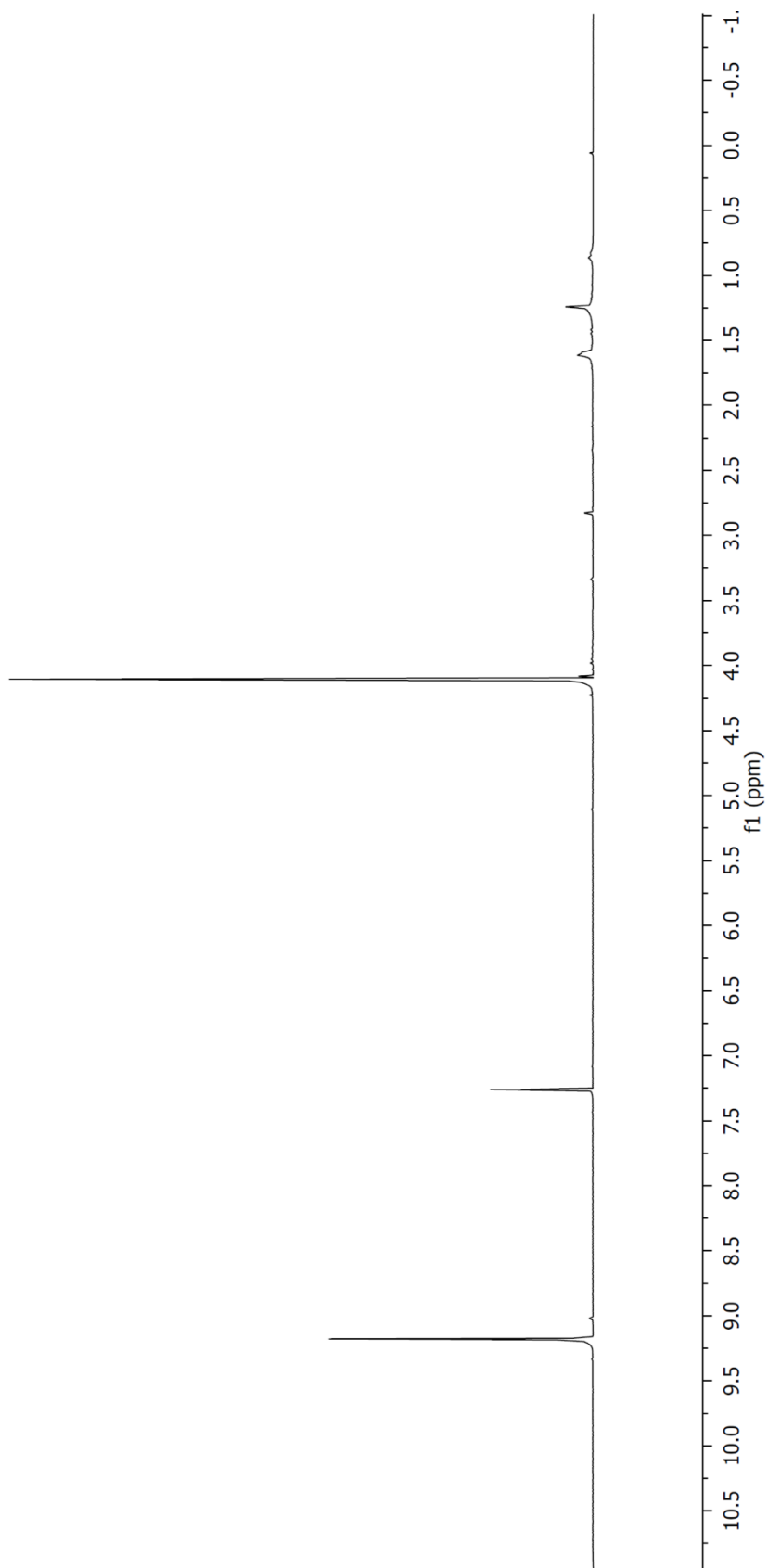


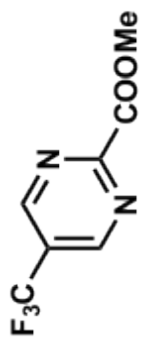
Compound 11  
19F NMR, 376 MHz



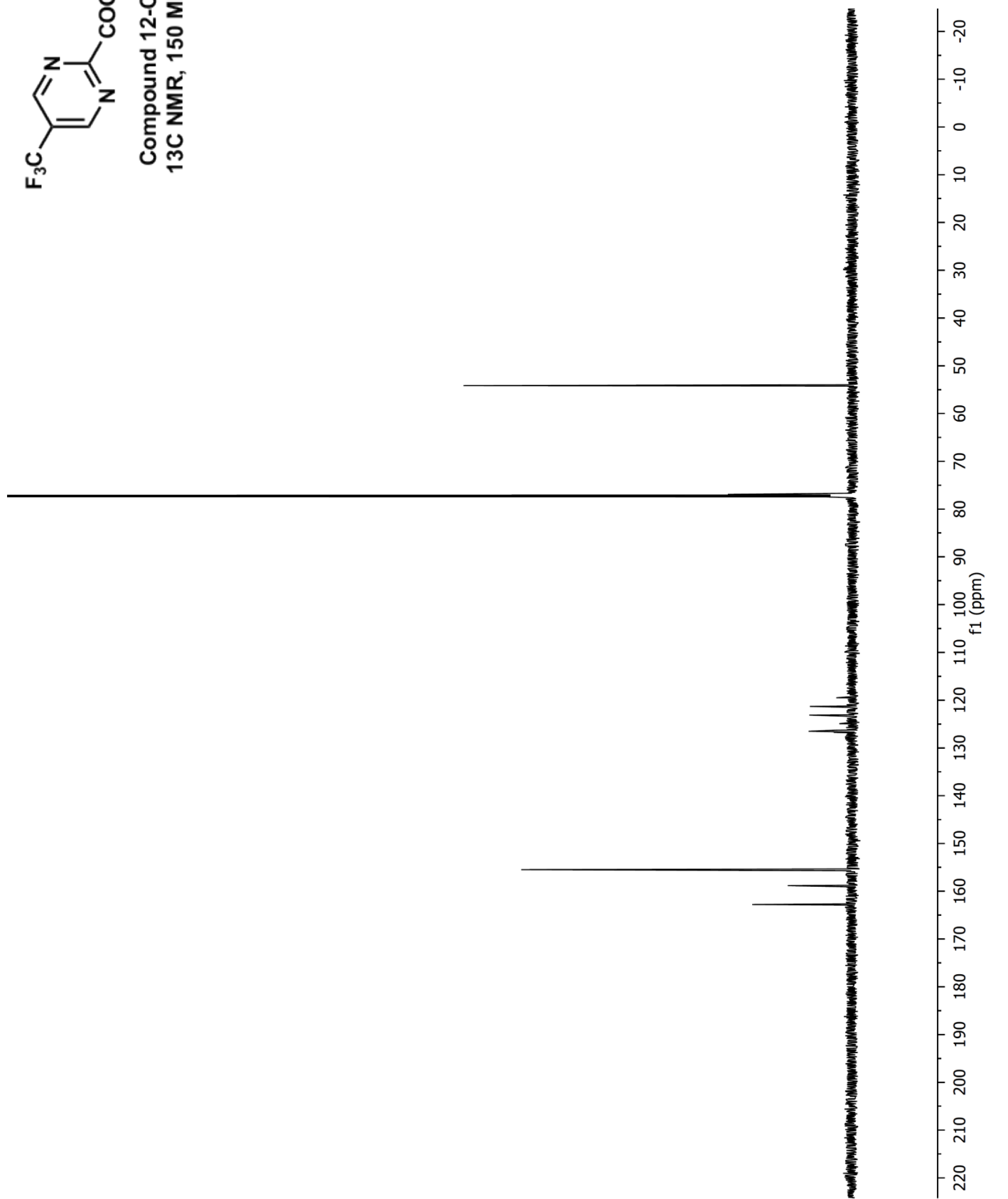


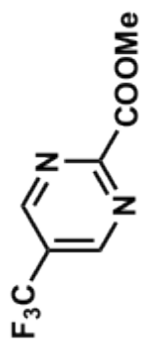
Compound 12-C5  
1H NMR, 400 MHz



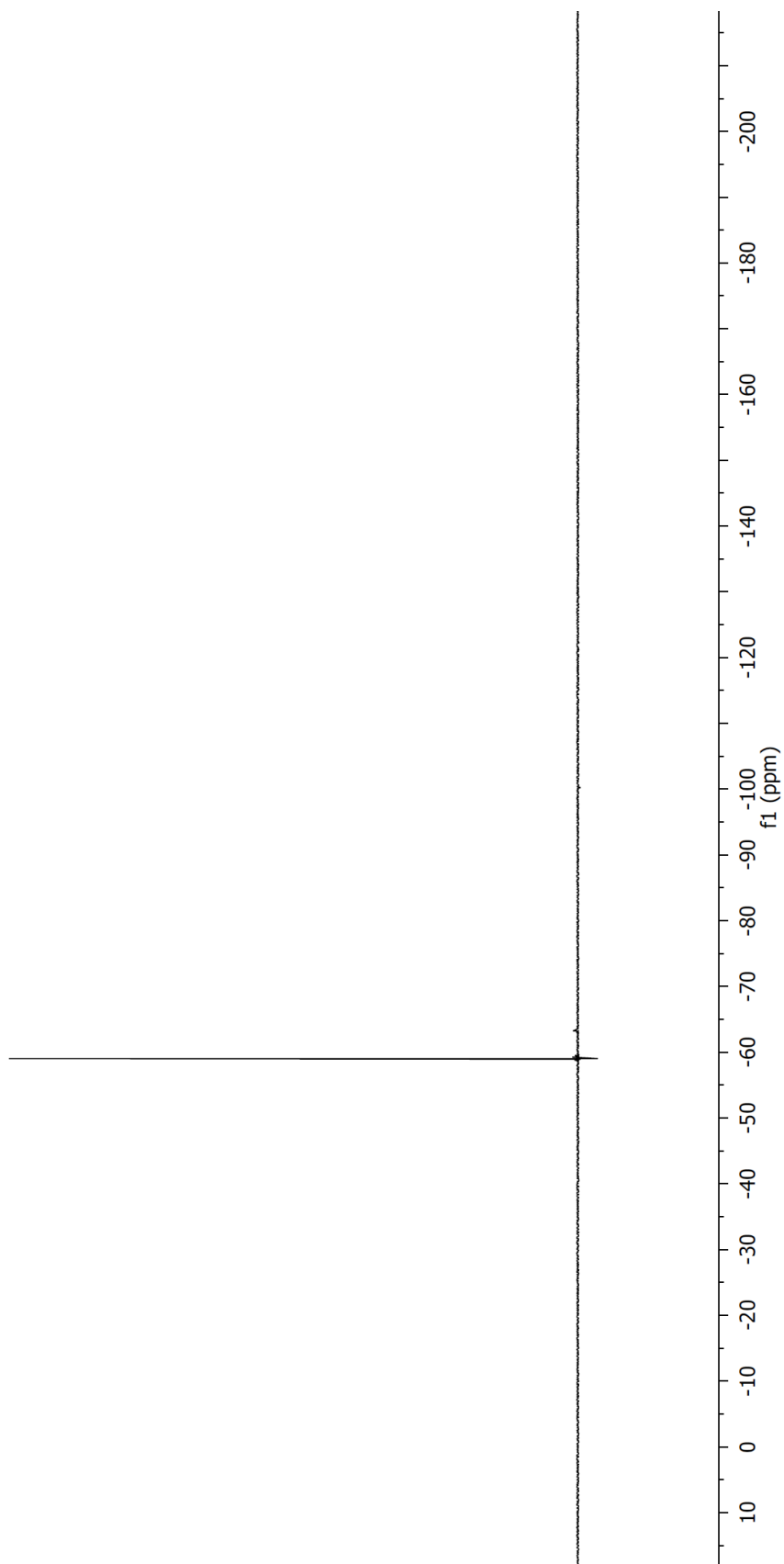


Compound 12-C5  
13C NMR, 150 MHz

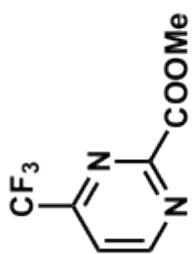




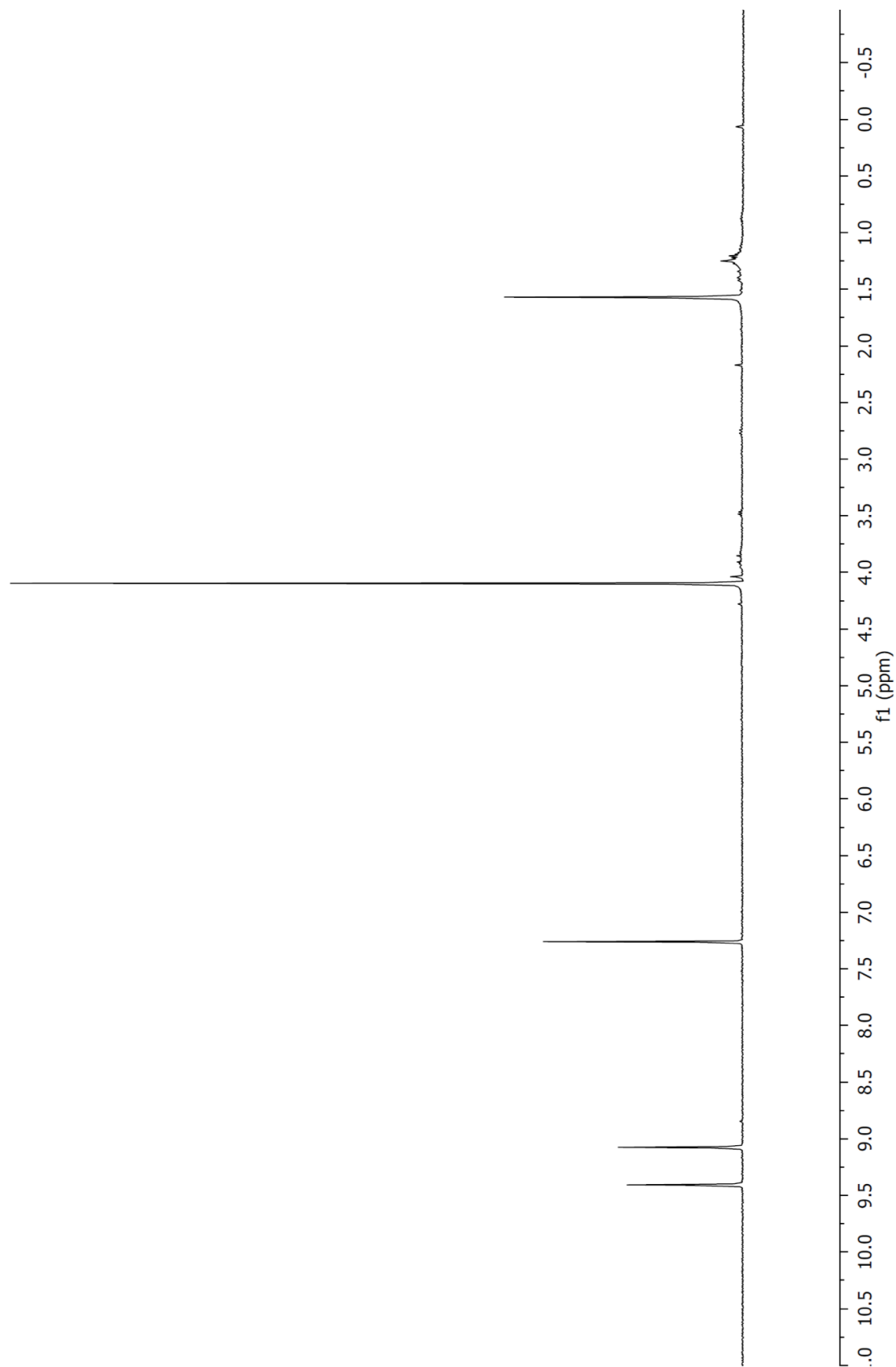
Compound 12-C5  
19F NMR, 376 MHz

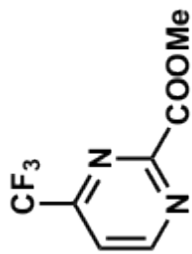




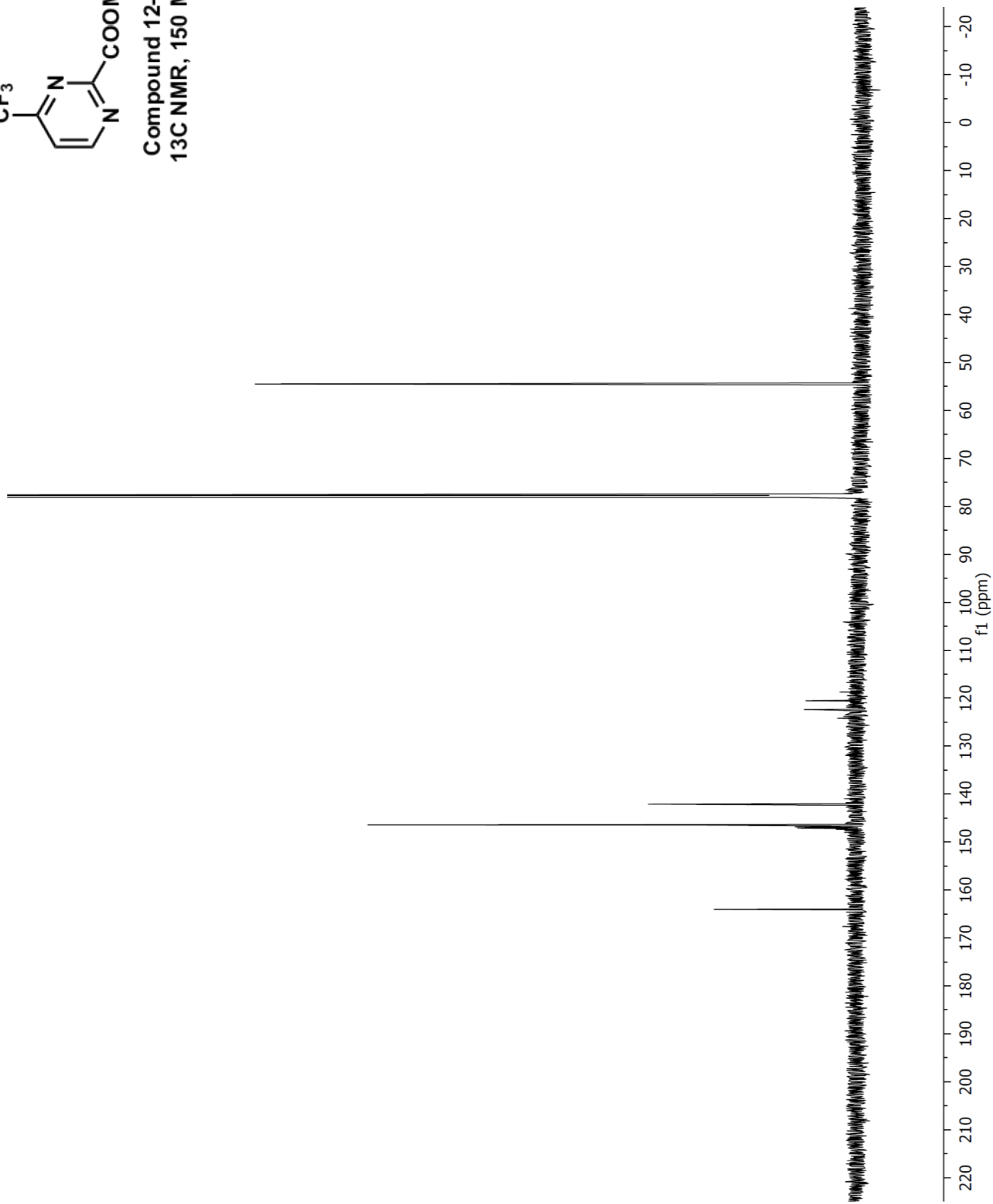


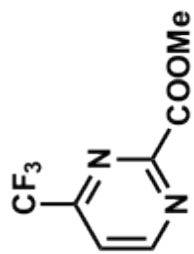
Compound 12-C4  
1H NMR, 400 MHz



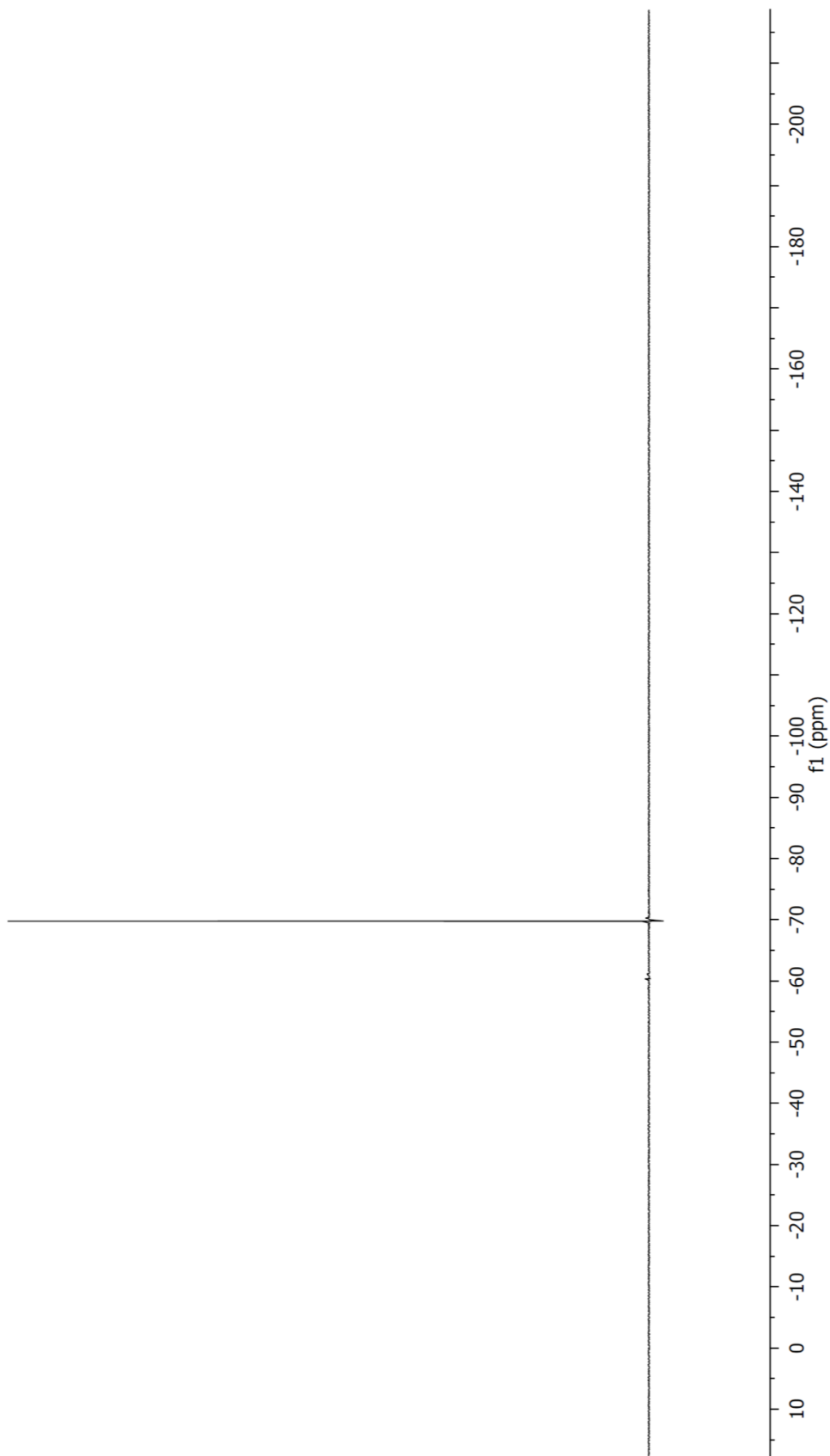


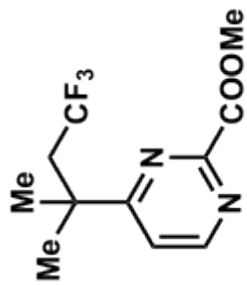
Compound 12-C4  
13C NMR, 150 MHz



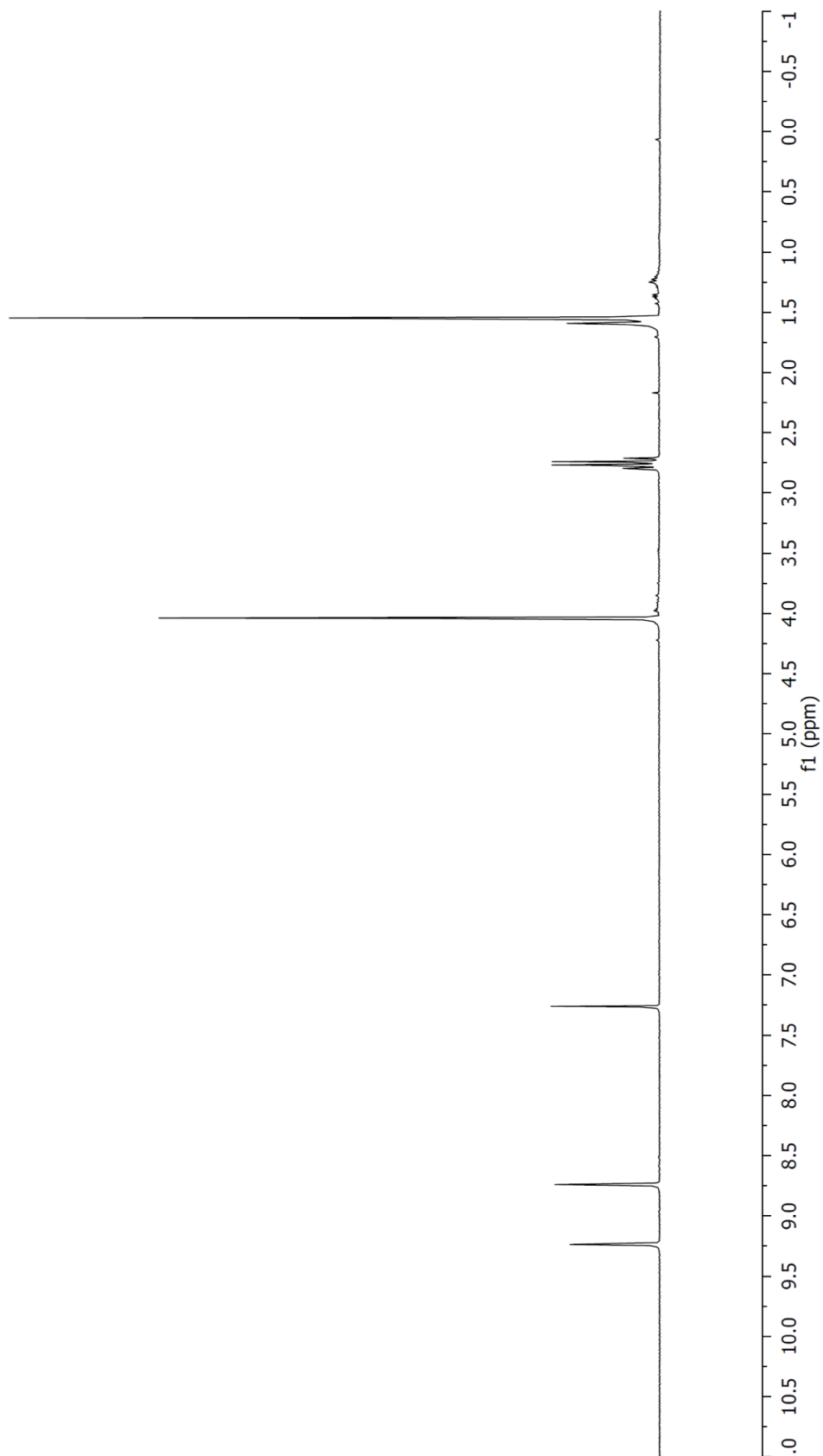


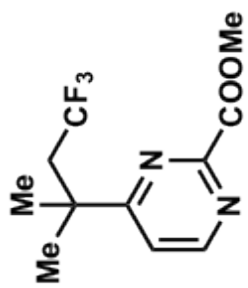
Compound 12-C4  
19F NMR, 376 MHz



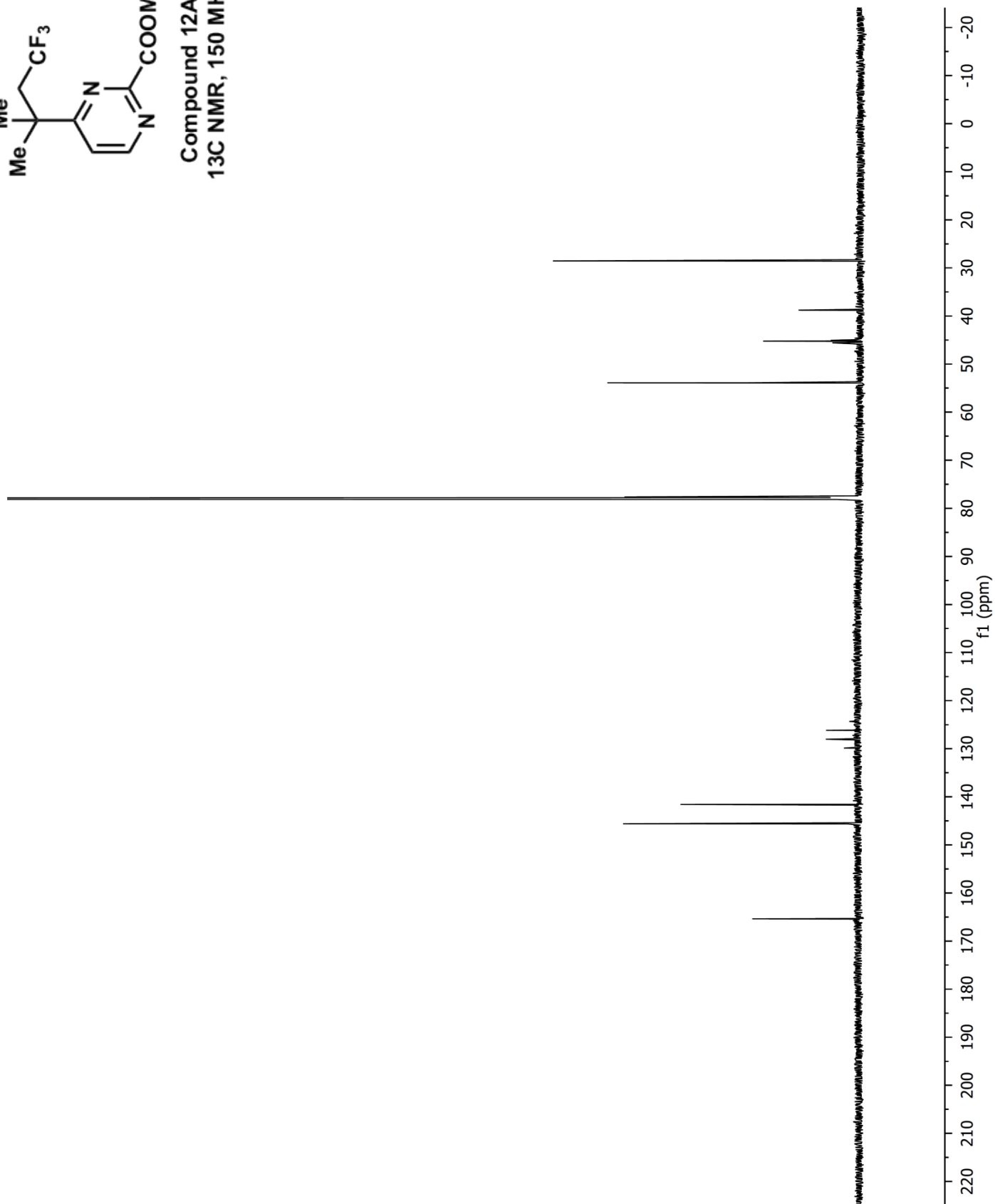


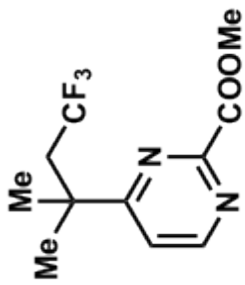
Compound 12A  
1H NMR, 400 MHz



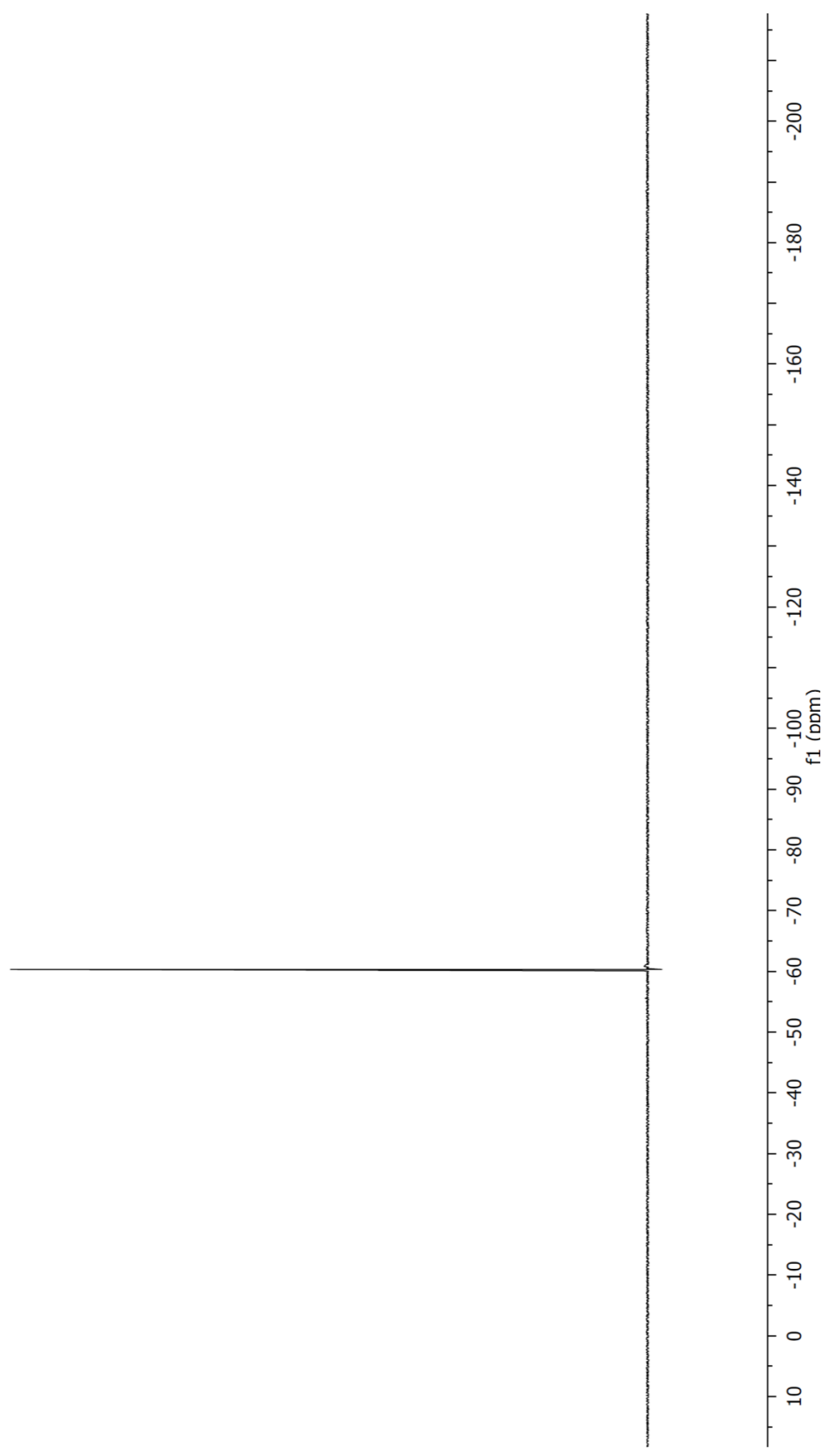


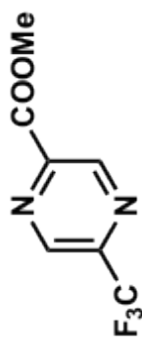
Compound 12A  
13C NMR, 150 MHz



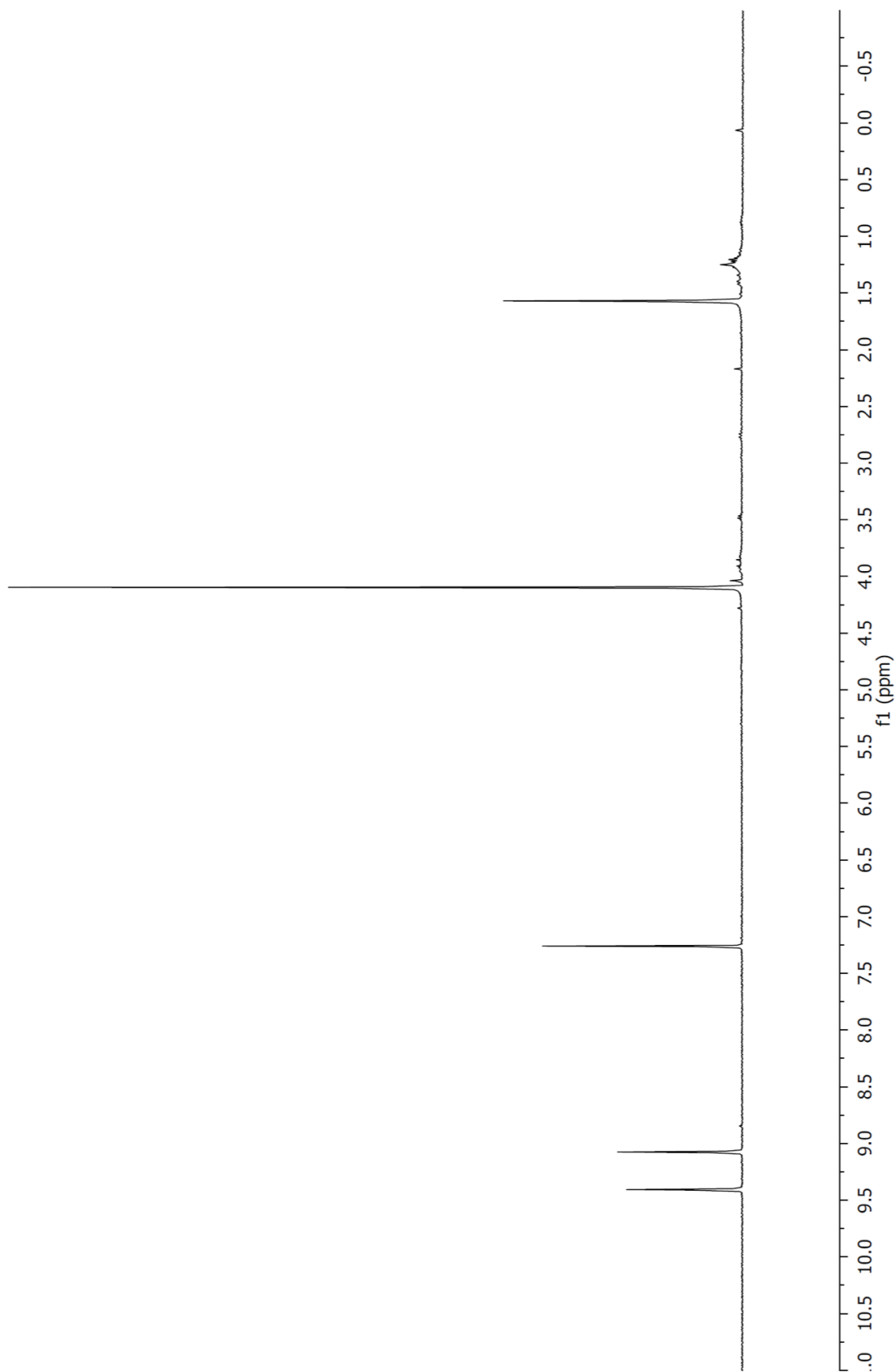


