

Nickel-Catalyzed Borylation of Halides and Pseudo-Halides with Tetrahydroxydiboron [$\text{B}_2(\text{OH})_4$]

Supporting Information

*Gary A. Molander**[†], *Livia N. Cavalcanti*[†] and *Carolina García-García*[‡]

[†]Roy and Diana Vagelos Laboratories and Penn/Merck Laboratory for High Throughput Experimentation, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, United States

[‡] Departamento de Química Orgánica (C-I), Universidad Autónoma de Madrid Cantoblanco, 28049, Madrid, Spain

gmolandr@sas.upenn.edu

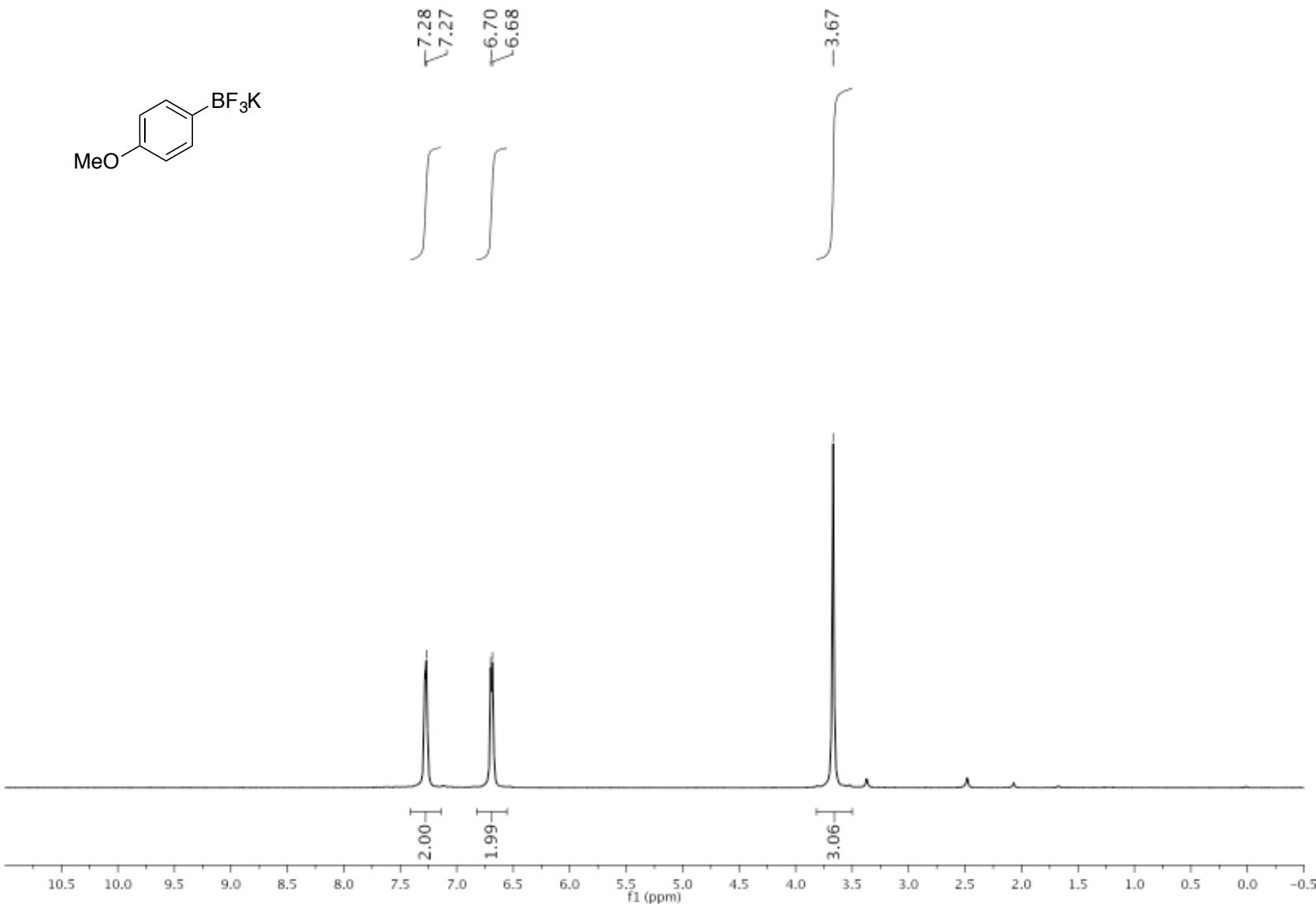
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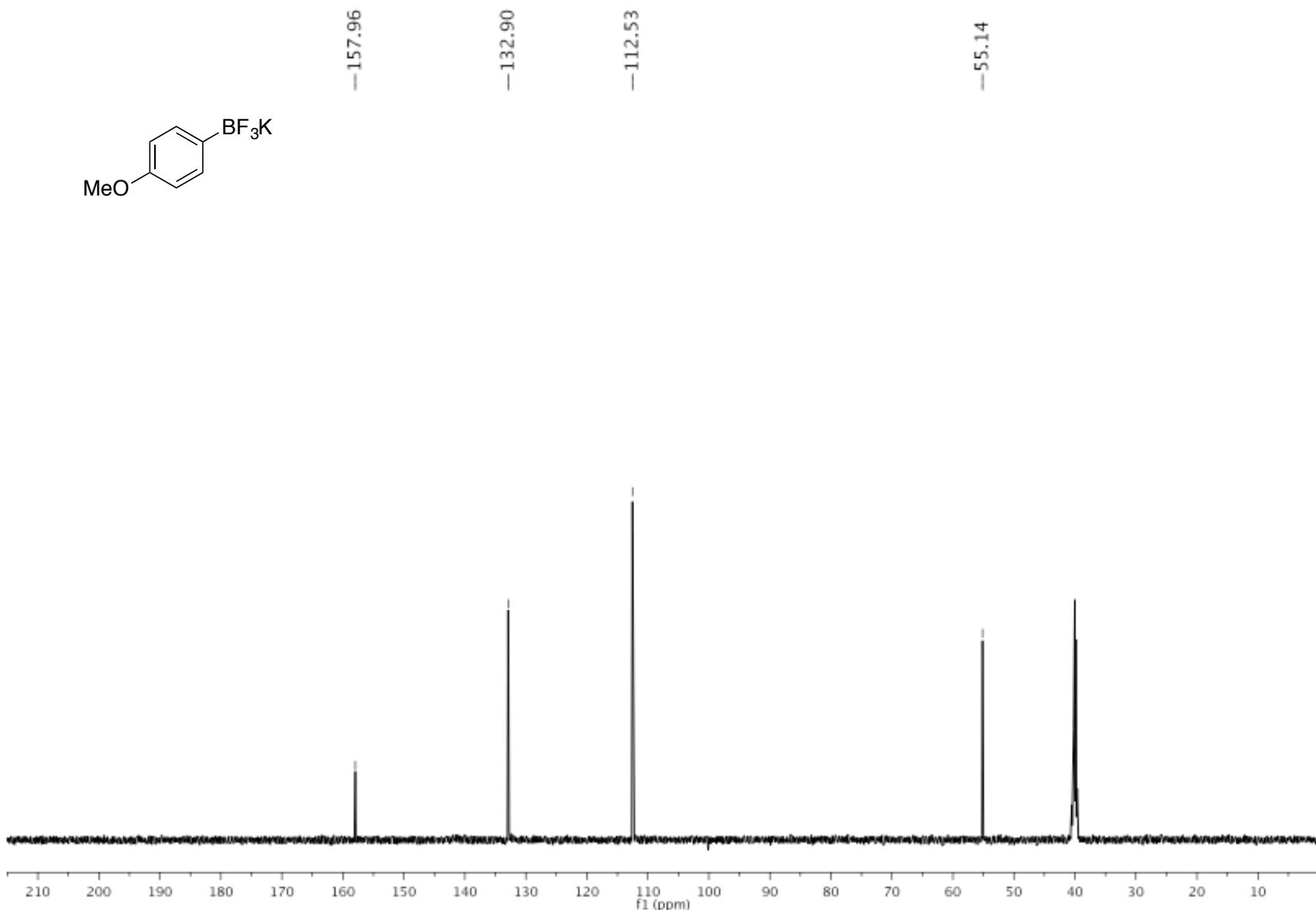
General Considerations

Reagents: All reactions were carried out under and atmosphere of argon. Ethanol (200 proof, non-anhydrous) was degassed (1 h) with argon prior to use. Aryl halides were purchased from commercial sources and used as received. Tetrahydroxydiboron (BBA) was provided by AllyChem co. Ltd. The catalyst and ligand used in this method were purchased from commercial sources and used without purification. BBA, NiCl₂(dppp), and PPh₃ were stored on a bench-top desiccator.

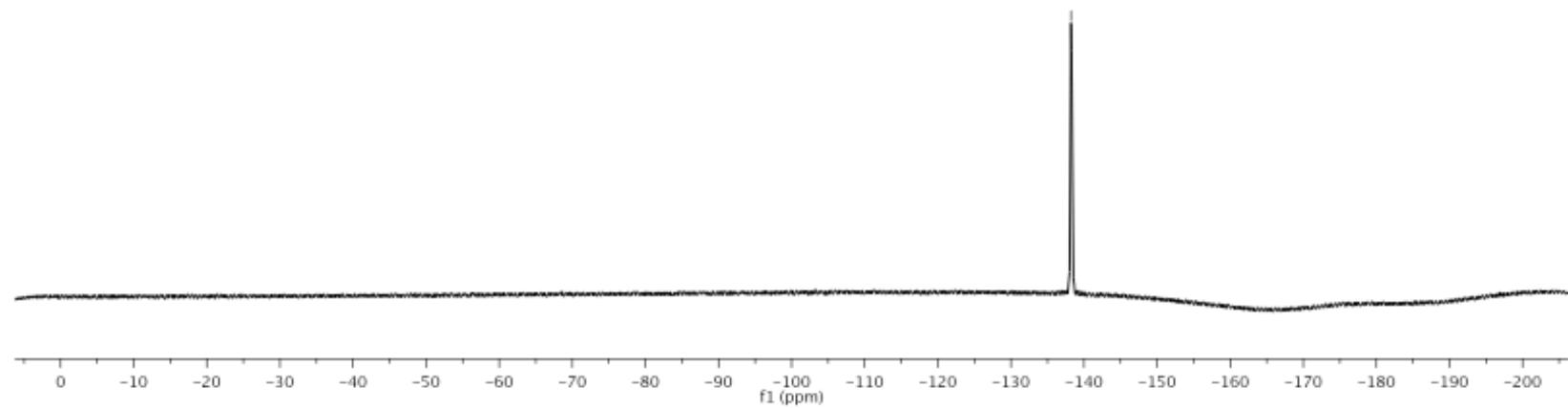
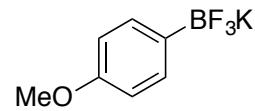
Analytical Methods: Melting points (°C) are uncorrected. All known compounds were characterized by ¹H, ¹³C, ¹⁹F, and ¹¹B NMR spectra, and melting point determination (for solids) and compared with literature values. All new compounds were characterized by ¹H, ¹³C, ¹⁹F, and ¹¹B NMR spectra, IR spectroscopy, high-resolution mass spectrometry (HRMS) and melting point determination (for solids). ¹H, ¹³C, ¹⁹F and ¹¹B NMR spectra were recorded at 500.4, 125.8, 470.8 and 128.4 MHz, respectively. ¹⁹F NMR chemical shifts were referenced to external CFCl₃ (0.0 ppm). ¹¹B NMR chemical shifts were referenced to external BF₃•OEt₂ (0.0 ppm) with a negative sign indicating an upfield shift. HRMS (CI) data were obtained in Pos mode, using methane as the ionizing gas. HRMS (ESI) data were obtained in Pos or Neg mode.



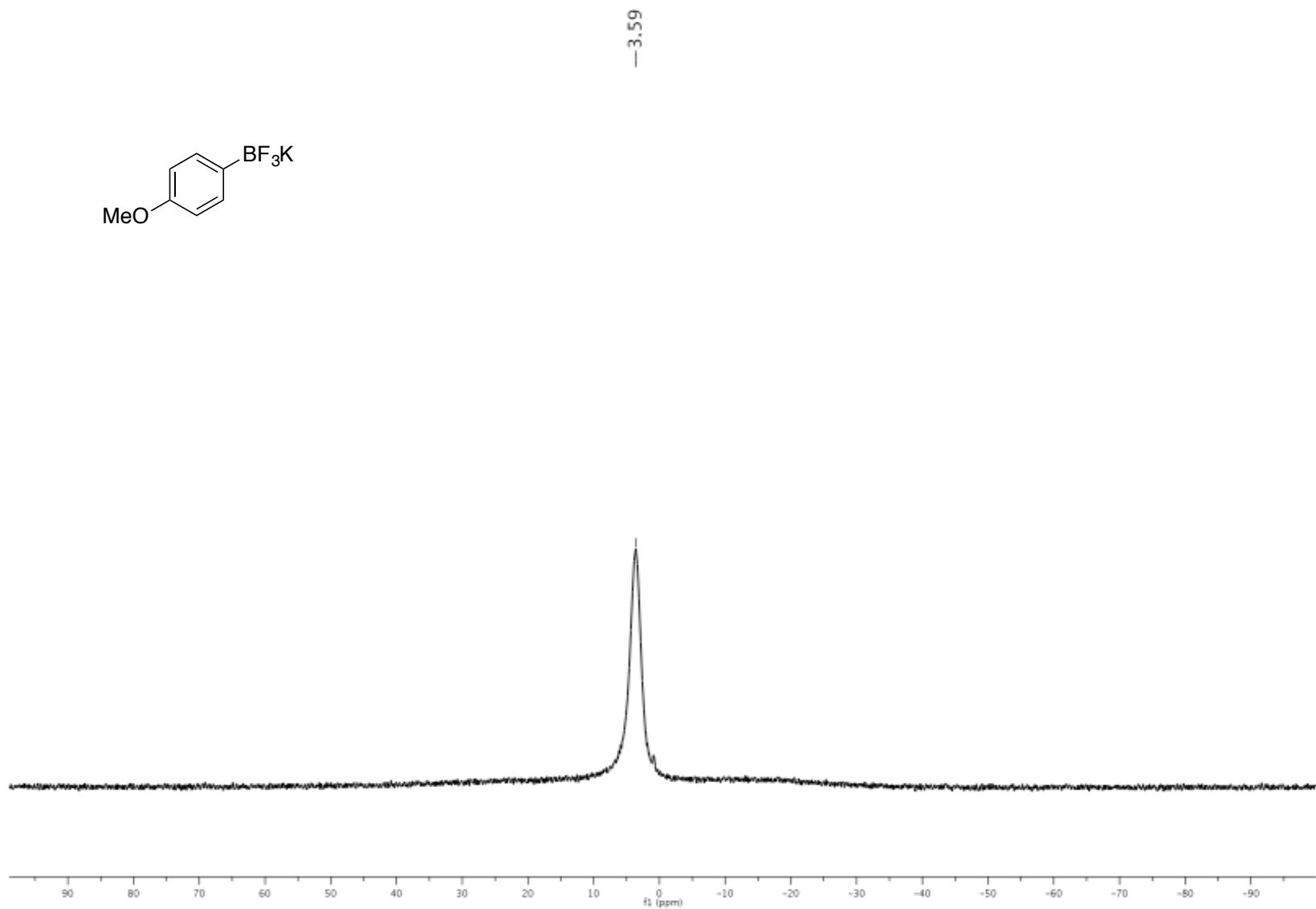
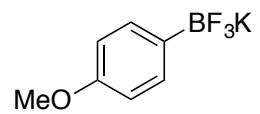
^1H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-methoxyphenyl)borate (1a, Table 1, entry 1)



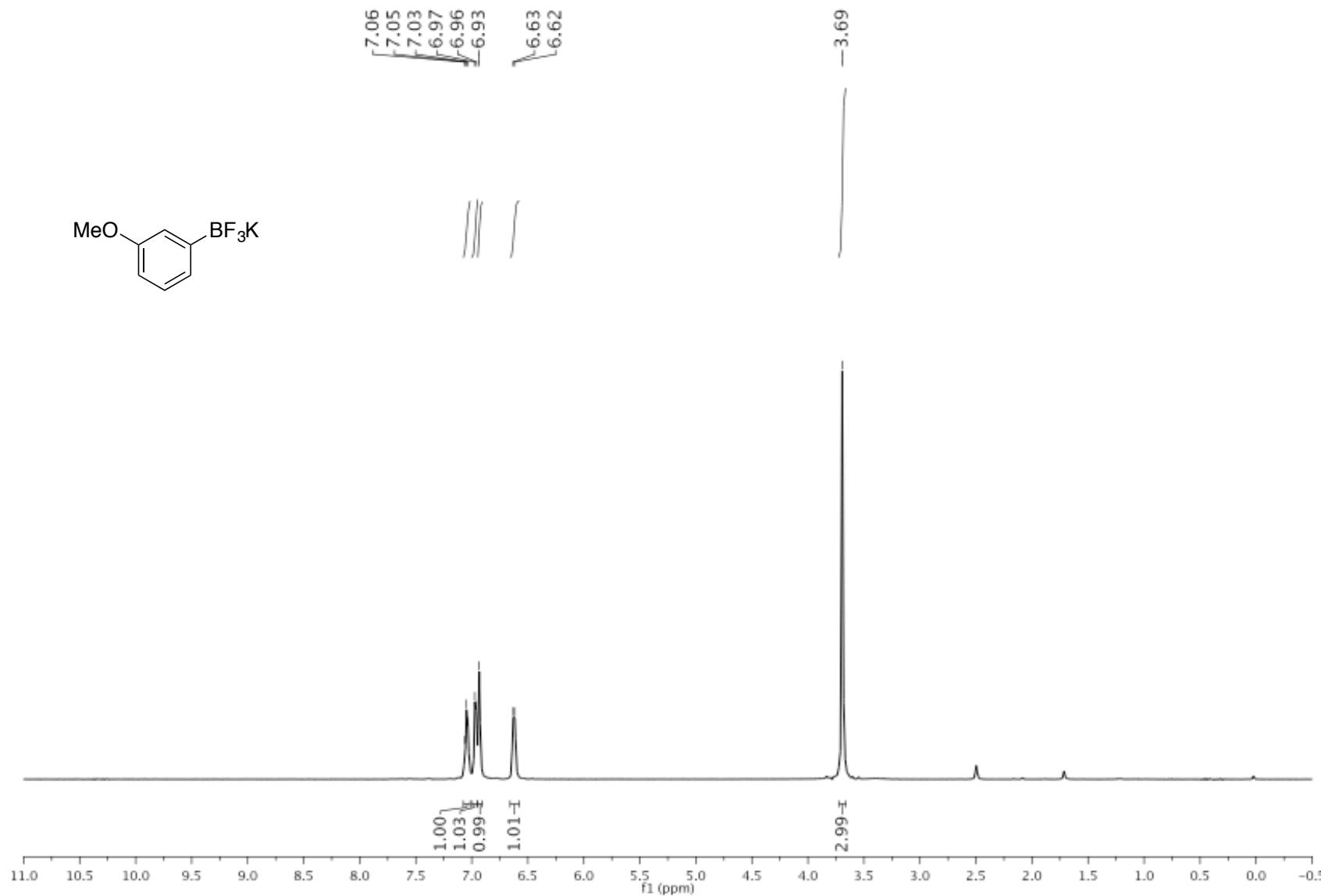
¹³C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-methoxyphenyl)borate (1a, Table 1, entry 1)



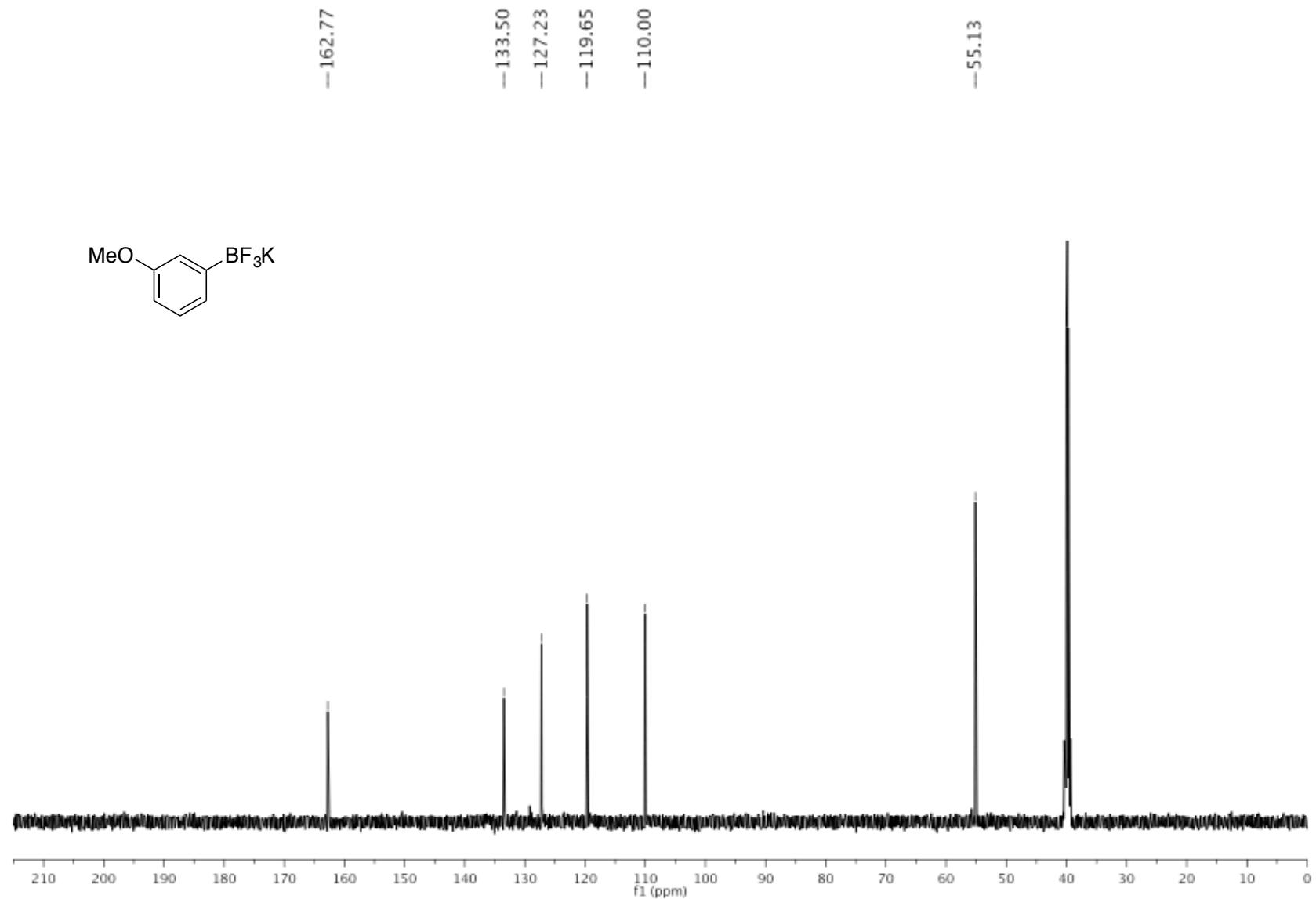
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-methoxyphenyl)borate (1a, Table 1, entry 1)



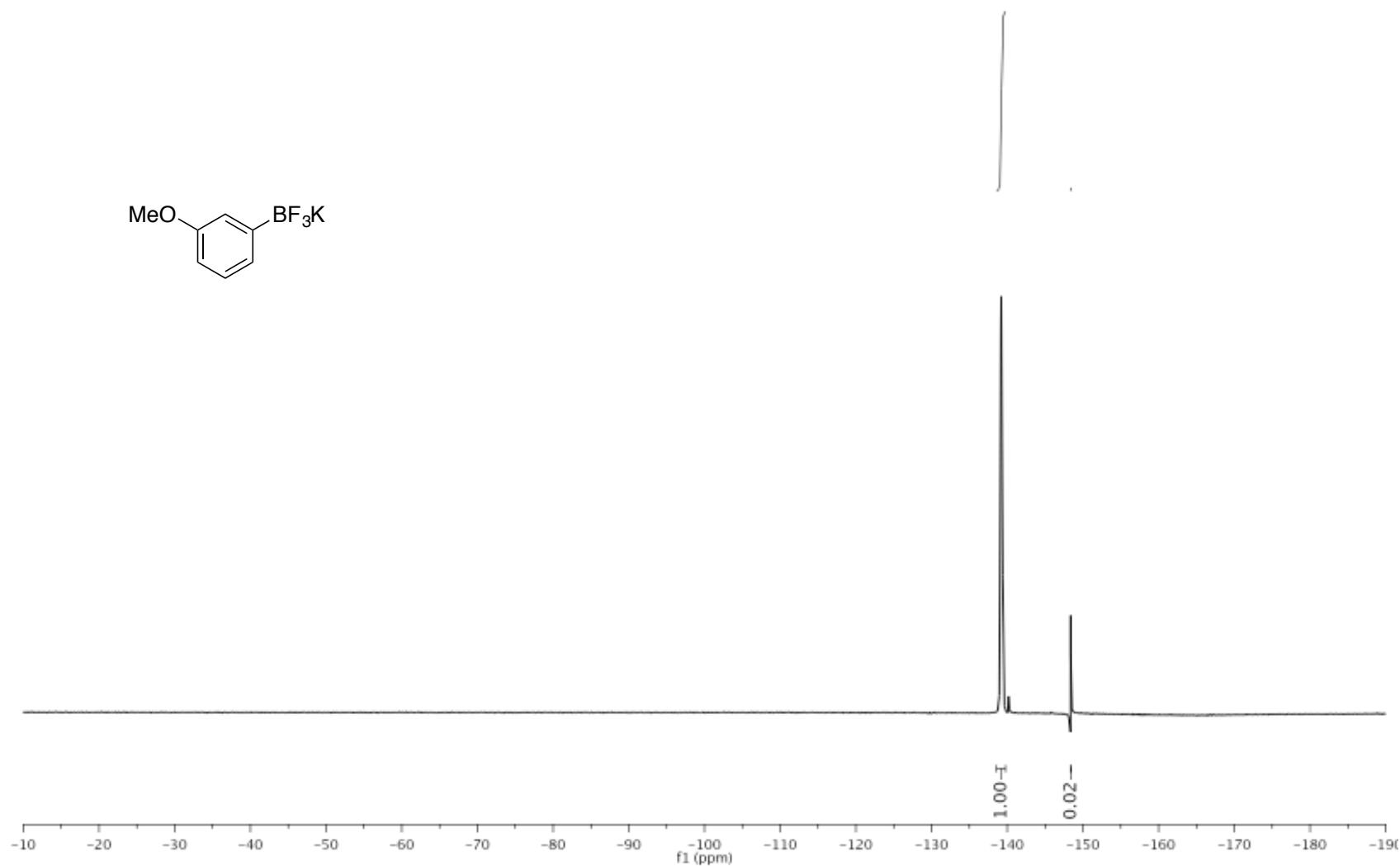
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-methoxyphenyl)borate (1a, Table 1, entry 1)



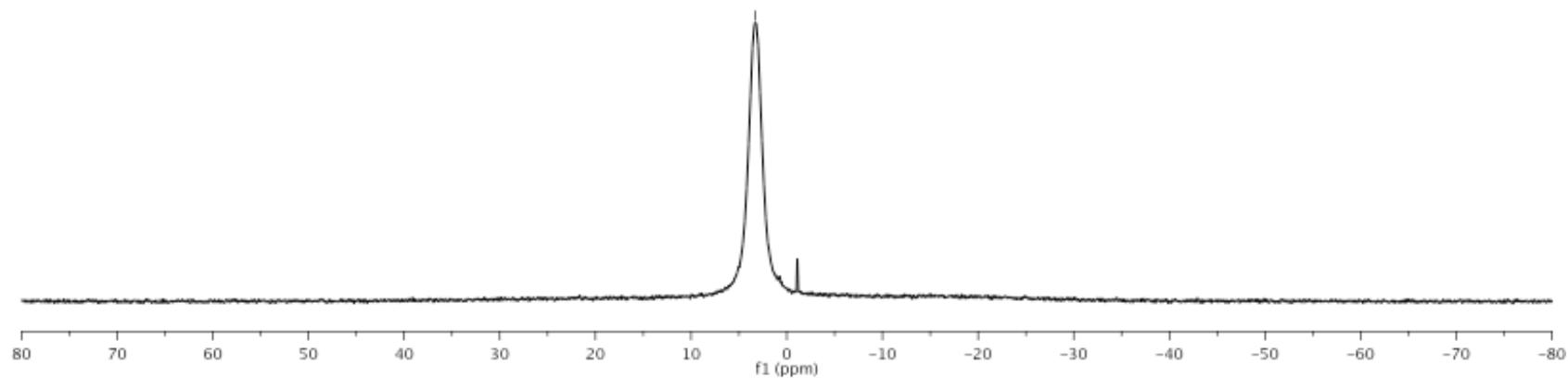
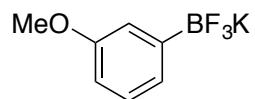
^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(3-methoxyphenyl)borate (1b, Table 1, entry 2)



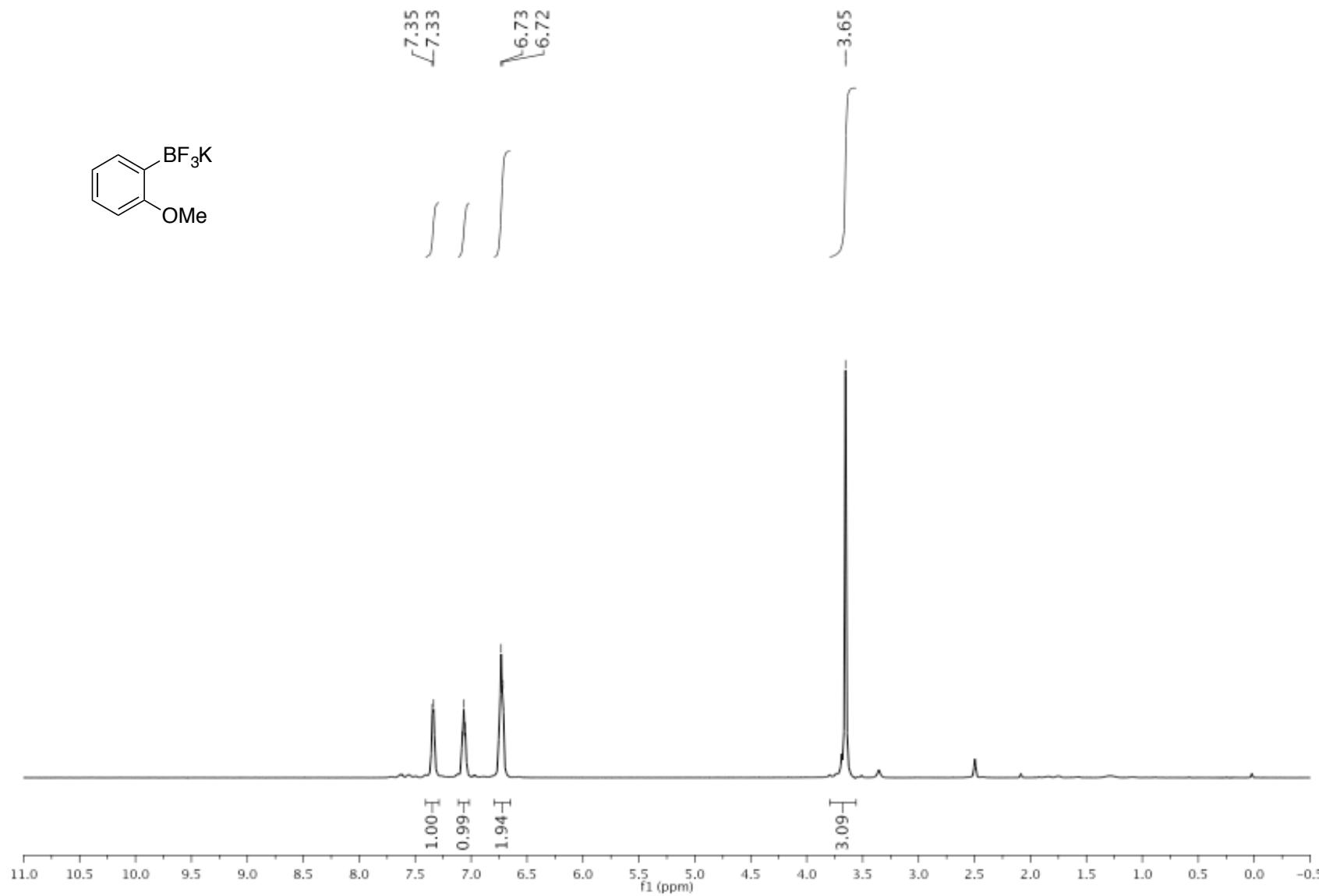
^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(3-methoxyphenyl)borate (1b, Table 1, entry 2)



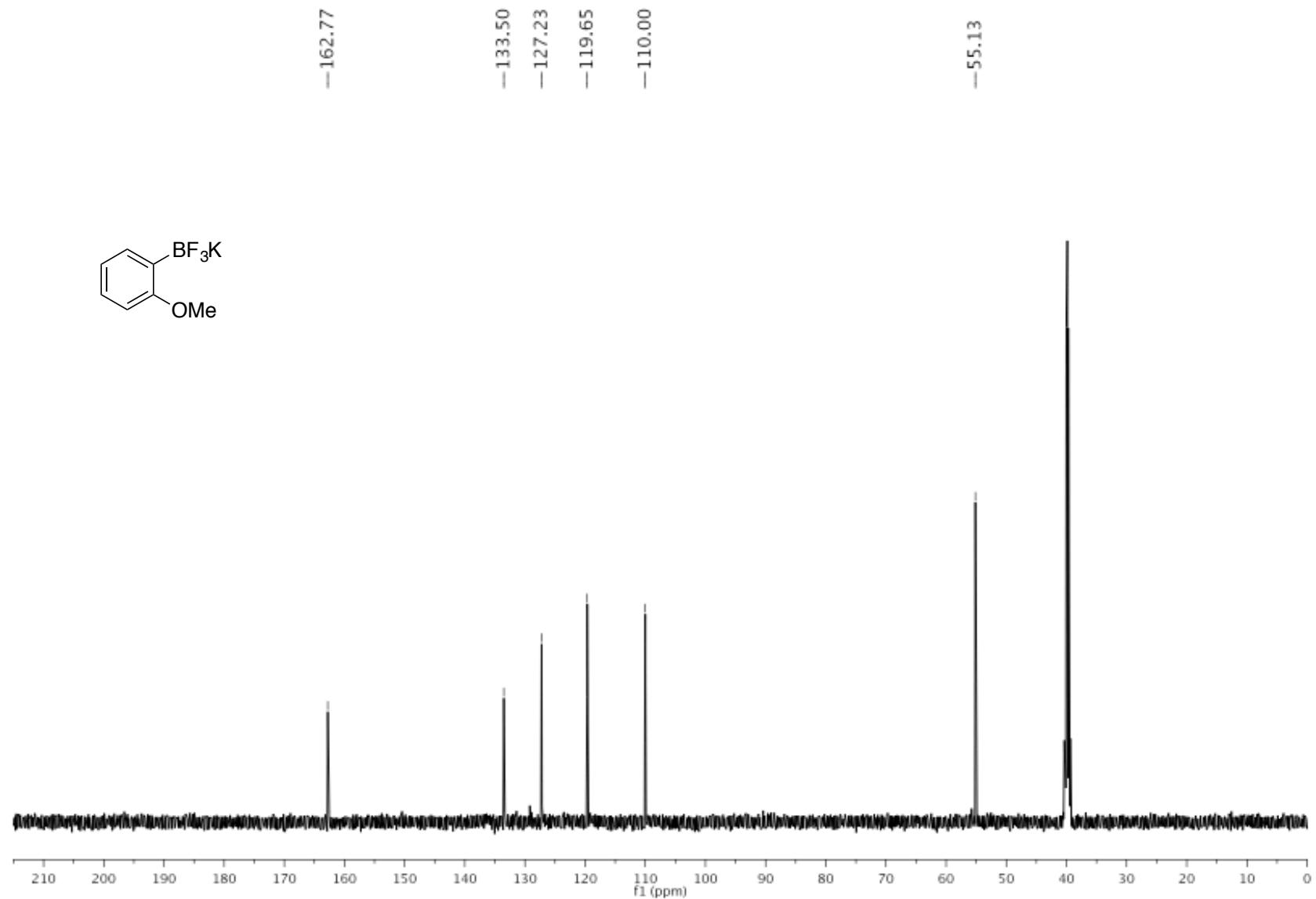
^{19}F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(3-methoxyphenyl)borate (1b, Table 1, entry 2)



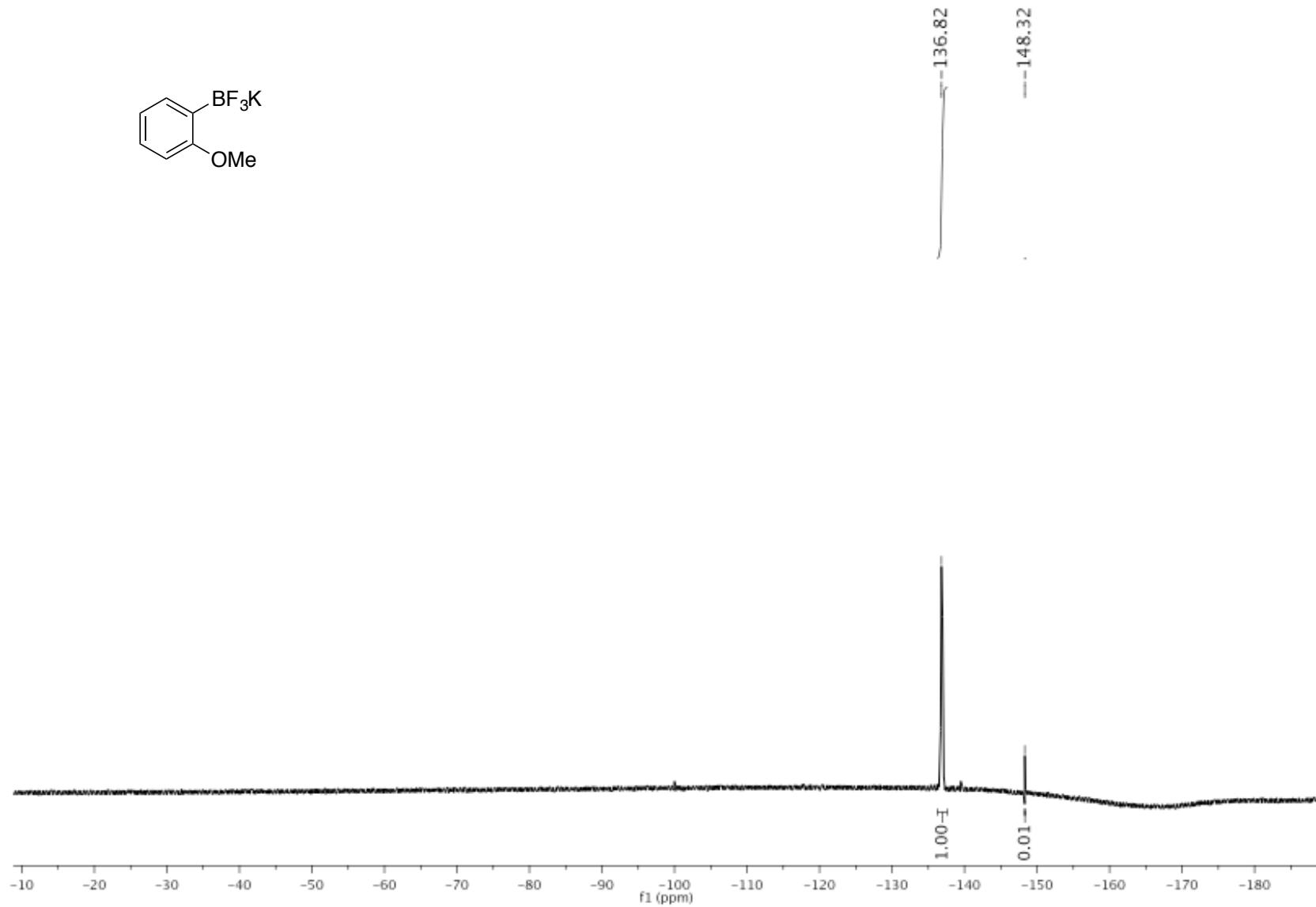
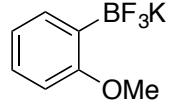
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(3-methoxyphenyl)borate (1b, Table 1, entry 2)



^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(2-methoxyphenyl)borate (1c, Table 1, entry 3)

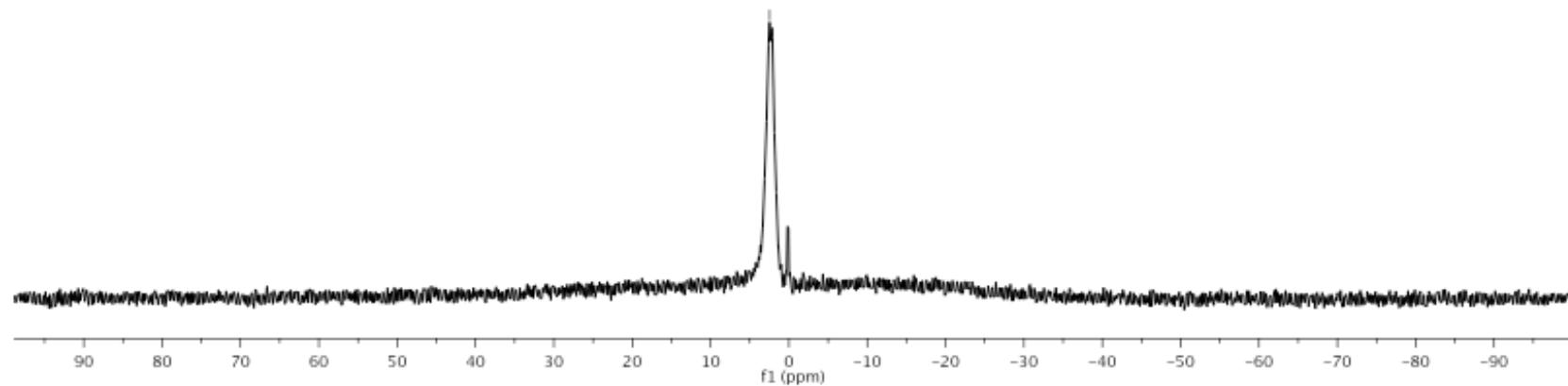
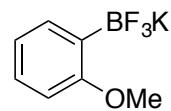


^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-methoxyphenyl)borate (1c, Table 1, entry 3)

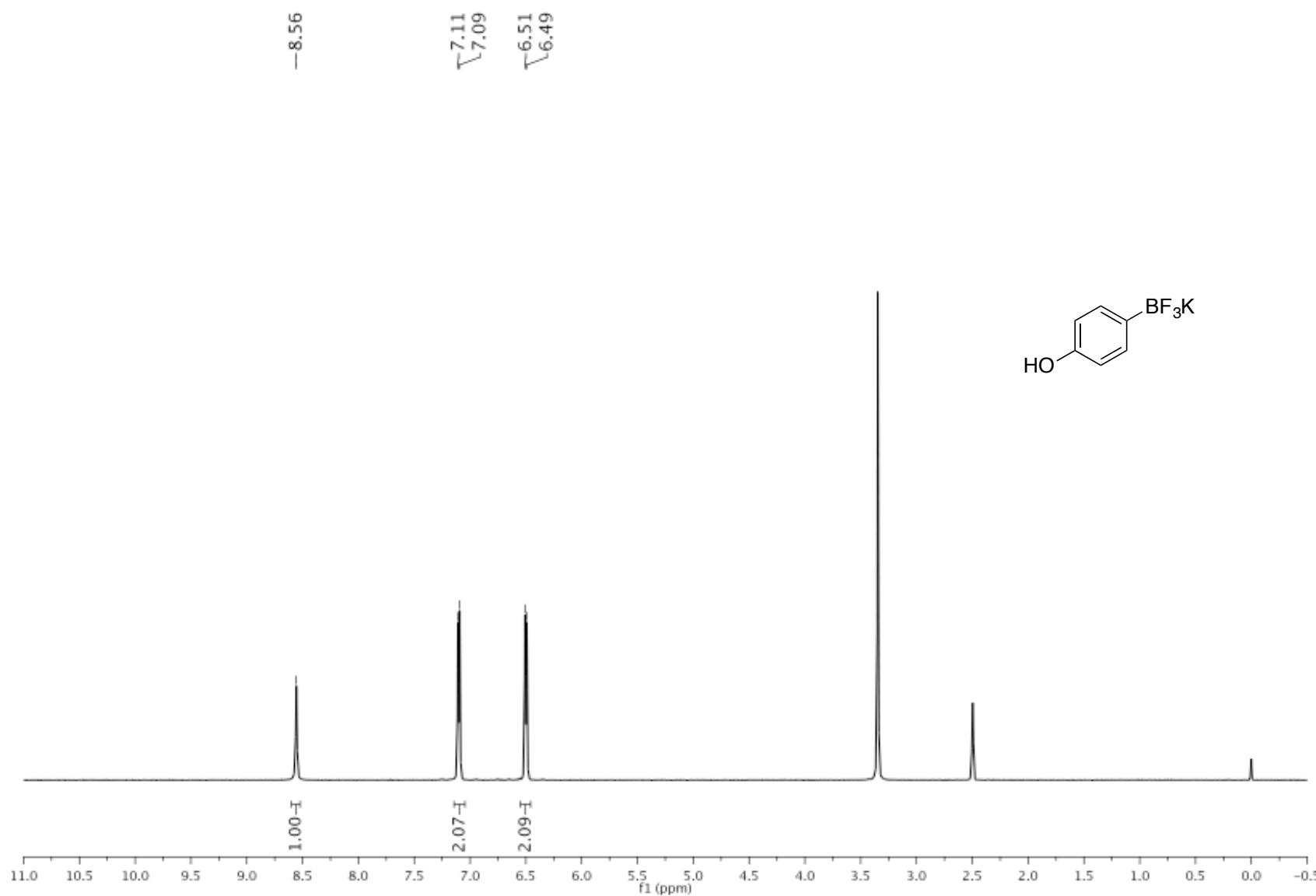


¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-methoxyphenyl)borate (1c, Table 1, entry 3)

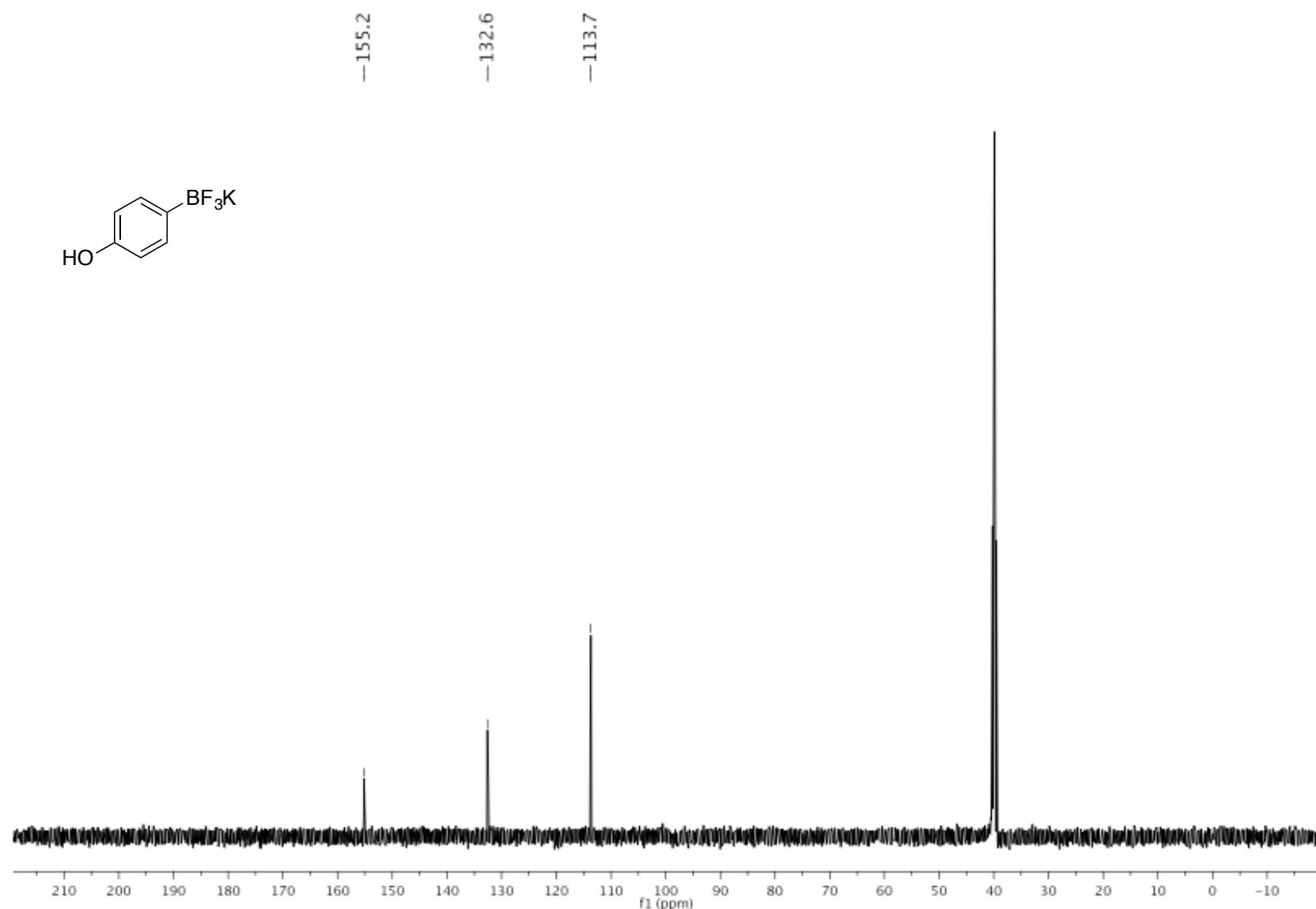
-2.47



¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-methoxyphenyl)borate (1c, Table 1, entry 3)

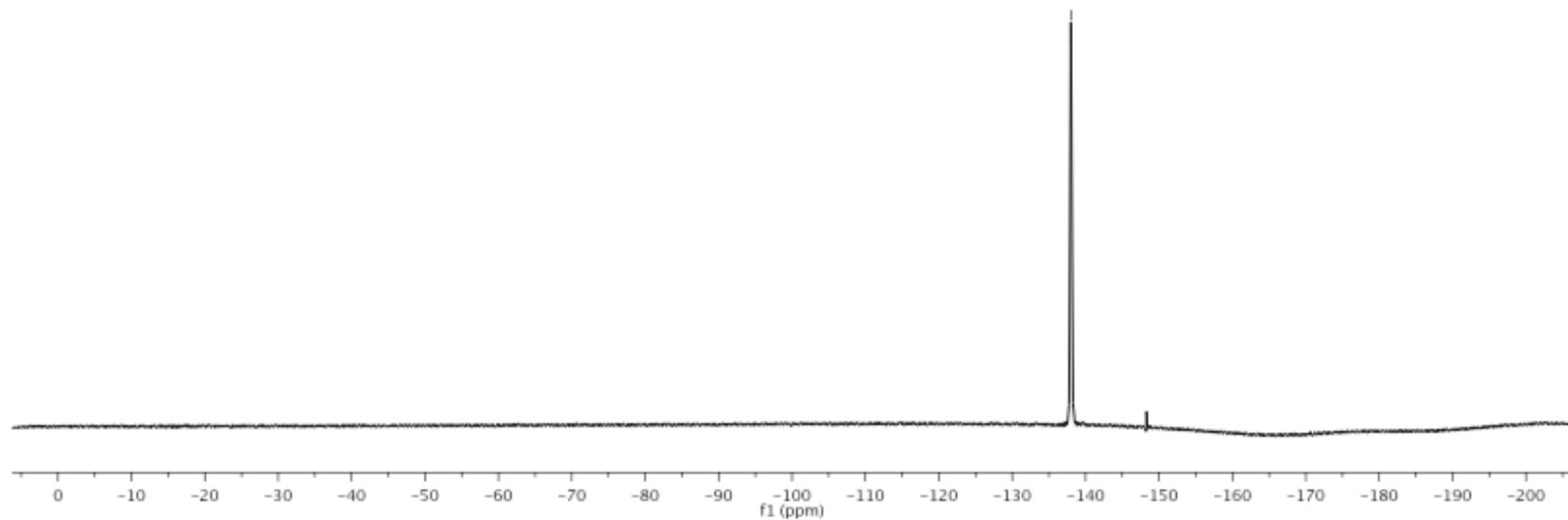
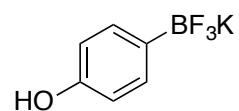


^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(4-hydroxyphenyl)borate (1d, Table 1, entry 4)

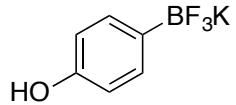


^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-hydroxyphenyl)borate (1d, Table 1, entry 4)

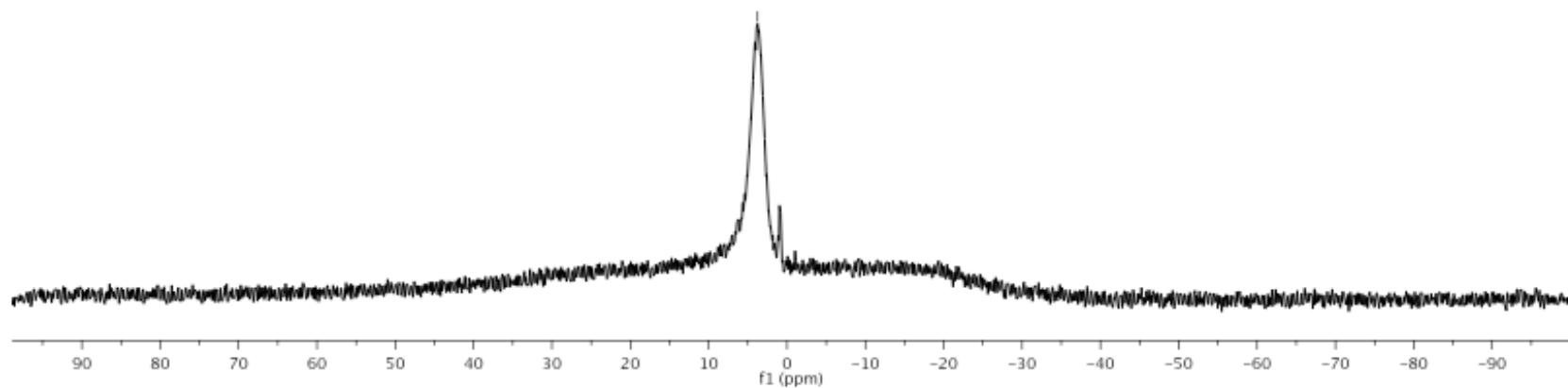
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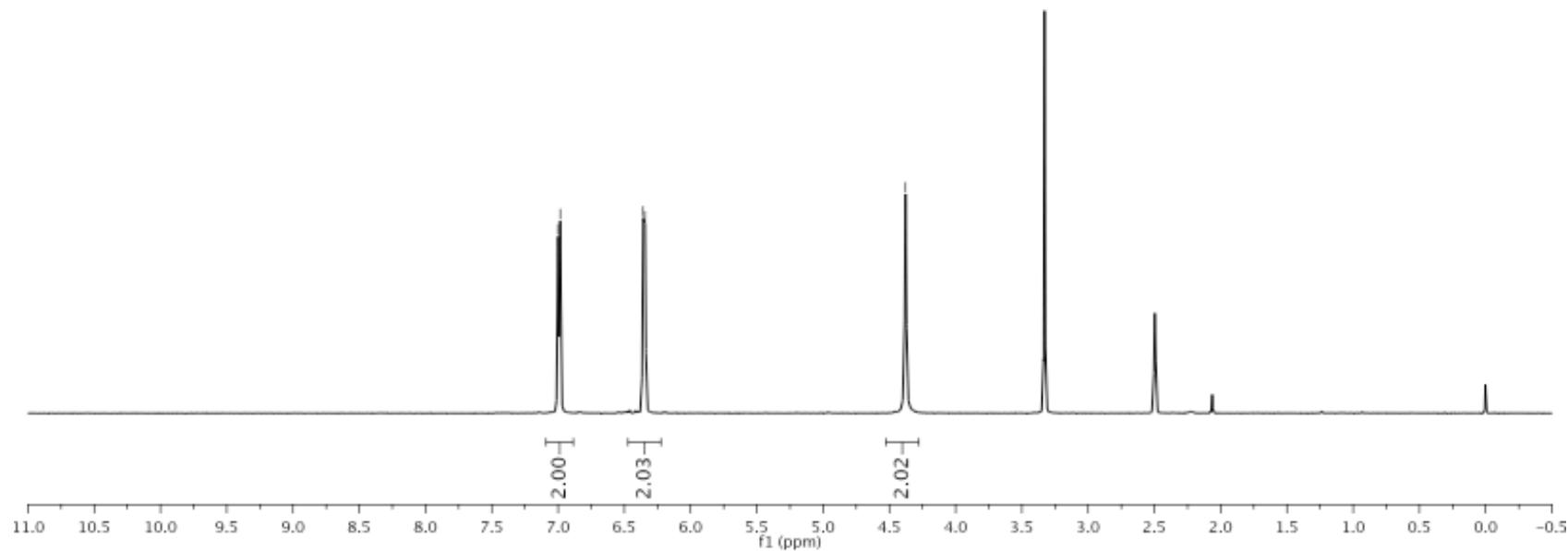
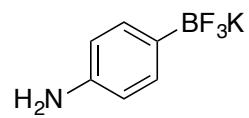
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-hydroxyphenyl)borate (1d, Table 1, entry 4)



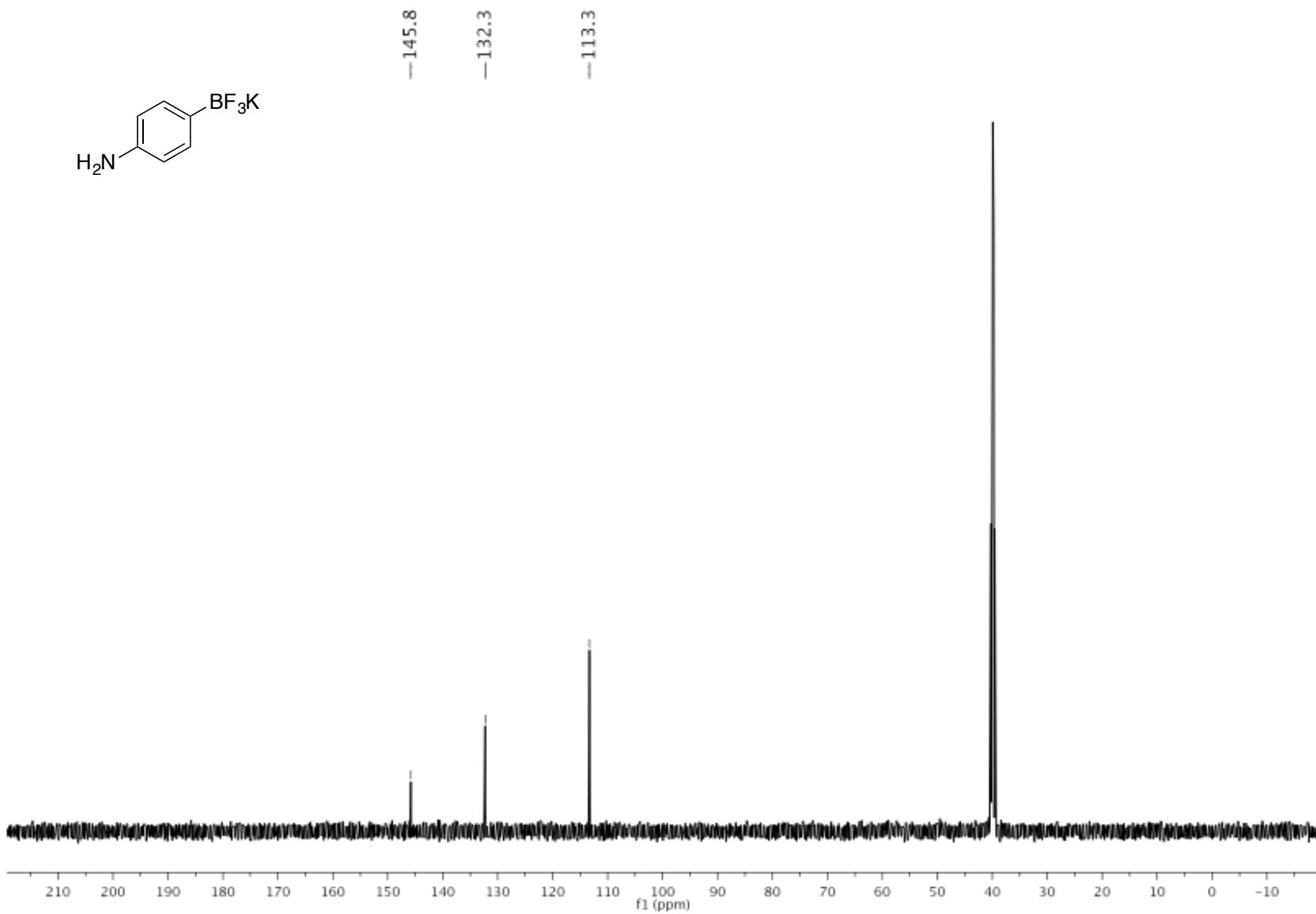
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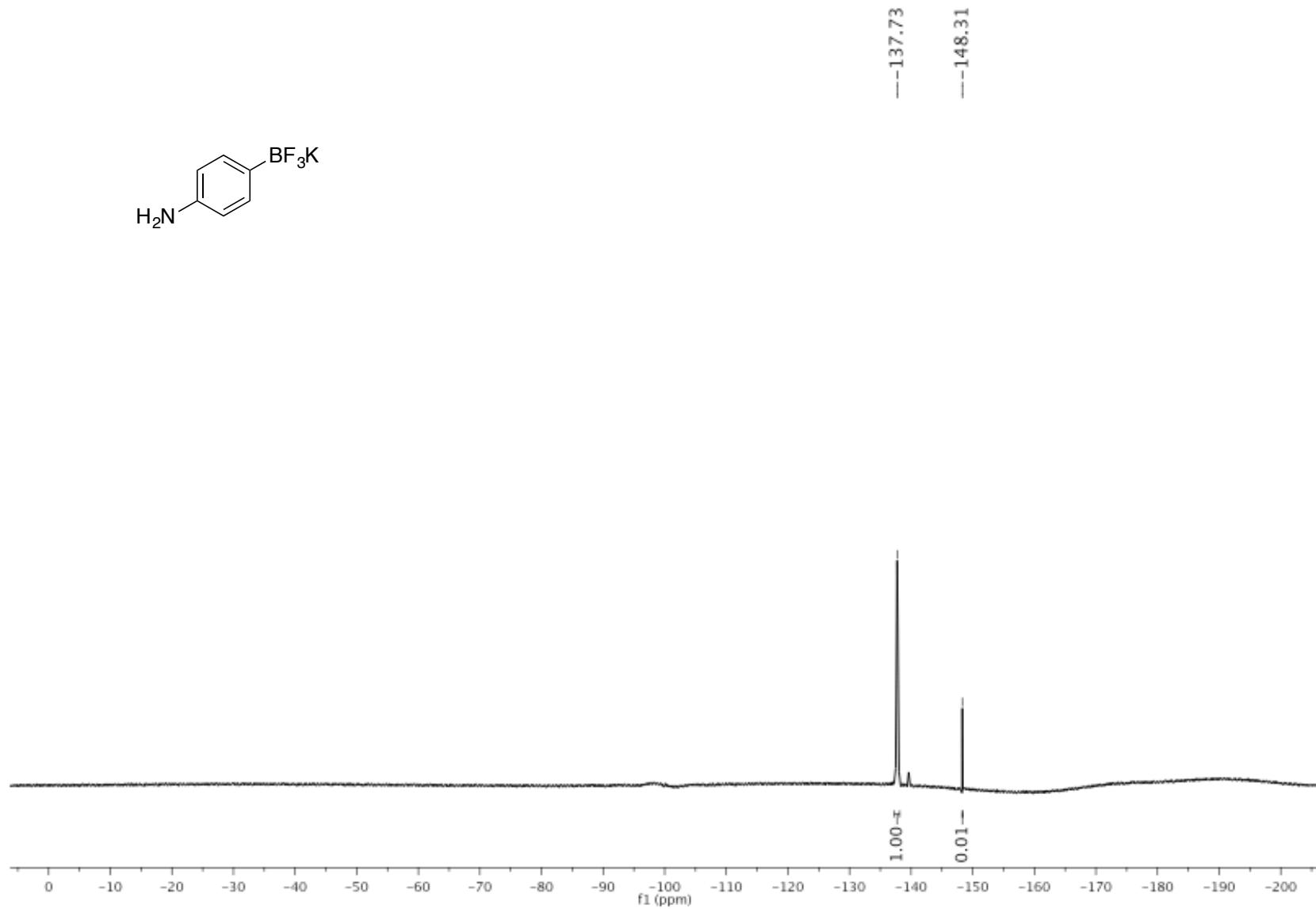
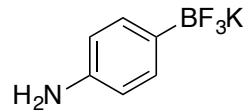
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-hydroxyphenyl)borate (1d, Table 1, entry 4)



