

***Para*-Selective Cu-Catalyzed C–H Aryloxylation of Electron-rich Arenes and Heteroarenes**

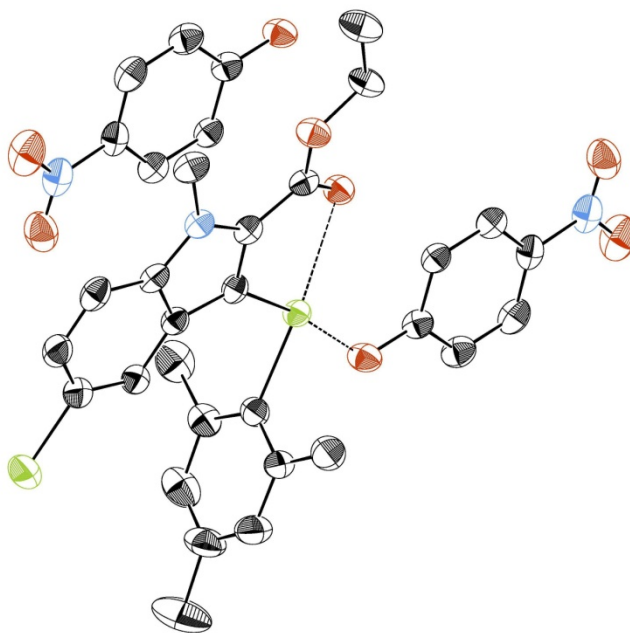
**Igors Sokolovs and Edgars Suna\***

*Latvian Institute of Organic Synthesis, Aizkraukles 21, LV-1006, Riga, Latvia*

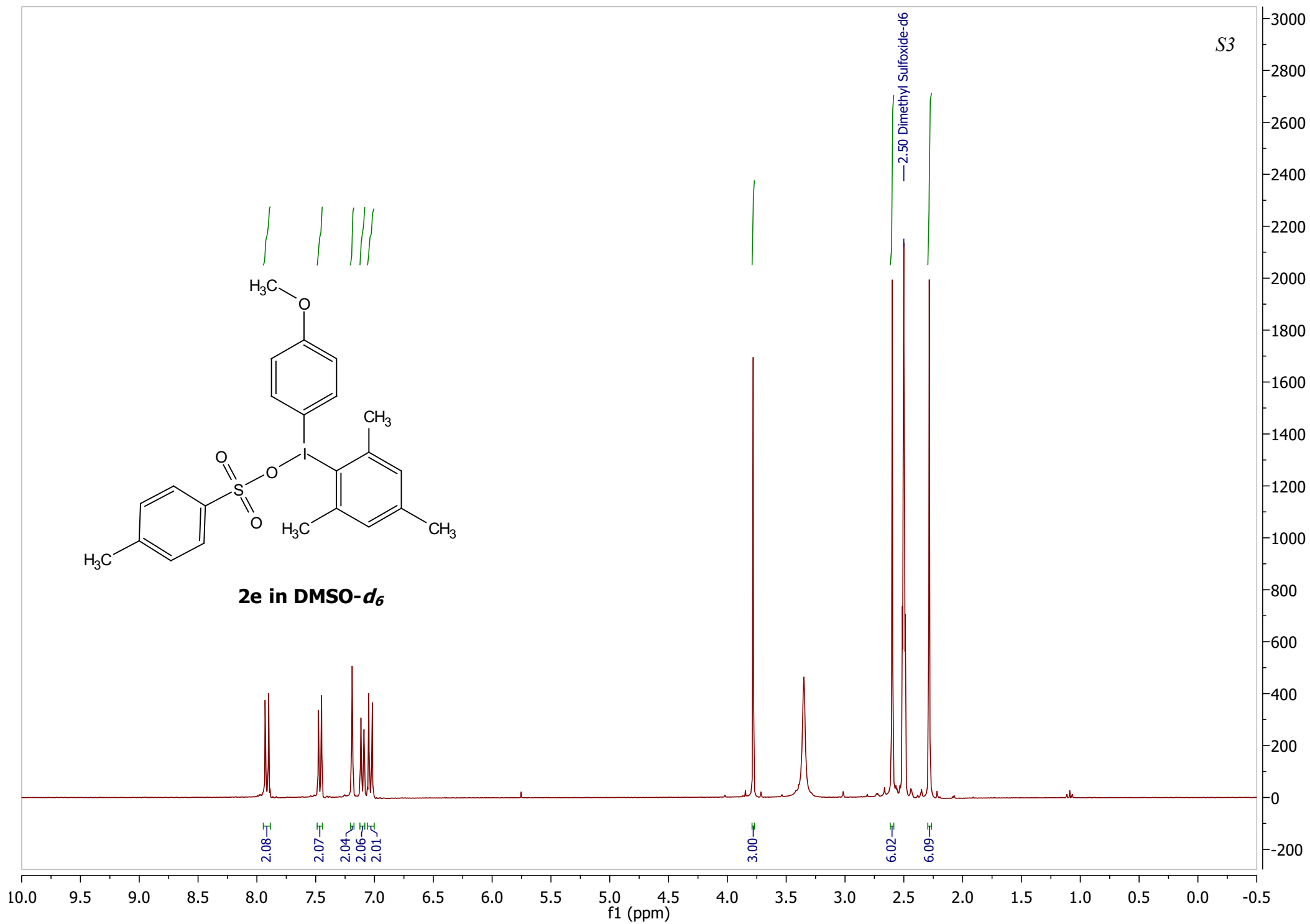
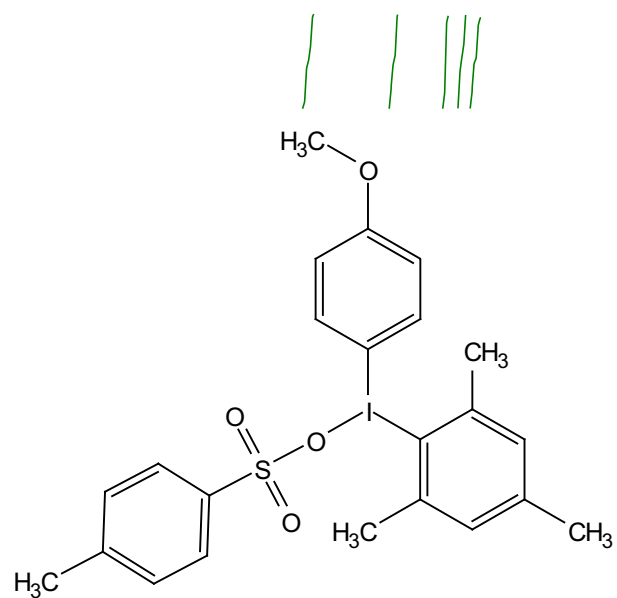
**edgars@osi.lv**