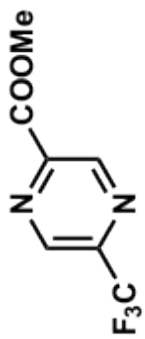
Compound 12A  
19F NMR, 376 MHz





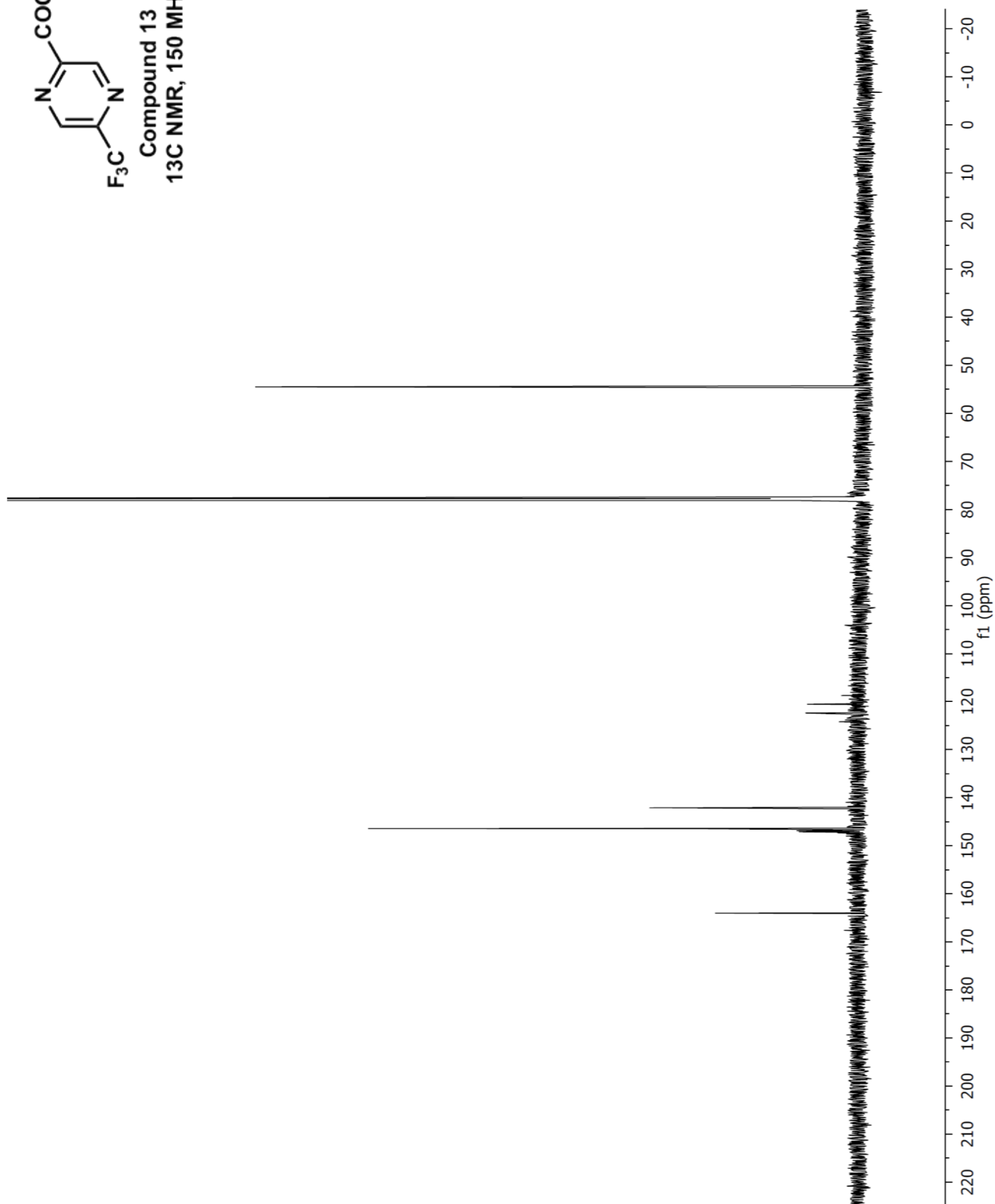
Compound 13  
1H NMR, 400 MHz



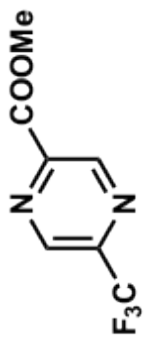


Compound 13

$^{13}\text{C}$  NMR, 150 MHz

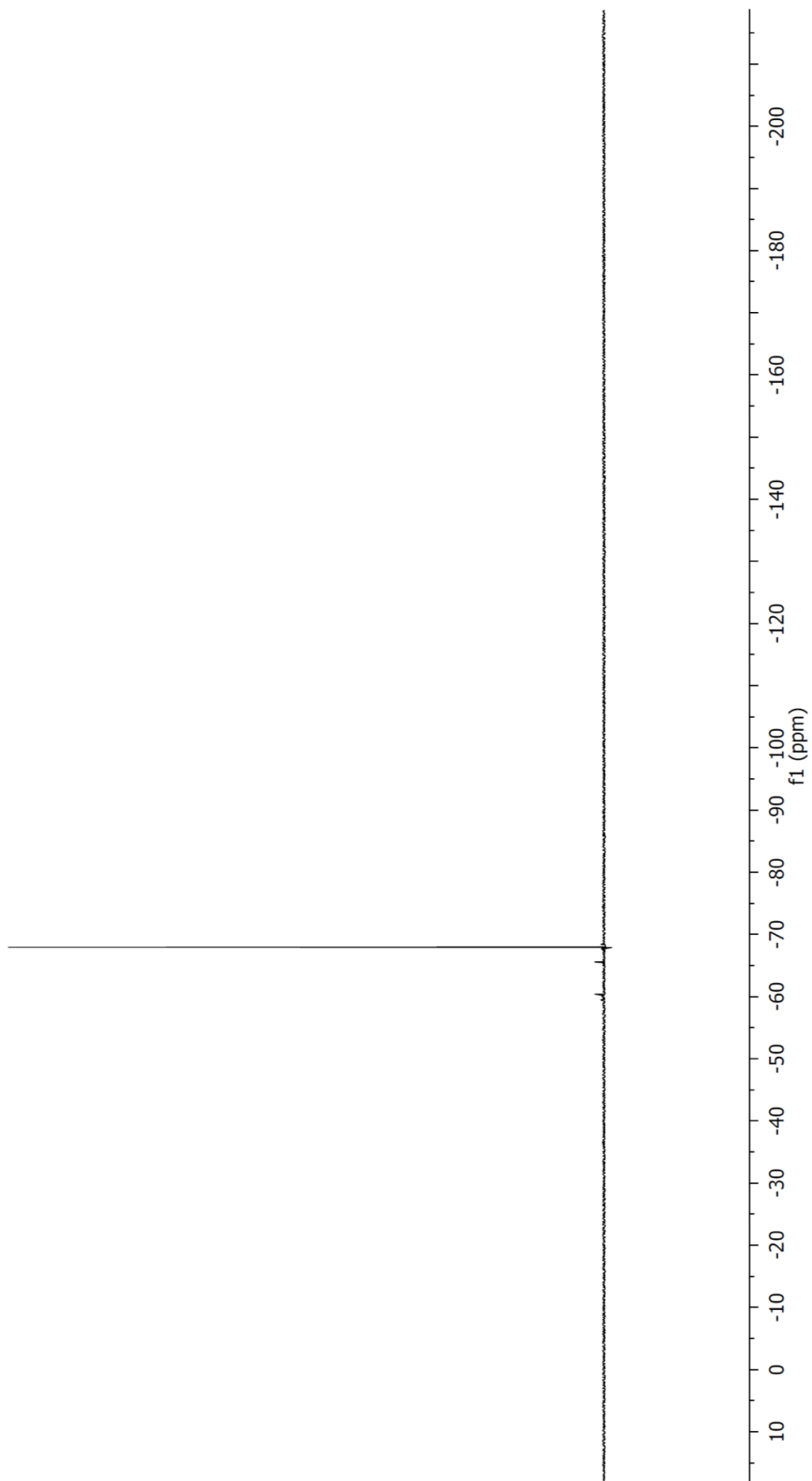


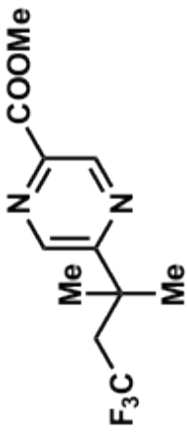




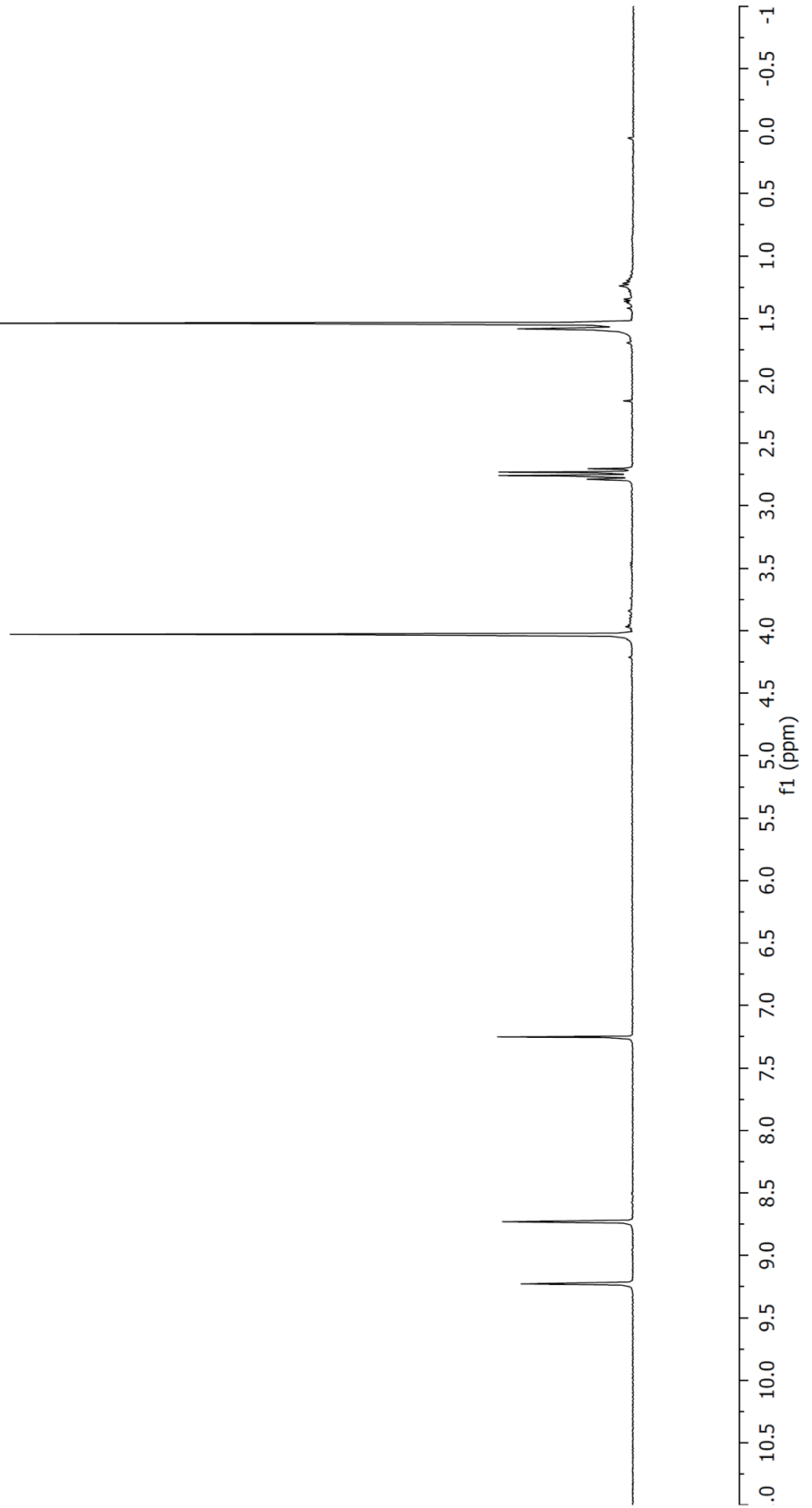
Compound 13

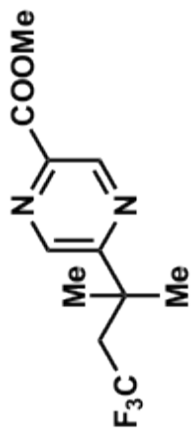
$^{19}\text{F}$  NMR, 376 MHz



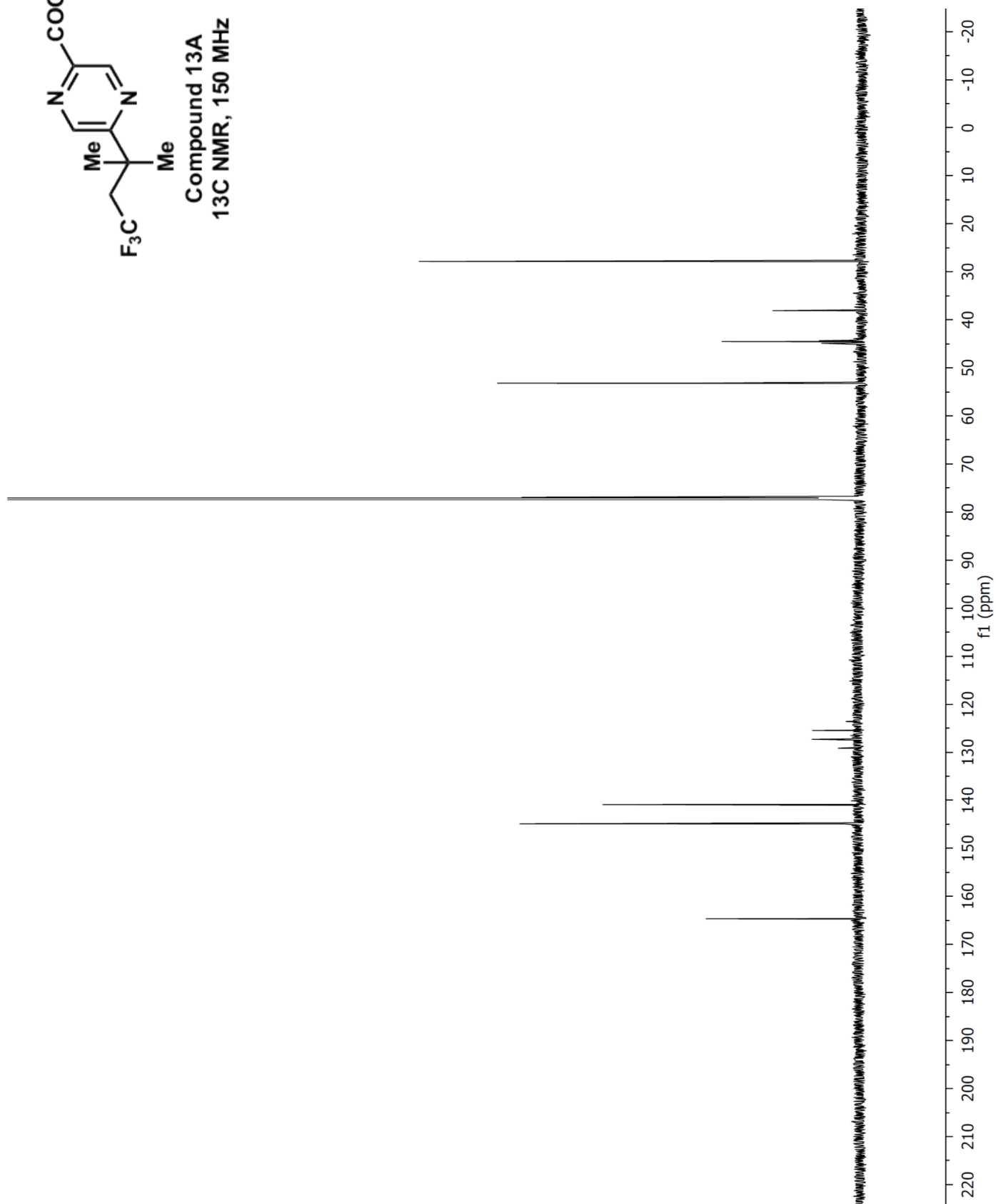


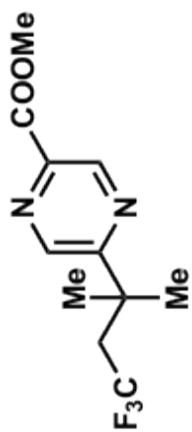
Compound 13A  
1H NMR, 400 MHz



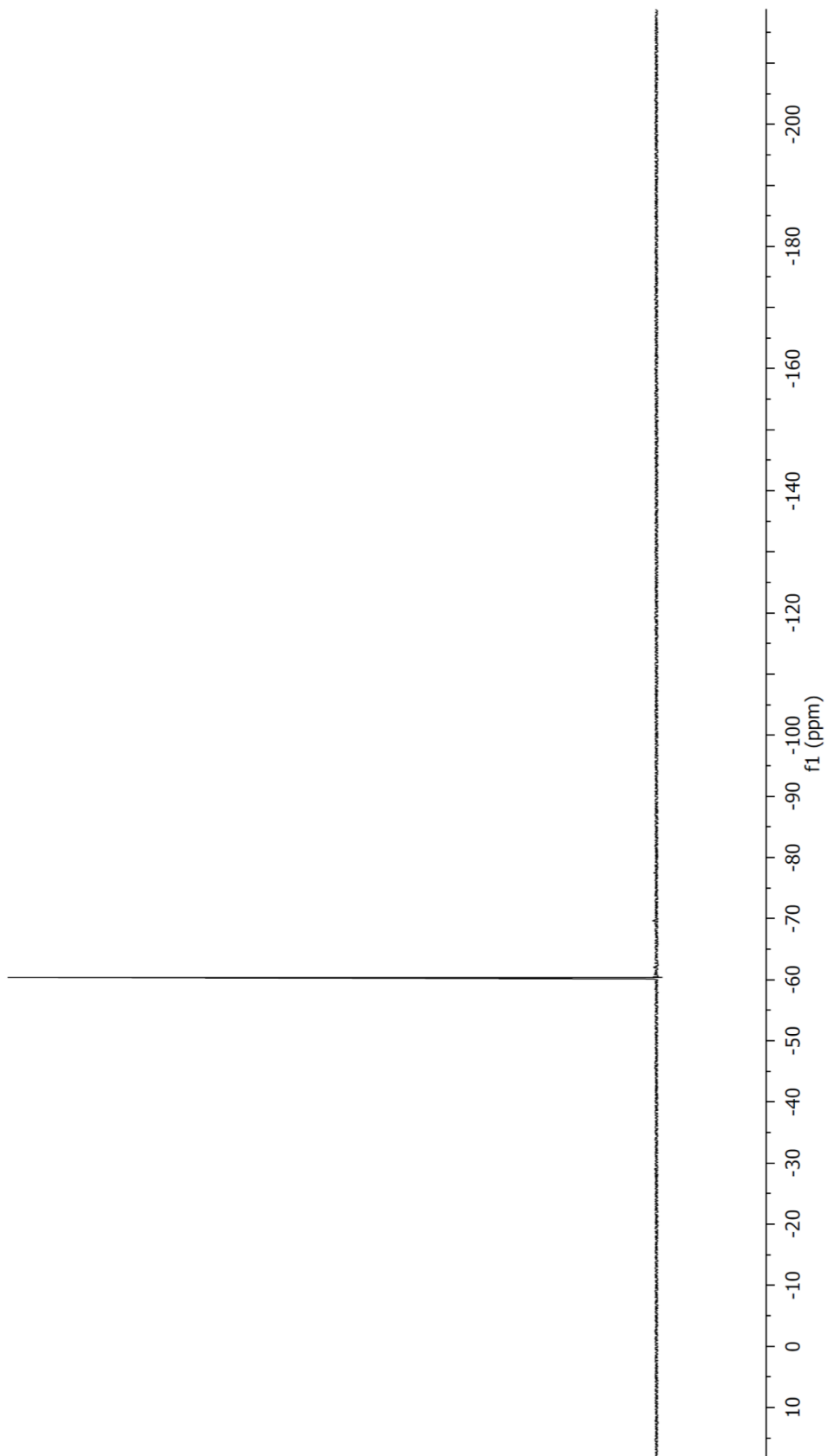


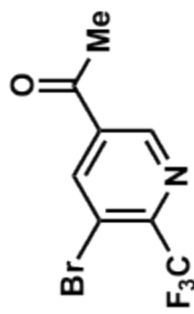
Compound 13A  
13C NMR, 150 MHz



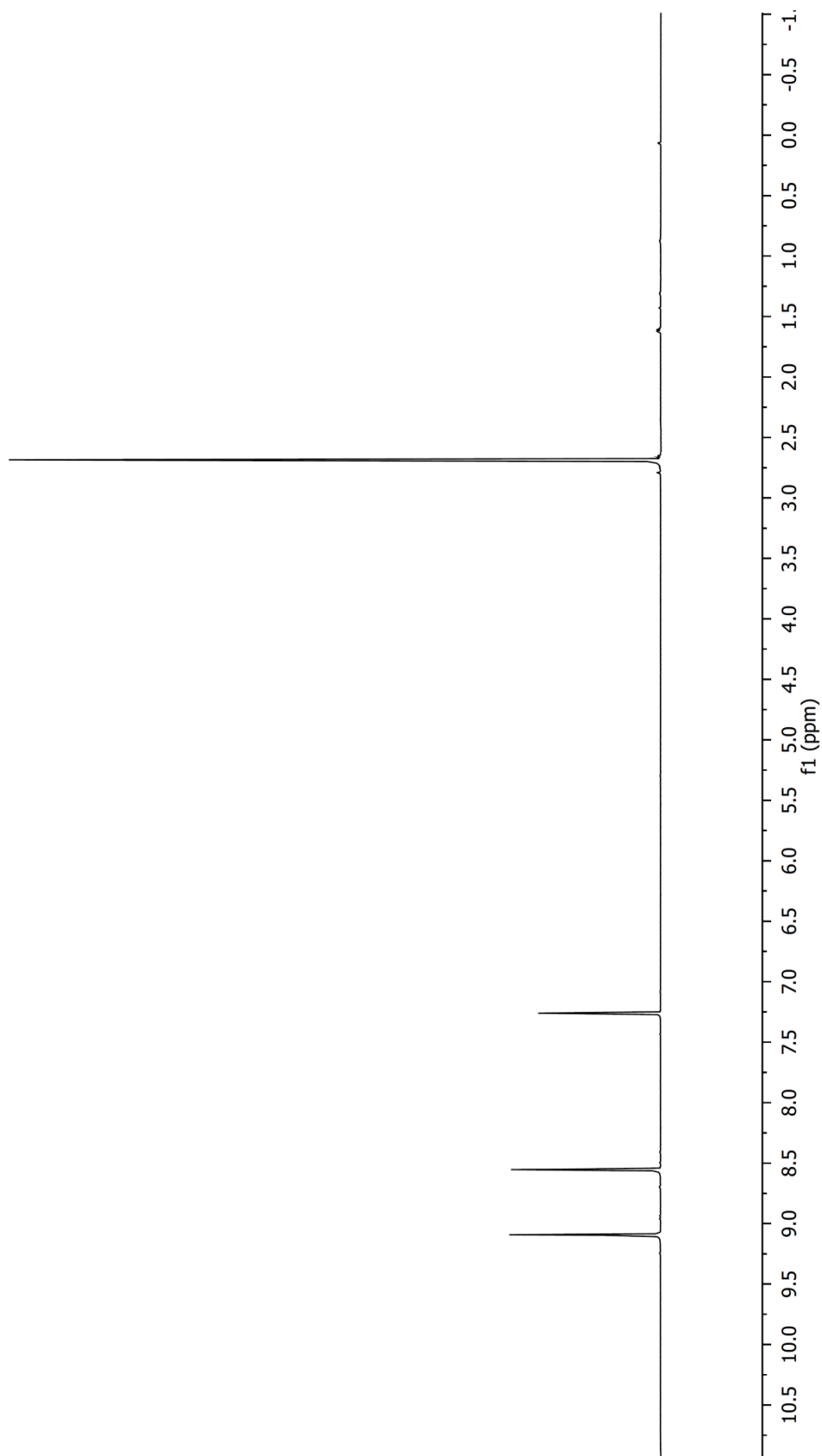


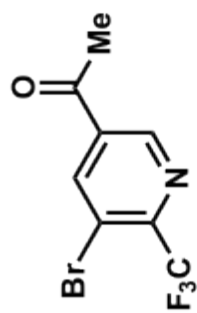
Compound 13A  
19F NMR, 376 MHz



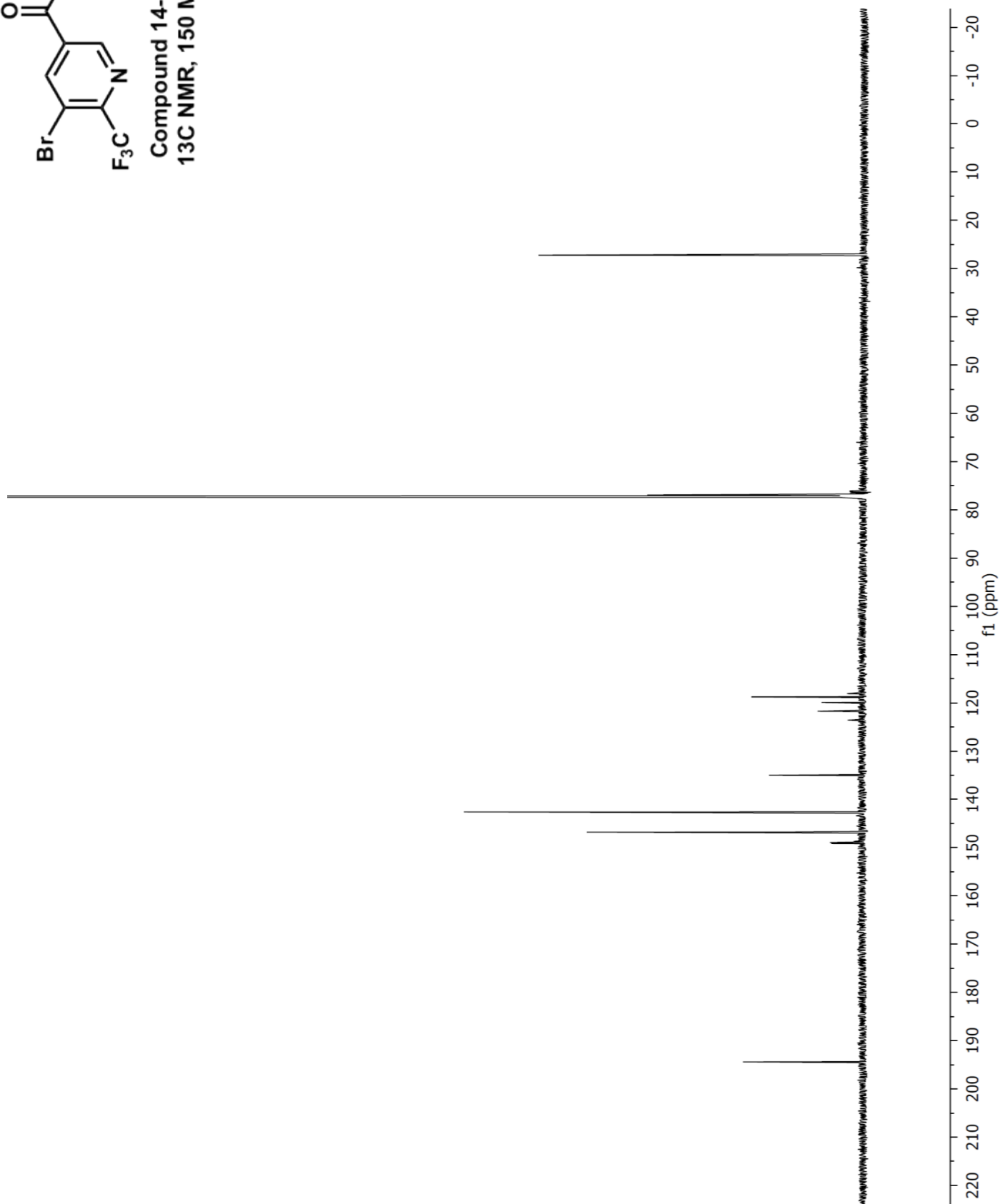


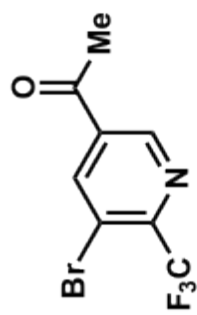
Compound 14-C2  
1H NMR, 400 MHz



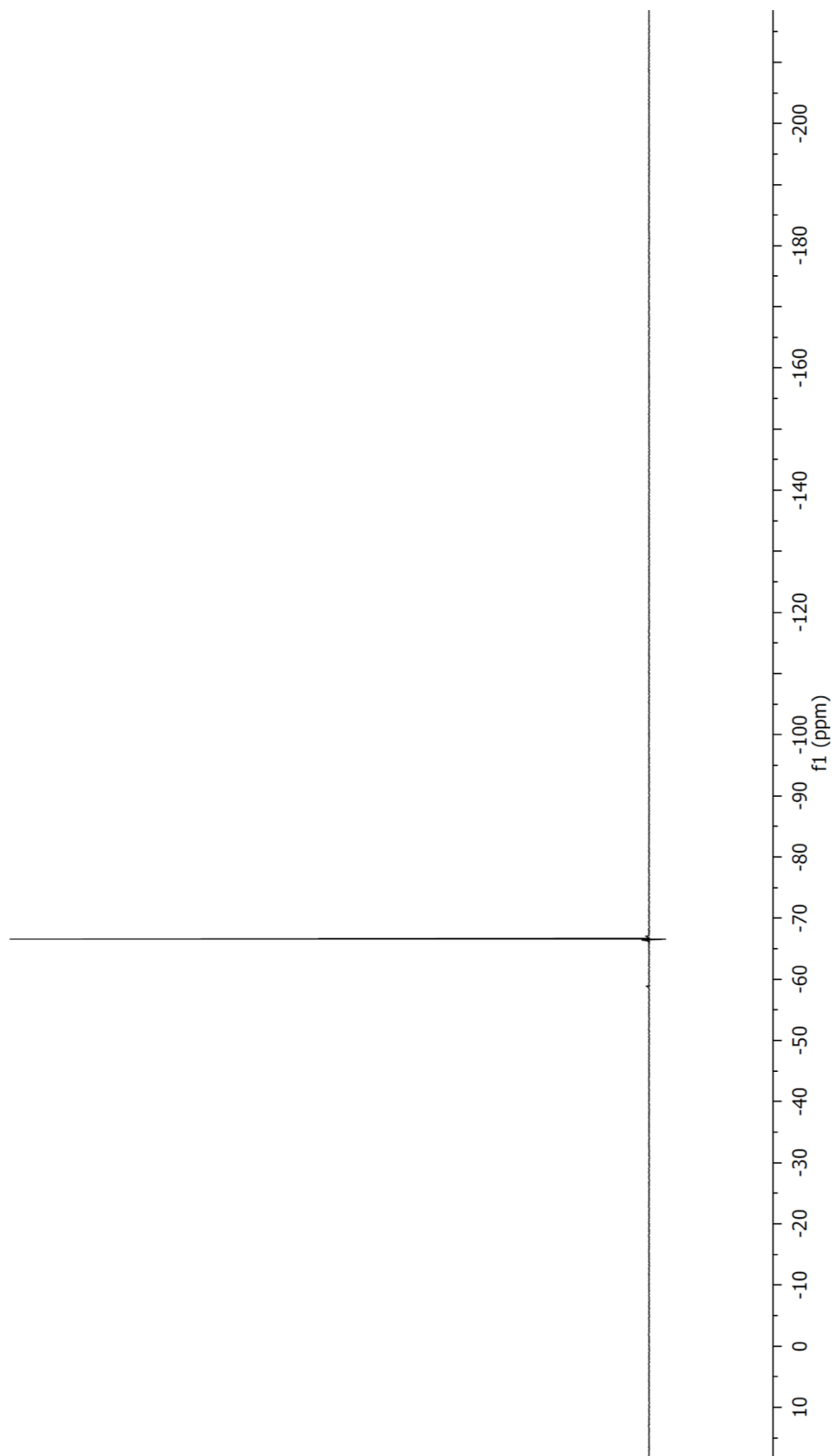


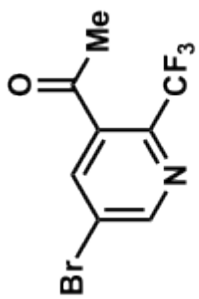
Compound 14-C2  
13C NMR, 150 MHz



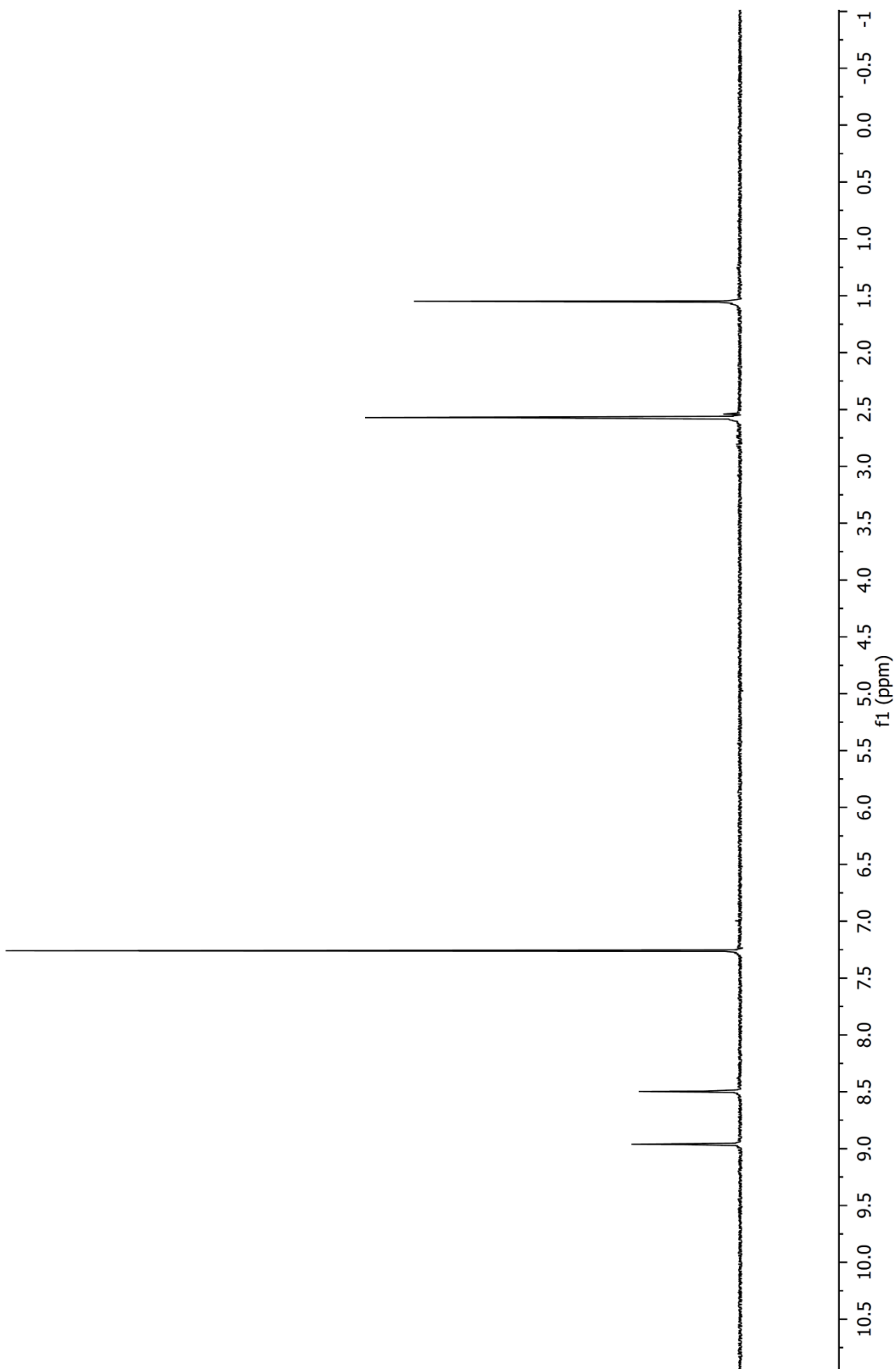


Compound 14-C2  
19F NMR, 376 MHz