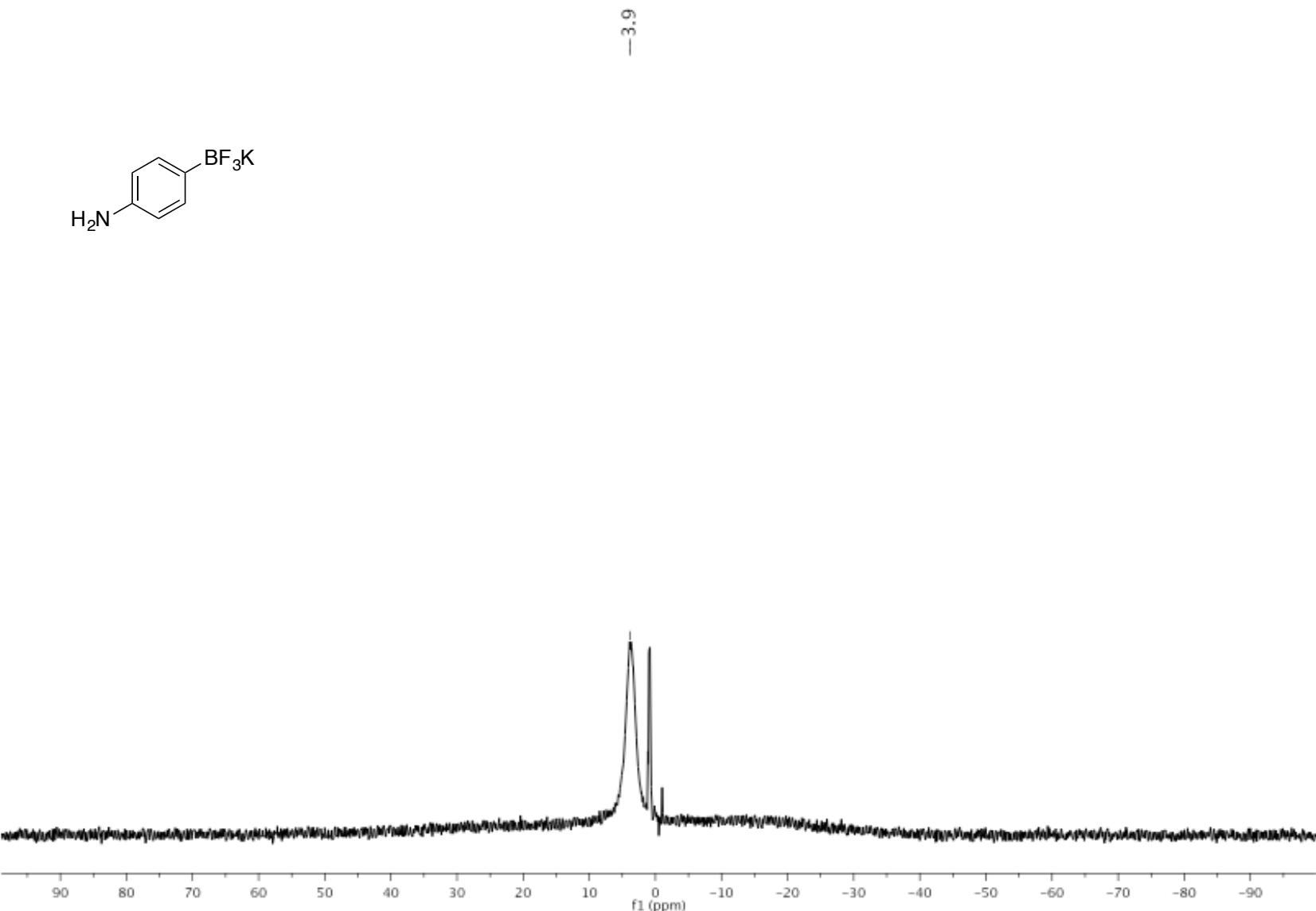
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium (4-Aminophenyl)trifluoroborate (1e, Table 1, entry 5)



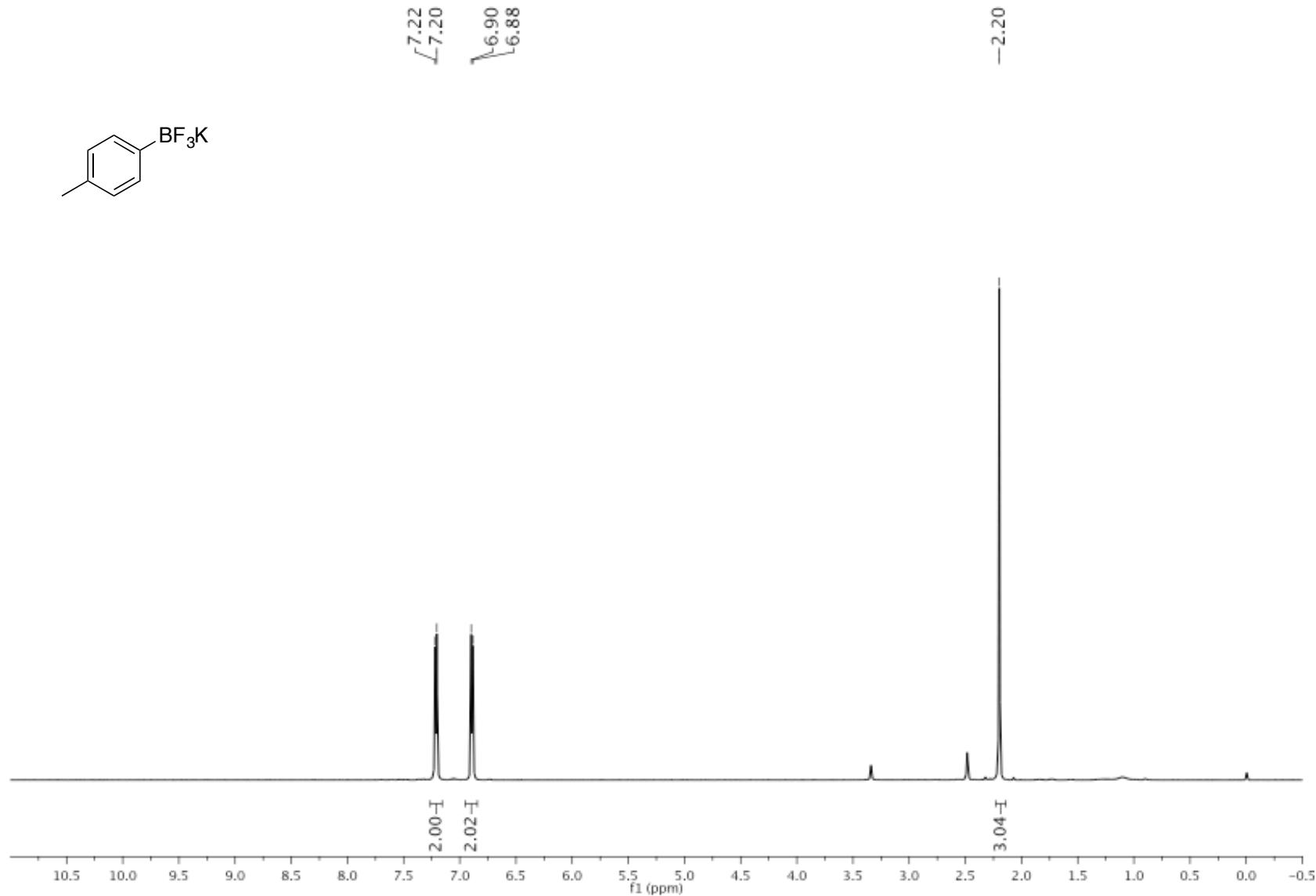
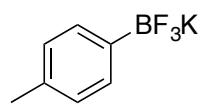
^{13}C NMR (128.5 MHz, DMSO-d_6) Spectrum of Potassium (4-Aminophenyl)trifluoroborate (1e, Table 1, entry 5)



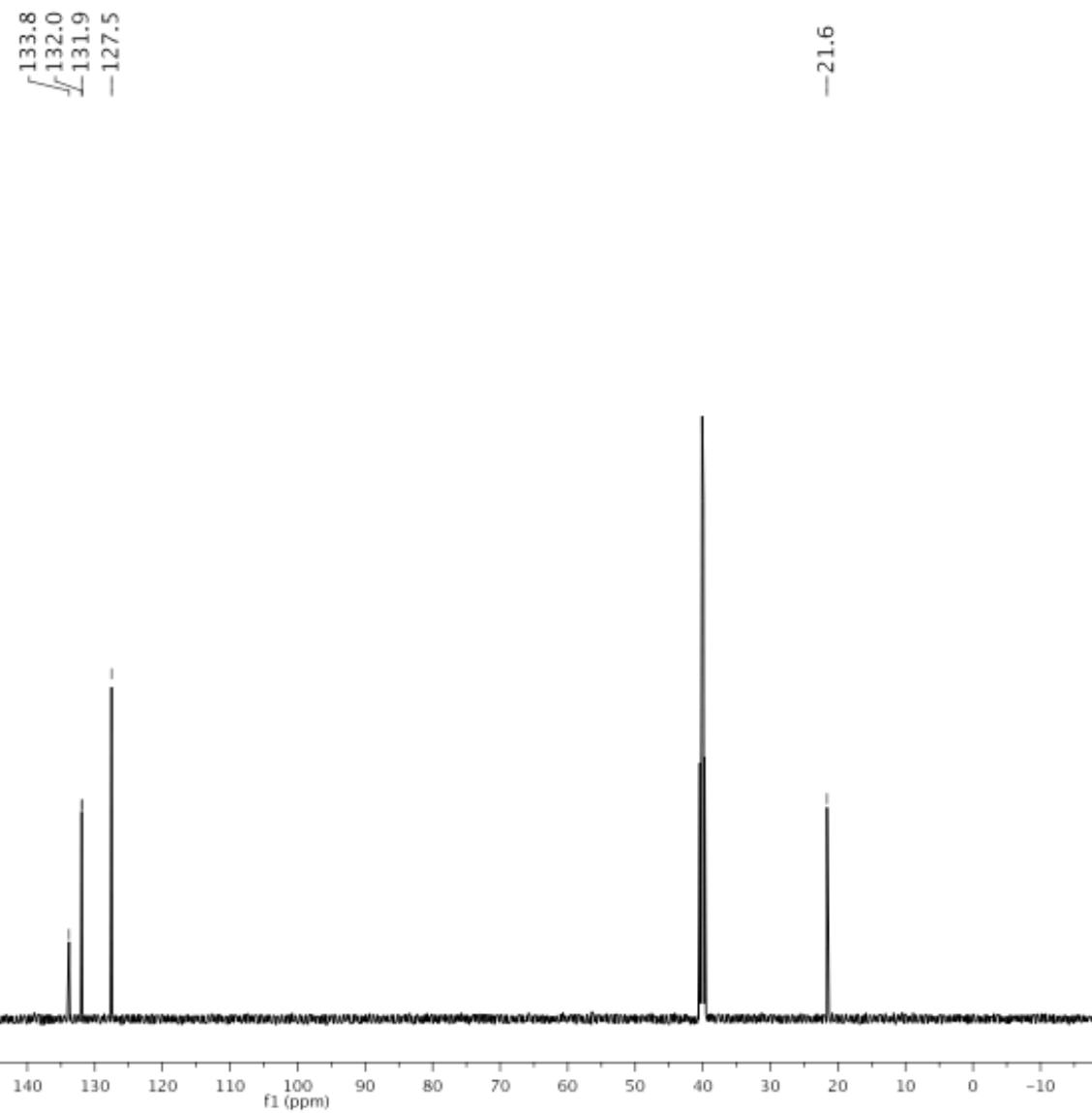
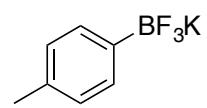
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium (4-Aminophenyl)trifluoroborate (1e, Table 1, entry 5)



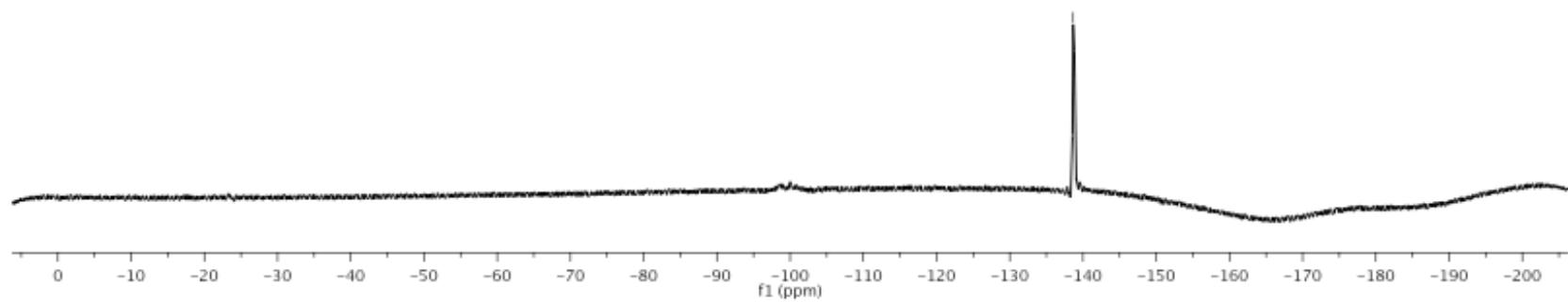
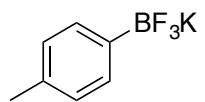
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium (4-Aminophenyl)trifluoroborate (1e, Table 1, entry 5)



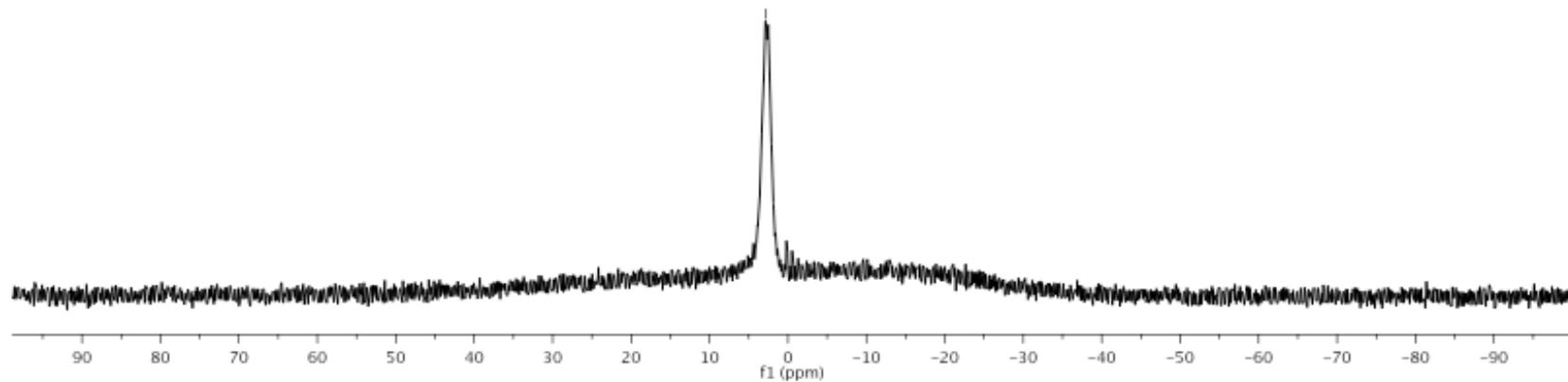
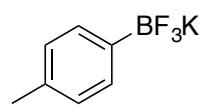
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(*p*-tolyl)borate (1f, Table 1, entry 6)



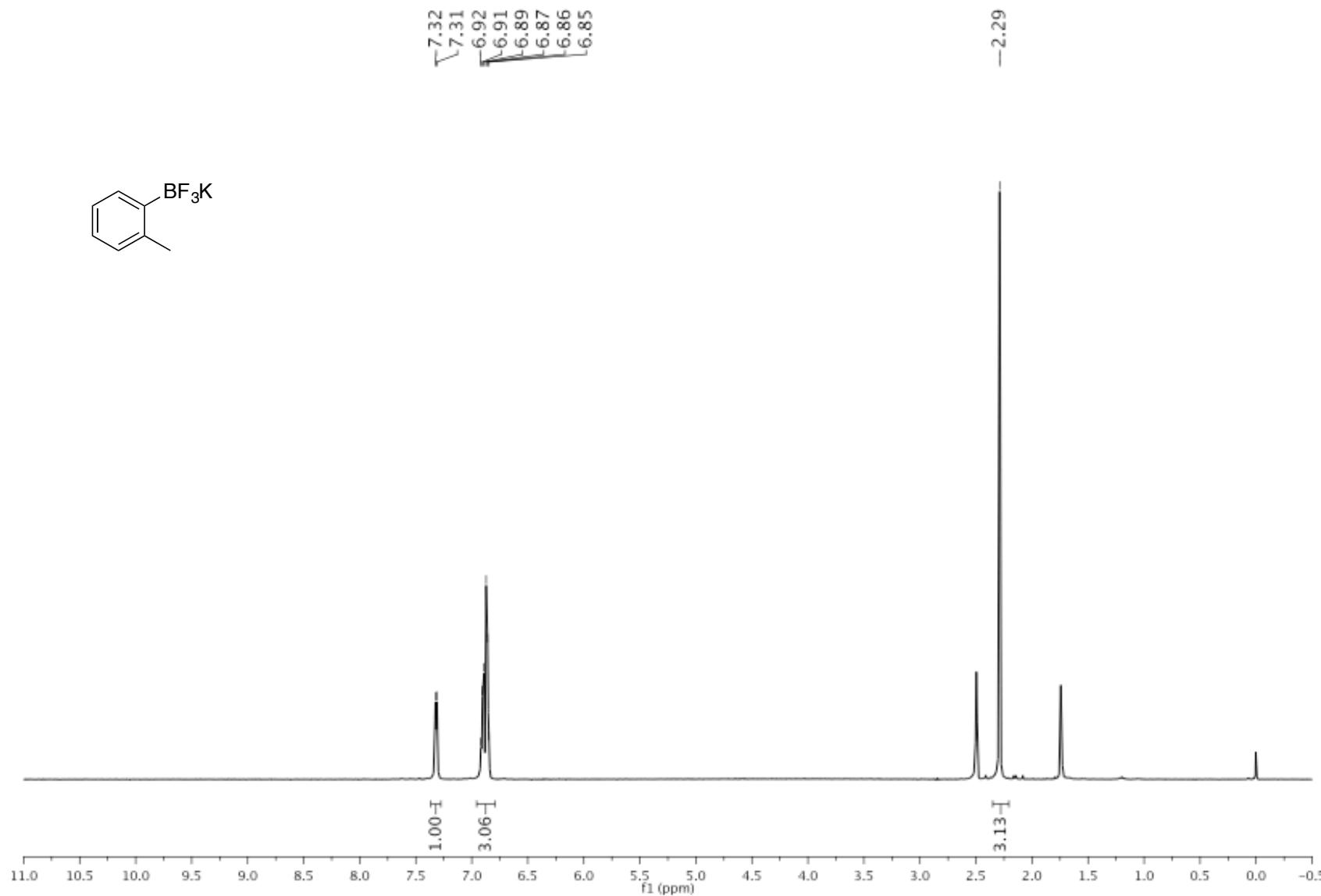
^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(*p*-tolyl)borate (1f, Table 1, entry 6)



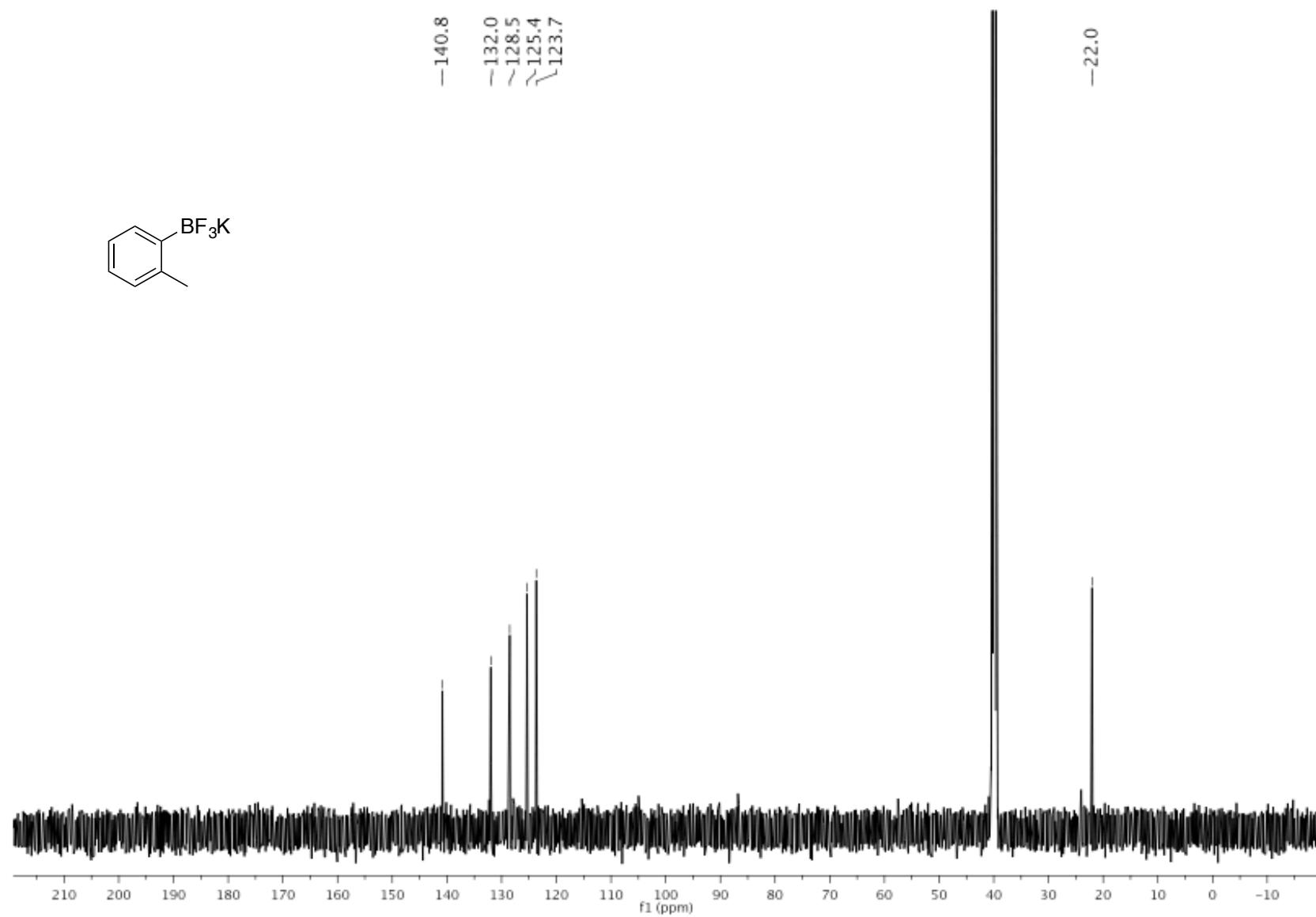
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(*p*-tolyl)borate (1f, Table 1, entry 6)



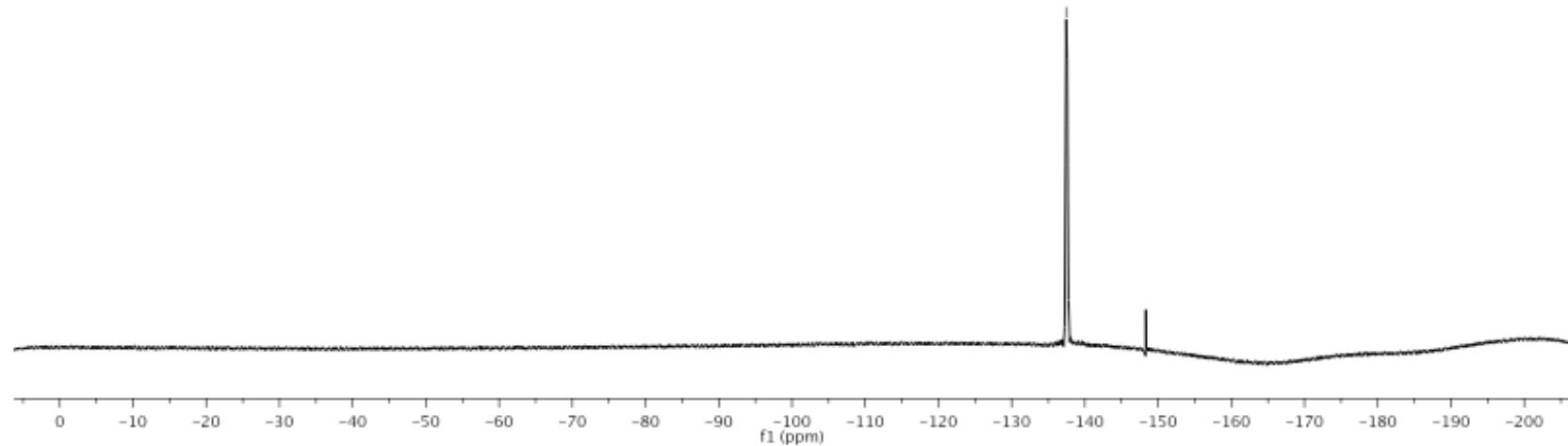
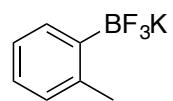
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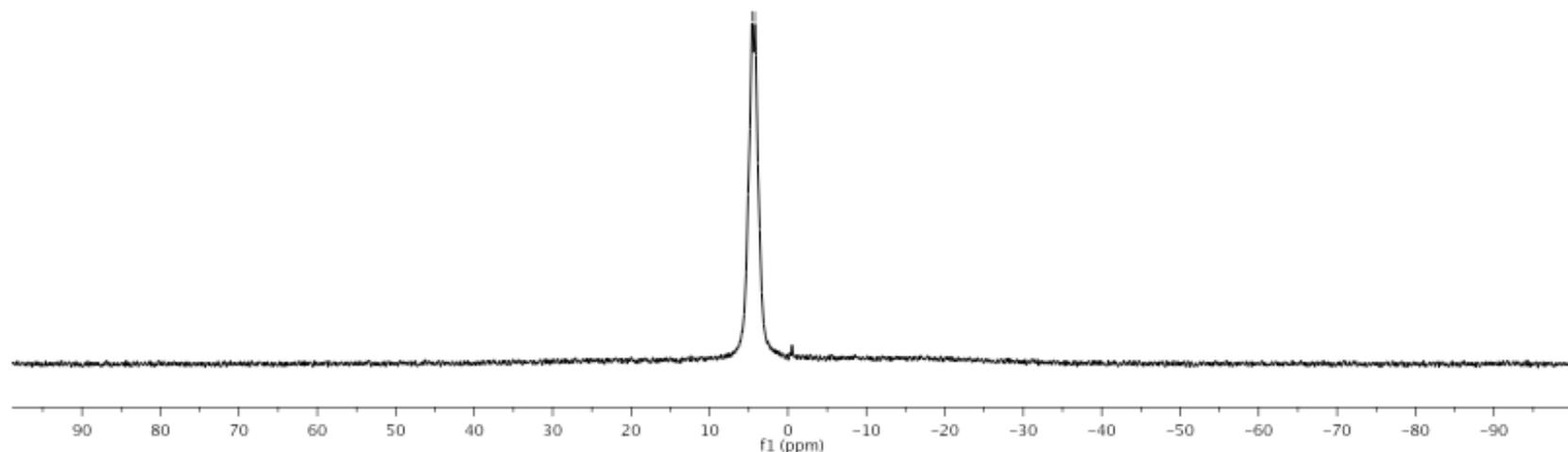
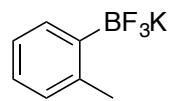
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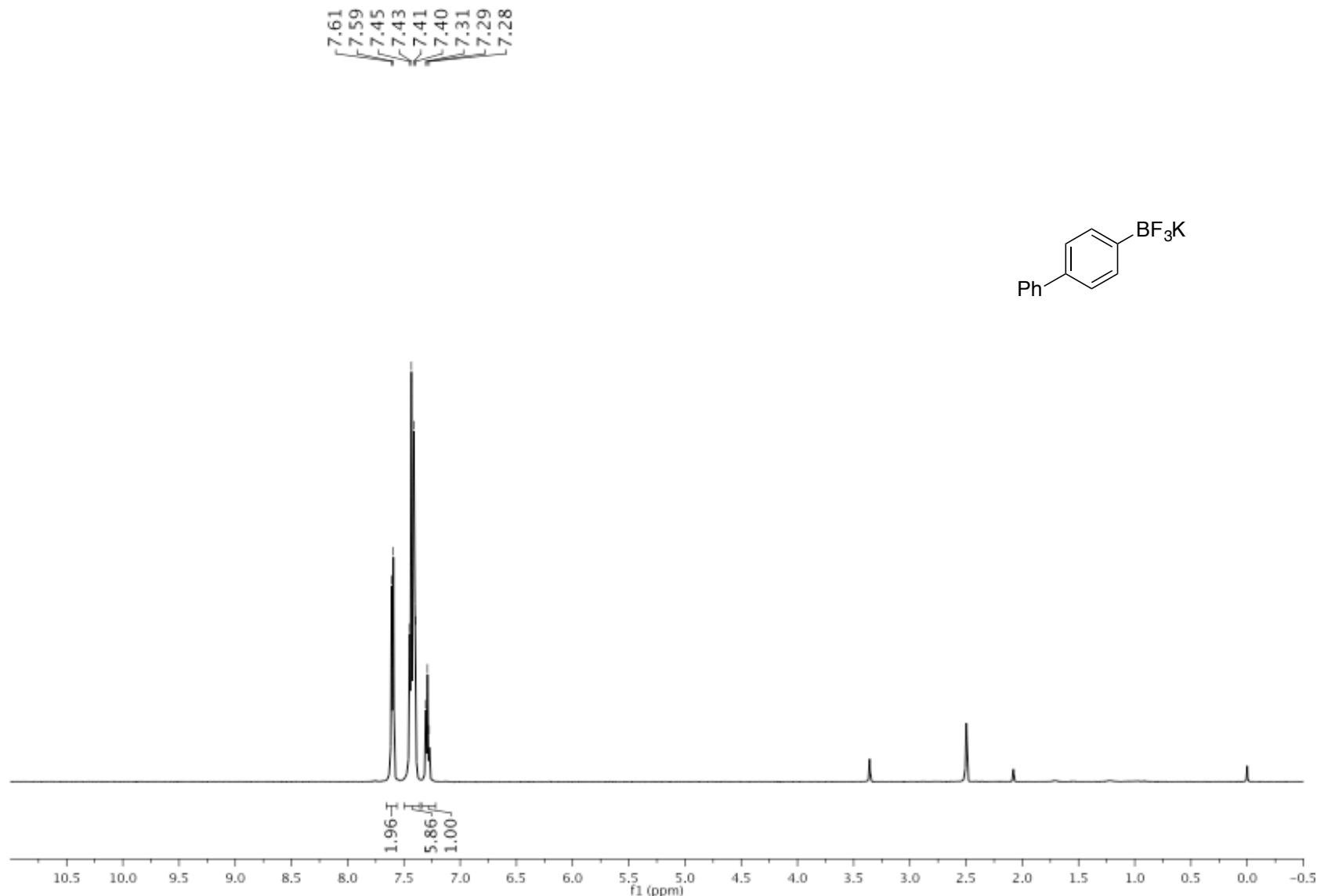
^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(*o*-tolyl)borate (1g, Table 1, entry 7)

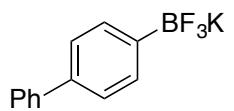


¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(*o*-tolyl)borate (1g, Table 1, entry 7)

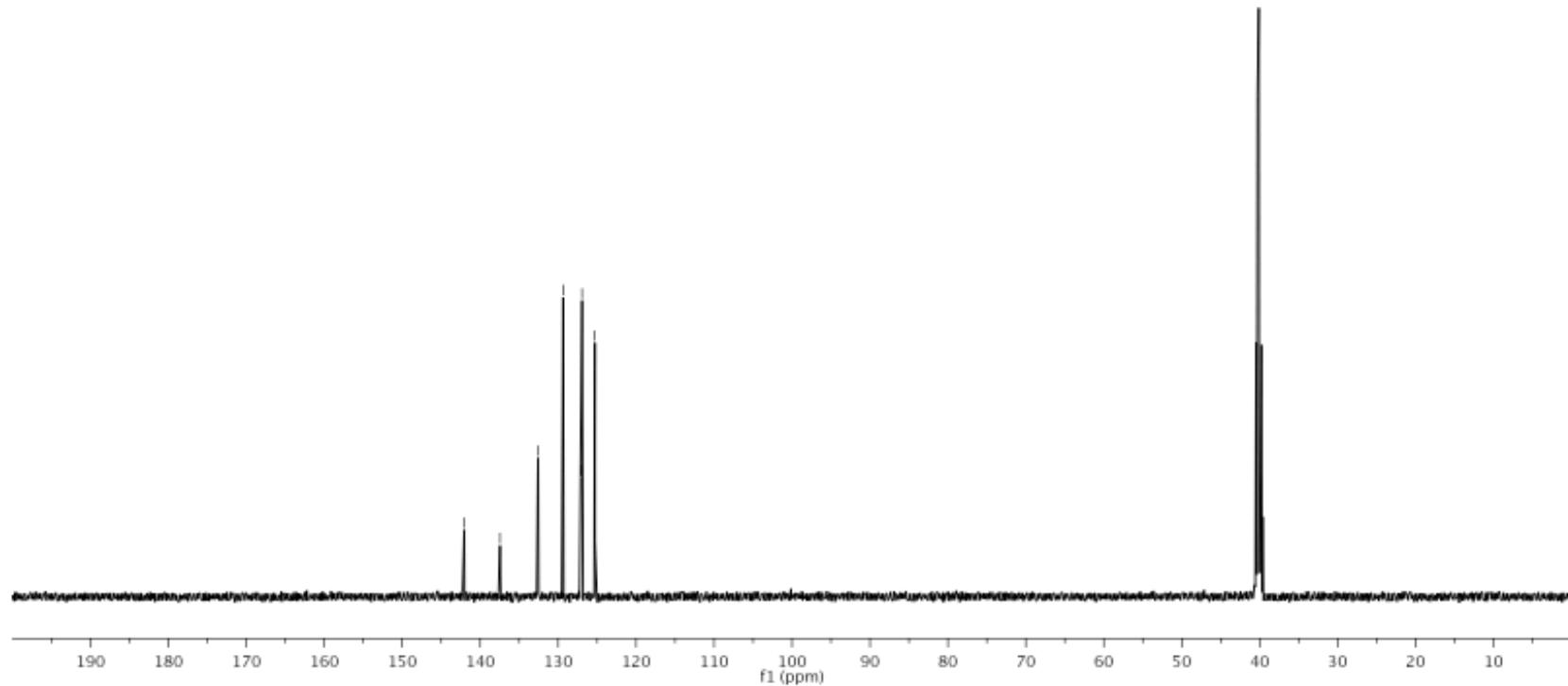


^{11}B NMR (128.4 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(*o*-tolyl)borate (1g, Table 1, entry 7)



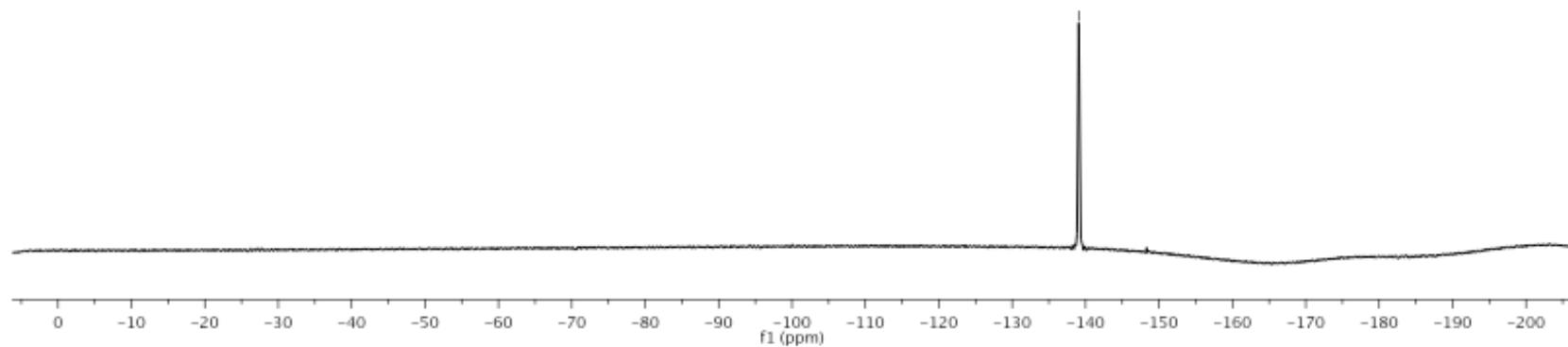
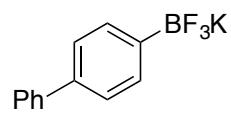


-142.0
-137.5
132.6
129.4
127.1
126.9
125.3

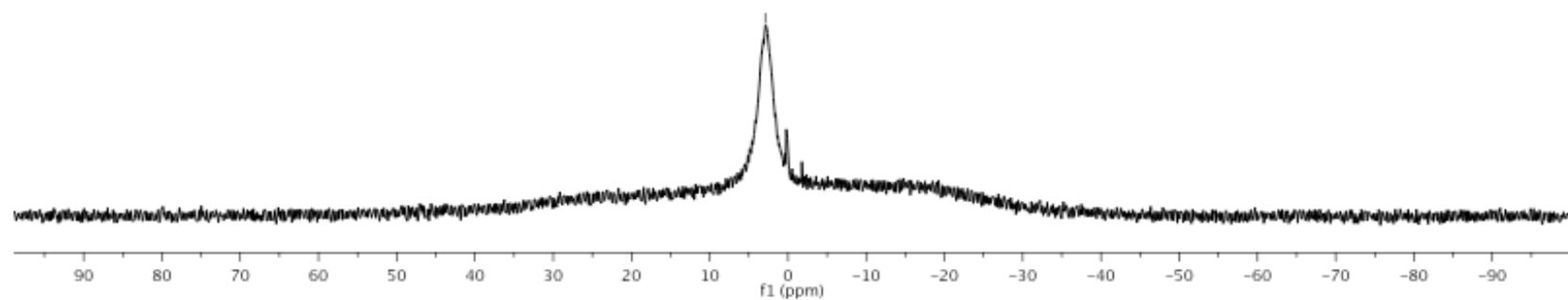
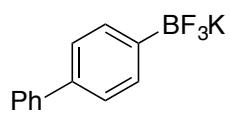


¹³C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium [1,1'-Biphenyl]-4-yltrifluoroborate (1h, Table 1, entry 8)

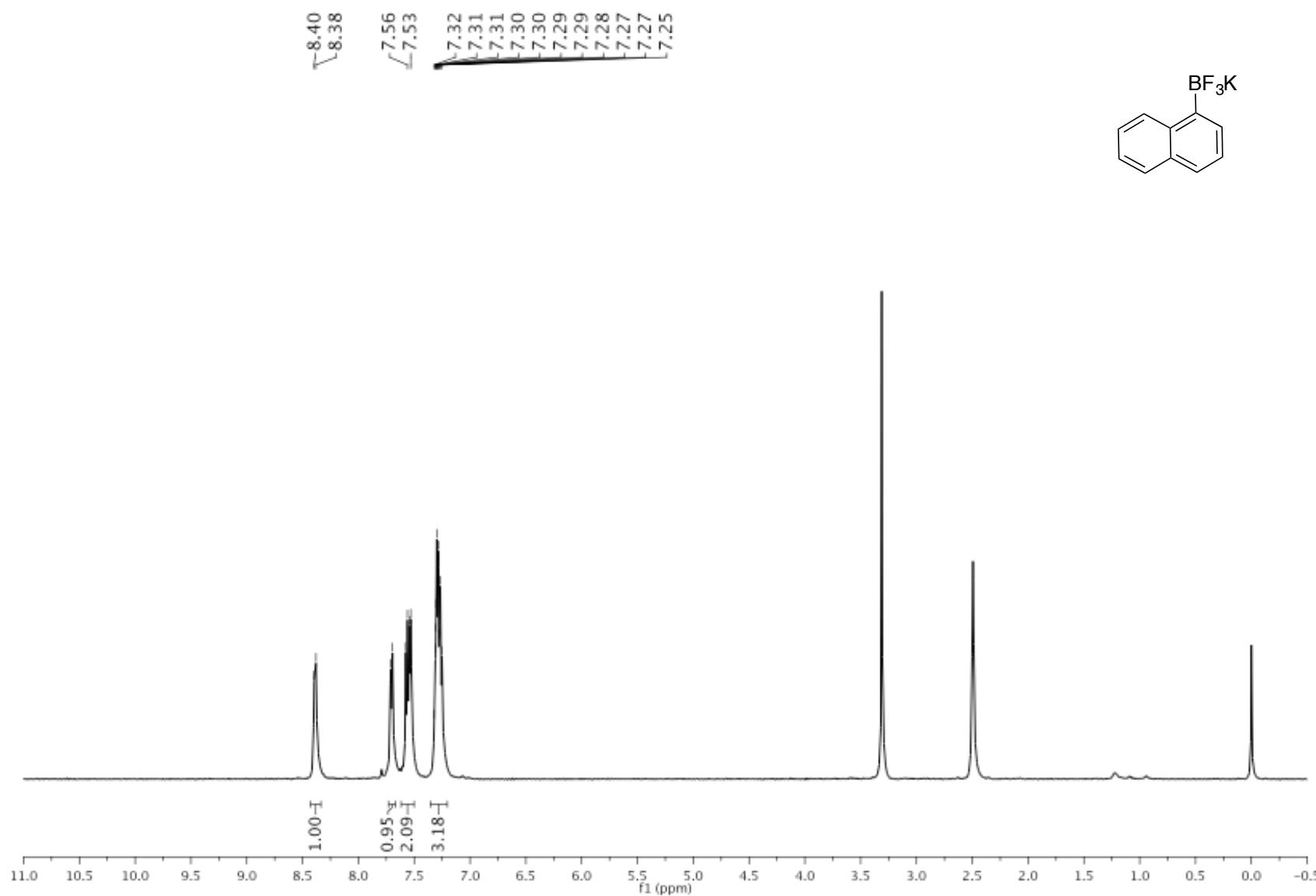
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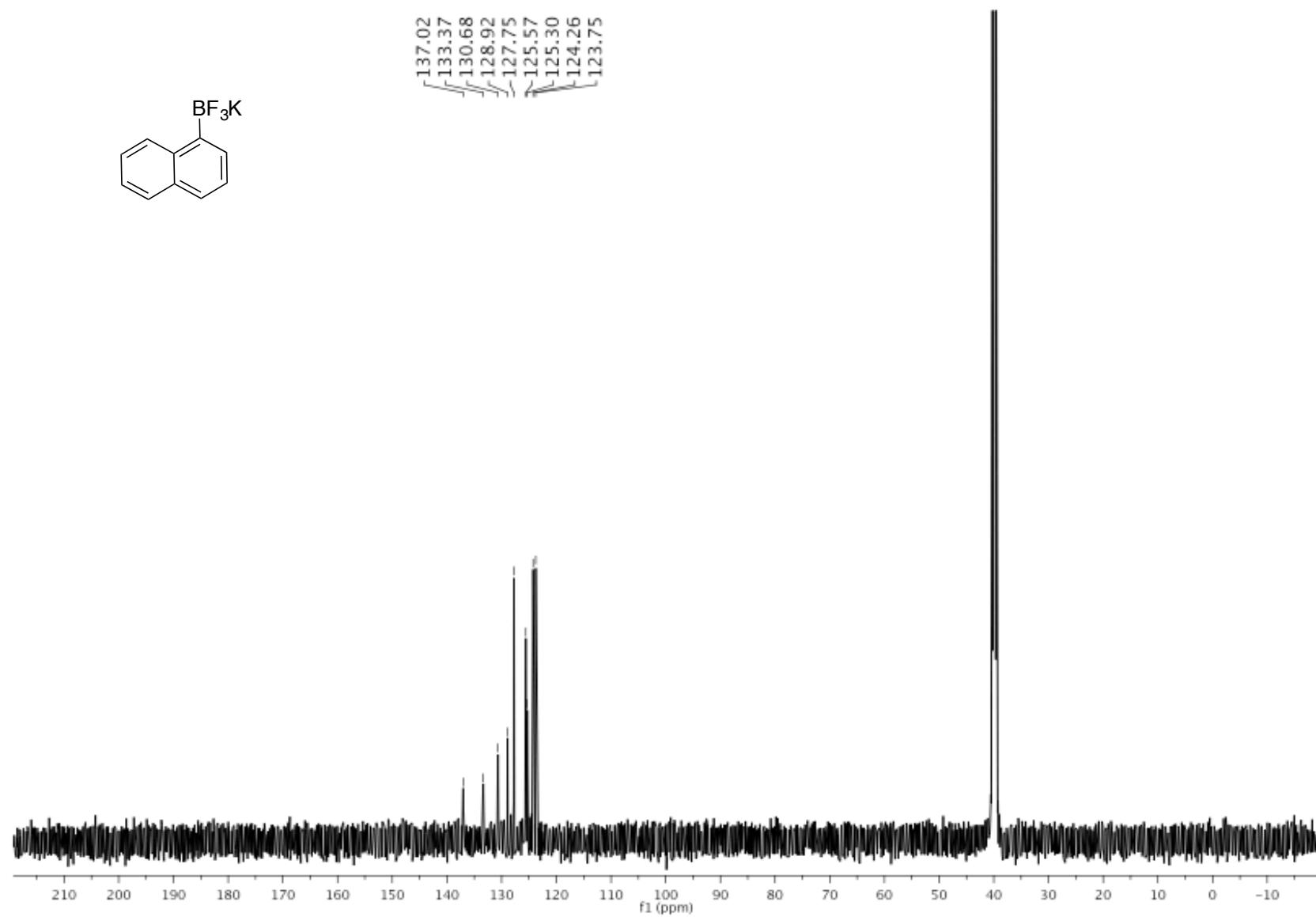
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium [1,1'-Biphenyl]-4-yltrifluoroborate (1h, Table 1, entry 8)



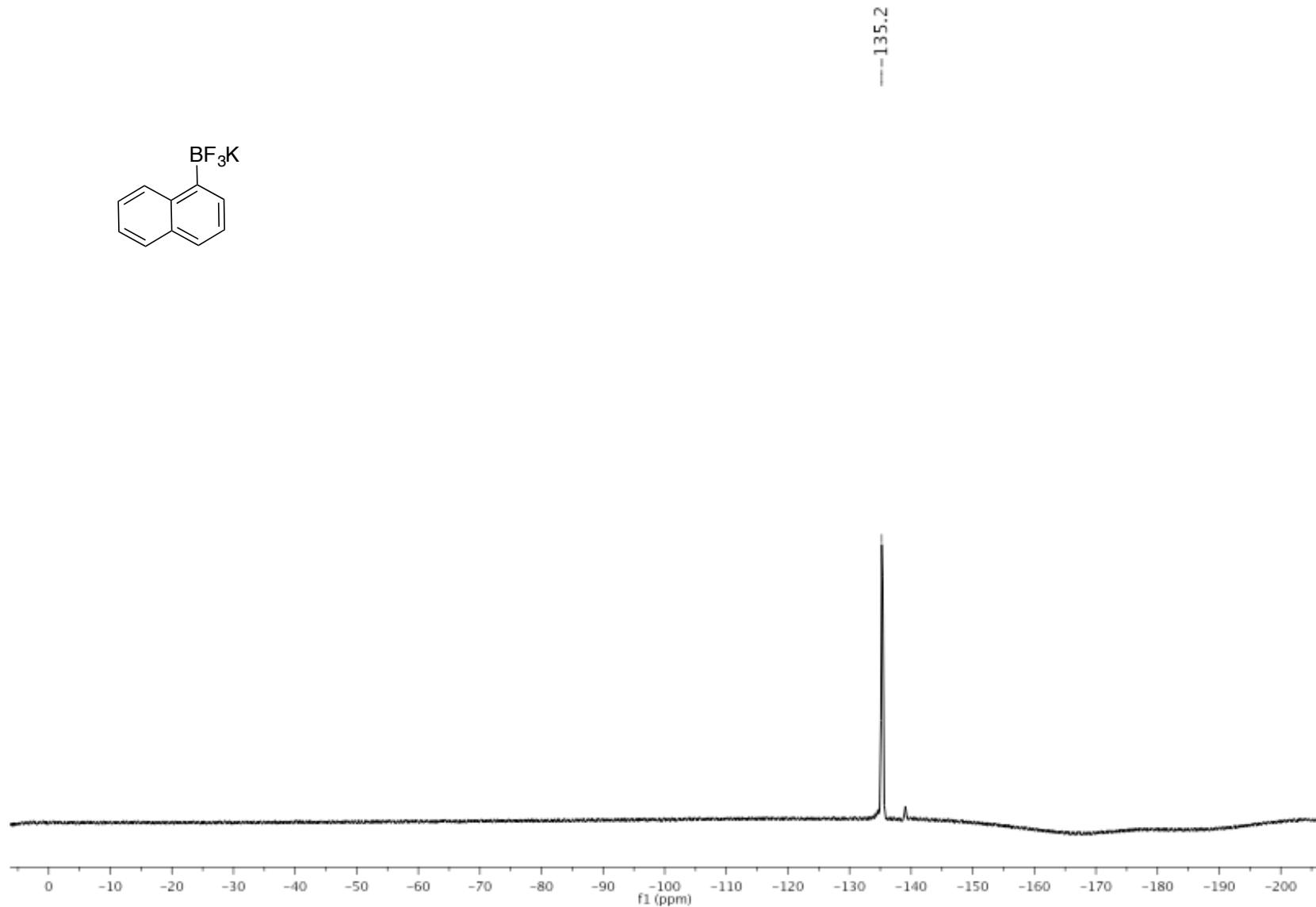
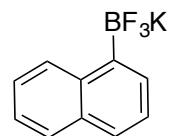
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium [1,1'-Biphenyl]-4-yltrifluoroborate (1h, Table 1, entry 8)



^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(naphthalen-1-yl)borate (1i, Table 1, entry 9)

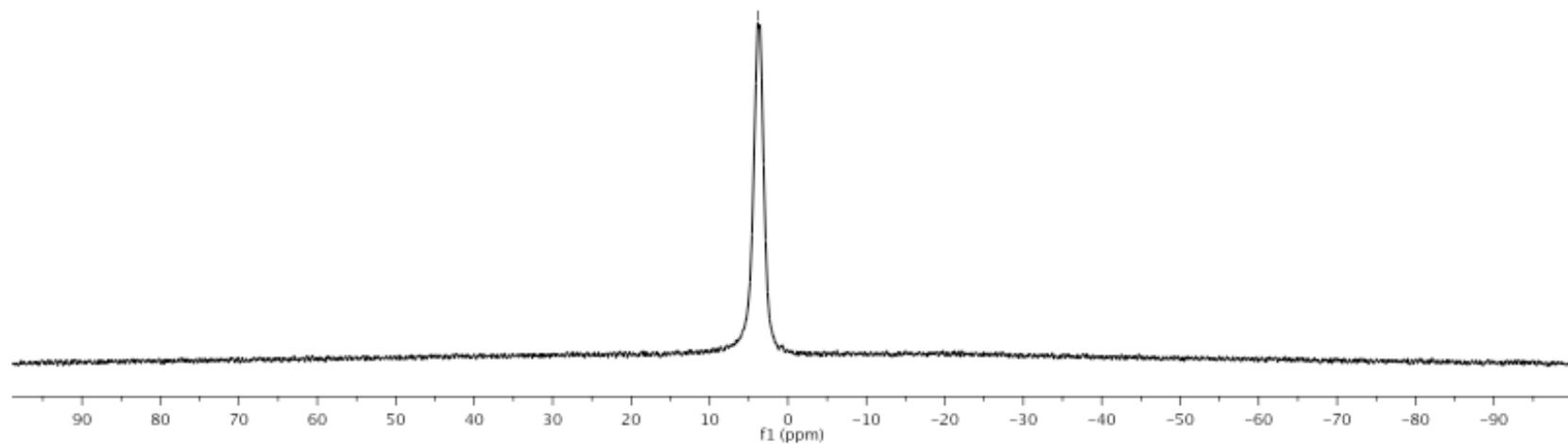
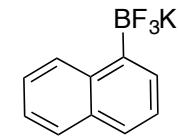


^{13}C NMR (128.5 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(naphthalen-1-yl)borate (1i, Table 1, entry 9)

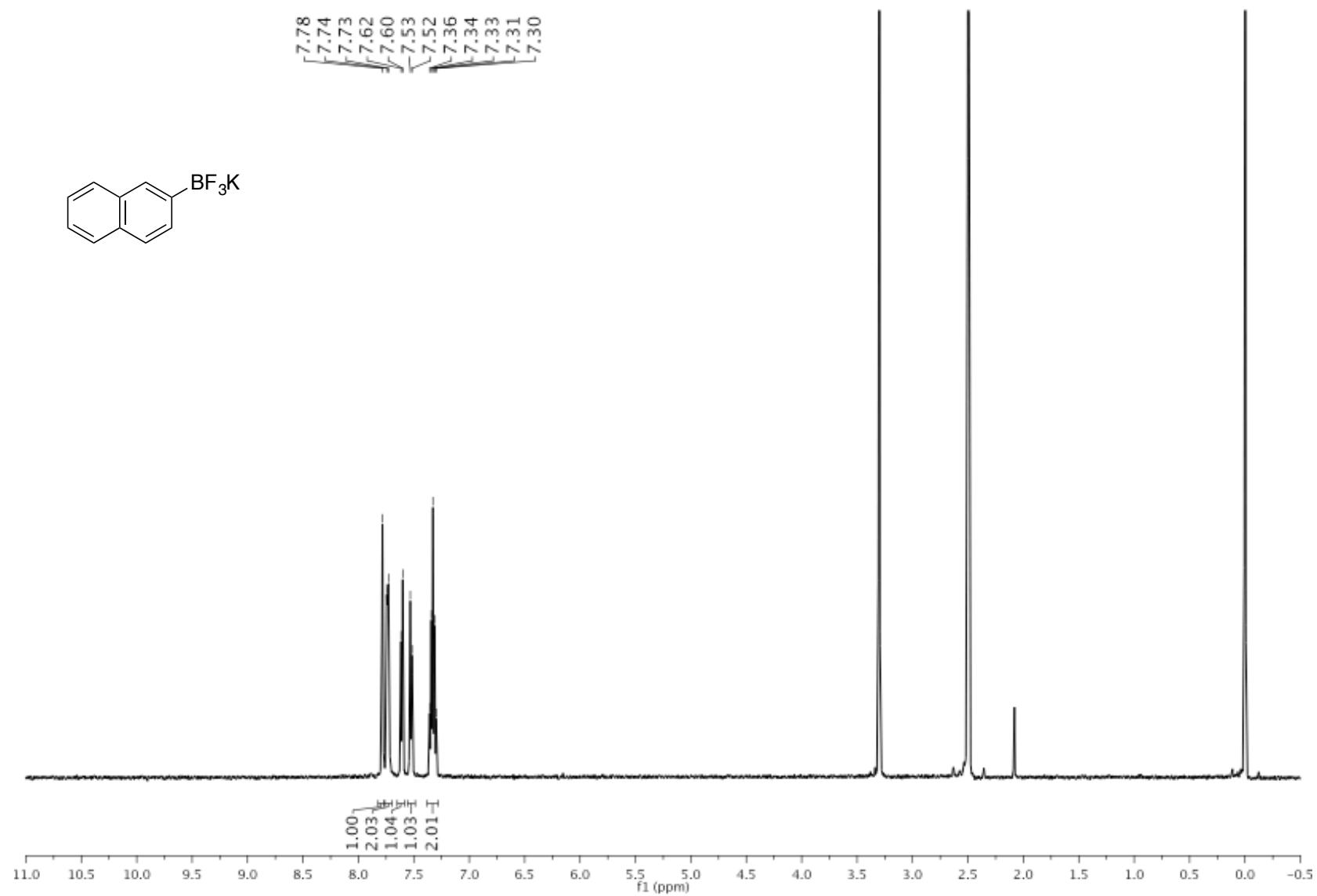


^{19}F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(naphthalen-1-yl)borate (1i, Table 1, entry 9)

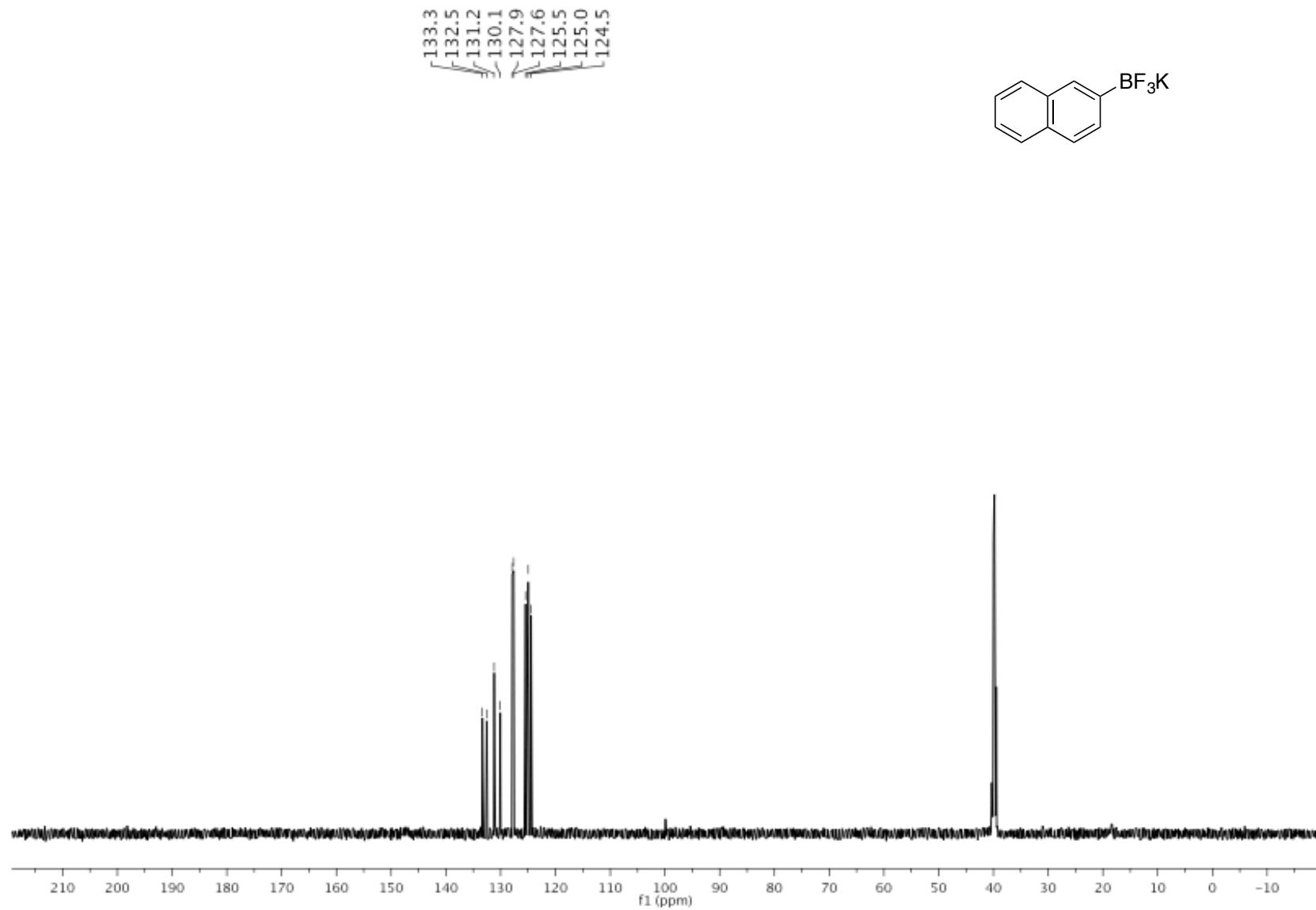
-3.9



¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(naphthalen-1-yl)borate (1i, Table 1, entry 9)

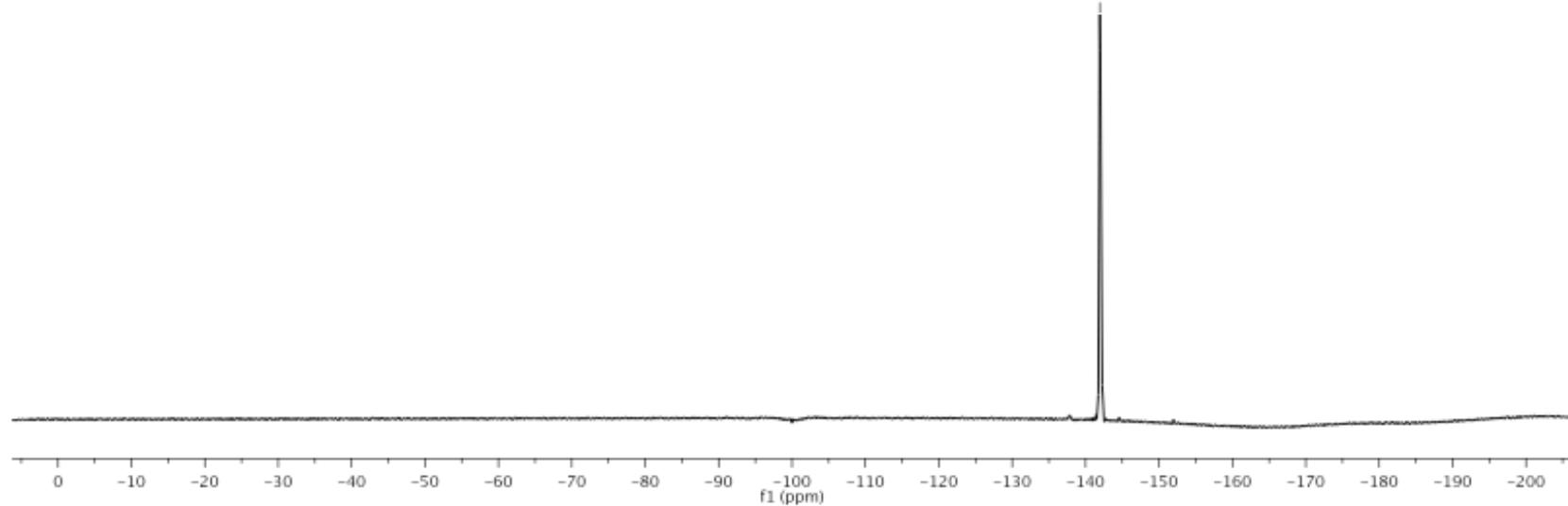
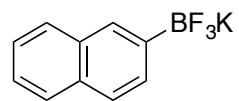


^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(naphthalen-2-yl)borate (1j, Table 1, entry 10)

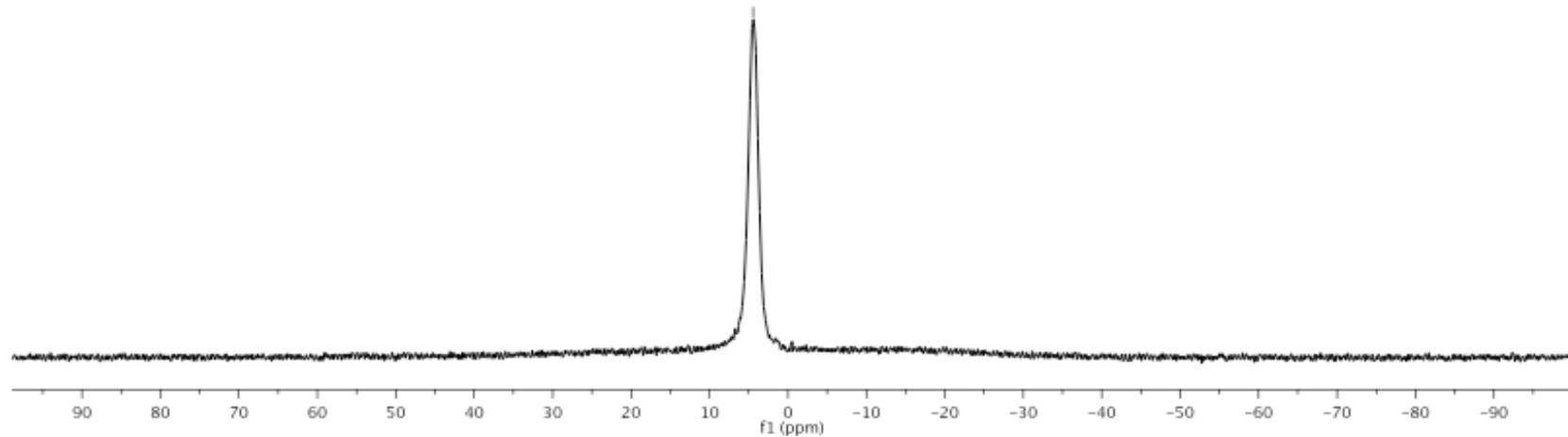
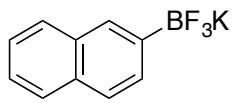


^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(naphthalen-2-yl)borate (1j, Table 1, entry 10)

-141.9

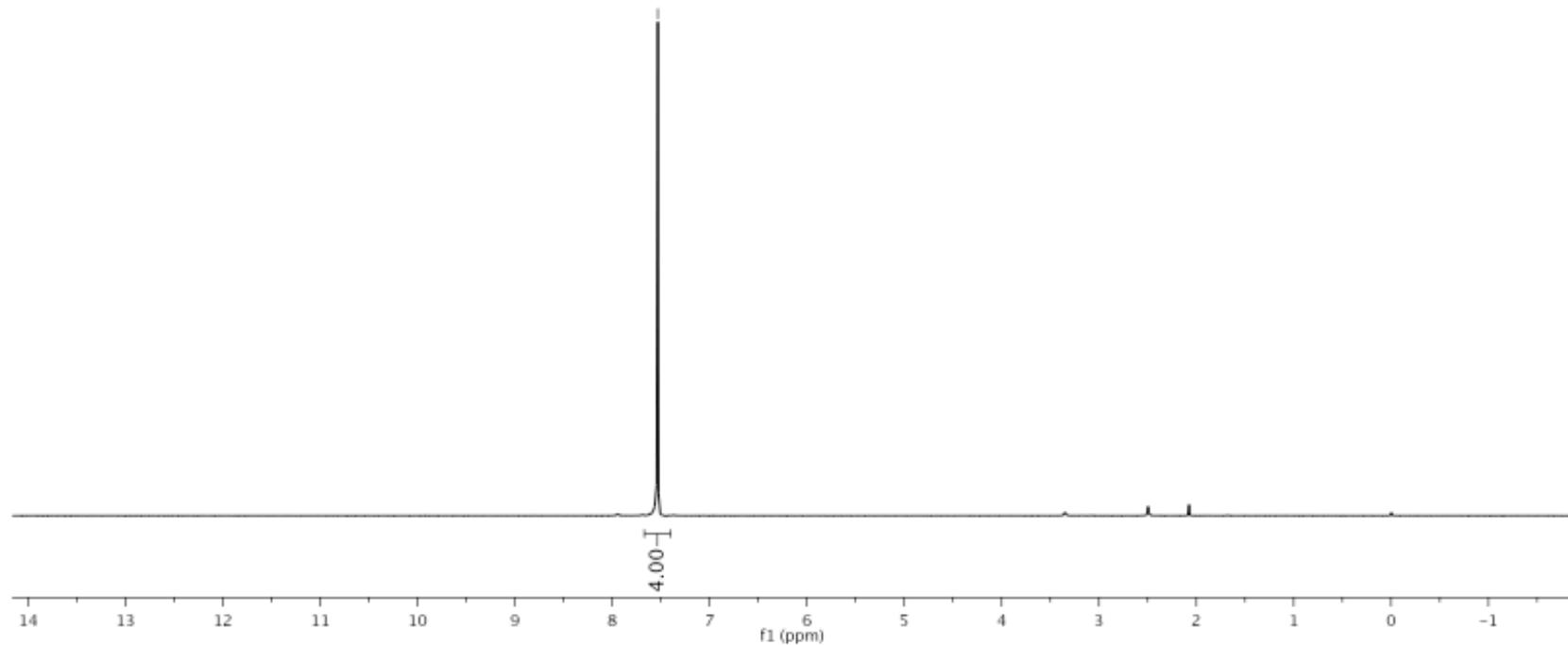
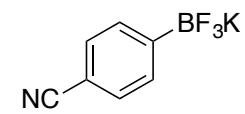


^{19}F NMR (470.8 MHz, acetone- d_6) Spectrum of Potassium Trifluoro(naphthalen-2-yl)borate (1j, Table 1, entry 10)