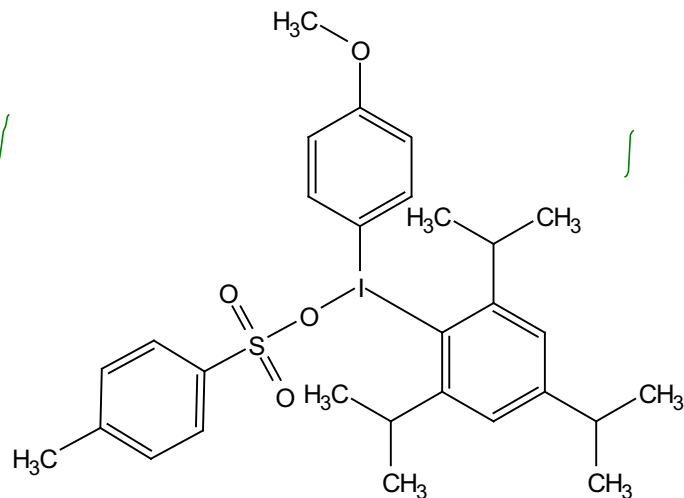
**CONTENTS**

X-Ray Structure, Crystal Data and Structure Refinements for <b>20</b> .....	2
Spectroscopic Data for $\lambda^3$ -Iodanes <b>2e</b> , <b>2e-TIPP</b> , <b>2e-Ph</b> and <b>20</b> .....	3
Spectroscopic Data for Compounds <b>4e-19e</b> (Table 2).....	8
Spectroscopic Data for Compounds <b>4a-r</b> (Table 3).....	28