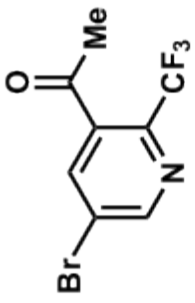




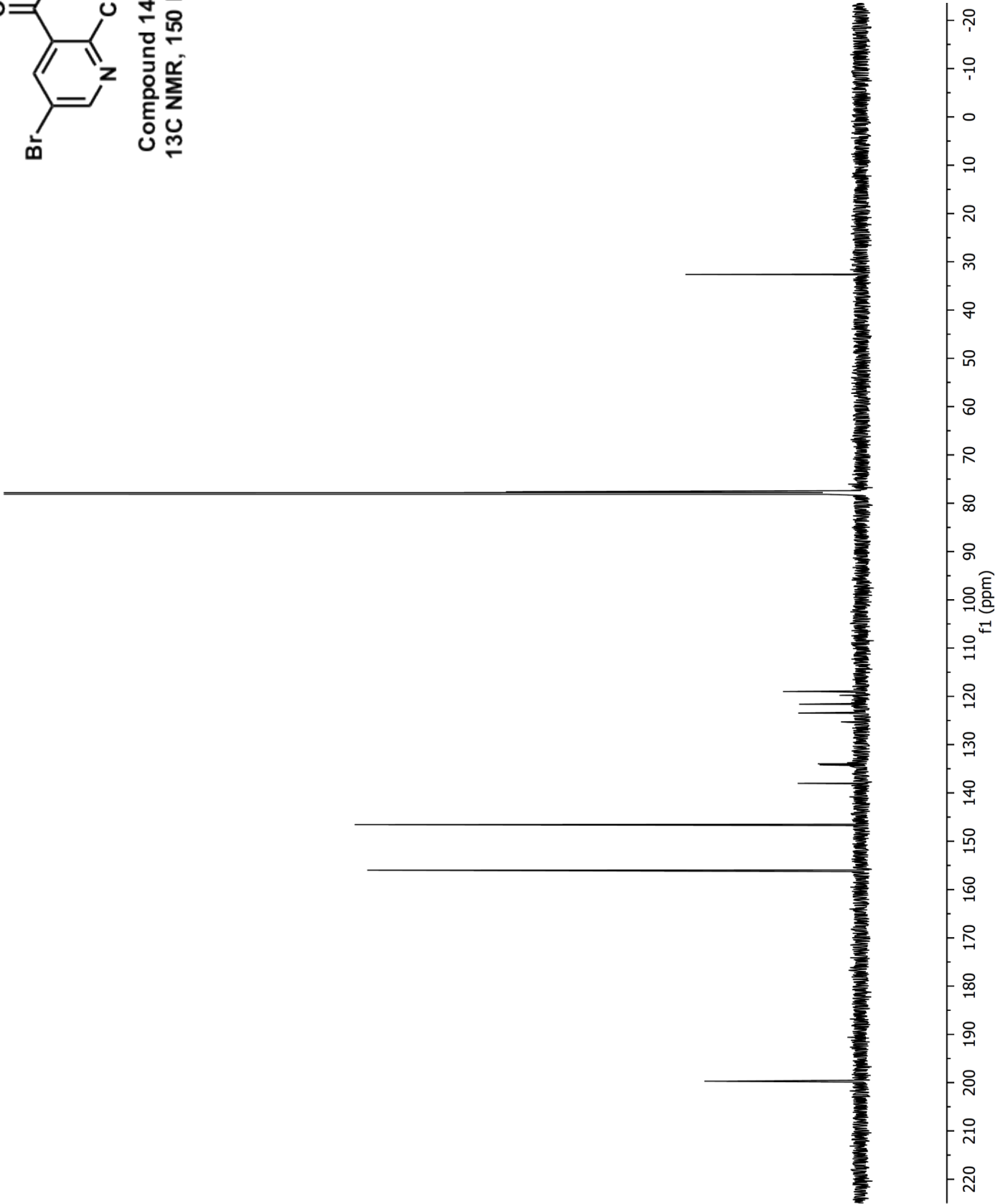
Compound 14-C6  
1H NMR, 400 MHz

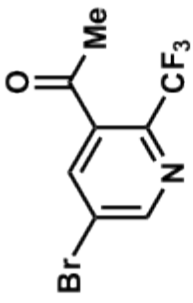




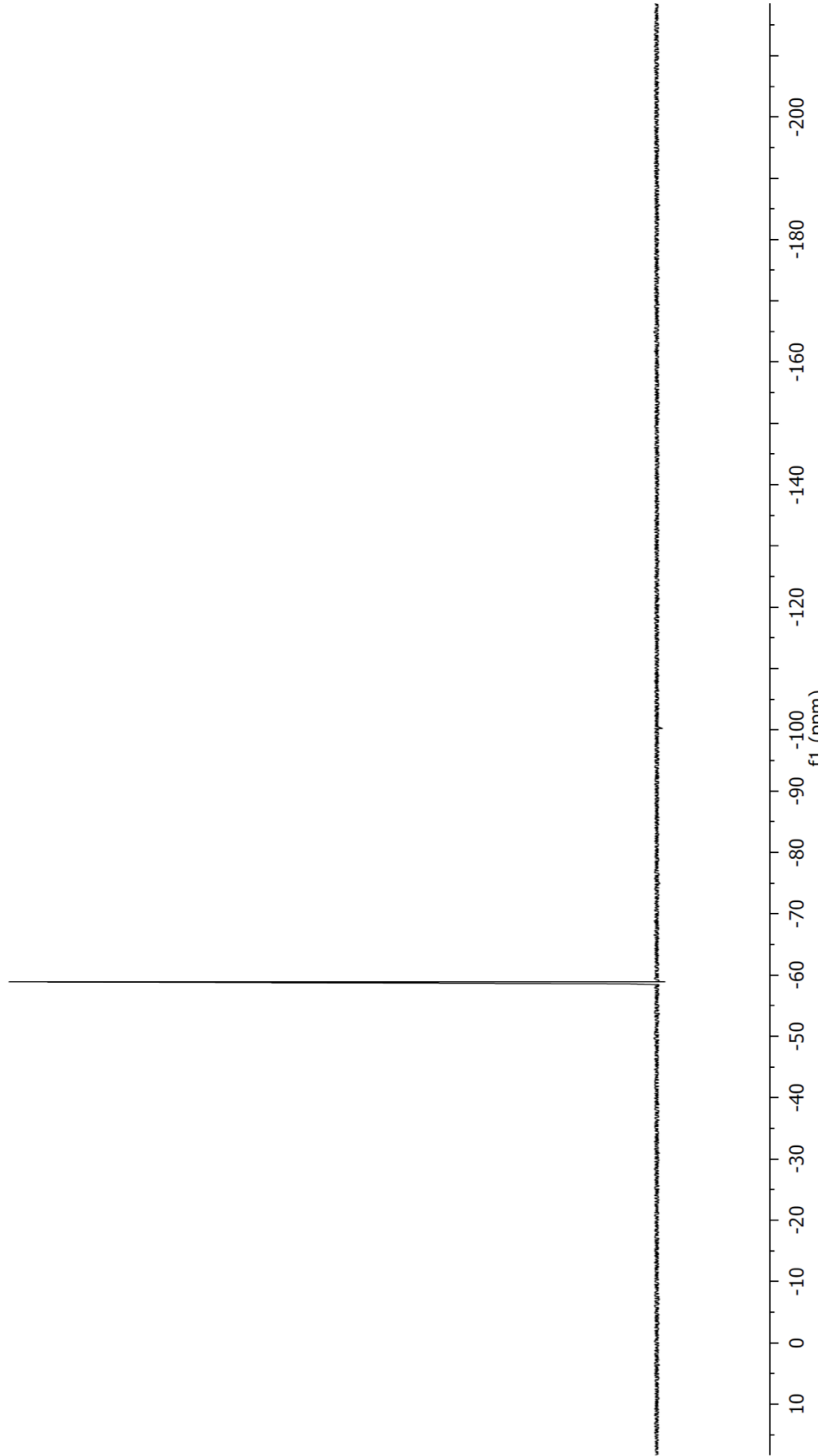


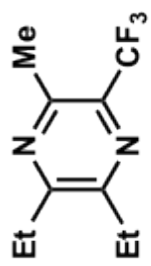
Compound 14-C6  
13C NMR, 150 MHz



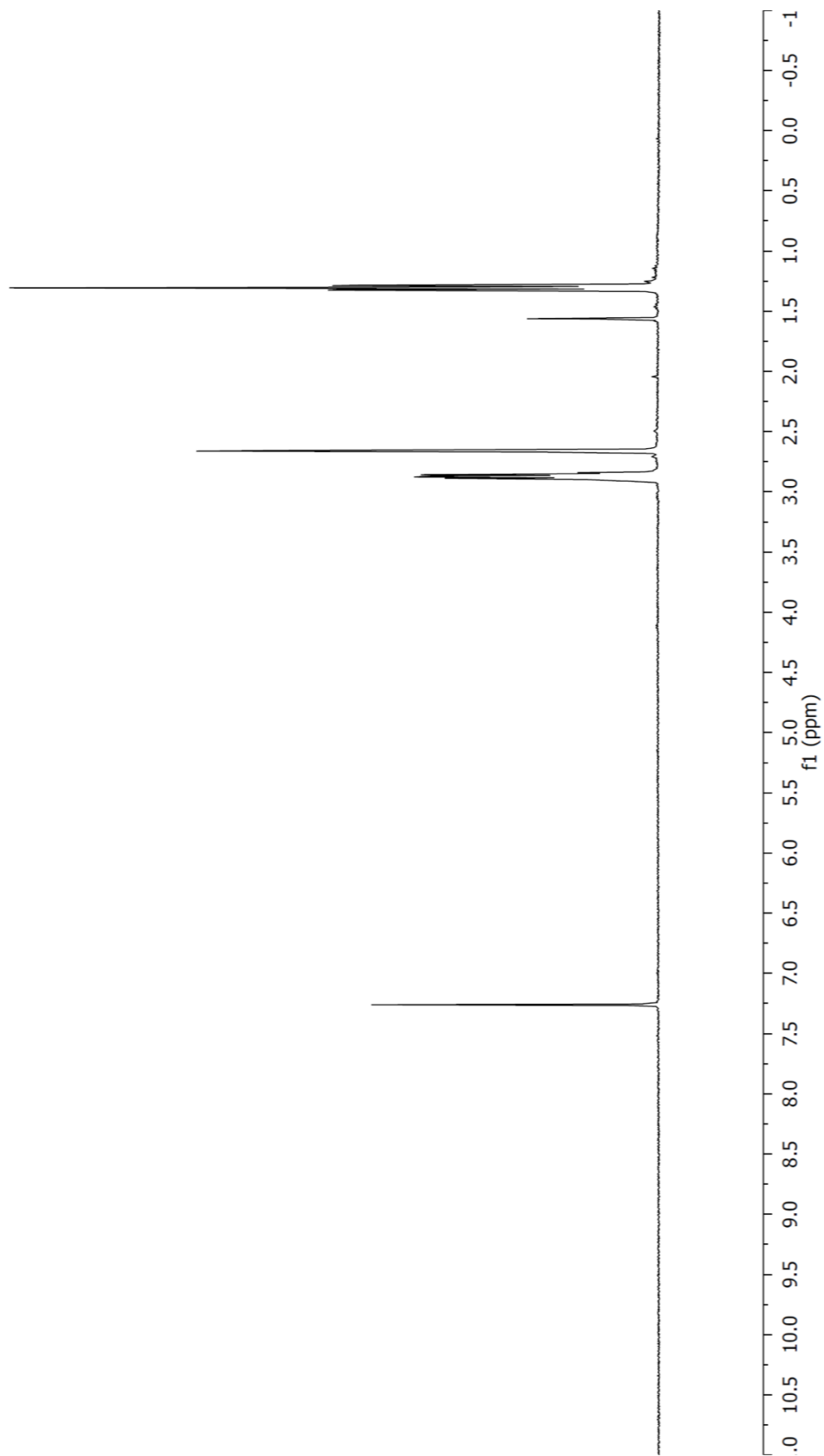


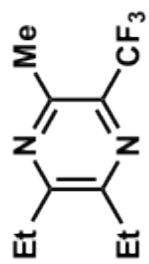
Compound 14-C6  
19F NMR, 376 MHz



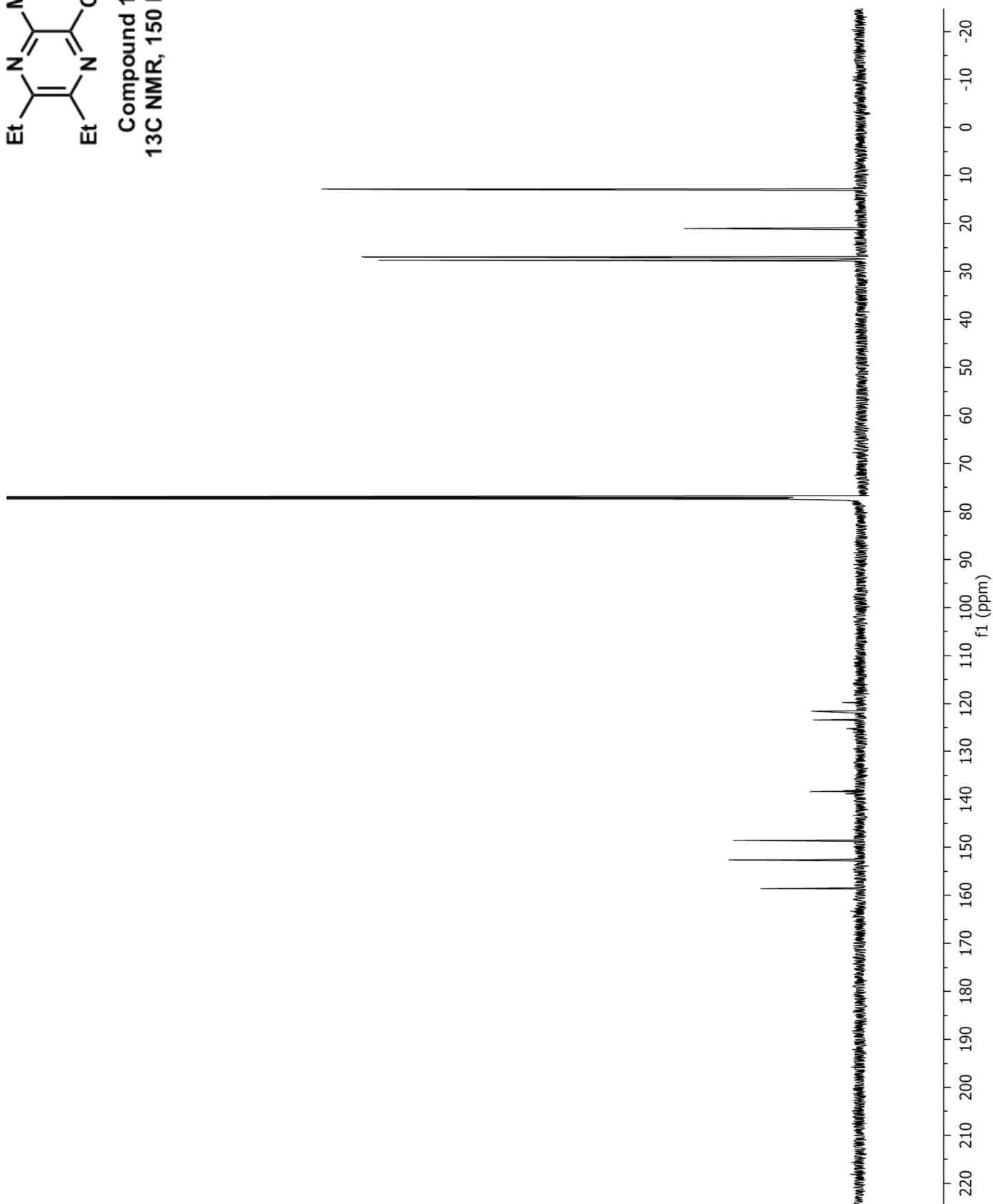


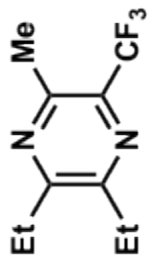
Compound 15  
1H NMR, 400 MHz



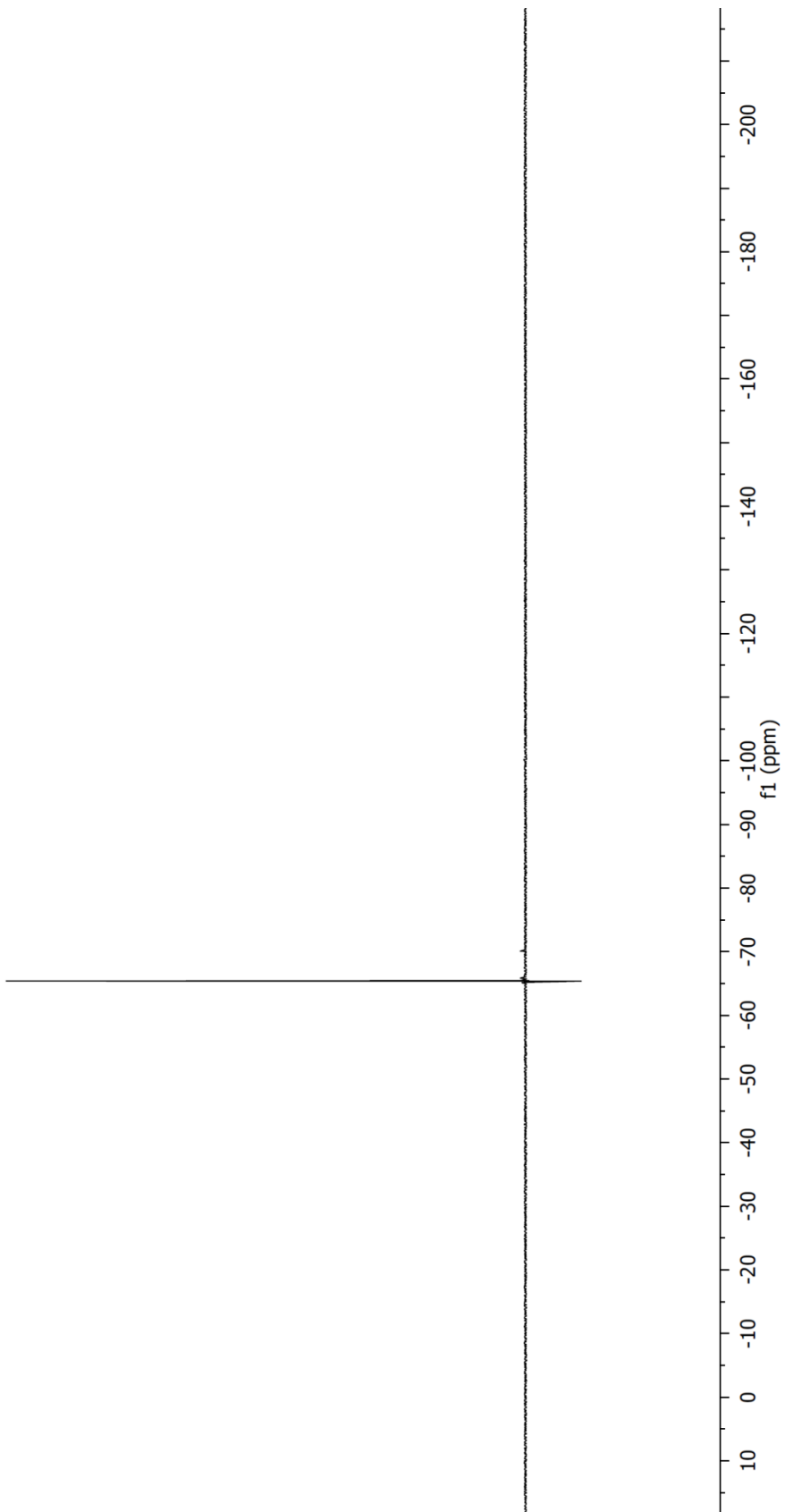


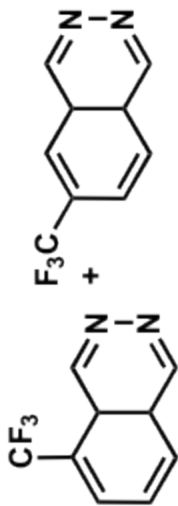
Compound 15  
13C NMR, 150 MHz



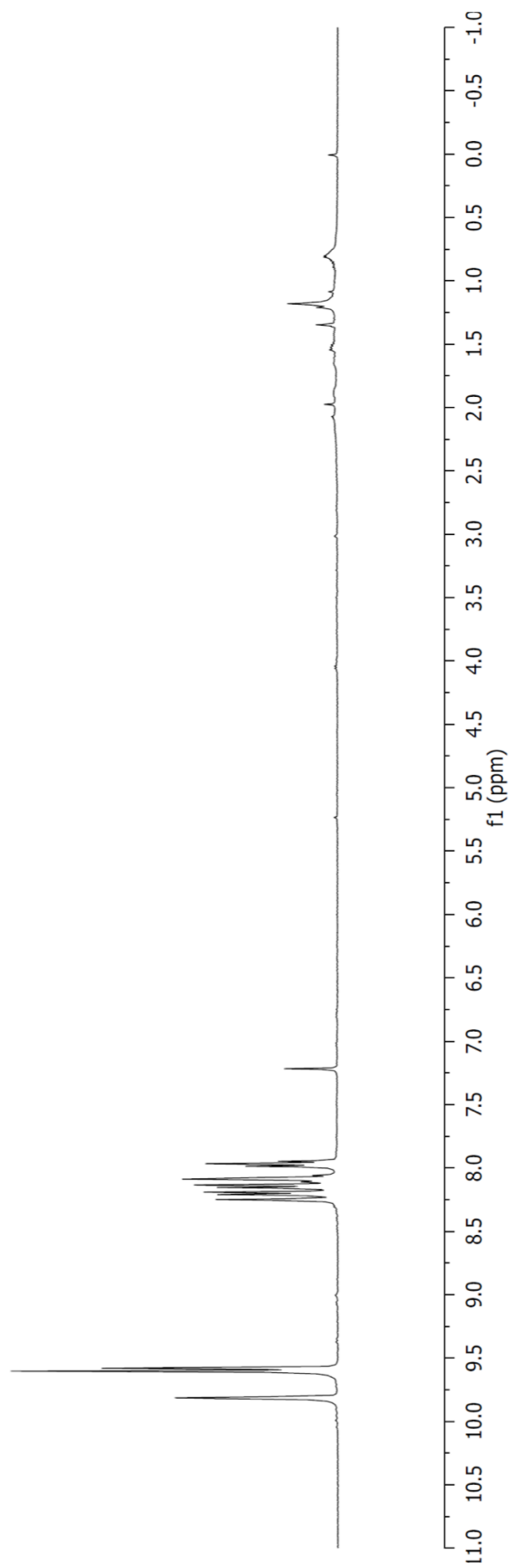


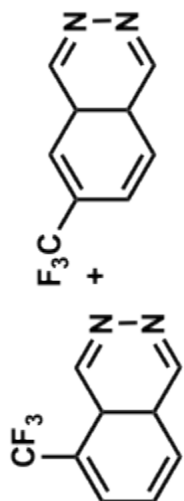
Compound 15  
19F NMR, 376 MHz



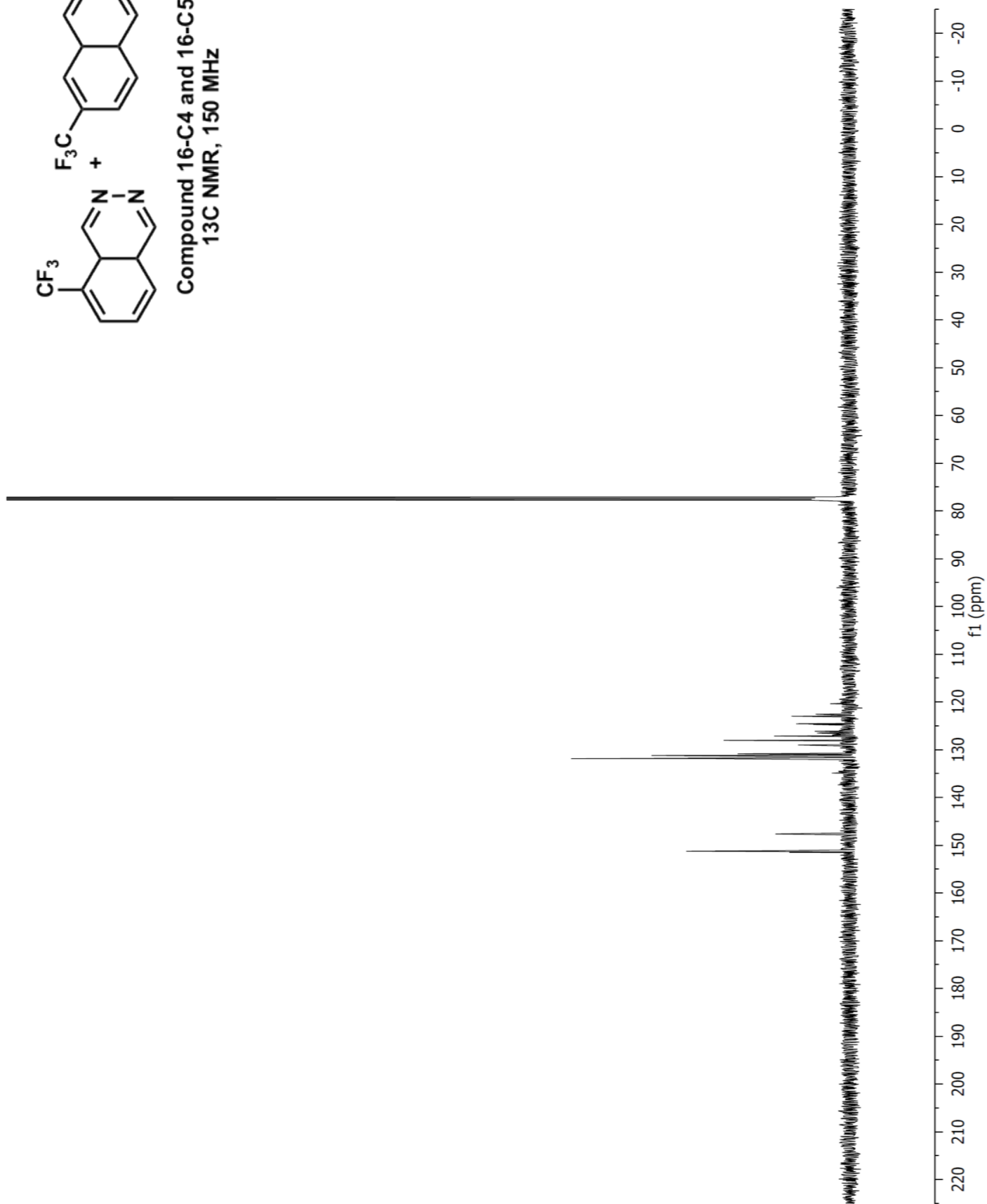


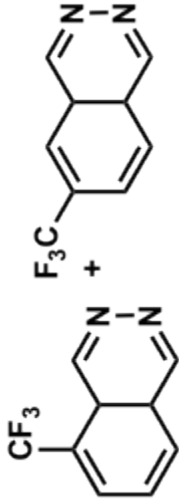
Compound 16-C4 and 16-C5  
<sup>1</sup>H NMR, 400 MHz



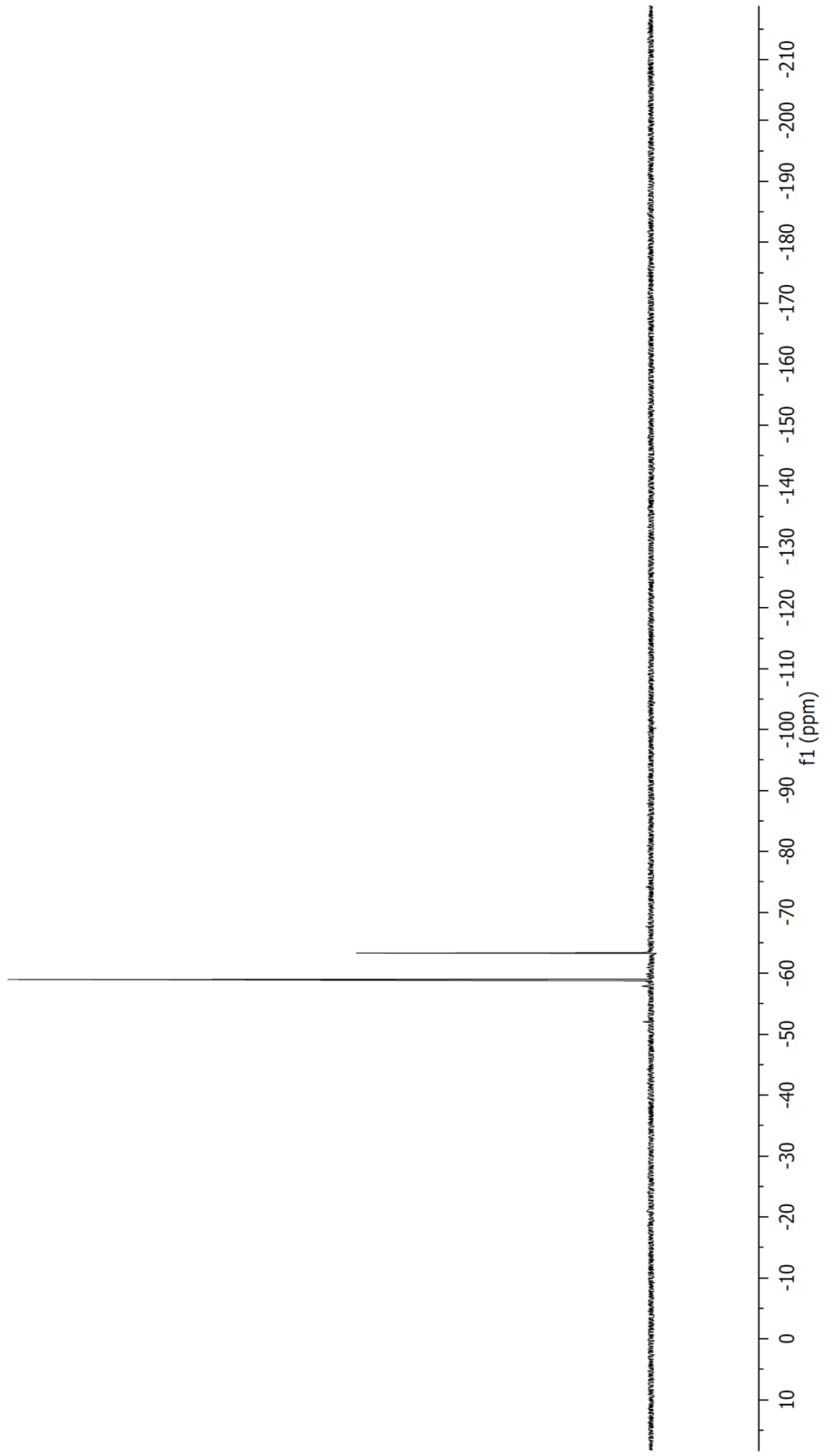


Compound 16-C4 and 16-C5  
13C NMR, 150 MHz

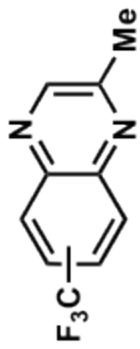




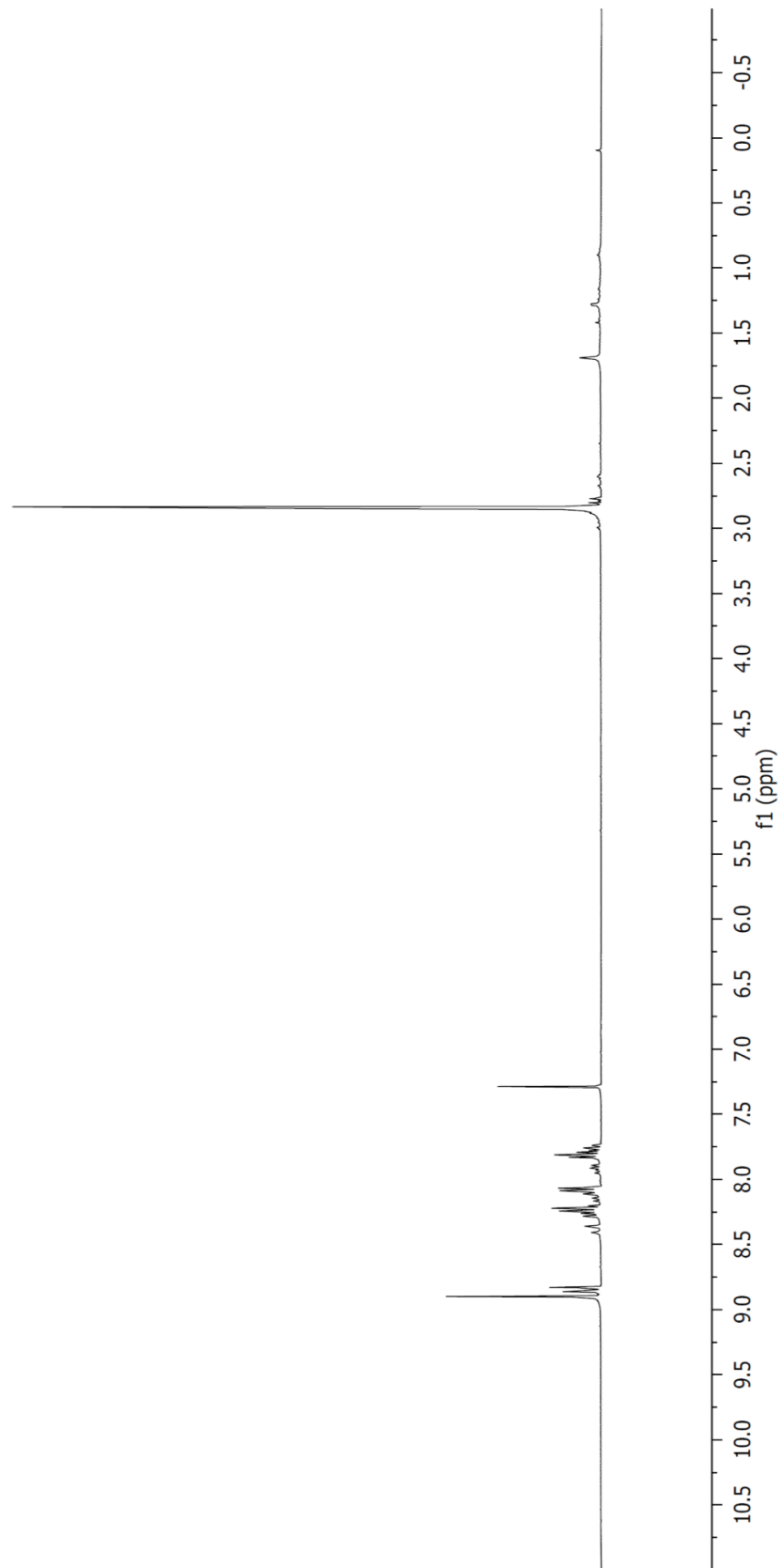
Compound 16-C4 and 16-C5  
19F NMR, 376 MHz