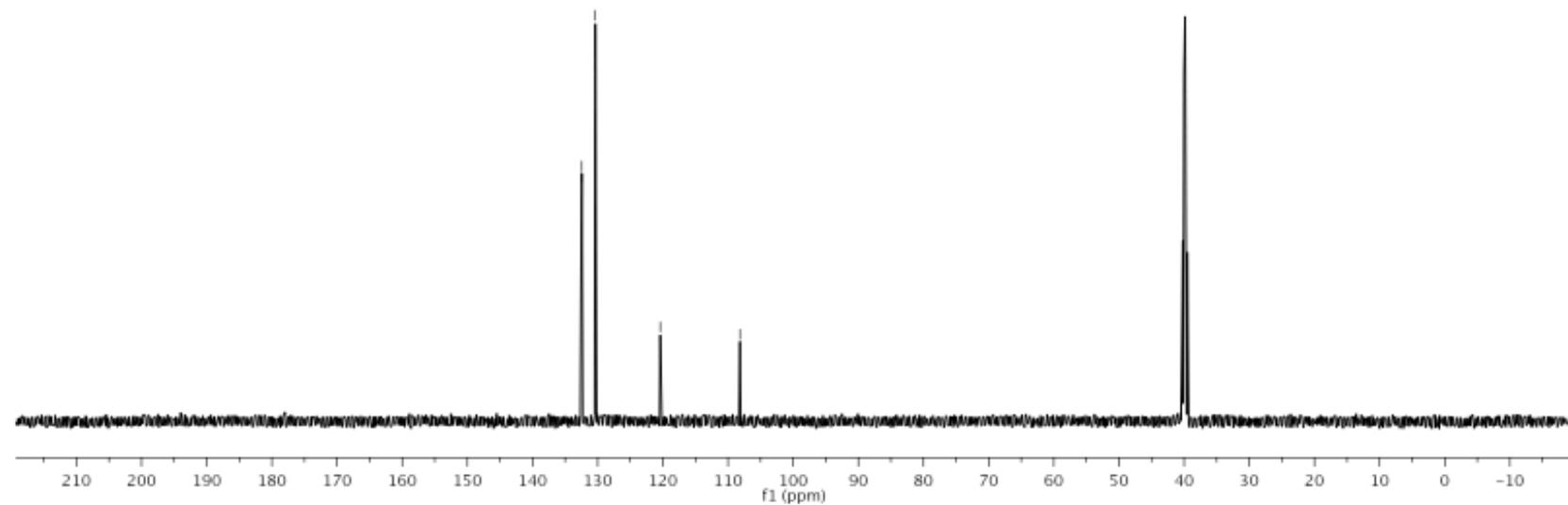
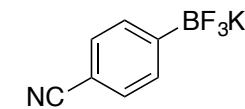
¹¹B NMR (128.4 MHz, acetone-d₆) Spectrum of Potassium Trifluoro(naphthalen-2-yl)borate (1j, Table 1, entry 10)

-7.53



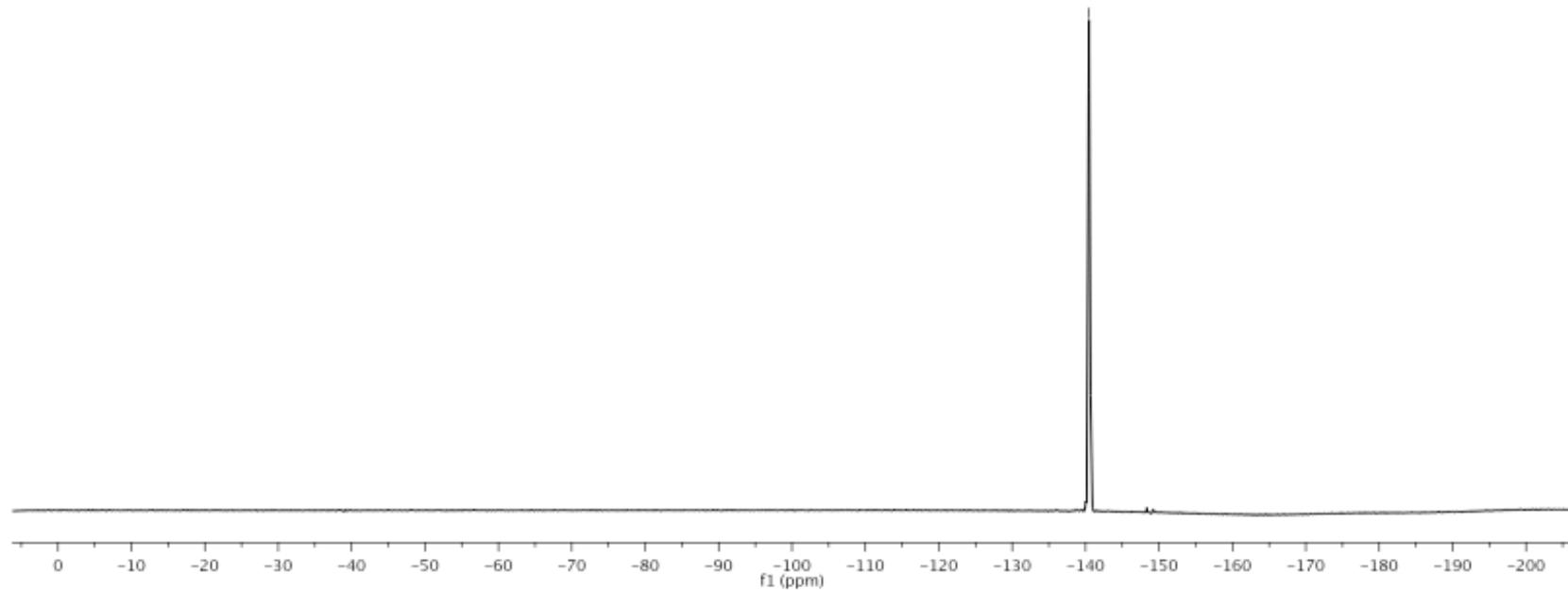
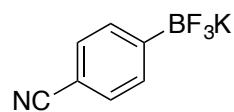
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium (4-Cyanophenyl)trifluoroborate (2a, Table 2, entry 1)

132.4
132.4
130.4
-120.4
-108.2

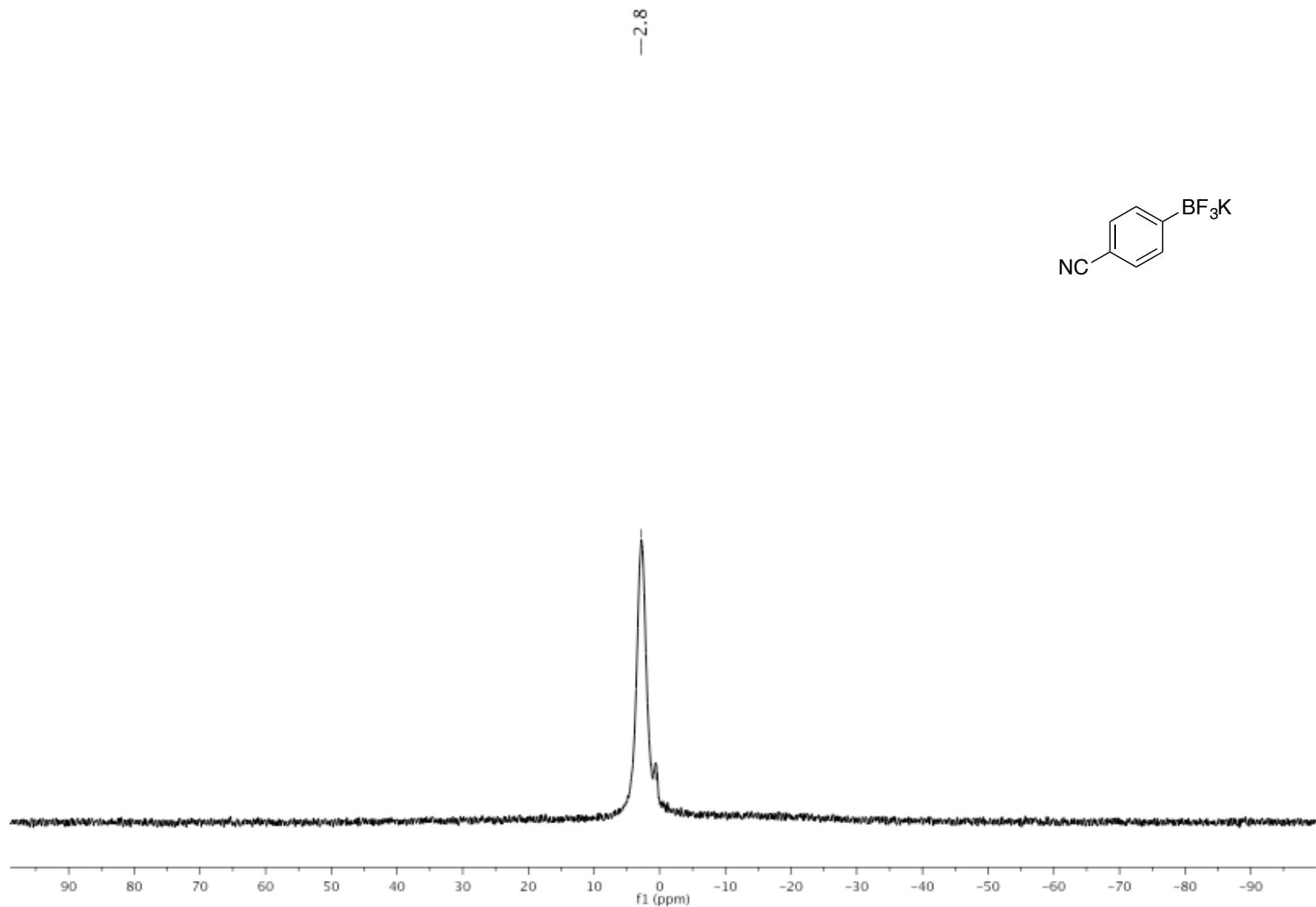
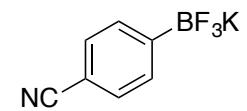


¹³C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium (4-Cyanophenyl)trifluoroborate (2a, Table 2, entry 1)

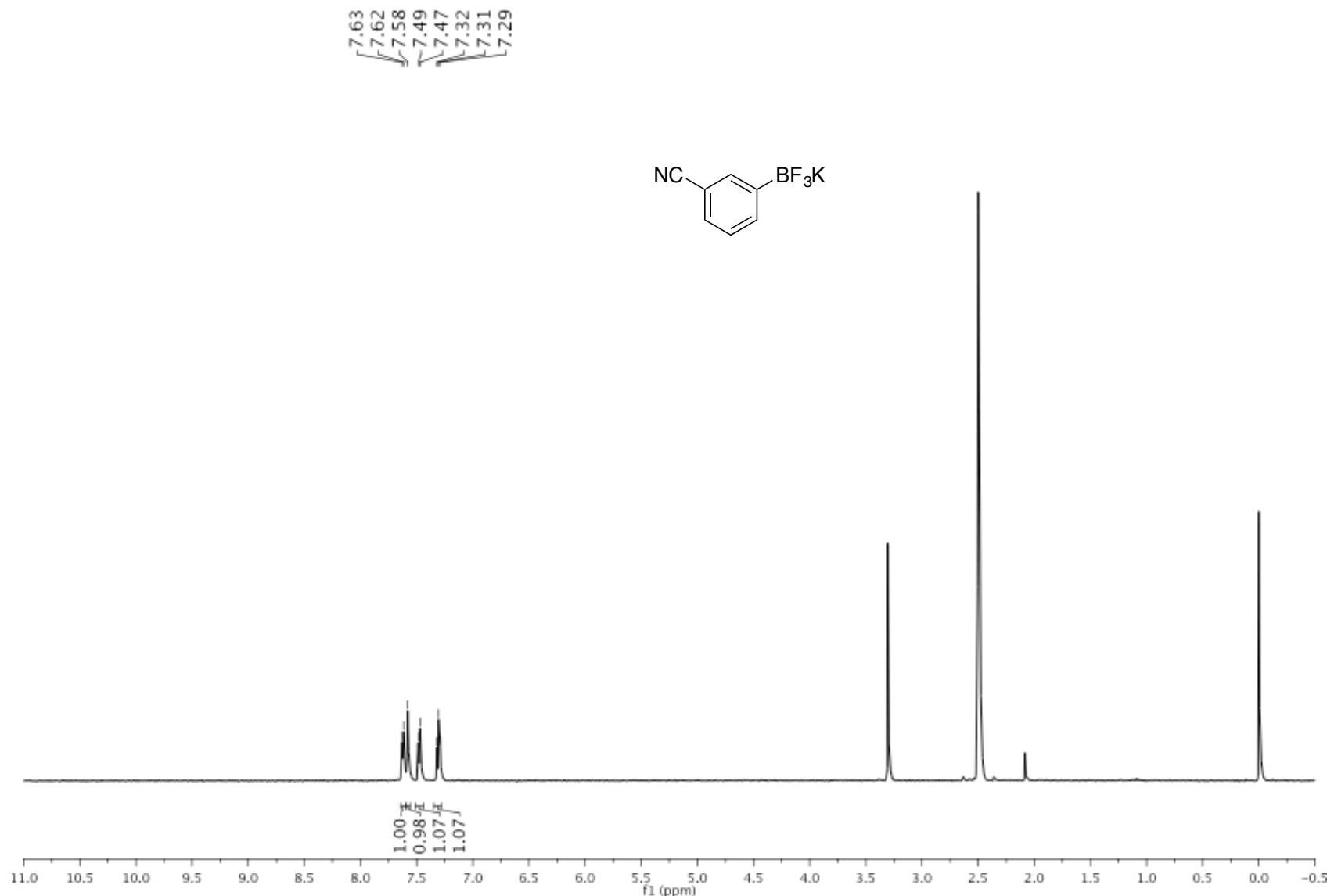
-140.5



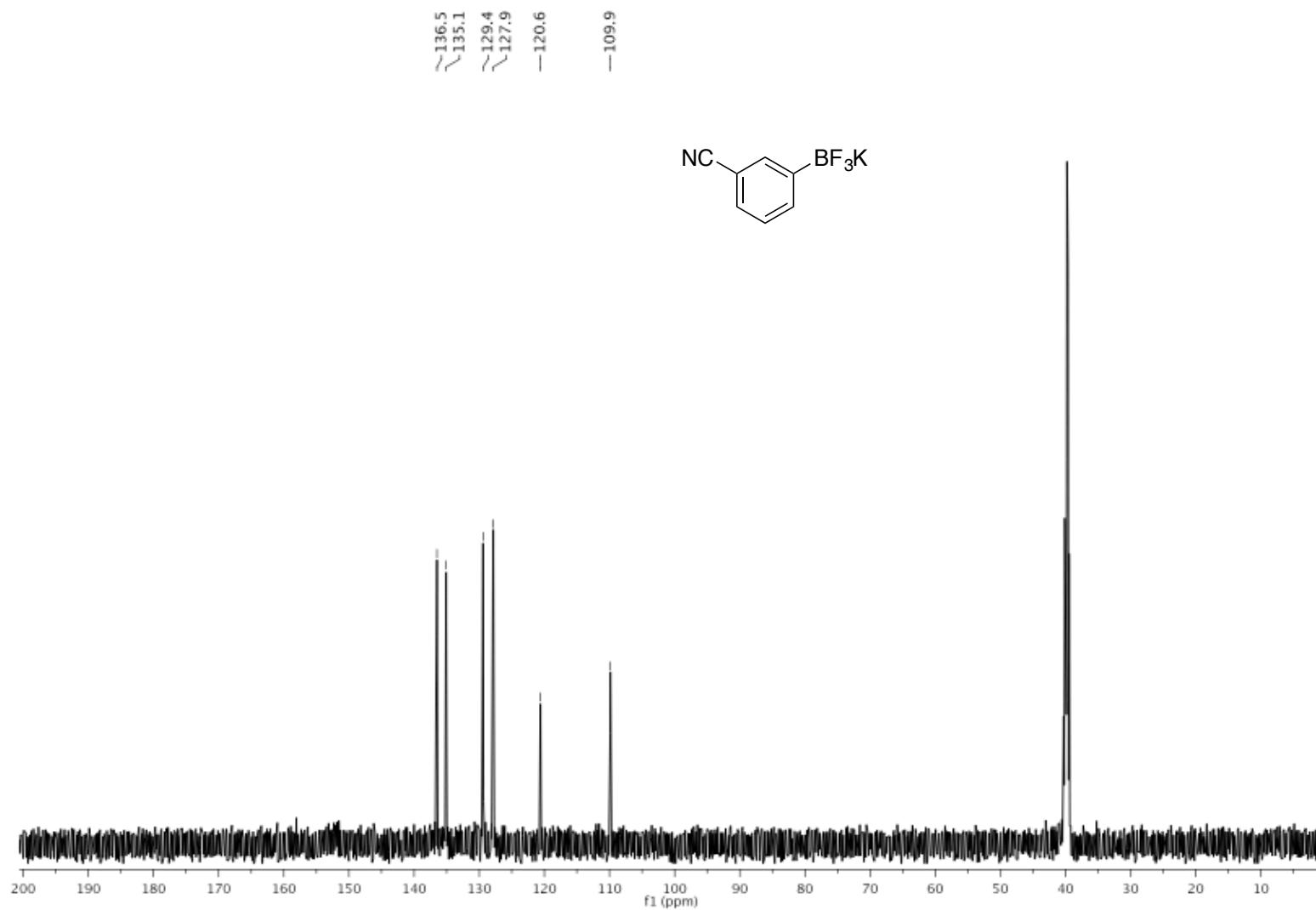
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium (4-Cyanophenyl)trifluoroborate (2a, Table 2, entry 1)



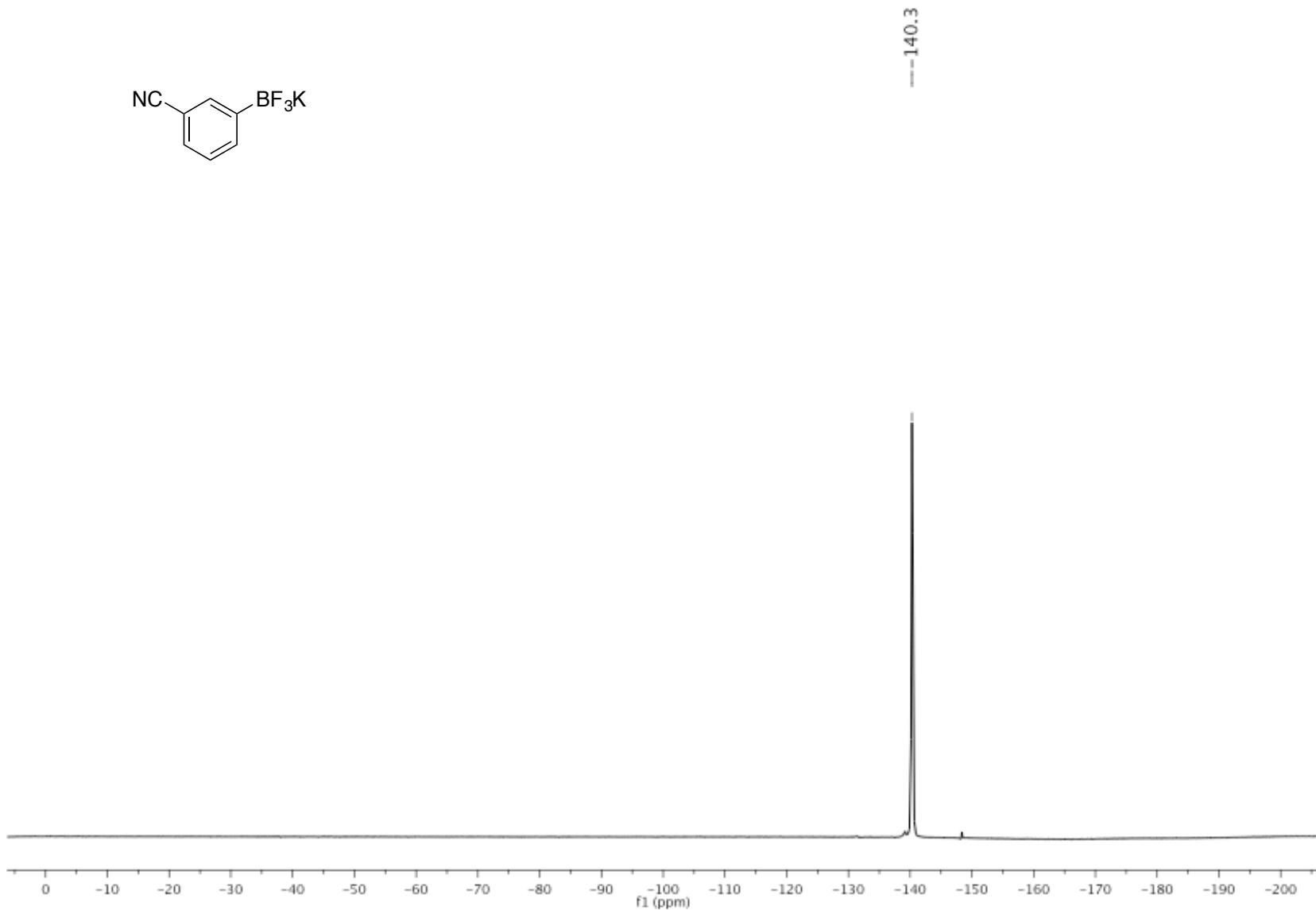
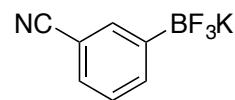
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium (4-Cyanophenyl)trifluoroborate (2a, Table 2, entry 1)



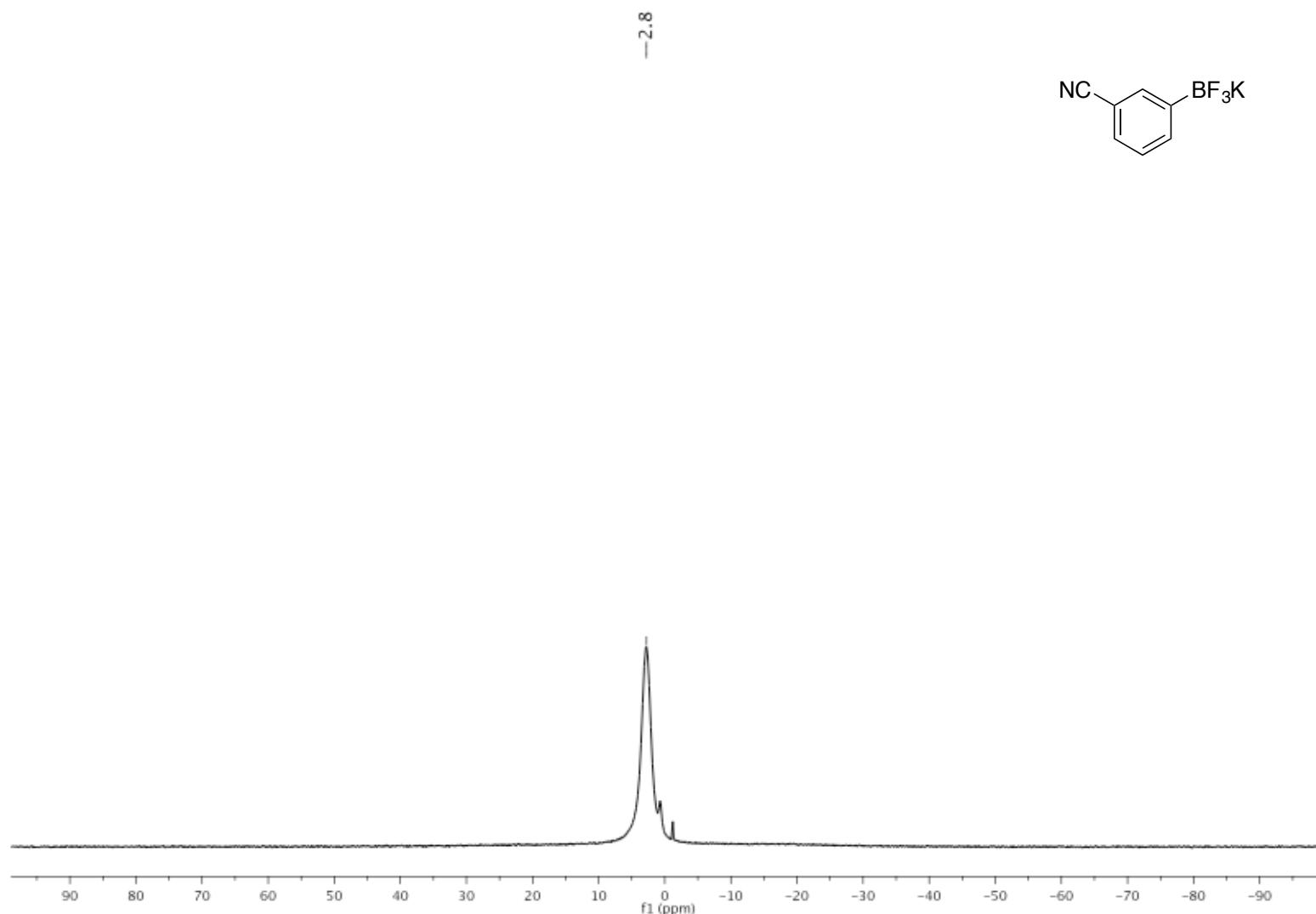
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium (3-Cyanophenyl)trifluoroborate (2b, Table 2, entry 2)



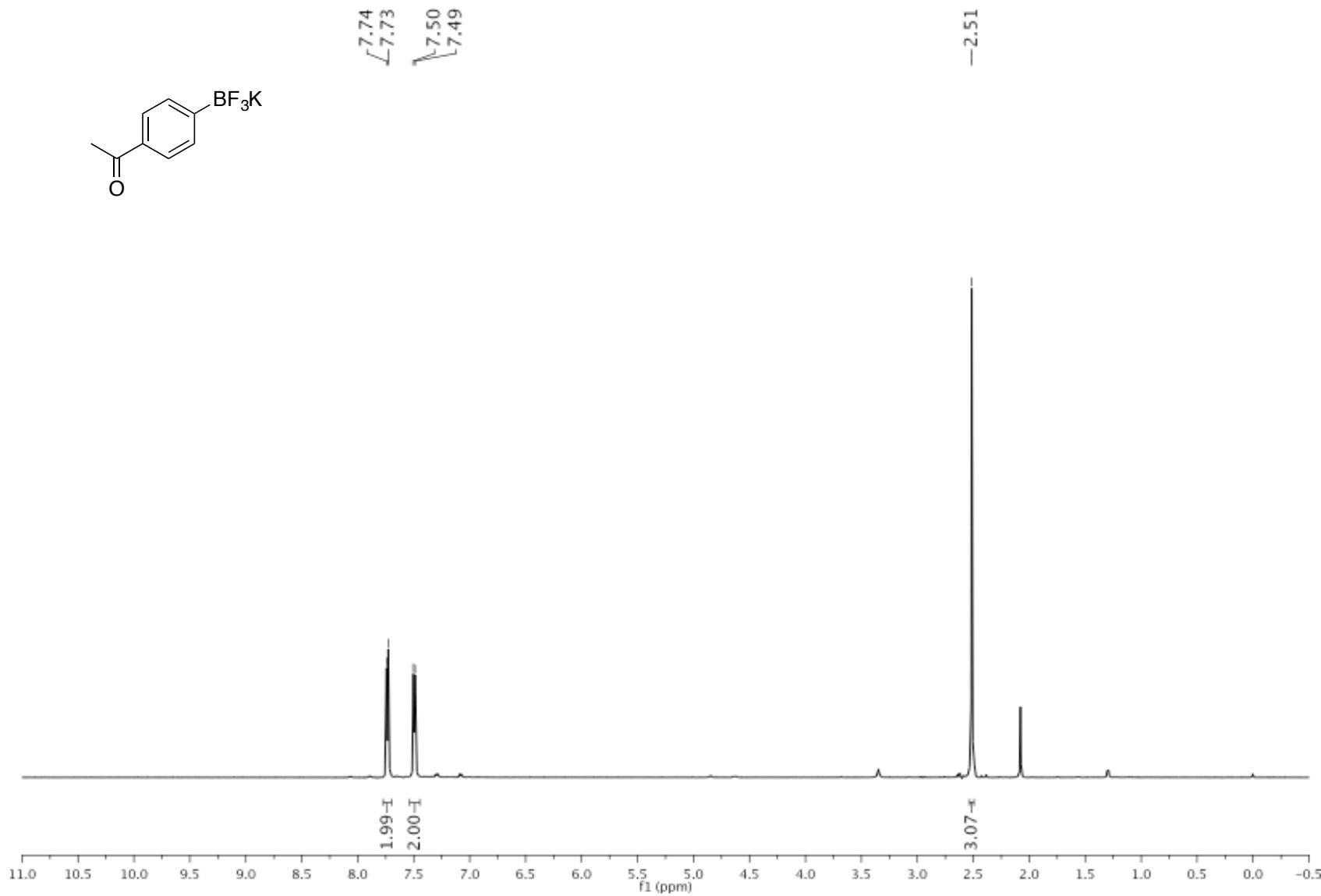
^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium (3-Cyanophenyl)trifluoroborate (2b, Table 2, entry 2)



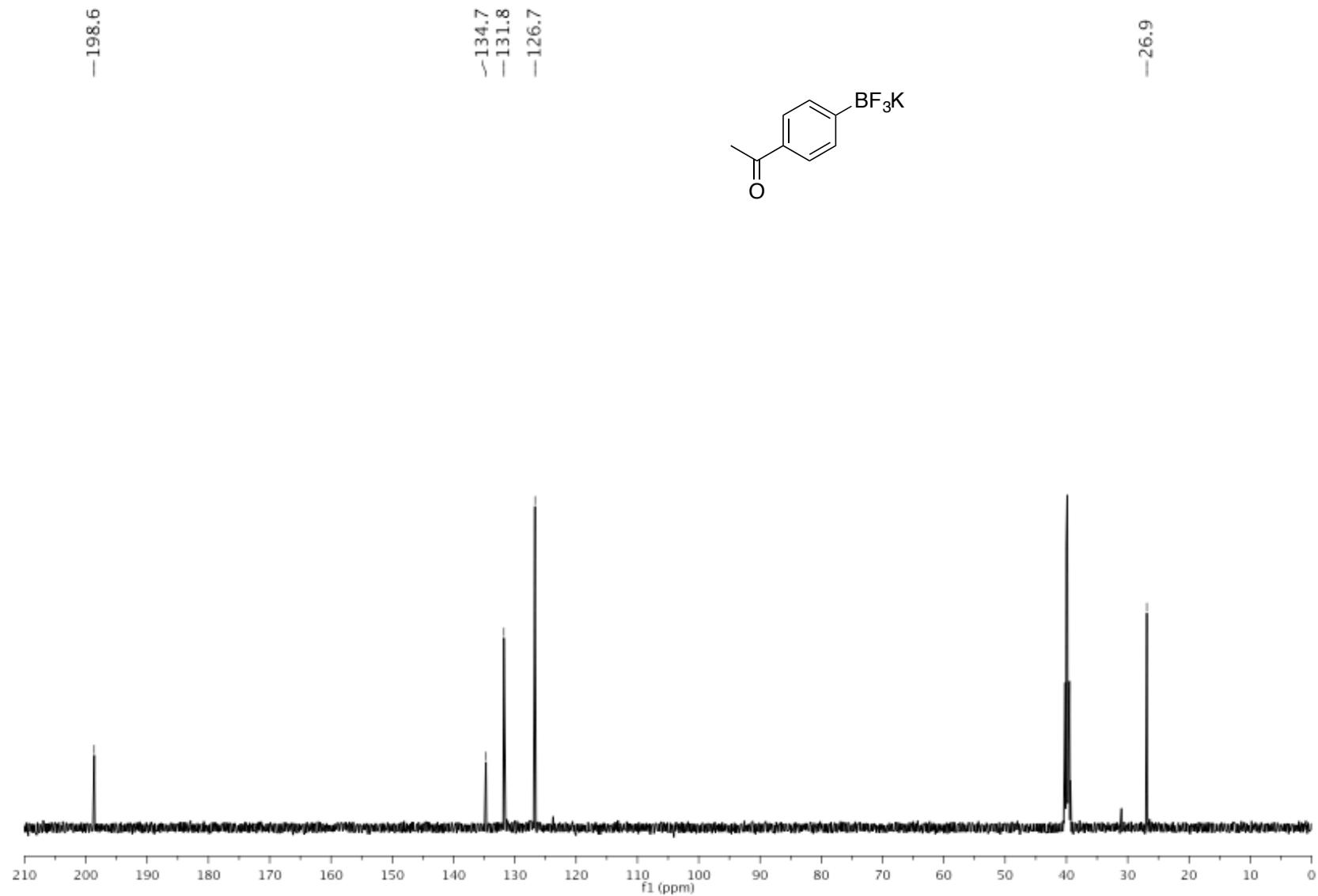
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium (3-Cyanophenyl)trifluoroborate (2b, Table 2, entry 2)



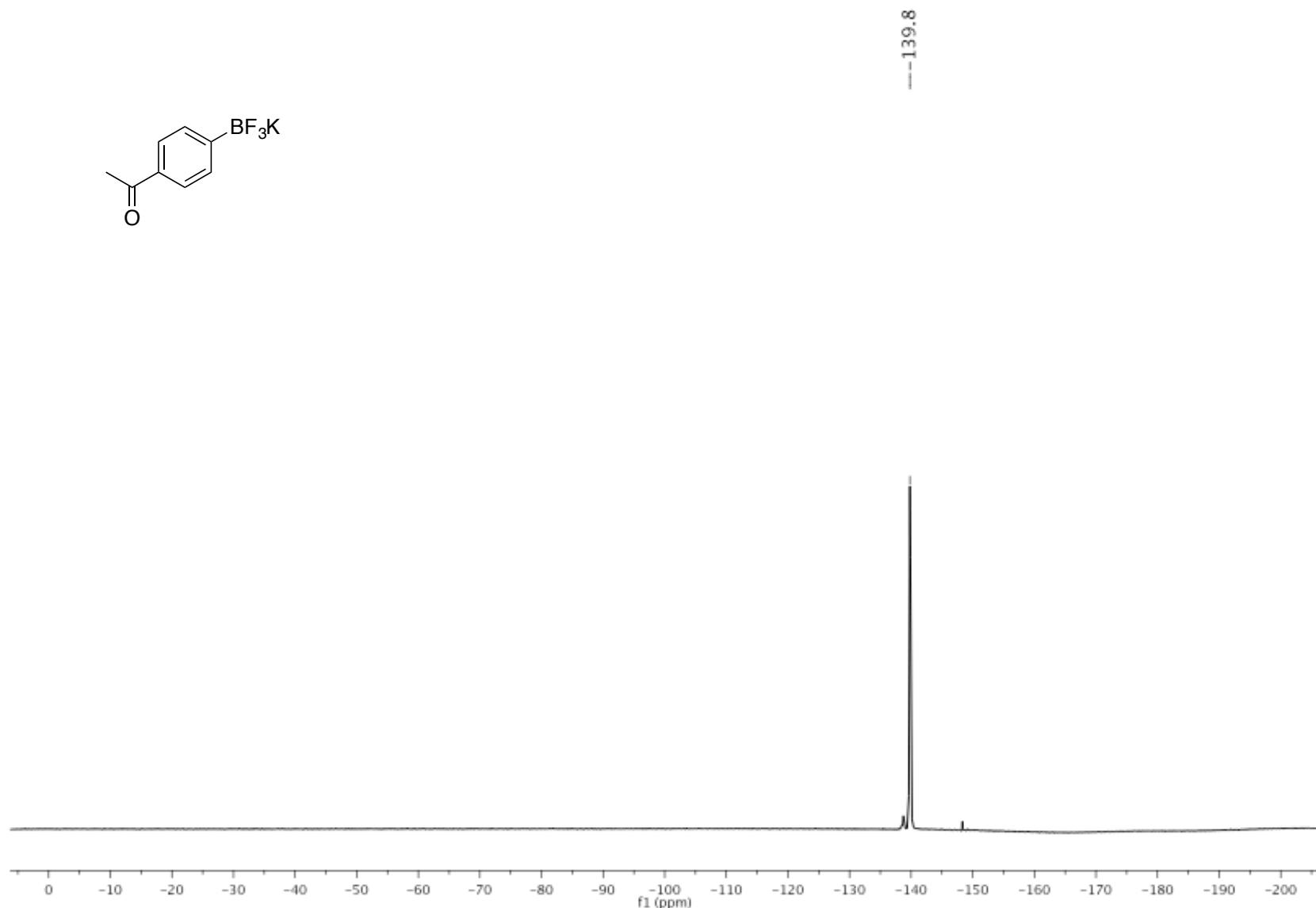
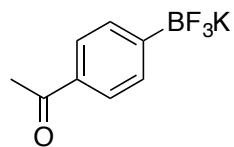
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium (3-Cyanophenyl)trifluoroborate (2b, Table 2, entry 2)



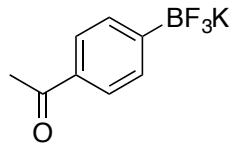
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium (4-Acetylphenyl)trifluoroborate (2c, Table 2, entry 3)



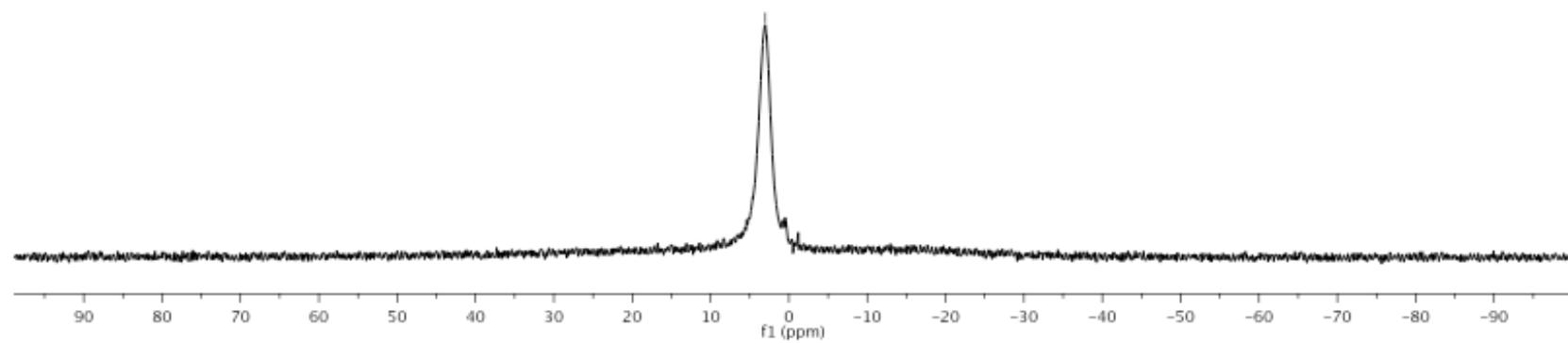
^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium (4-Acetylphenyl)trifluoroborate (2c, Table 2, entry 3)



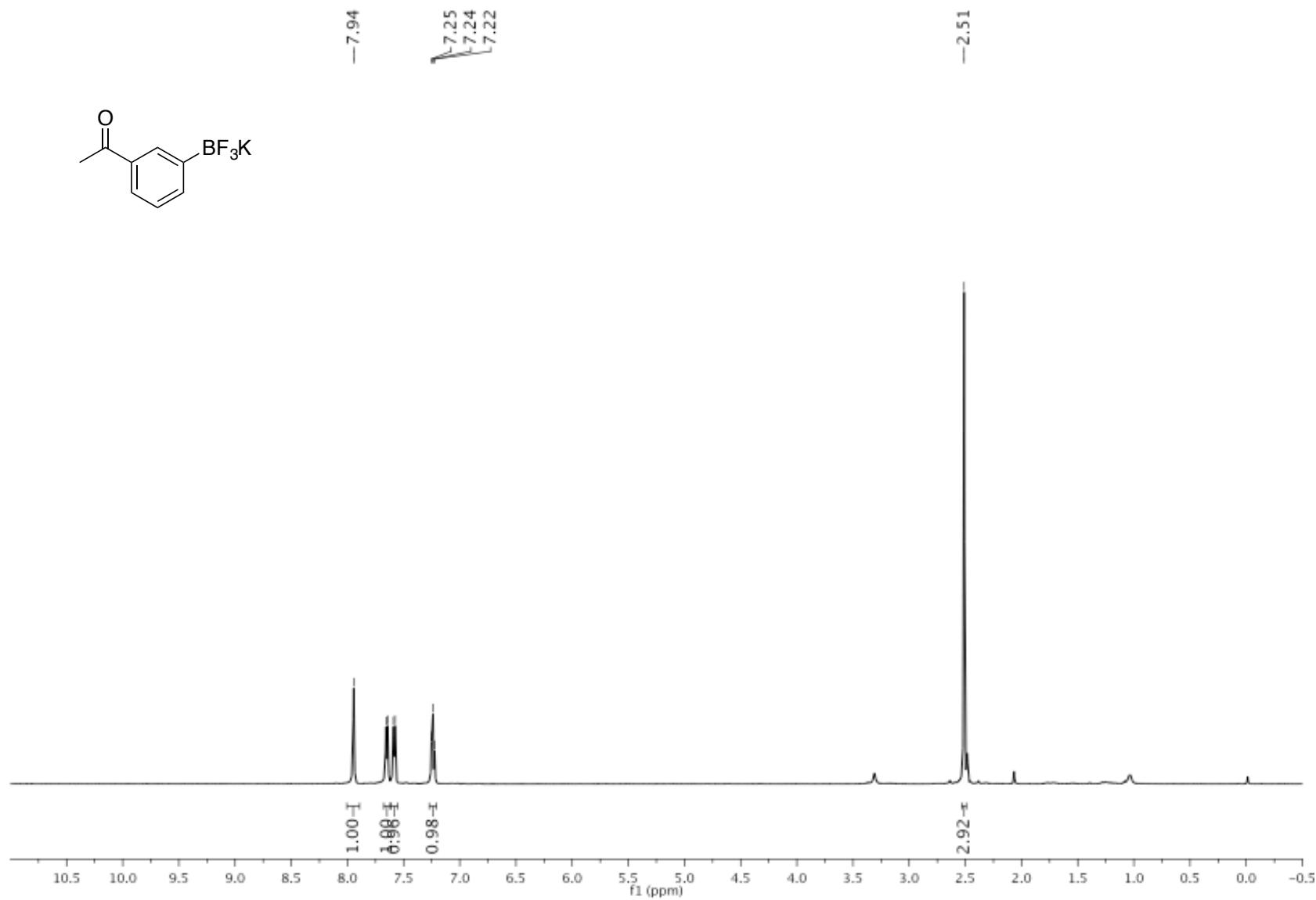
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium (4-Acetylphenyl)trifluoroborate (2c, Table 2, entry 3)



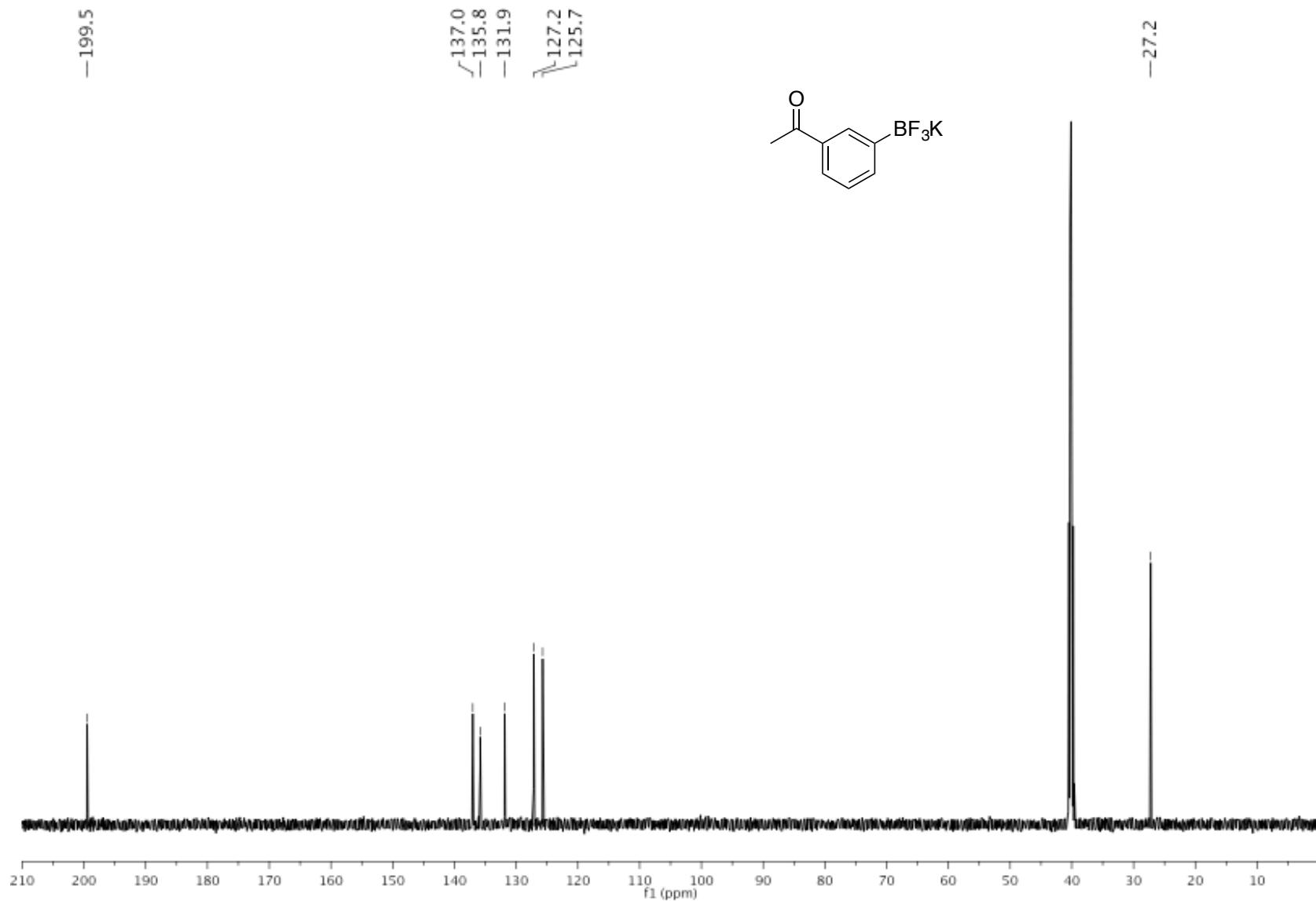
-3.0



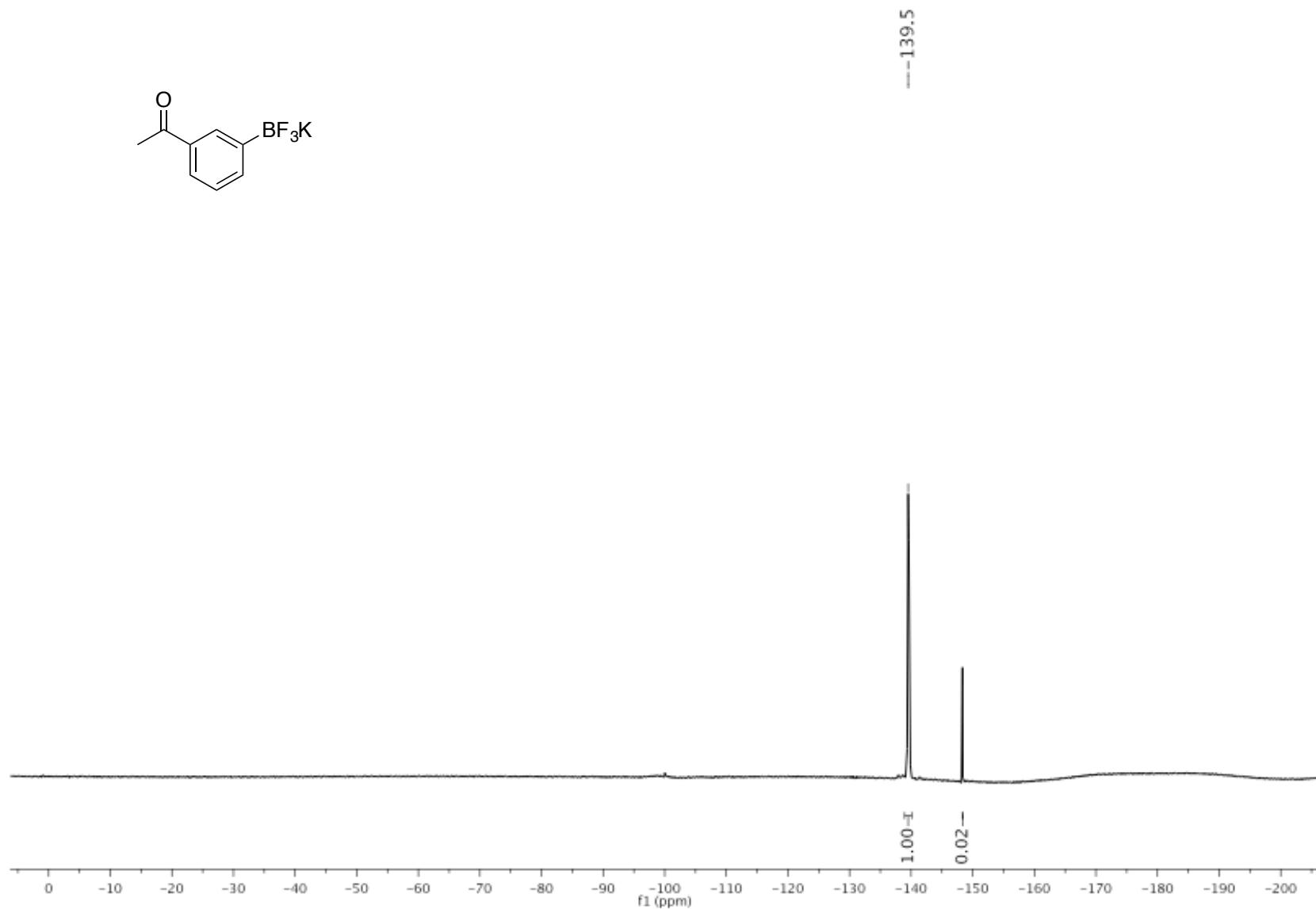
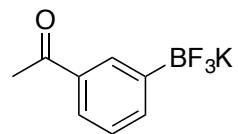
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium (4-Acetylphenyl)trifluoroborate (2c, Table 2, entry 3)



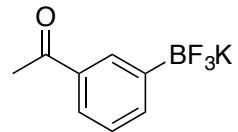
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium (3-Acetylphenyl)trifluoroborate (2d, Table 2, entry 4)



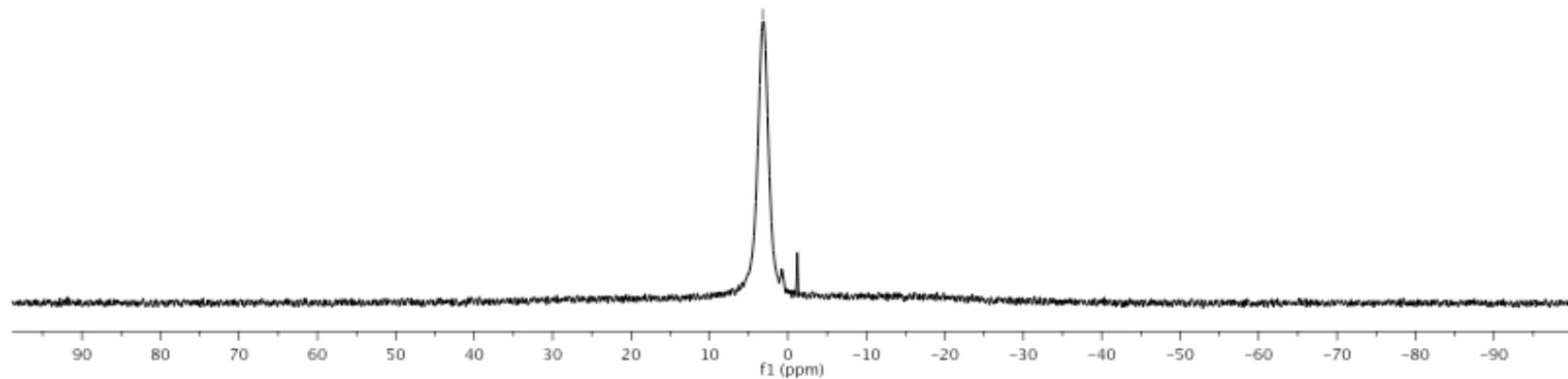
^{13}C NMR (128.5 MHz, DMSO-d_6) Spectrum of Potassium (3-Acetylphenyl)trifluoroborate (2d, Table 2, entry 4)



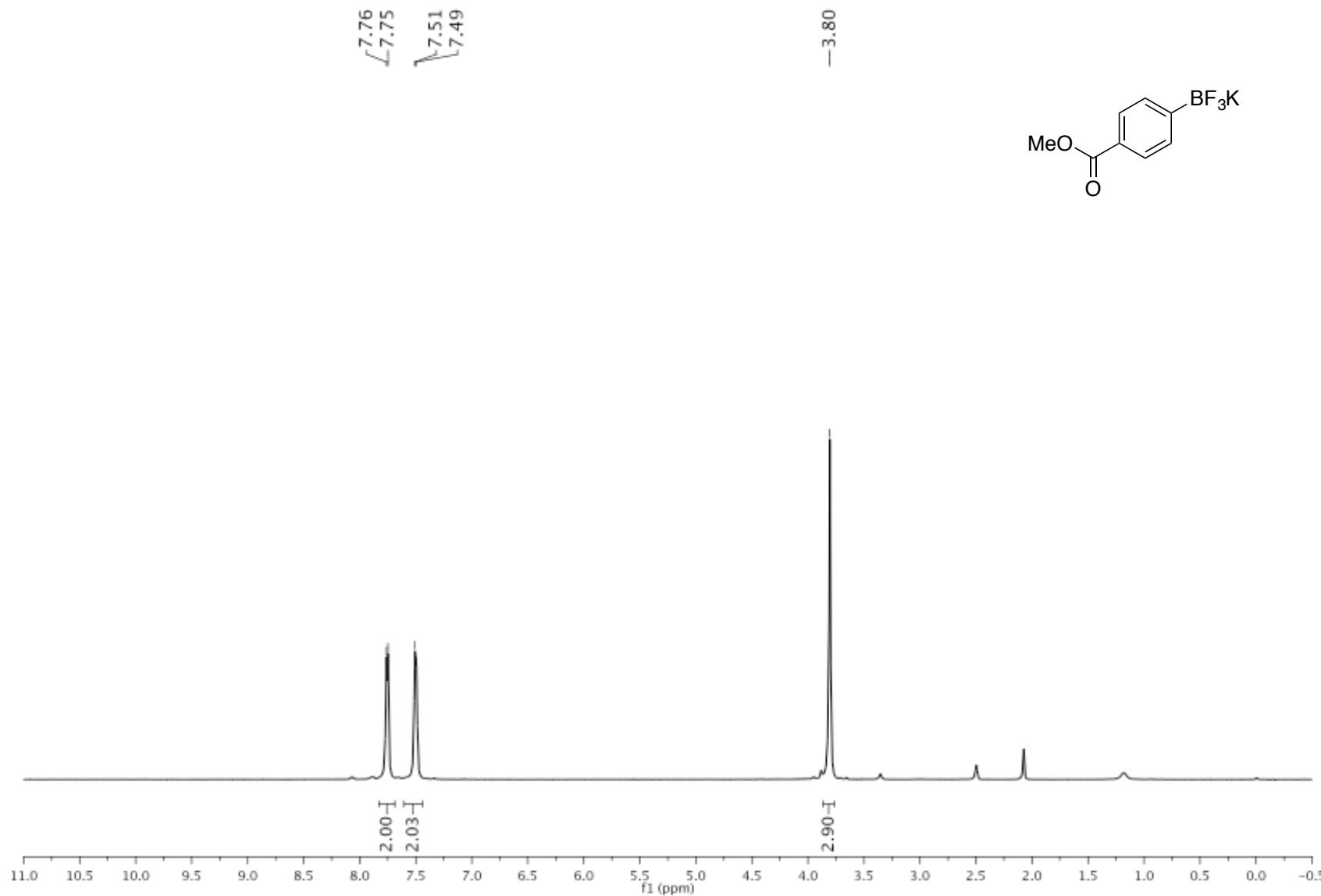
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium (3-Acetylphenyl)trifluoroborate (2d, Table 2, entry 4)



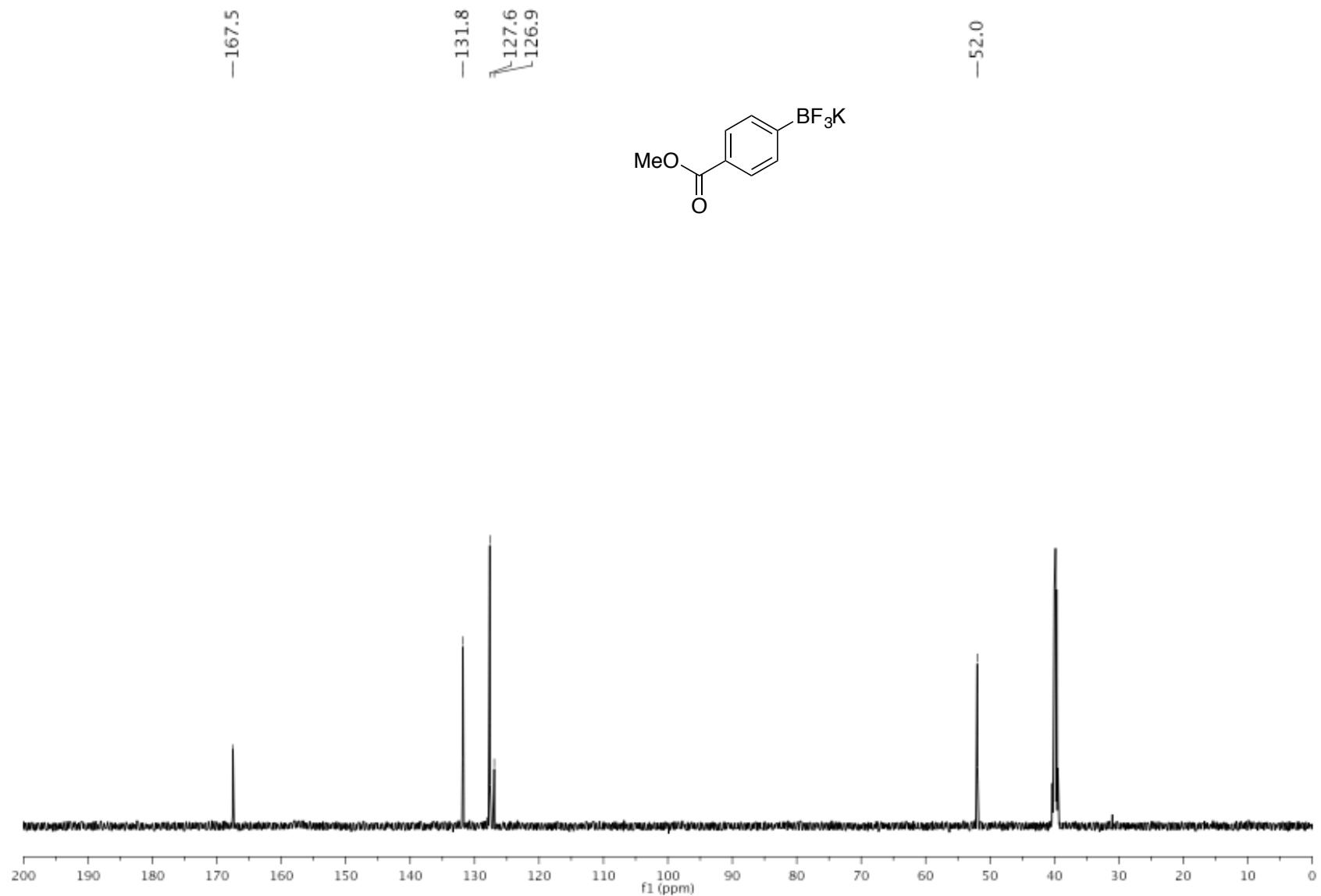
-3.2



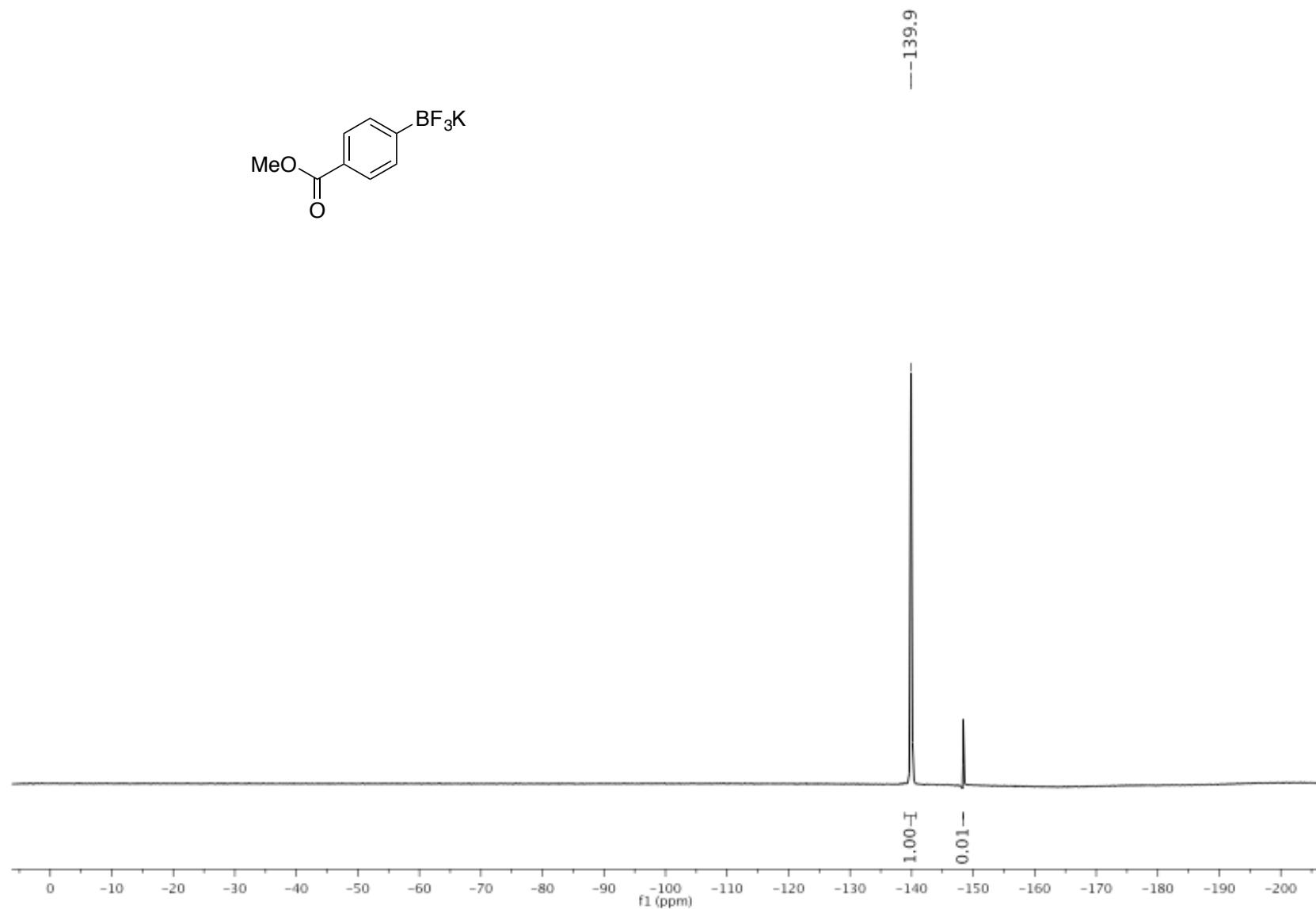
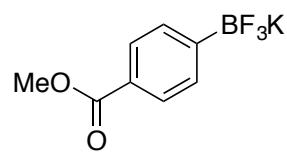
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium (3-Acetylphenyl)trifluoroborate (2d, Table 2, entry 4)



¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-(methoxycarbonyl)phenyl)borate (2e, Table 2, entry 5)

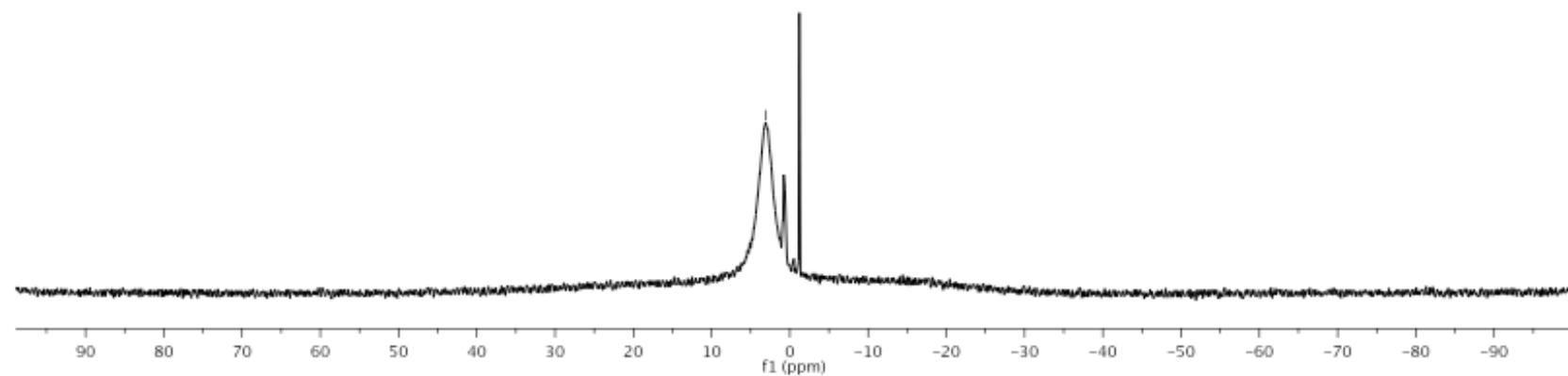
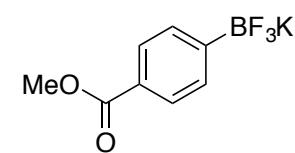


^{13}C NMR (128.5 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(4-(methoxycarbonyl)phenyl)borate (2e, Table 2, entry 5)