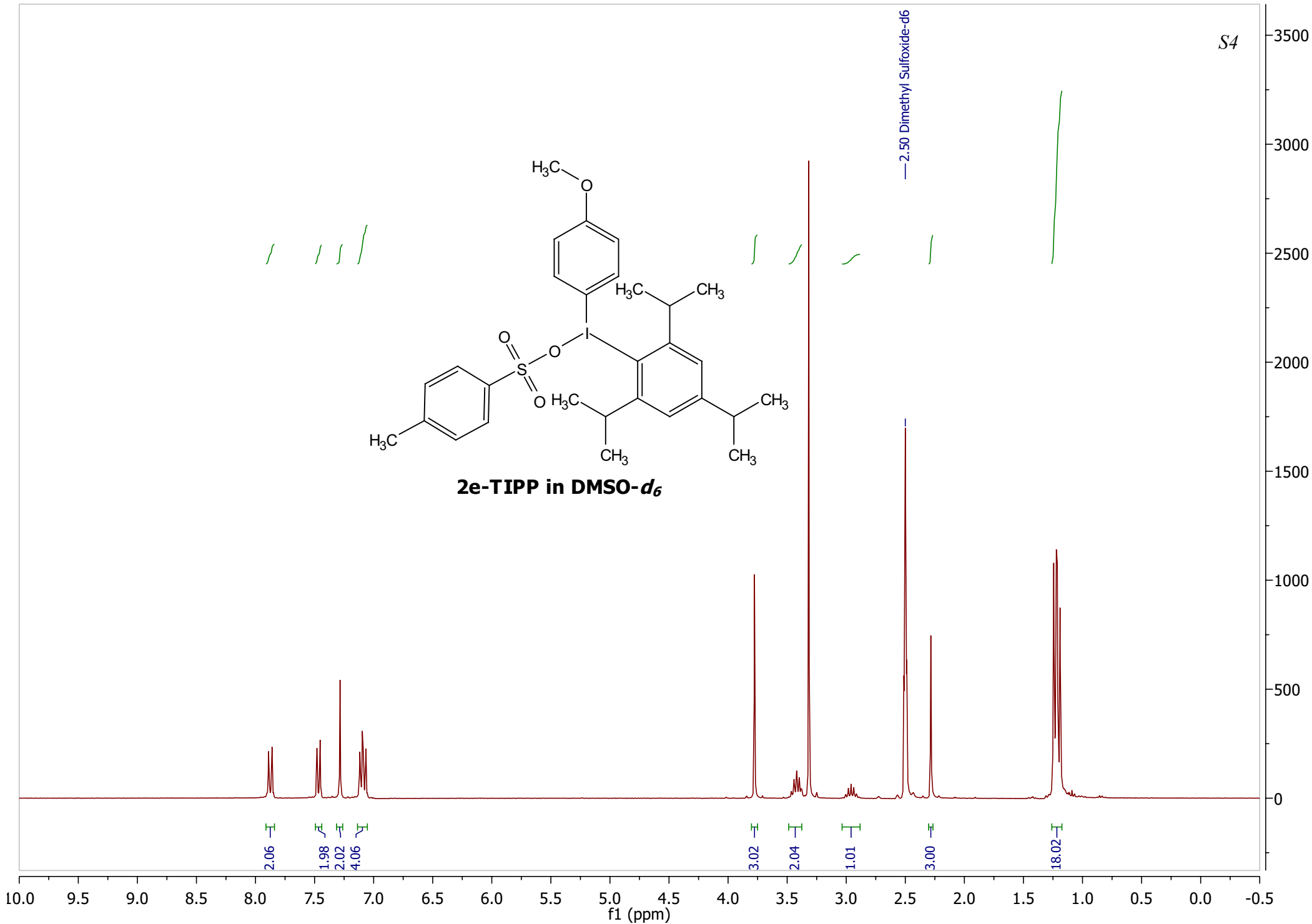
**X-Ray Structure, Crystal Data and Structure Refinements for 20****Crystal data and structure refinement for 20**

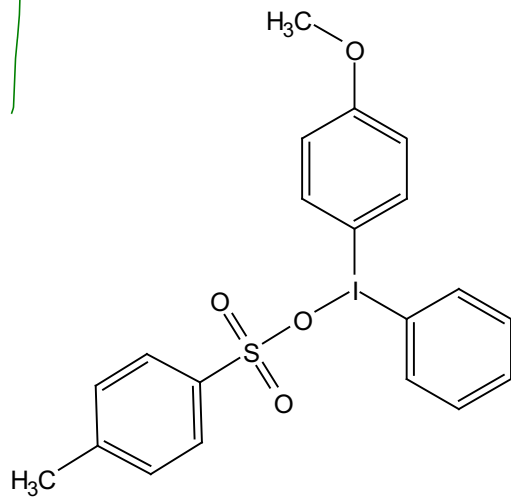
Identification code	Dmitry
Empirical formula	C <sub>21</sub> H <sub>22</sub> Br I N O <sub>2</sub> , C <sub>6</sub> H <sub>4</sub> N O <sub>3</sub> , C <sub>6</sub> H <sub>5</sub> N O <sub>3</sub>
Formula weight	804.428
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 8.7052(1) Å    alpha = 75.2788(7) deg. b = 12.2035(2) Å    beta = 88.3395(7) deg. c = 16.0777(4) Å    gamma = 83.2541(12) deg.
Volume	1640.49(5) Å <sup>3</sup>
Z	2
Density (calculated)	1.629 Mg/m <sup>3</sup>
Absorption coefficient	2.25 mm <sup>-1</sup>
F(000)	804
Crystal size	0.16 x 0.17 x 0.19 mm
Two-theta max. for data	58.0 deg.
Index ranges	-11<=h<=11, -14<=k<=16, -20<=l<=21
Reflections collected	11515
Independent reflections	8629 [R(int) = 0.025]
Absorption correction	None
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	7266 / 0 / 415
Goodness-of-fit on F <sup>2</sup>	1.009
Final R indices [I>2sigma(I)]	R1 = 0.034, wR2 = 0.066
R indices (all data)	R1 = 0.043, wR2 = 0.068
Absolute structure parameter	0.02(10)
Largest diff. peak and hole	0.85 and -1.35 e.Å <sup>-3</sup>