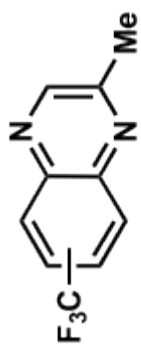




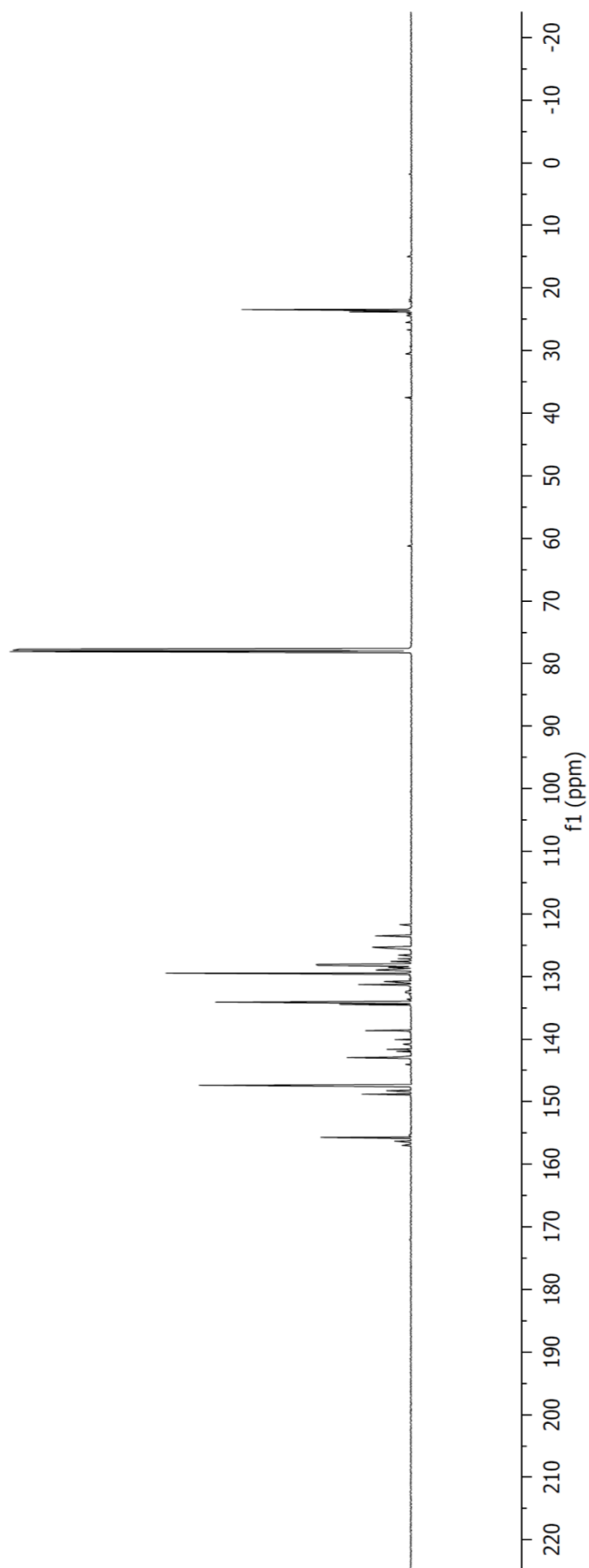


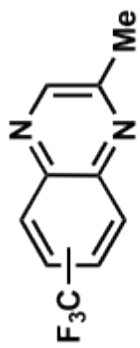
Compound 17  
1H NMR, 400 MHz



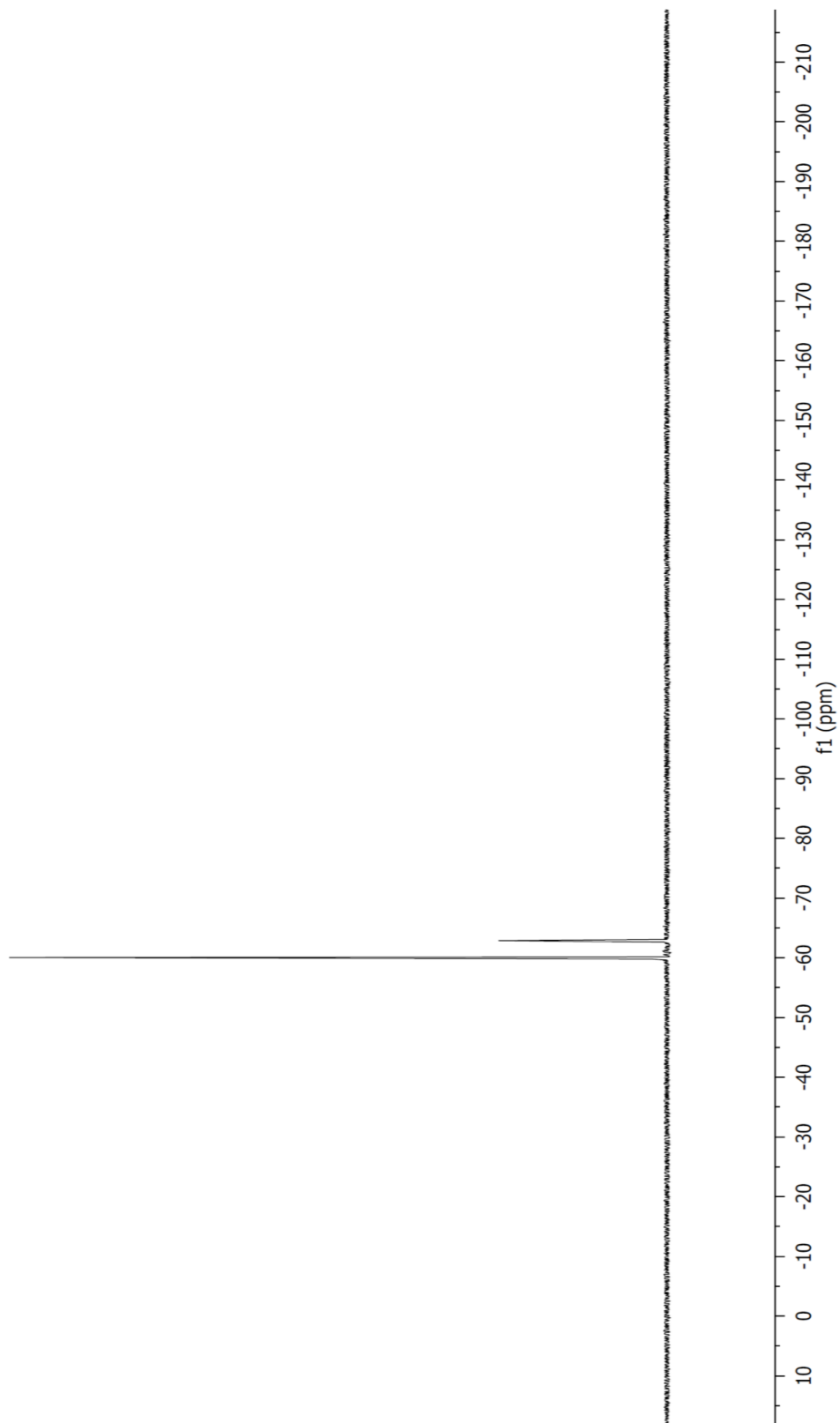


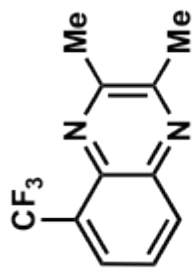
Compound 17  
13C NMR, 150 MHz



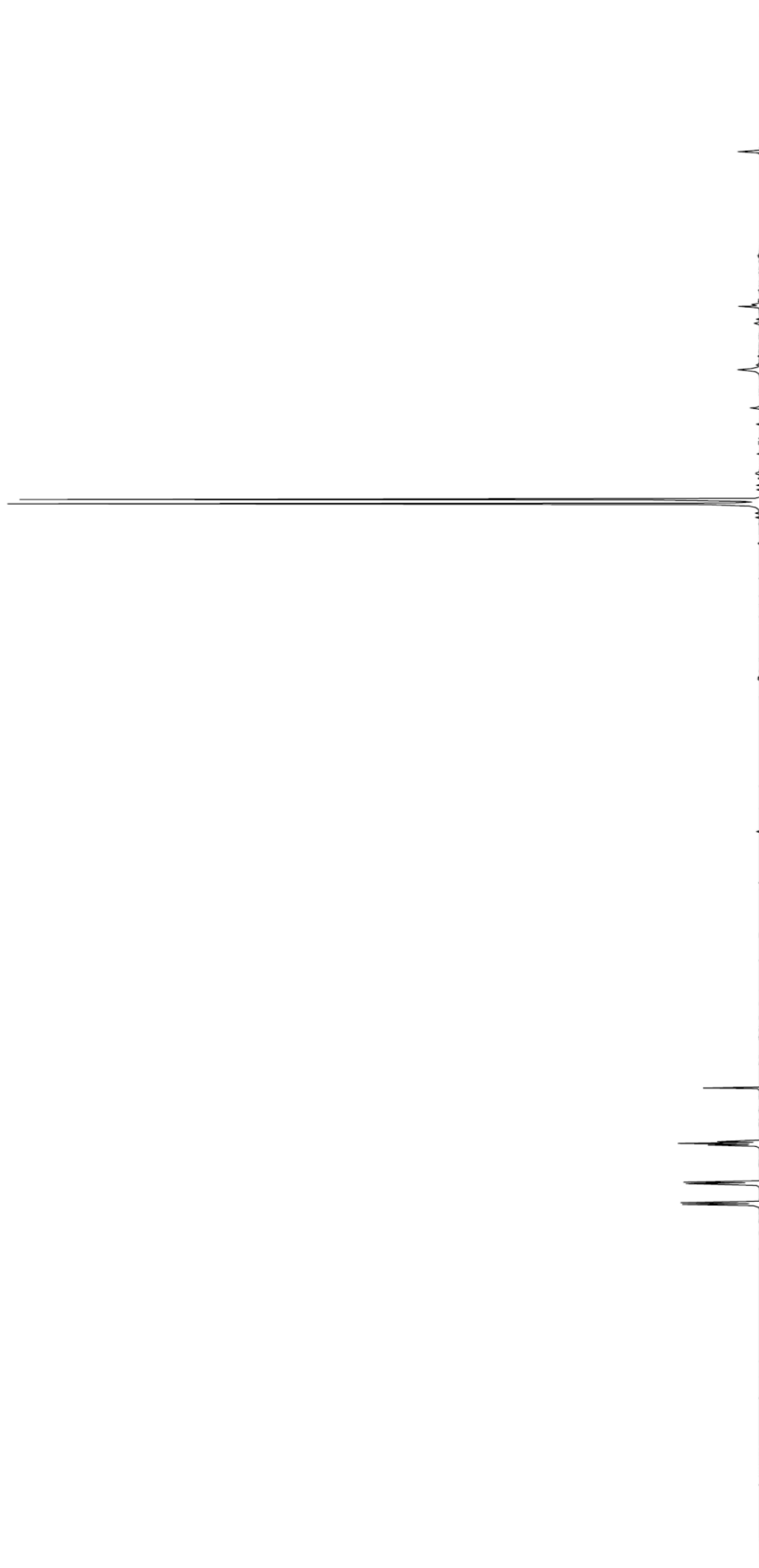


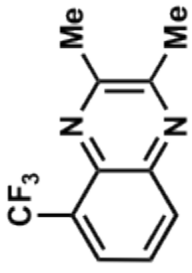
Compound 17  
19F NMR, 376 MHz



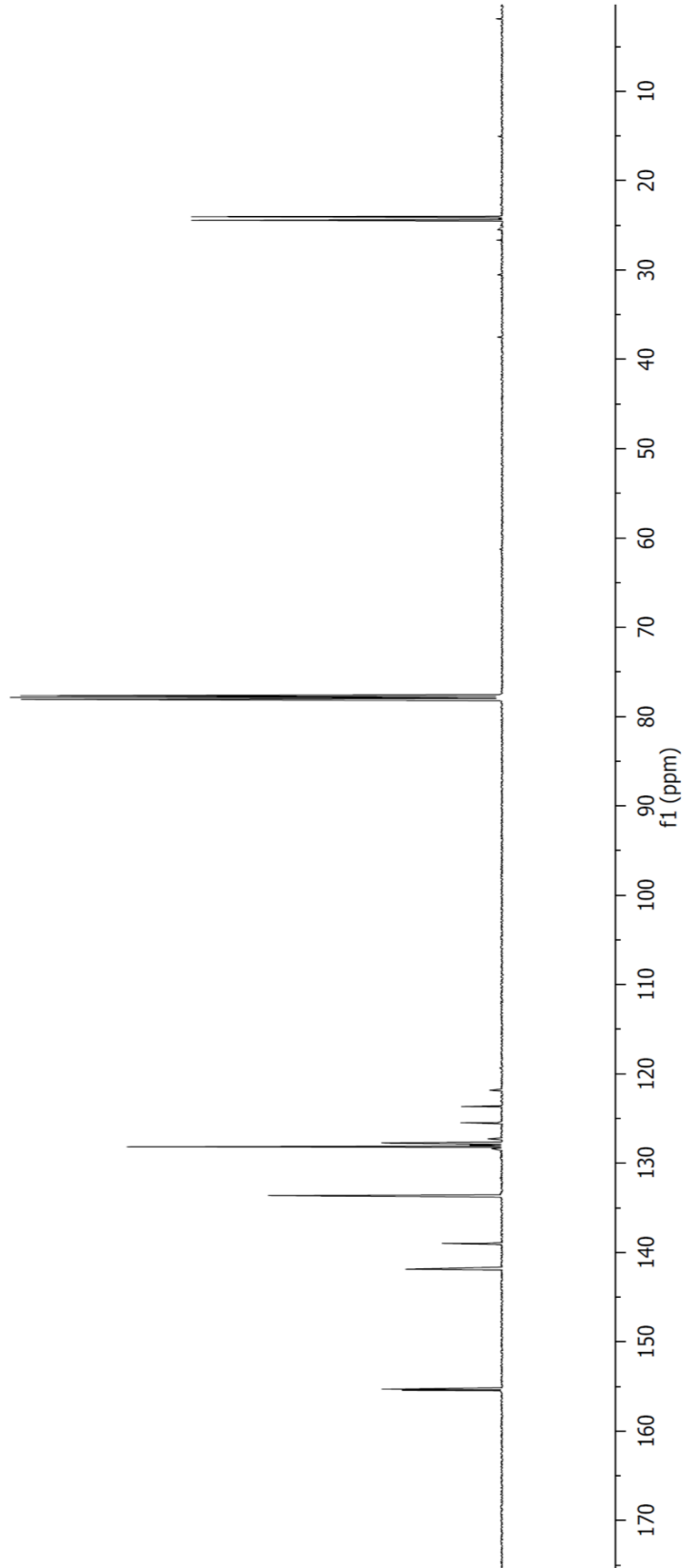


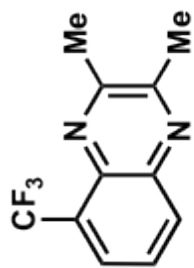
Compound 18-C5  
1H NMR, 400 MHz



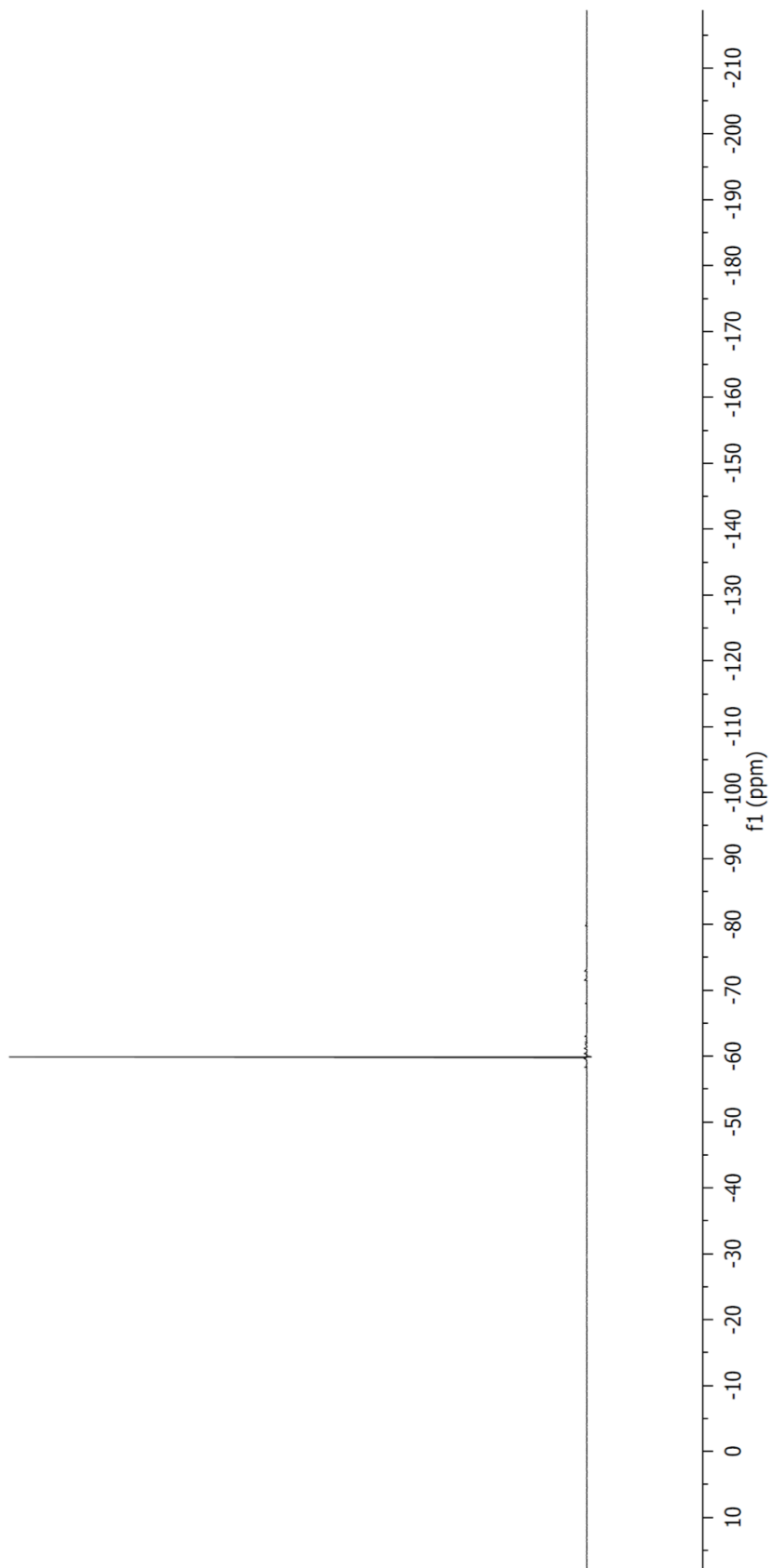


Compound 18-C5  
13C NMR, 150 MHz



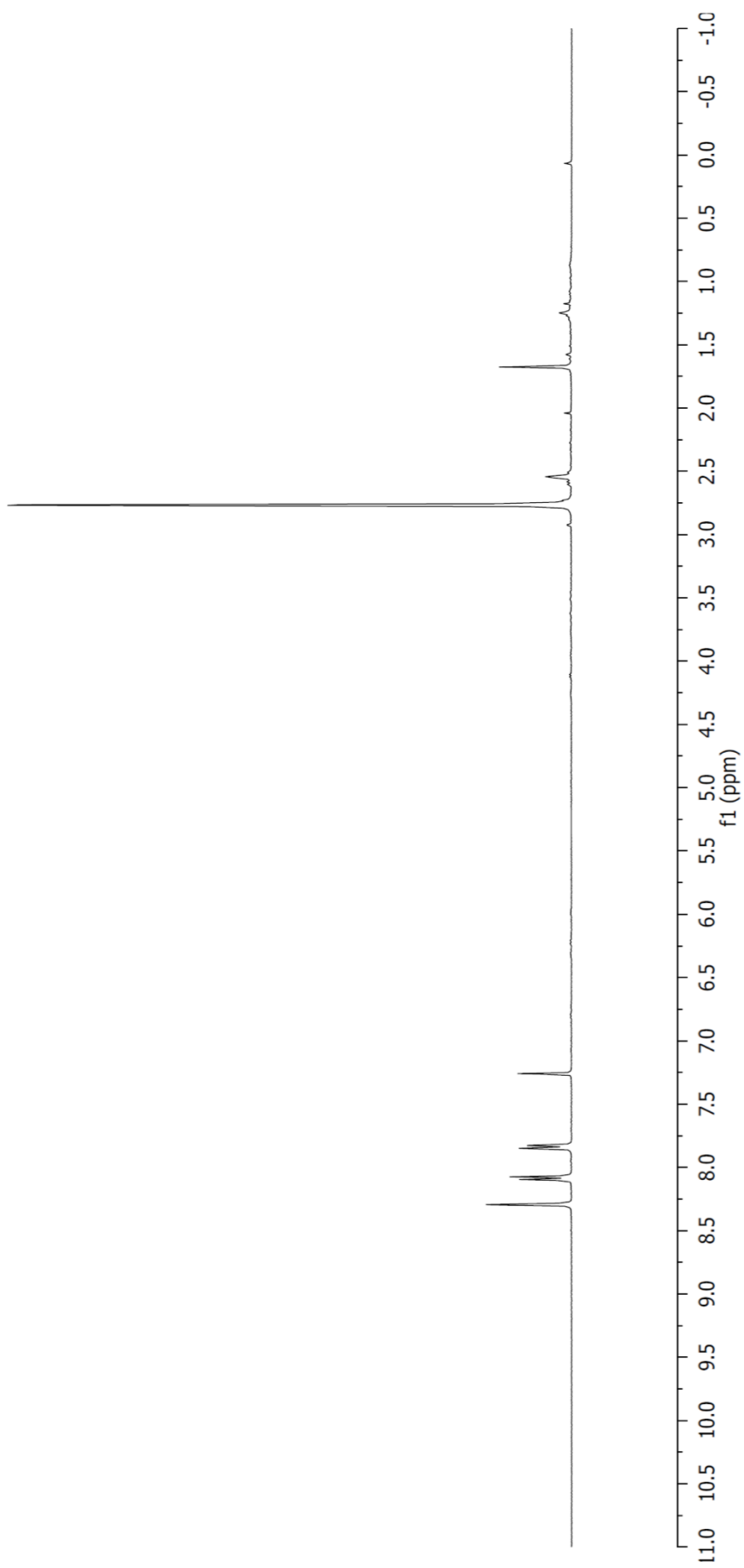


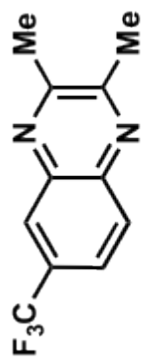
Compound 18-C5  
19F NMR, 376 MHz



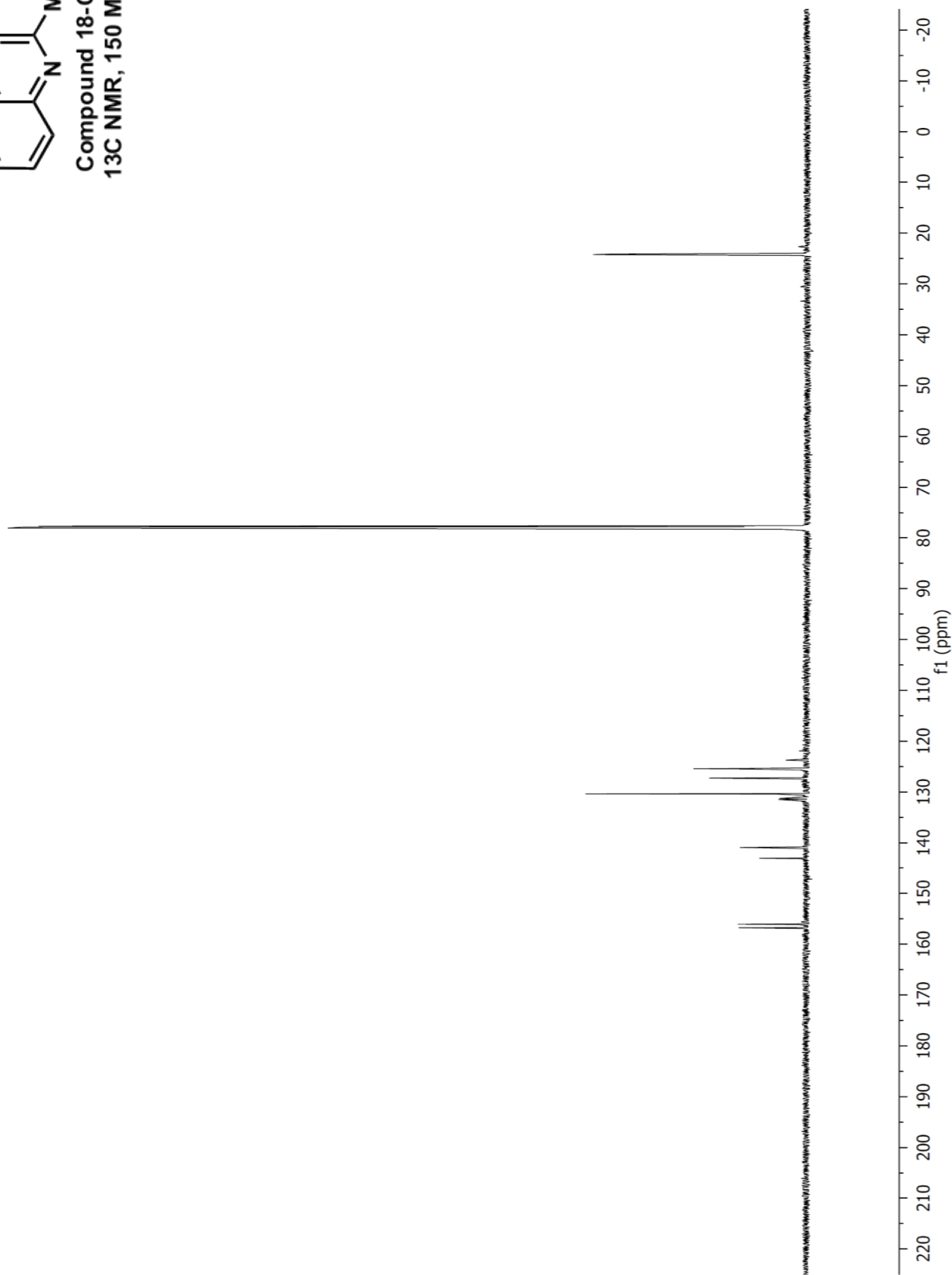


Compound 18-C6  
1H NMR, 400 MHz





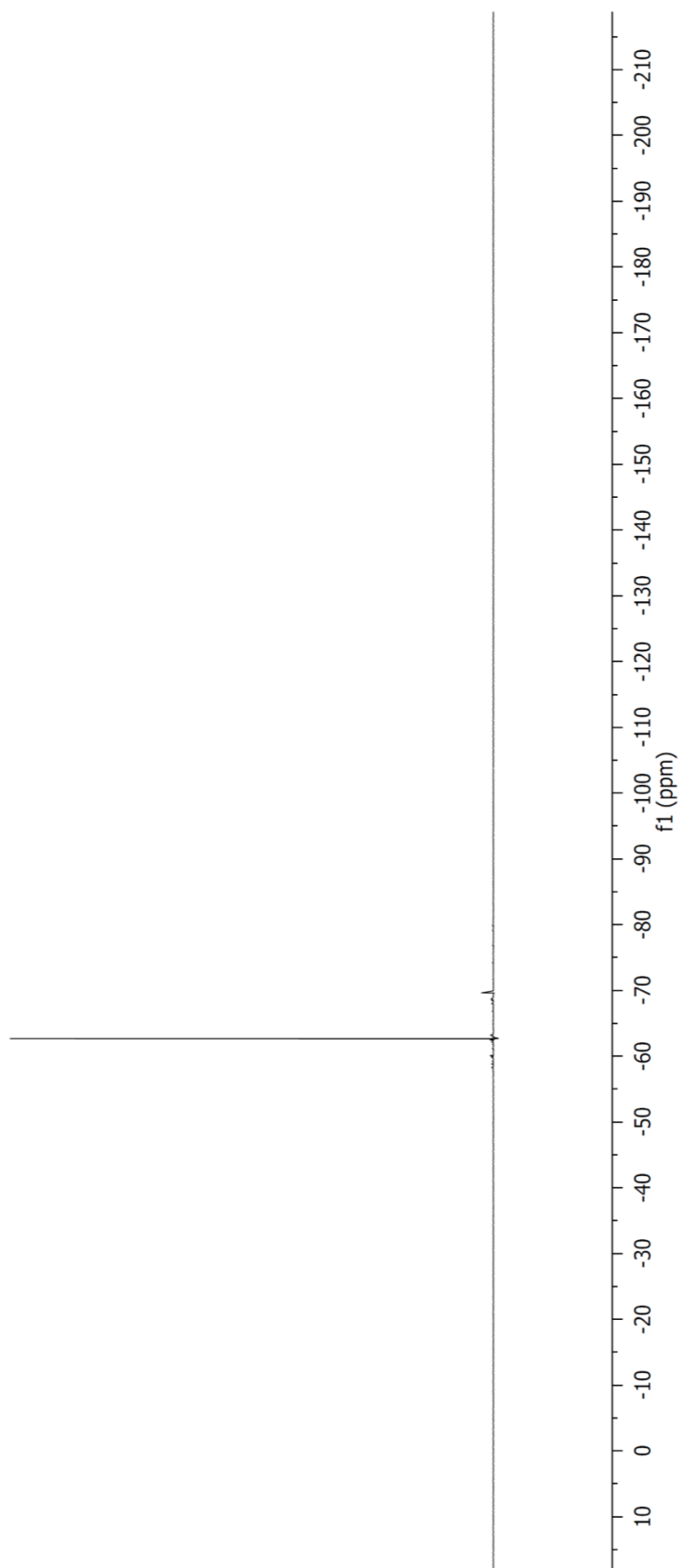
Compound 18-C6  
13C NMR, 150 MHz

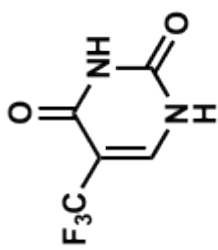




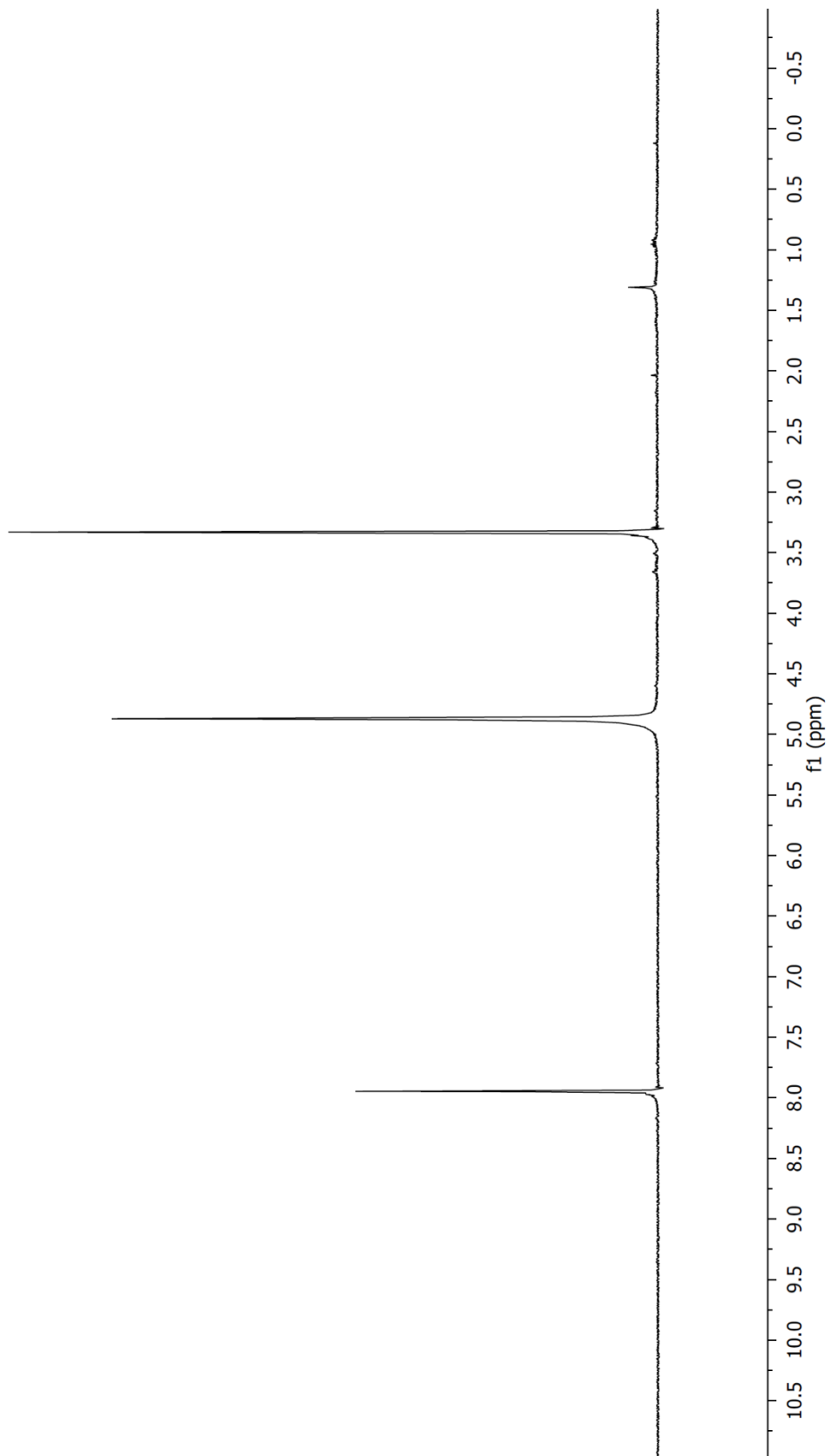


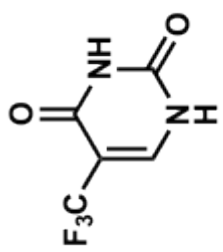
Compound 18-C6  
19F NMR, 376 MHz



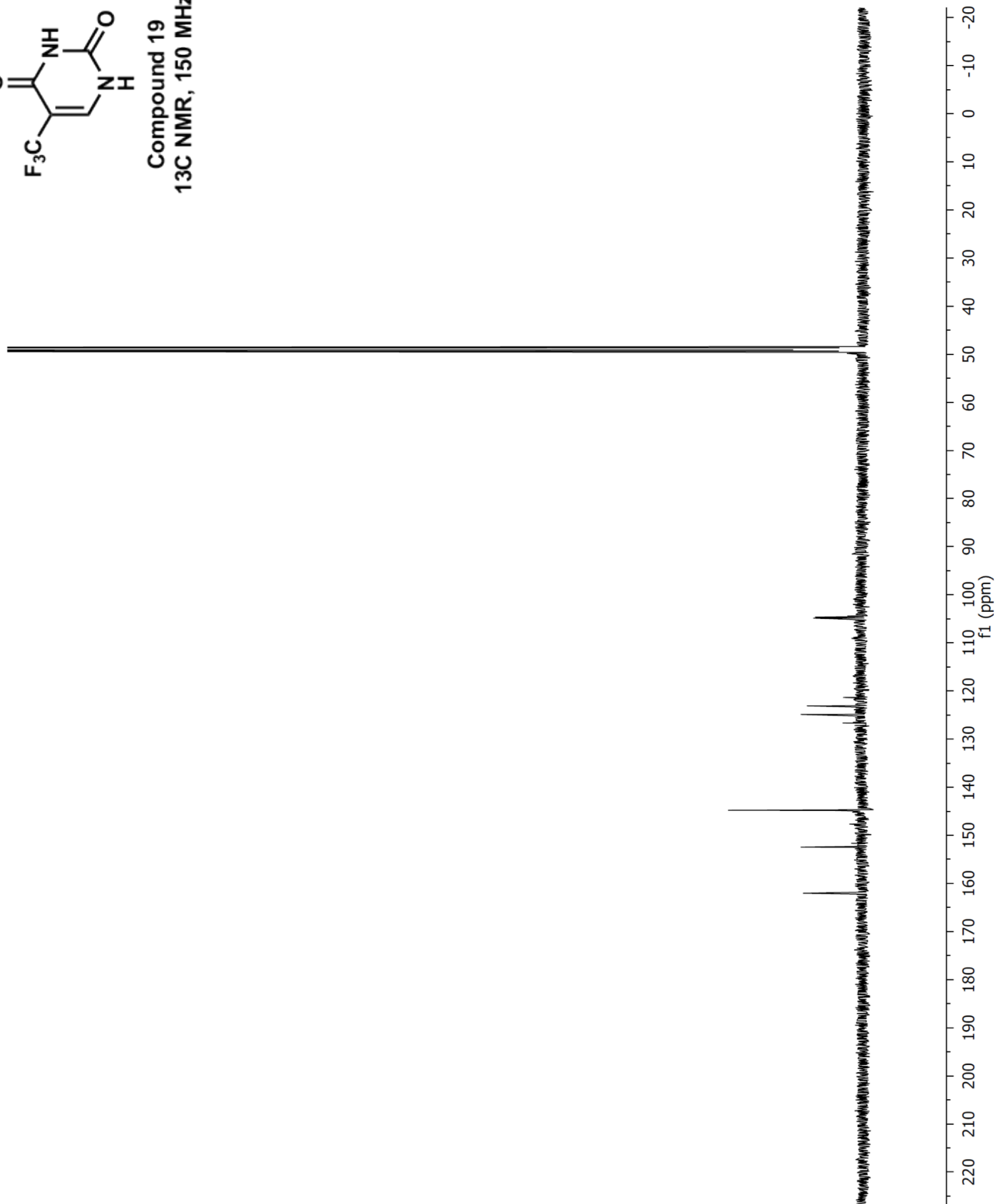


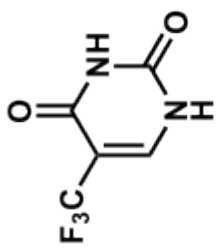
Compound 19  
1H NMR, 400 MHz



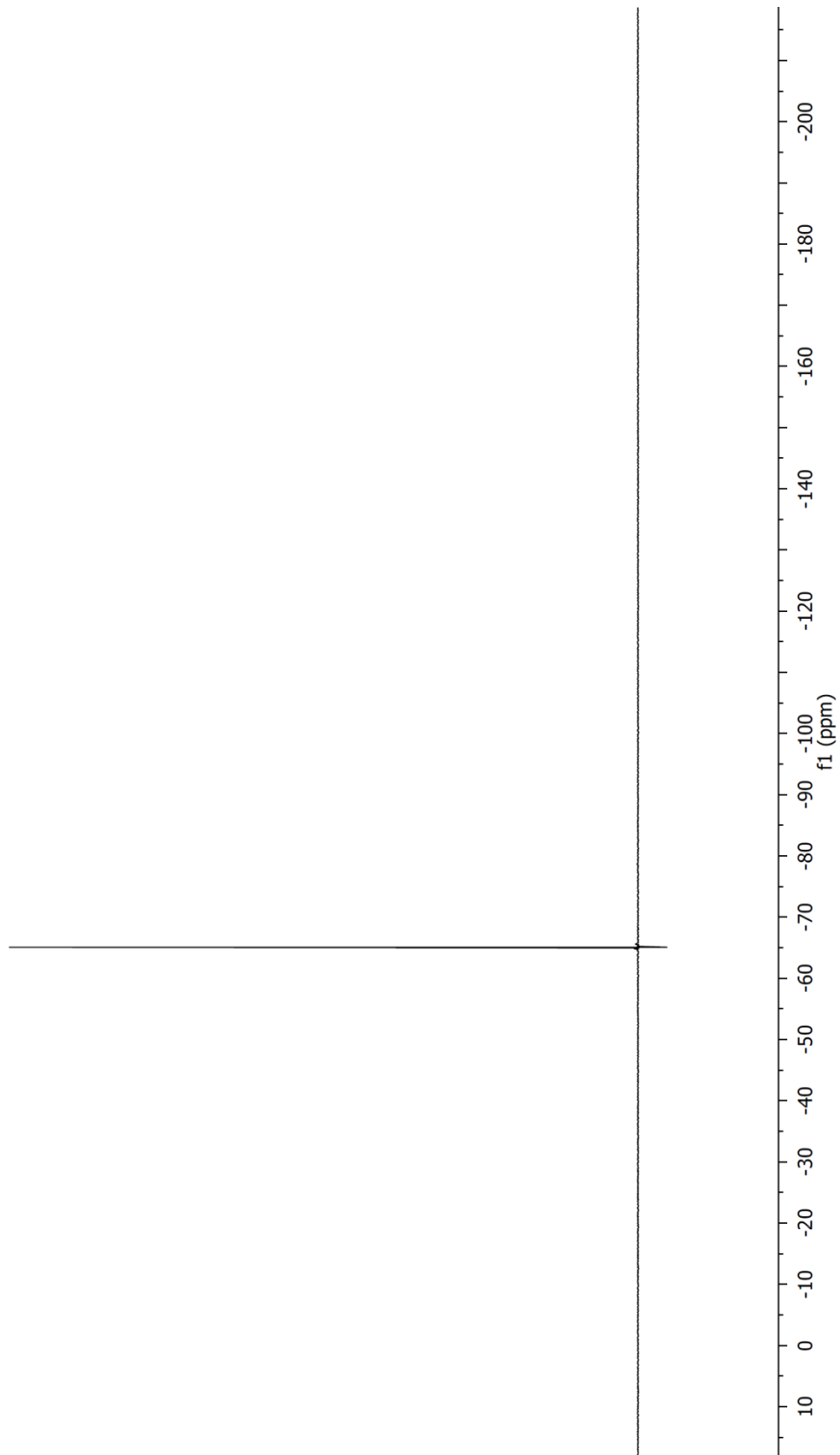


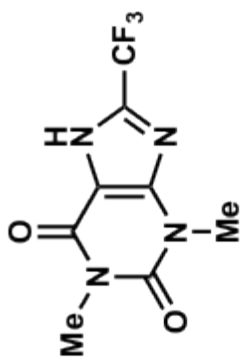