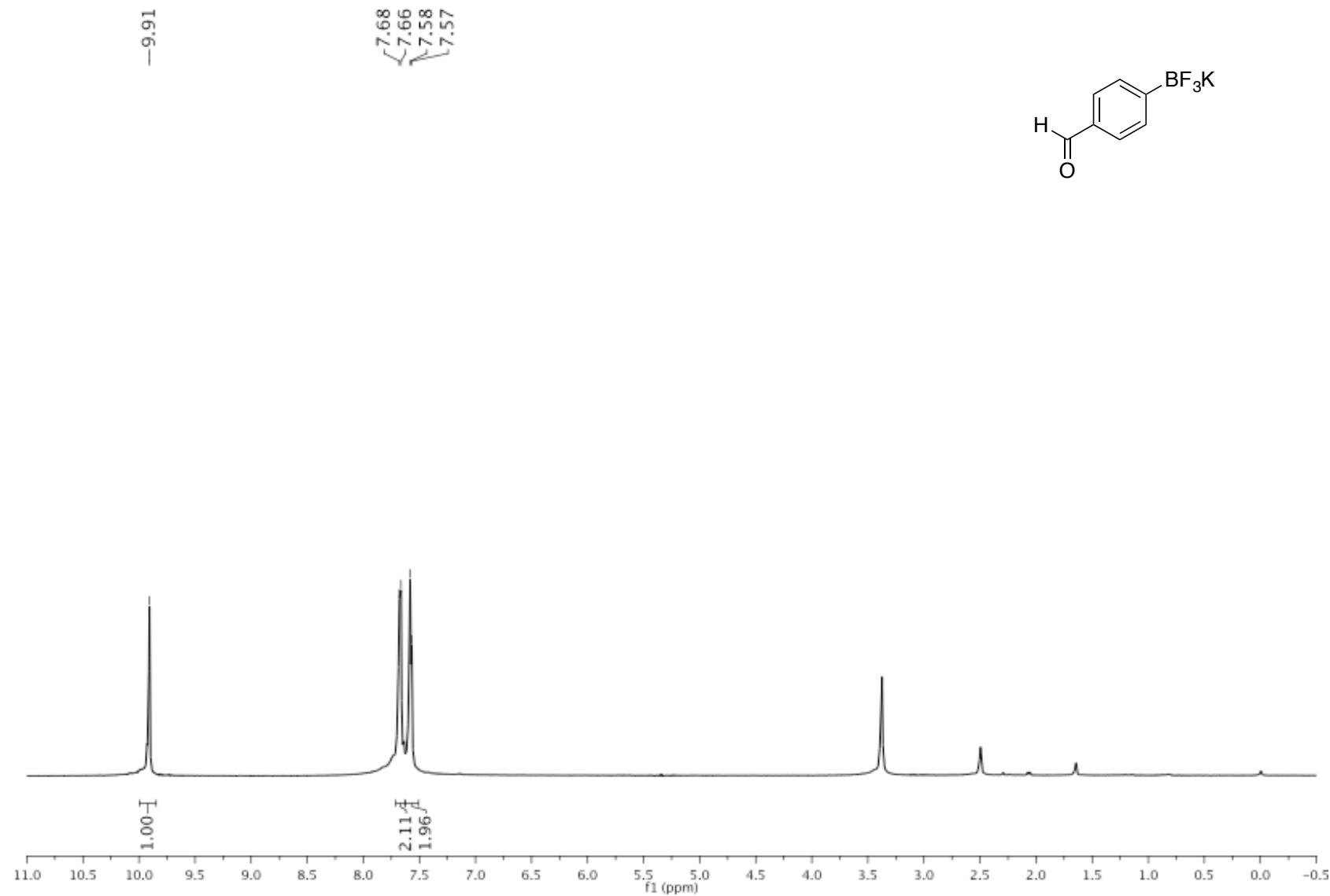


^{19}F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-(methoxycarbonyl)phenyl)borate (2e, Table 2, entry 5)

-3.1



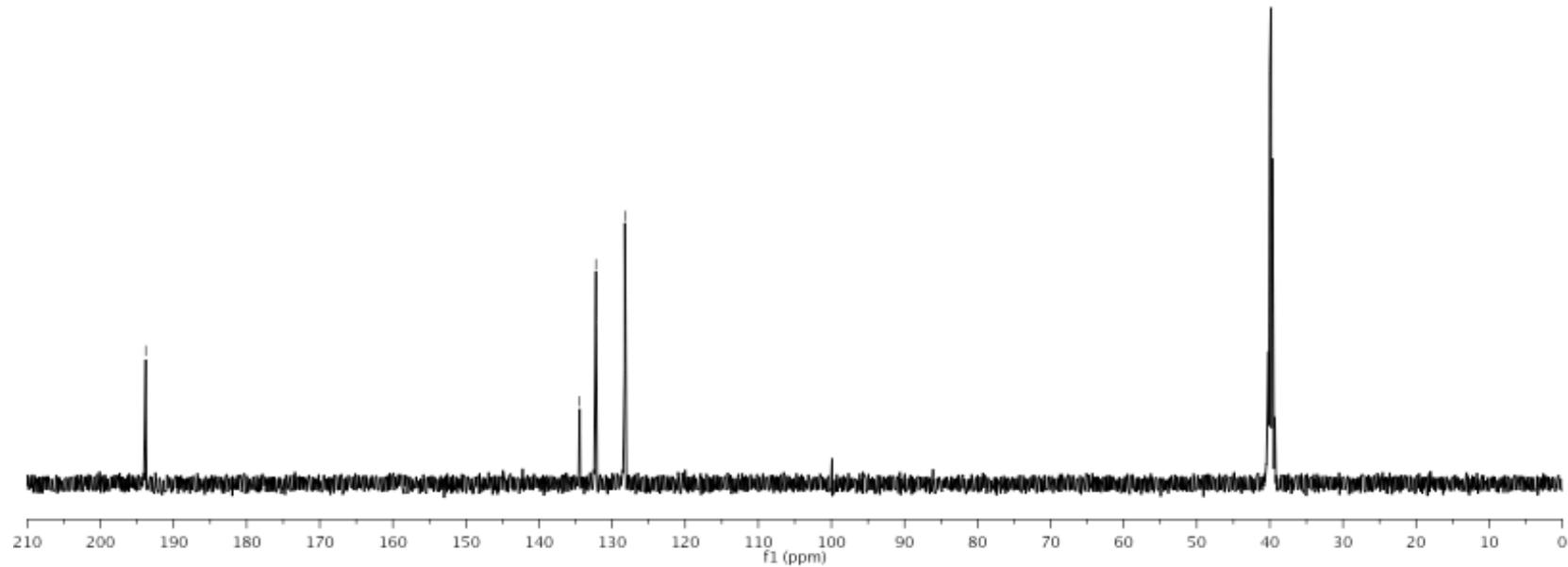
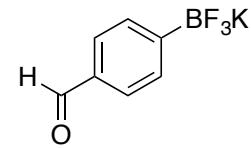
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-(methoxycarbonyl)phenyl)borate (2e, Table 2, entry 5)



¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-formylphenyl)borate (2f, Table 2, entry 6)

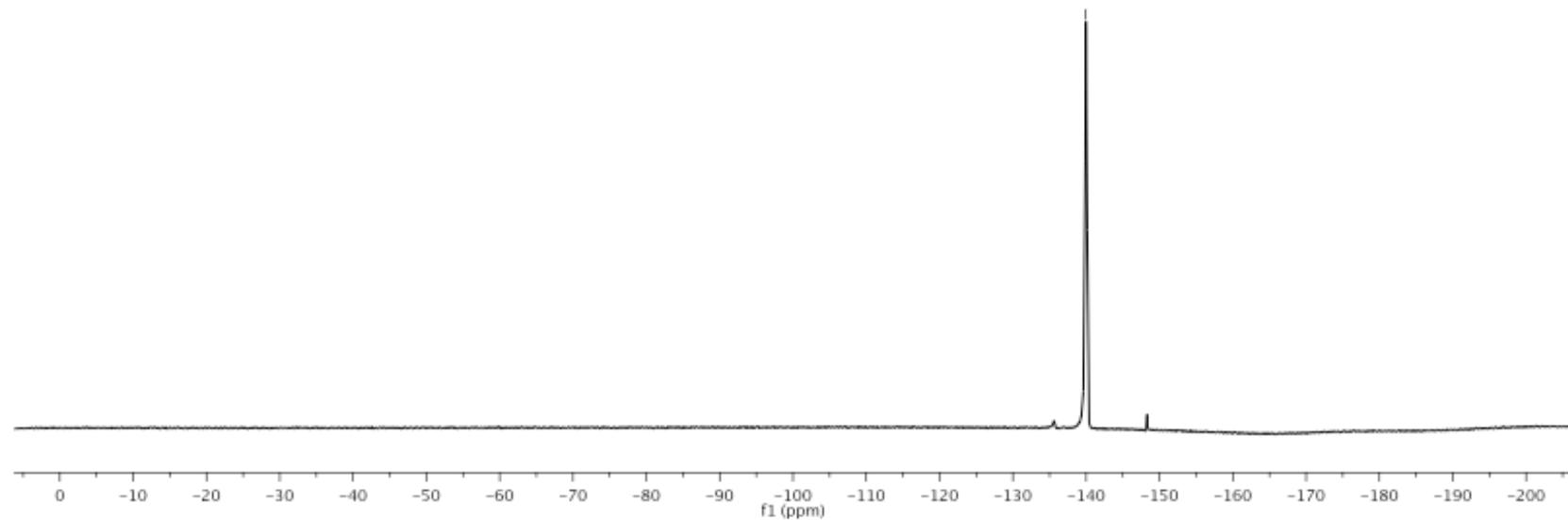
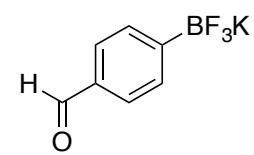
-193.8

✓ 134.4
— 132.2
— 128.2



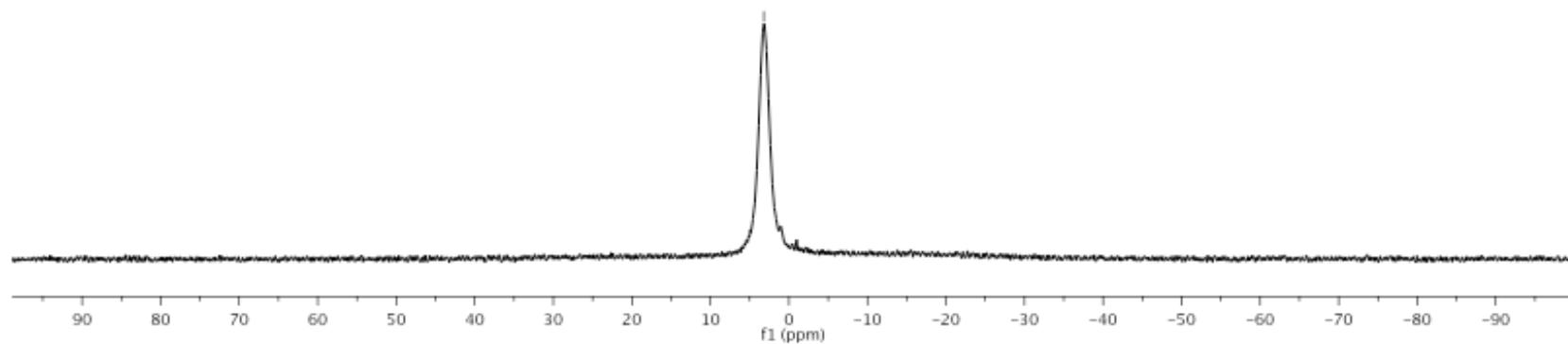
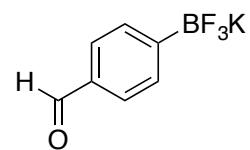
^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-formylphenyl)borate (2f, Table 2, entry 6)

-140.0

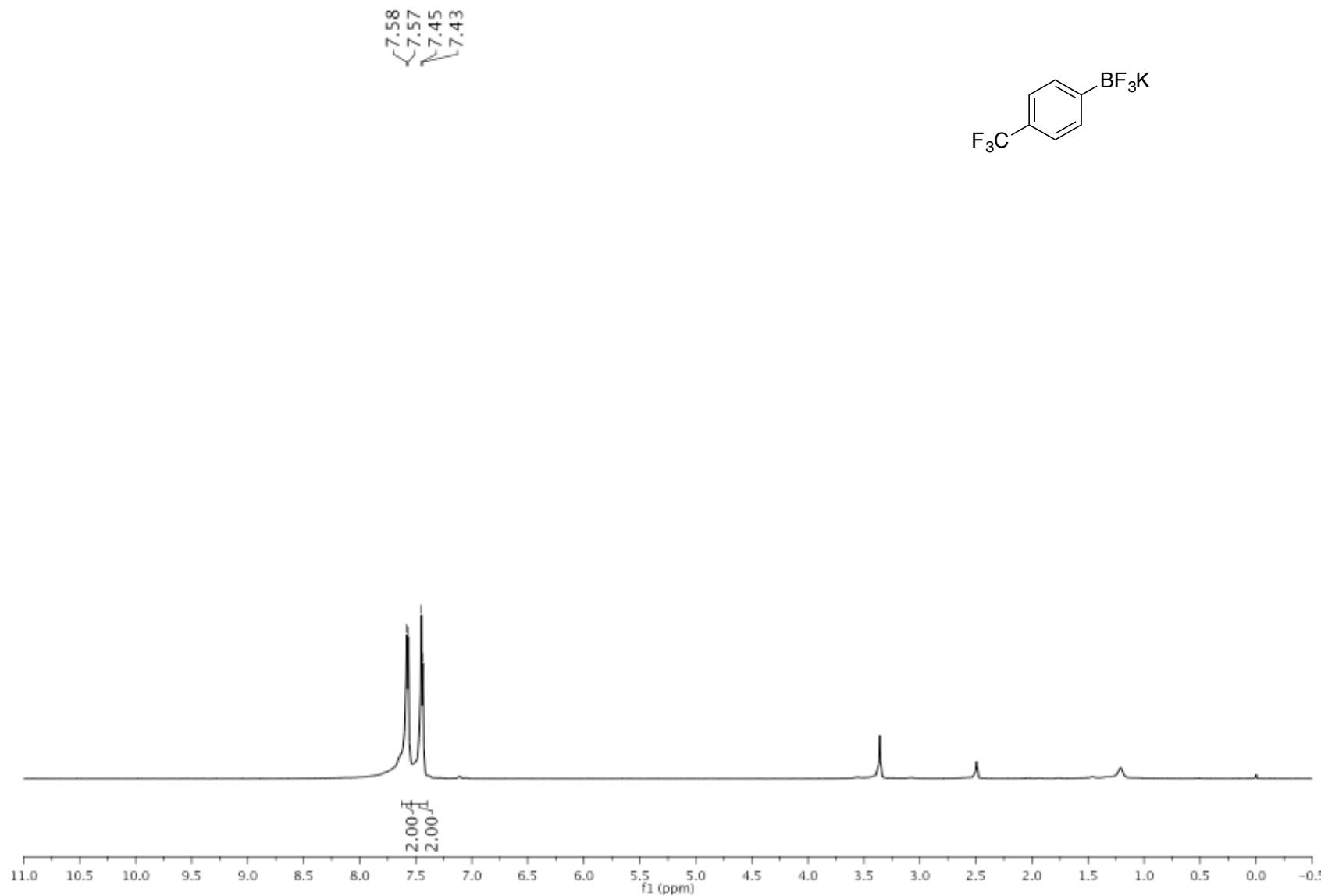


¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-formylphenyl)borate (2f, Table 2, entry 6)

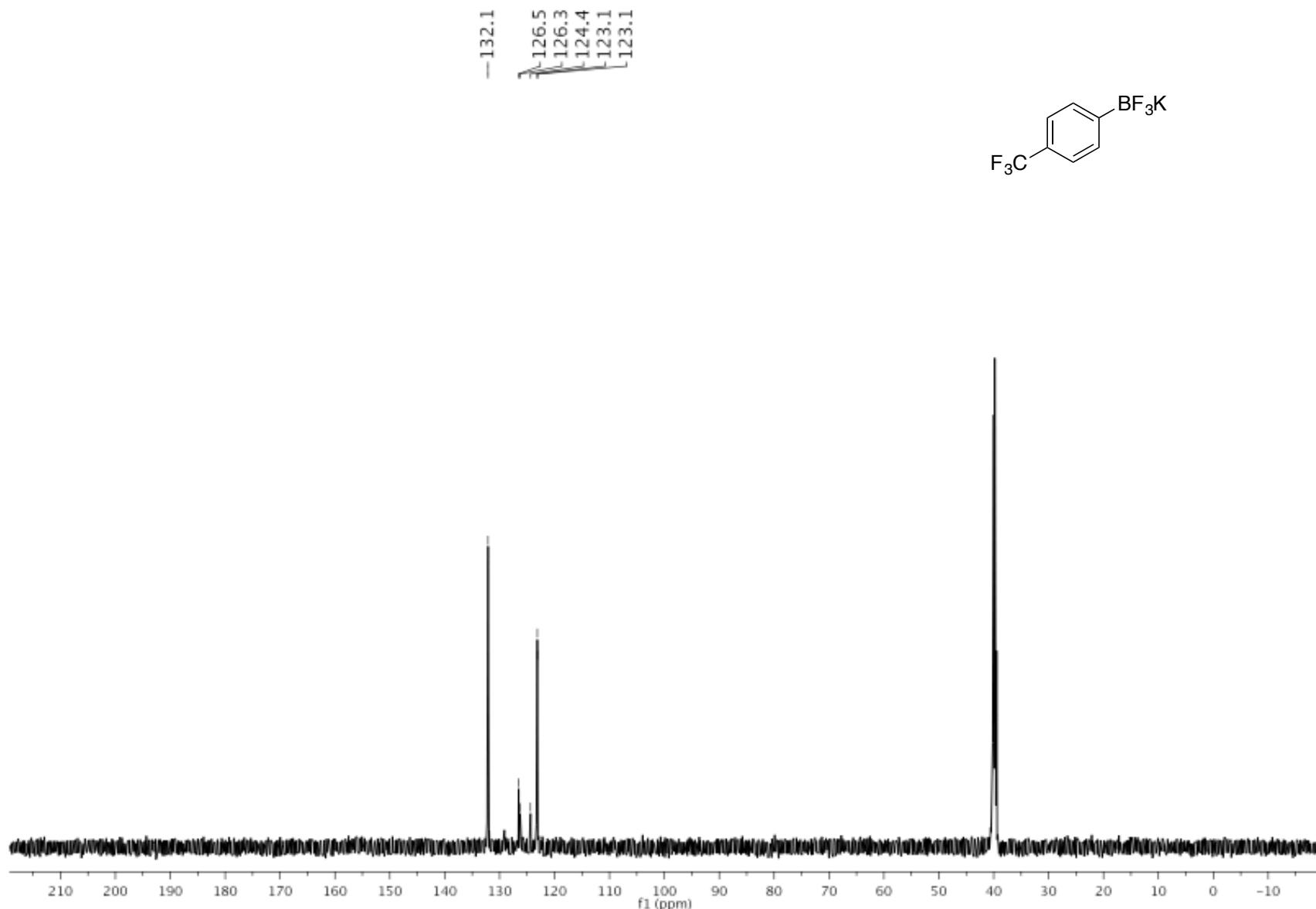
-3.2



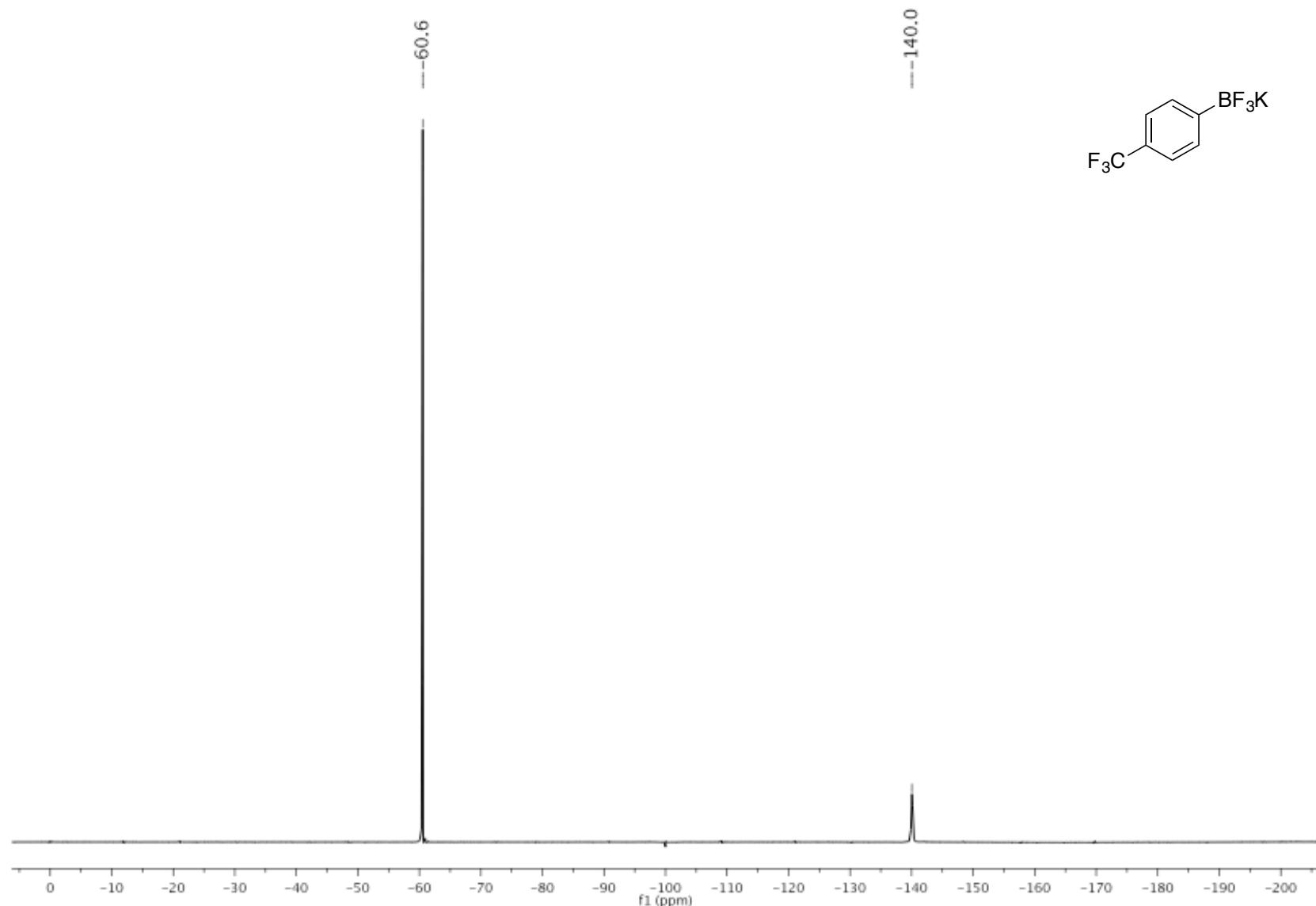
^{11}B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-formylphenyl)borate (2f, Table 2, entry 6)



^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(4-(trifluoromethyl)phenyl)borate (2g, Table 2, entry 7)

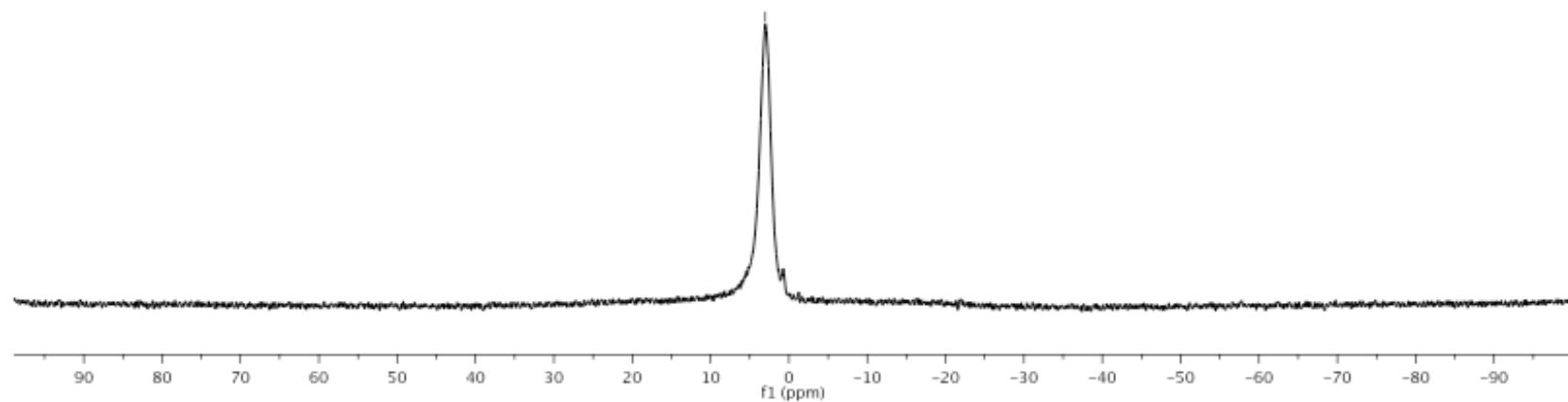
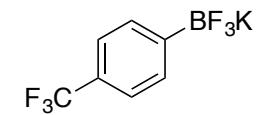


^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-(trifluoromethyl)phenyl)borate (2g, Table 2, entry 7)

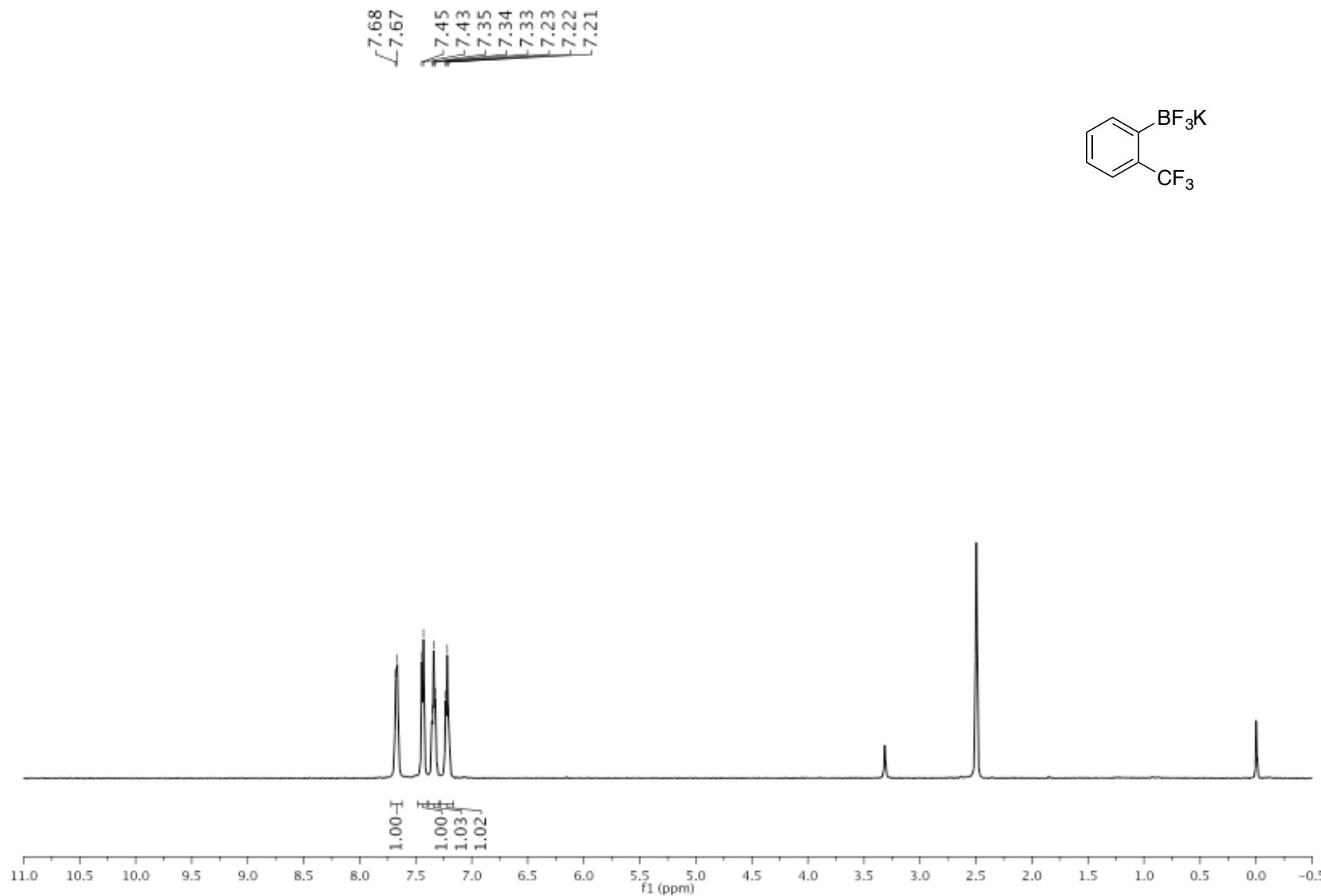


^{19}F NMR (470.8 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(4-(trifluoromethyl)phenyl)borate (2g, Table 2, entry 7)

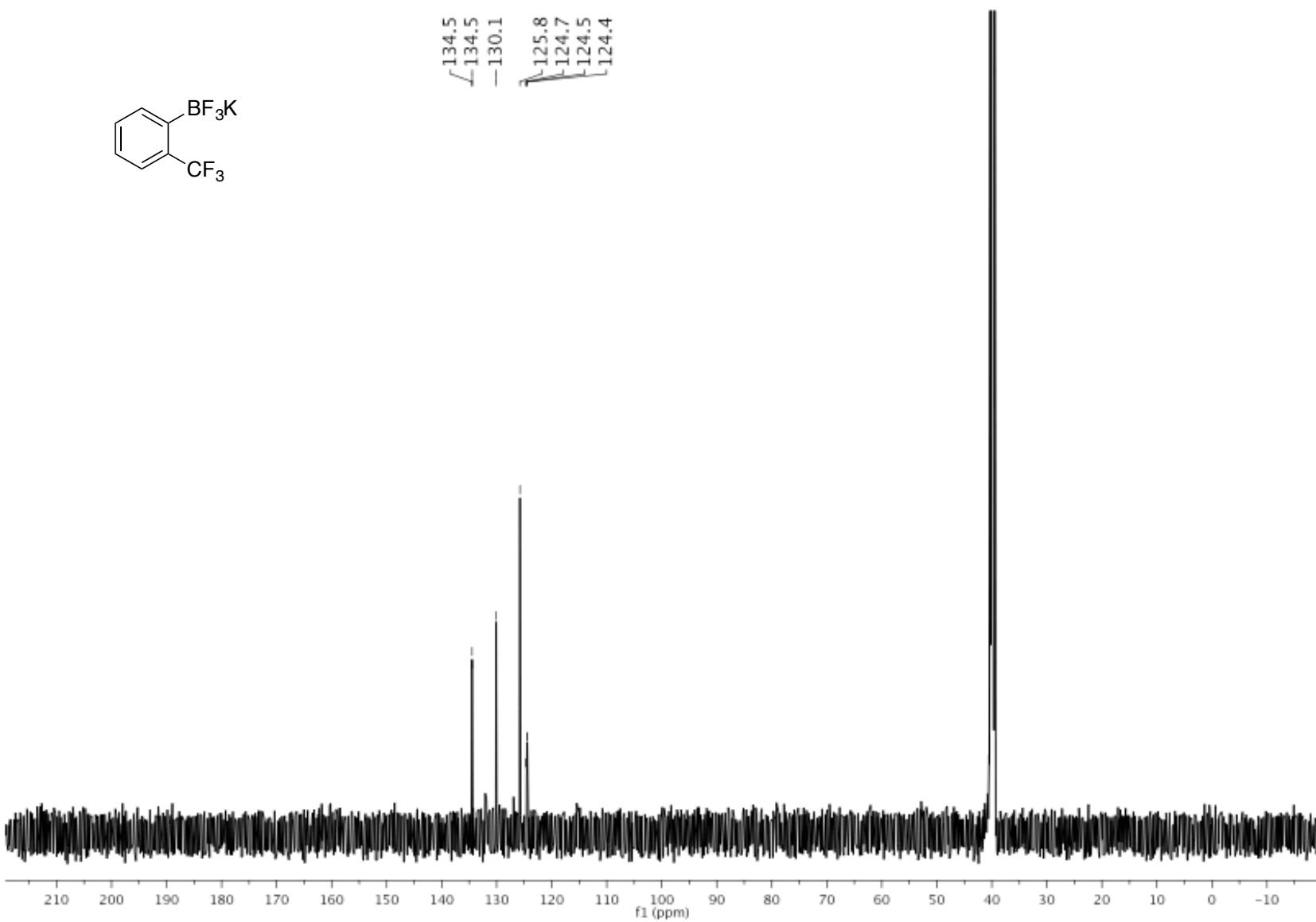
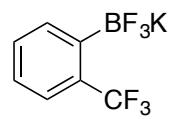
-3.0



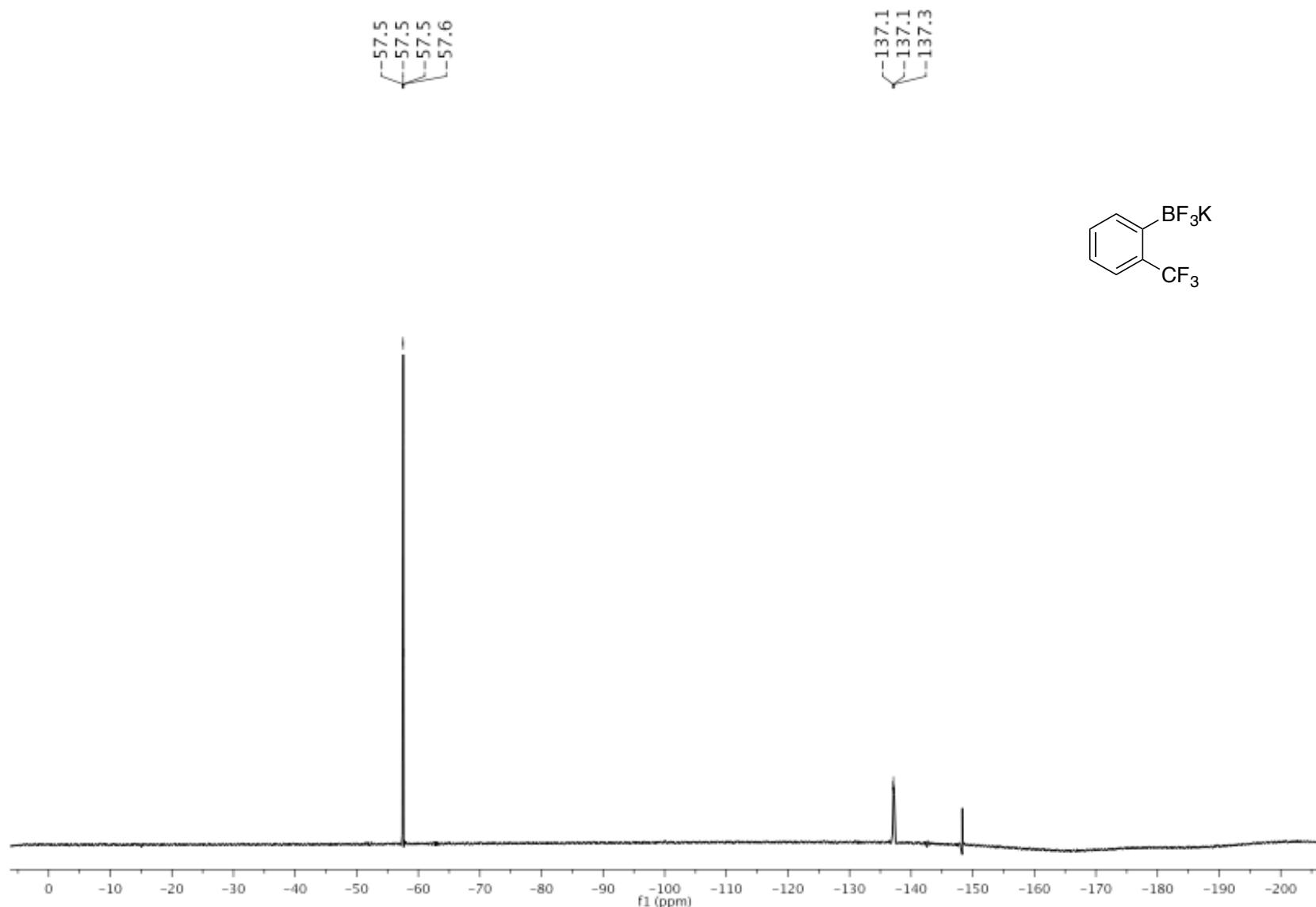
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-(trifluoromethyl)phenyl)borate (2g, Table 2, entry 7)



¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-(trifluoromethyl)phenyl)borate (2h, Table 2, entry 8)

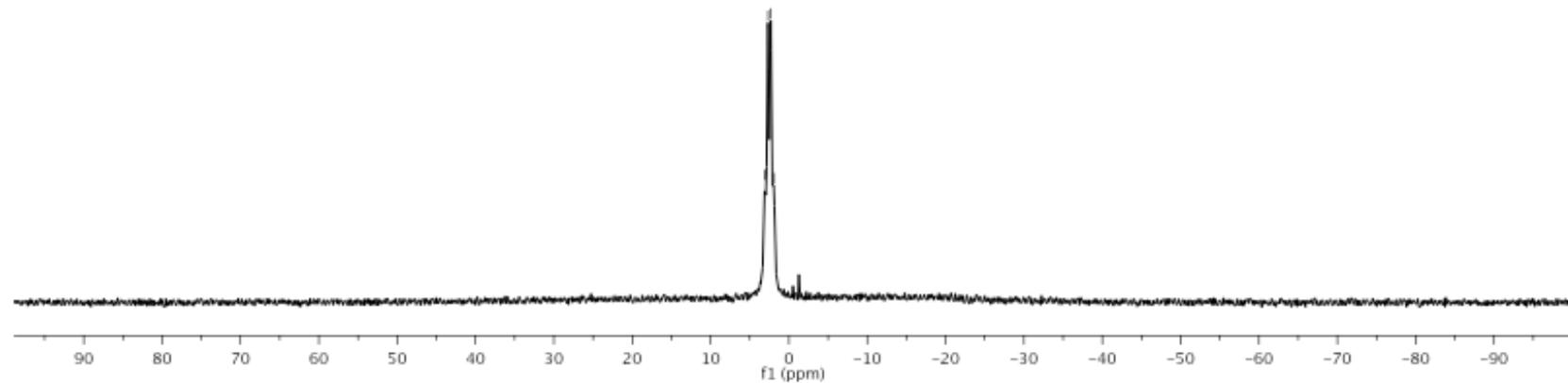
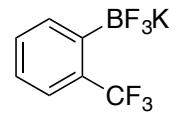


¹³C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-(trifluoromethyl)phenyl)borate (2h, Table 2, entry 8)



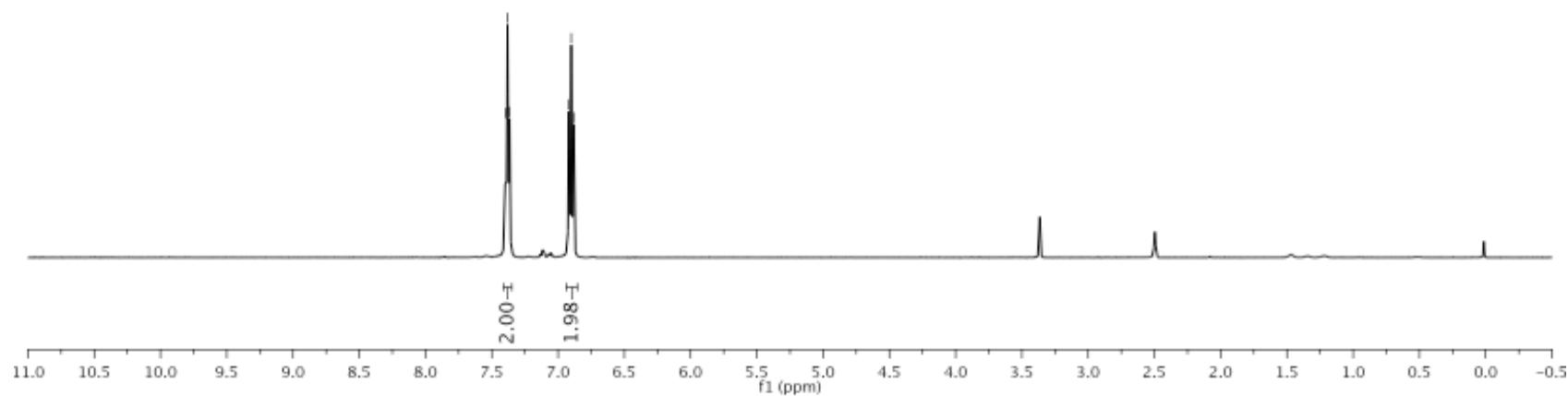
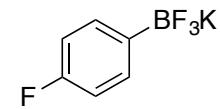
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-(trifluoromethyl)phenyl)borate (2h, Table 2, entry 8)

3.06
2.69
2.31
1.93

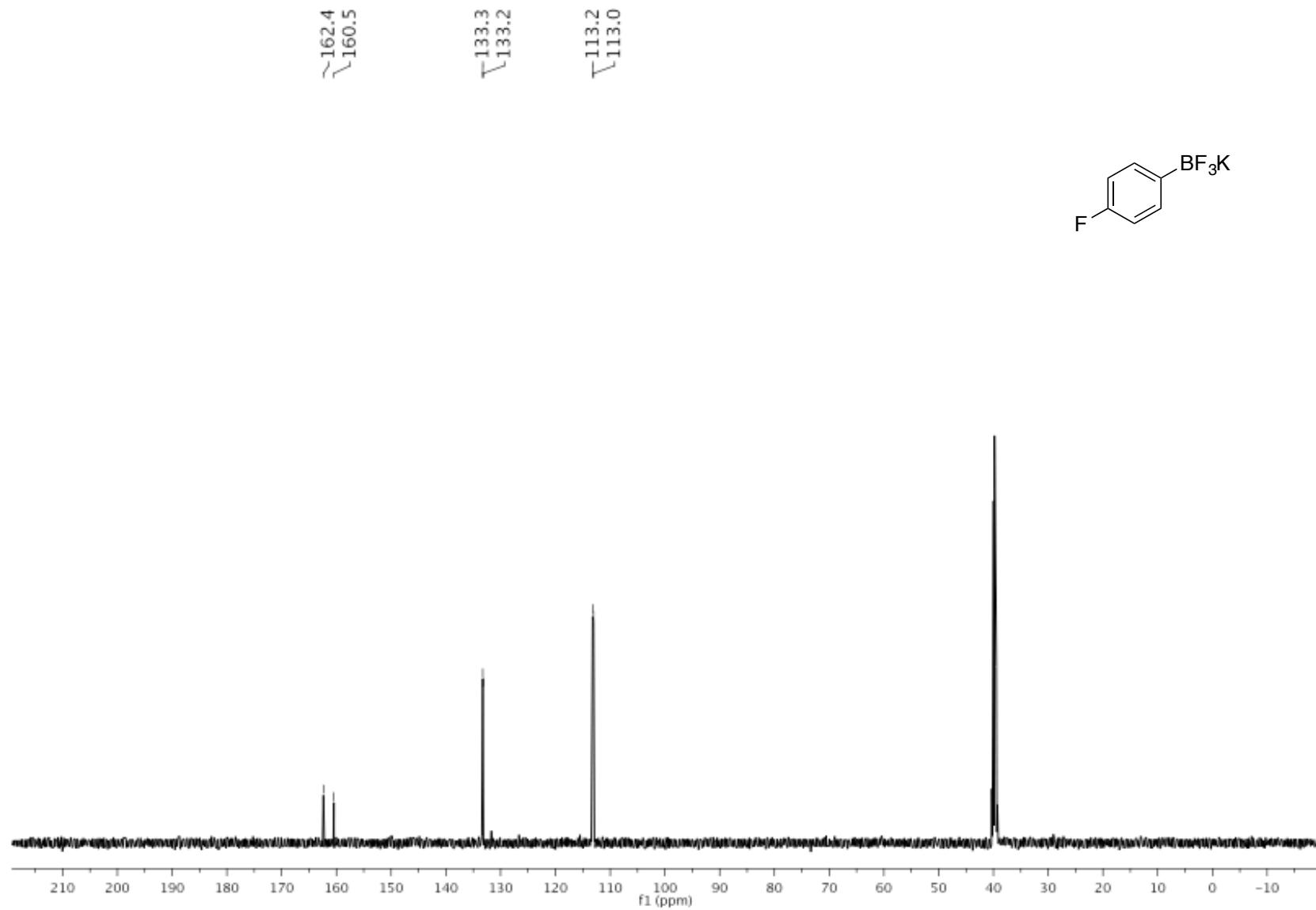


¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-(trifluoromethyl)phenyl)borate (2h, Table 2, entry 8)

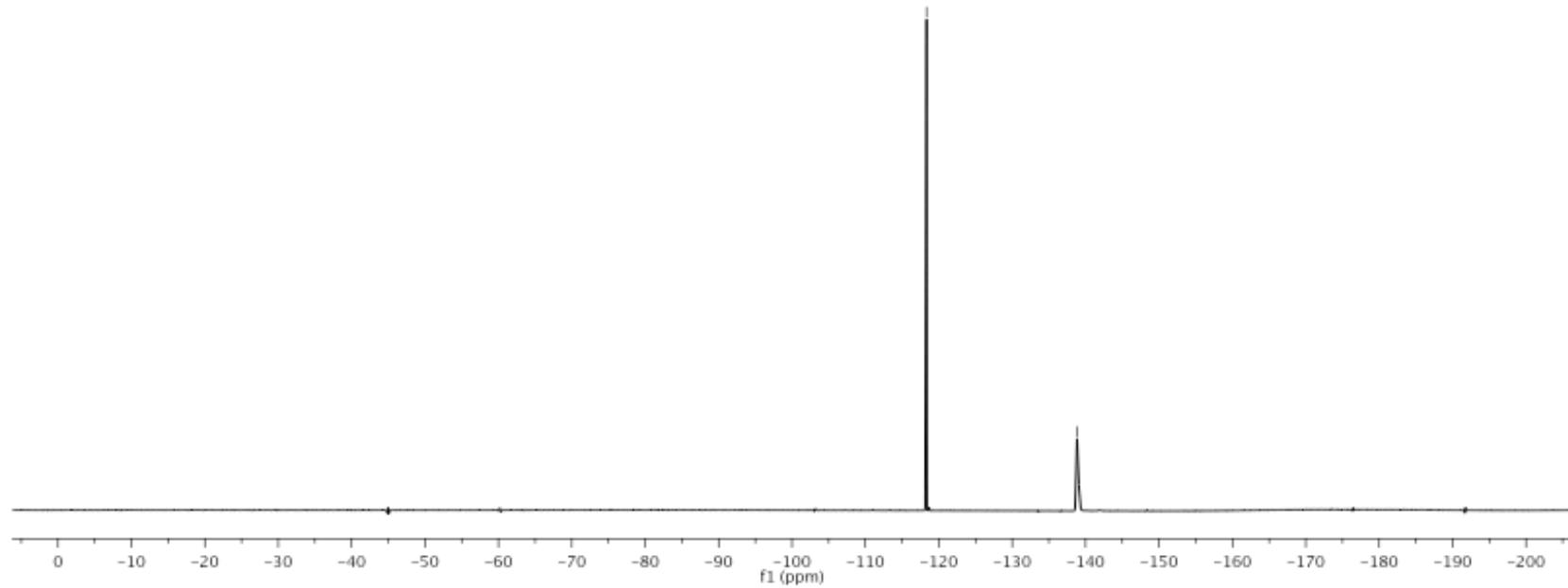
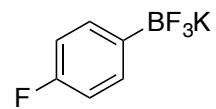
7.40
7.38
7.37
6.92
6.90
6.88



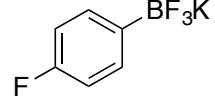
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-fluorophenyl)borate (2i, Table 2, entry 9)



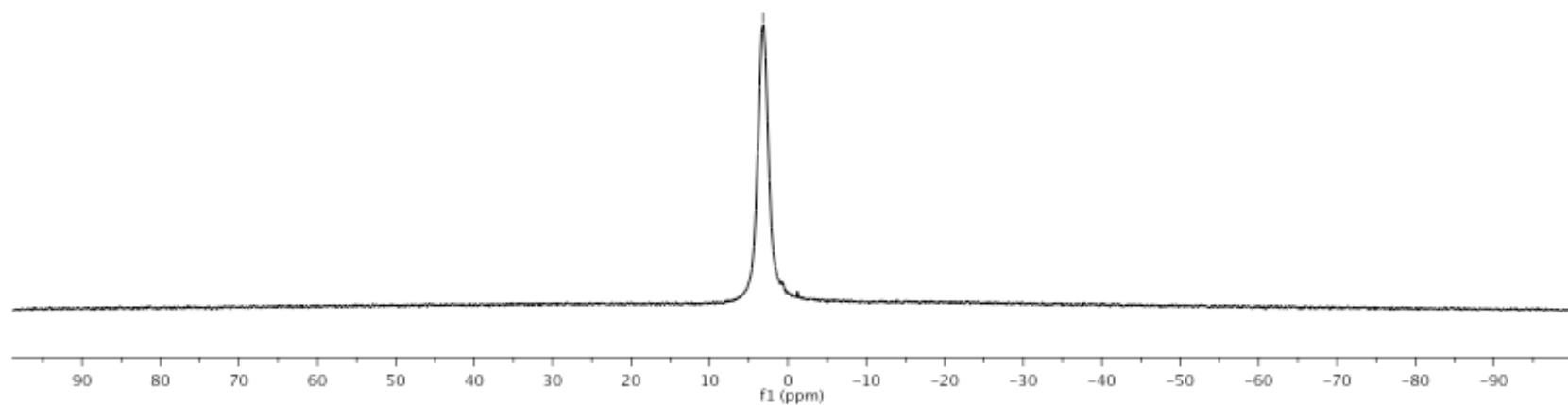
^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-fluorophenyl)borate (2i, Table 2, entry 9)



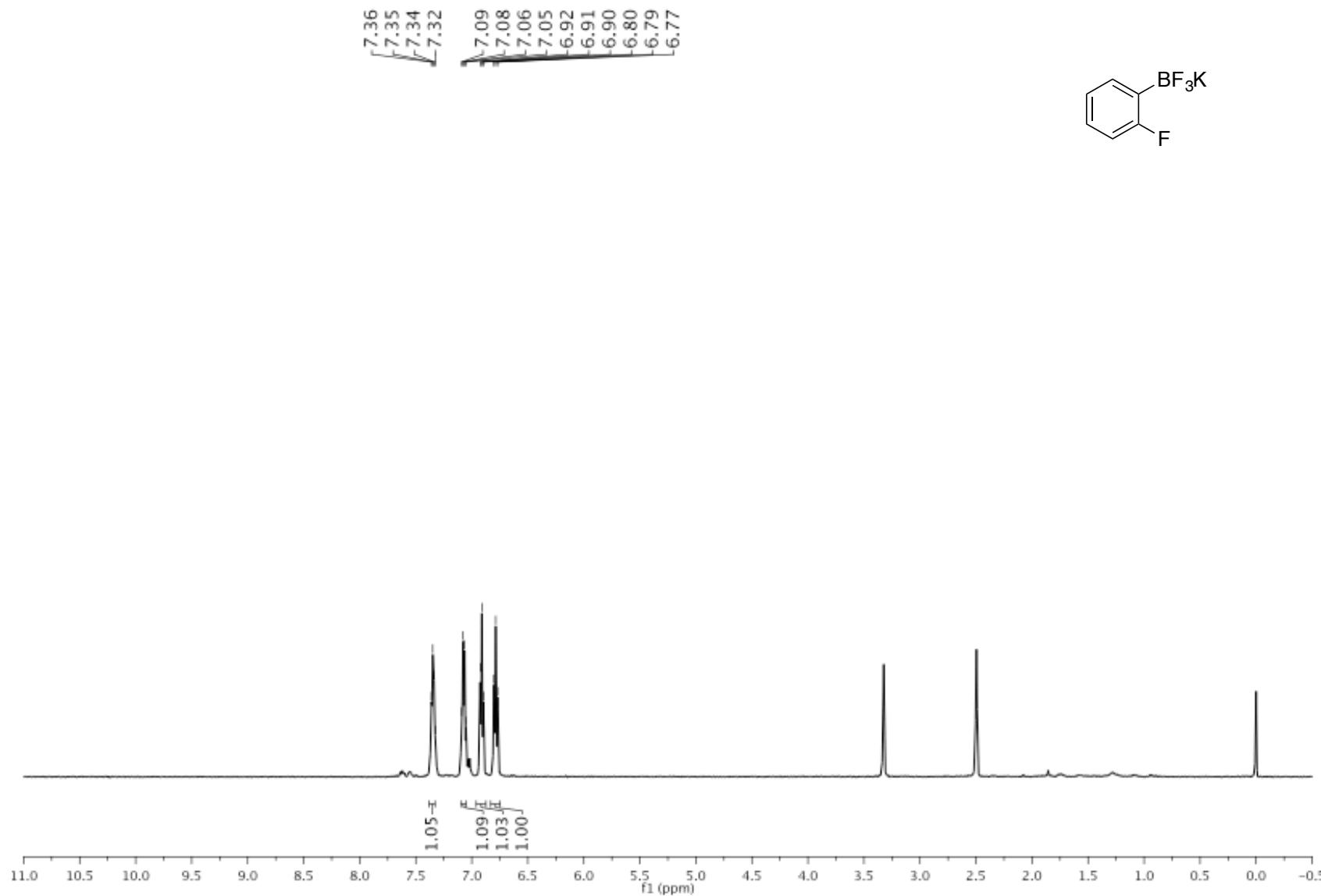
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-fluorophenyl)borate (2i, Table 2, entry 9)



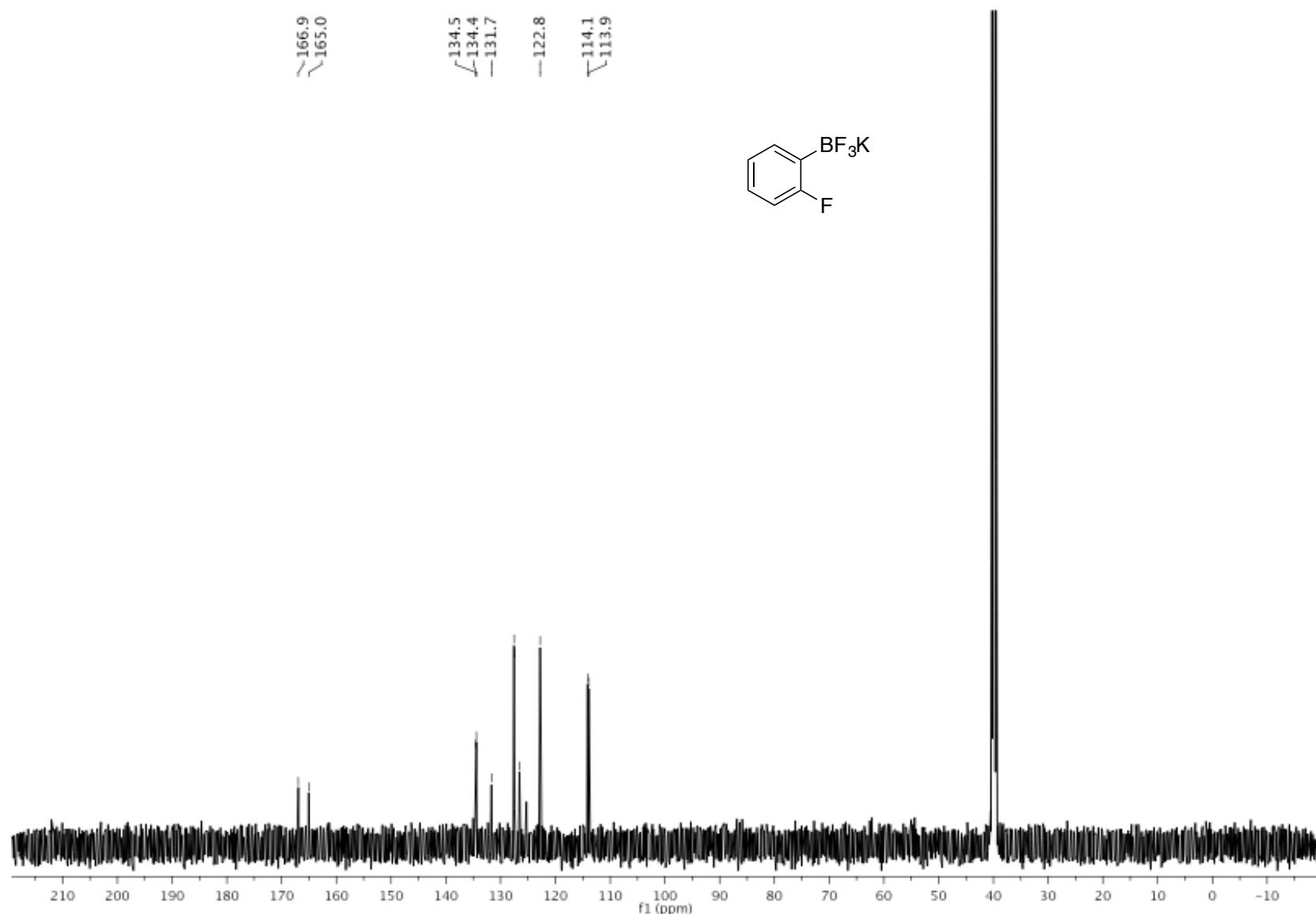
-3.2



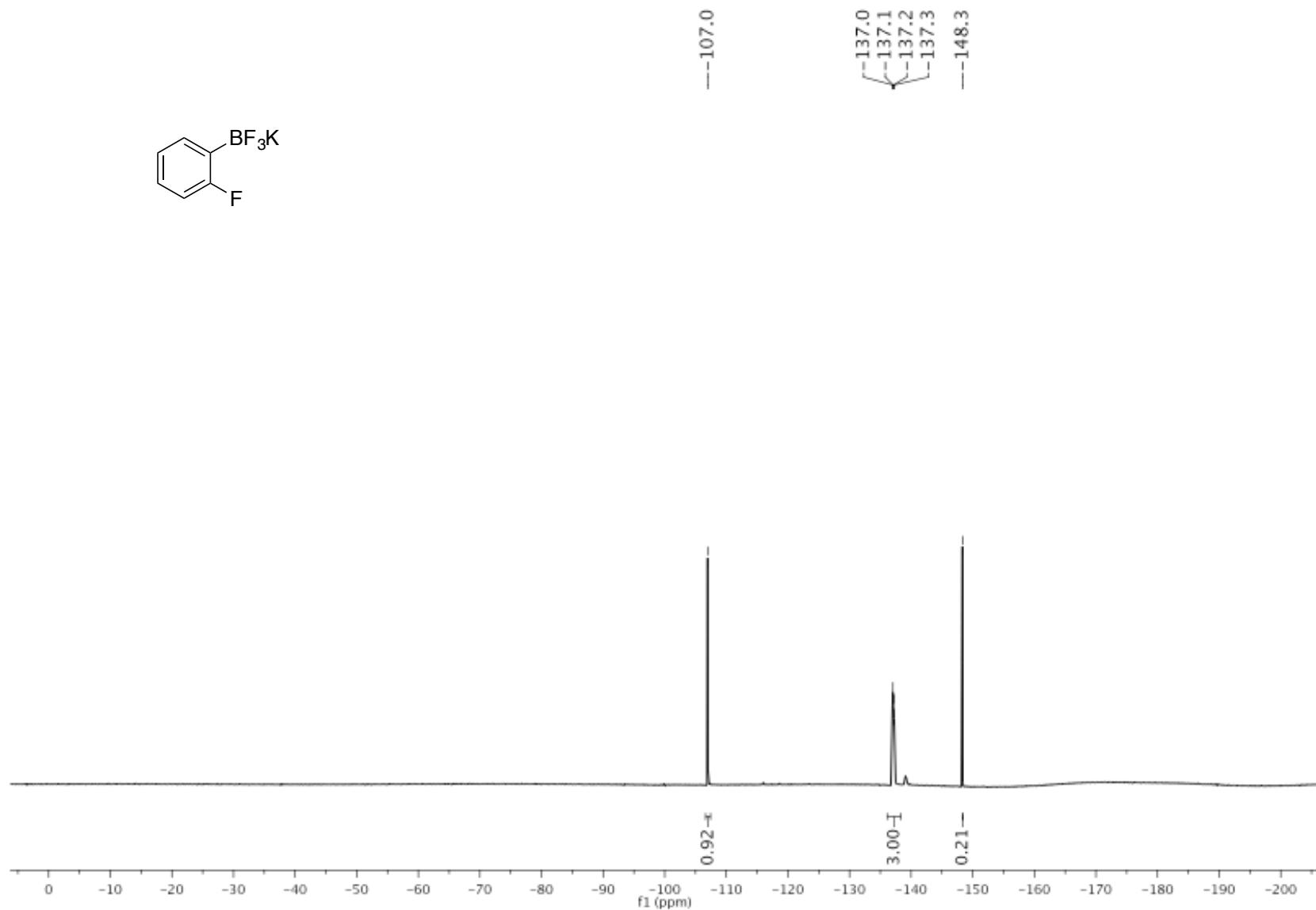
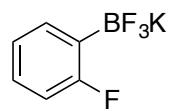
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-fluorophenyl)borate (2i, Table 2, entry 9)



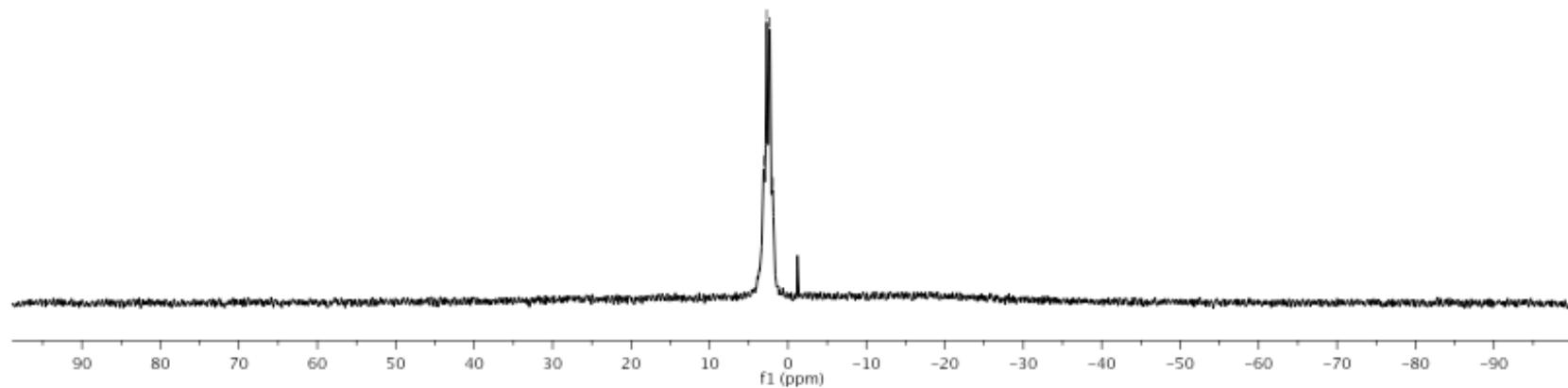
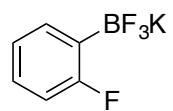
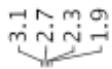
^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(2-fluorophenyl)borate (2j, Table 2, entry 10)



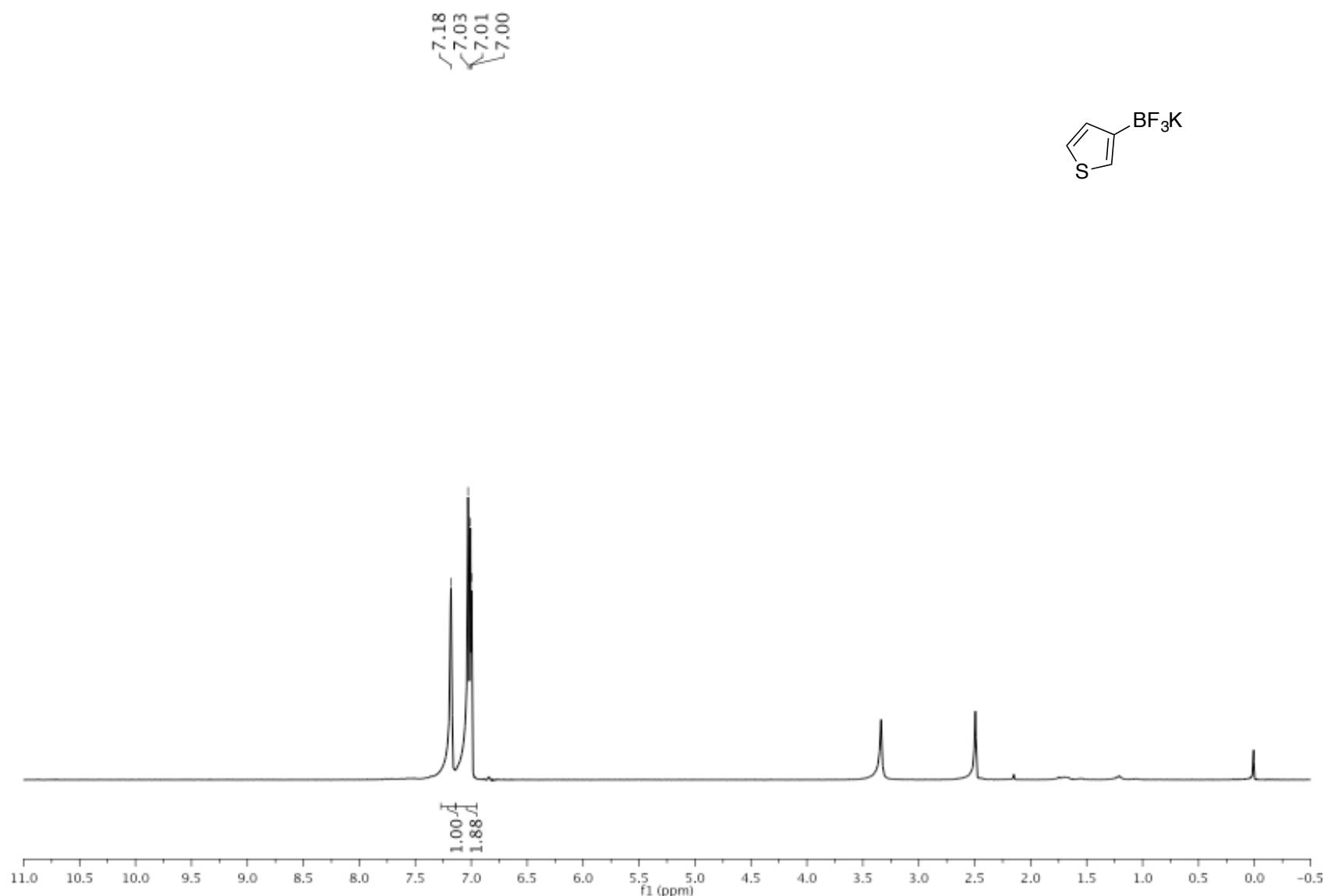
¹³C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-fluorophenyl)borate (2j, Table 2, entry 10)