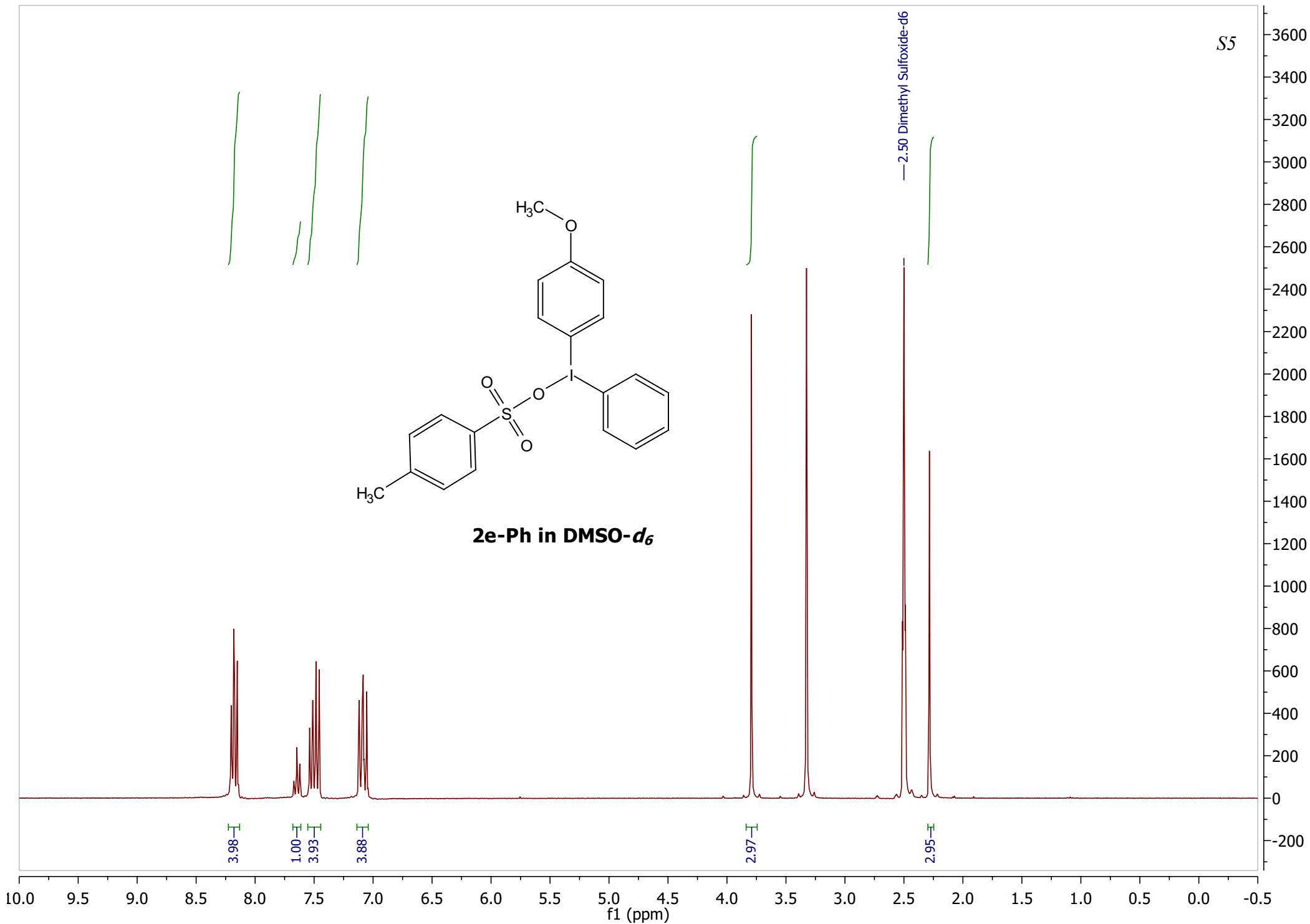


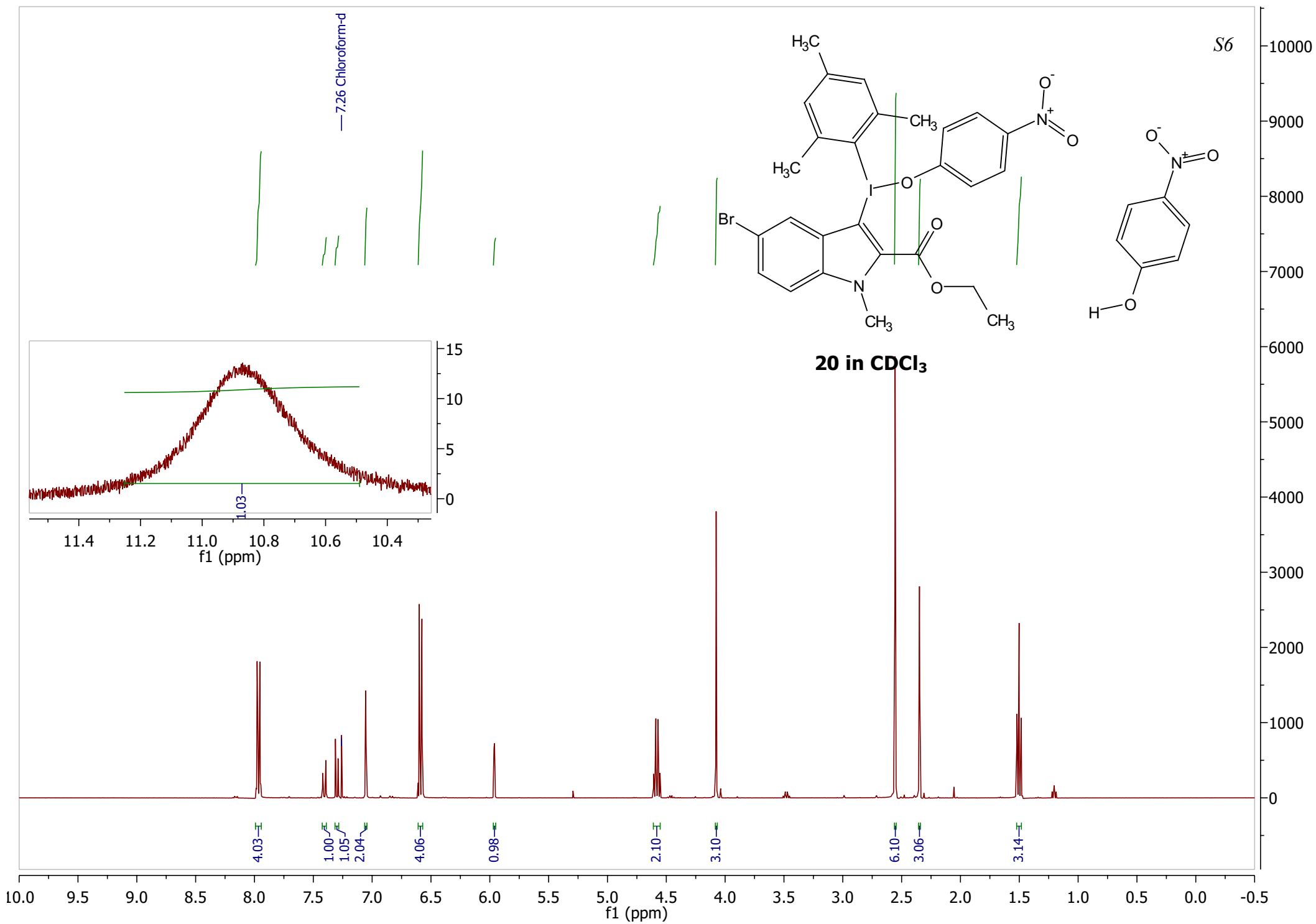
**2e-TIPP in DMSO-d<sub>6</sub>**

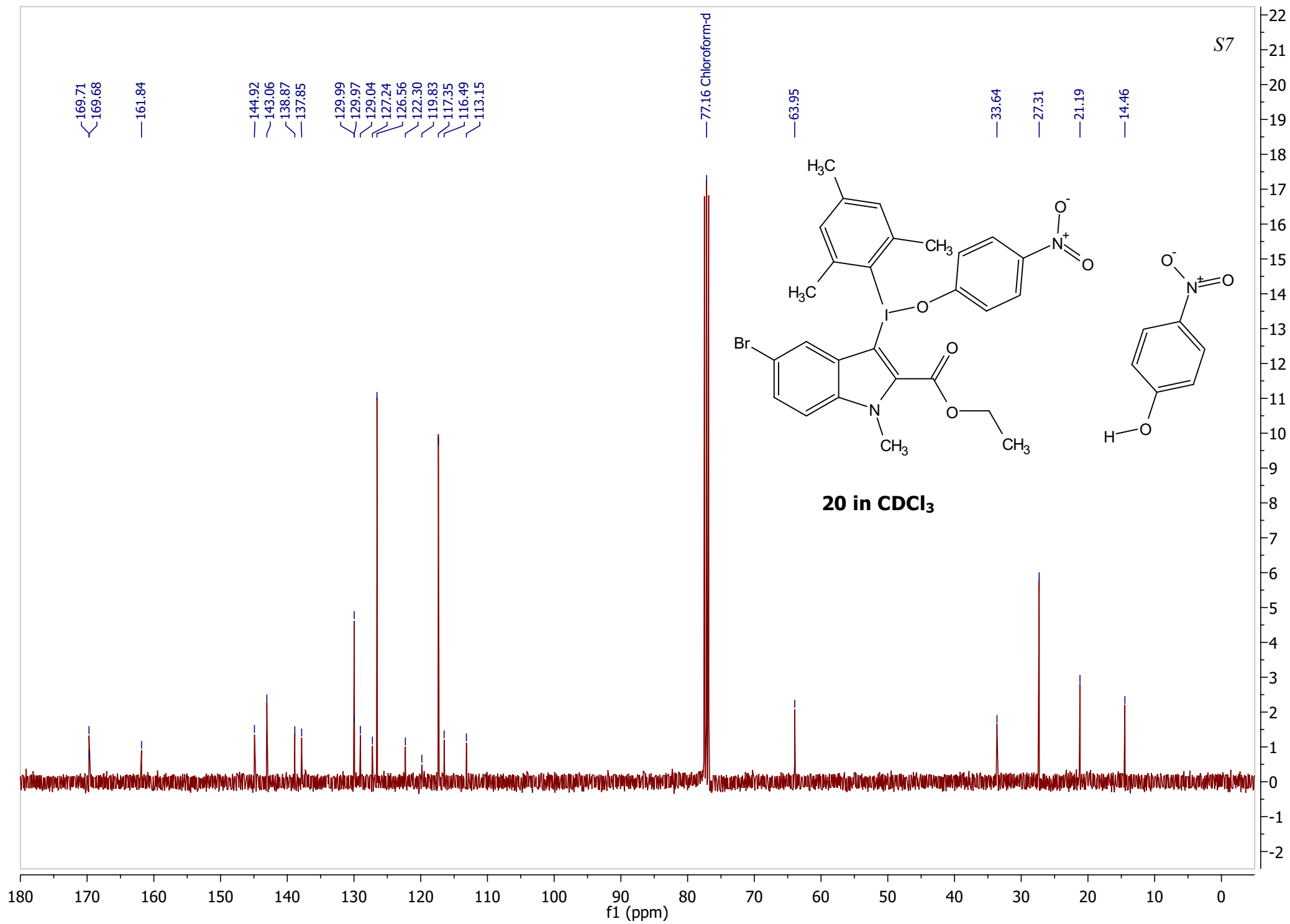




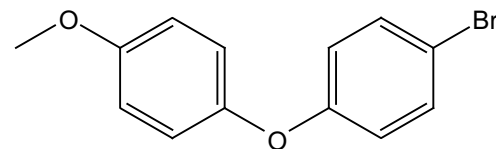
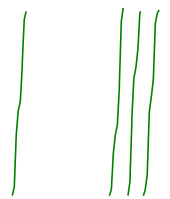
**2e-Ph in DMSO-d<sub>6</sub>**







— 7.26 Chloroform-d

**4e in CDCl<sub>3</sub>**

1.98

2.02

1.99

2.00

2.99

8.5

8.0

7.5

7.0

6.5

6.0

5.5

5.0

4.5

f1 (ppm)