Compound 19  
13C NMR, 150 MHz



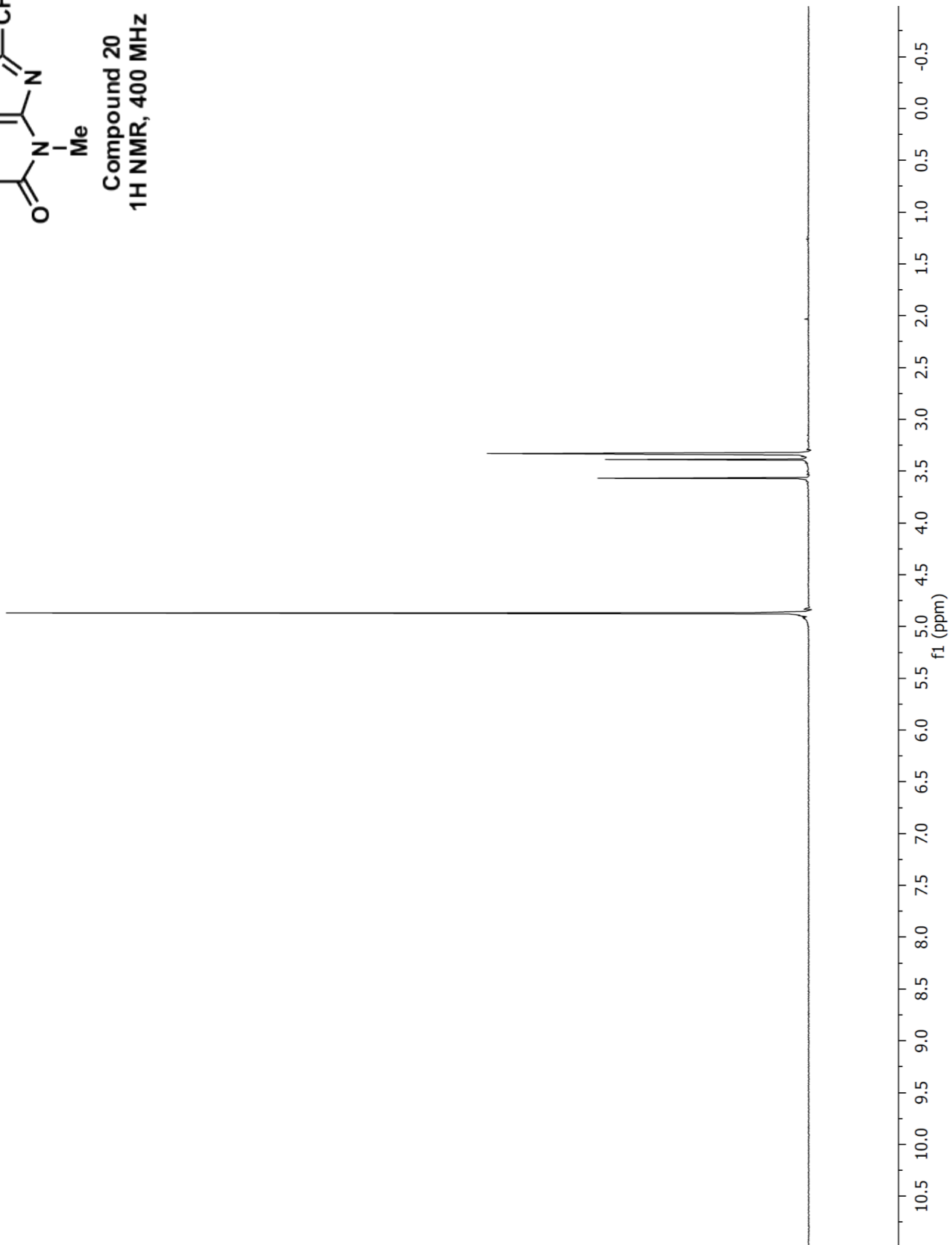


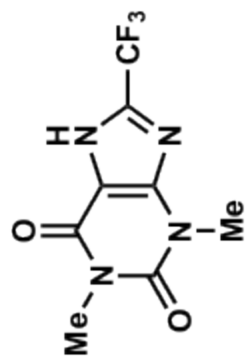
Compound 19  
19F NMR, 376 MHz



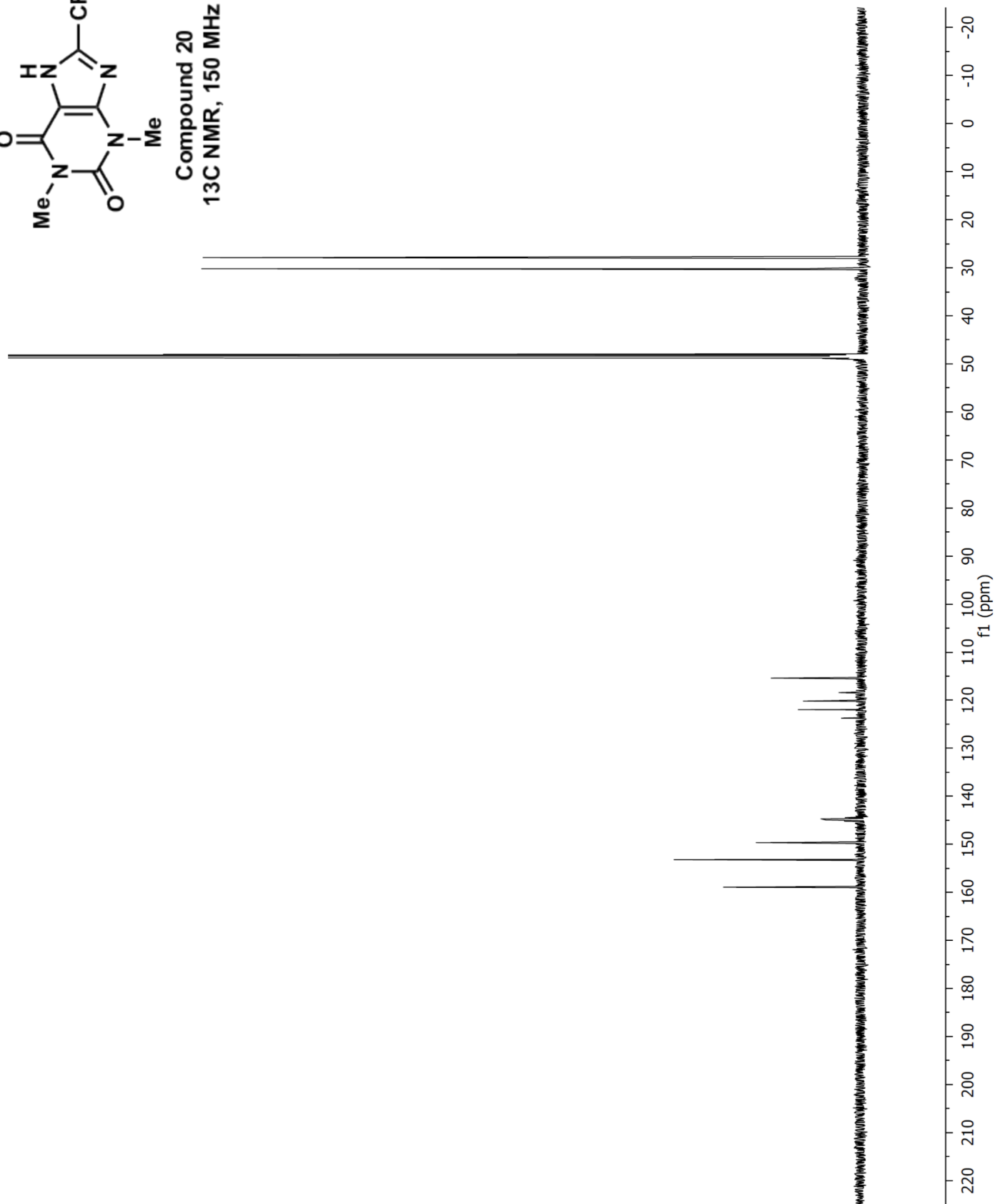


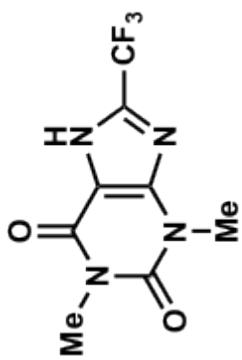
Compound 20  
1H NMR, 400 MHz



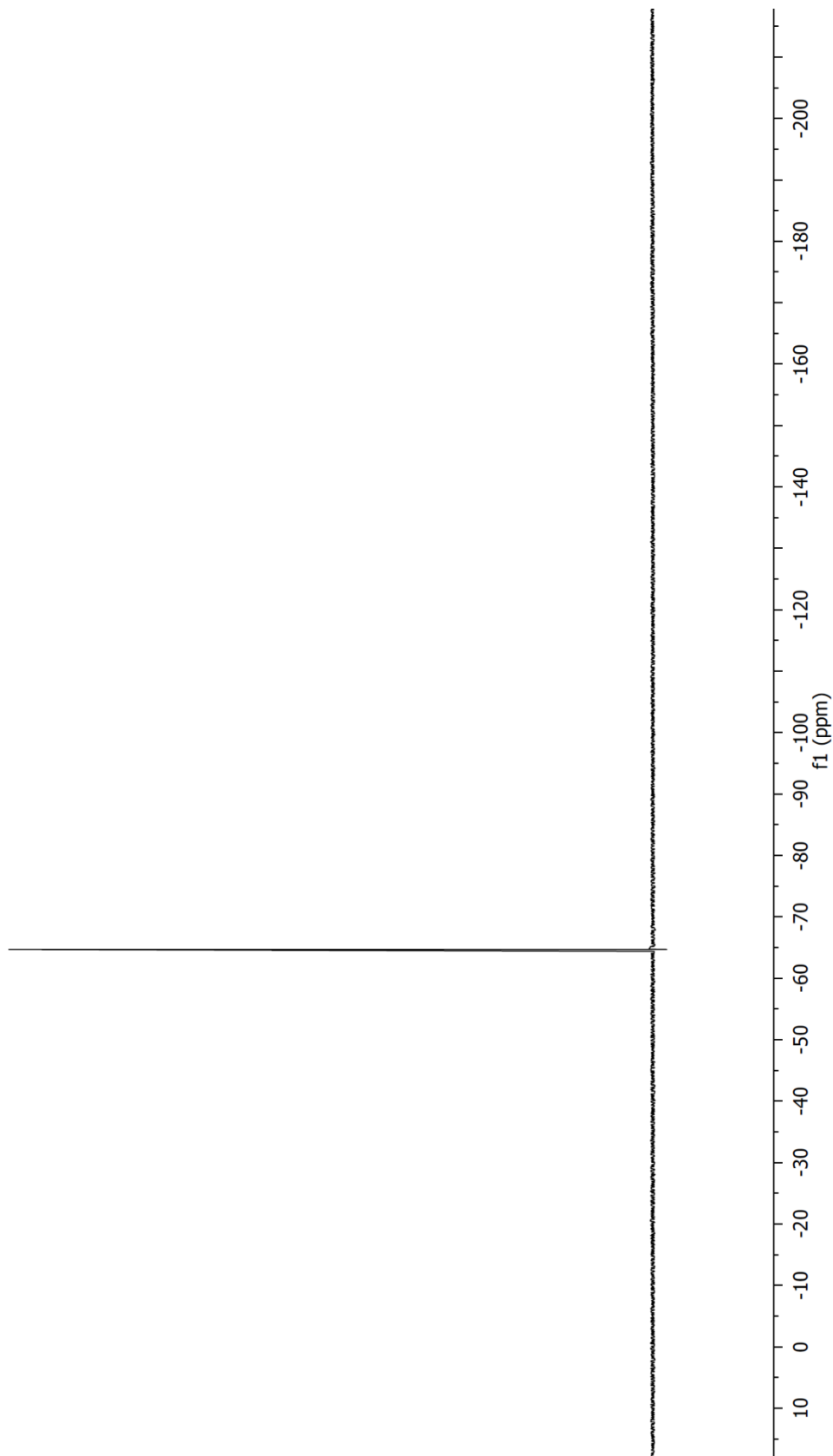


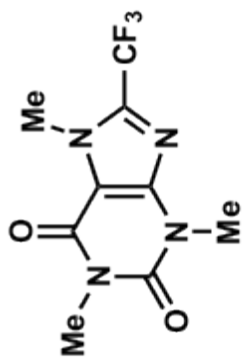
Compound 20  
13C NMR, 150 MHz



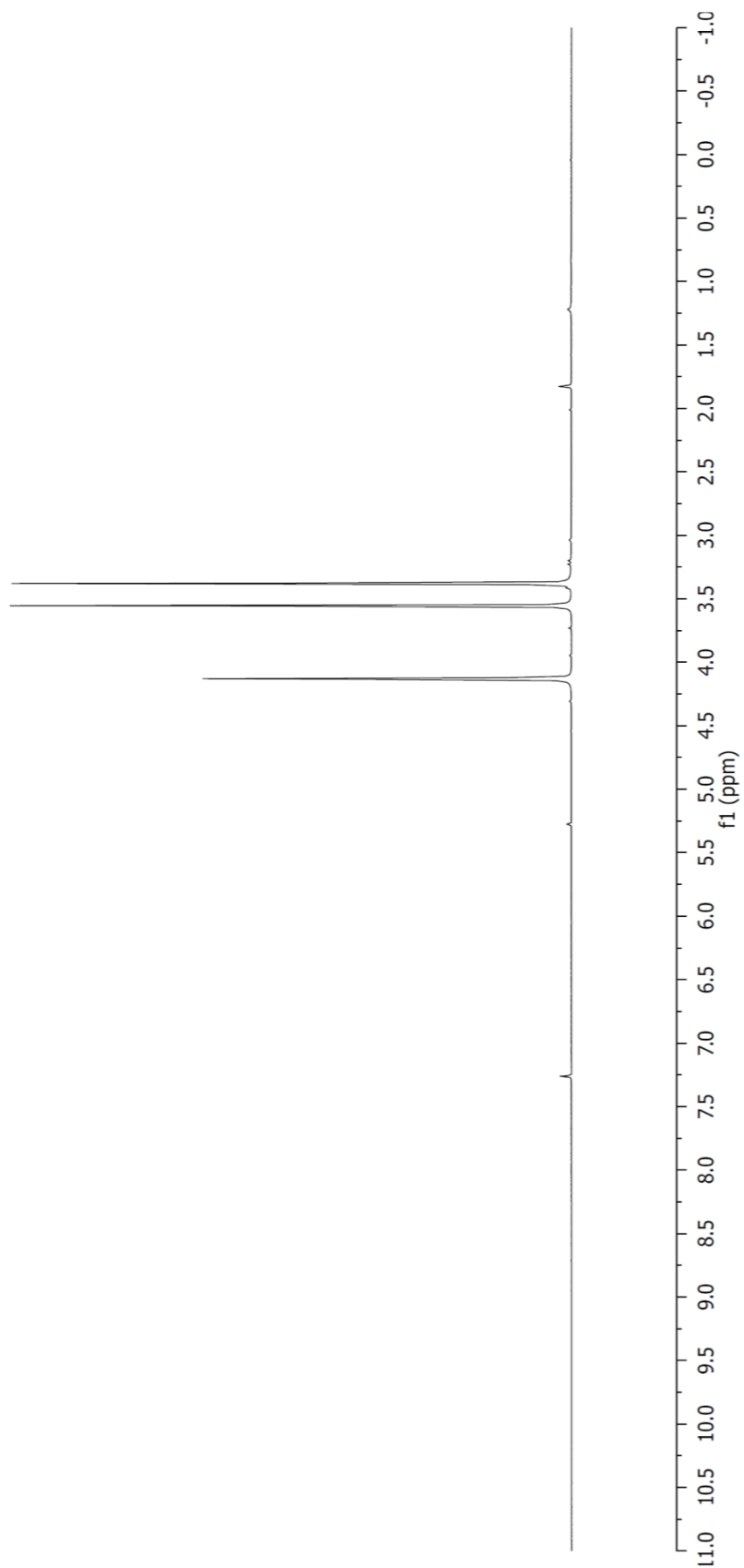


Compound 20  
19F NMR, 376 MHz

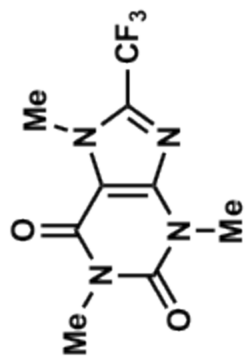




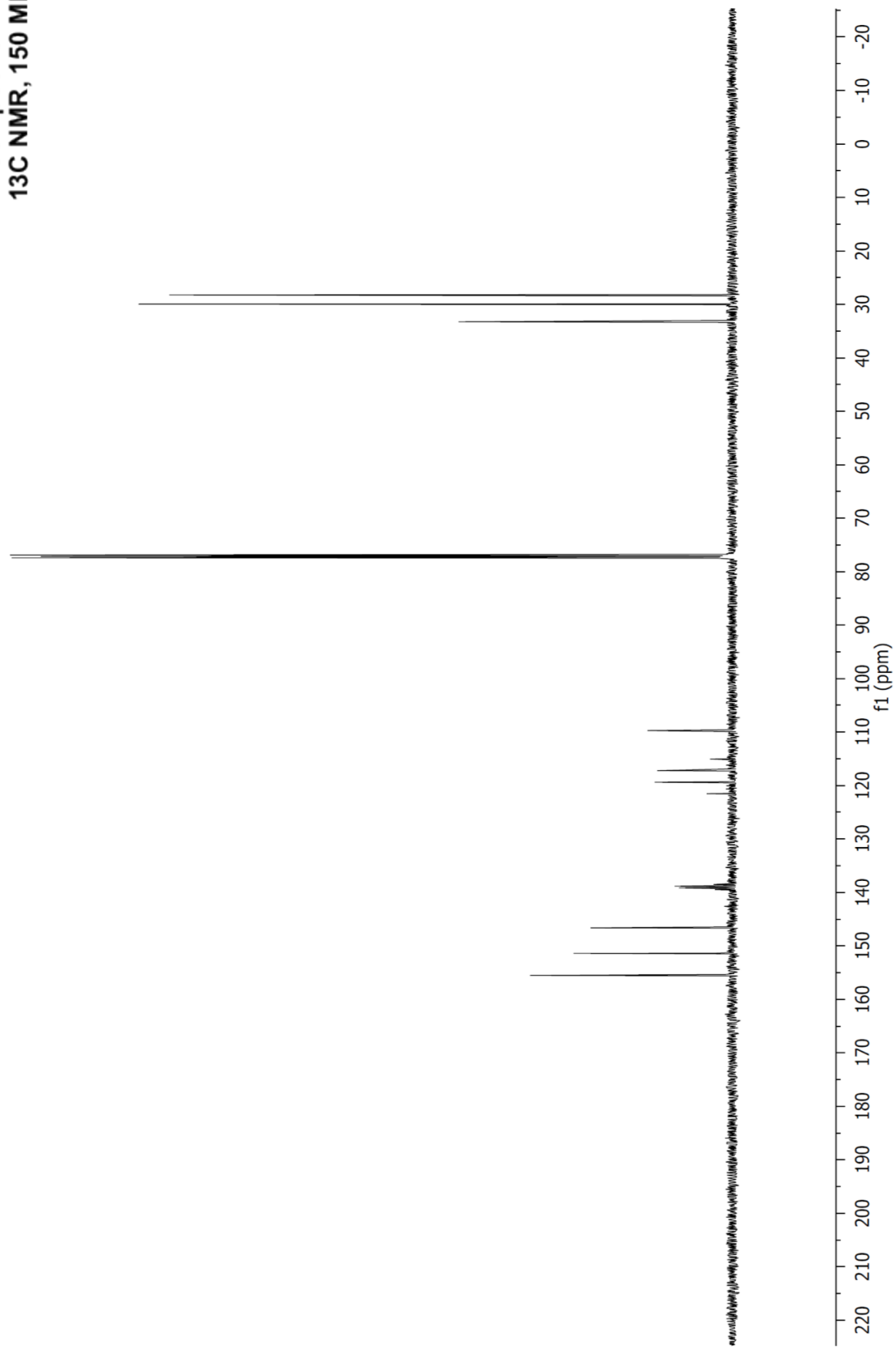
Compound 21  
1H NMR, 400 MHz

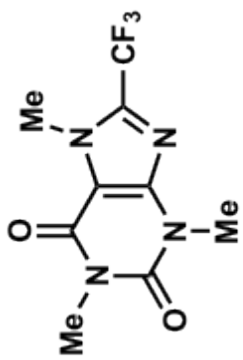




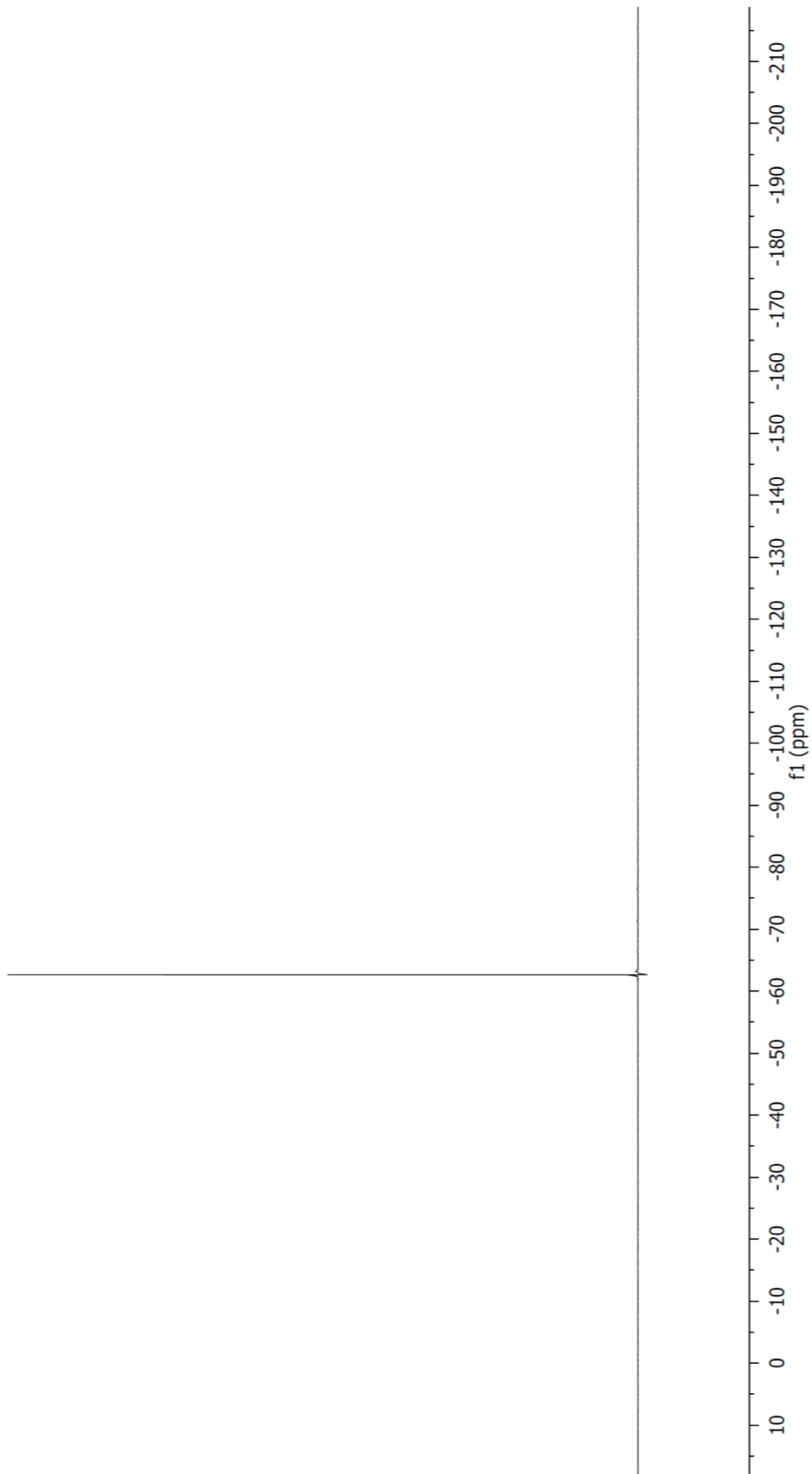


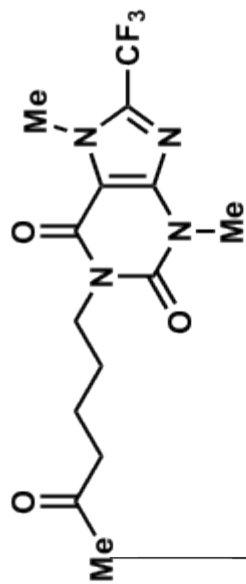
Compound 21  
13C NMR, 150 MHz



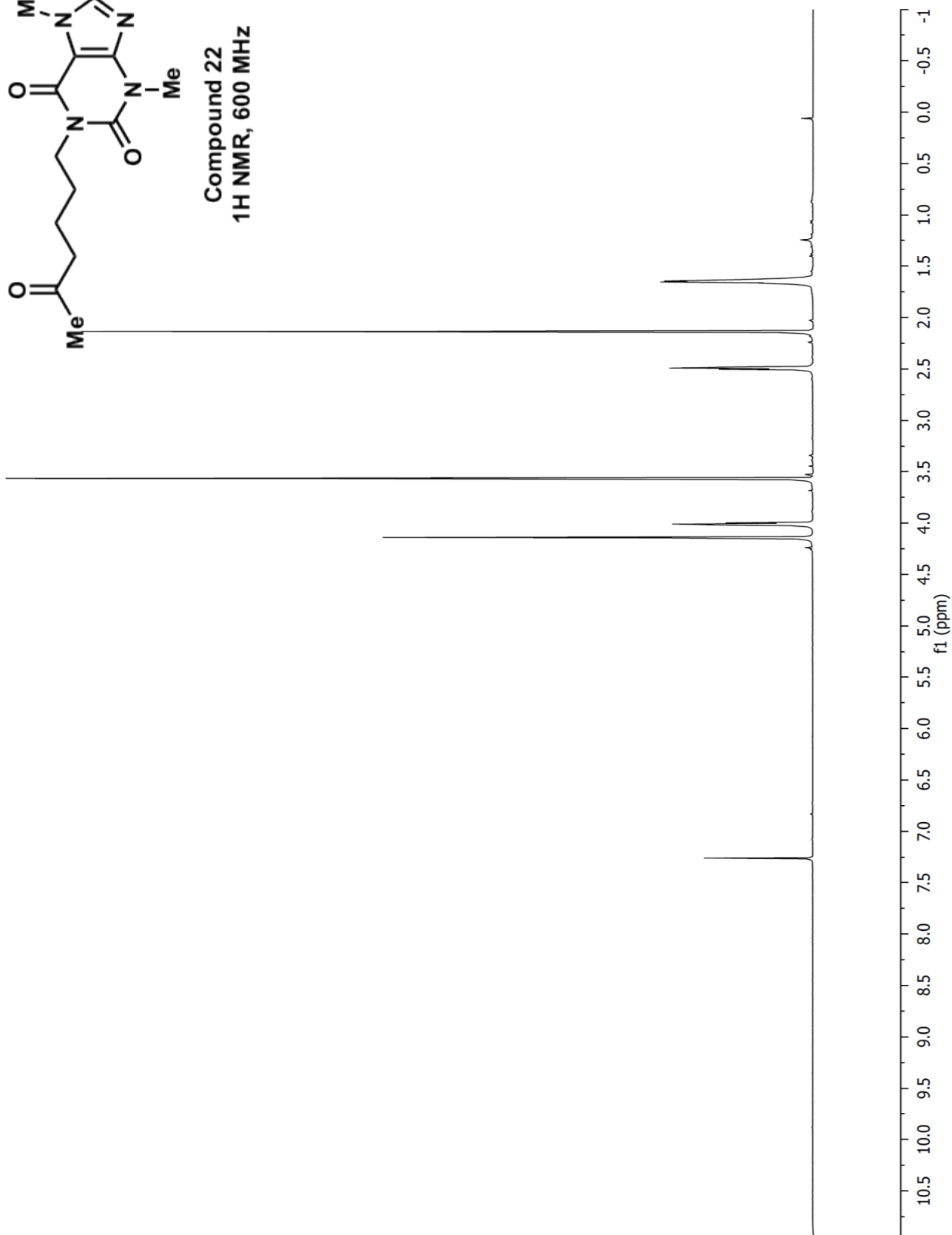


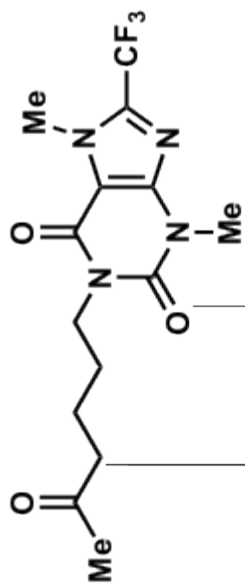
Compound 21  
19F NMR, 376 MHz



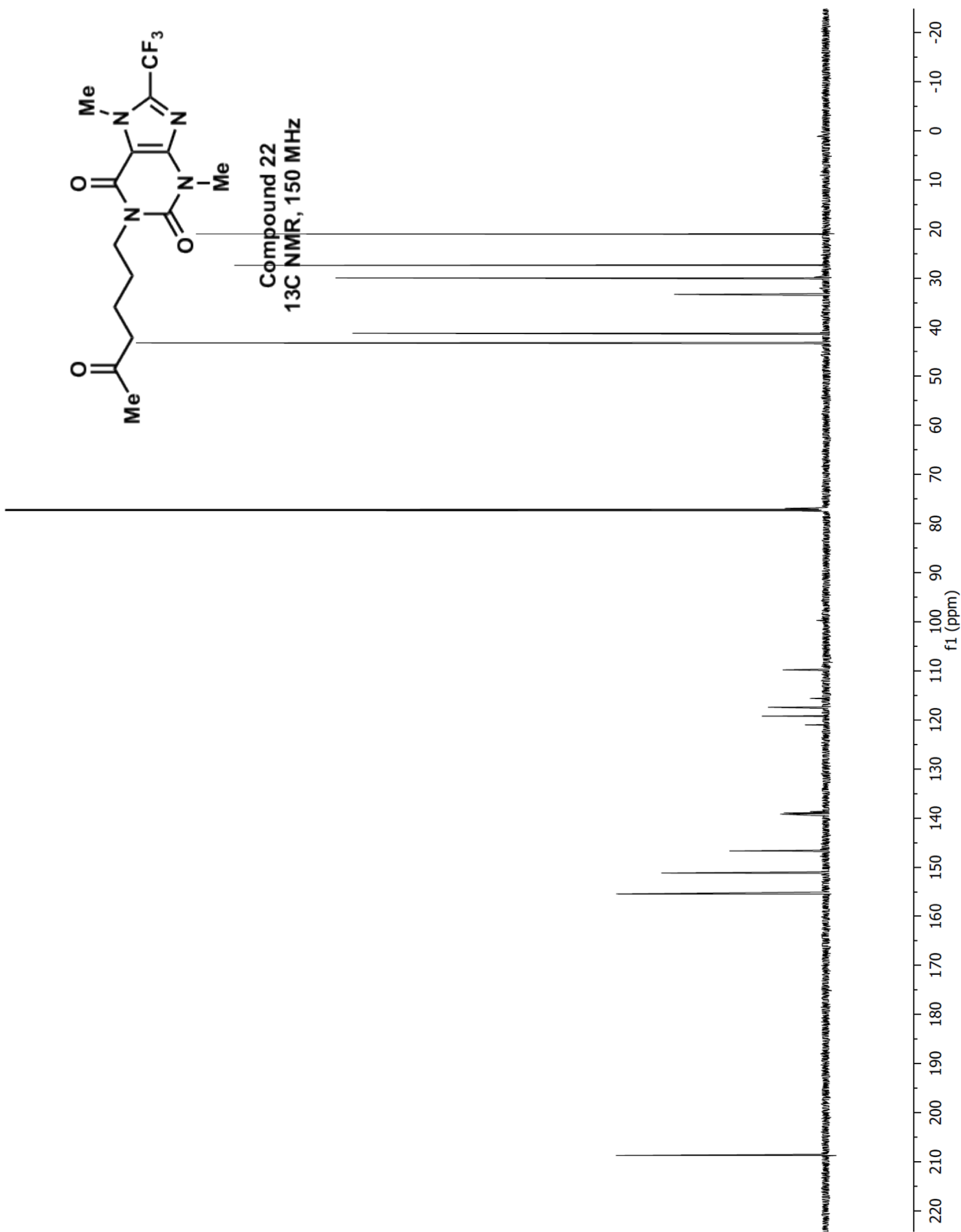


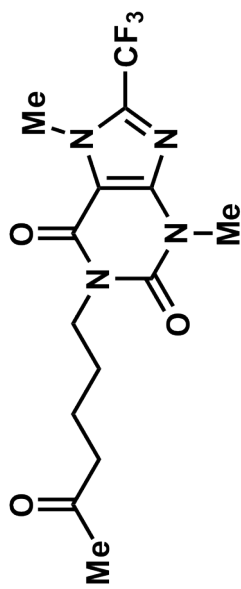
Compound 22  
1H NMR, 600 MHz



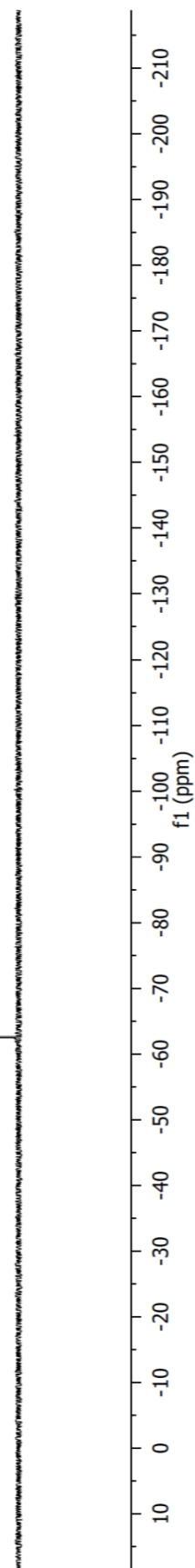


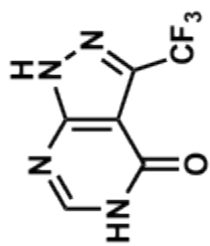
Compound 22  
13C NMR, 150 MHz



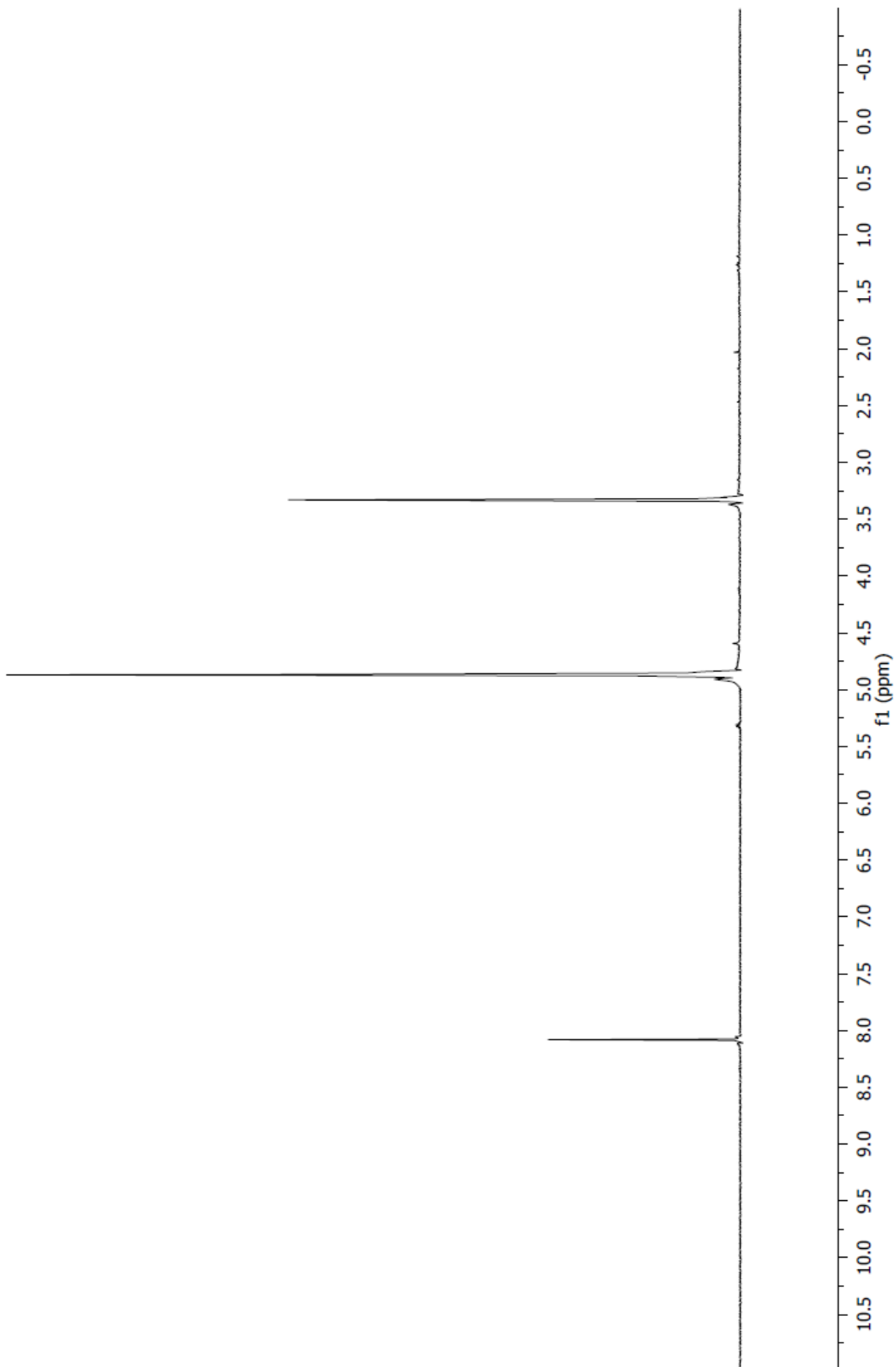


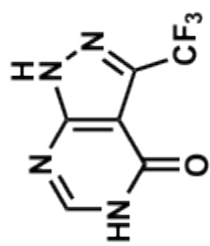
Compound 22  
19F NMR, 376 MHz