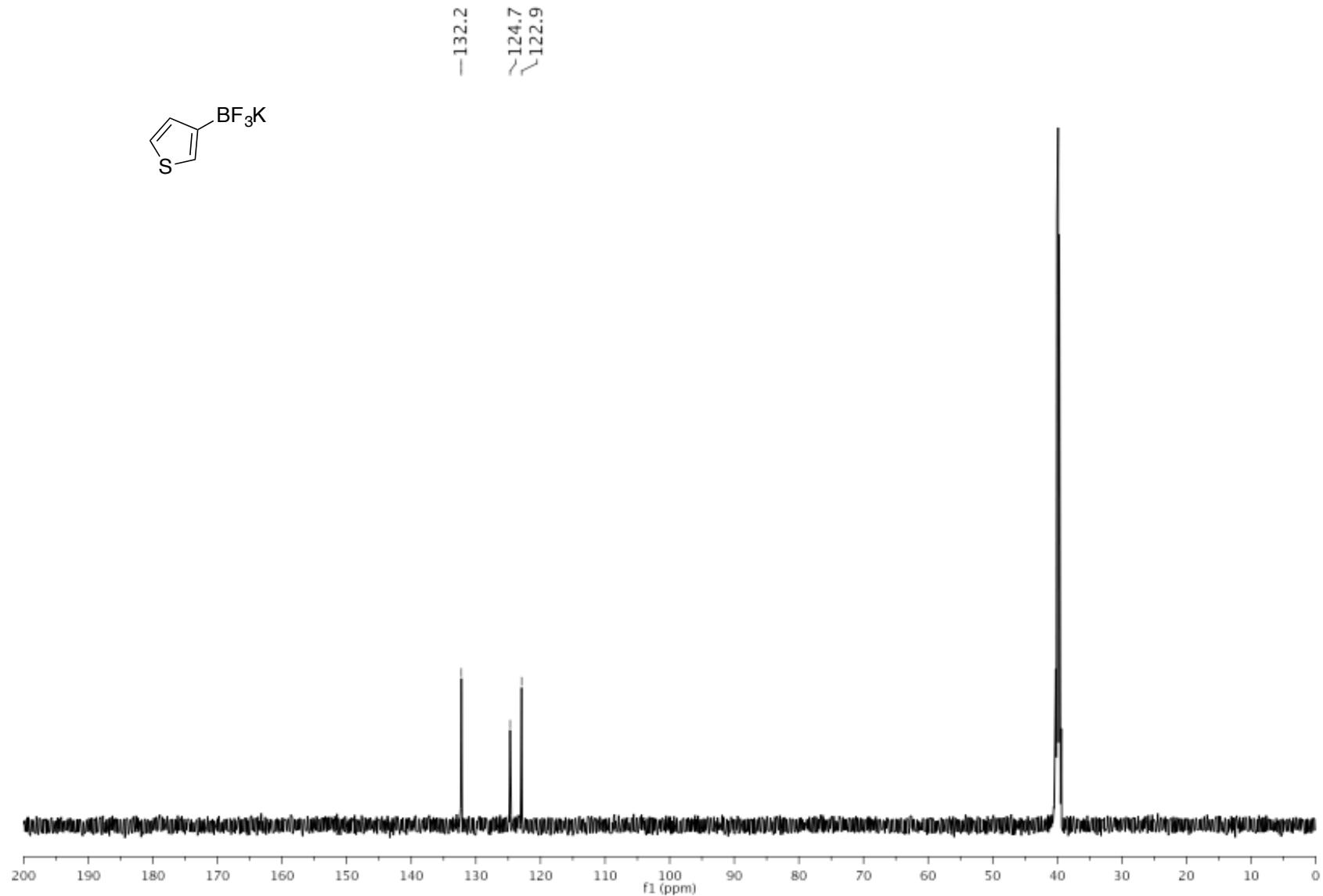
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-fluorophenyl)borate (2j, Table 2, entry 10)



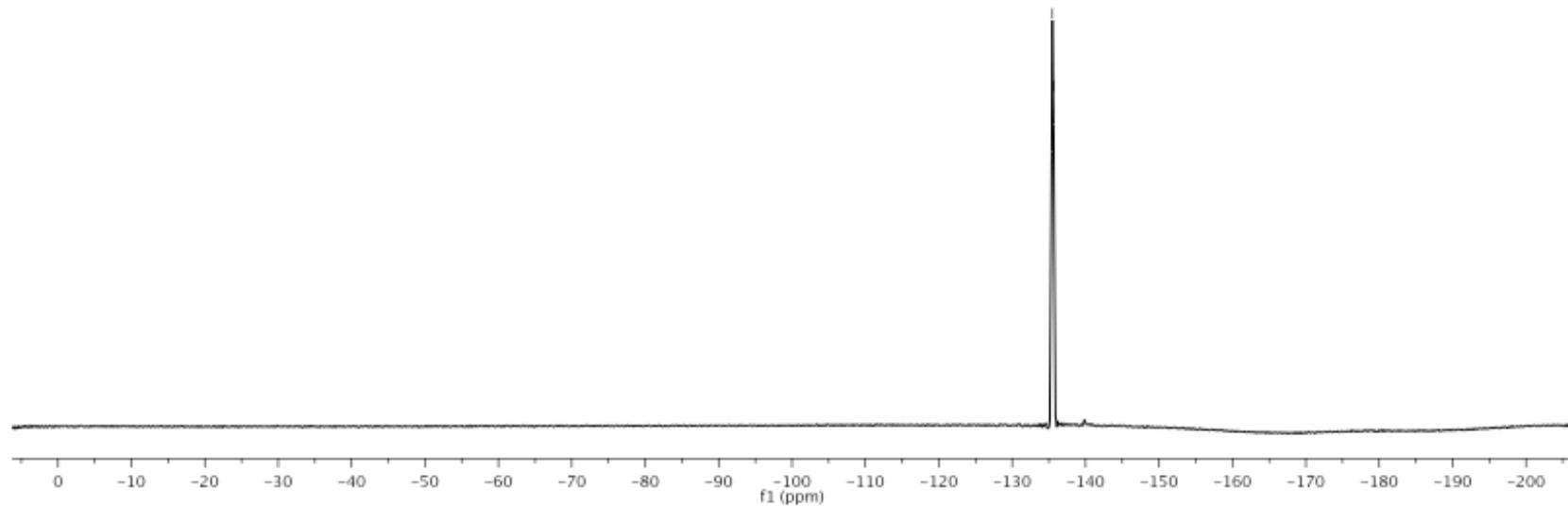
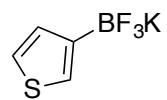
^{11}B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-fluorophenyl)borate (2j, Table 2, entry 10)



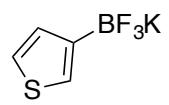
^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(thien-3-yl)borate (3a, Table 3, entry 1)



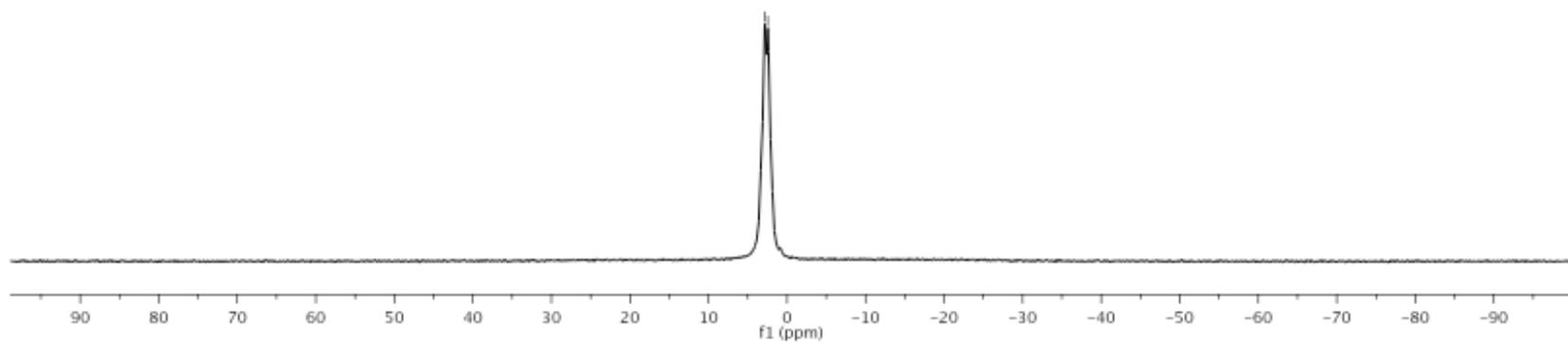
^{13}C NMR (128.5 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(thien-3-yl)borate (3a, Table 3, entry 1)



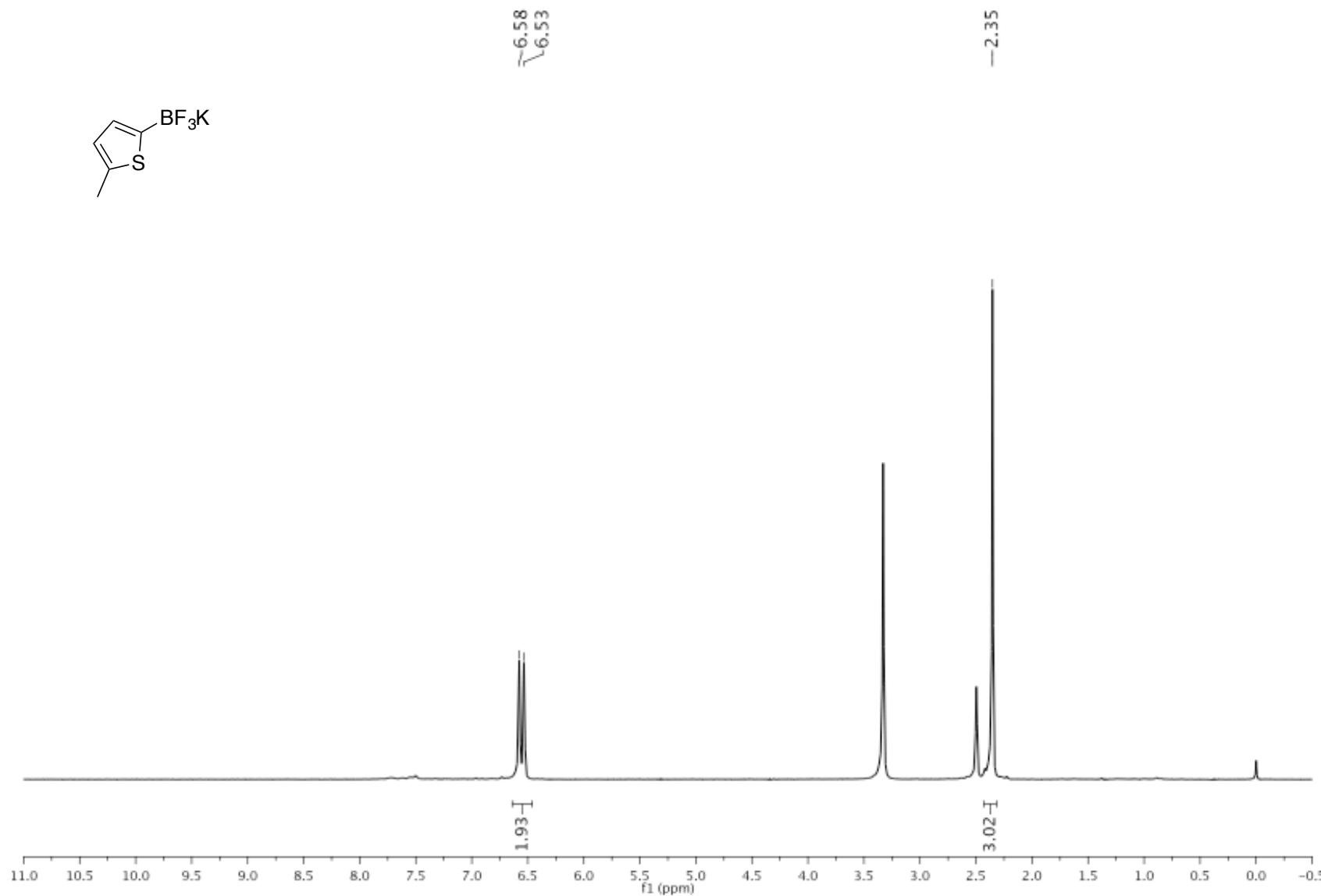
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(thien-3-yl)borate (3a, Table 3, entry 1)



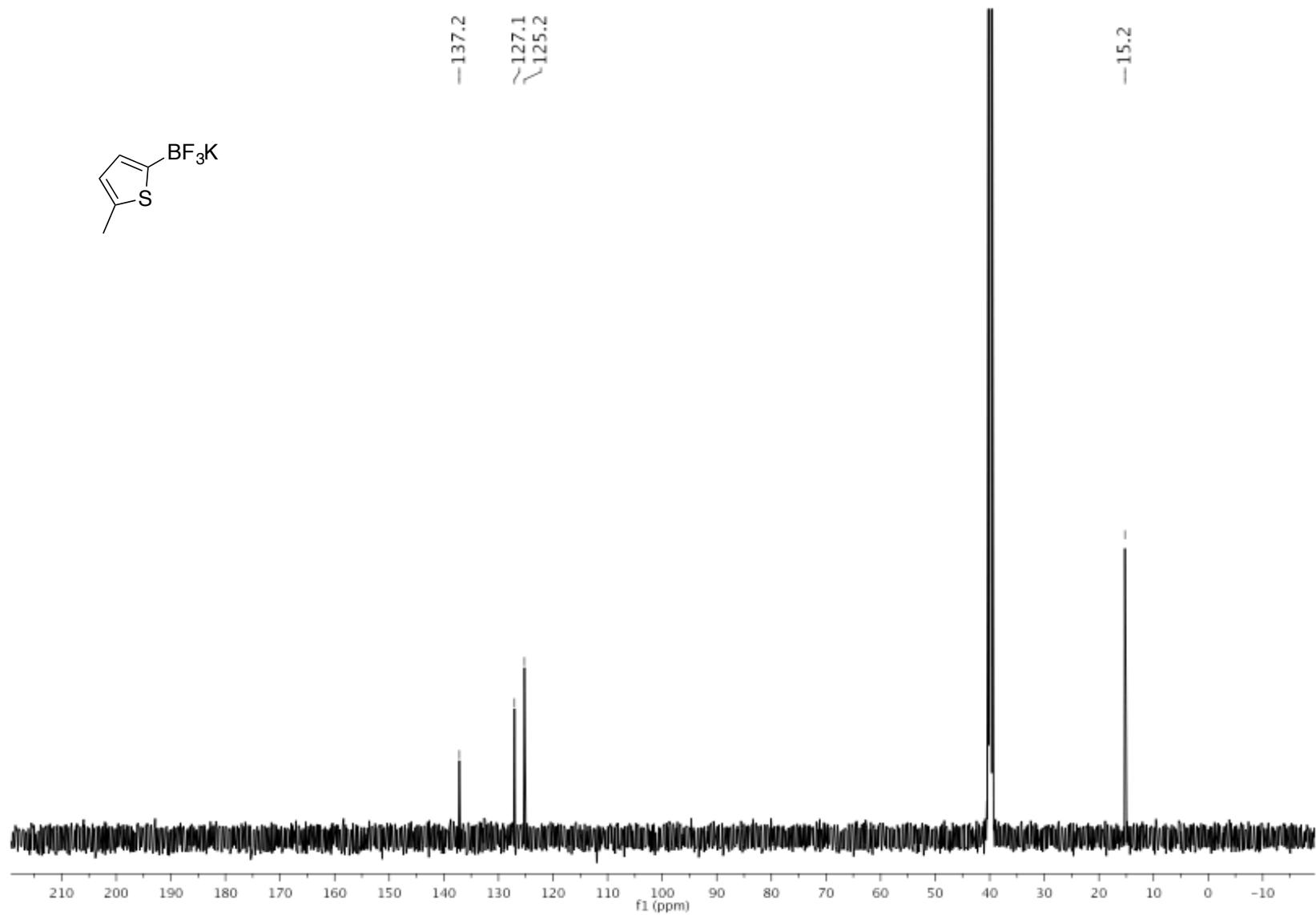
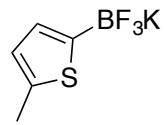
2.8
2.4



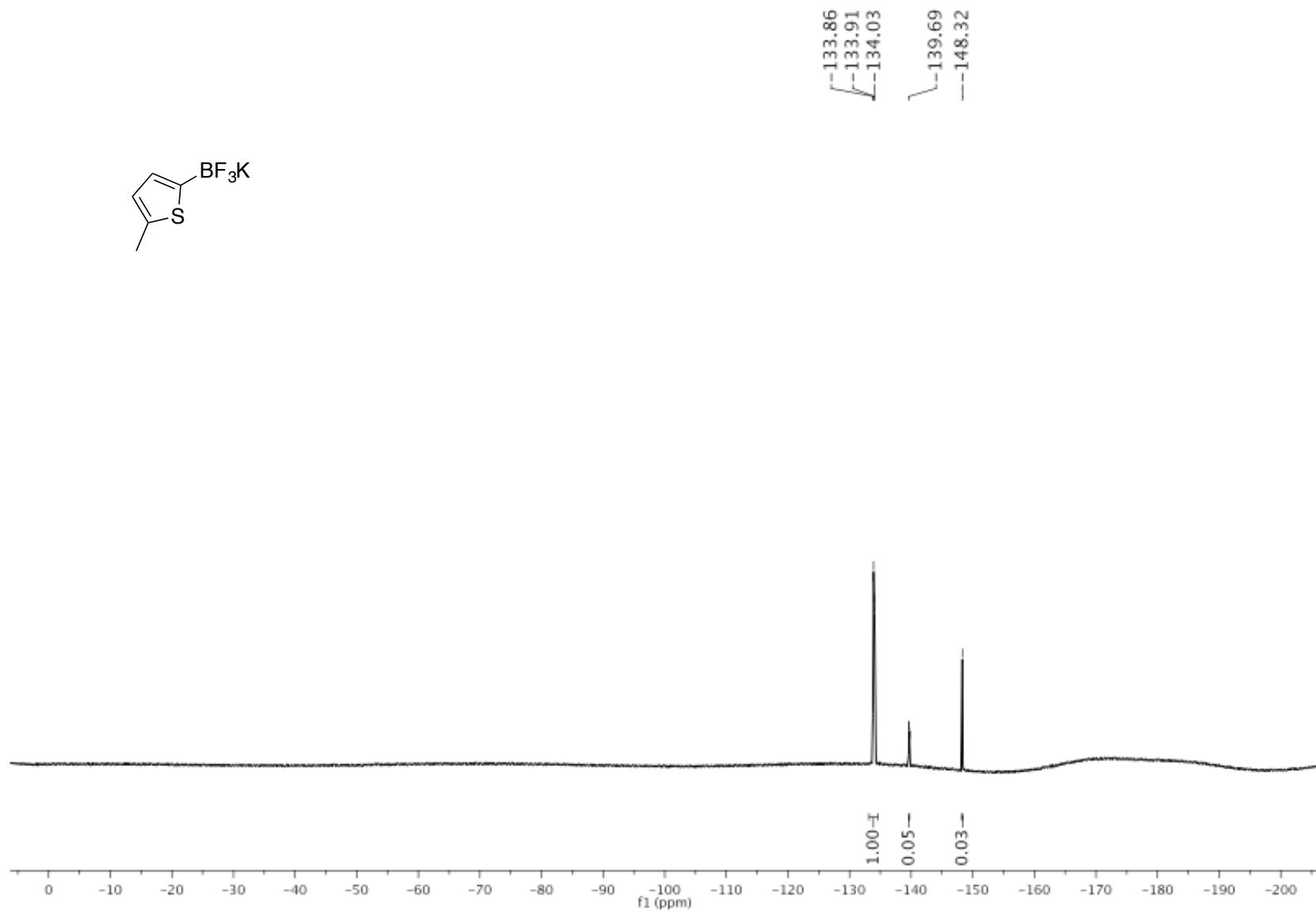
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(thien-3-yl)borate (3a, Table 3, entry 1)



¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(5-methylthien-2-yl)borate (3b, Table 3, entry 2)

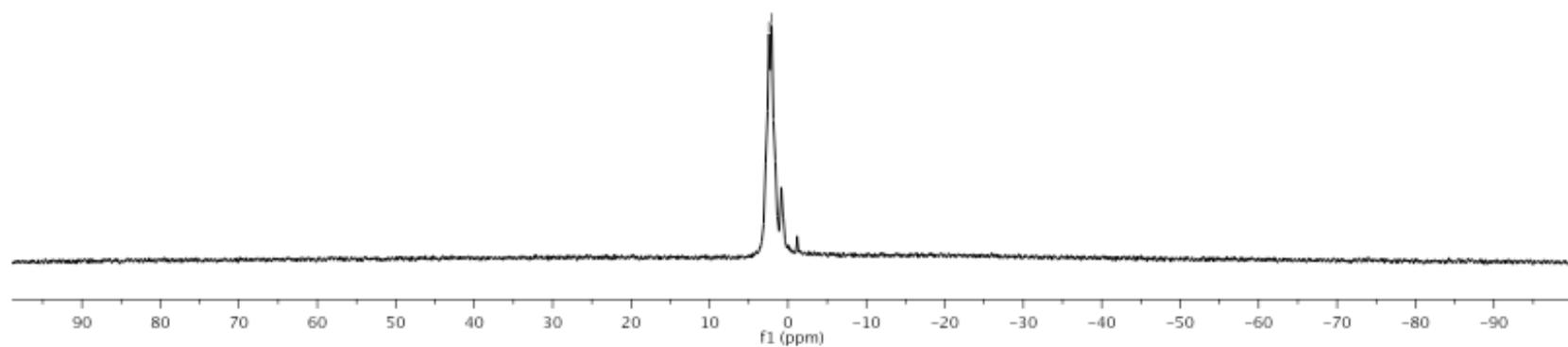
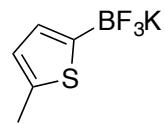


¹³C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(5-methylthien-2-yl)borate (3b, Table 3, entry 2)

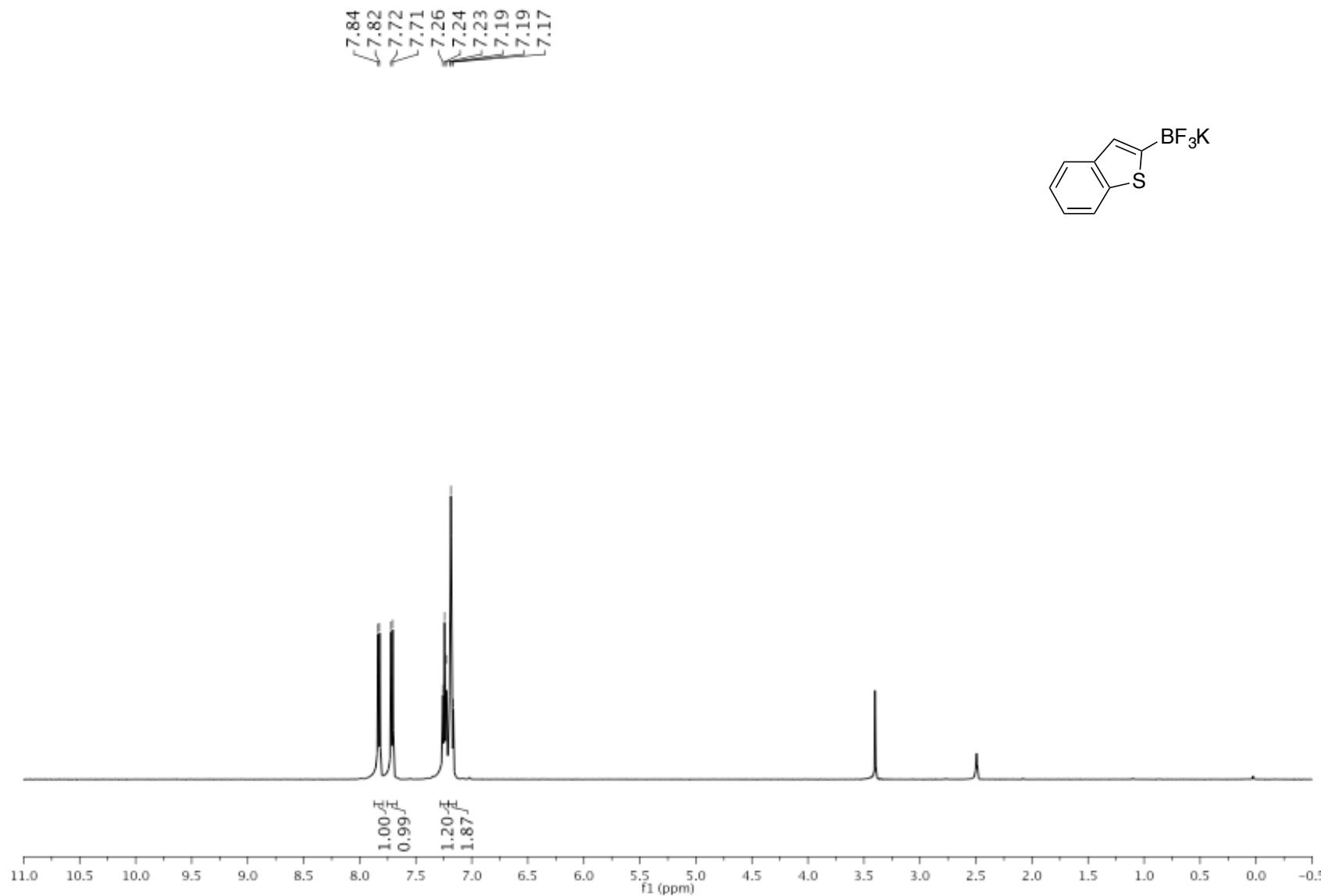


¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(5-methylthien-2-yl)borate (3b, Table 3, entry 2)

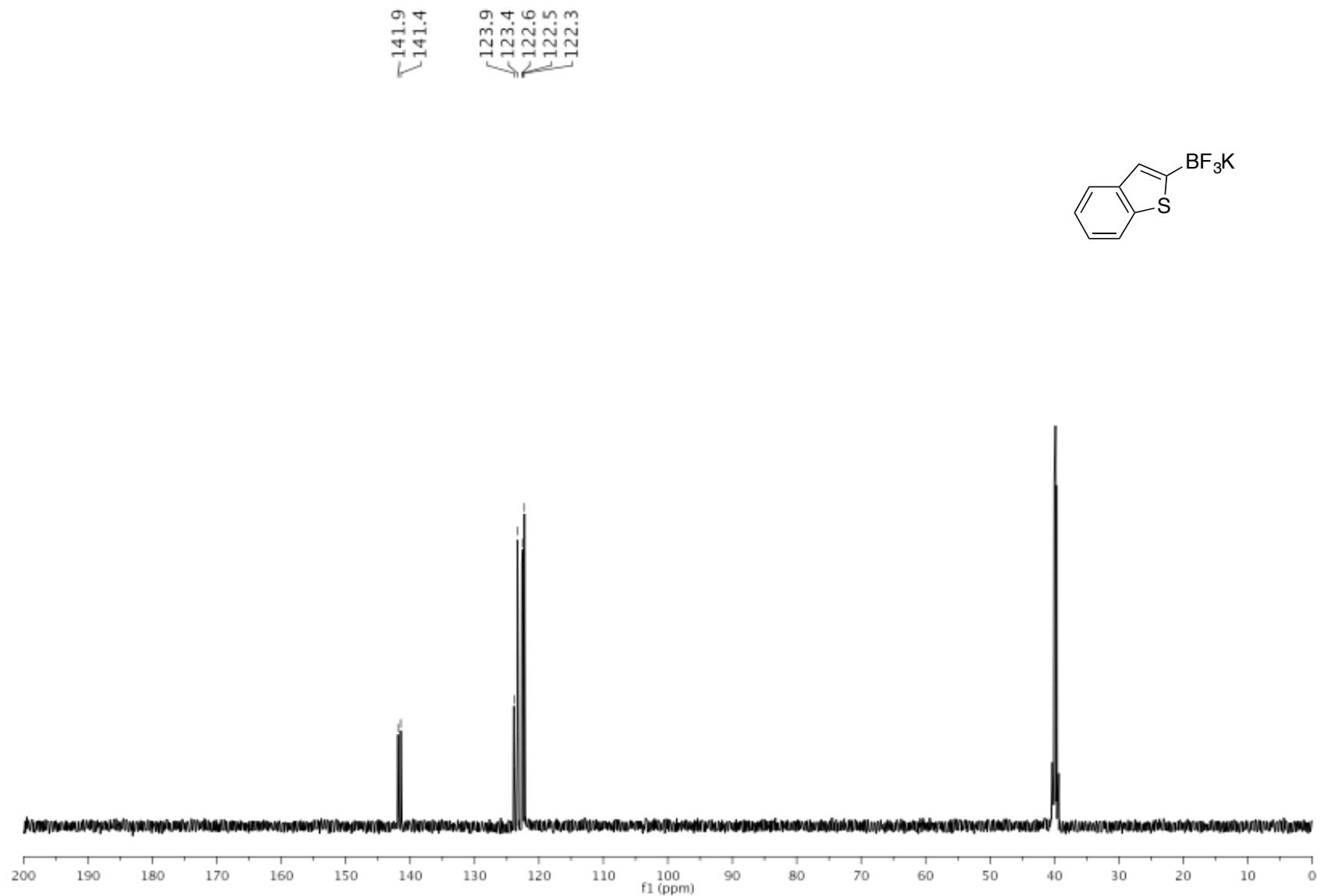
$\sqrt{2.4}$
 $\sqrt{2.1}$



^{11}B NMR (128.4 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(5-methylthien-2-yl)borate (3b, Table 3, entry 2)

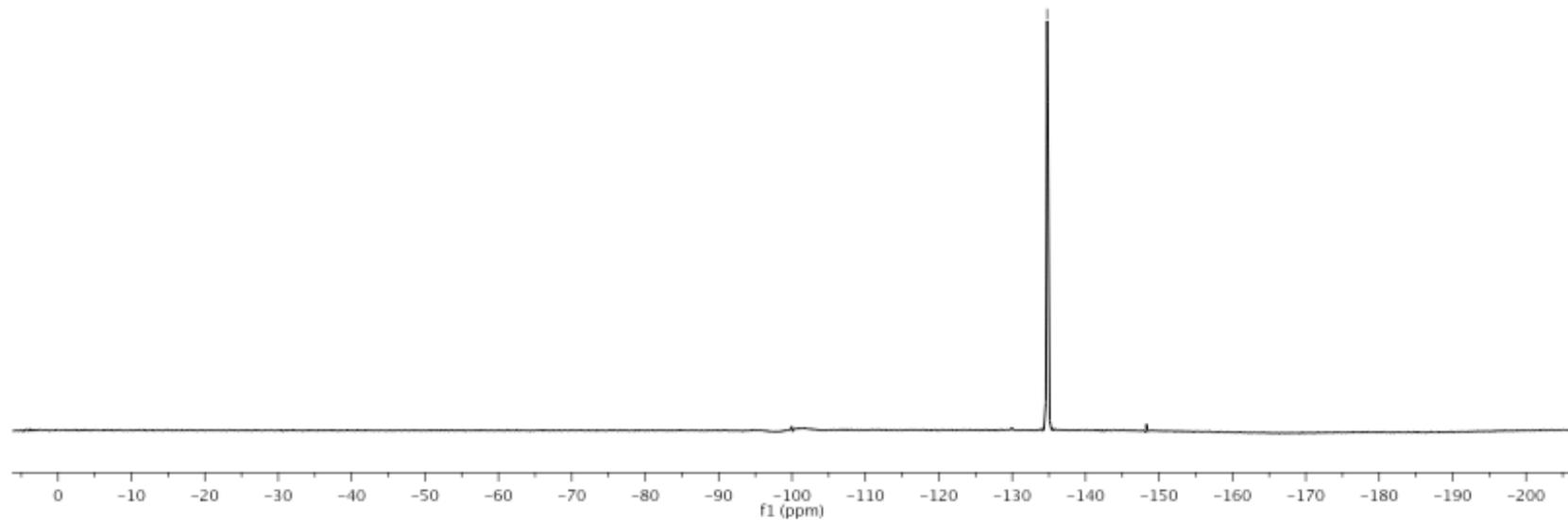
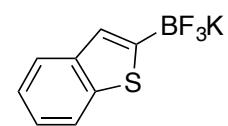


^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Benzo[b]thien-2-yltrifluoroborate (3c, Table 3, entry 3)



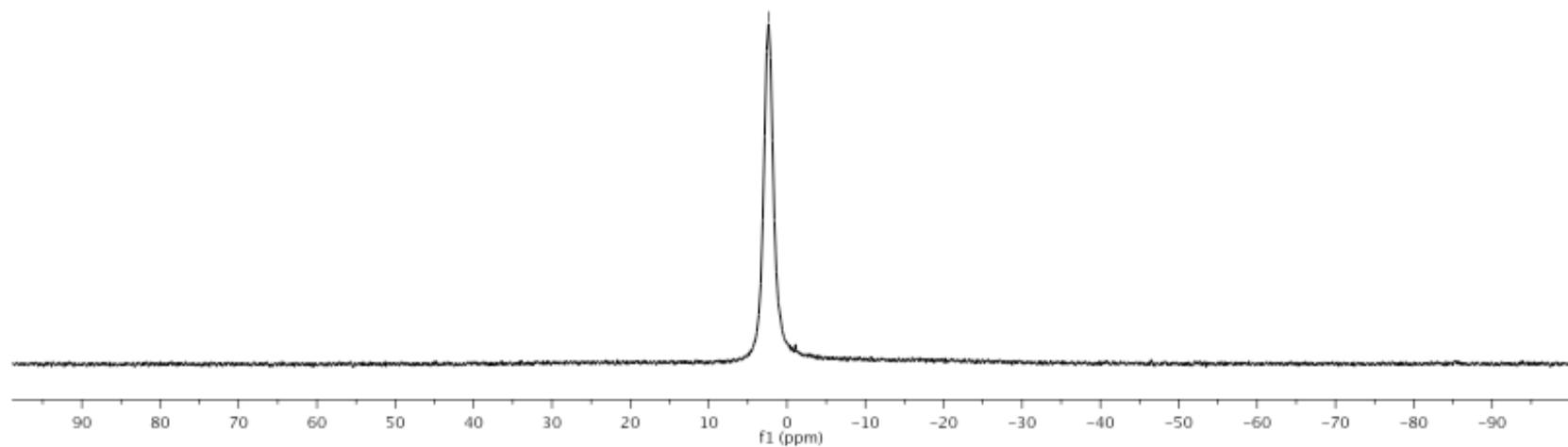
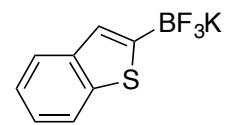
^{13}C NMR (128.5 MHz, DMSO-d_6) Spectrum of Potassium Benzo[*b*]thien-2-yltrifluoroborate (**3c**, Table 3, entry 3)

—134.8

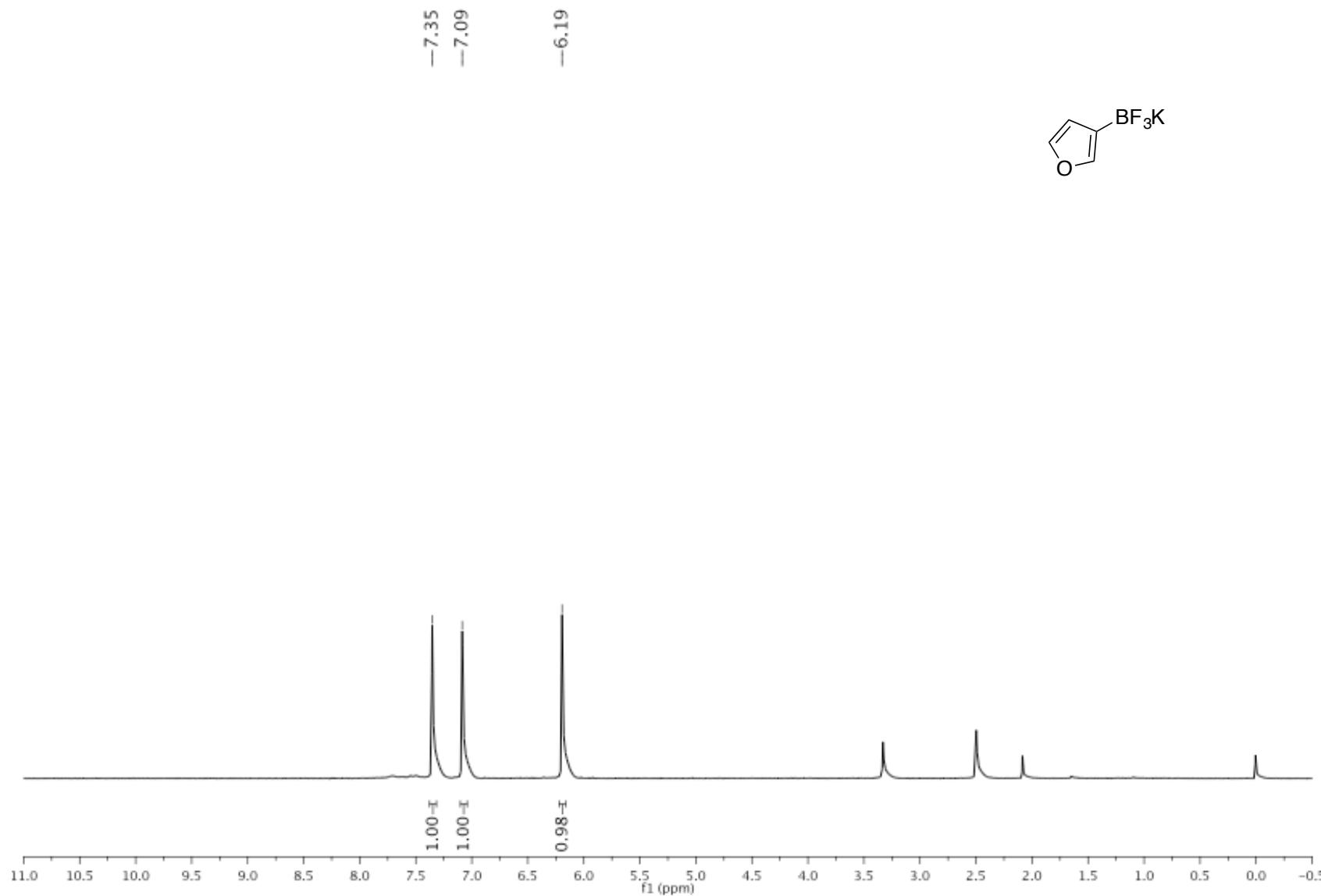


^{19}F NMR (470.8 MHz, DMSO- d_6) Spectrum of Potassium Benzo[*b*]thien-2-yltrifluoroborate (**3c**, Table 3, entry 3)

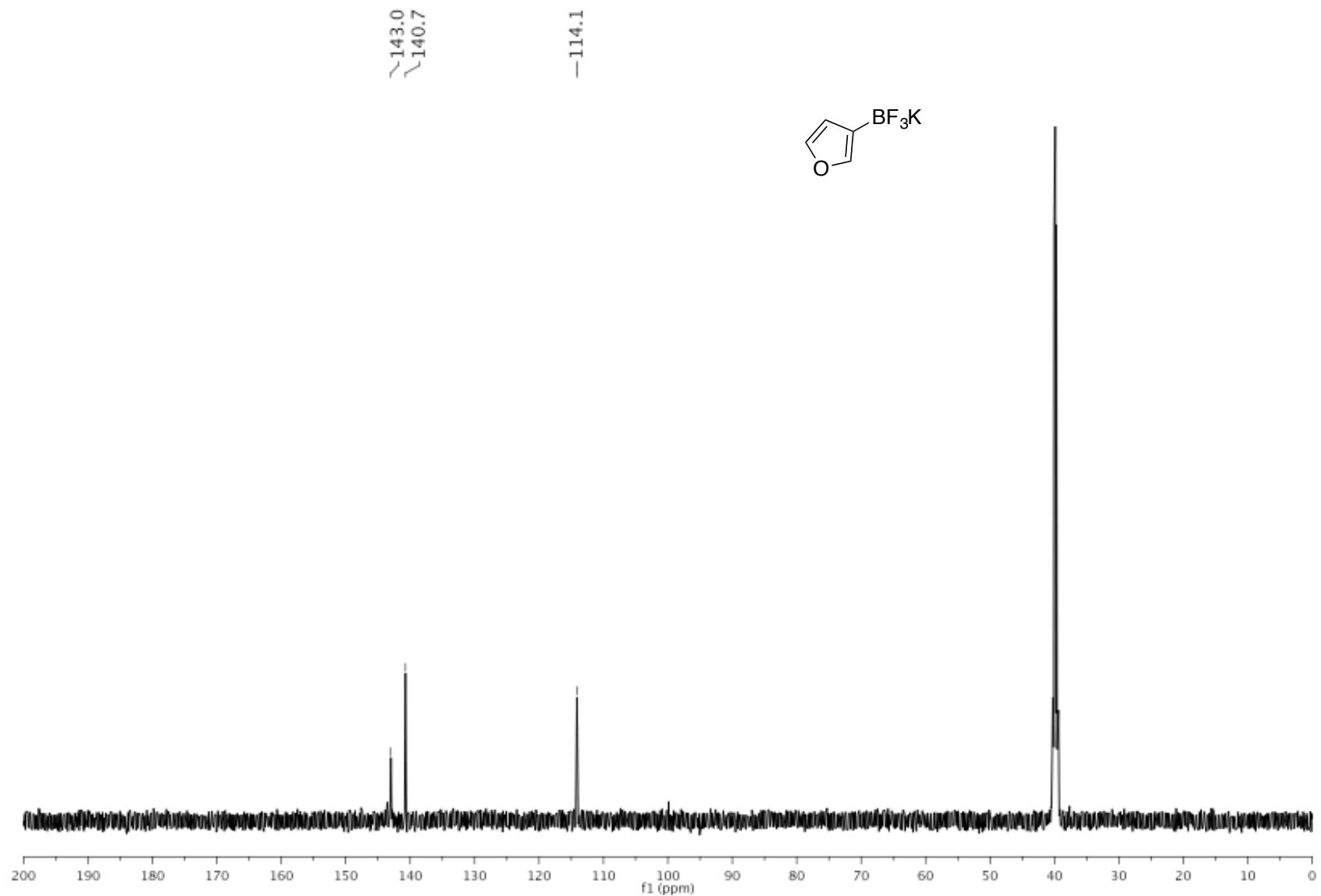
-2.4



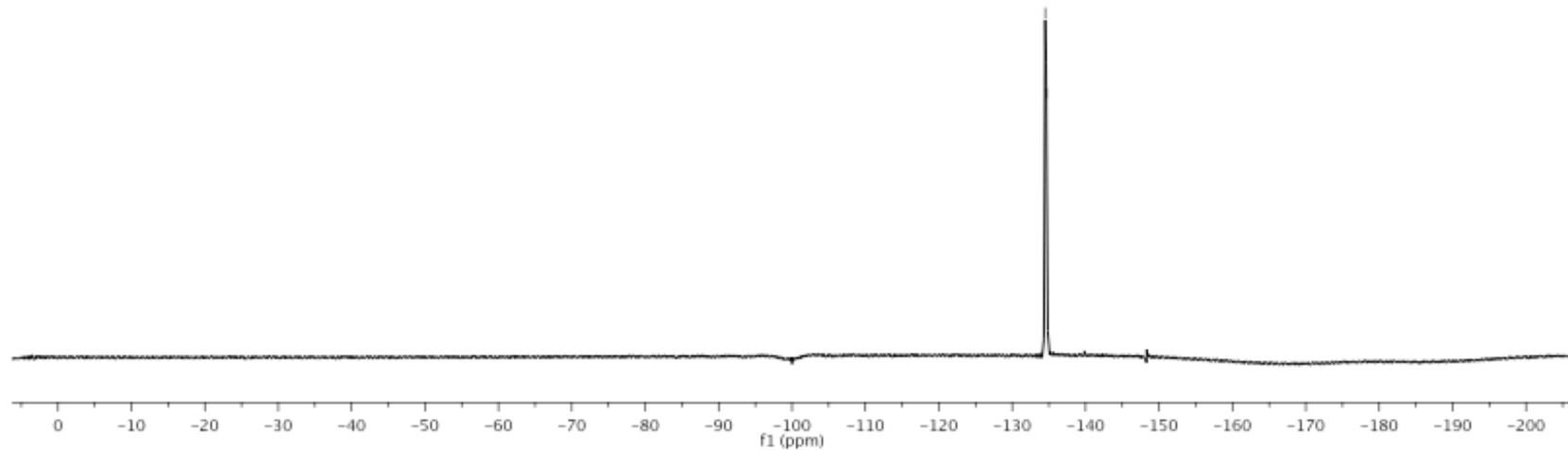
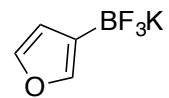
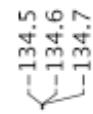
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Benzo[b]thien-2-yltrifluoroborate (3c, Table 3, entry 3)



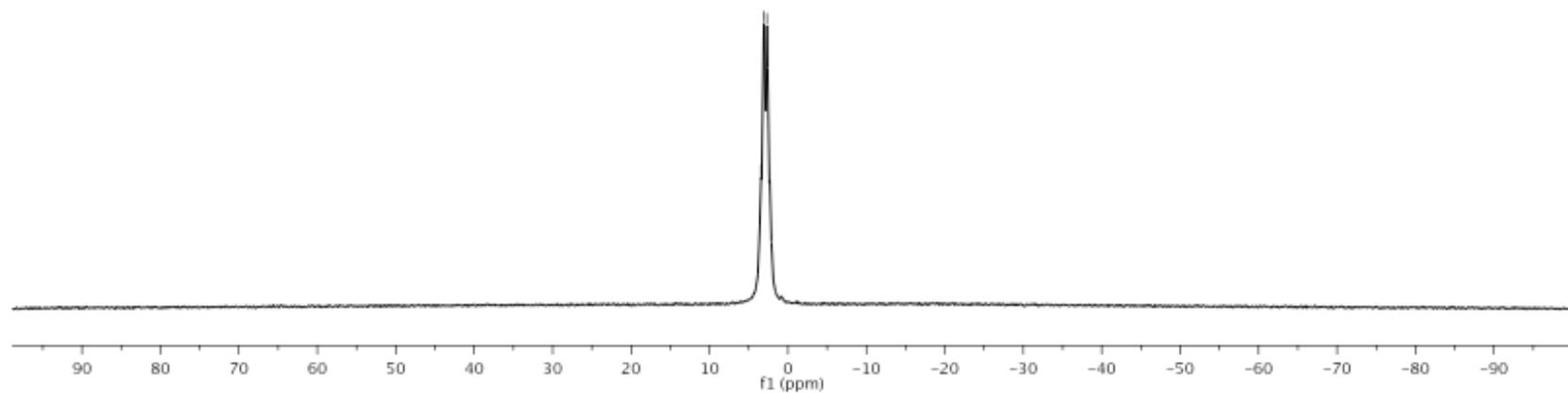
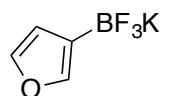
^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(furan-3-yl)borate (3d, Table 3, entry 4)



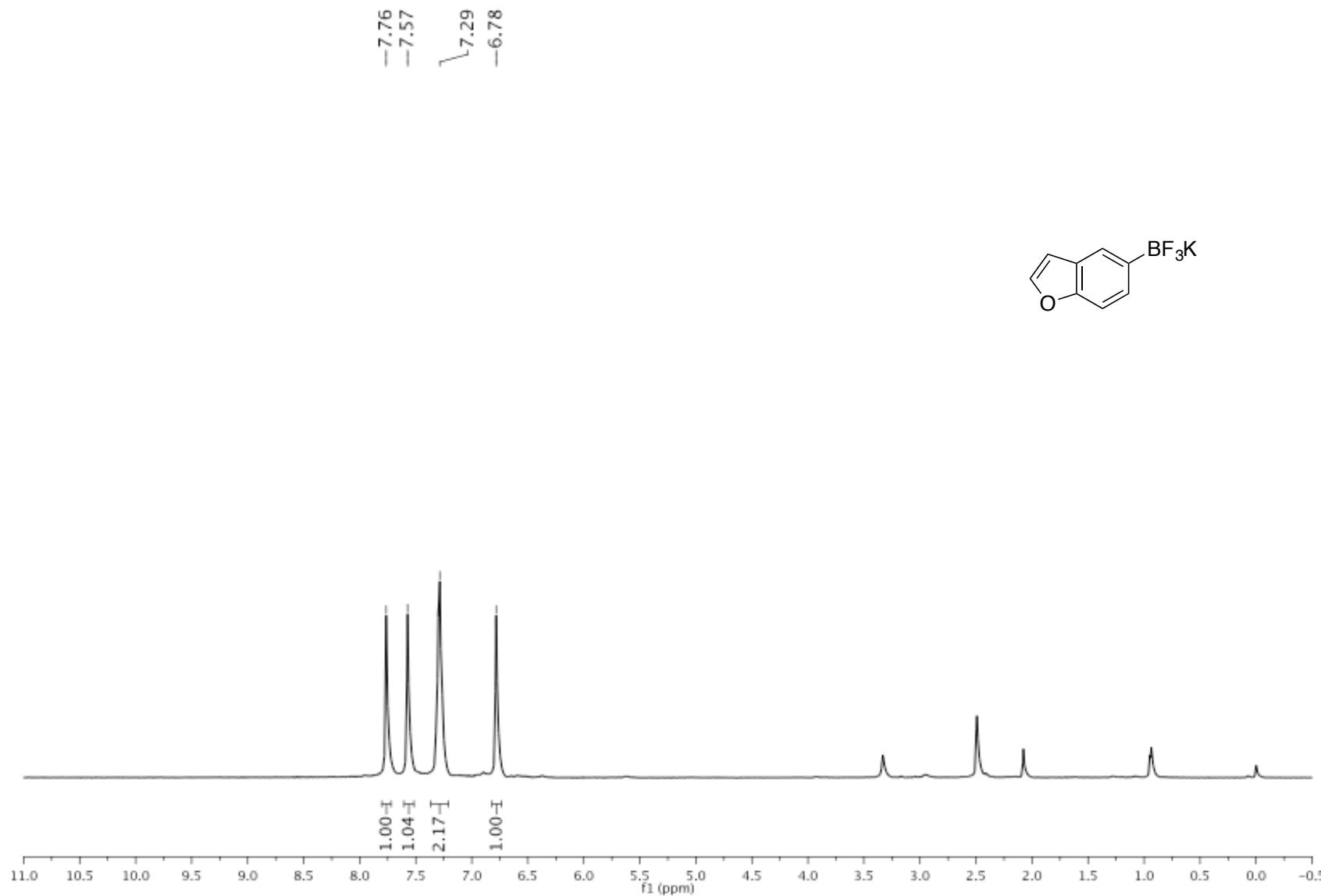
^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(furan-3-yl)borate (3d, Table 3, entry 4)



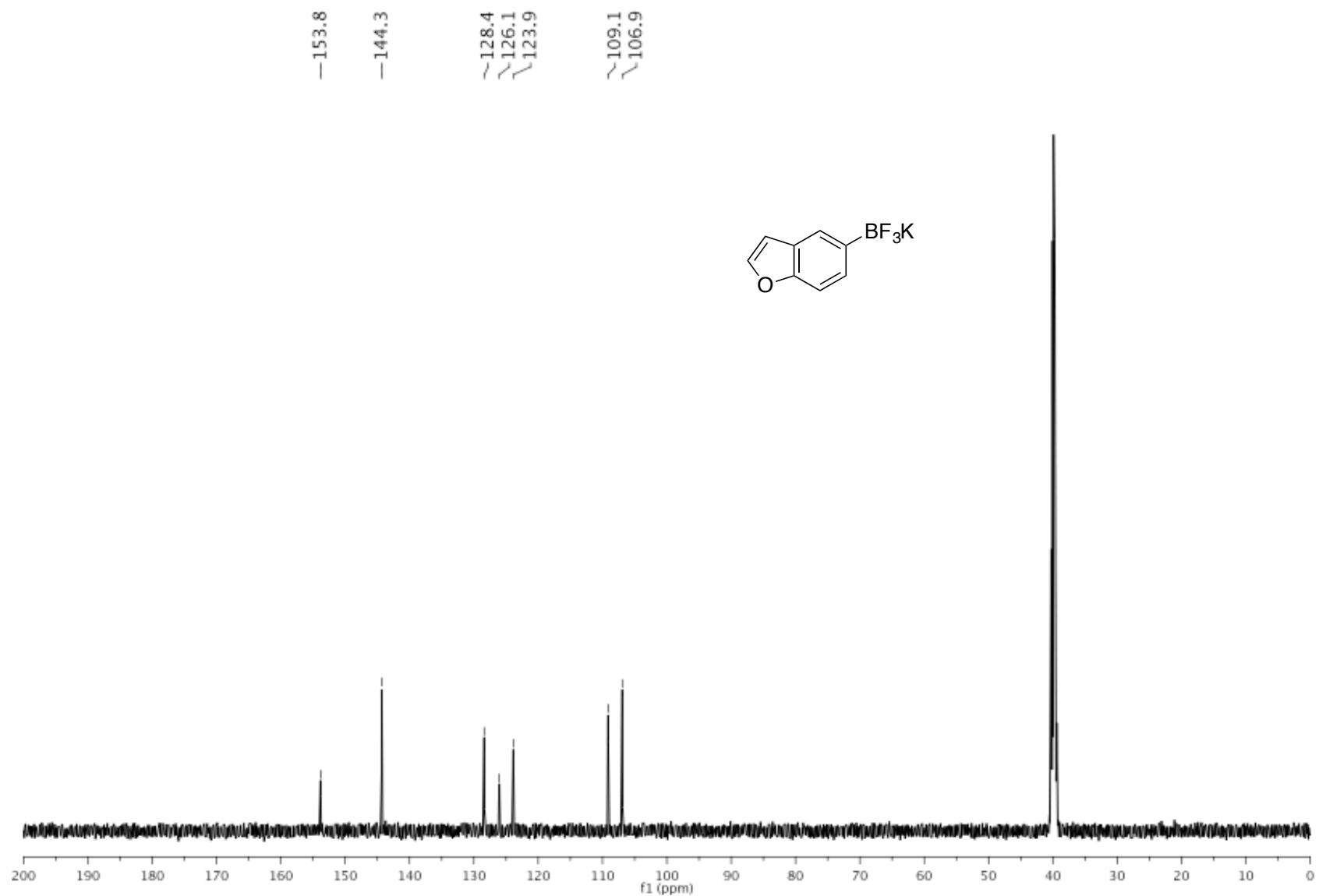
¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(furan-3-yl)borate (3d, Table 3, entry 4)



¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(furan-3-yl)borate (3d, Table 3, entry 4)

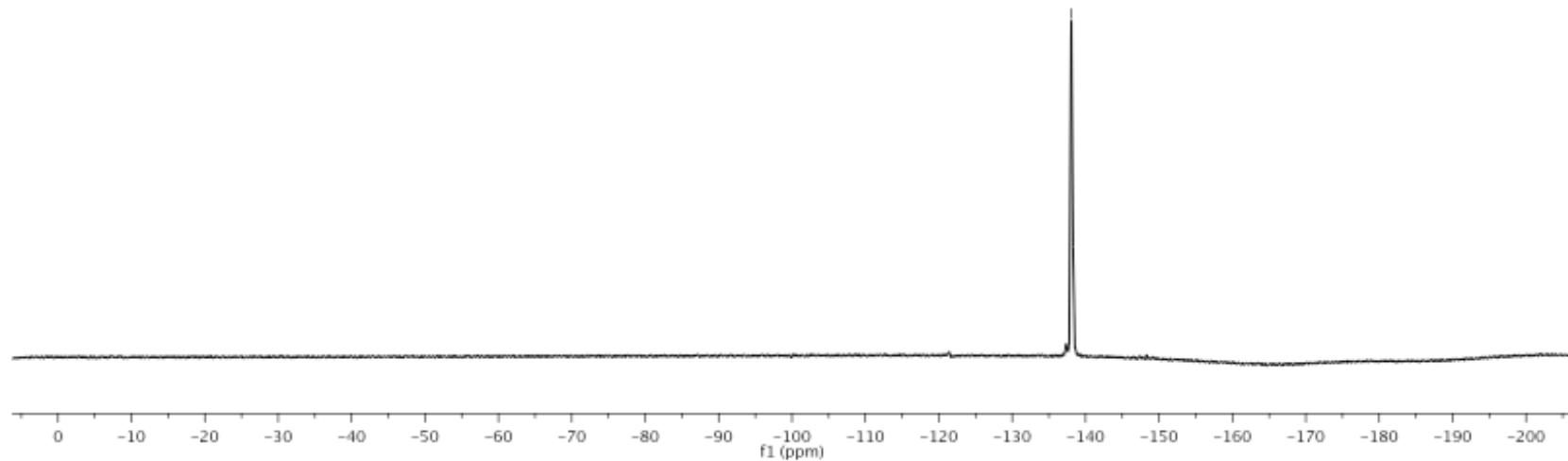
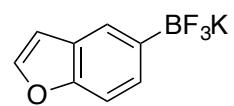


^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Benzofuran-5-yltrifluoroborate (3e, Table 3, entry 5)

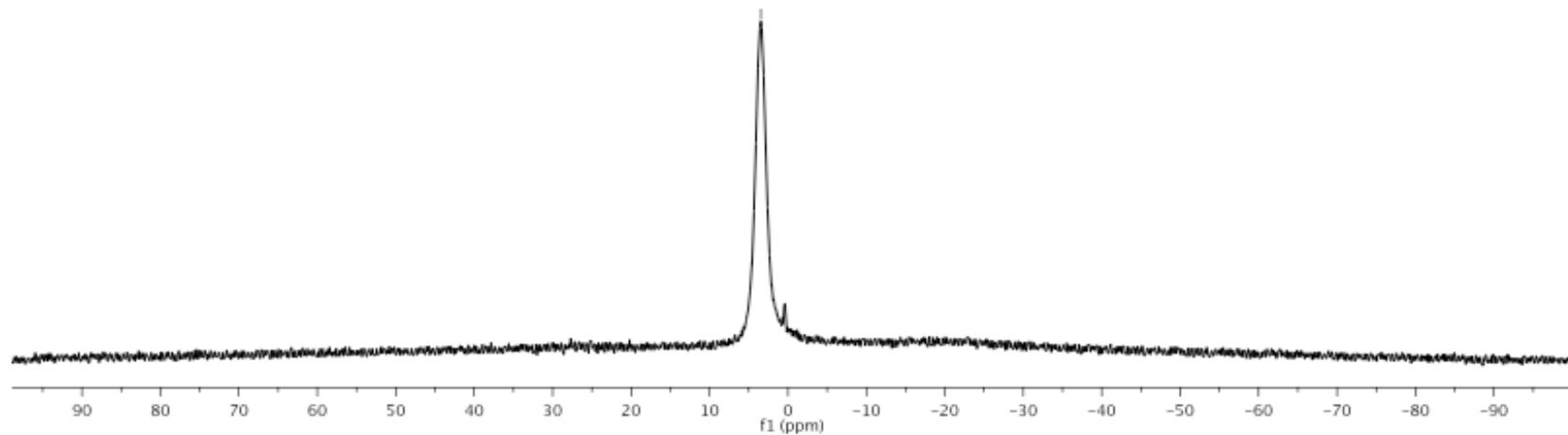
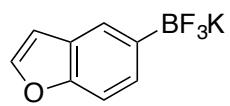


^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Benzofuran-5-yltrifluoroborate (3e, Table 3, entry 5)

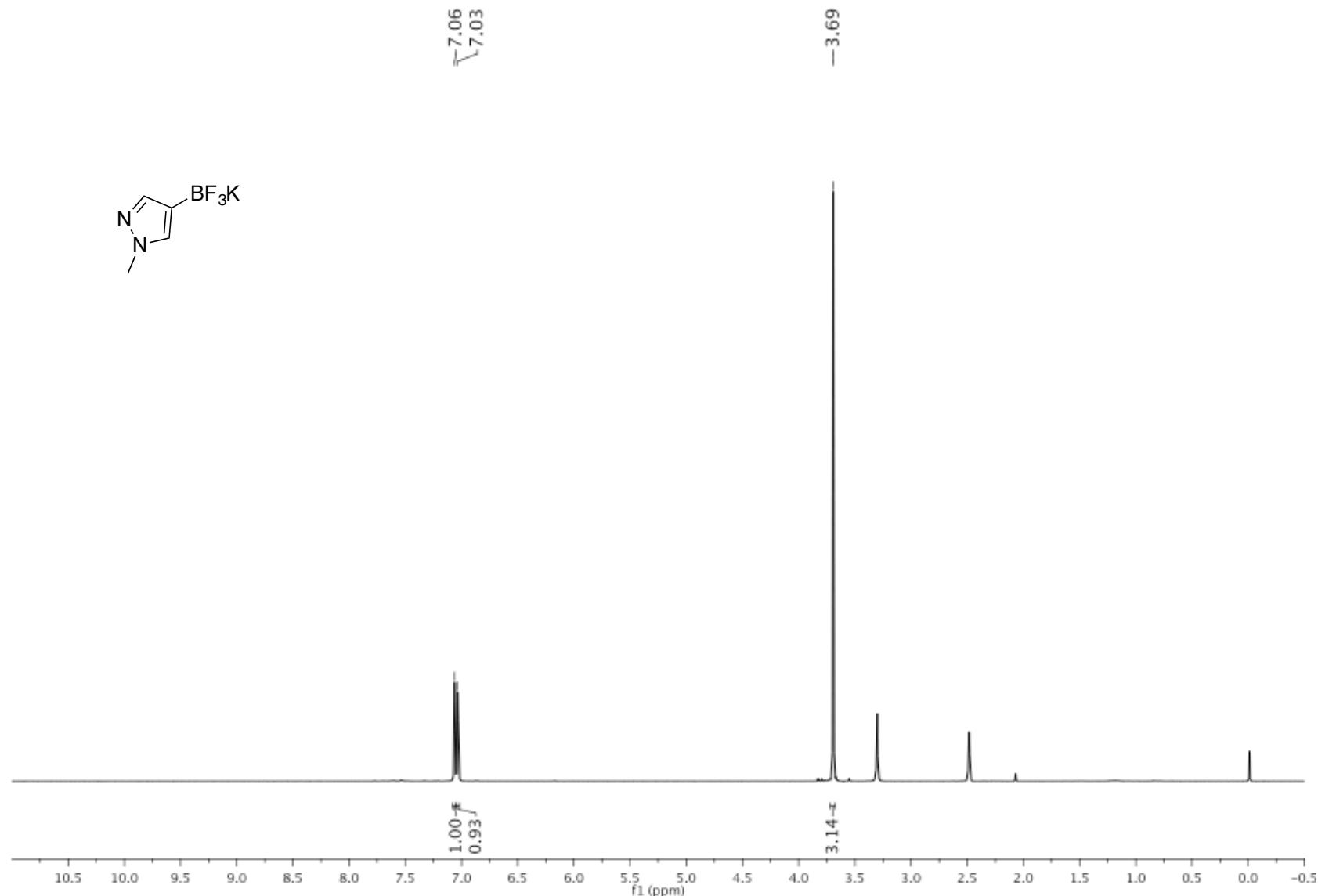
—138.1



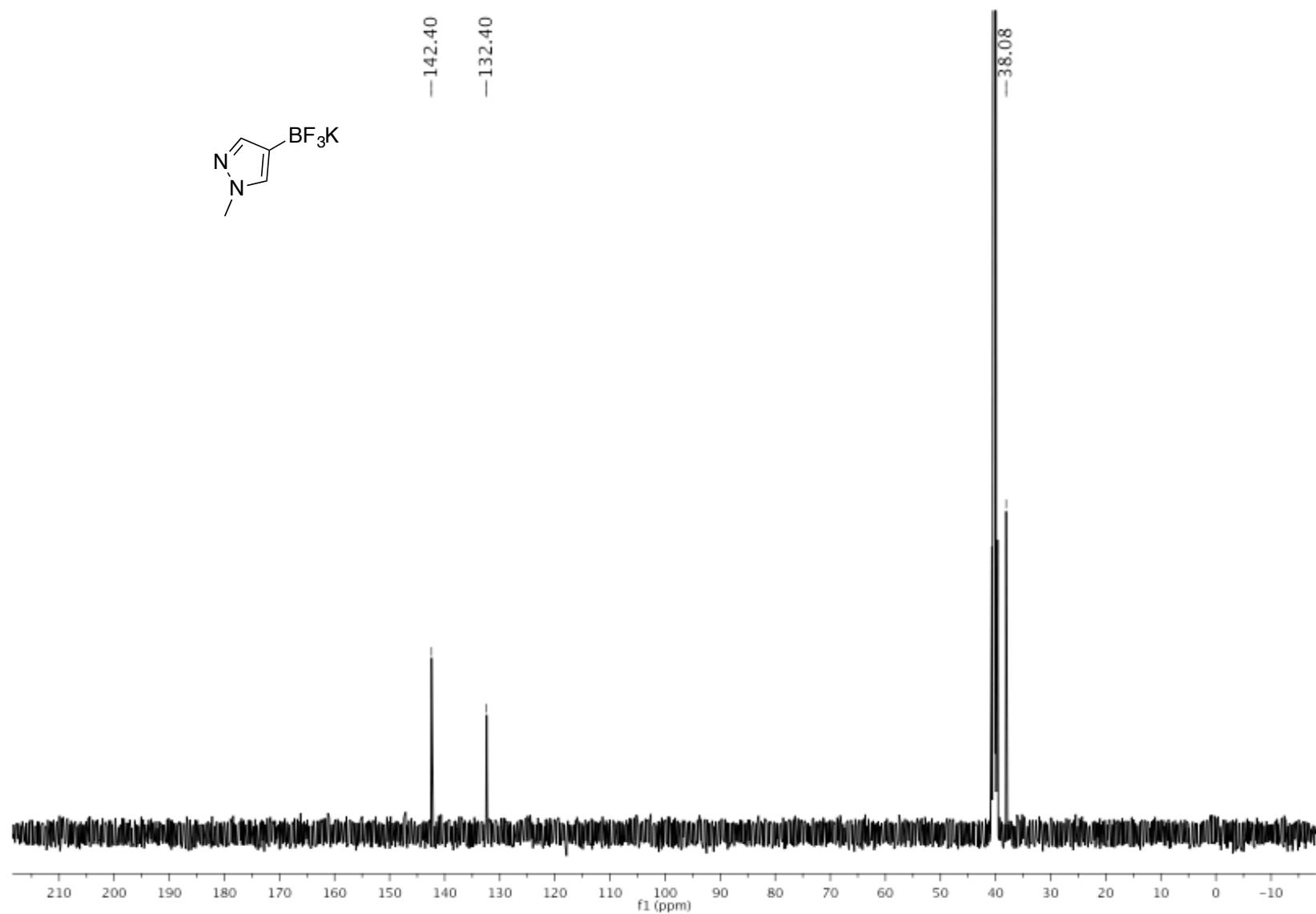
${}^{19}\text{F}$ NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Benzofuran-5-yltrifluoroborate (3e, Table 3, entry 5)