4.0

3.5

3.0

2.5

2.0

1.5

1.0

0.5

9000

8500

8000

7500

7000

6500

6000

5500

5000

4500

4000

3500

3000

2500

2000

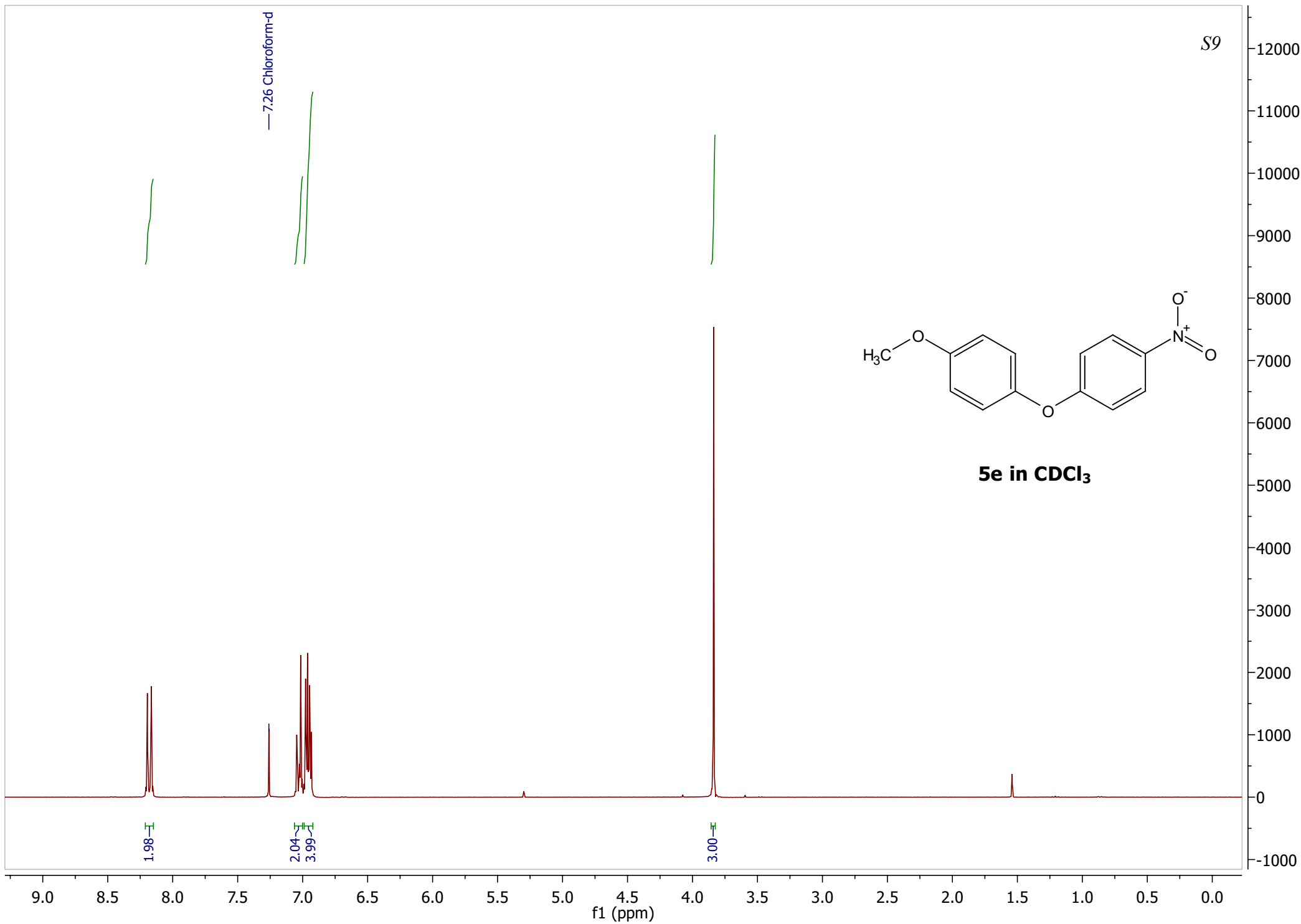
1500

1000

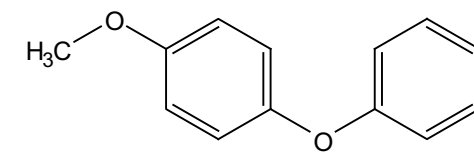
500

0

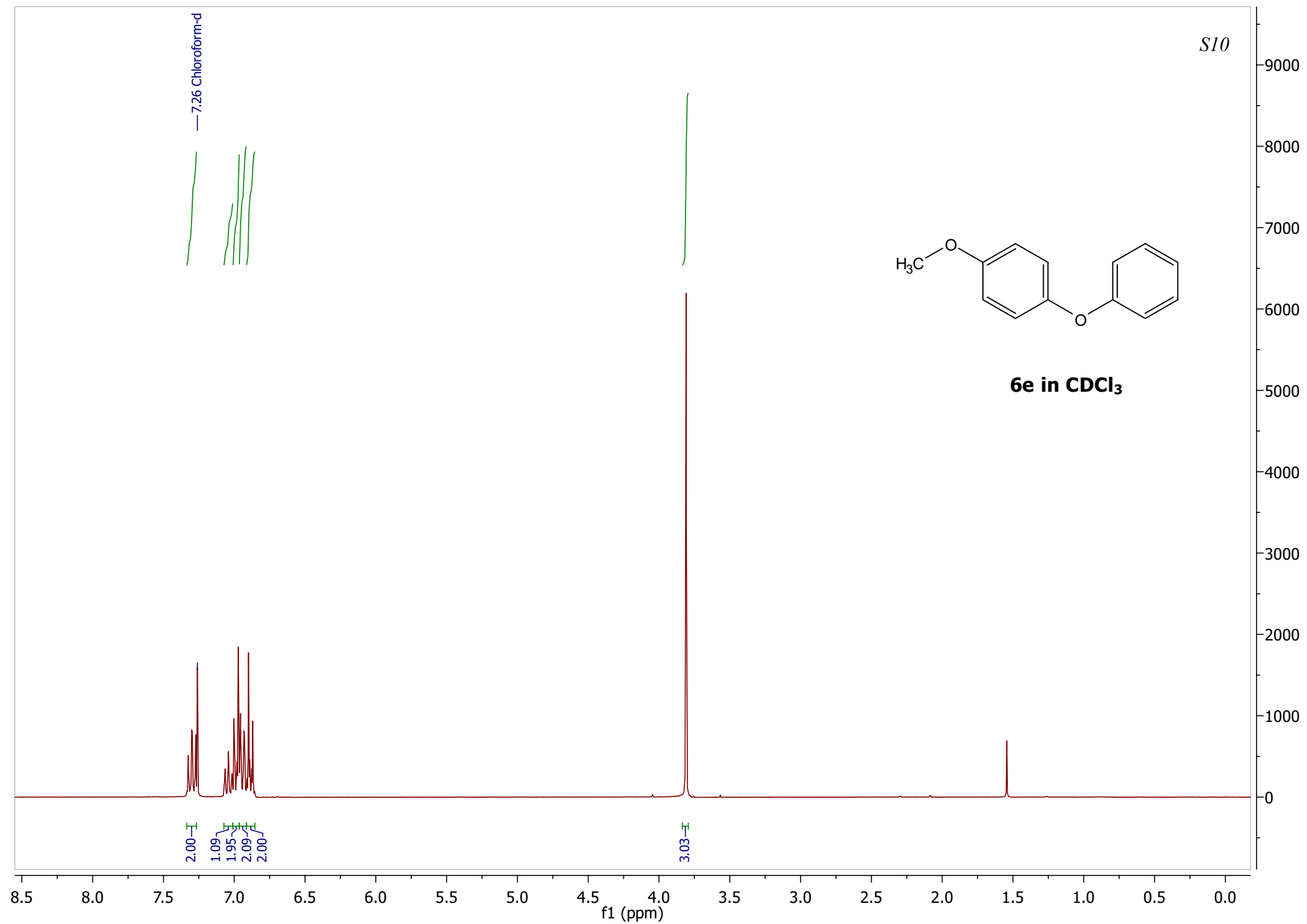
-500