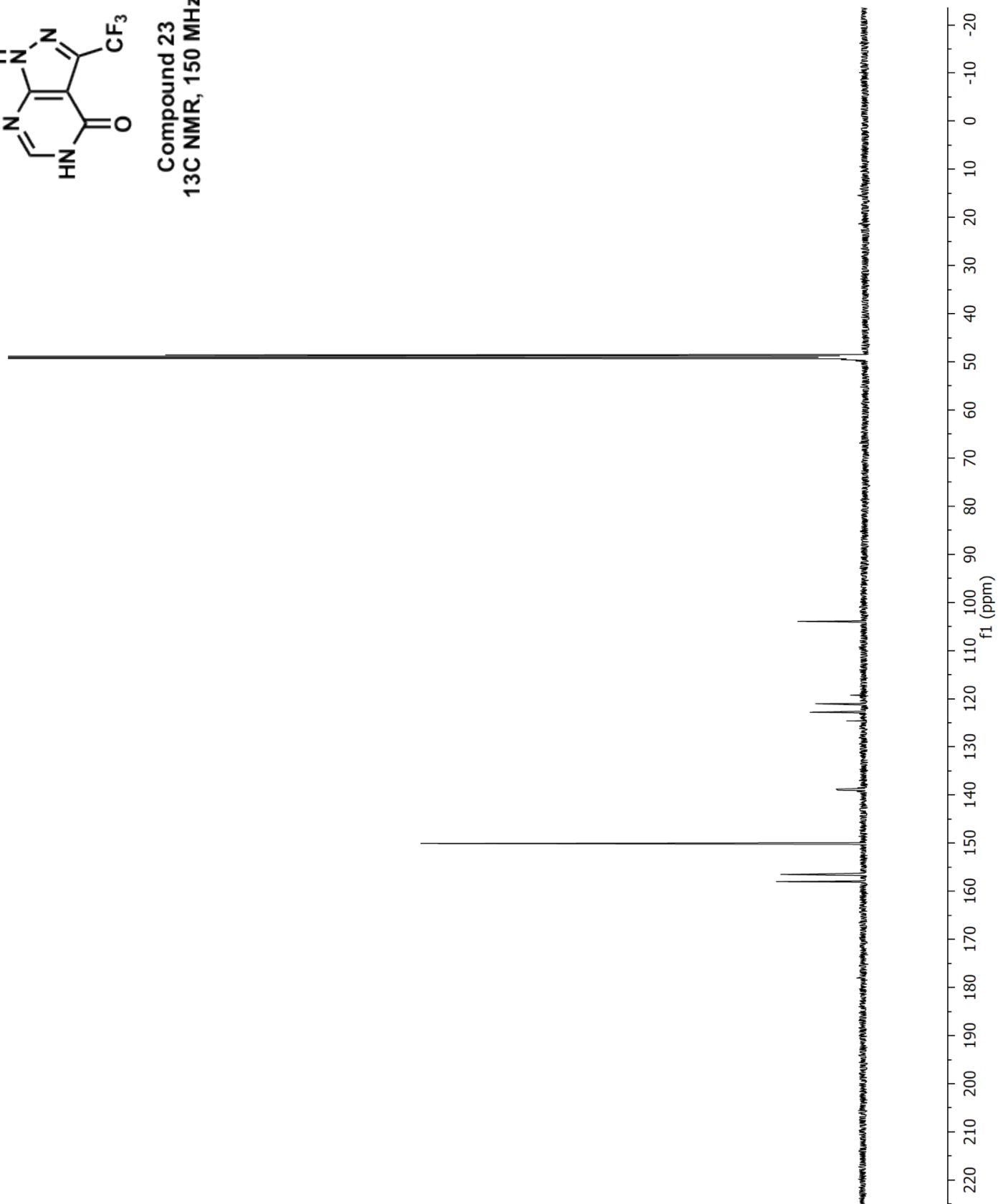


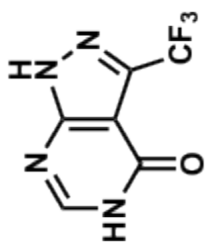
Compound 23  
1H NMR, 400 MHz



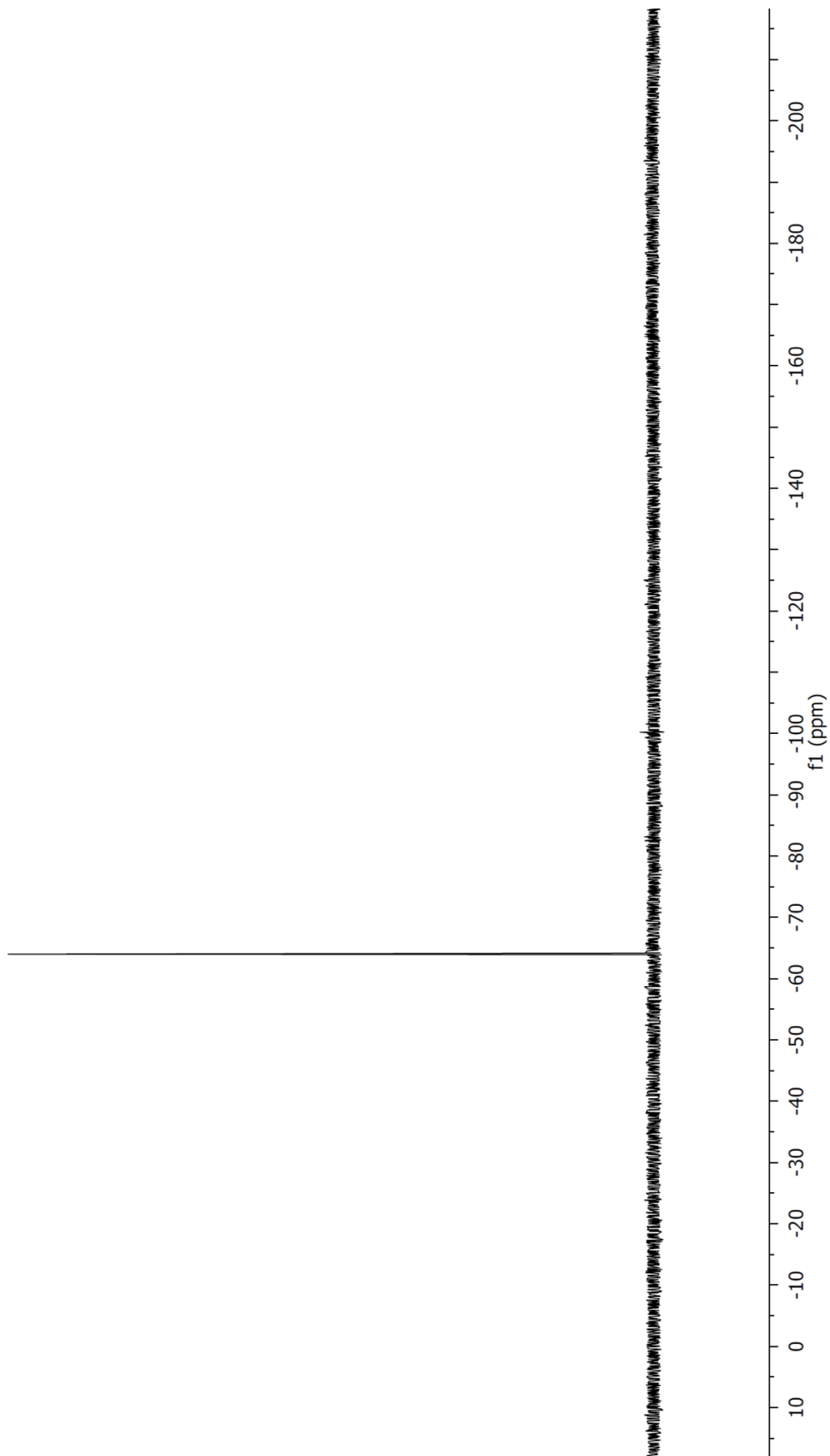


Compound 23  
13C NMR, 150 MHz

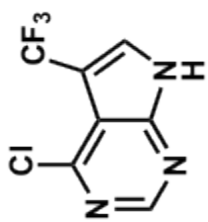




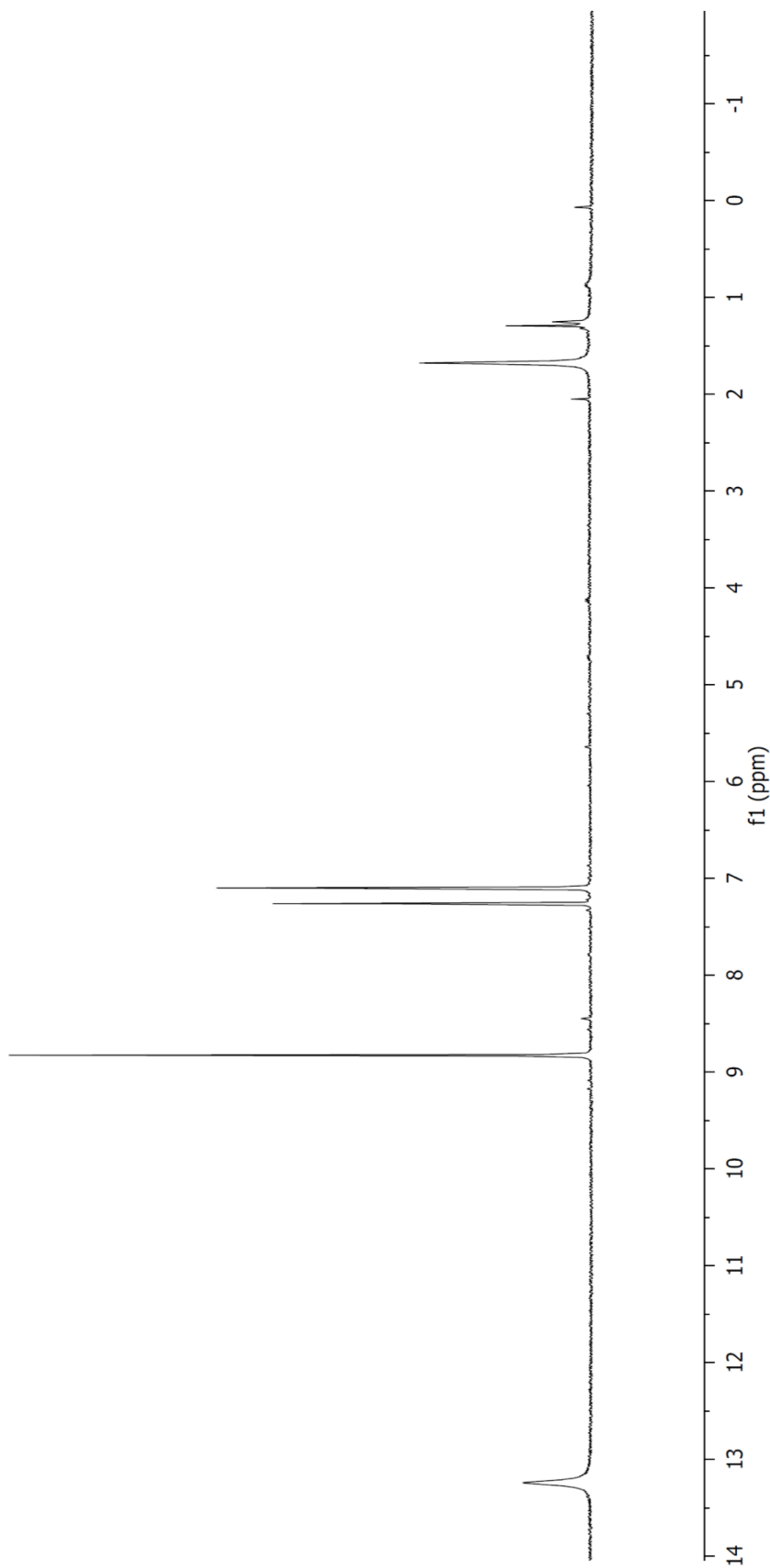
Compound 23  
19F NMR, 376 MHz

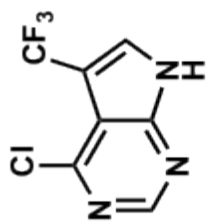




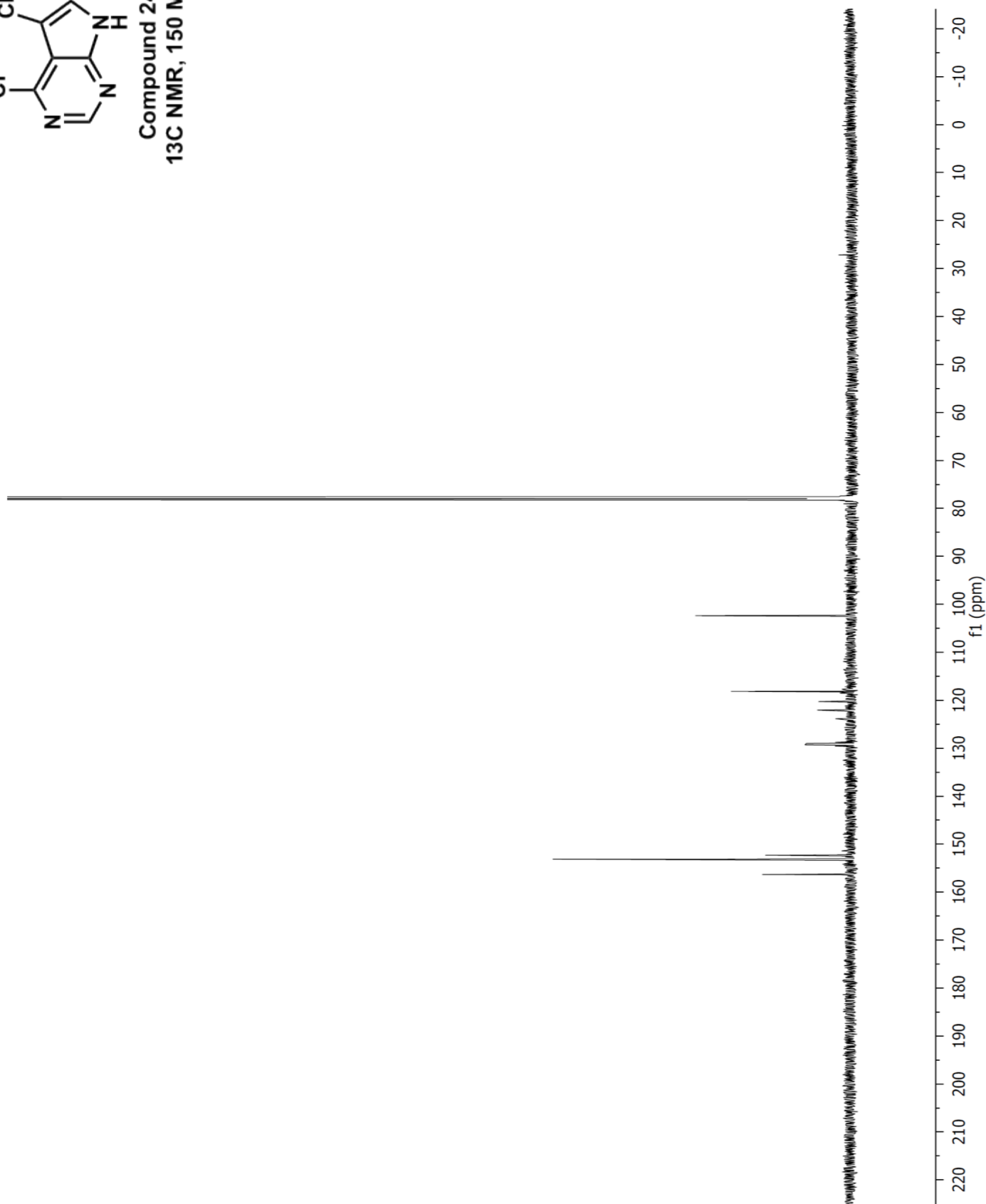


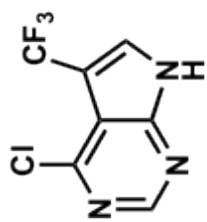
Compound 24  
1H NMR, 400 MHz



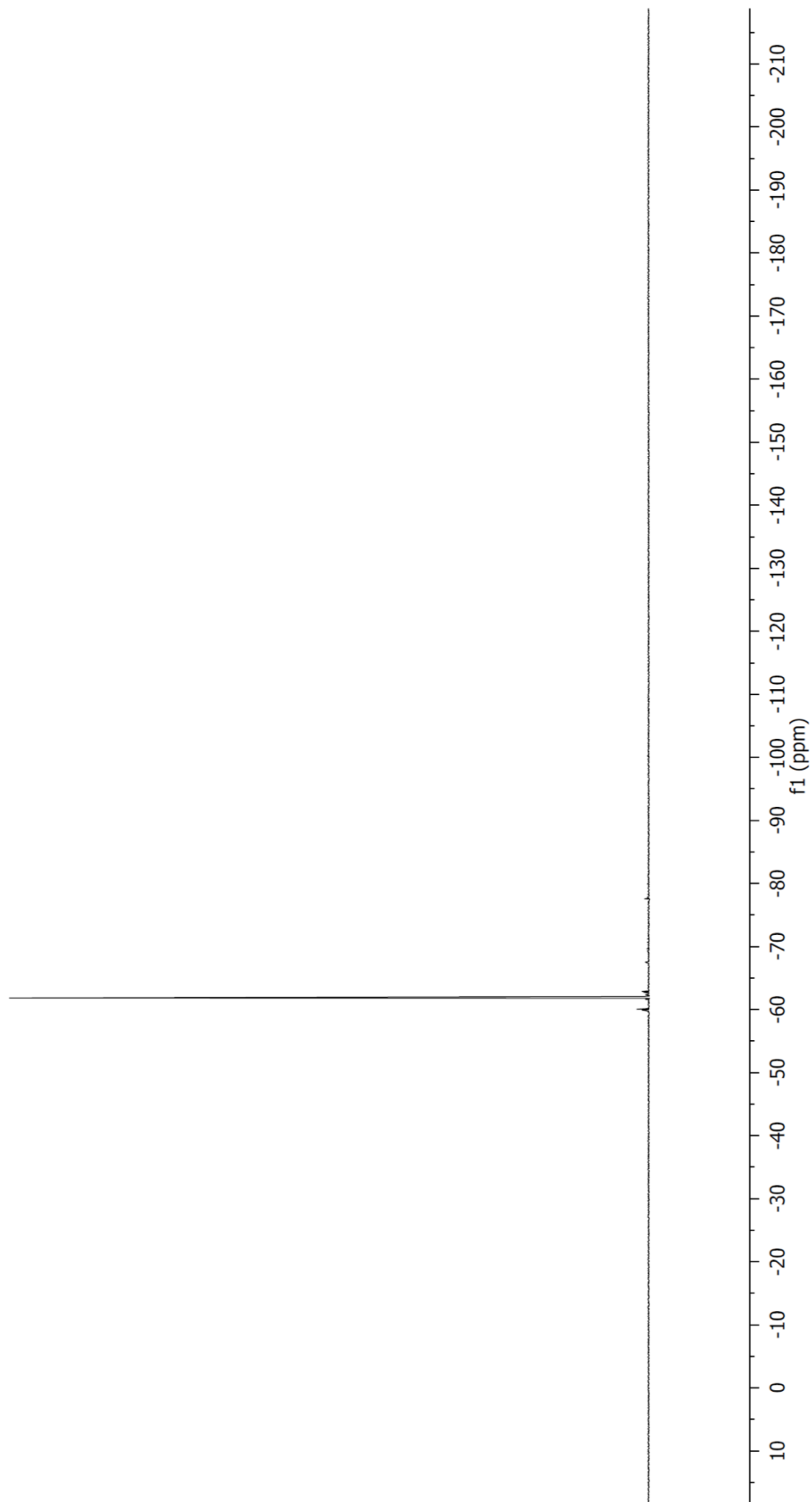


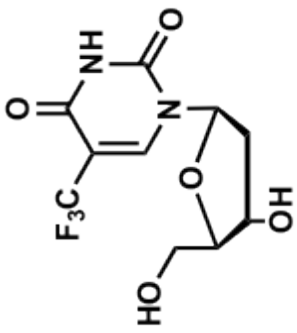
Compound 24  
13C NMR, 150 MHz



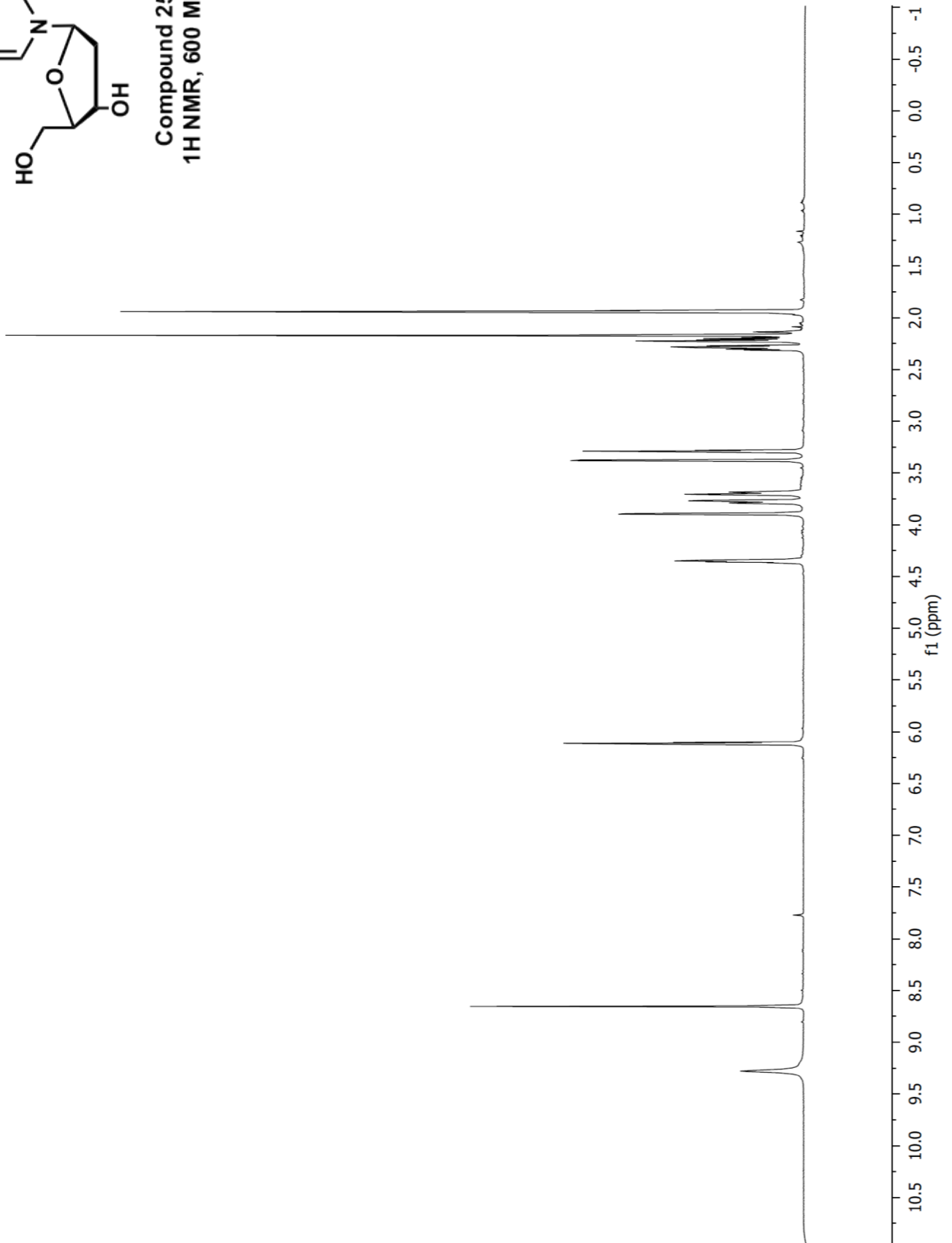


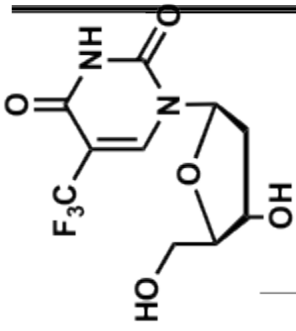
Compound 24  
19F NMR, 376 MHz



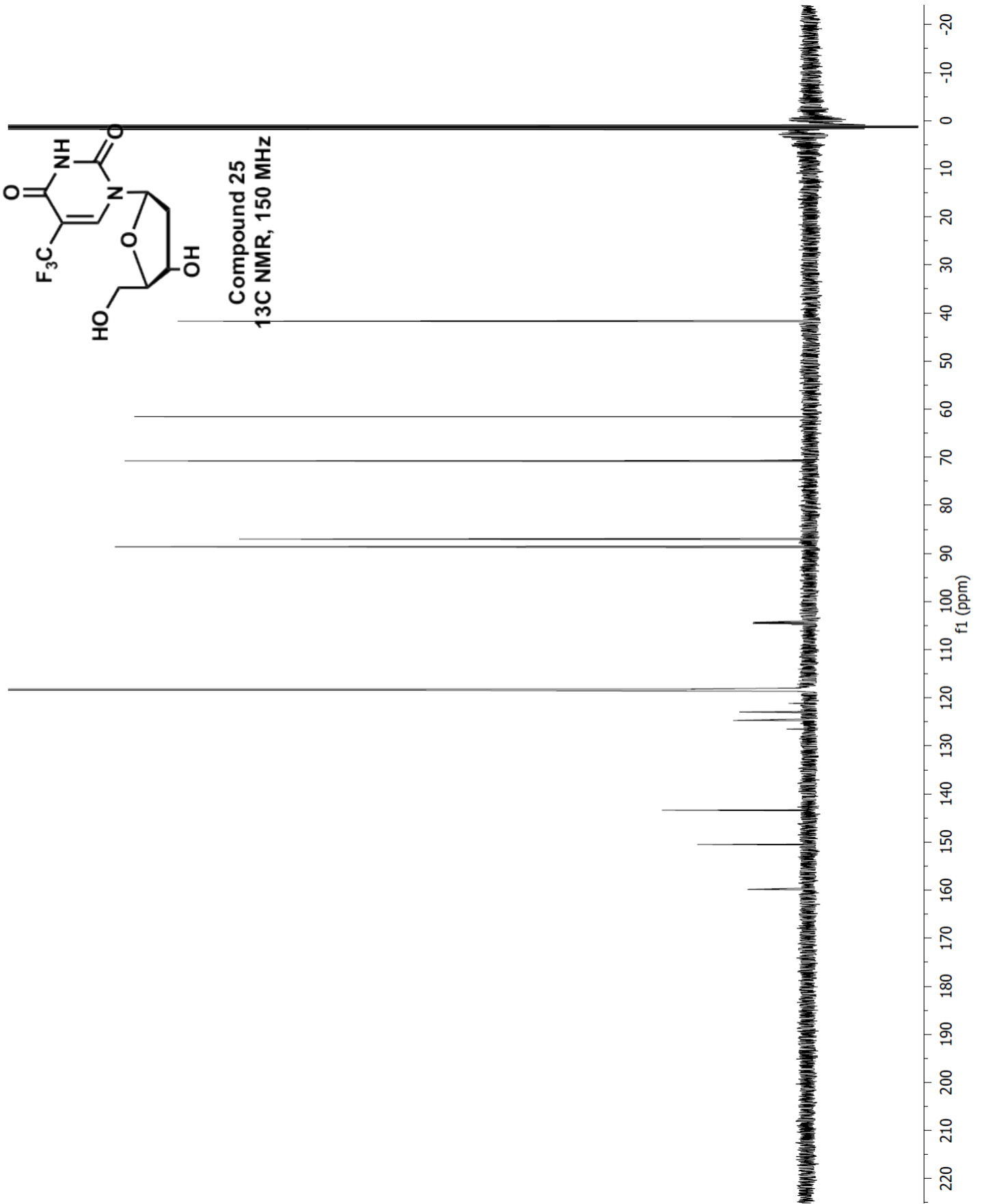


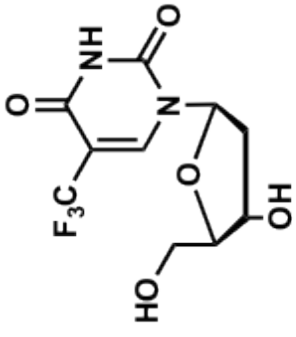
Compound 25  
1H NMR, 600 MHz



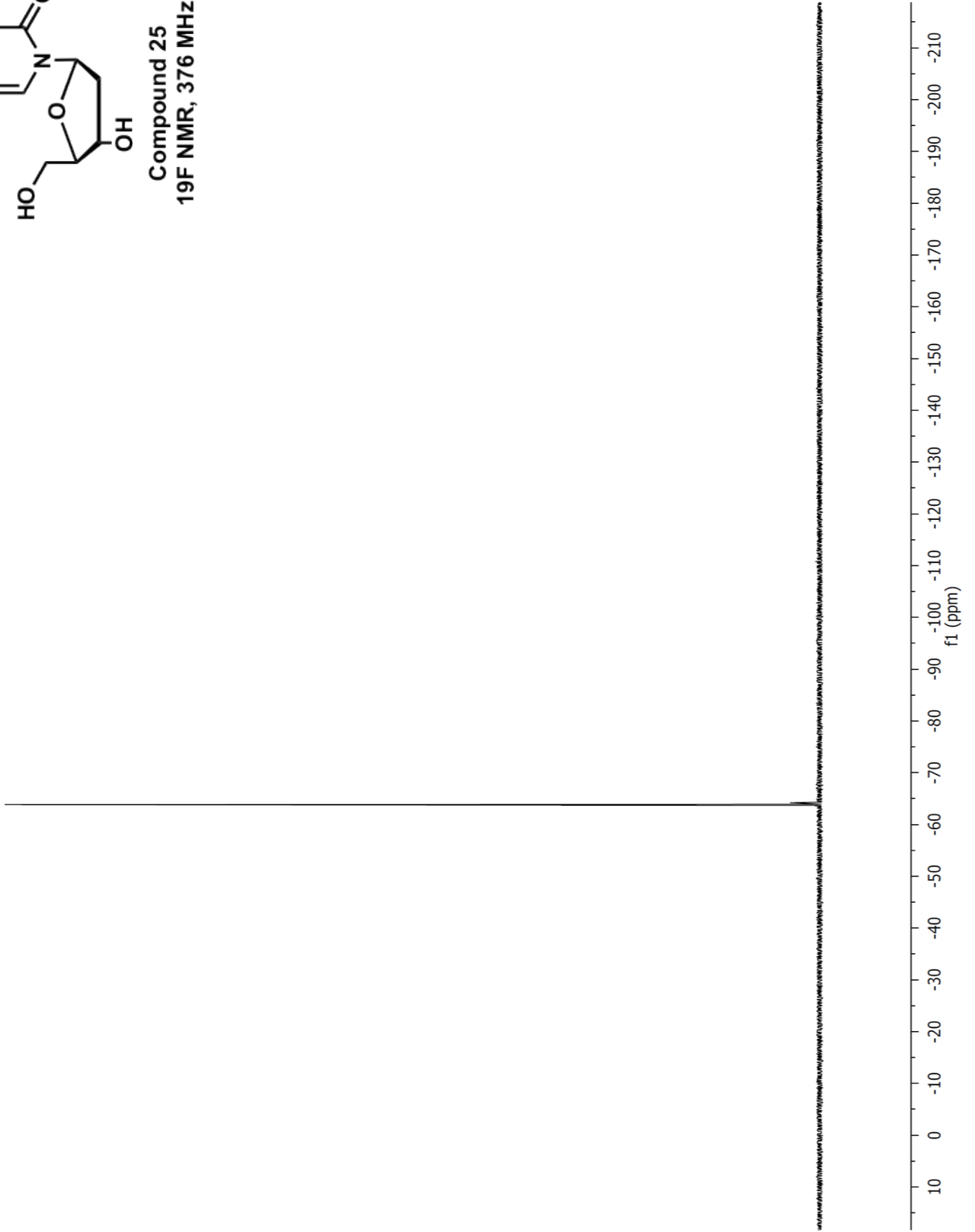


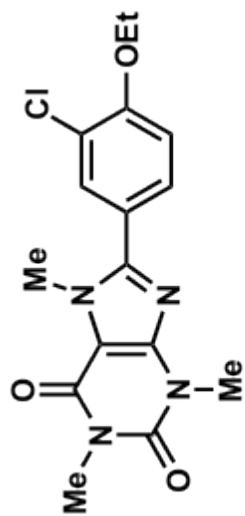
Compound 25  
 $^{13}C$  NMR, 150 MHz



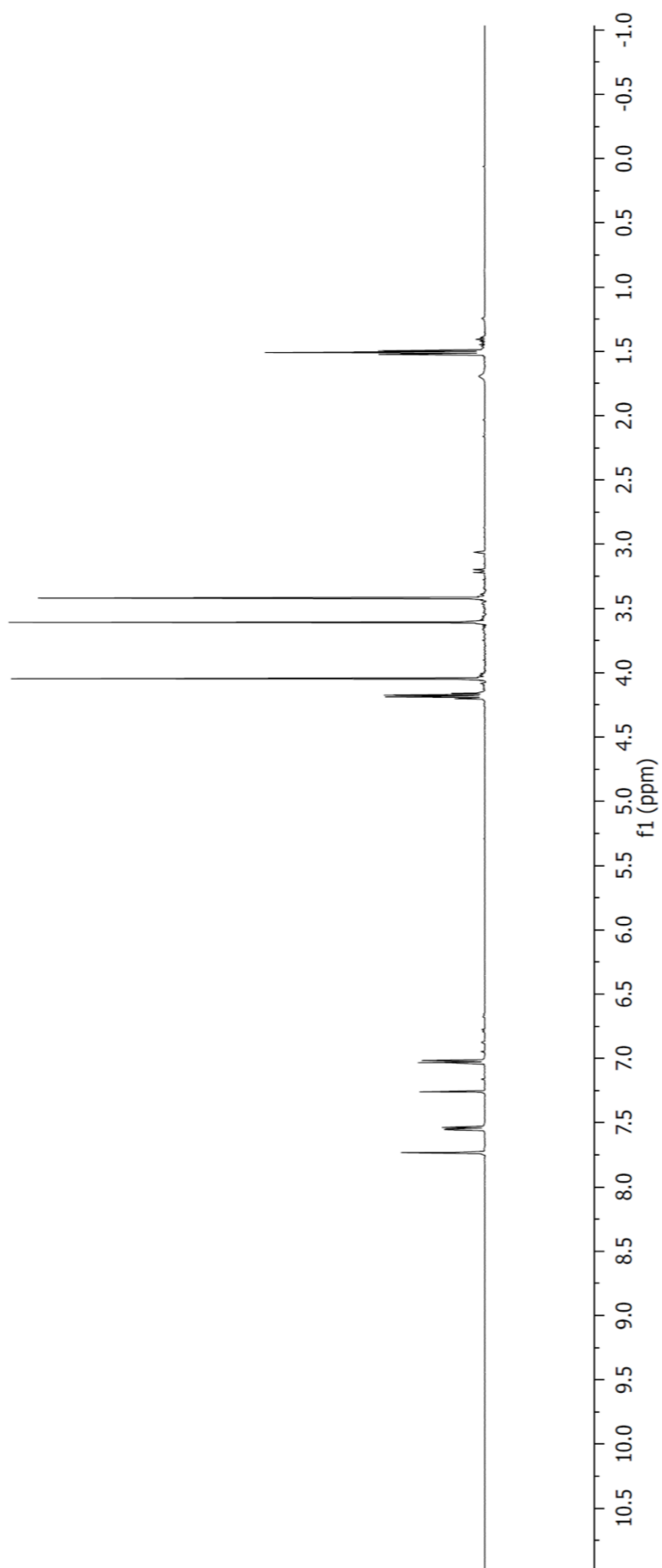


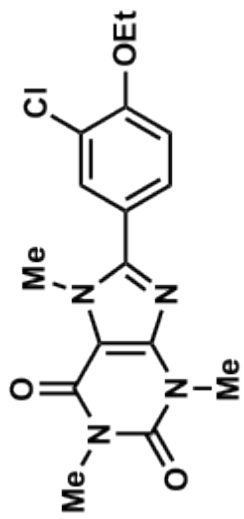
Compound 25  
19F NMR, 376 MHz



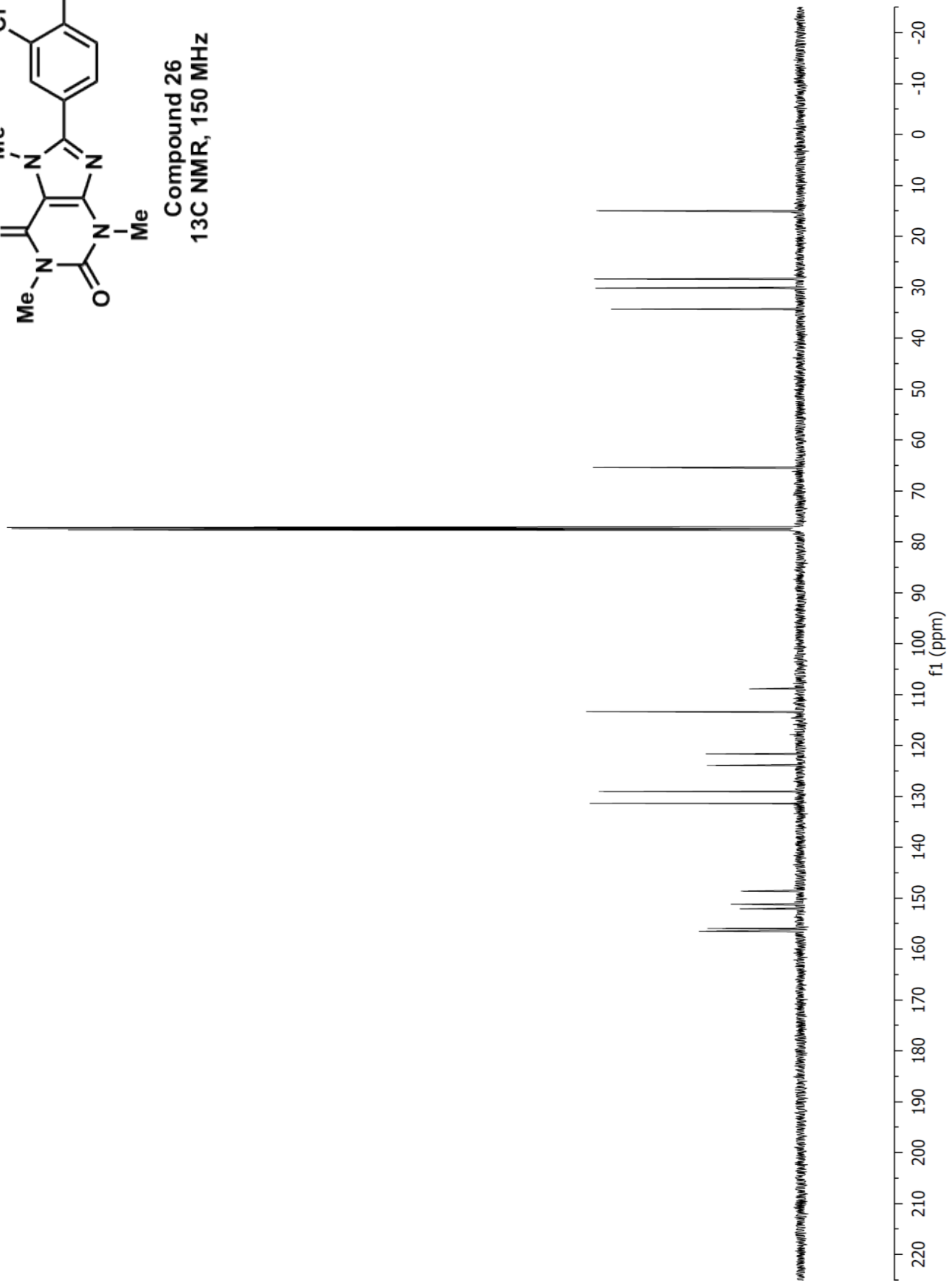


Compound 26  
1H NMR, 400 MHz

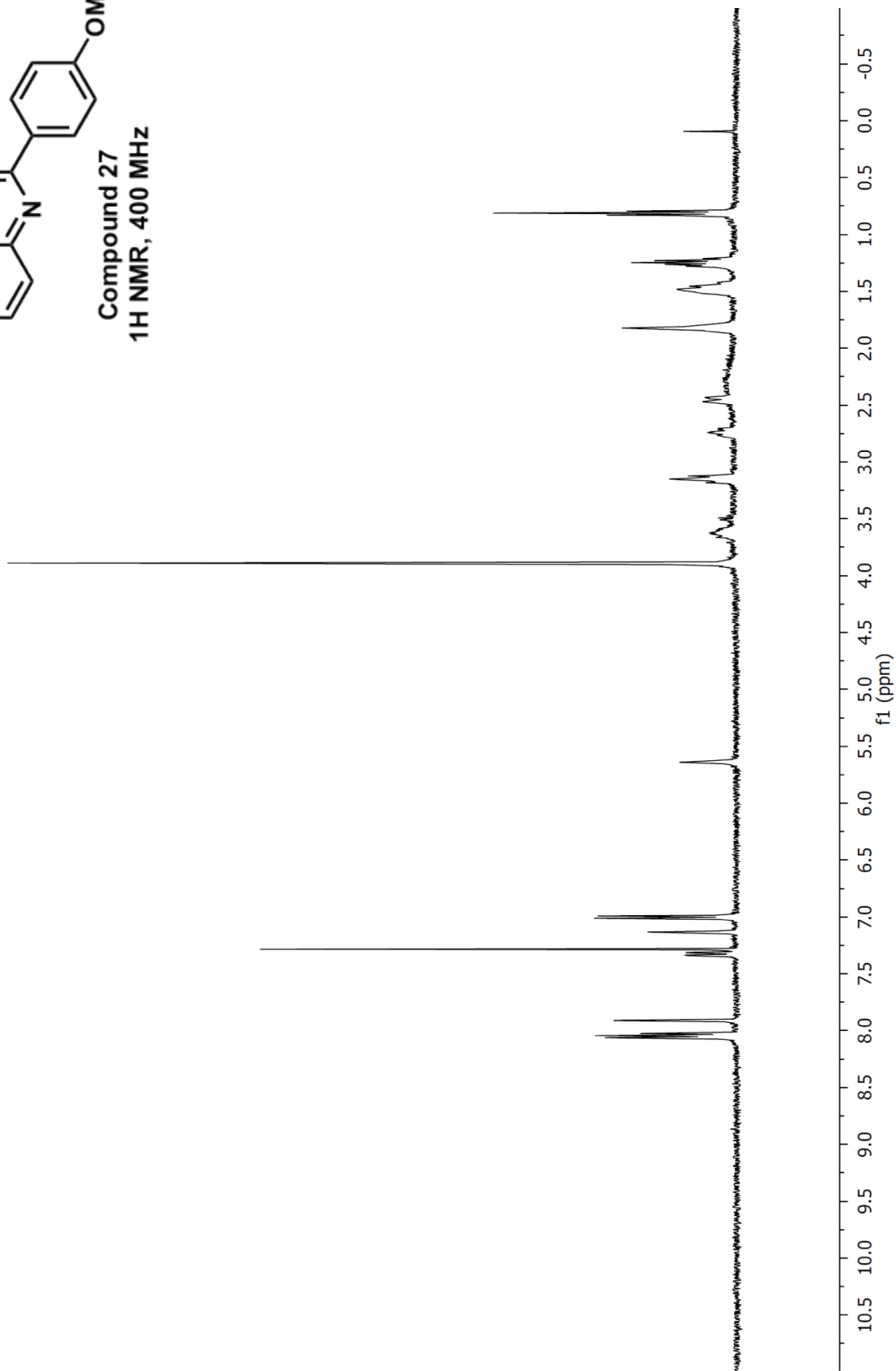
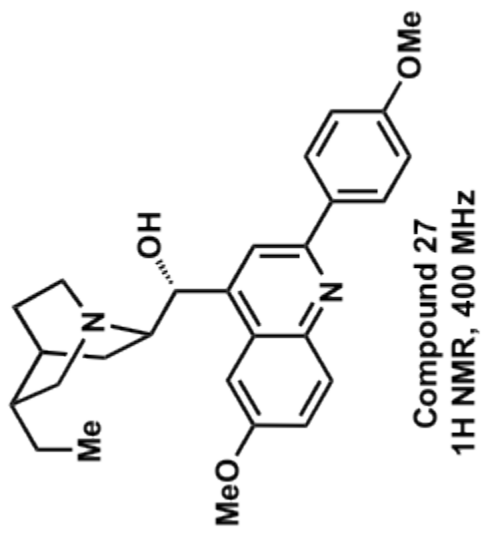