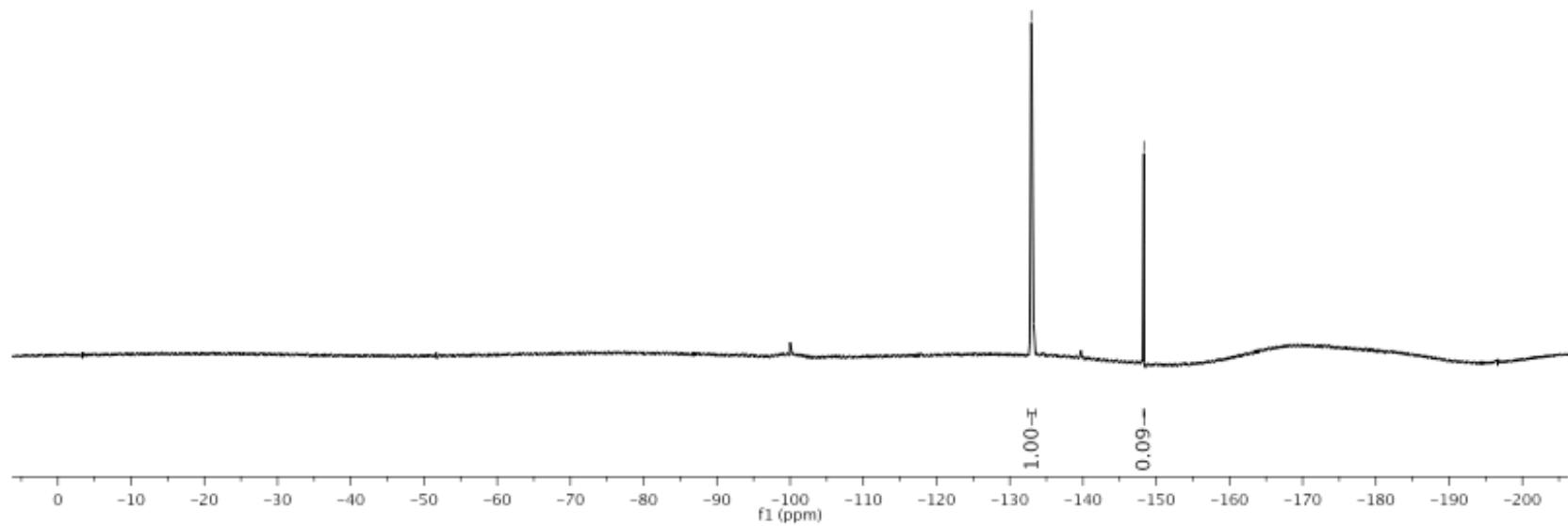
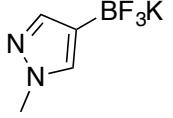
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Benzofuran-5-yltrifluoroborate (3e, Table 3, entry 5)



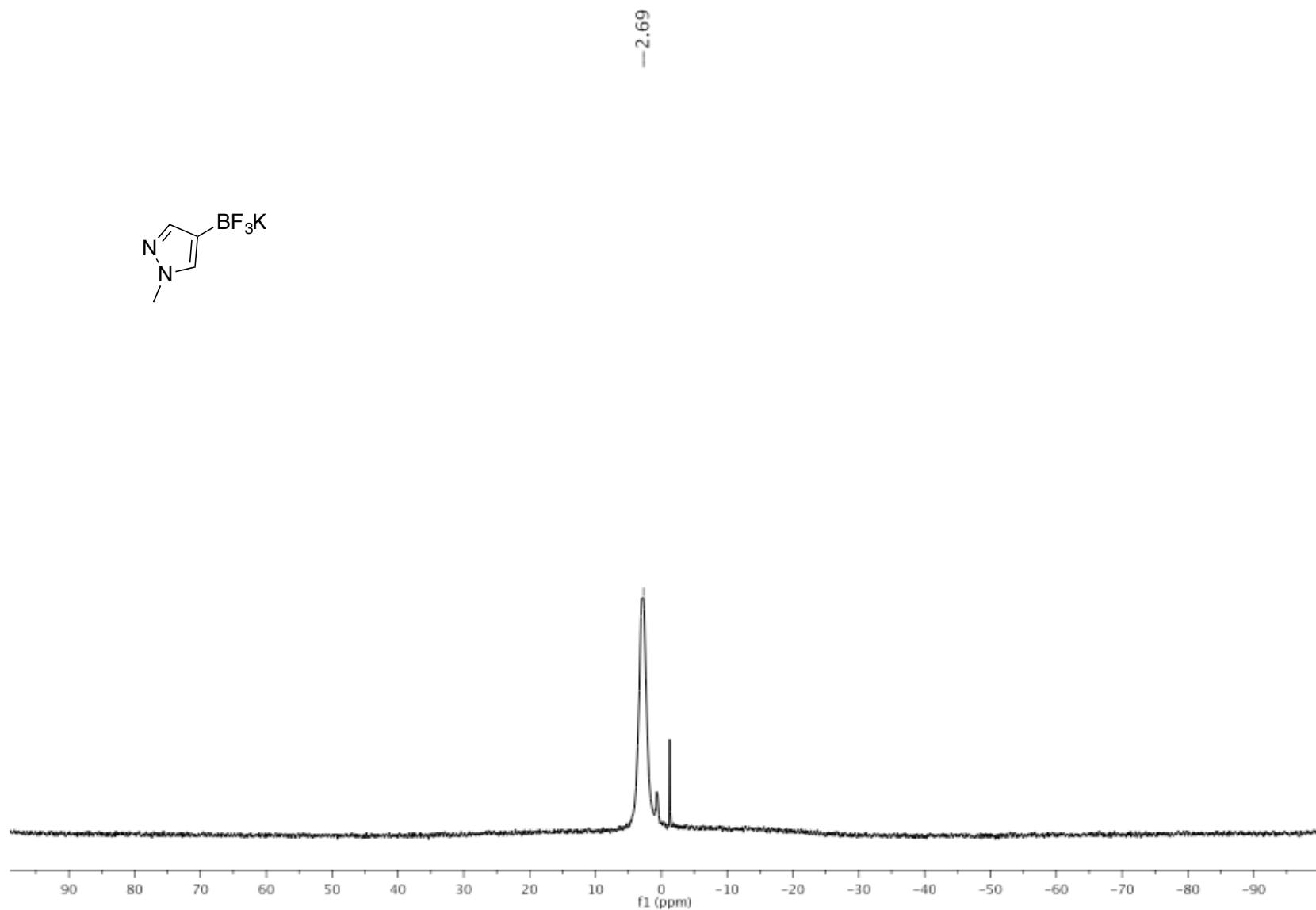
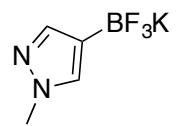
^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(1-methyl-1*H*-pyrazol-4-yl)borate (3f, Table 3, entry 6)



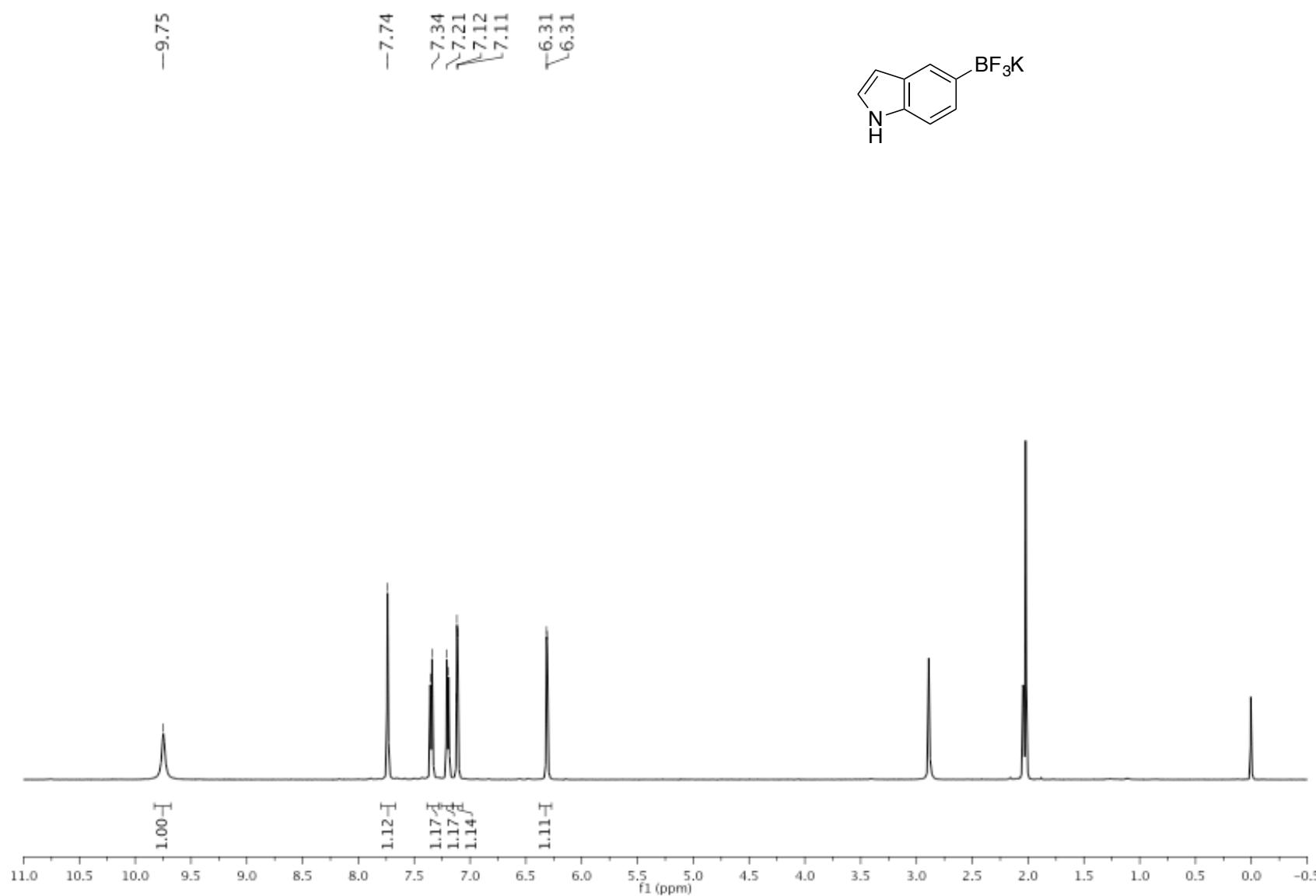
^{13}C NMR (128.5 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(1-methyl-1*H*-pyrazol-4-yl)borate (3f, Table 3, entry 6)

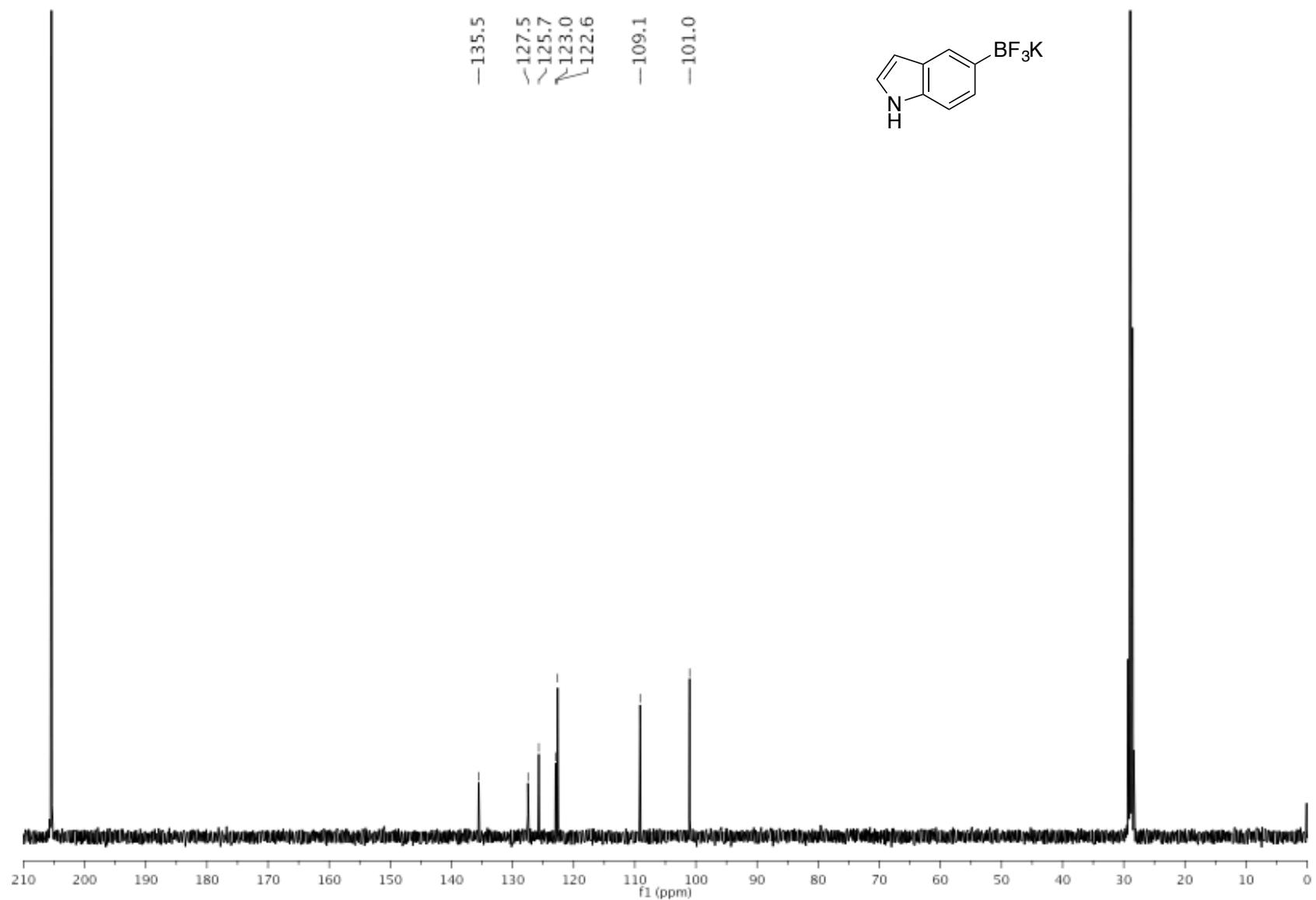


¹⁹F NMR (470.8 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(1-methyl-1*H*-pyrazol-4-yl)borate (3f, Table 3, entry 6)

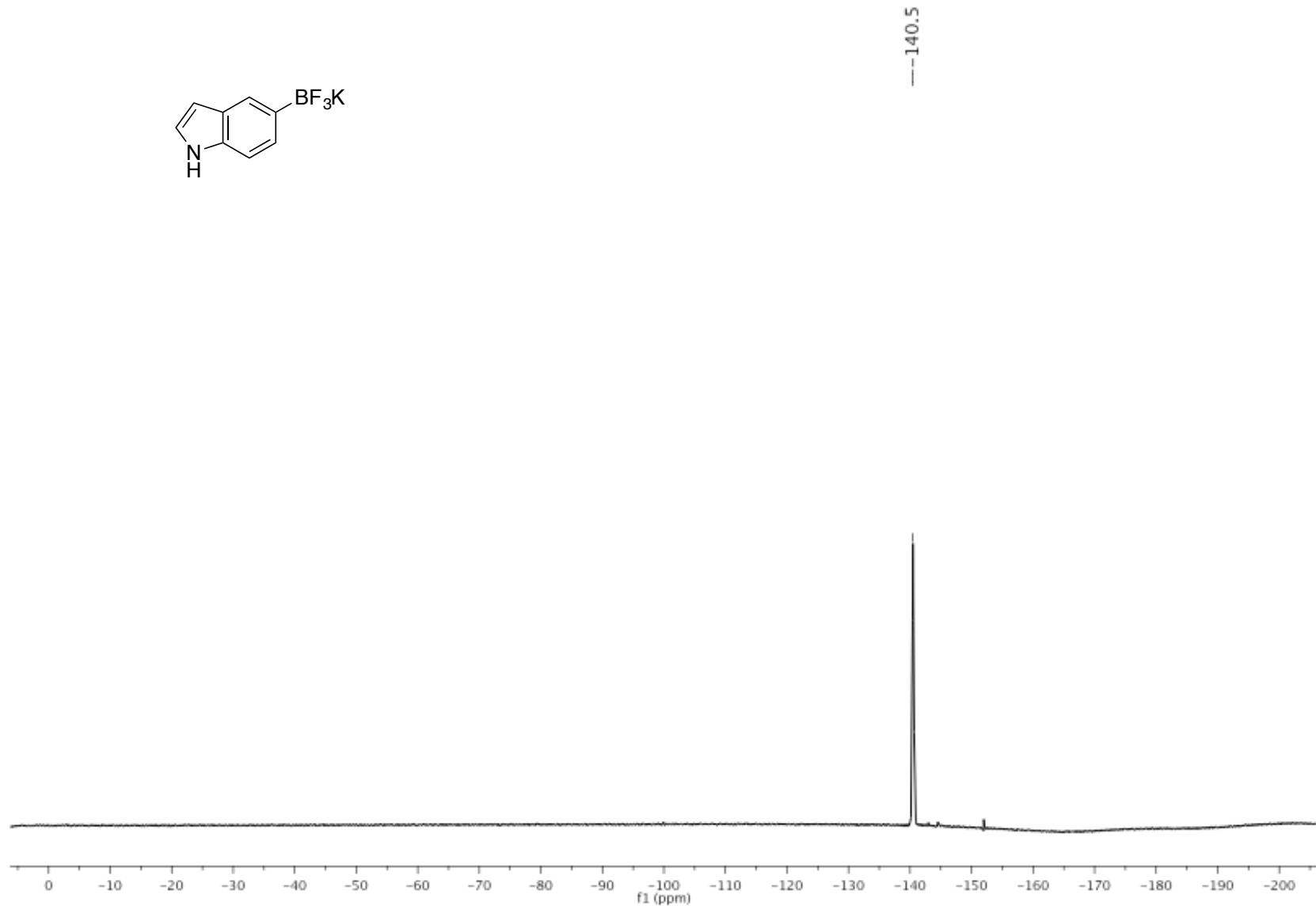
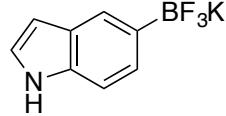


¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(1-methyl-1*H*-pyrazol-4-yl)borate (3f, Table 3, entry 6)

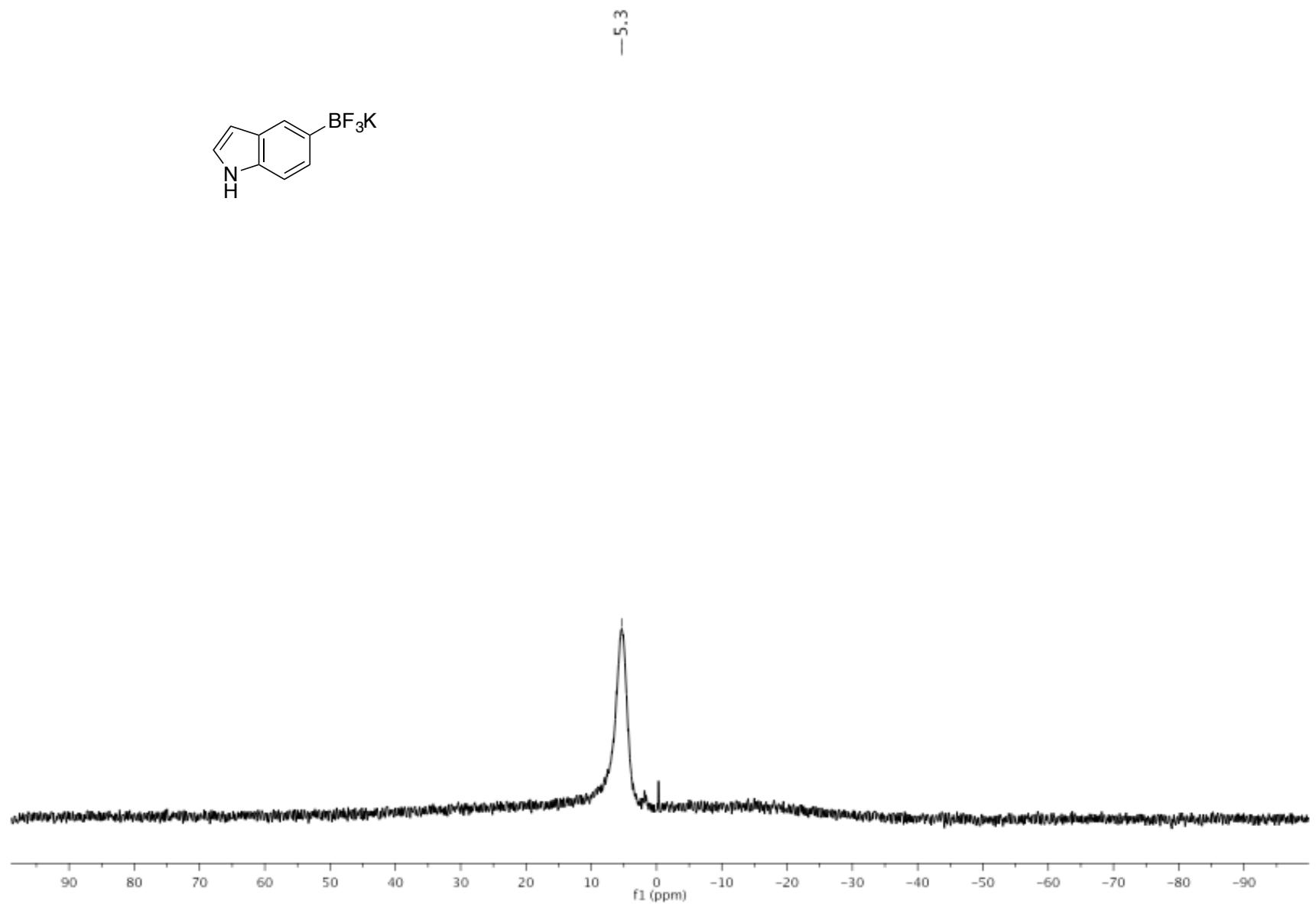




^{13}C NMR (128.5 MHz, acetone- d_6) Spectrum of Potassium Trifluoro(1*H*-indol-5-yl)borate (3g, Table 3, entry 7)



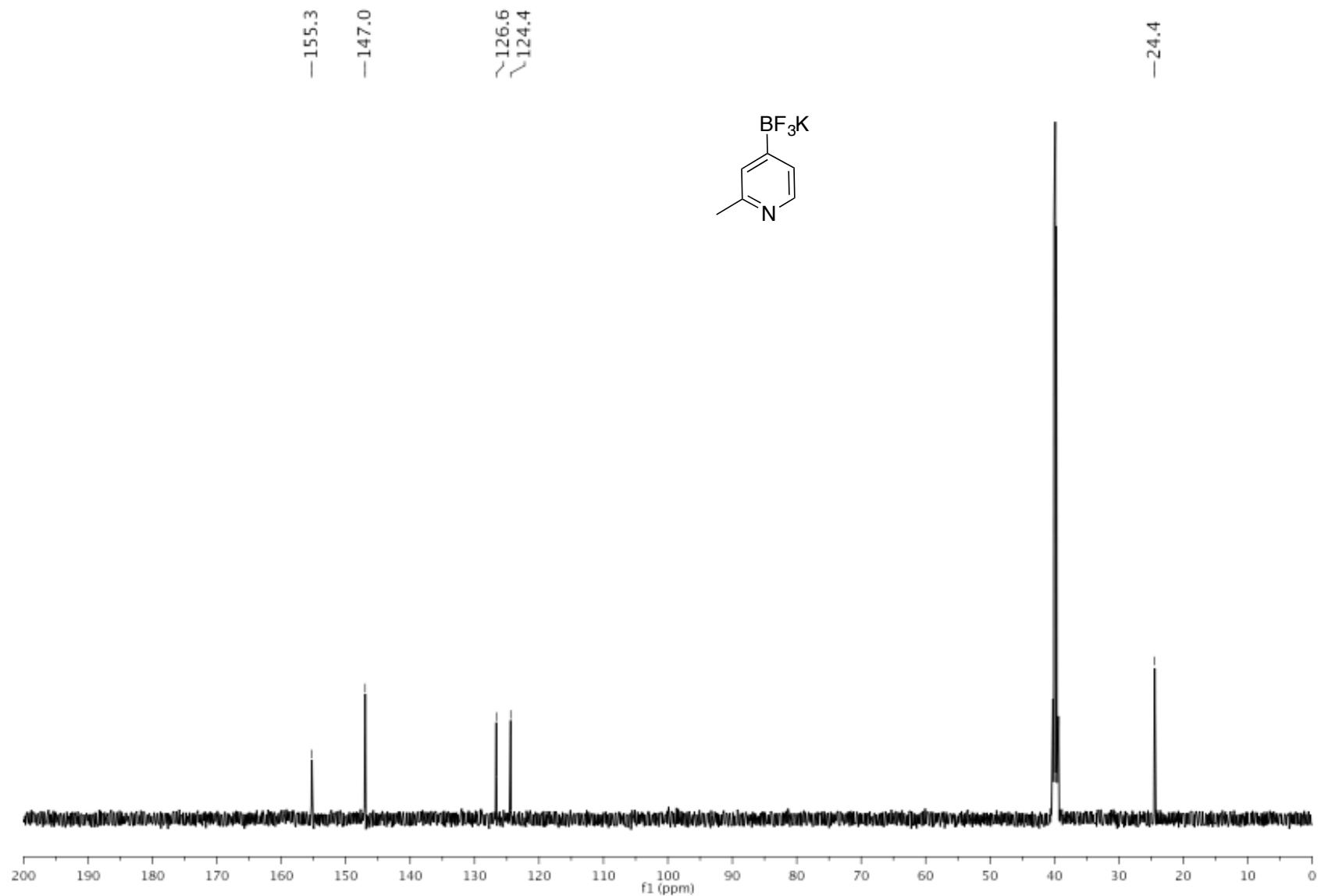
^{19}F NMR (470.8 MHz, acetone - d_6) Spectrum of Potassium Trifluoro(1*H*-indol-5-yl)borate (3g, Table 3, entry 7)



¹¹B NMR (128.4 MHz, acetone-d₆) Spectrum of Potassium Trifluoro(1*H*-indol-5-yl)borate (3g, Table 3, entry 7)

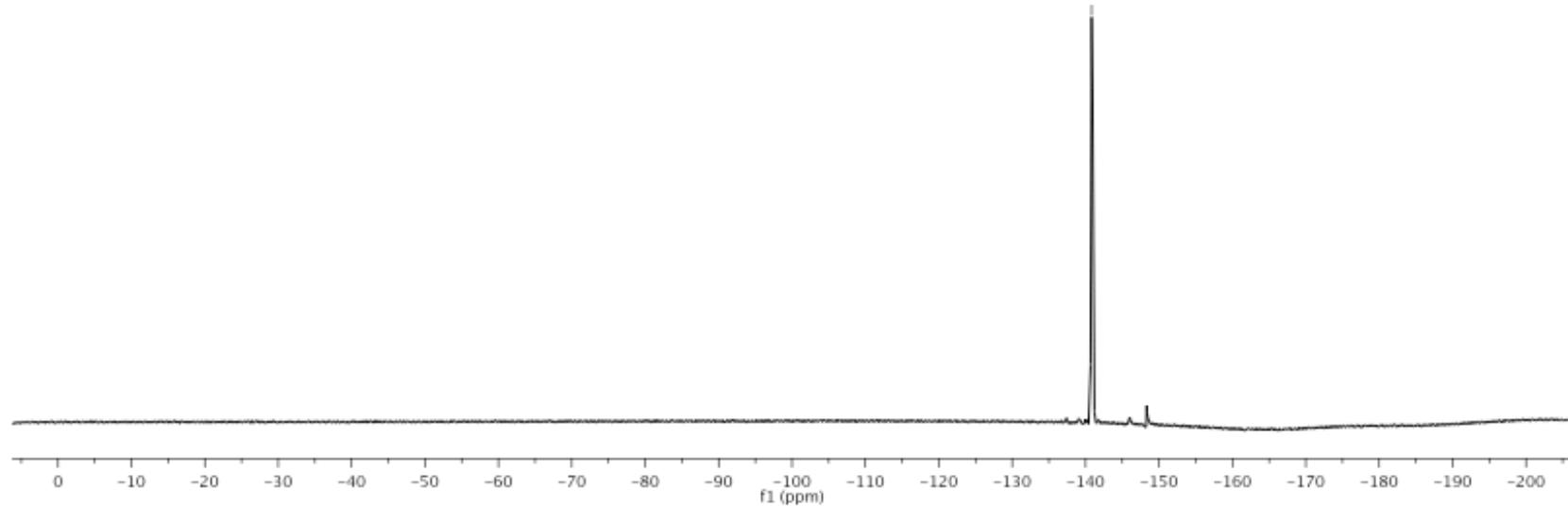
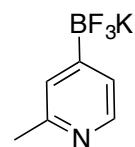


^1H NMR (500 MHz, DMSO - d_6) Spectrum of Potassium Trifluoro(2-methylpyridin-4-yl)borate (3h, Table 3, entry 8)



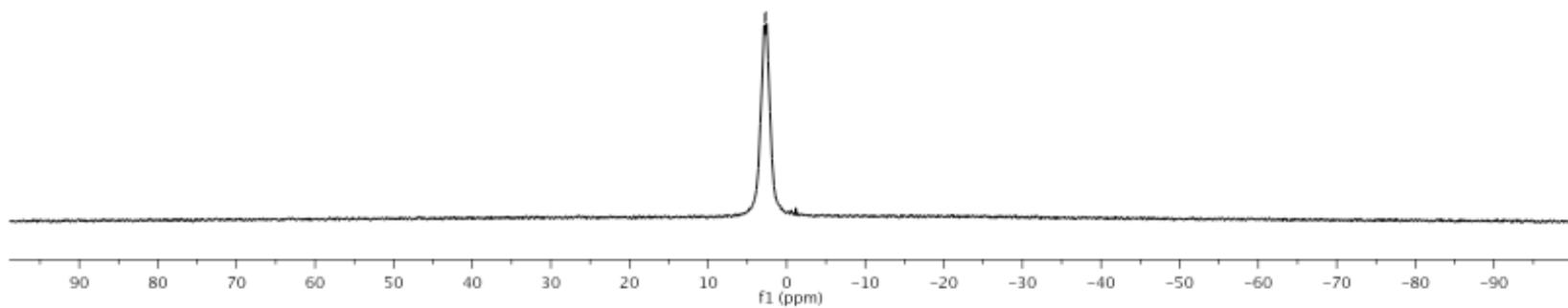
^{13}C NMR (128.5 MHz, DMSO - d_6) Spectrum of Potassium Trifluoro(2-methylpyridin-4-yl)borate (3h, Table 3, entry 8)

— -140.8

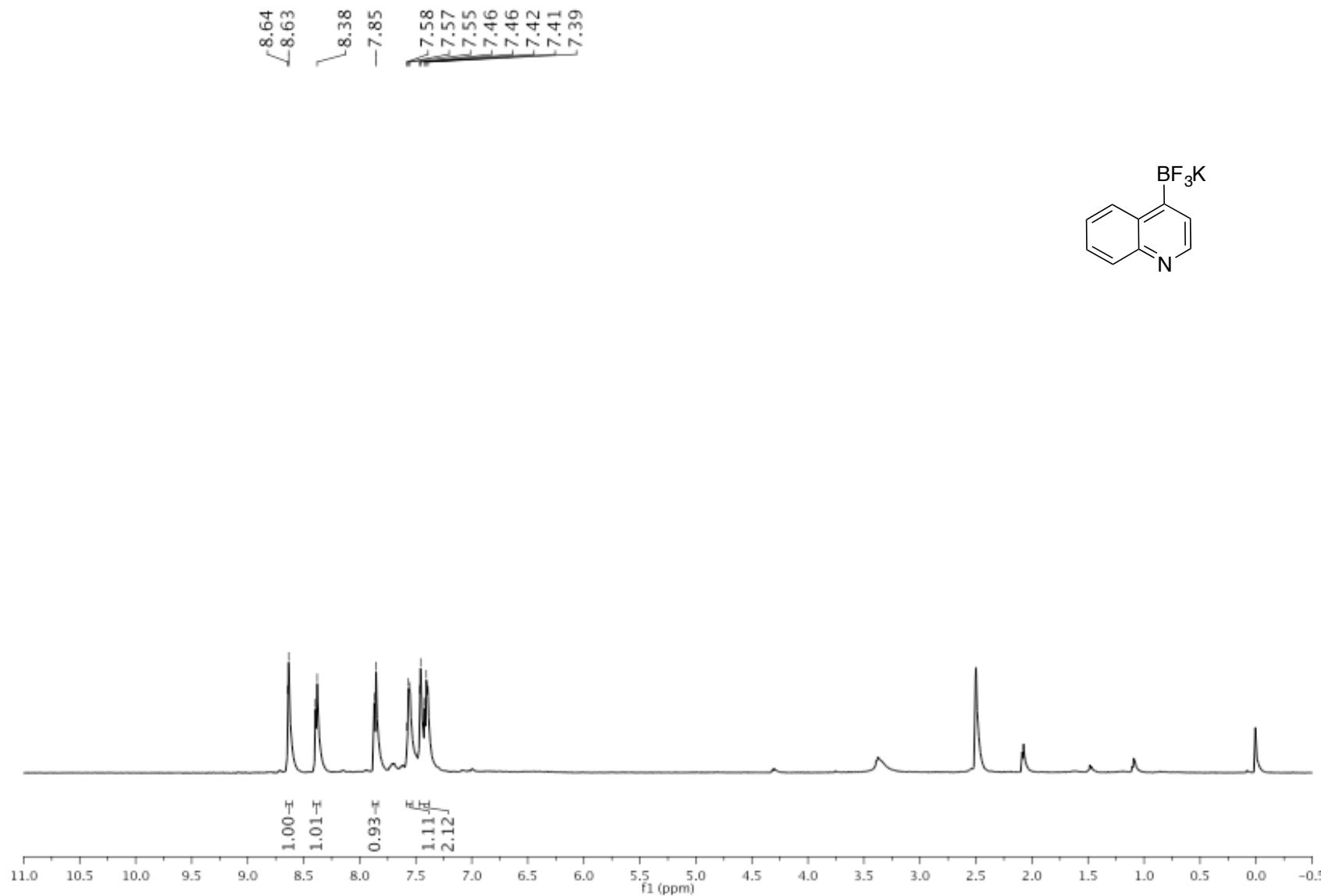


¹⁹F NMR (470.8 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(2-methylpyridin-4-yl)borate (3h, Table 3, entry 8)

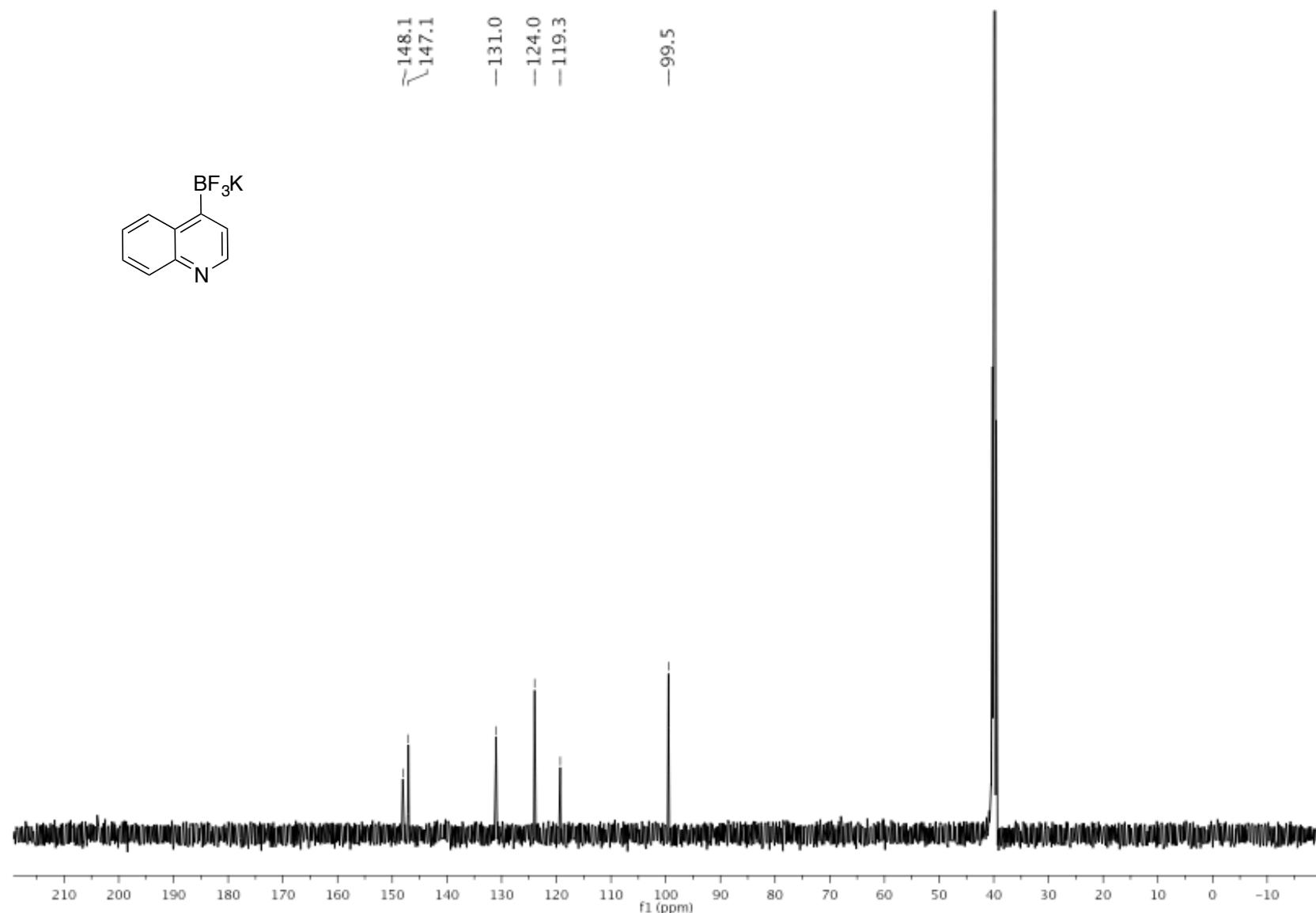
2.9
2.5



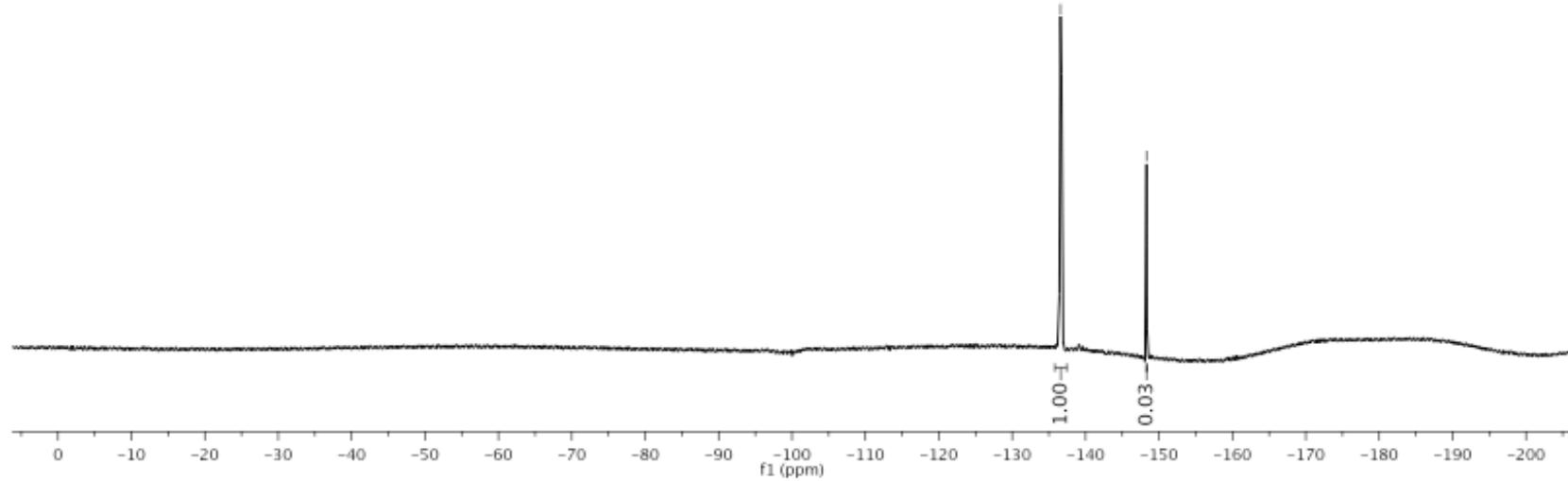
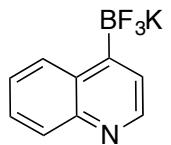
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(2-methylpyridin-4-yl)borate (3h, Table 3, entry 8)



^1H NMR (500 MHz, $\text{DMSO}-\text{d}_6$) Spectrum of Potassium Trifluoro(quinolin-4-yl)borate (3i, Table 3, entry 9)

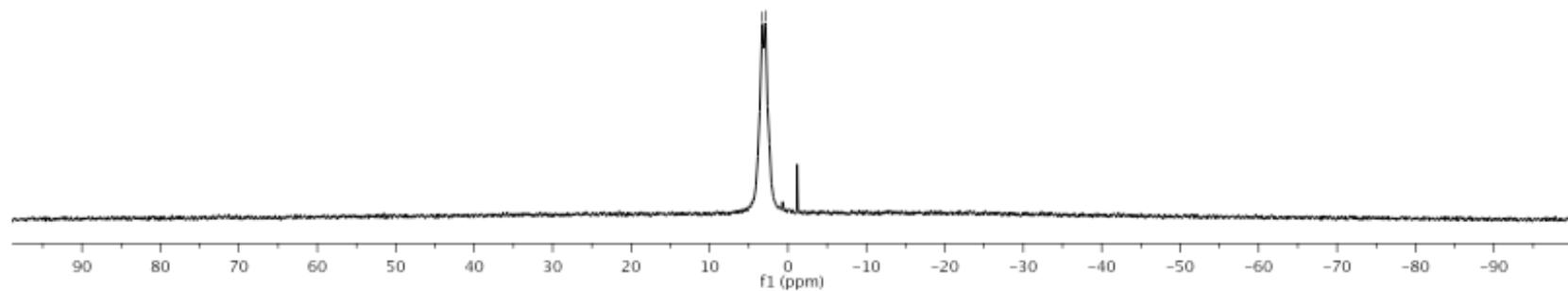
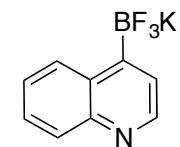


^{13}C NMR (128.5 MHz, DMSO - d_6) Spectrum of Potassium Trifluoro(quinolin-4-yl)borate (3i, Table 3, entry 9)



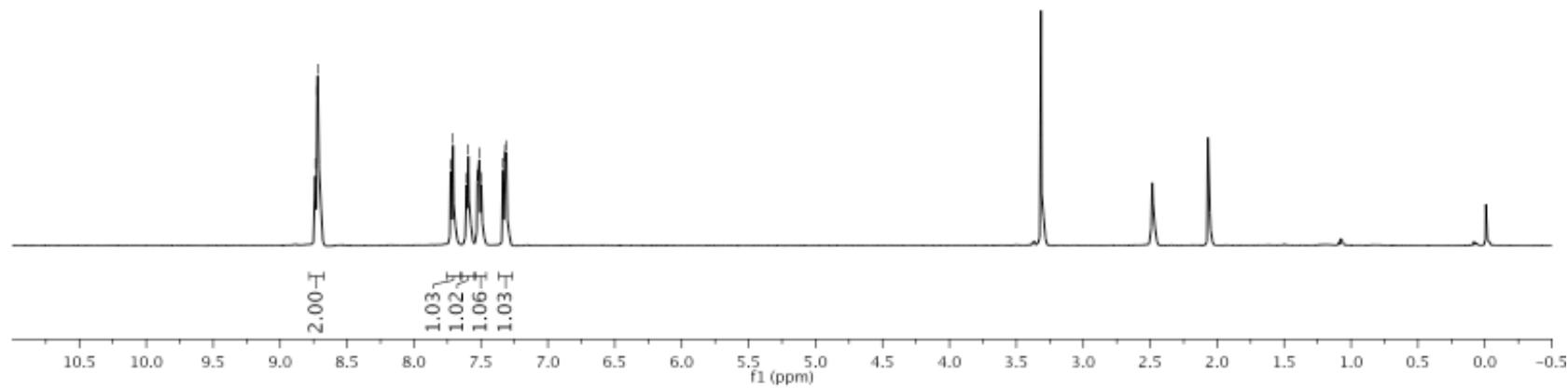
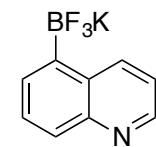
¹⁹F NMR (470.8 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(quinolin-4-yl)borate (3i, Table 3, entry 9)

3.3
2.9

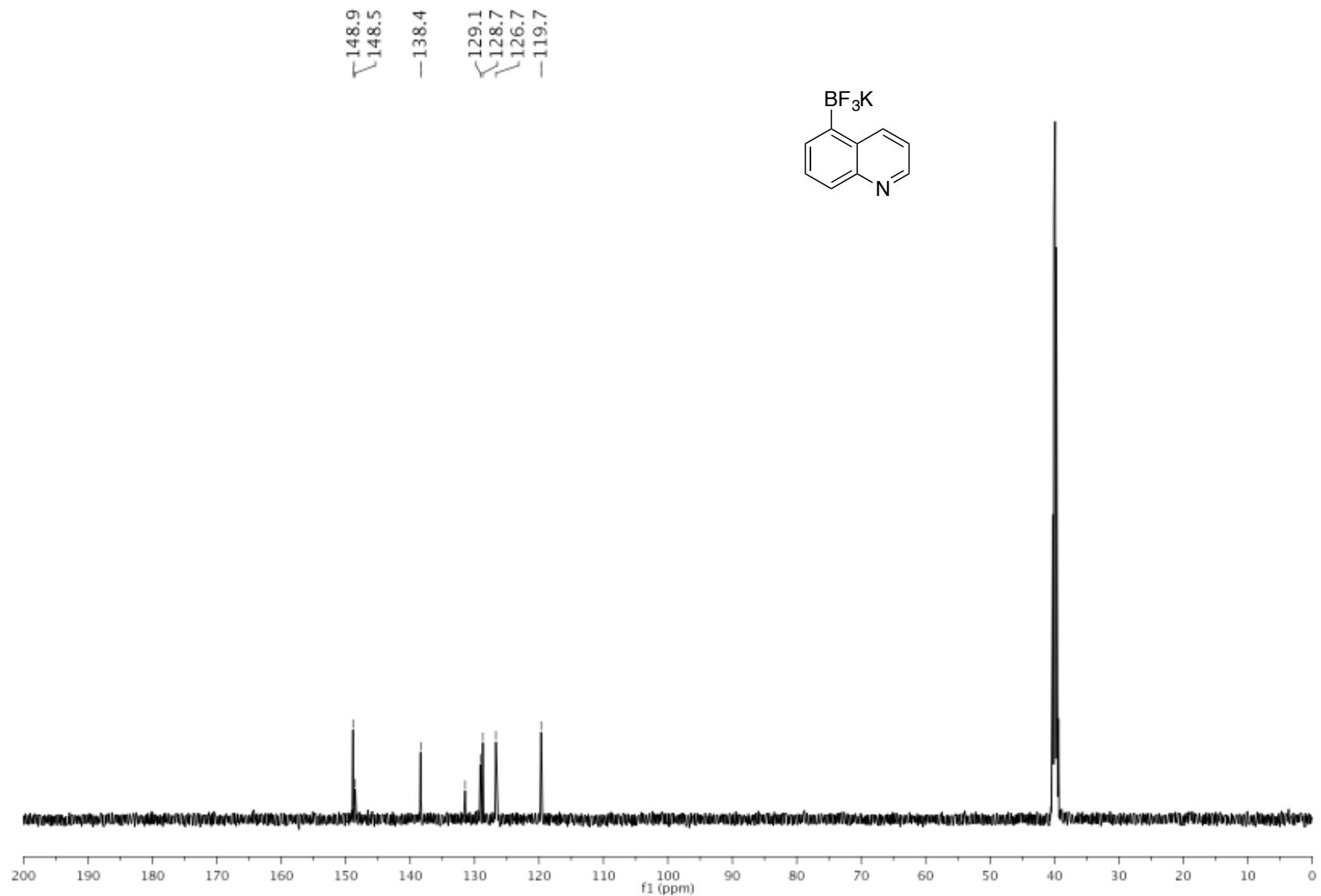


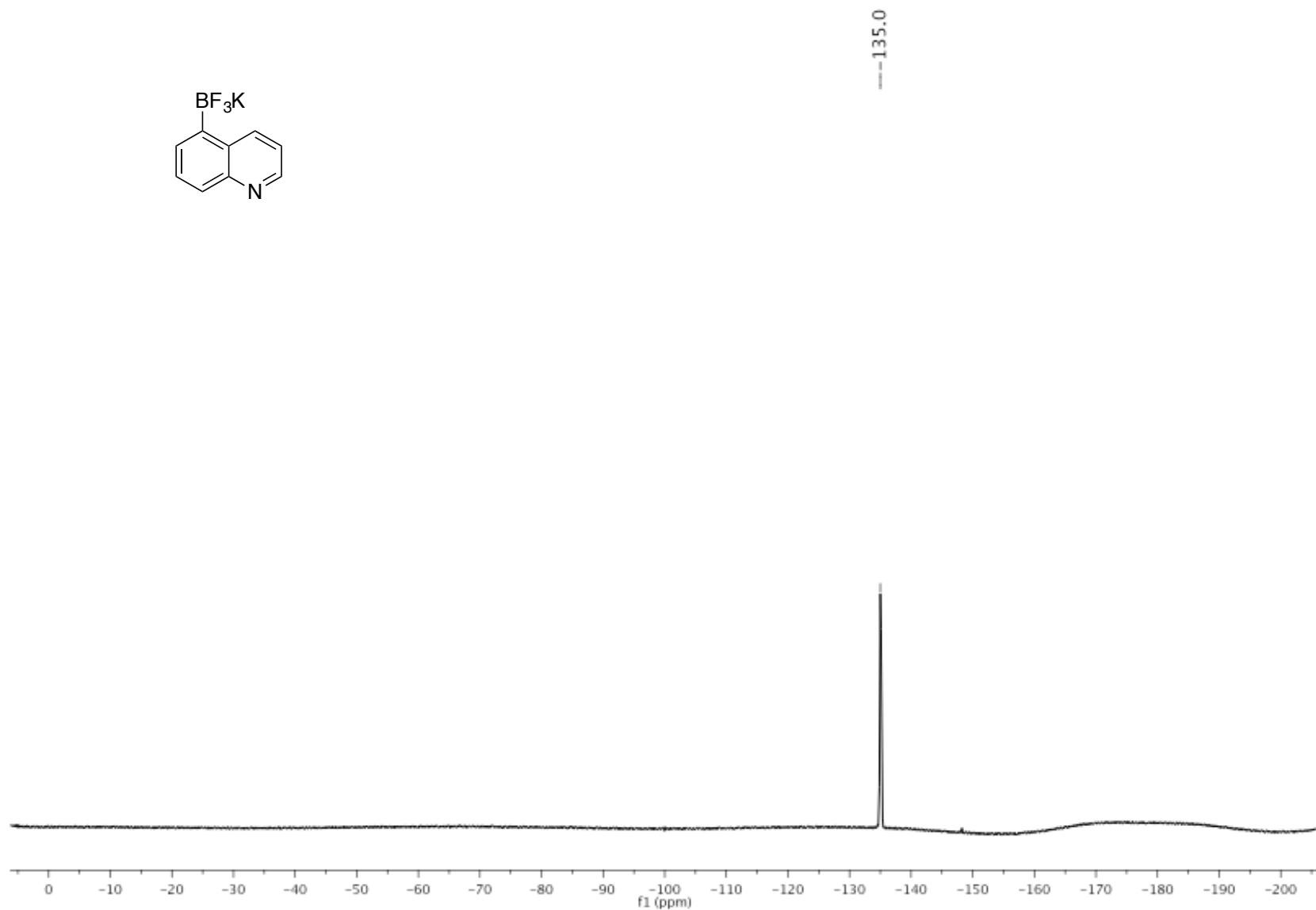
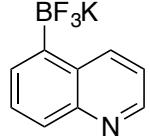
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(quinolin-4-yl)borate (3i, Table 3, entry 9)

8.74
8.72
8.71
7.73
7.71
7.61
7.59
7.53
7.51
7.50
7.33
7.33
7.32
7.31



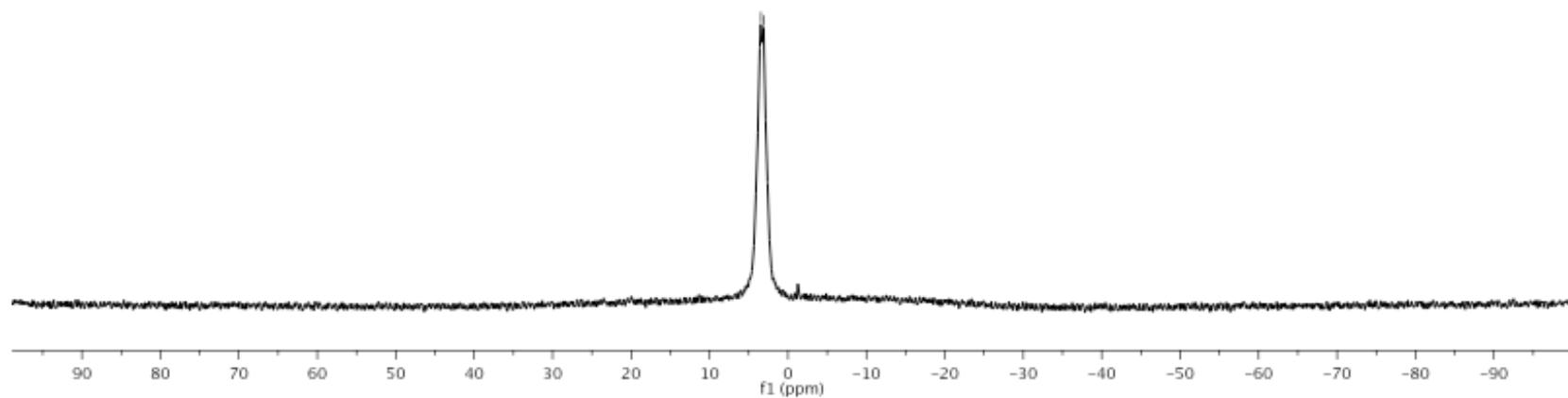
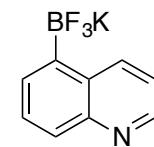
¹H NMR (500 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(quinolin-5-yl)borate (3j, Table 3, entry 10)



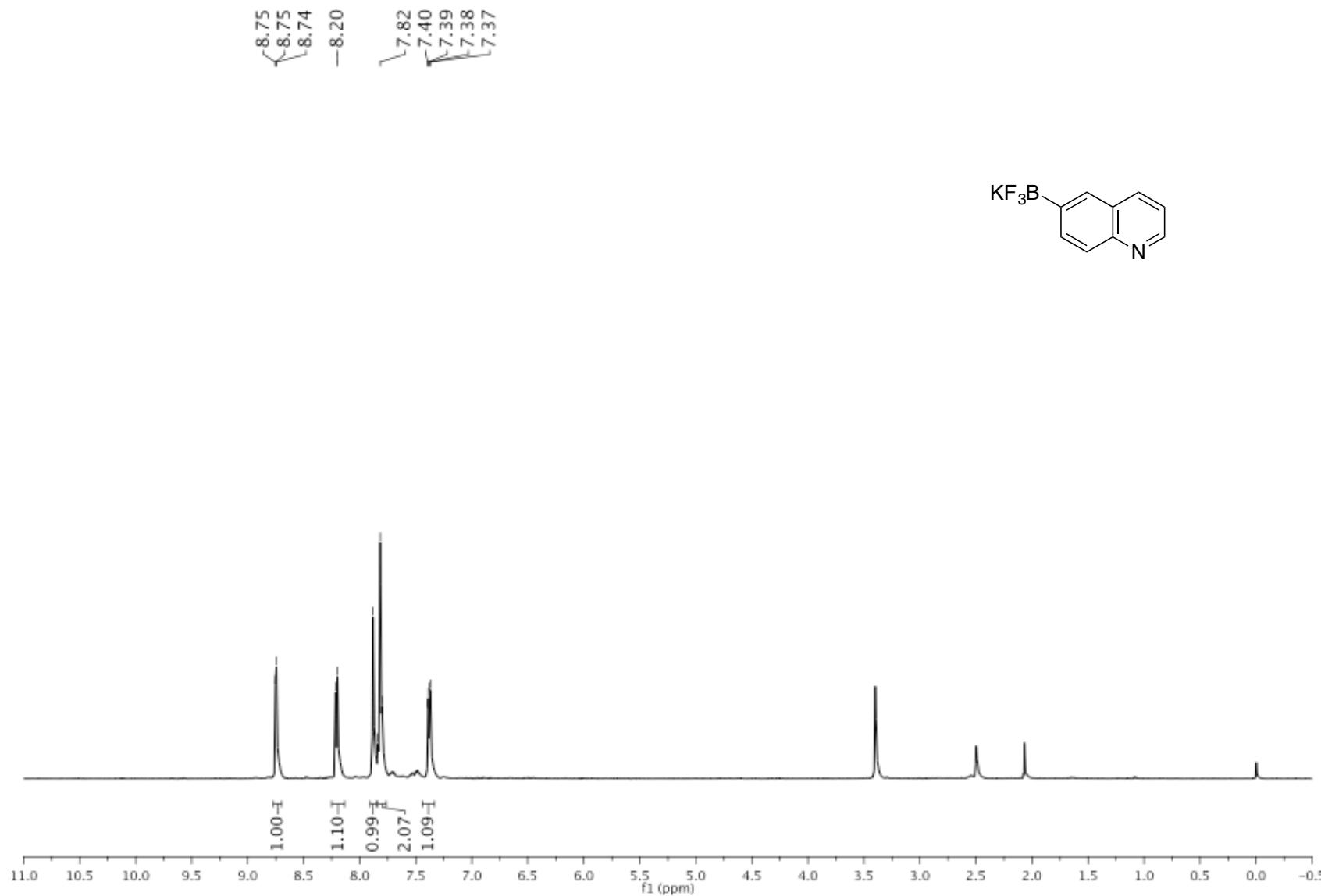


¹⁹F NMR (470.8 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(quinolin-5-yl)borate (3j, Table 3, entry 10)

$\sqrt{3.5}$
 $\sqrt{3.1}$

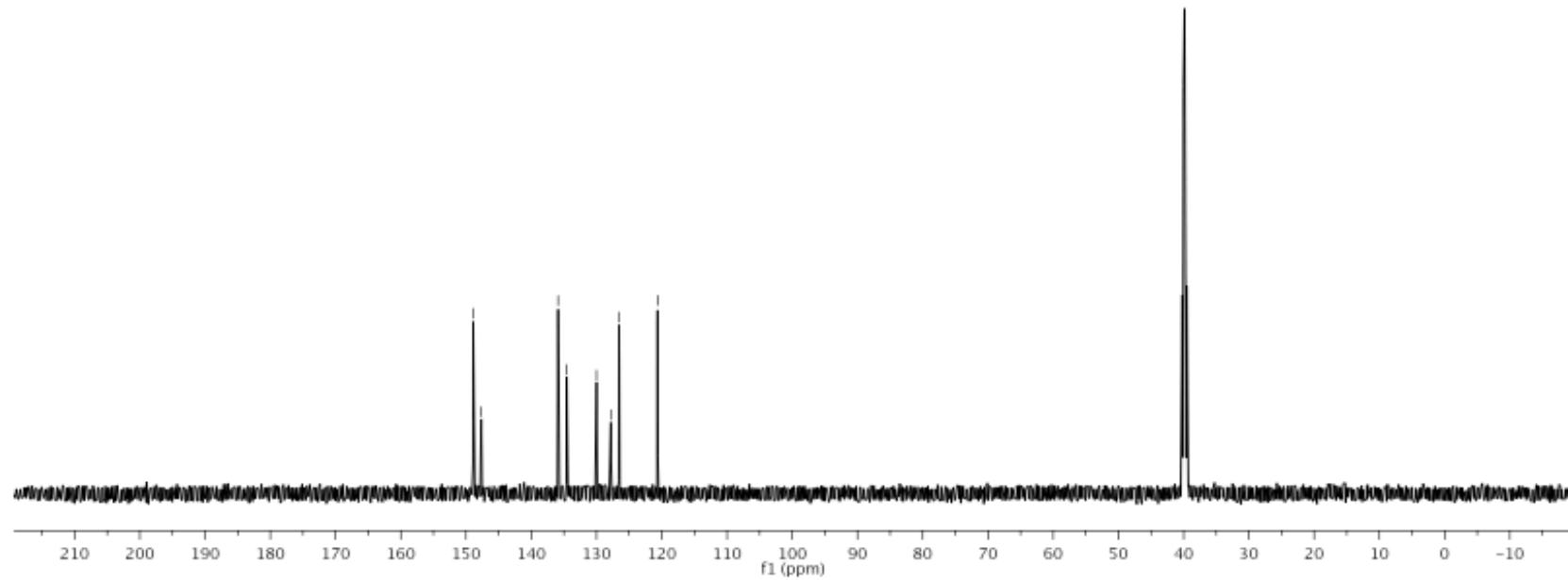
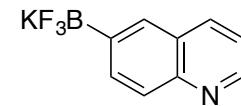


^{11}B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(quinolin-5-yl)borate (3j, Table 3, entry 10)



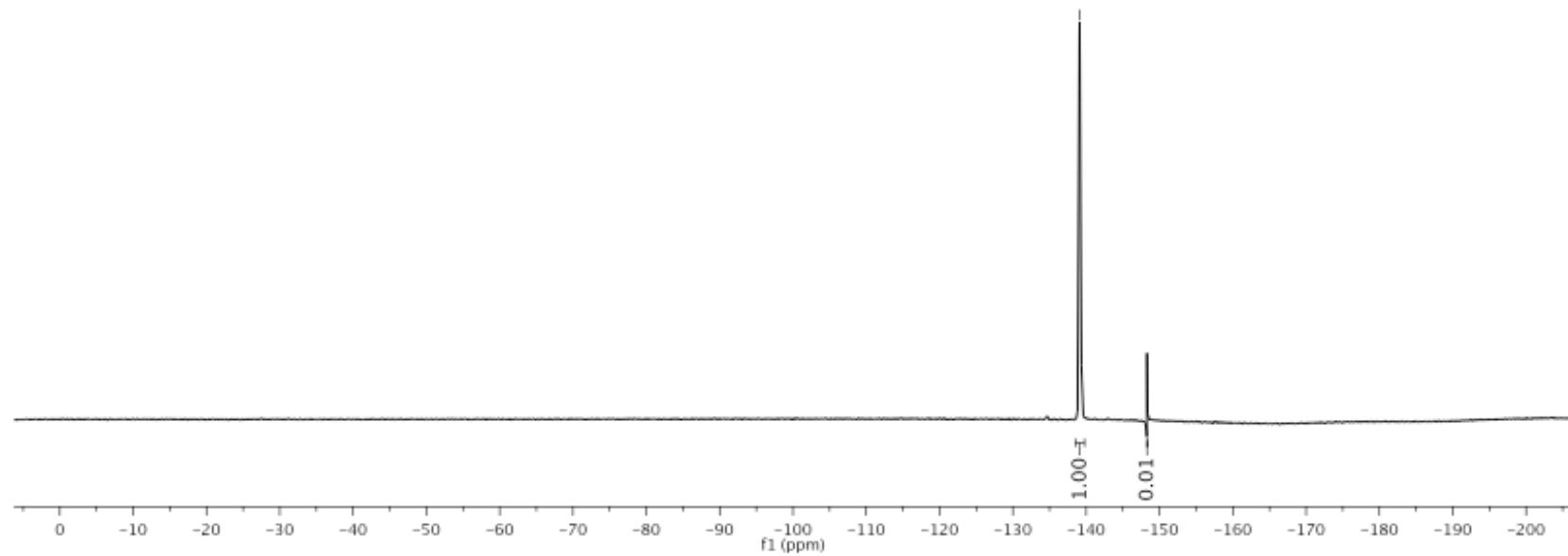
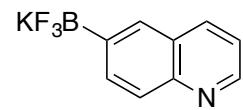
^1H NMR (500 MHz, $\text{DMSO}-\text{d}_6$) Spectrum of Potassium Trifluoro(quinolin-6-yl)borate (3k, Table 3, entry 11)

~148.9
~147.7
135.9
134.6
-126.5
-120.6

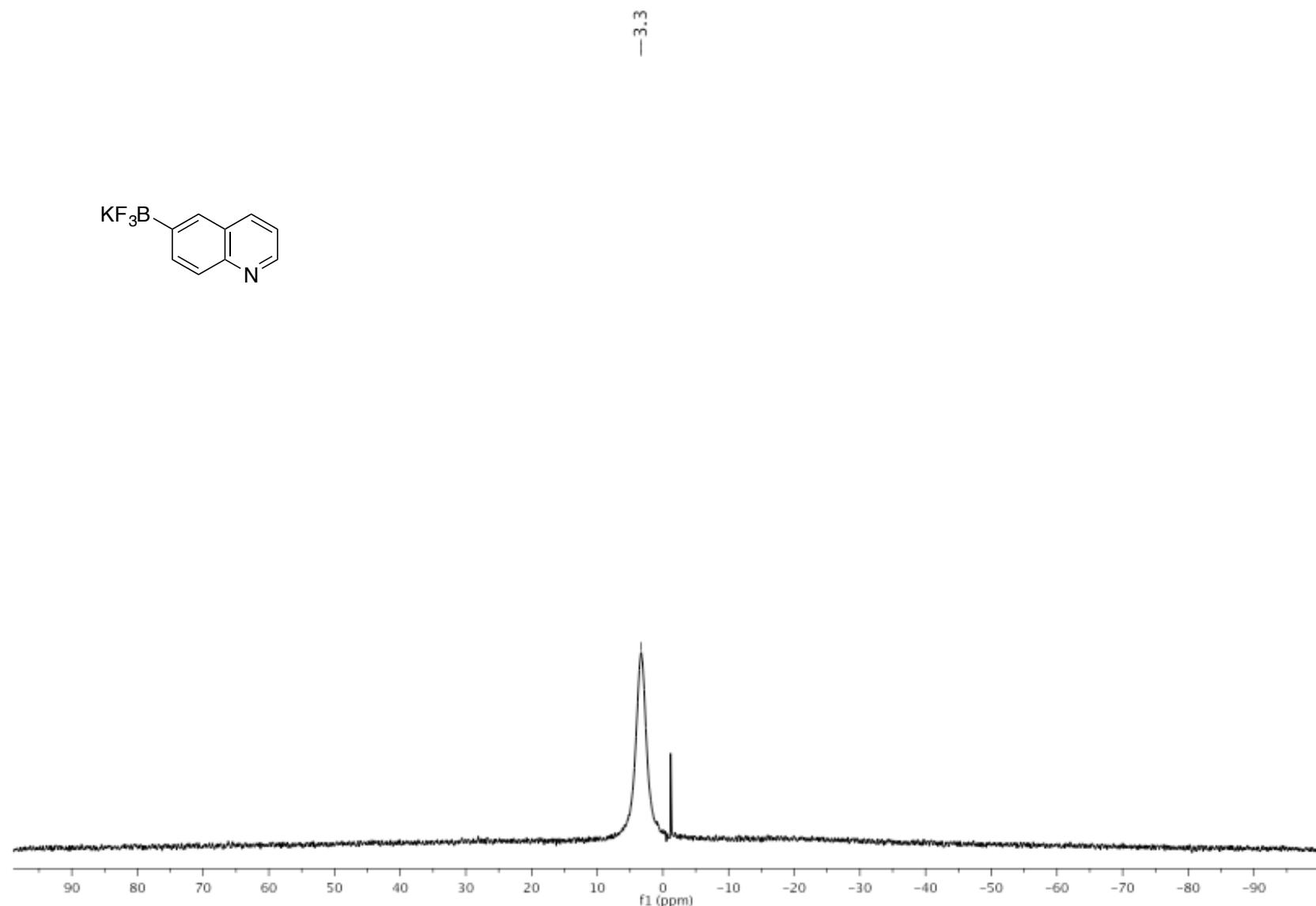


¹³C NMR (128.5 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(quinolin-6-yl)borate (3k, Table 3, entry 11)