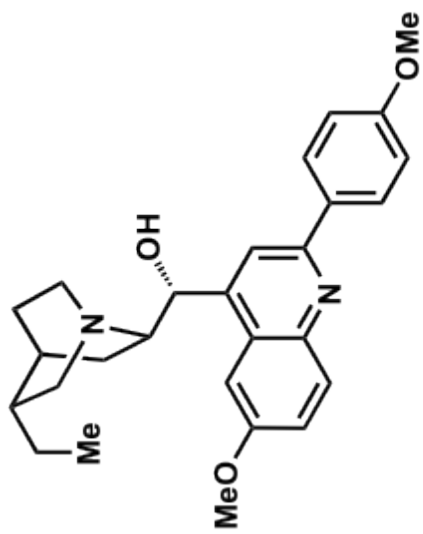


Compound 26  
13C NMR, 150 MHz

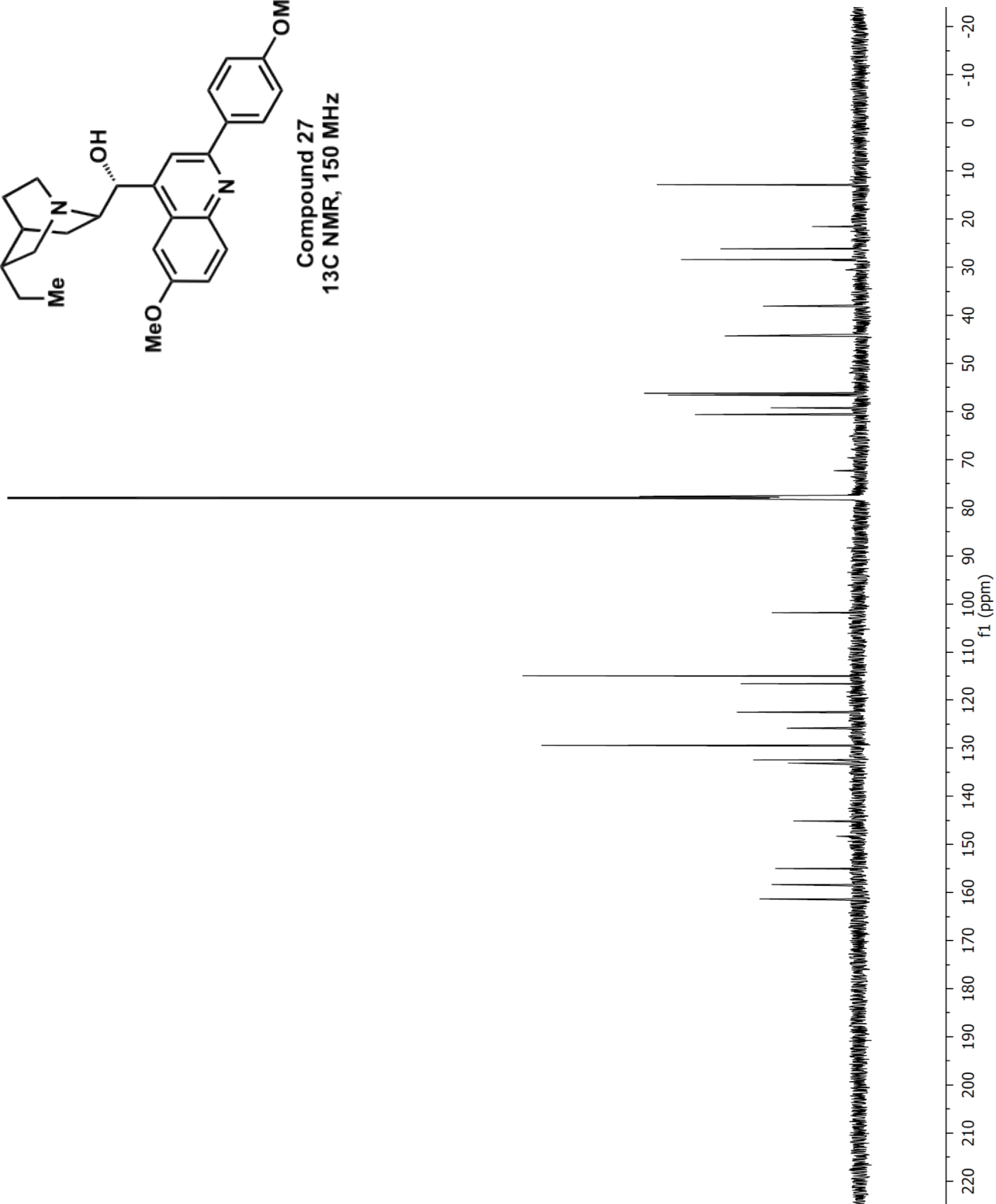


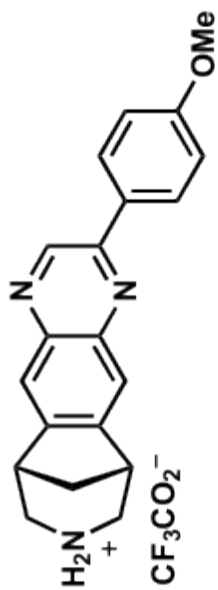




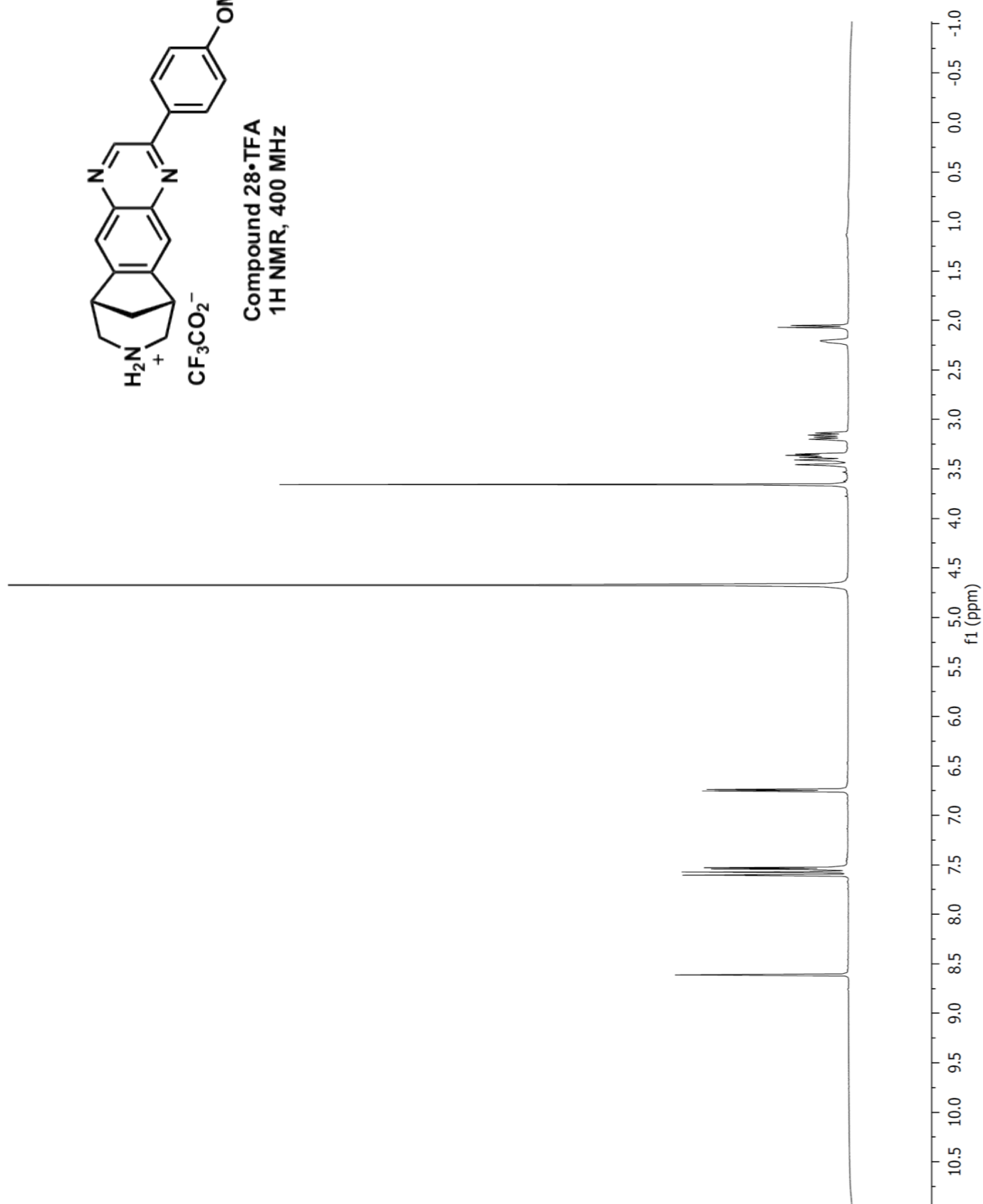


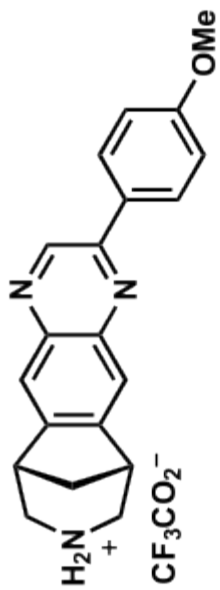
Compound 27  
13C NMR, 150 MHz



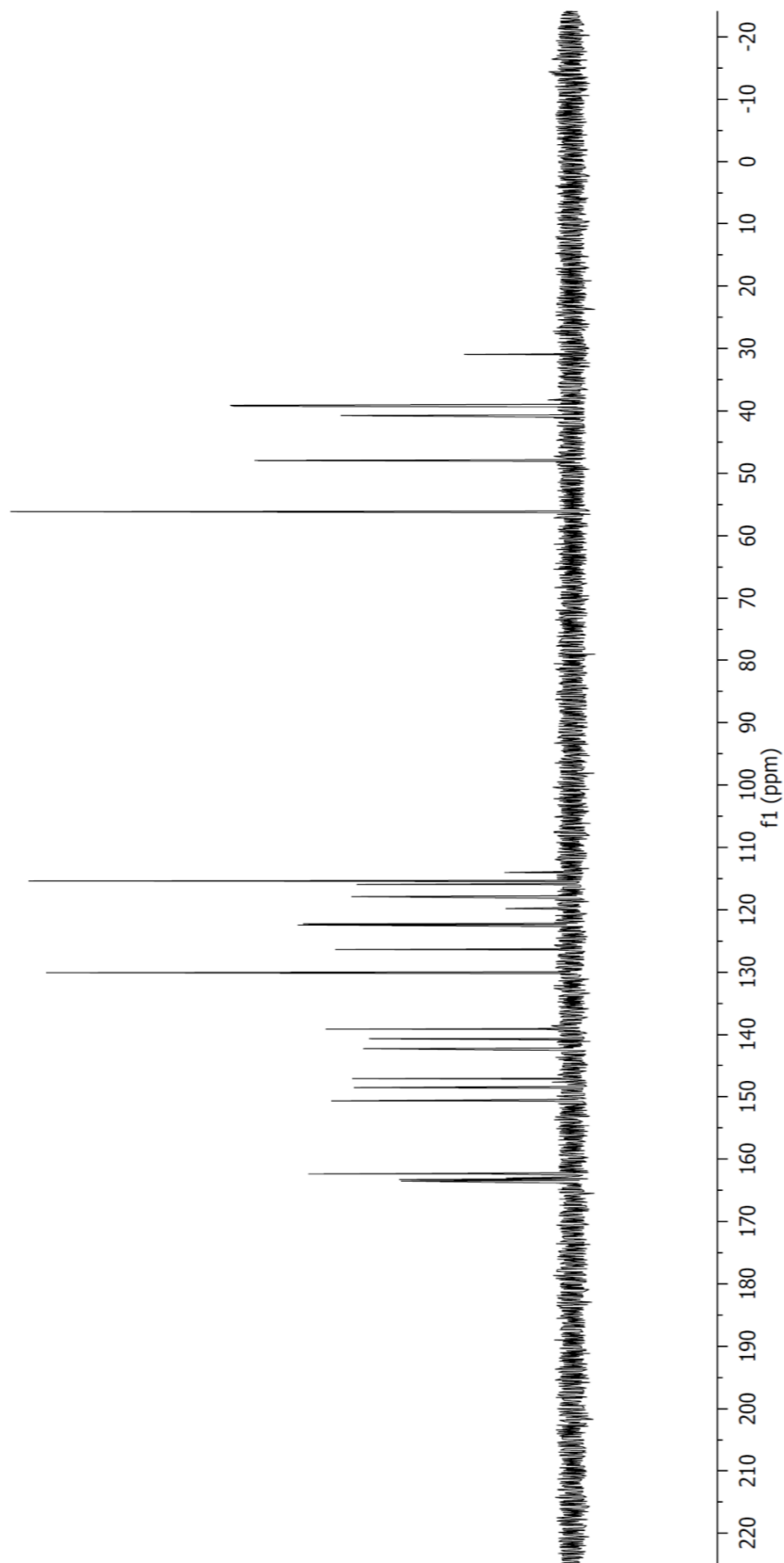


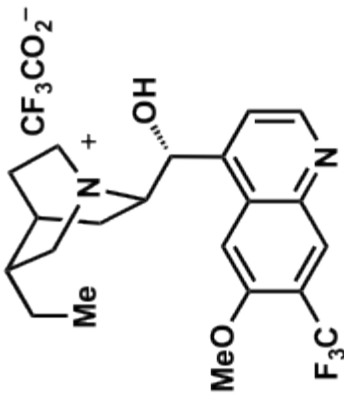
Compound 28•TFA  
1H NMR, 400 MHz



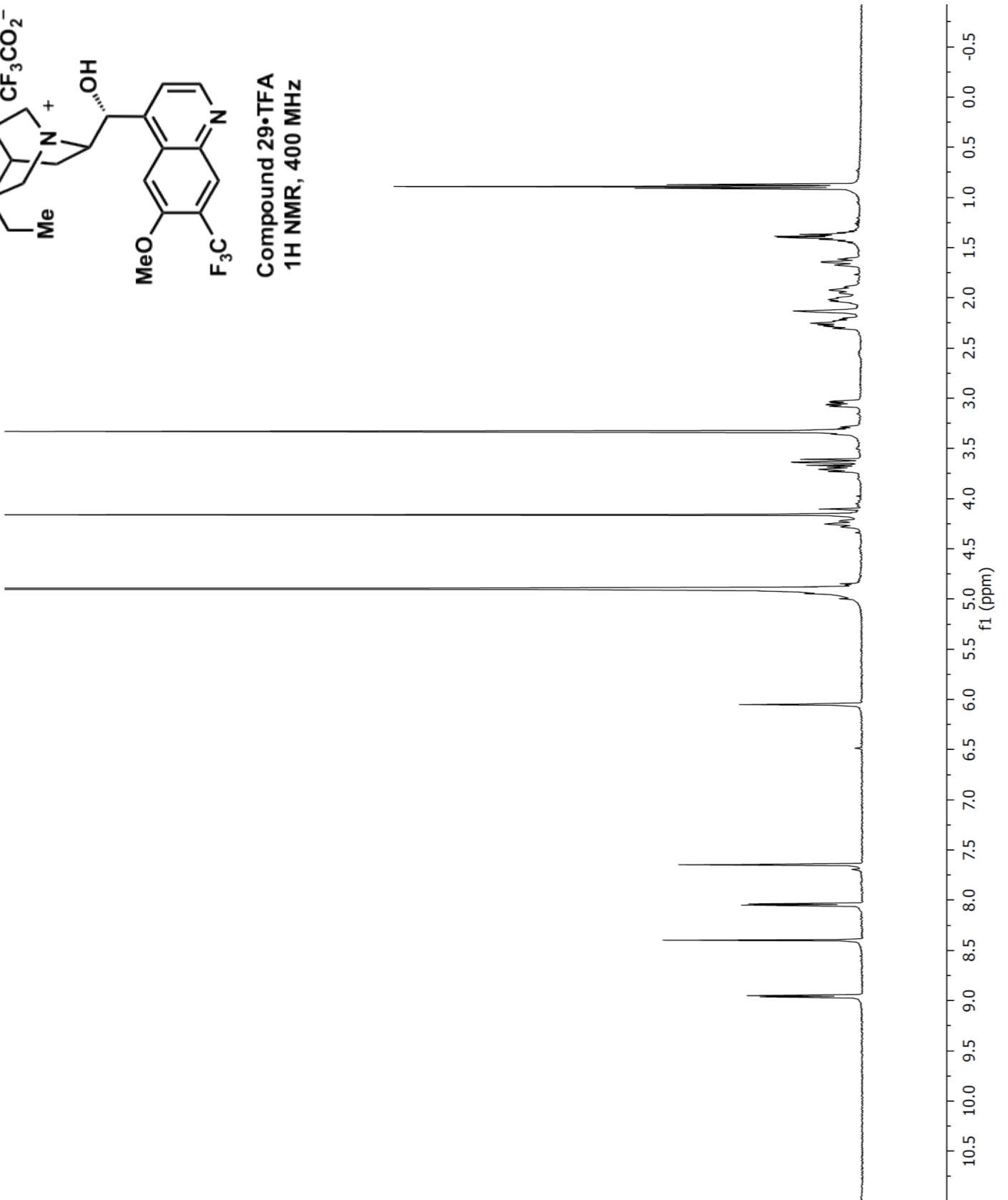


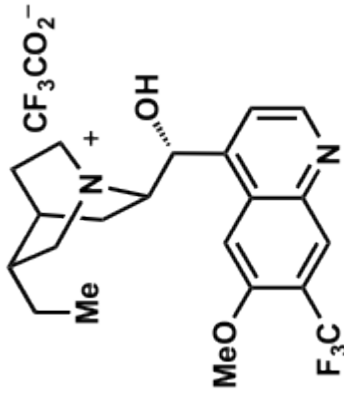
Compound 28•TFA  
13C NMR, 150 MHz



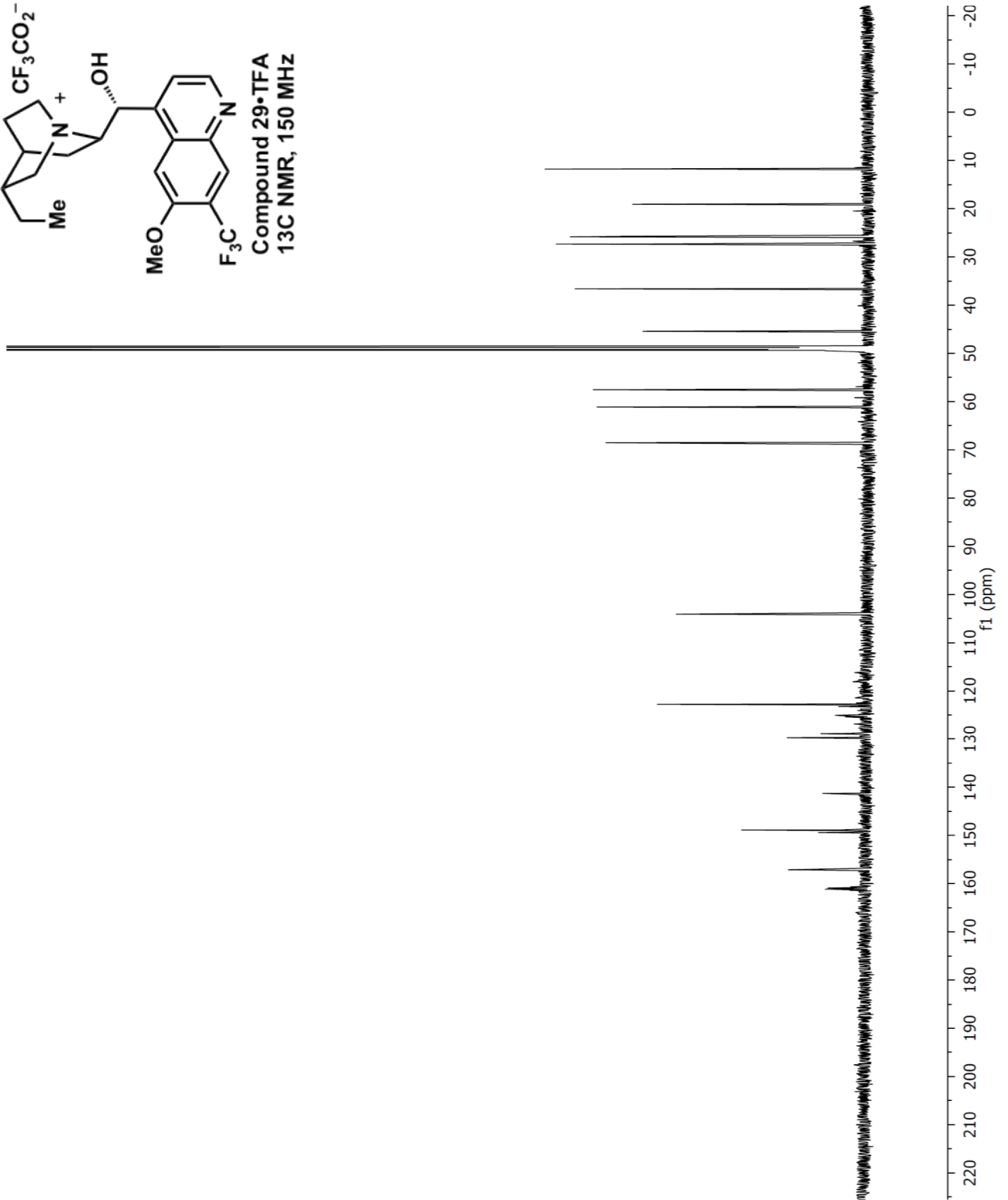


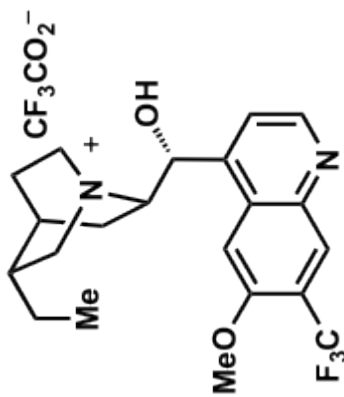
Compound 29•TFA  
1H NMR, 400 MHz



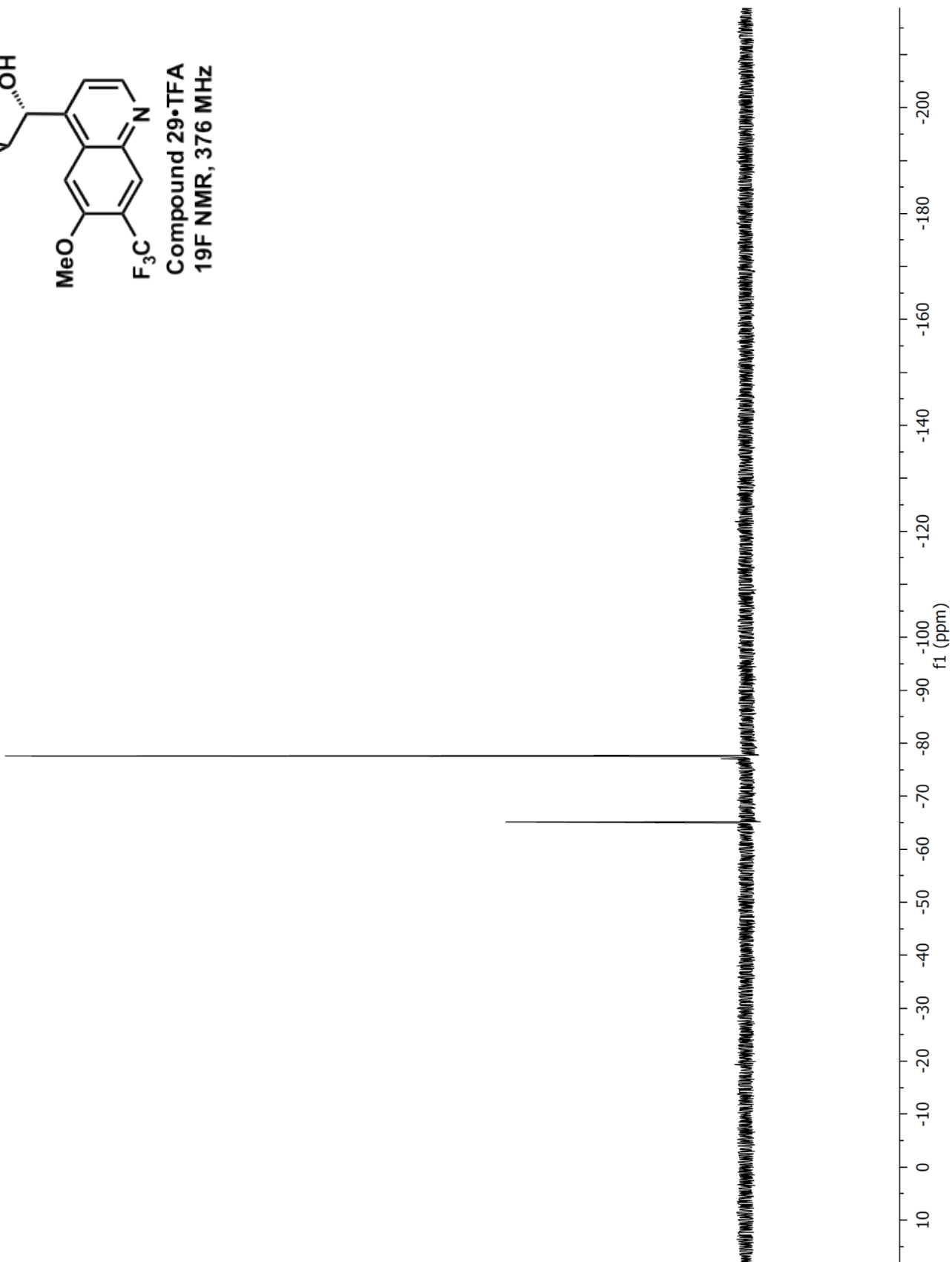


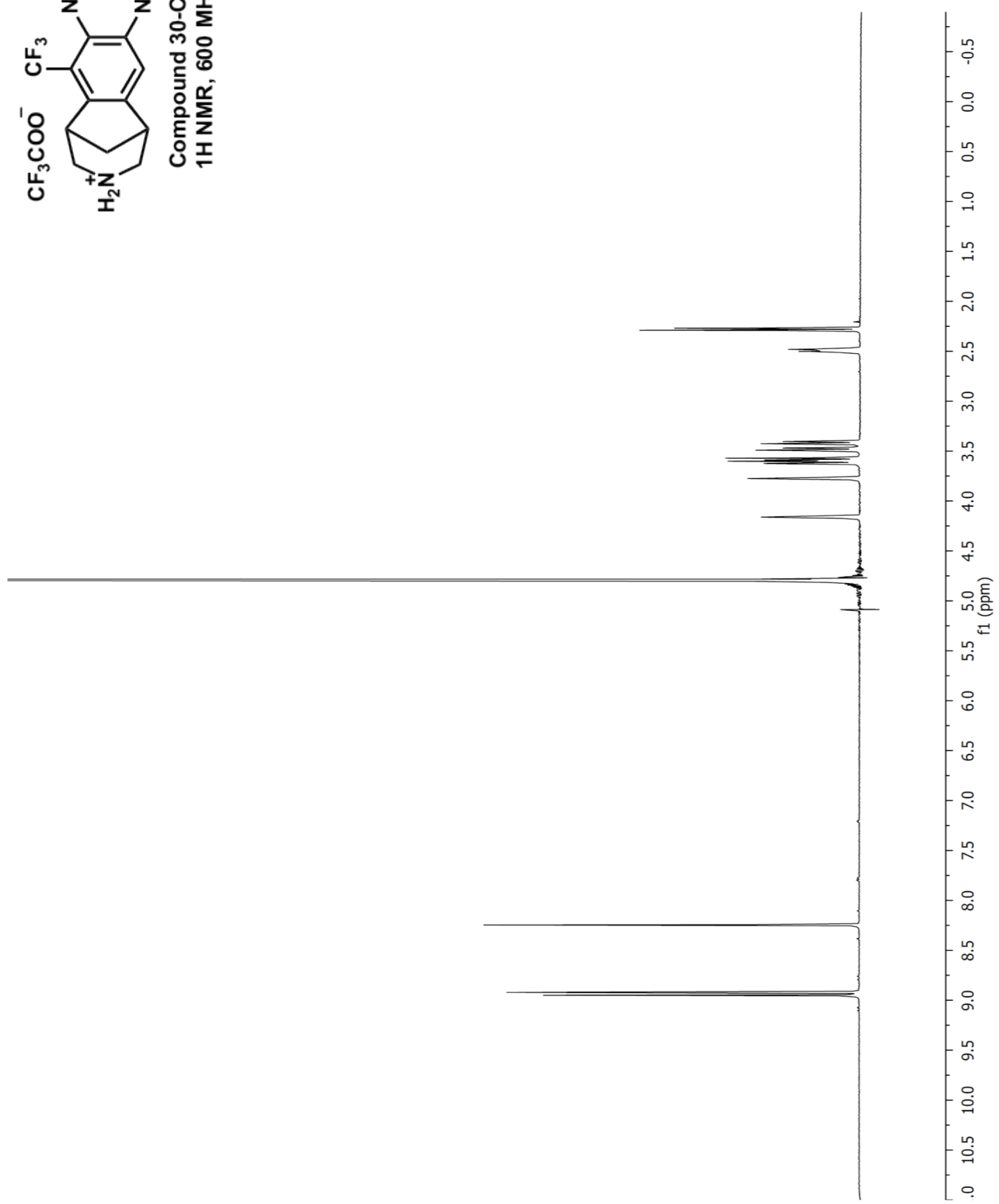
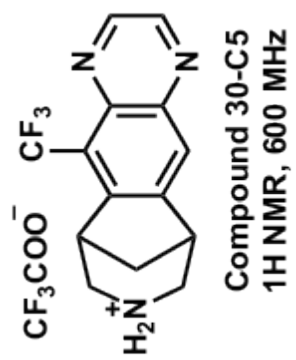
Compound 29•TFA  
13C NMR, 150 MHz



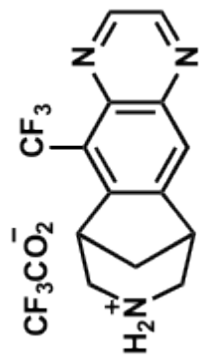


Compound 29•TFA  
19F NMR, 376 MHz

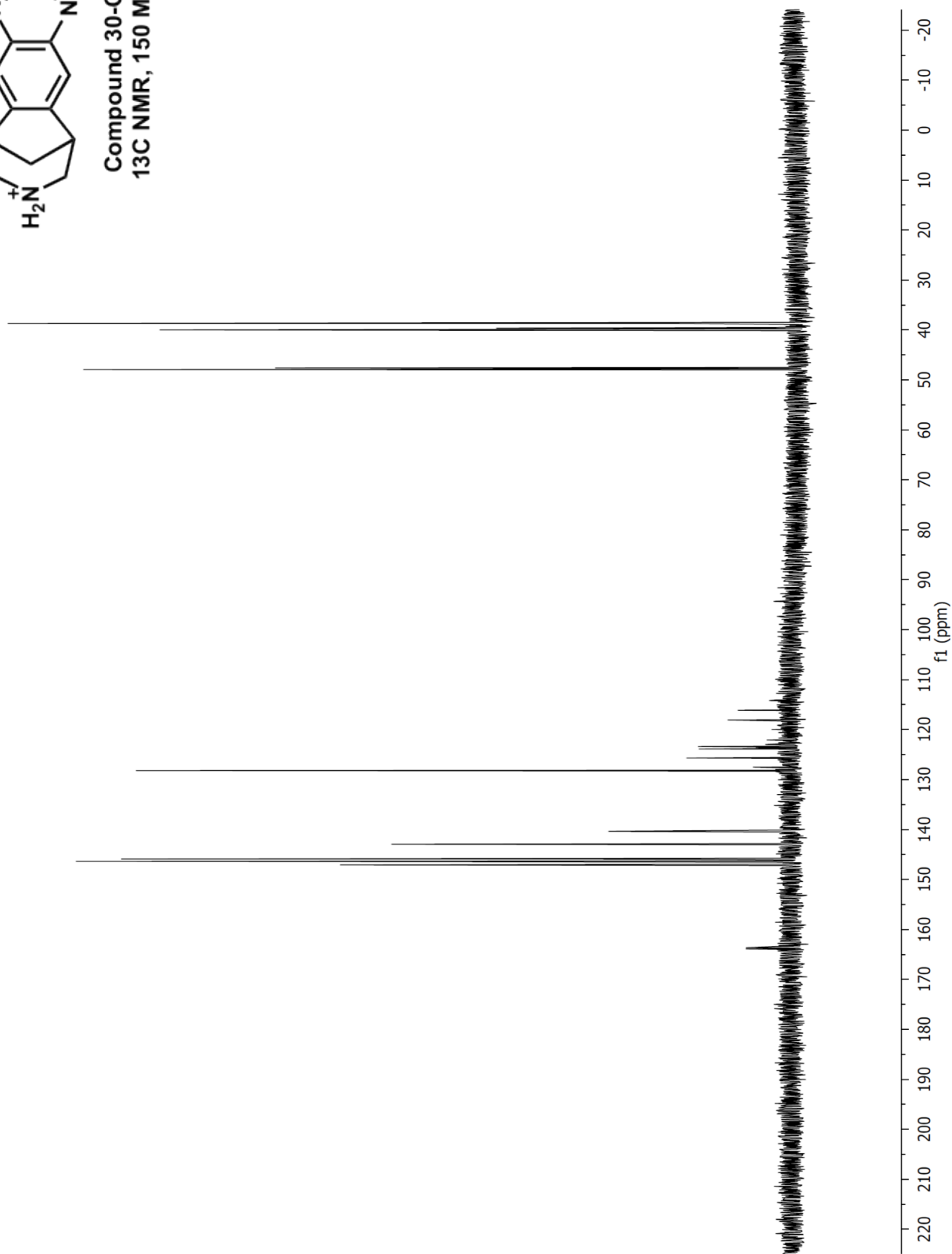