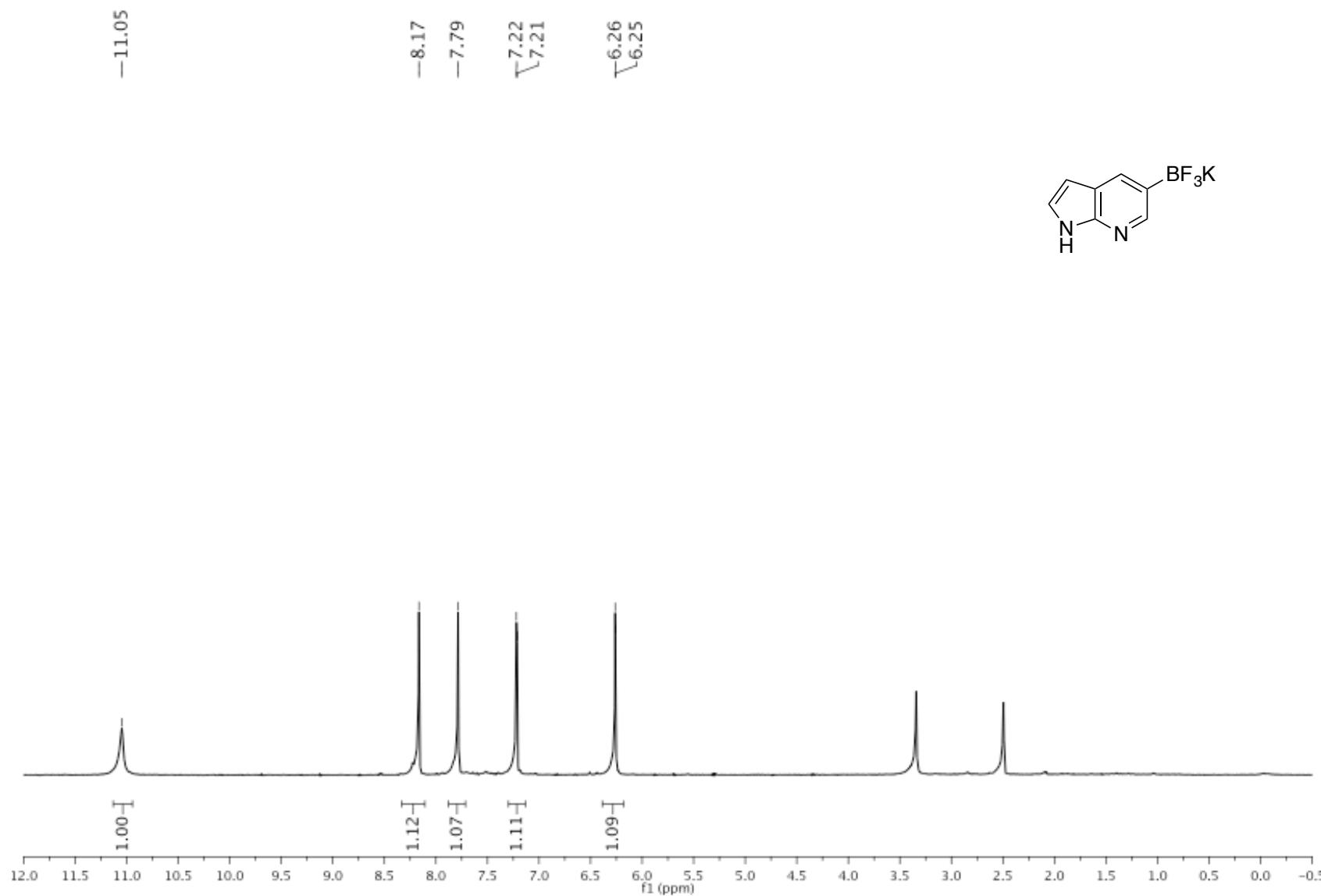
--139.1



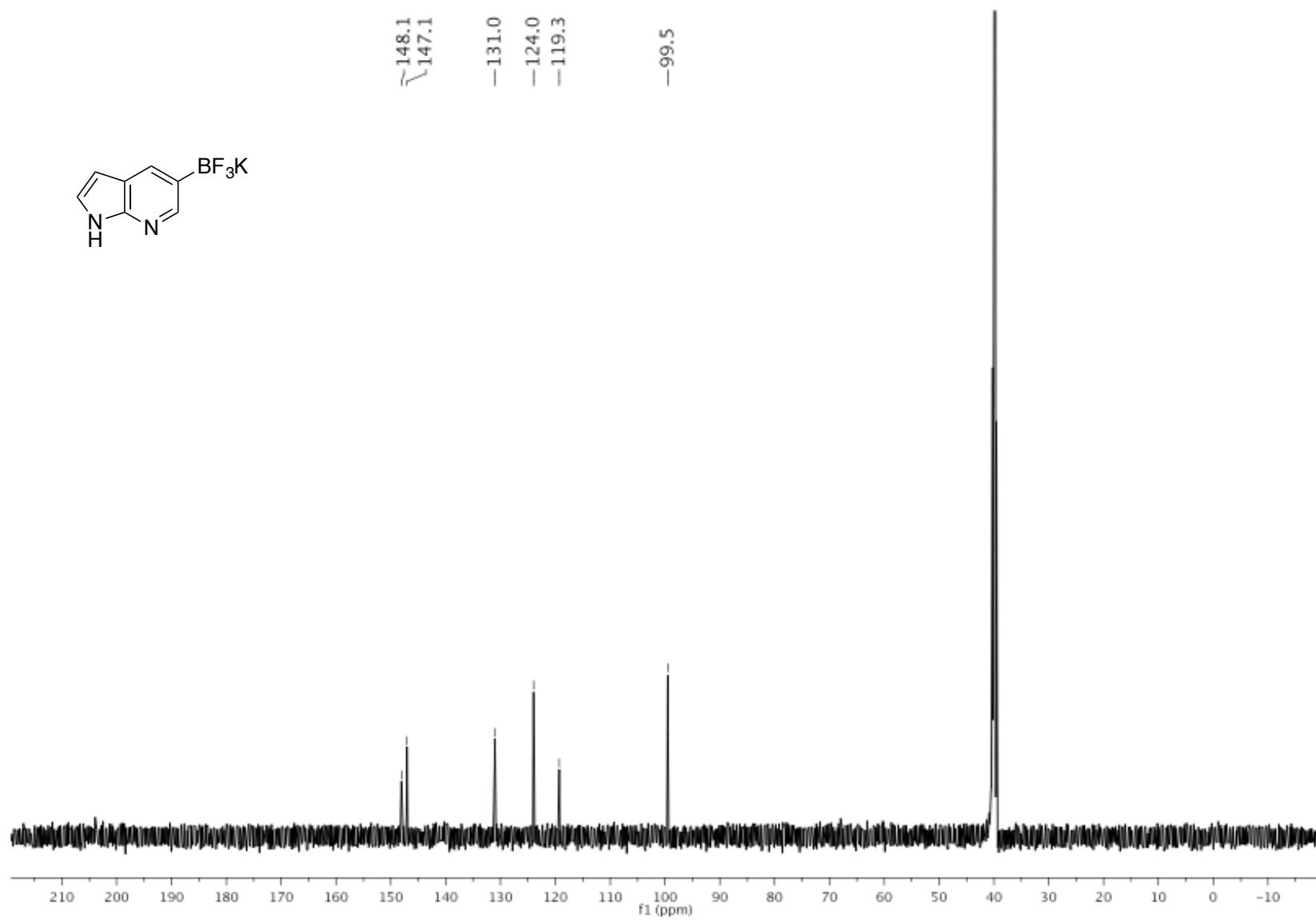
¹⁹F NMR (470.8 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(quinolin-6-yl)borate (3k, Table 3, entry 11)



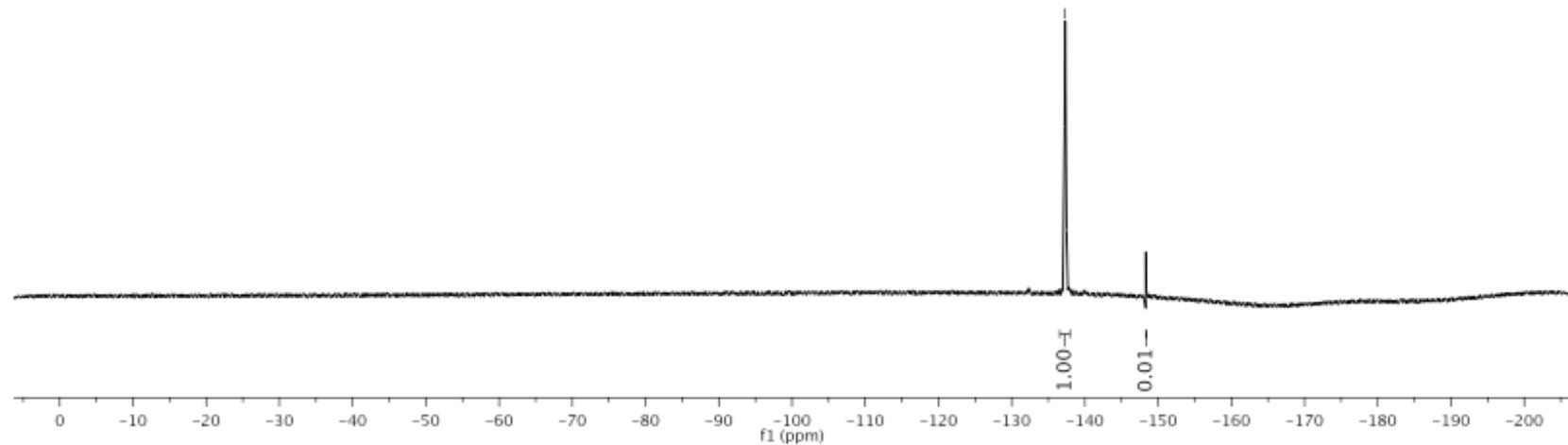
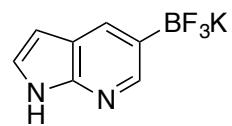
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(quinolin-6-yl)borate (3k, Table 3, entry 11)



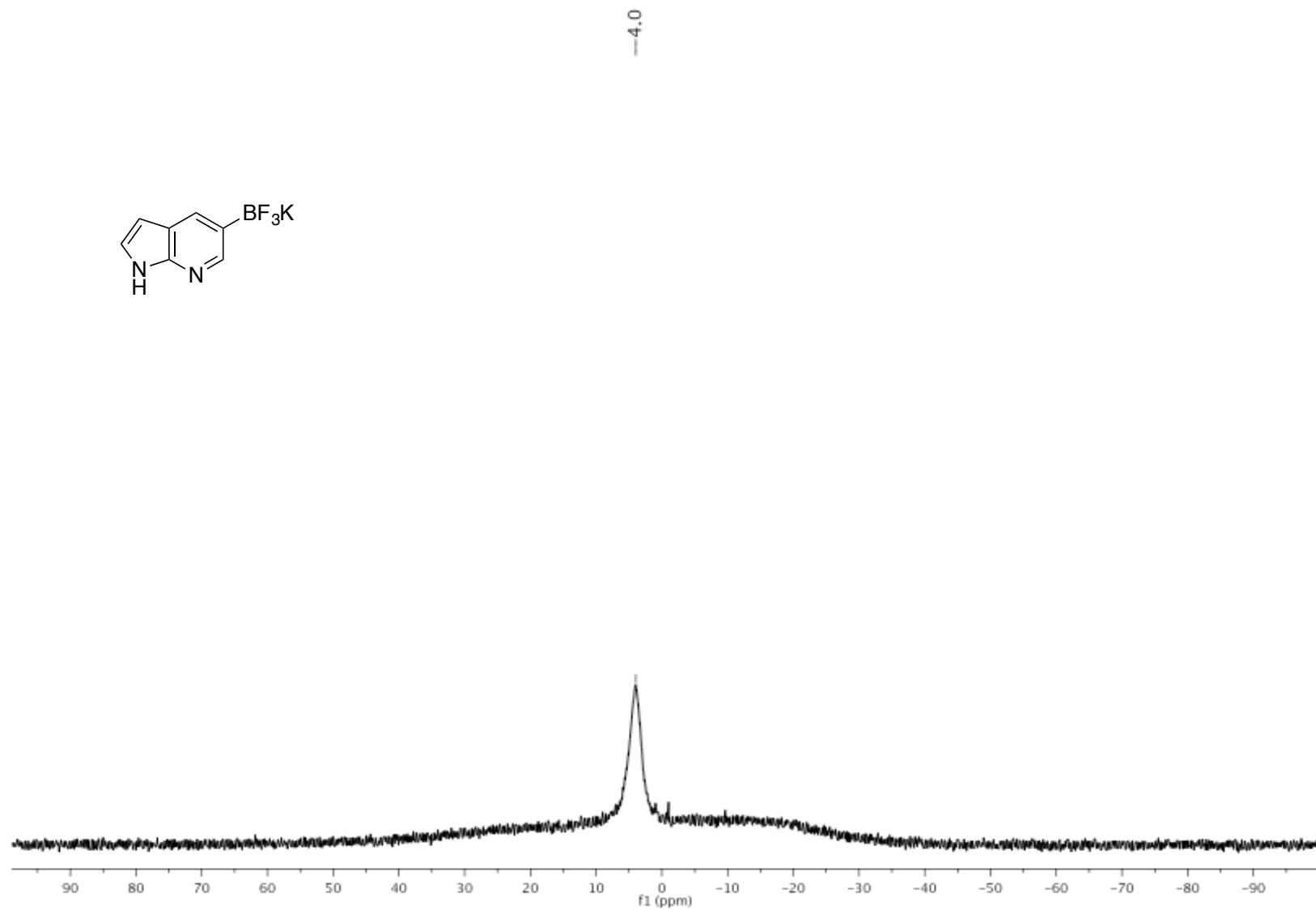
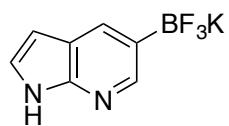
^1H NMR (500 MHz, DMSO - d_6) Spectrum of Potassium Trifluoro(1H -pyrrolo[2,3-*b*]pyridin-5-yl)borate (3l, Table 3, entry 12)



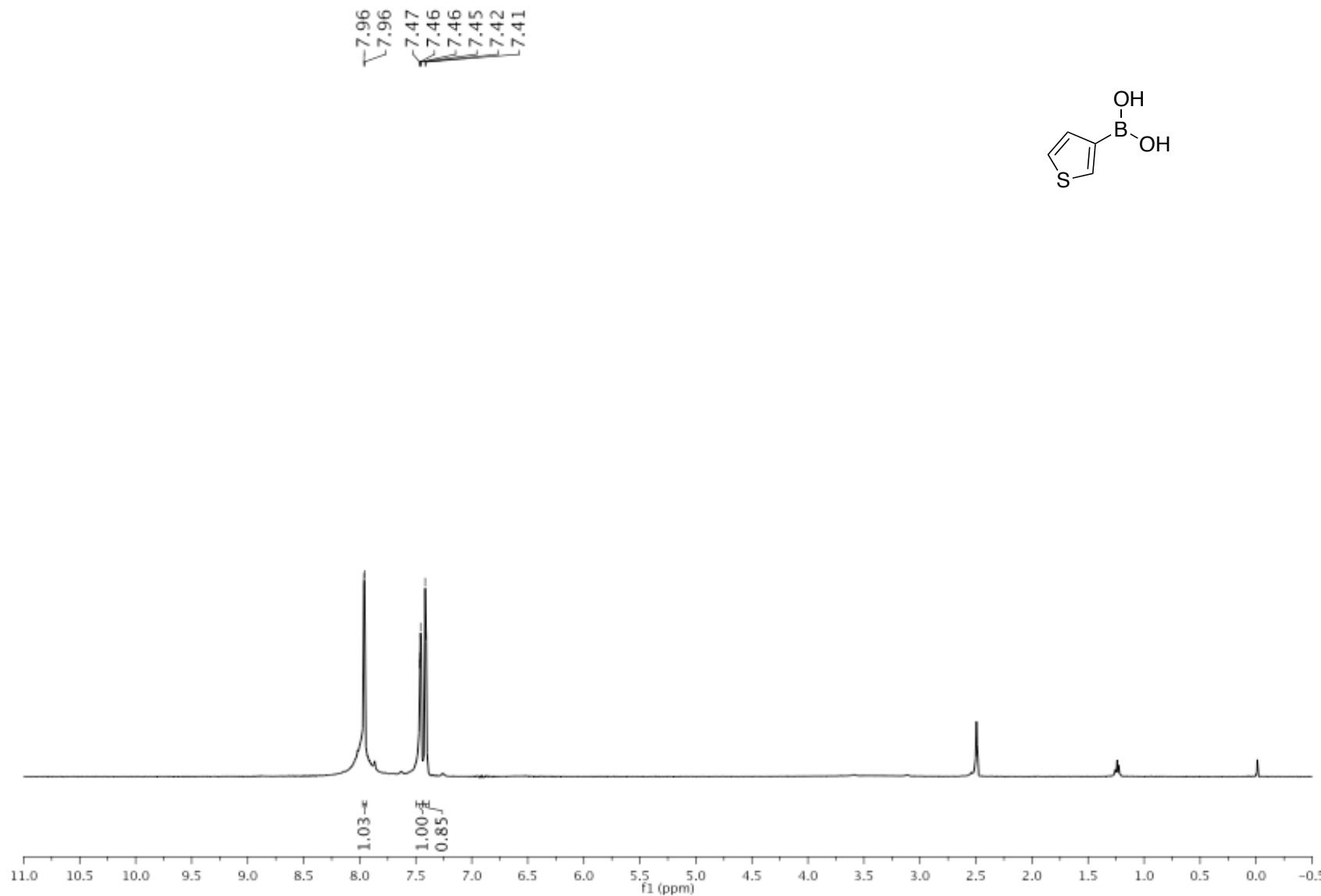
^{13}C NMR (128.5 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(1*H*-pyrrolo[2,3-*b*]pyridin-5-yl)borate (3l, Table 3, entry 12)



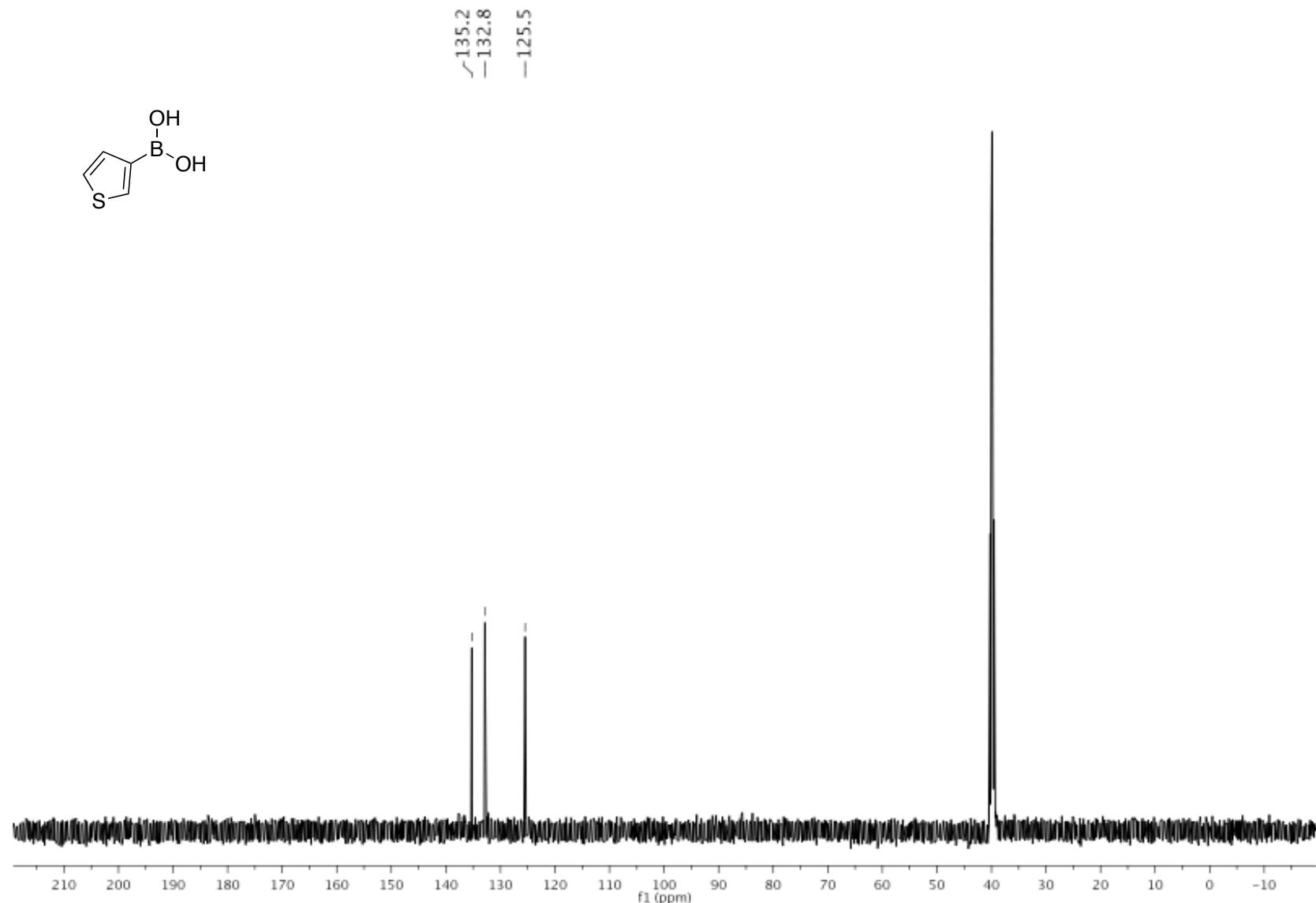
¹⁹F NMR (470.8 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(1*H*-pyrrolo[2,3-*b*]pyridin-5-yl)borate (3l, Table 3, entry 12)



¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(1*H*-pyrrolo[2,3-*b*]pyridin-5-yl)borate (3l, Table 3, entry 12)



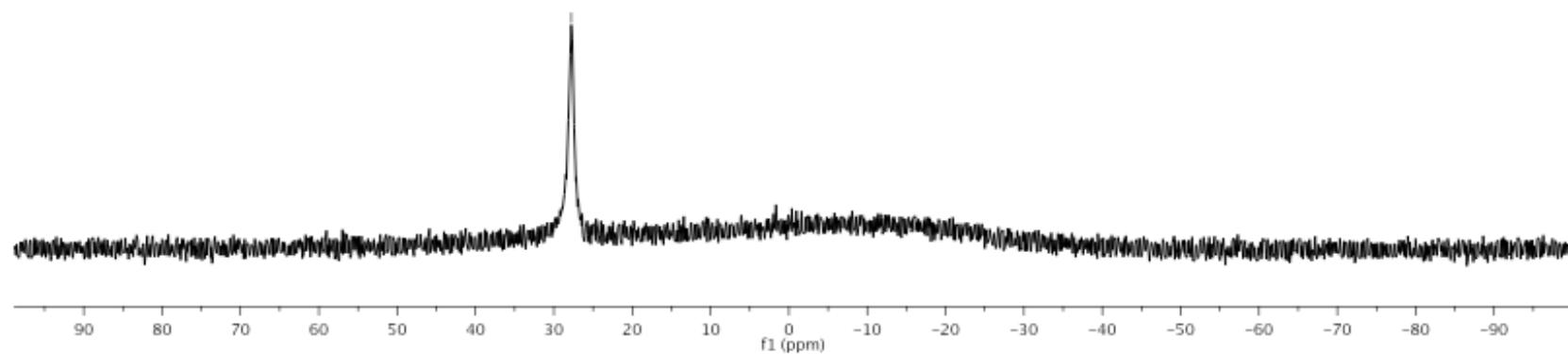
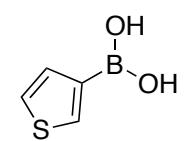
^1H NMR (500 MHz, $\text{DMSO}-\text{d}_6$) Spectrum of Thien-3-ylboronic acid (4a, Table 4, entry 1)



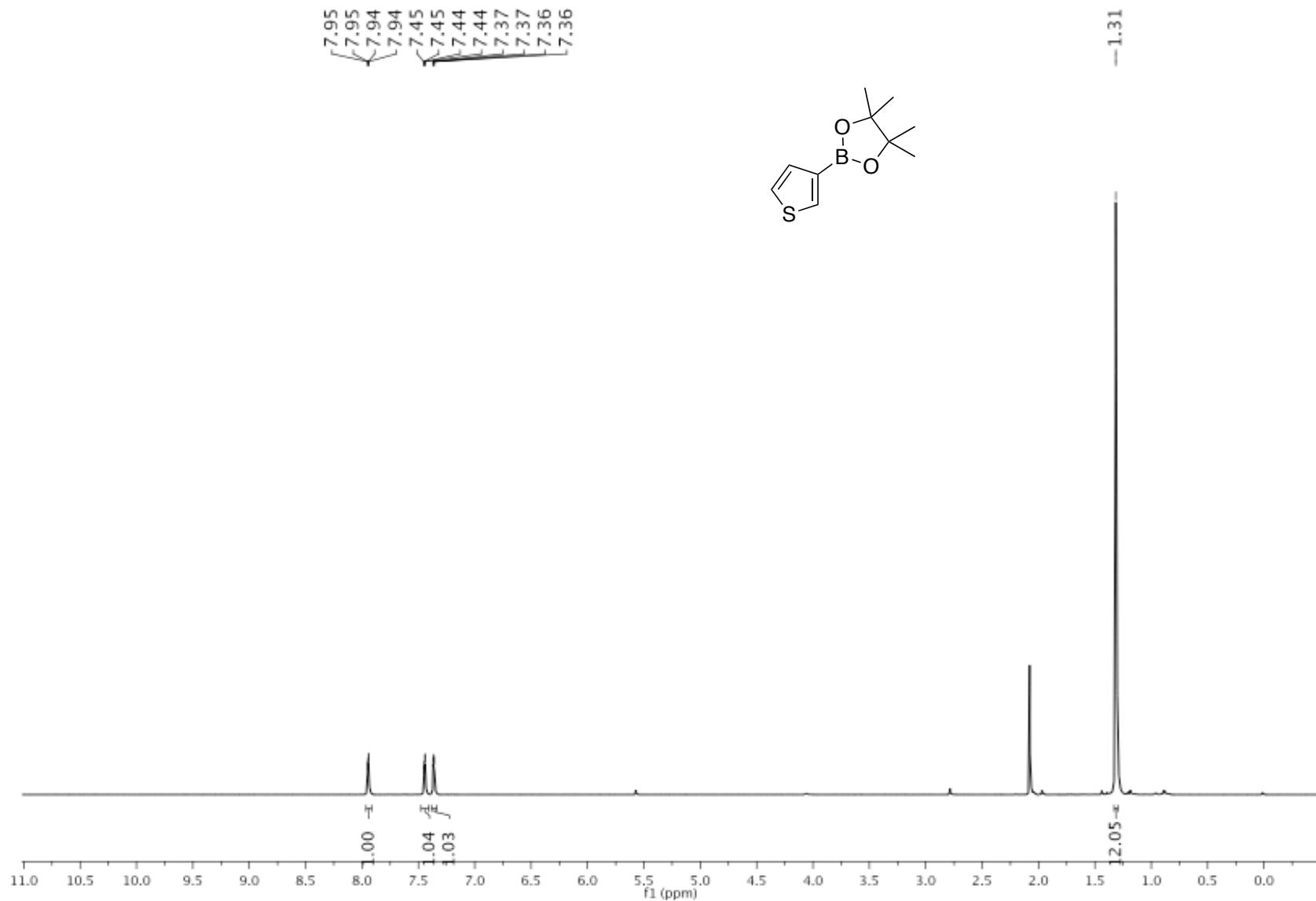
^{13}C NMR (128.5 MHz, DMSO-d_6) Spectrum of Thien-3-ylboronic acid (4a, Table 4, entry 1)

S-132

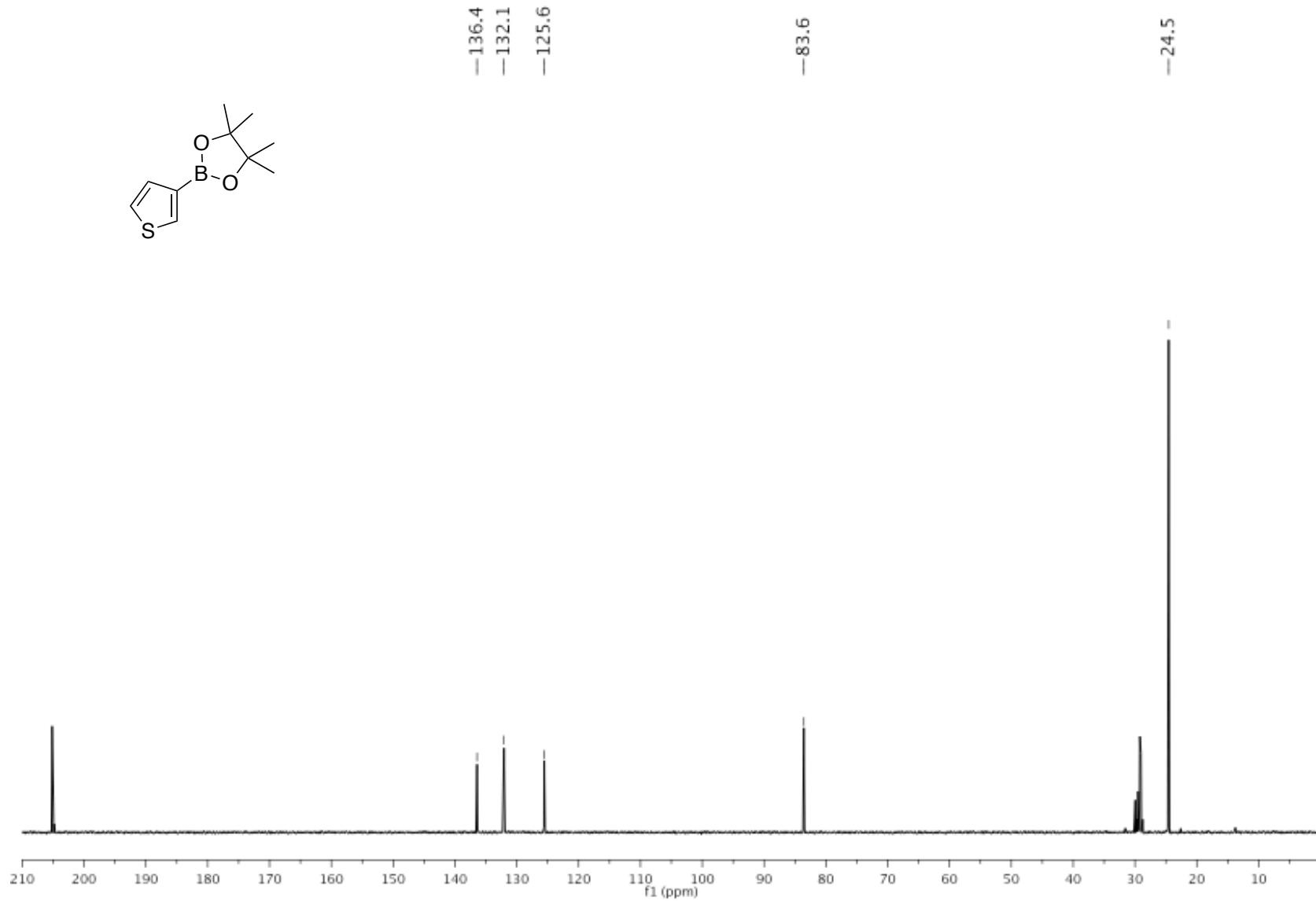
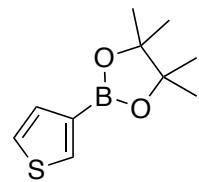
⁰B
—27.8



¹¹B NMR (128.4 MHz, acetone-d₆) Spectrum of Thien-3-ylboronic acid (4a, Table 4, entry 1)



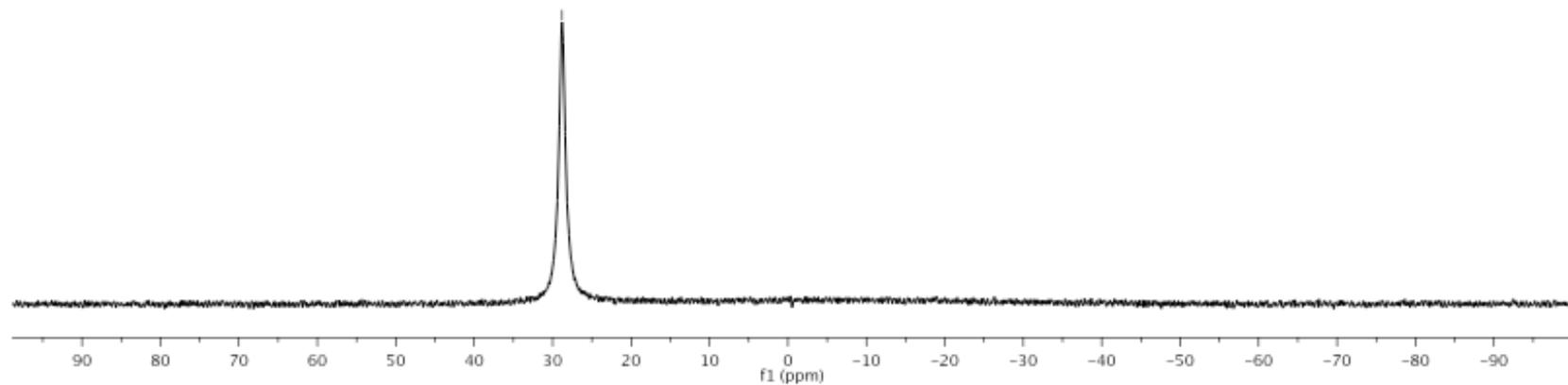
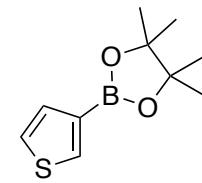
S-134



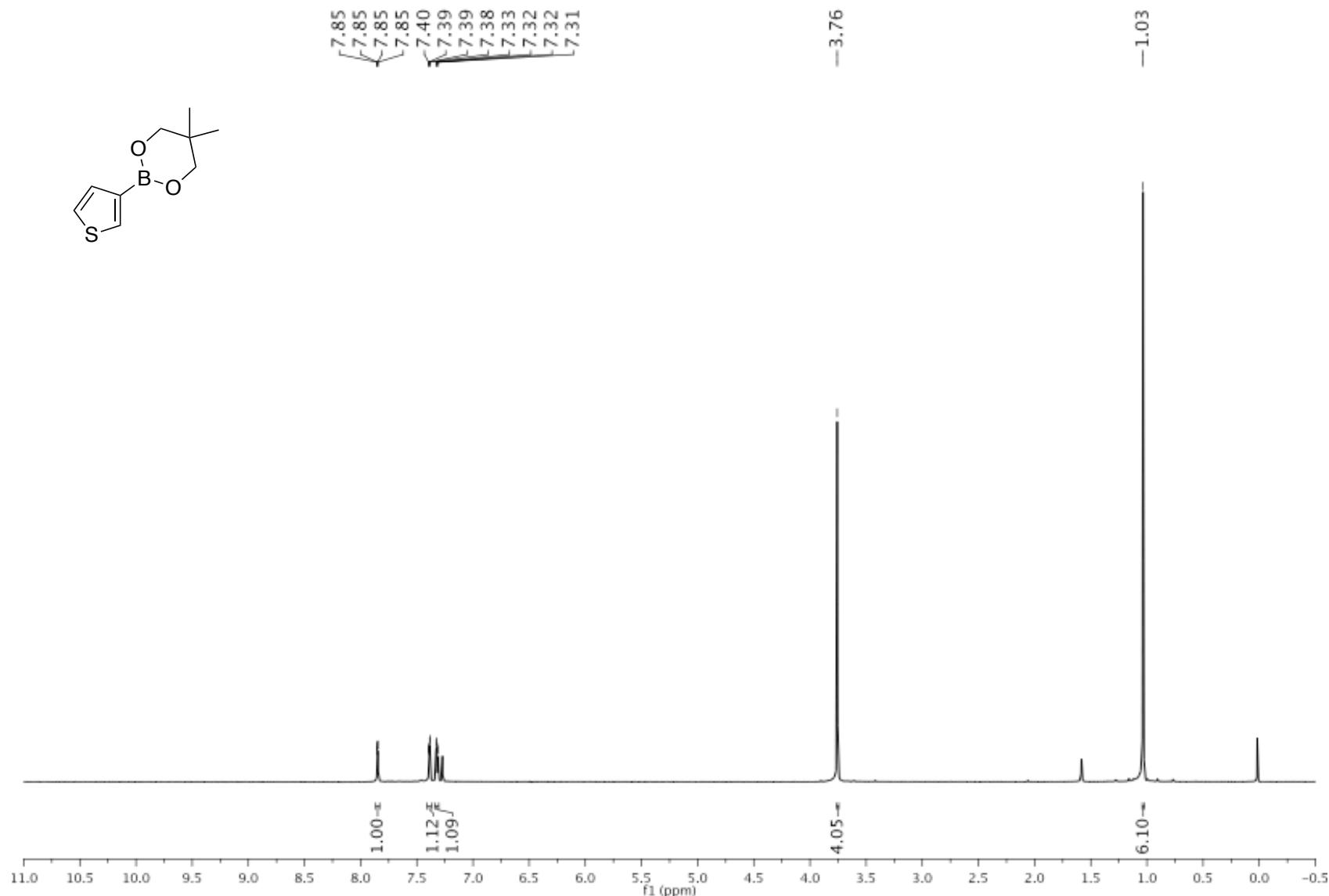
¹³C NMR (128.5 MHz, acetone -d₆) Spectrum of 4,4,5,5-Tetramethyl-2-(thien-3-yl)-1,3,2-dioxaborolane (4b, Table 4, entry 2)

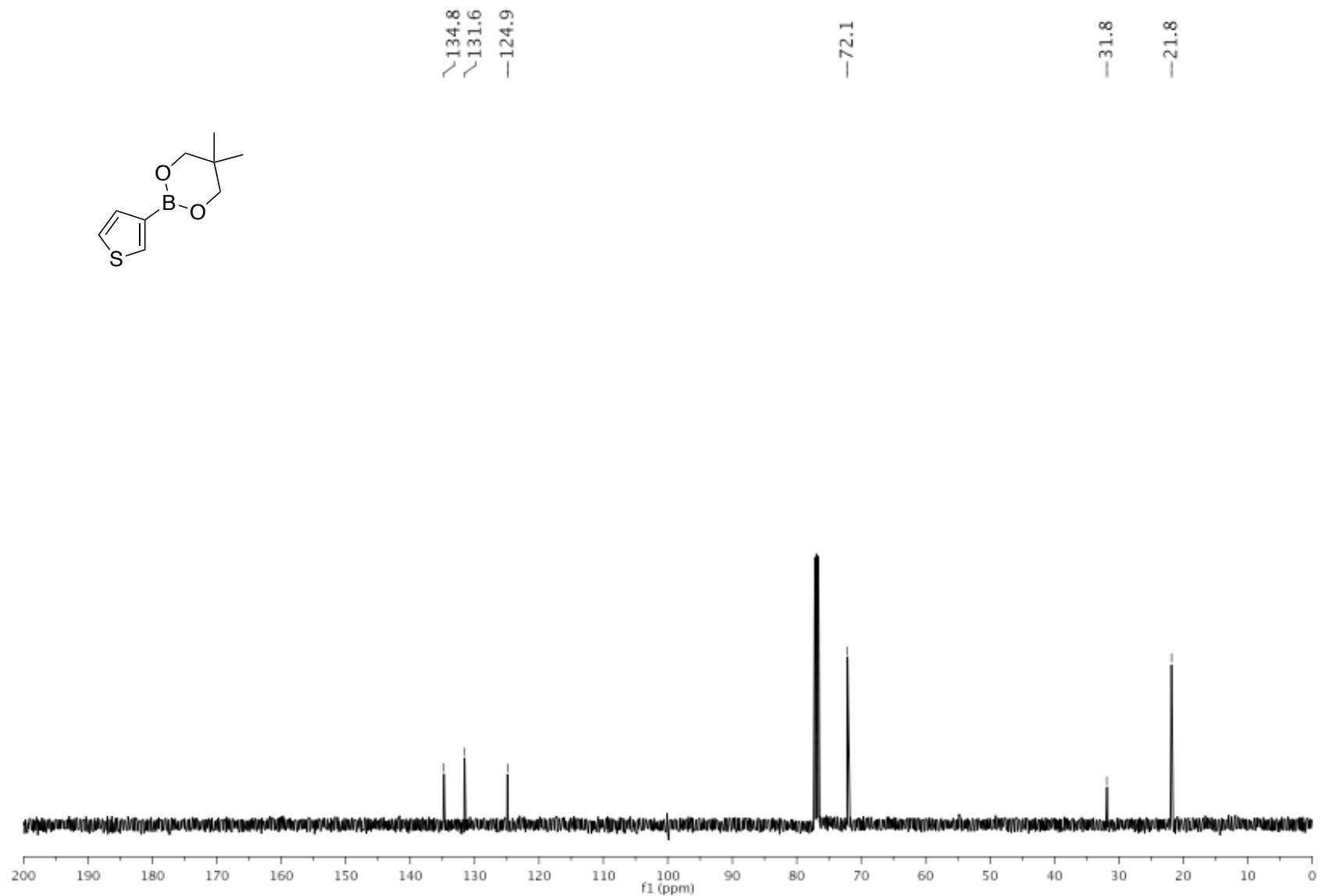
S-135

-28.8



¹¹B NMR (128.4 MHz, acetone-d₆) Spectrum of 4,4,5,5-Tetramethyl-2-(thien-3-yl)-1,3,2-dioxaborolane (4b, Table 4, entry 2)

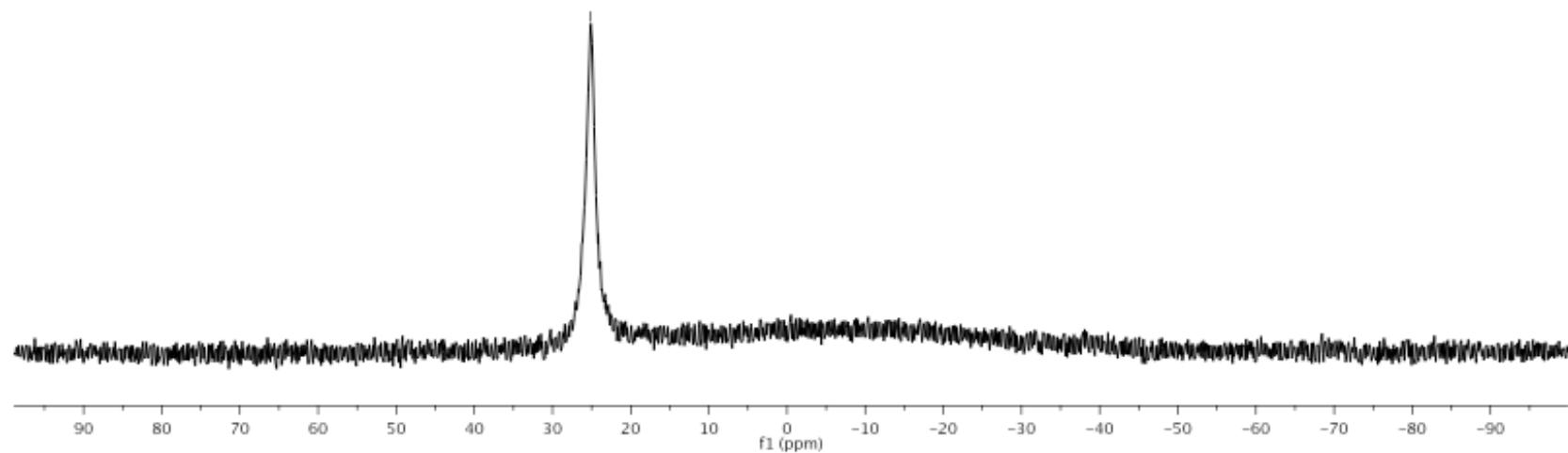
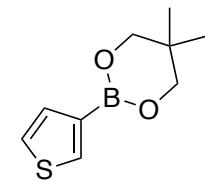




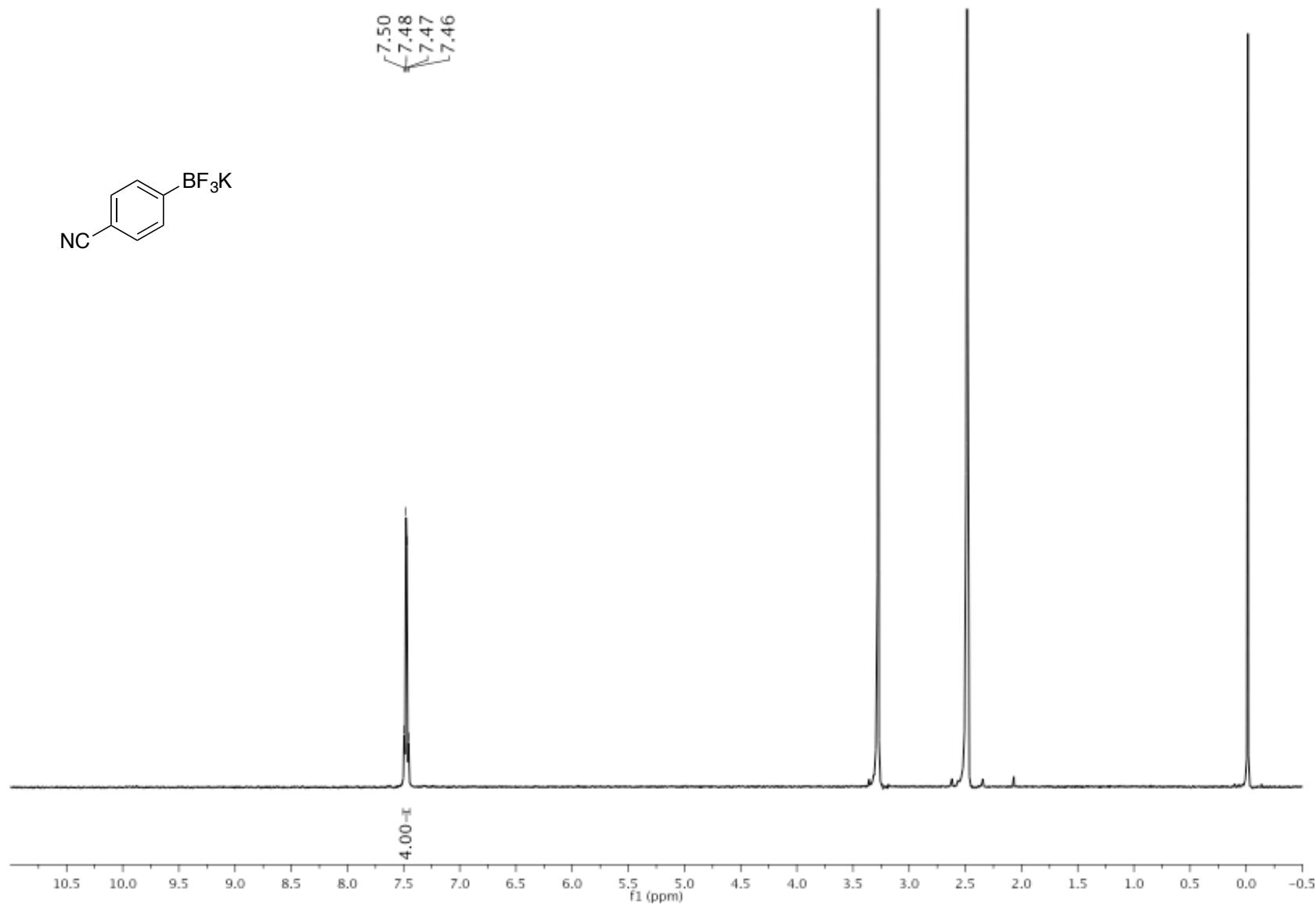
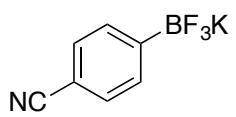
^{13}C NMR (128.5 MHz, acetone- d_6) Spectrum of 5,5-Dimethyl-2-(thien-3-yl)-1,3,2-dioxaborinane (4c, Table 4, entry 3)

S-138

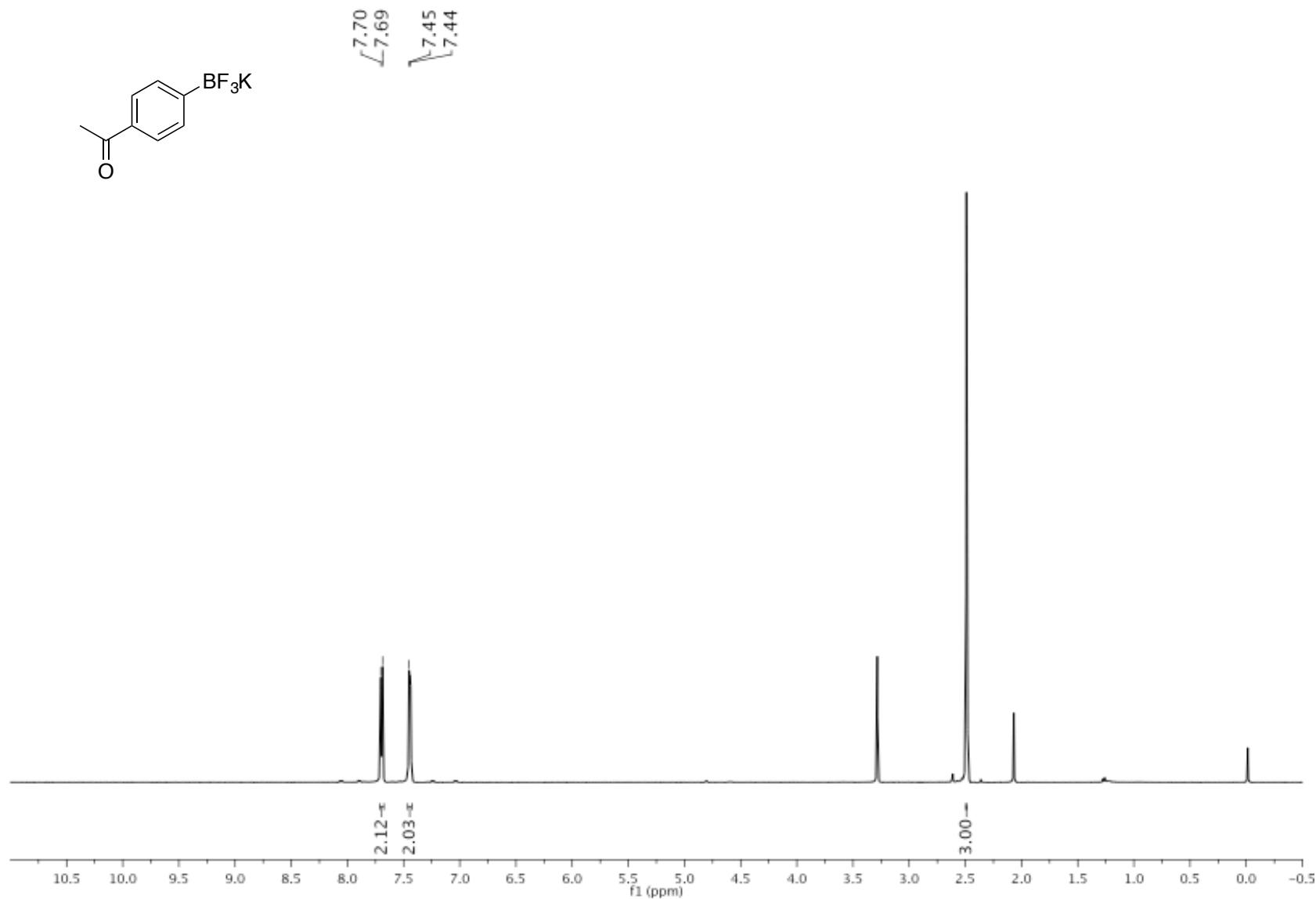
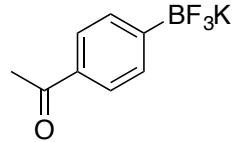
-25.11



¹¹B NMR (128.4 MHz, acetone-d₆) Spectrum of 5,5-Dimethyl-2-(thien-3-yl)-1,3,2-dioxaborinane (4c, Table 4, entry 3)



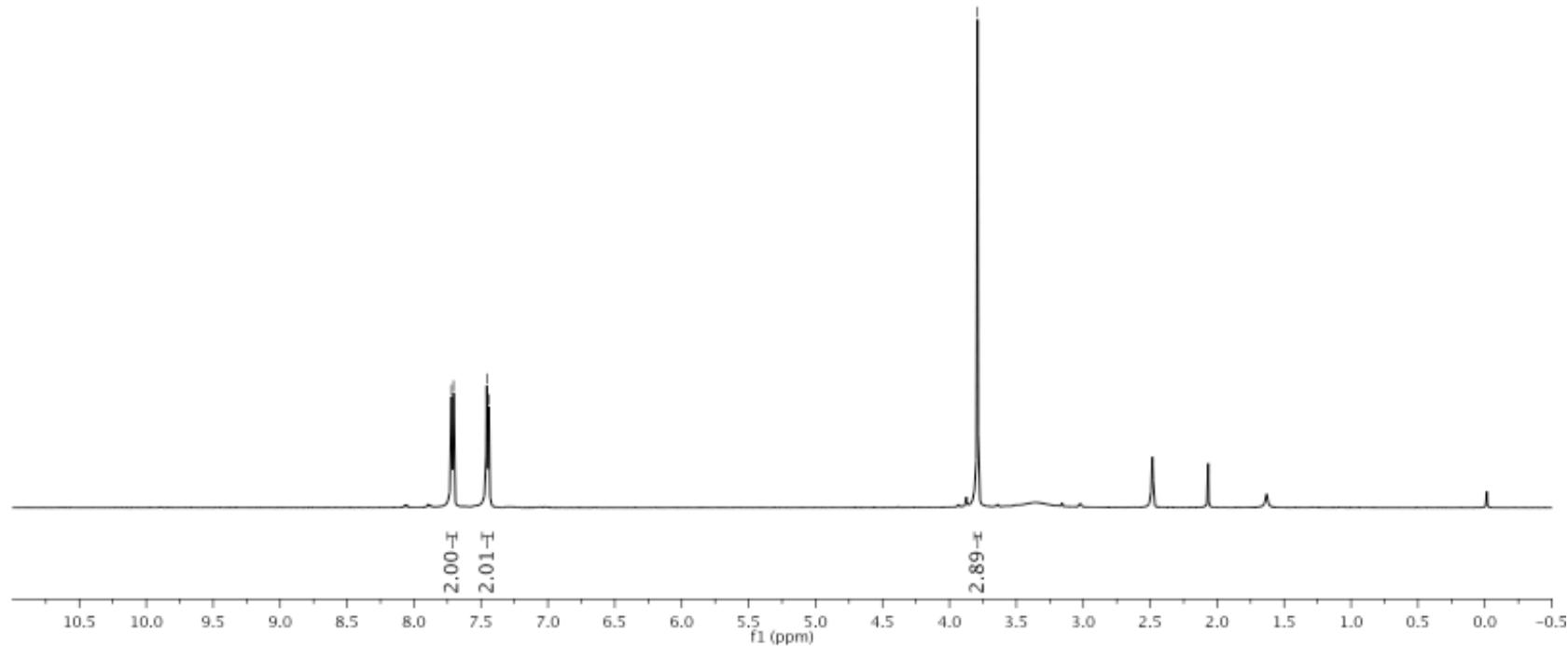
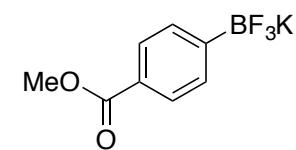
^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium (4-Cyanophenyl)trifluoroborate (2a, Table 5, entry 1)



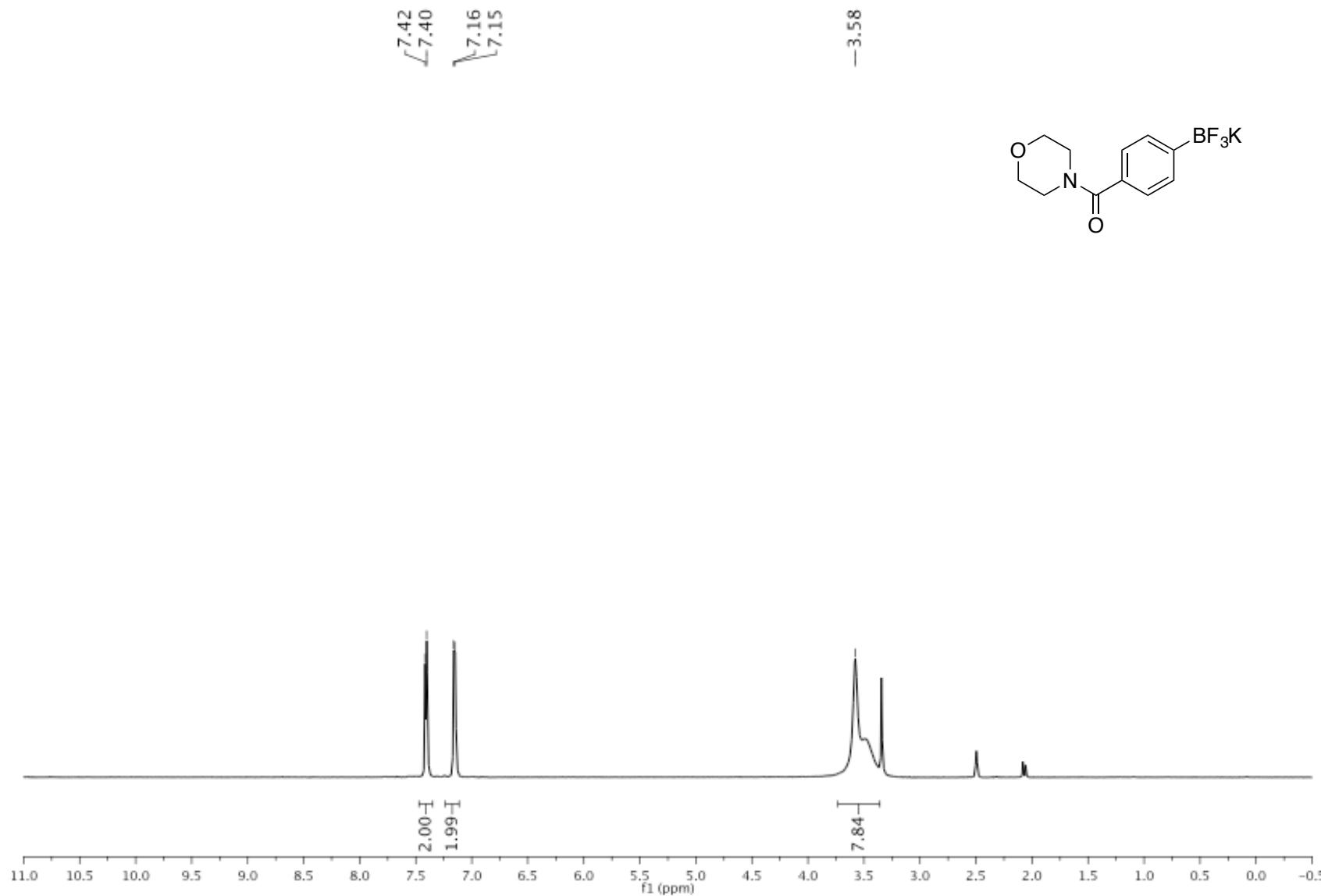
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium (4-Acetylphenyl)trifluoroborate (2c, Table 5, entry 2)

7.72
7.70
7.46
7.44

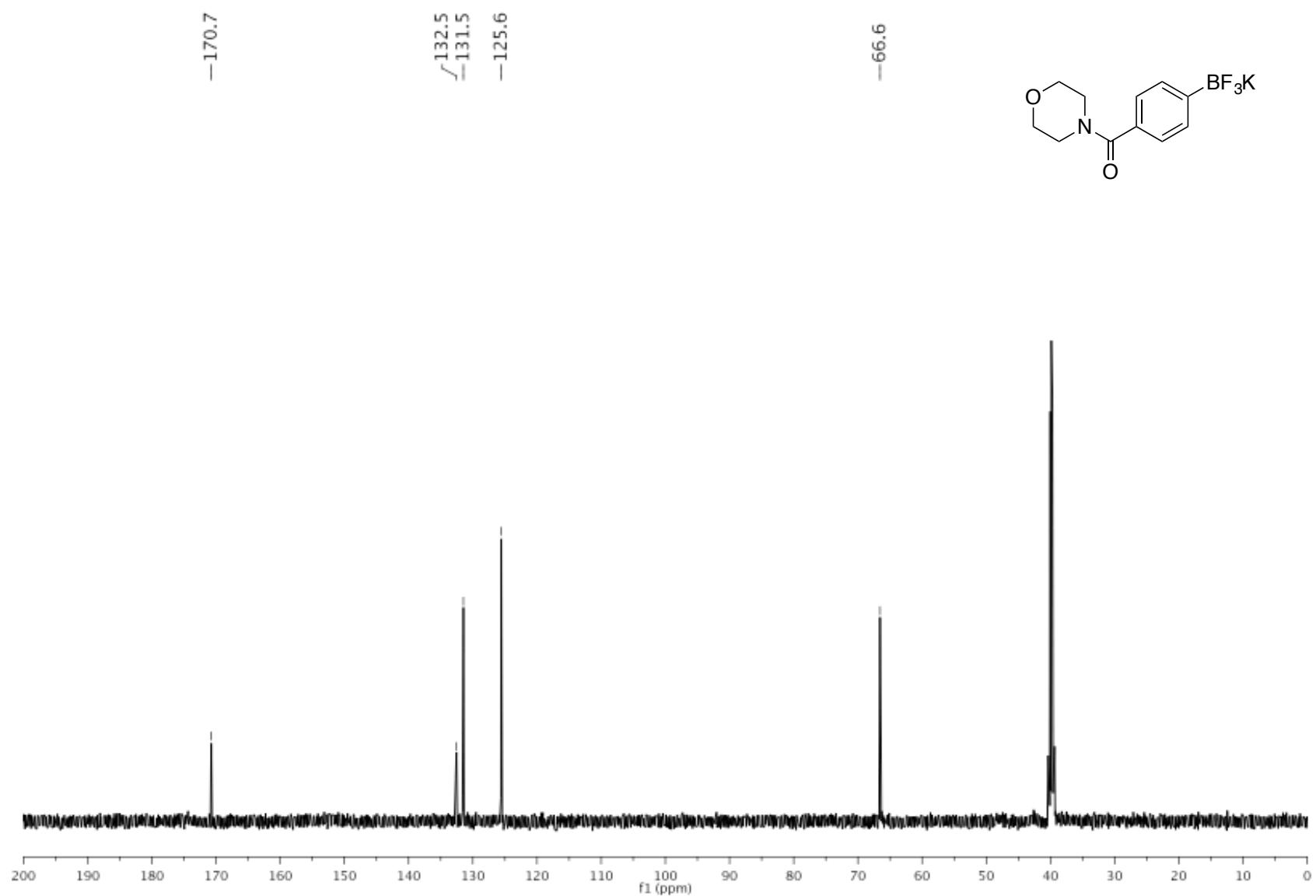
-3.79



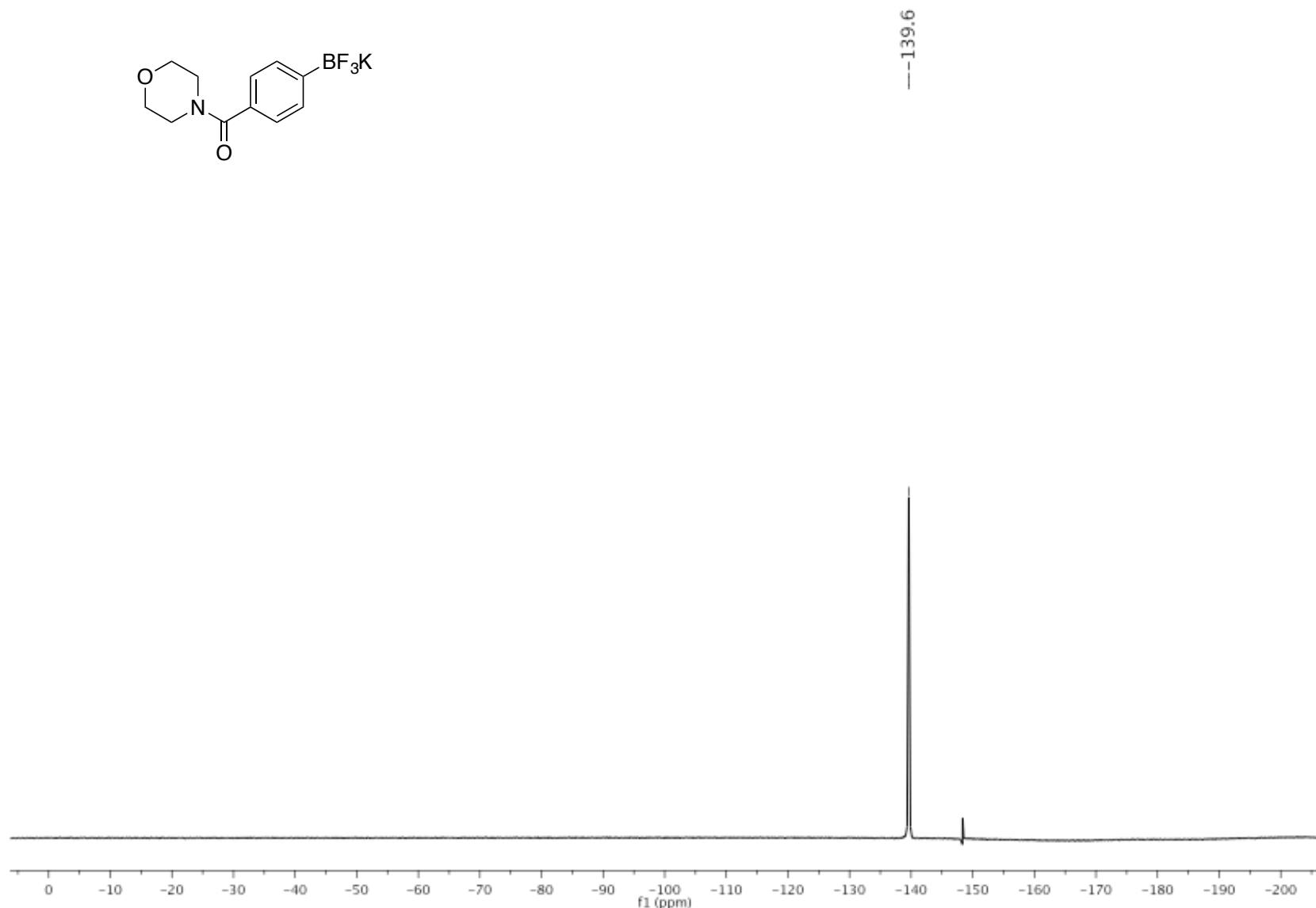
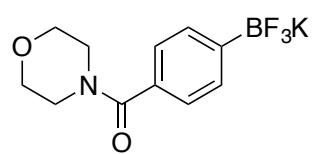
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-(methoxycarbonyl)phenyl)borate (2e, Table 5, entry 3)