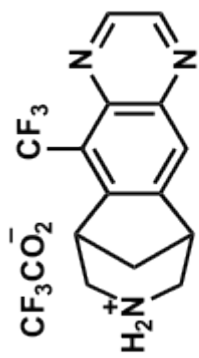




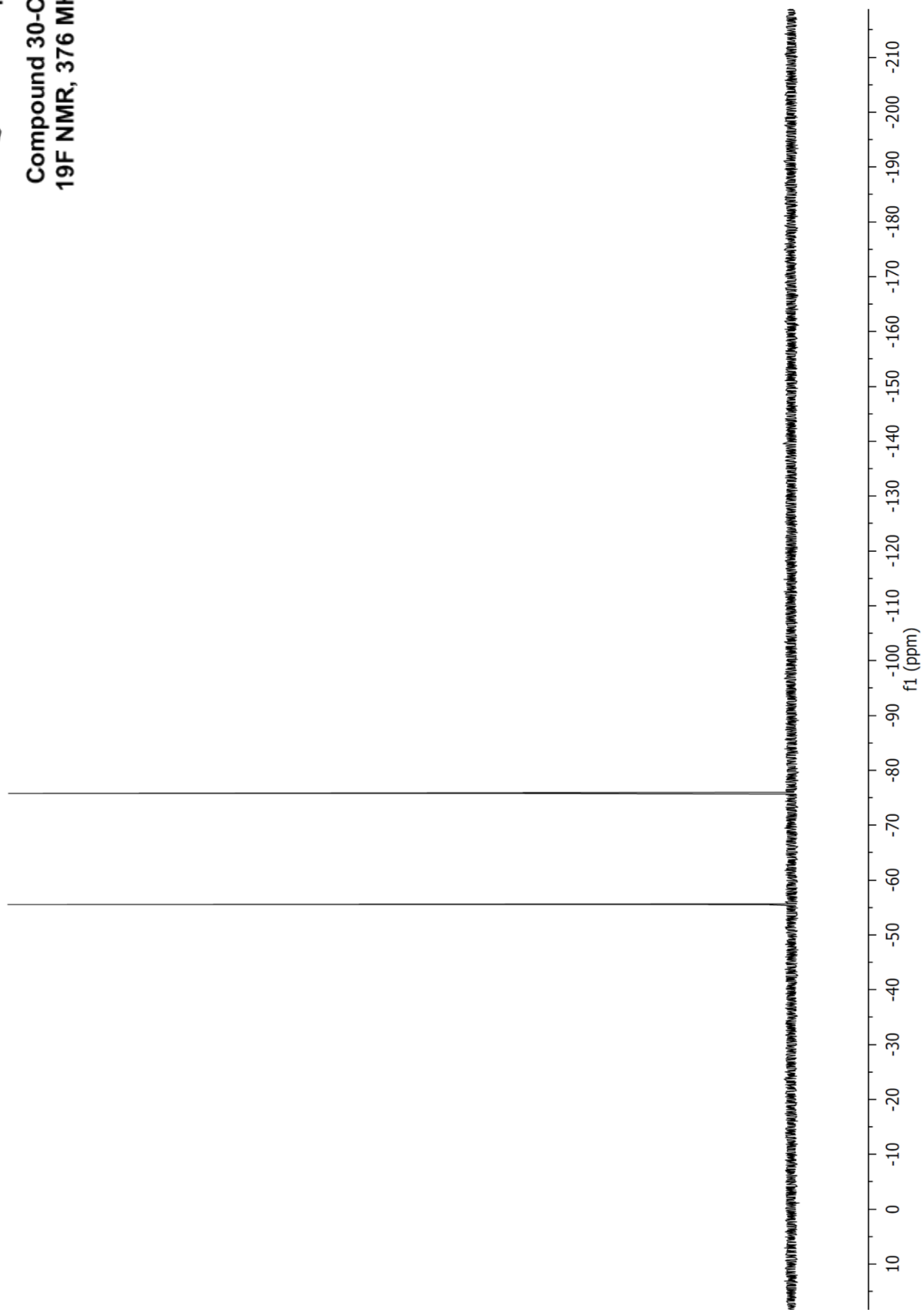


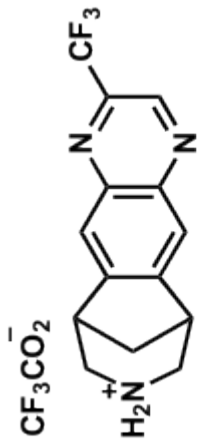
Compound 30-C5  
13C NMR, 150 MHz



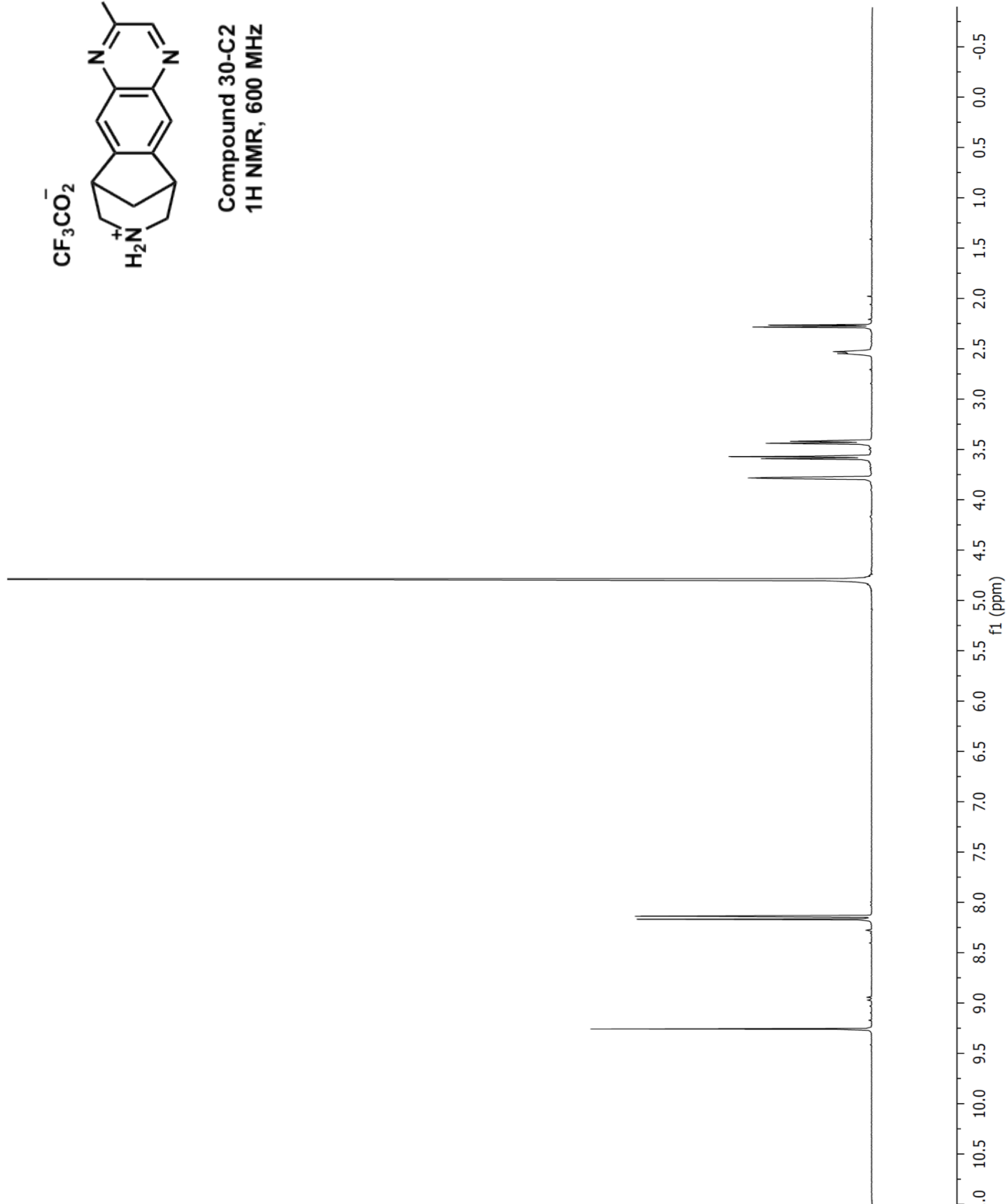


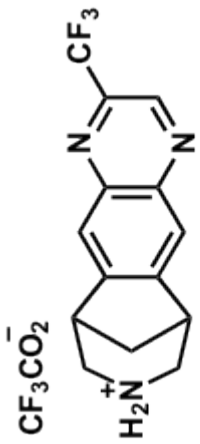
Compound 30-C5  
19F NMR, 376 MHz



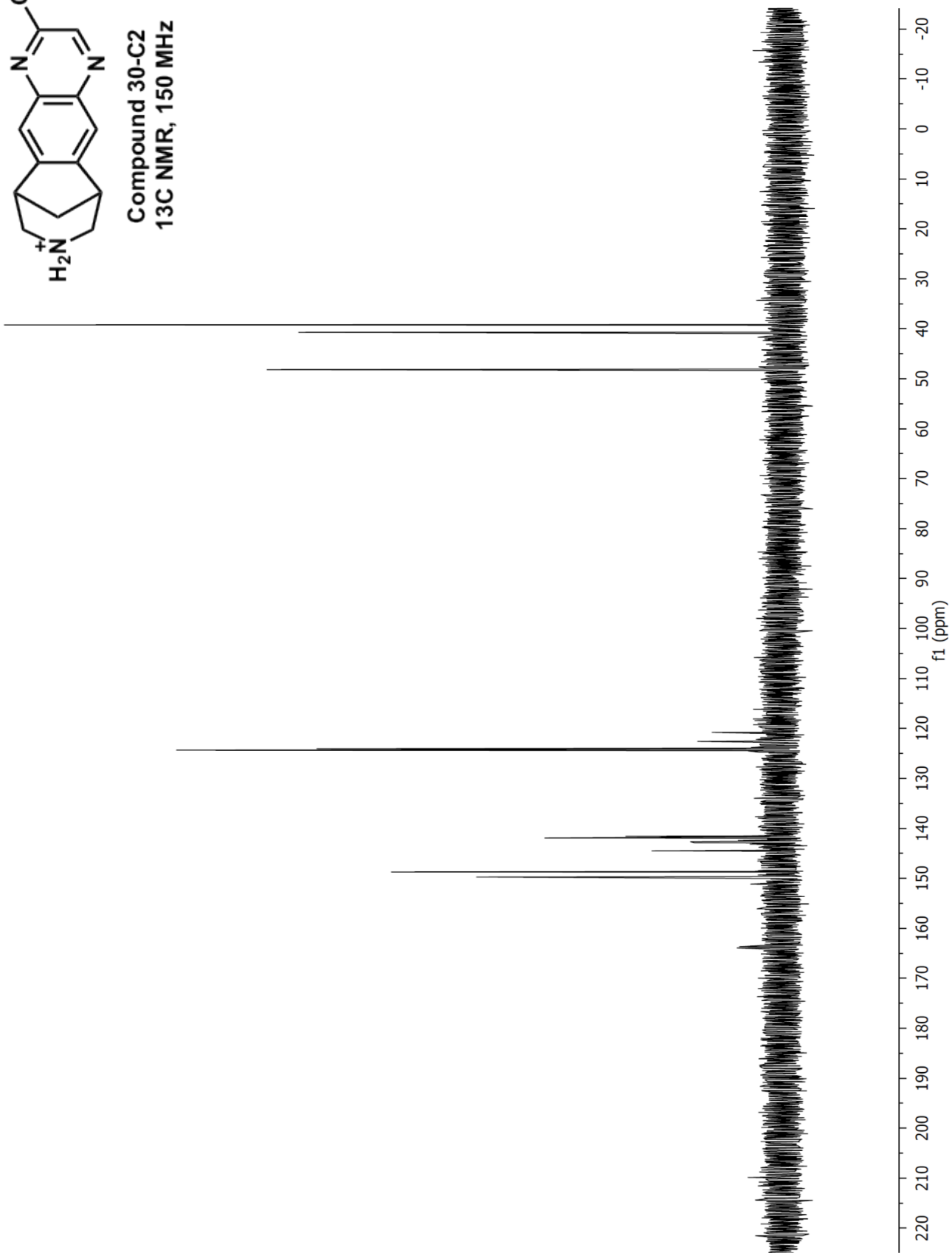


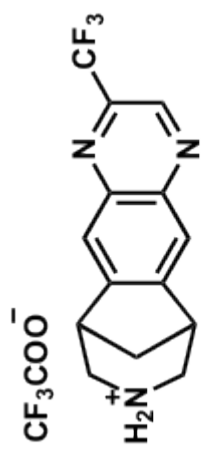
Compound 30-C2  
1H NMR, 600 MHz



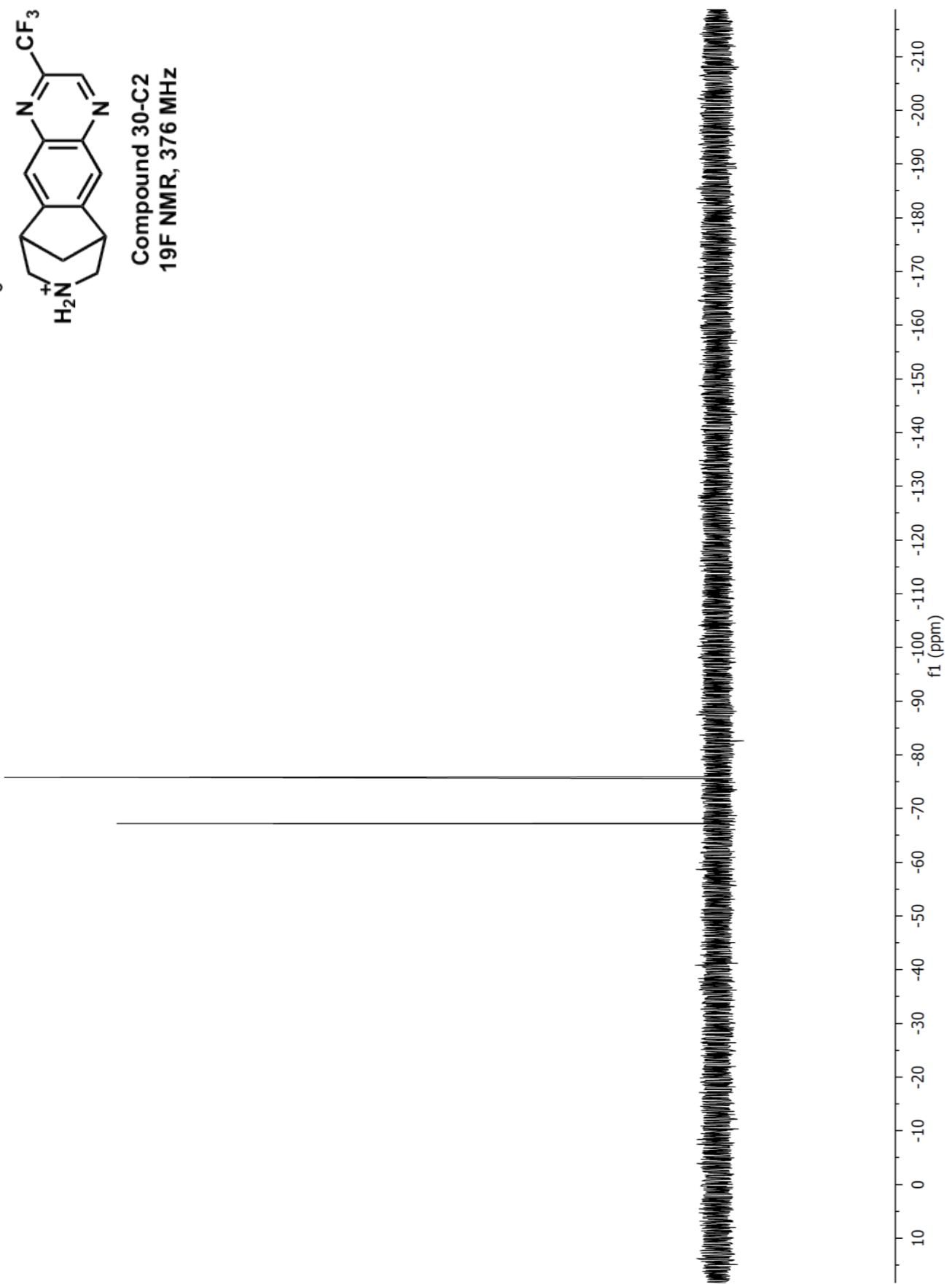


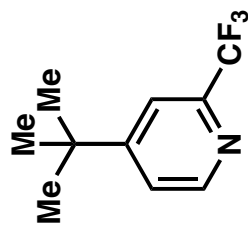
Compound 30-C2  
13C NMR, 150 MHz



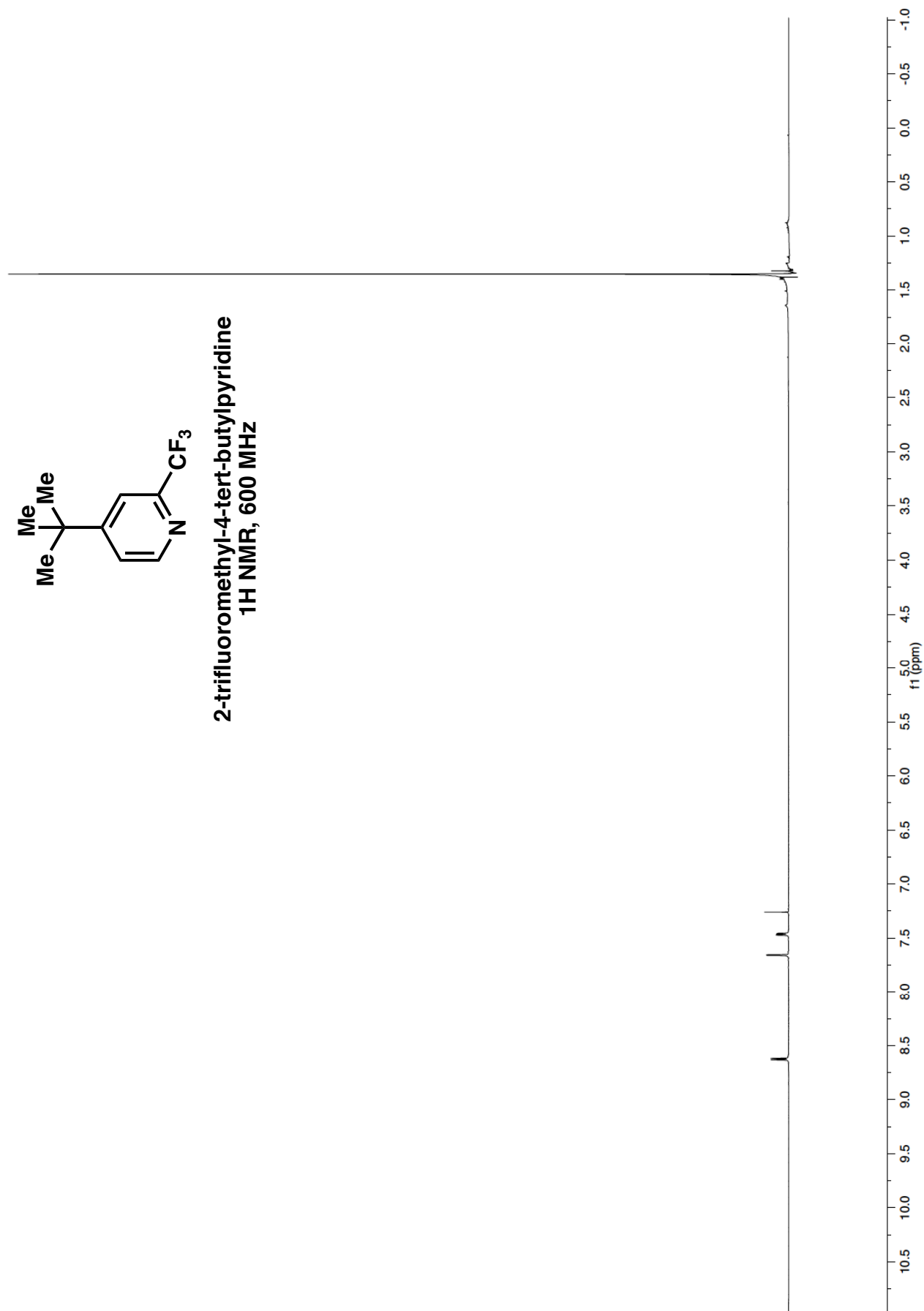


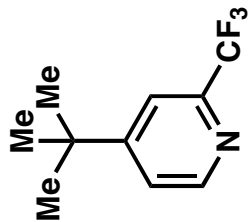
Compound 30-C2  
19F NMR, 376 MHz



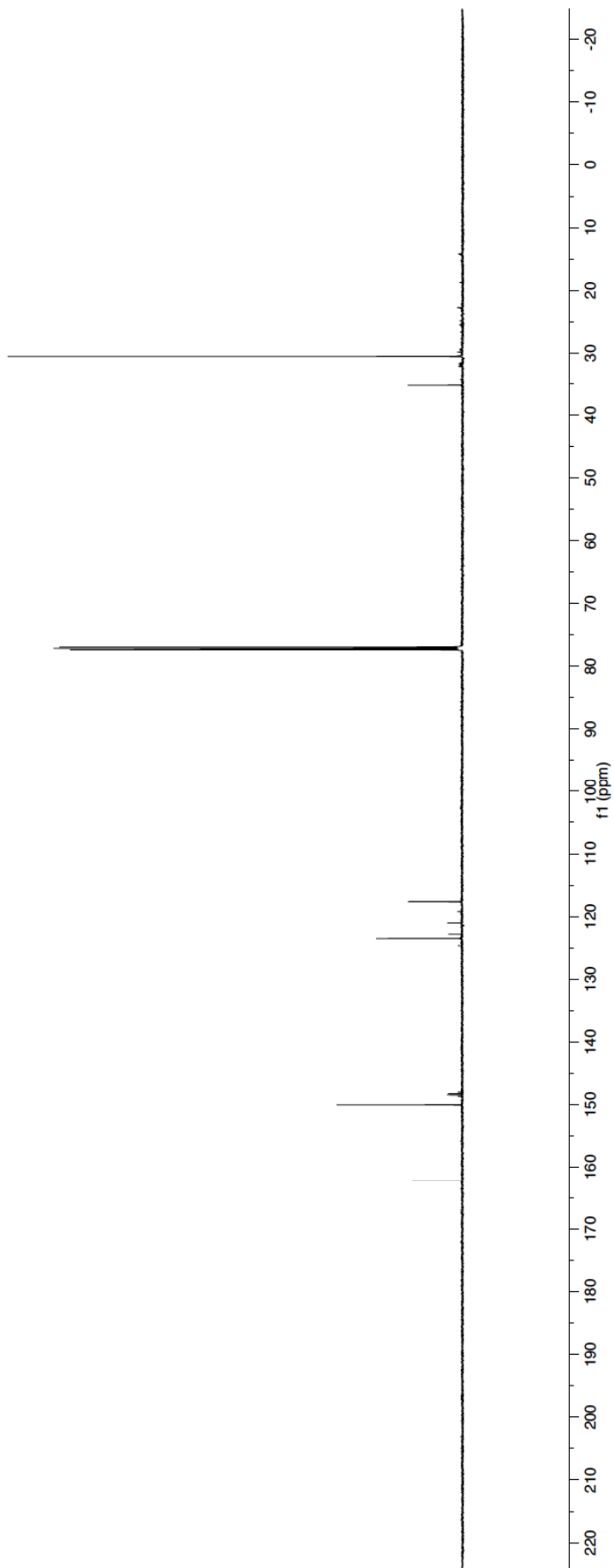


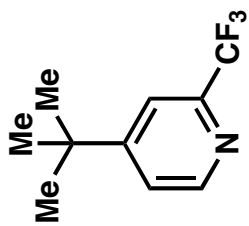
2-trifluoromethyl-4-tert-butylpyridine  
1H NMR, 600 MHz





2-tert-butyl-4-(trifluoromethyl)pyridine  
13C NMR, 150 MHz





2-(tert-butyl)-4-(trifluoromethyl)pyridine  
19F NMR, 376 MHz