¹H NMR (500 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(4-(morpholine-4-carbonyl)phenyl)borate (5a, Table 5, entry 4)

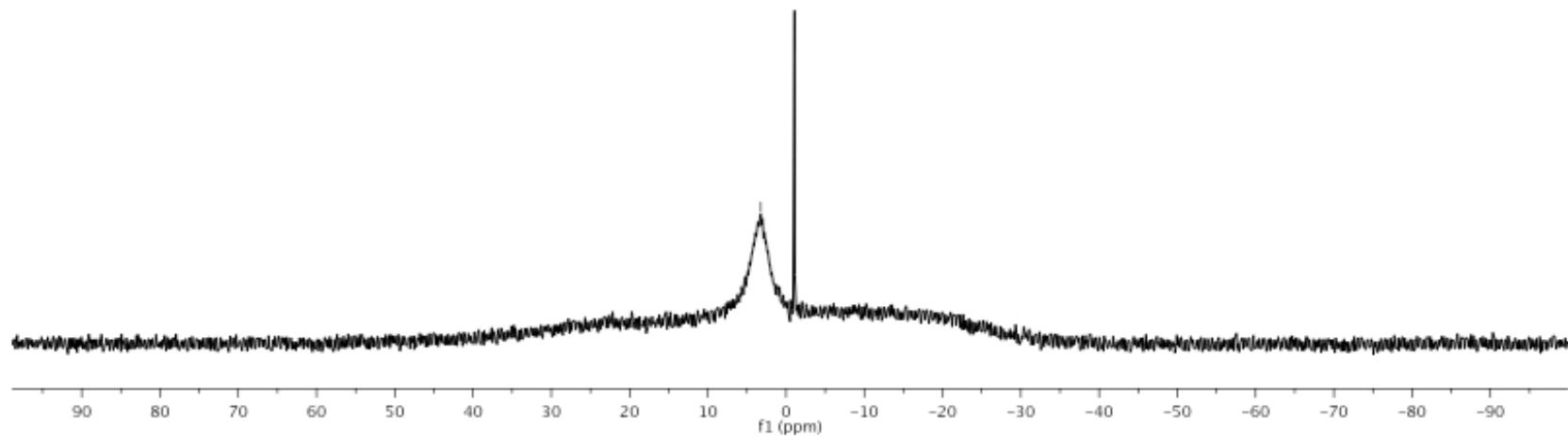
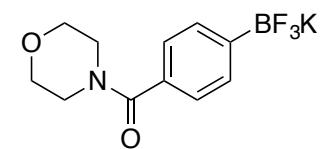


^{13}C NMR (128.5 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(4-(morpholine-4-carbonyl)phenyl)borate (5a, Table 5, entry 4)

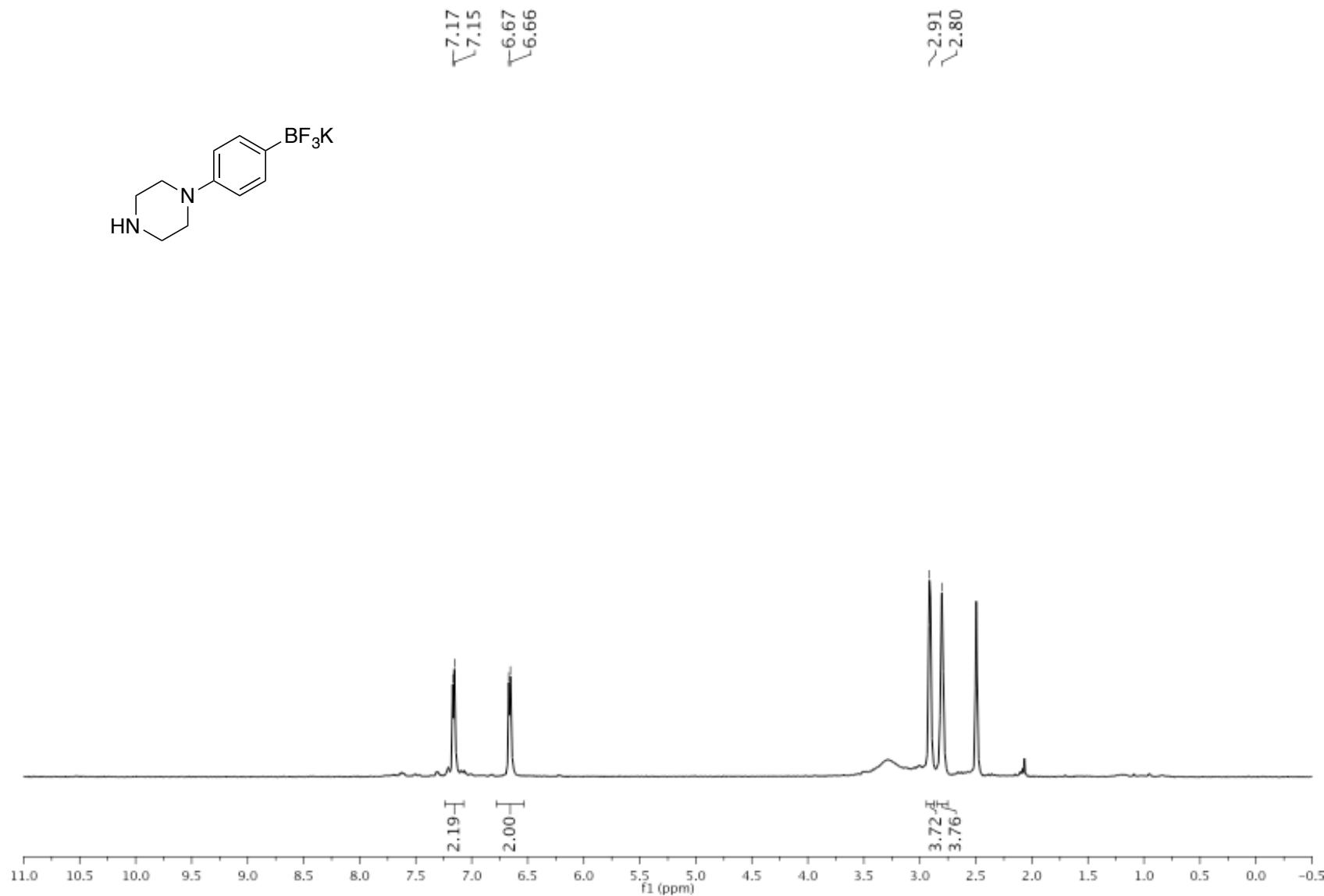
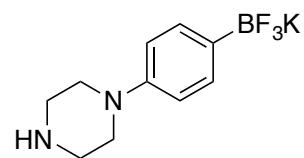


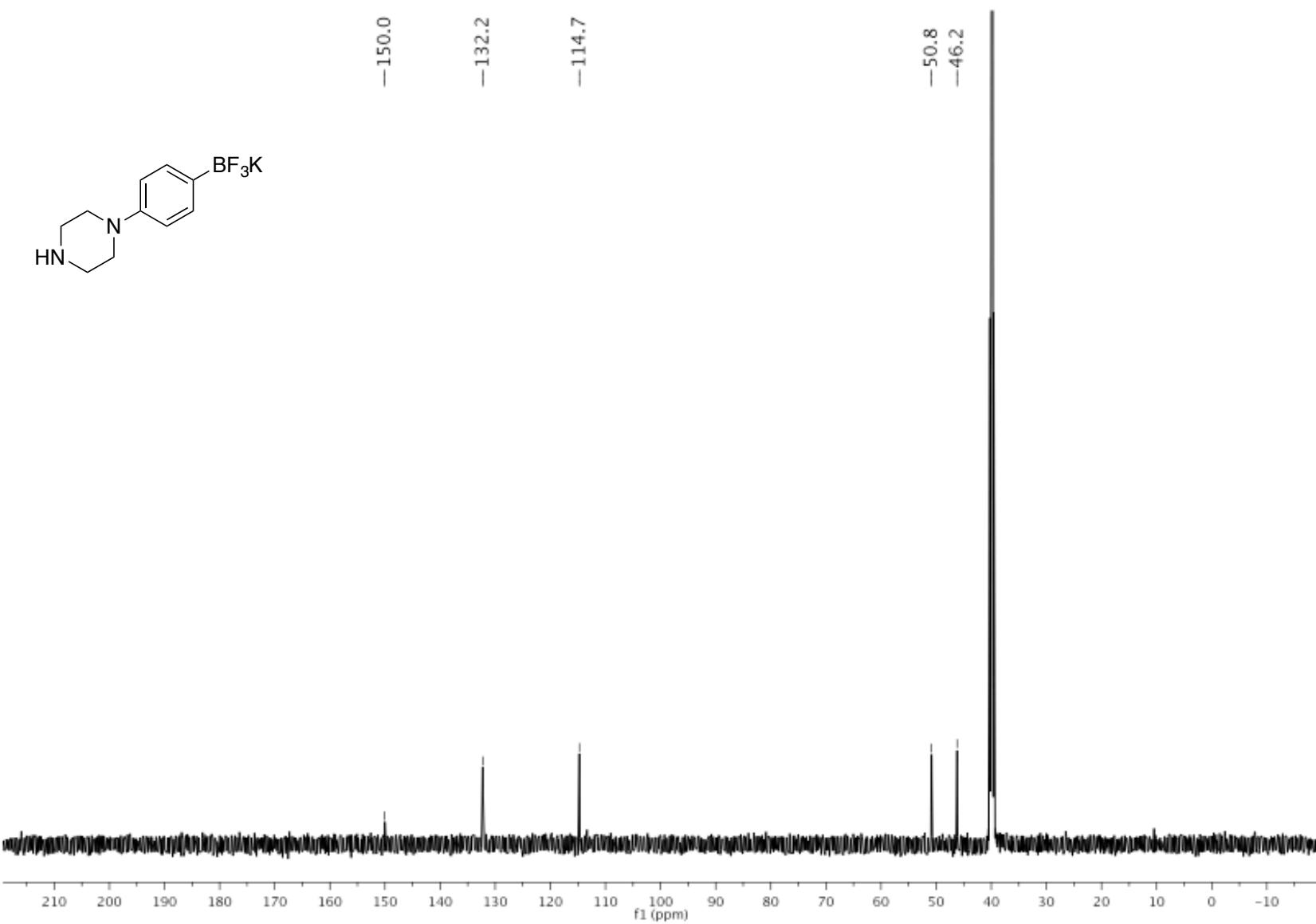
${}^{19}\text{F}$ NMR (470.8 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(4-(morpholine-4-carbonyl)phenyl)borate (5a, Table 5, entry 4)

-3.2

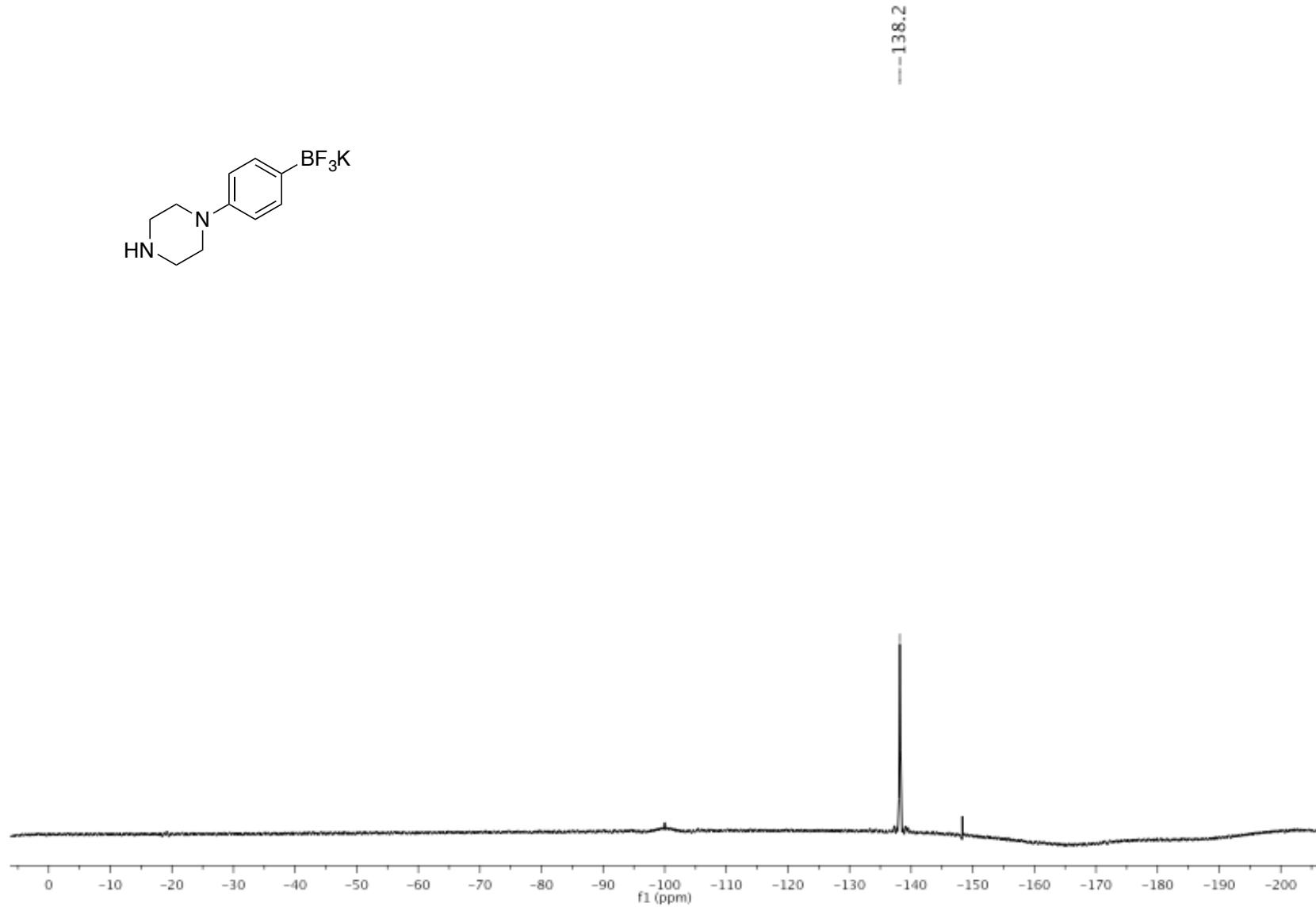
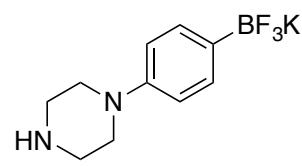


¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-(morpholine-4-carbonyl)phenyl)borate (5a, Table 5, entry 4)

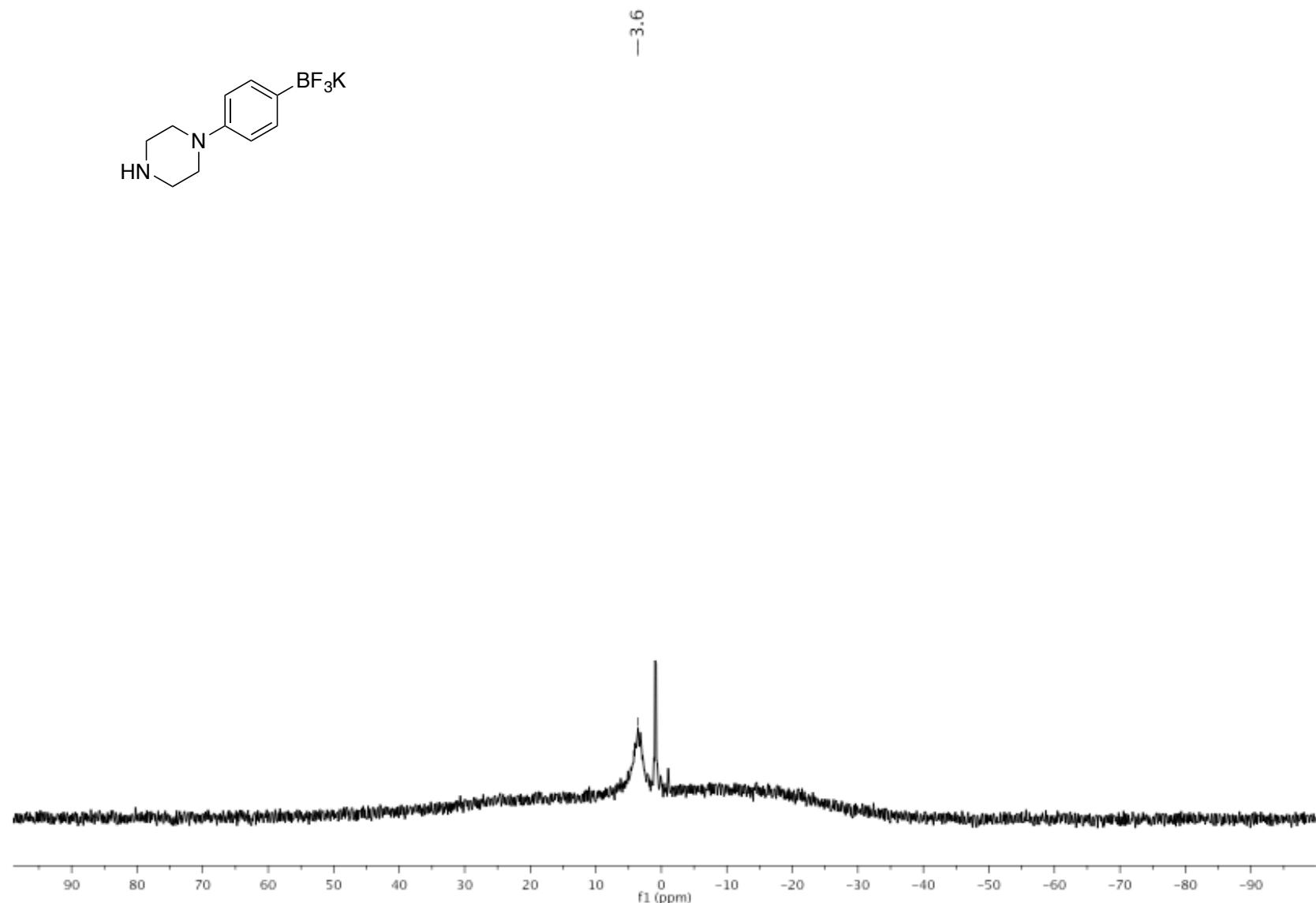




^{13}C NMR (128.5 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(4-(piperazin-1-yl)phenyl)borate (5b, Table 5, entry 5)

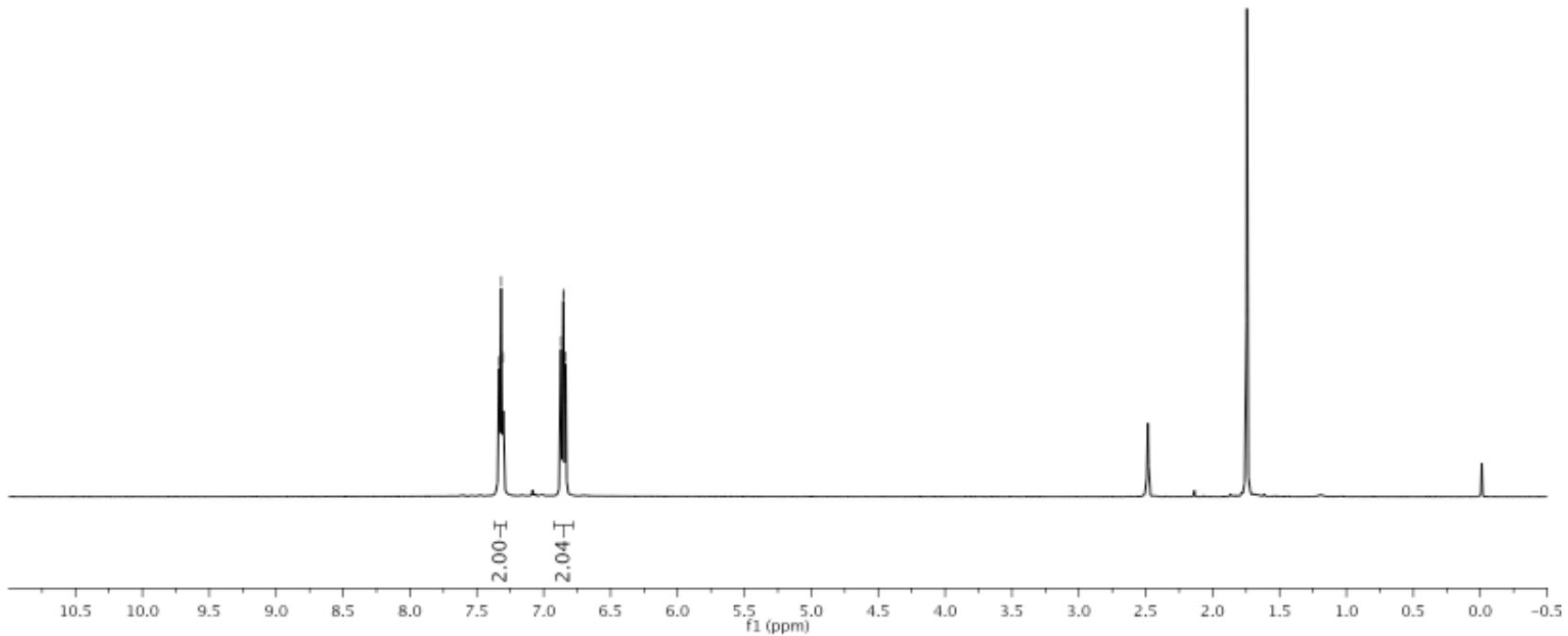
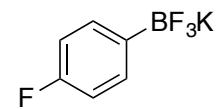


¹⁹F NMR (470.8 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(4-(piperazin-1-yl)phenyl)borate (5b, Table 5, entry 5)

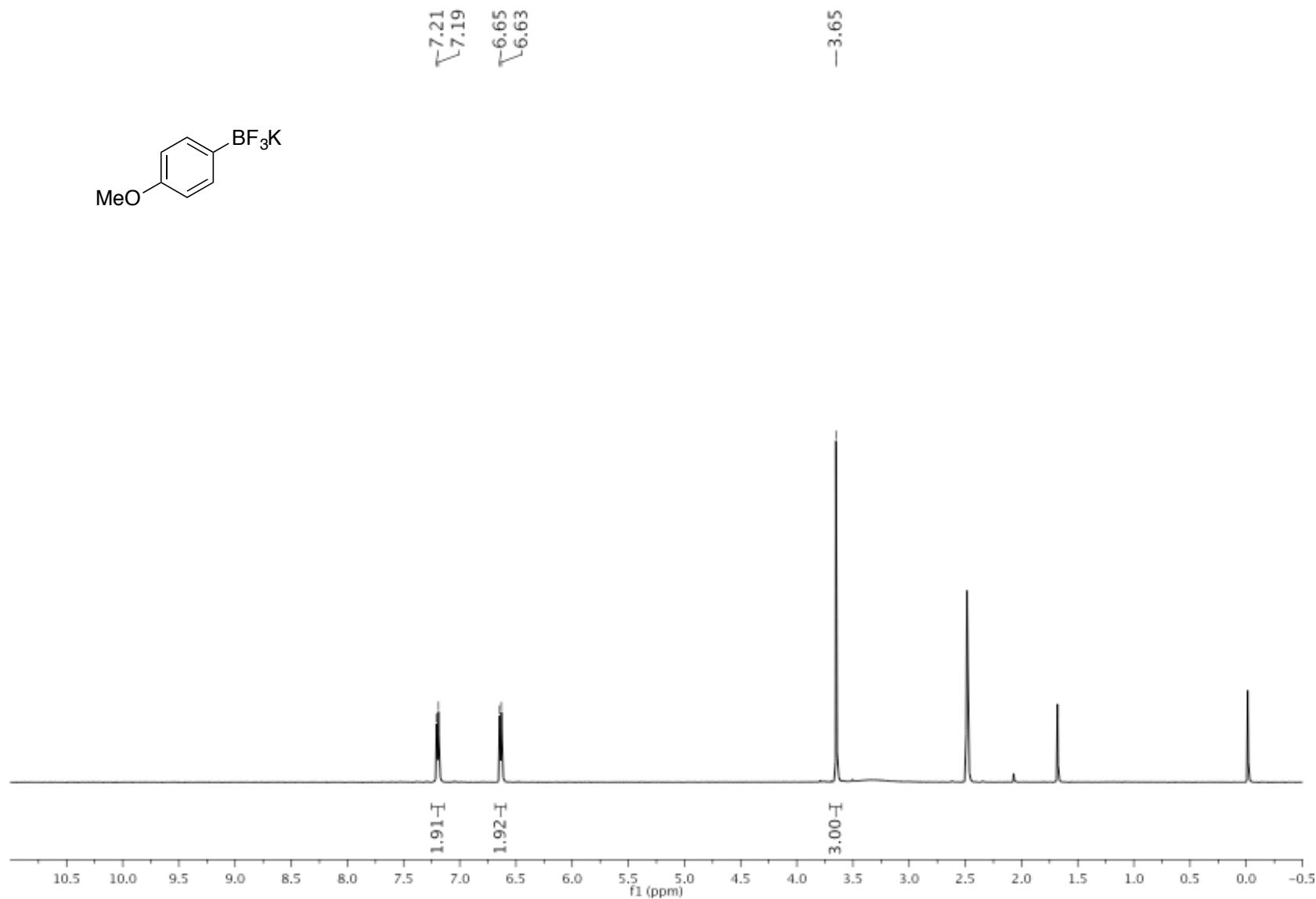
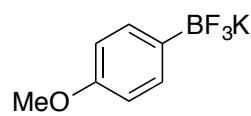


^{11}B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-(piperazin-1-yl)phenyl)borate (5b, Table 5, entry 5)

7.33
7.32
7.30
6.87
6.85
6.85
6.84



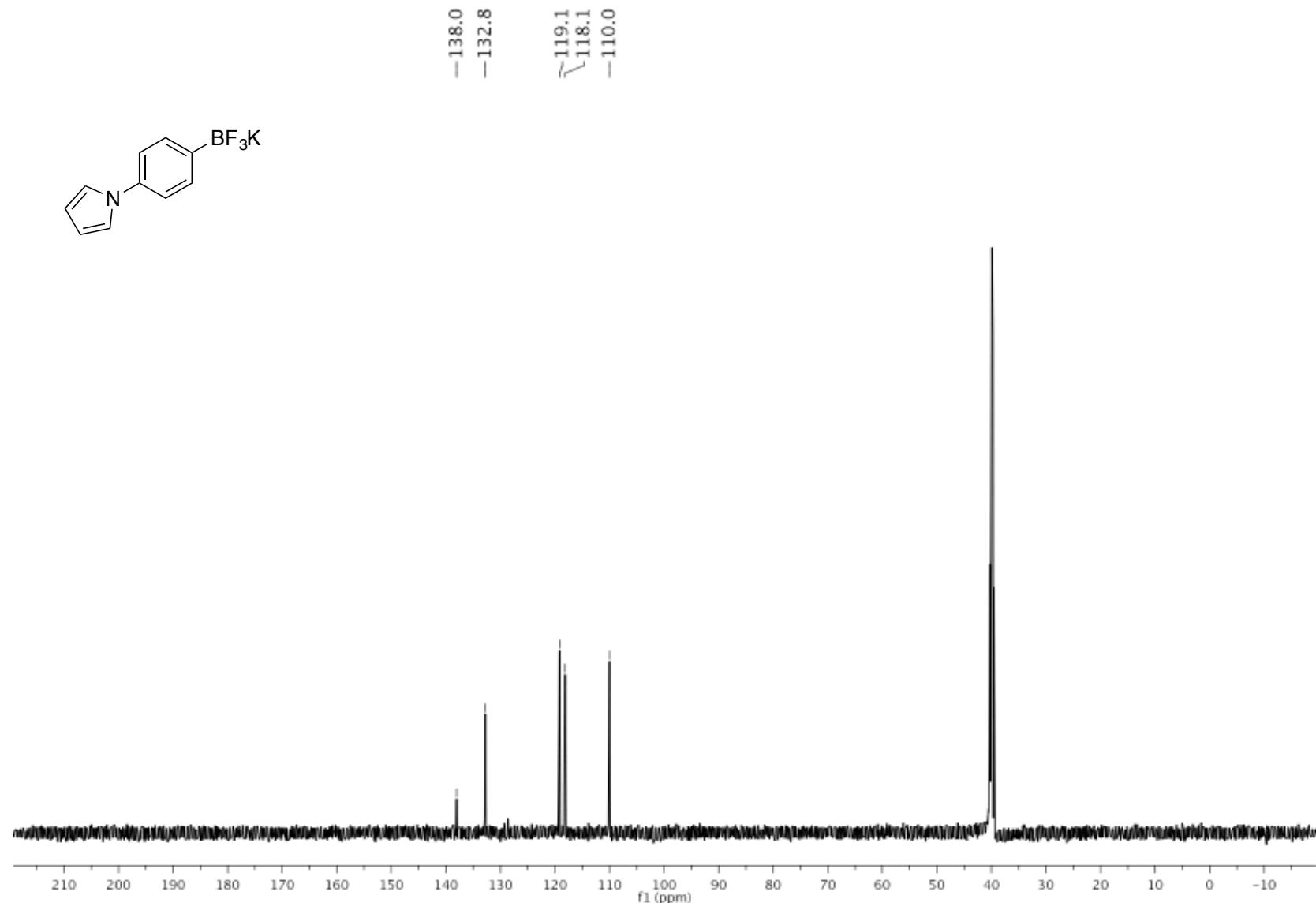
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-fluorophenyl)borate (2i, Table 5, entry 6)



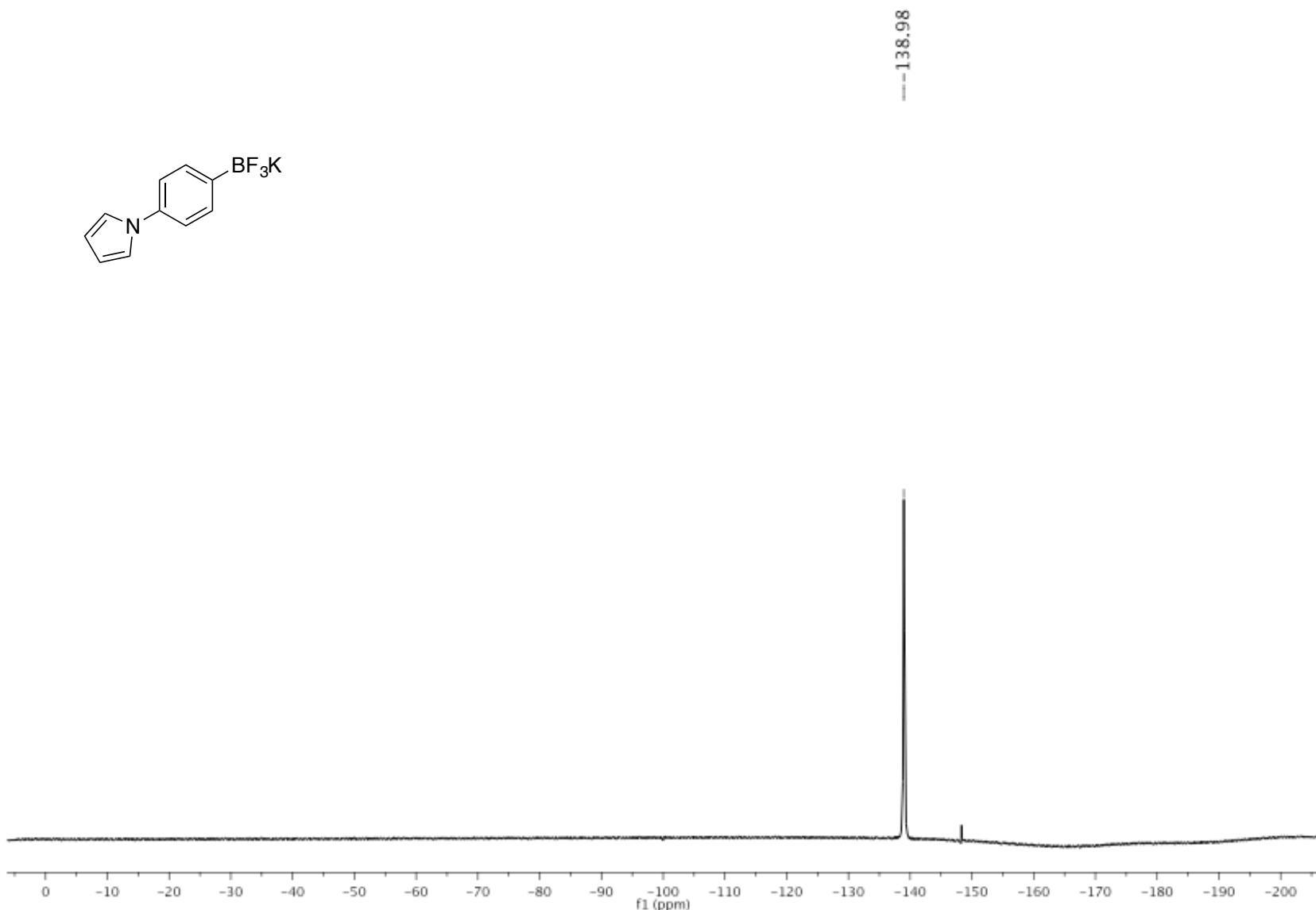
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-methoxyphenyl)borate (1a, Table 5, entry 7)



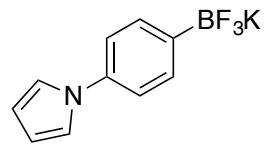
¹H NMR (500 MHz, DMSO -d₆) Spectrum of Potassium (4-(1H-Pyrrol-1-yl)phenyl)trifluoroborate (5c, Table 5, entry 8)



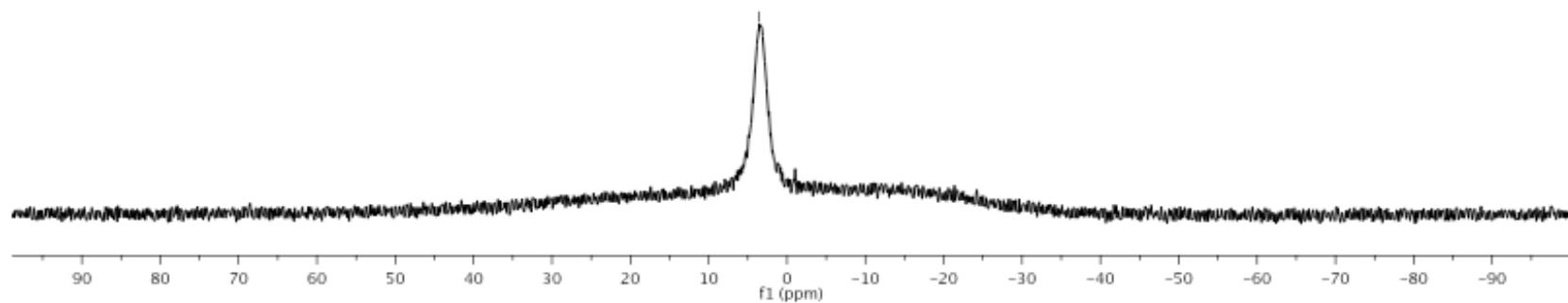
^{13}C NMR (128.5 MHz, DMSO -d₆) Spectrum of Potassium (4-(1*H*-Pyrrol-1-yl)phenyl)trifluoroborate (**5c**, Table 5, entry 8)



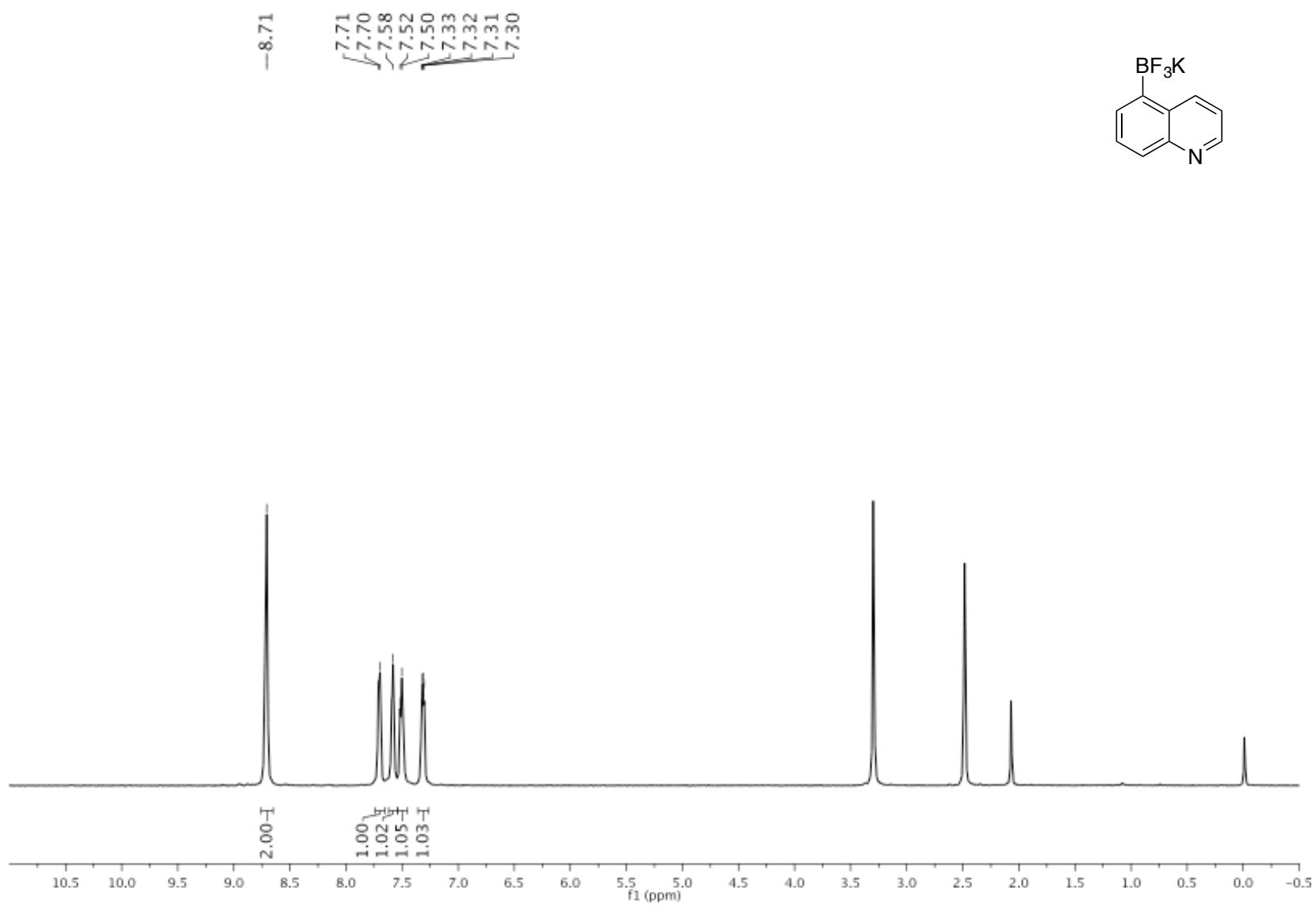
^{19}F NMR (470.8 MHz, DMSO -d₆) Spectrum of Potassium (4-(1*H*-Pyrrol-1-yl)phenyl)trifluoroborate (**5c**, Table 5, entry 8)



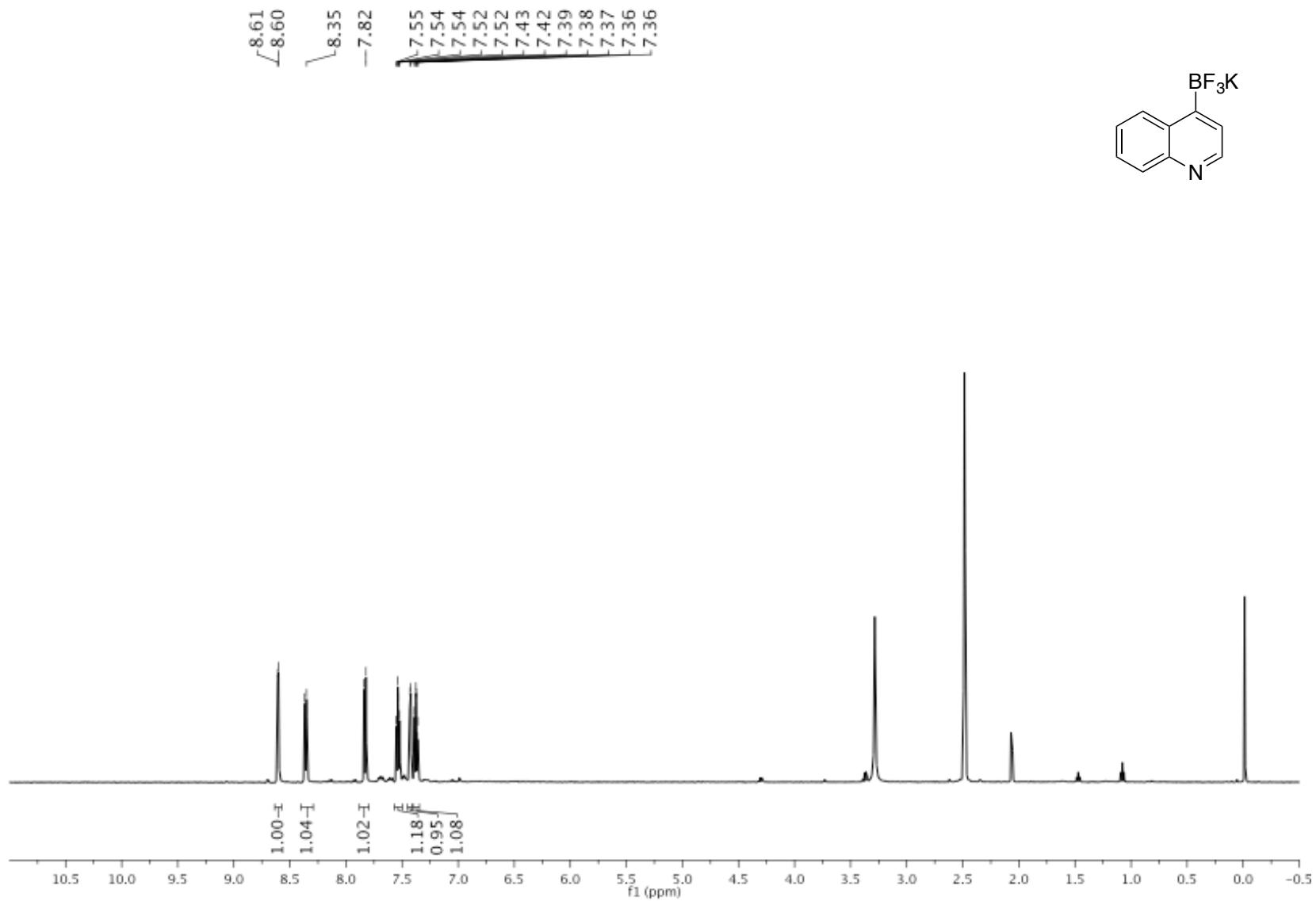
-3.6



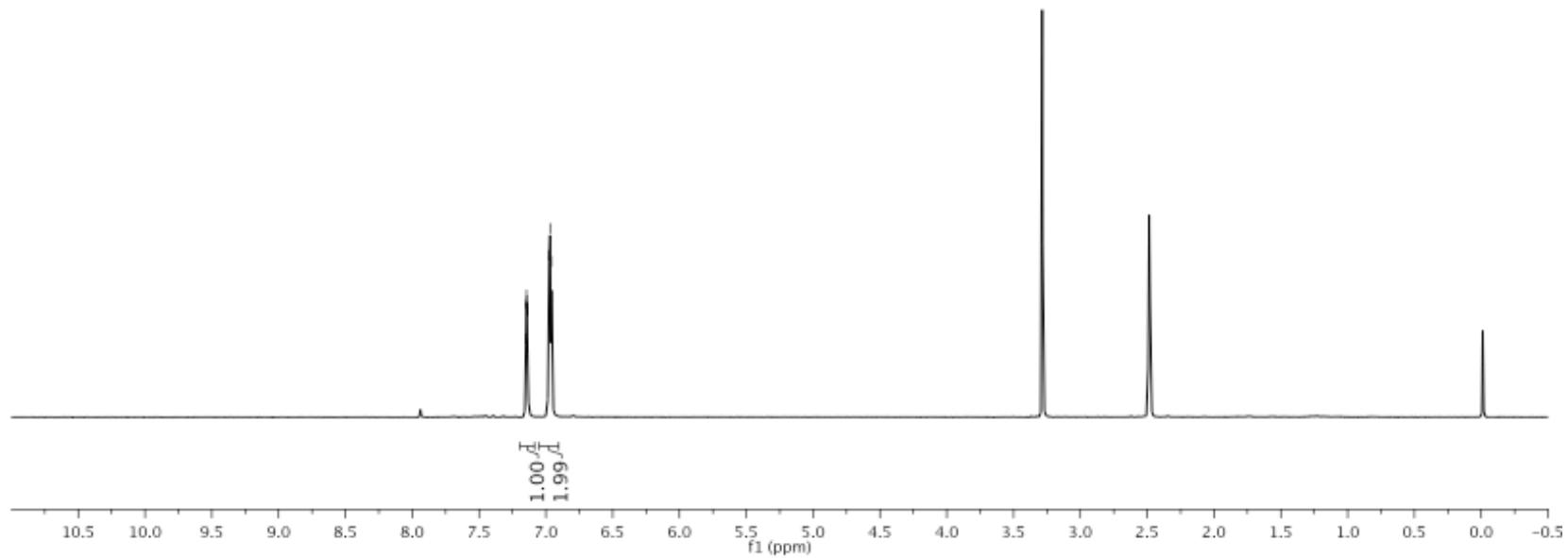
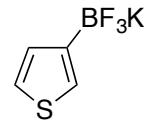
¹¹B NMR (128.4 MHz, DMSO-d₆) Spectrum of Potassium (4-(1H-Pyrrol-1-yl)phenyl)trifluoroborate (5c, Table 5, entry 8)



^1H NMR (500 MHz, $\text{DMSO}-\text{d}_6$) Spectrum of Potassium Trifluoro(quinolin-5-yl)borate (3j, Table 5, entry 9)

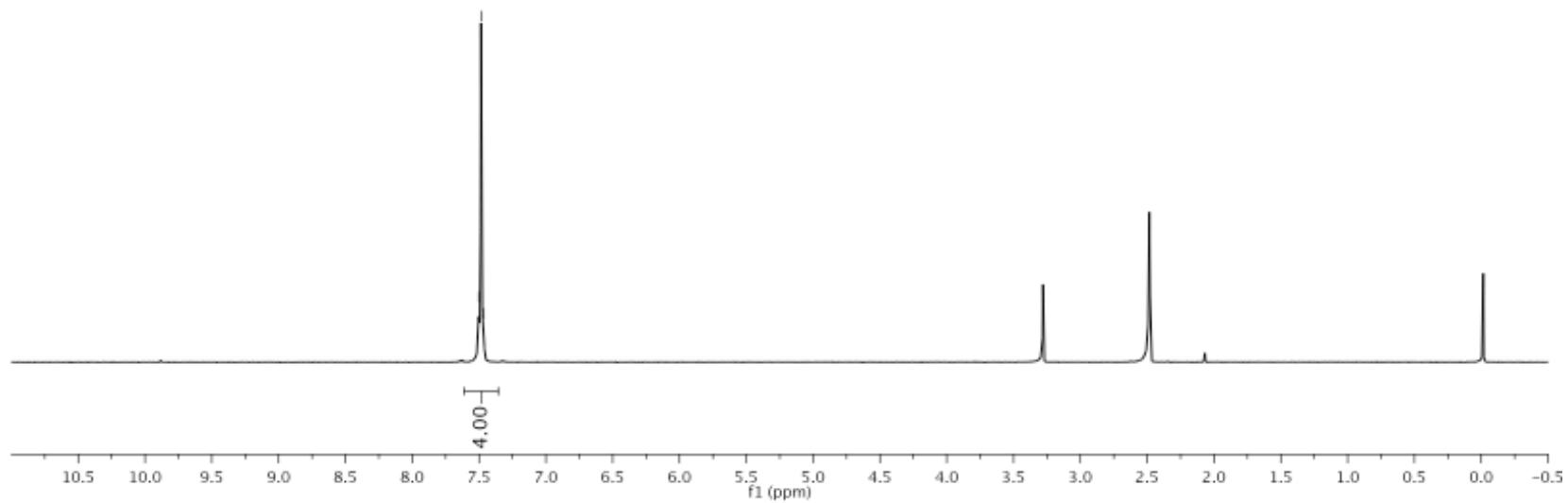
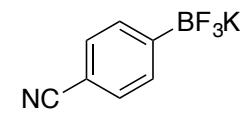


7.15
7.15
7.14
7.14
7.14
6.98
6.97
6.96



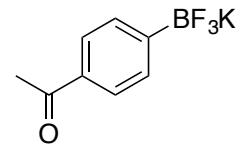
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(thien-3-yl)borate (3a, Table 5, entry 11)

7.50
7.49
7.48
7.46

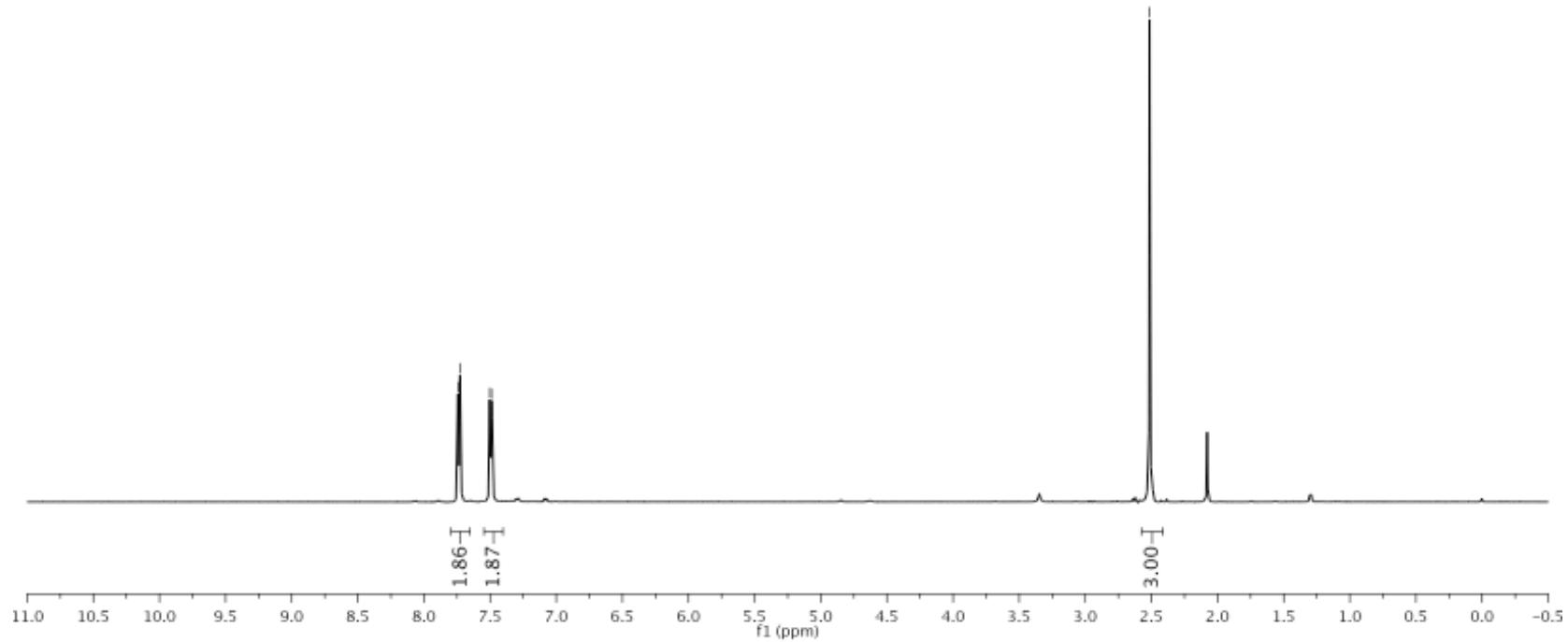


¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium (4-Cyanophenyl)trifluoroborate (2a, Table 7, entry 1)

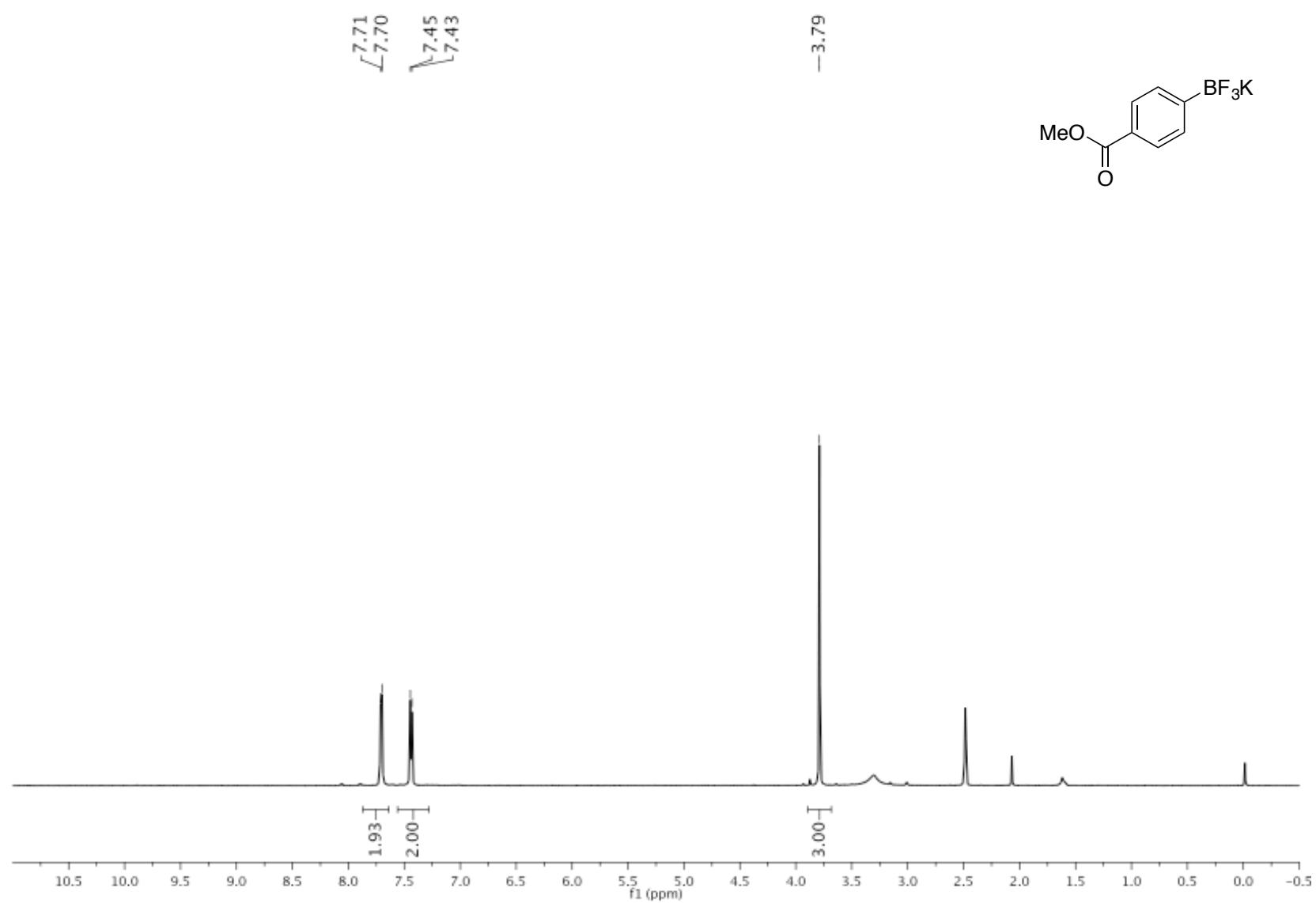
7.74
7.73
7.50
7.49



-2.51

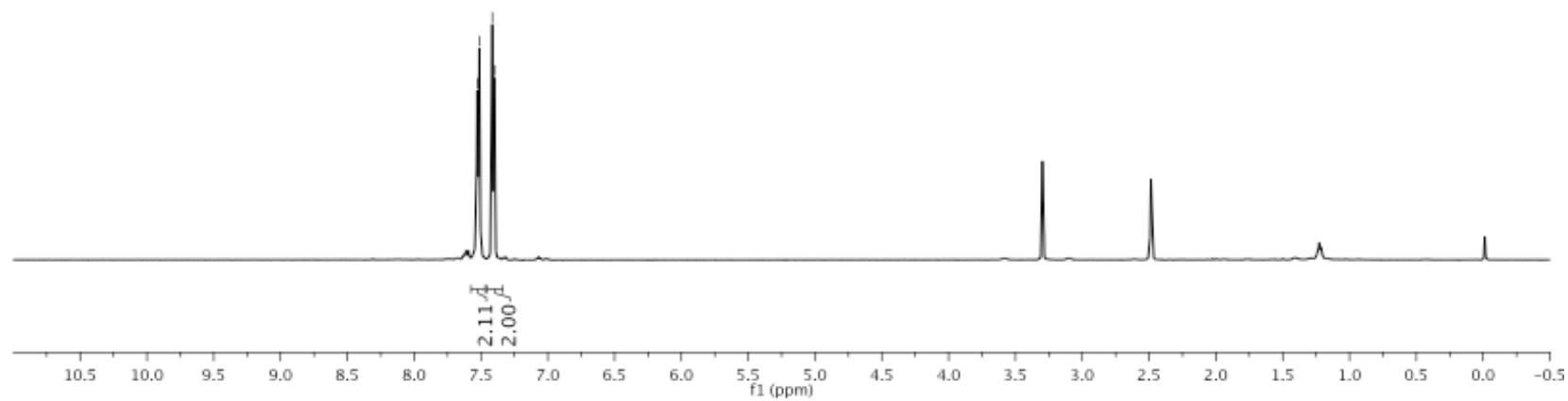
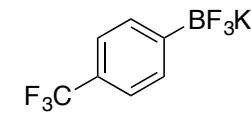


¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium (4-Acetylphenyl)trifluoroborate (2c, Table 7, entry 2)

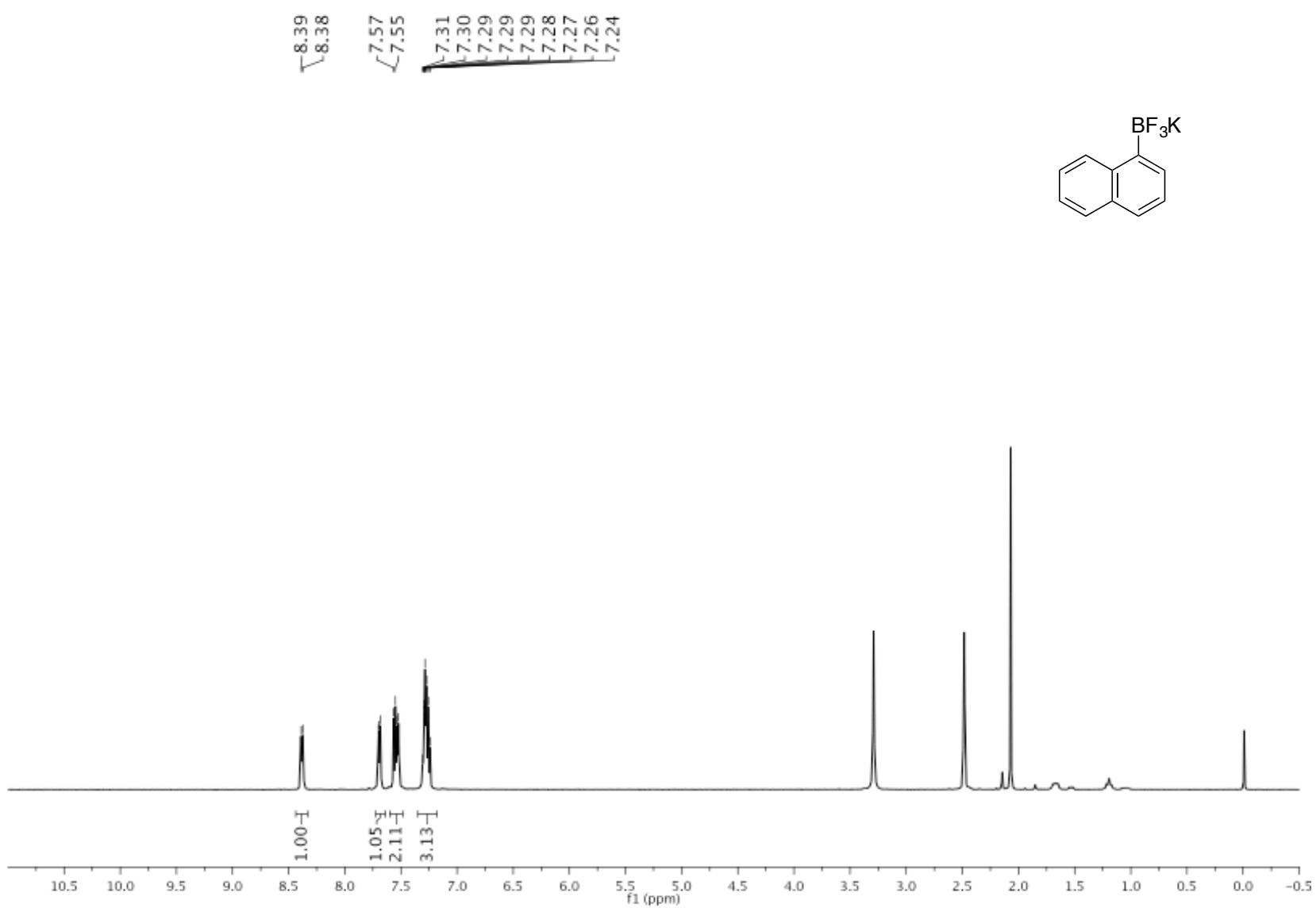


^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(4-(methoxycarbonyl)phenyl)borate (2e, Table 7, entry 3)

7.53
7.51
7.41
7.40



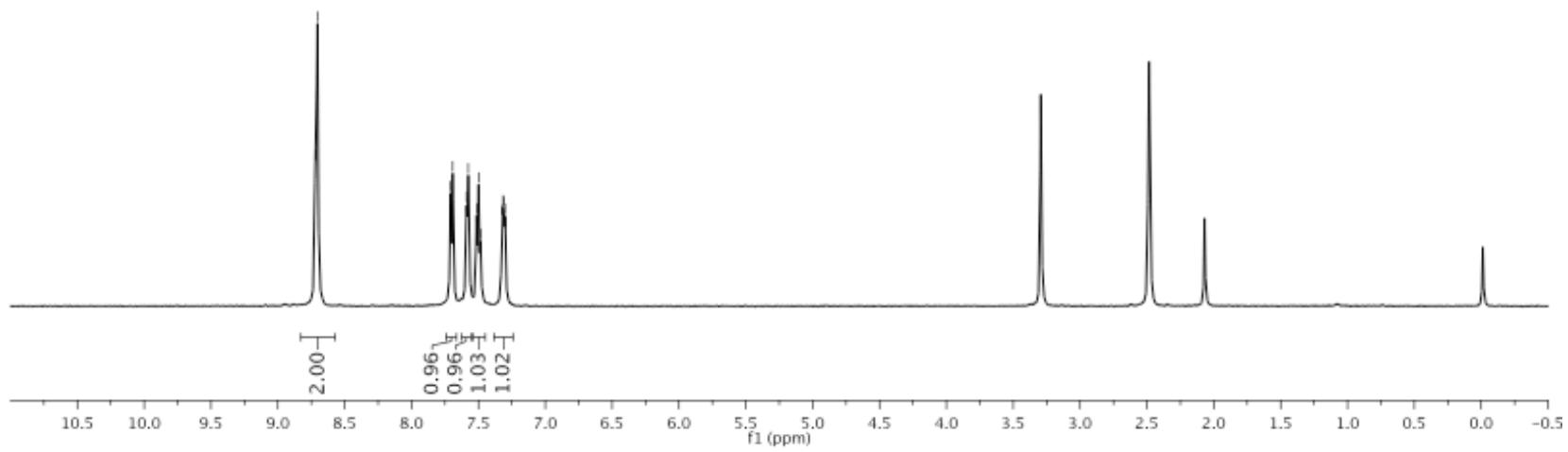
¹H NMR (500 MHz, DMSO-d₆) Spectrum of Potassium Trifluoro(4-(trifluoromethyl)phenyl)borate (2g, Table 7, entry 4)



^1H NMR (500 MHz, DMSO-d_6) Spectrum of Potassium Trifluoro(naphthalen-1-yl)borate (1i, Table 7, entry 5)

8.72
8.70

7.71
7.69
7.59
7.58
7.51
7.50
7.48
7.32
7.32
7.31
7.30



¹H NMR (500 MHz, DMSO -d₆) Spectrum of Potassium Trifluoro(quinolin-5-yl)borate (3j, Table 7, entry 6)