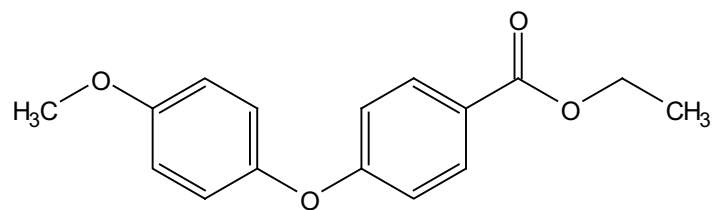
— 7.26 Chloroform-d



**6e in CDCl<sub>3</sub>**

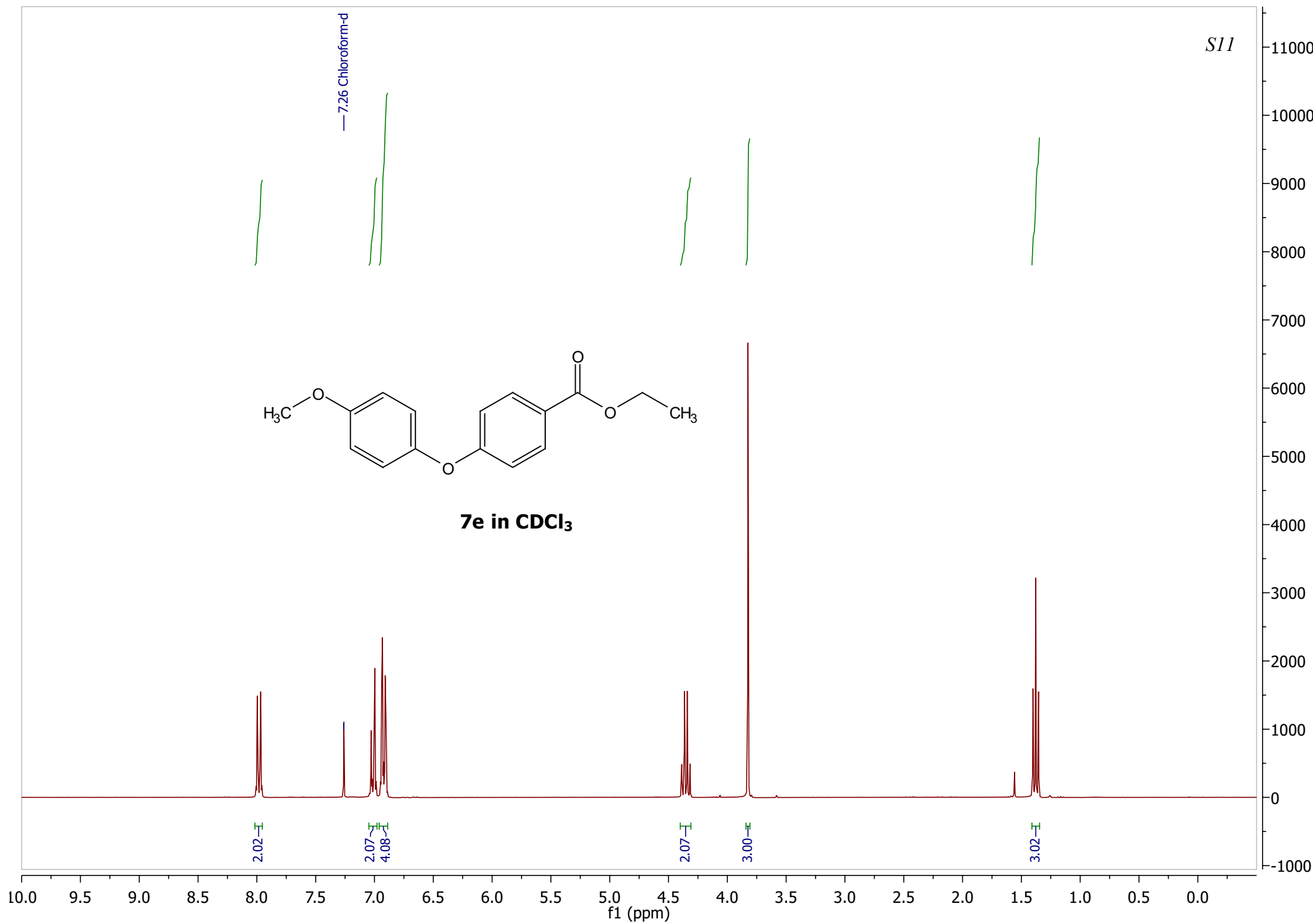


S11

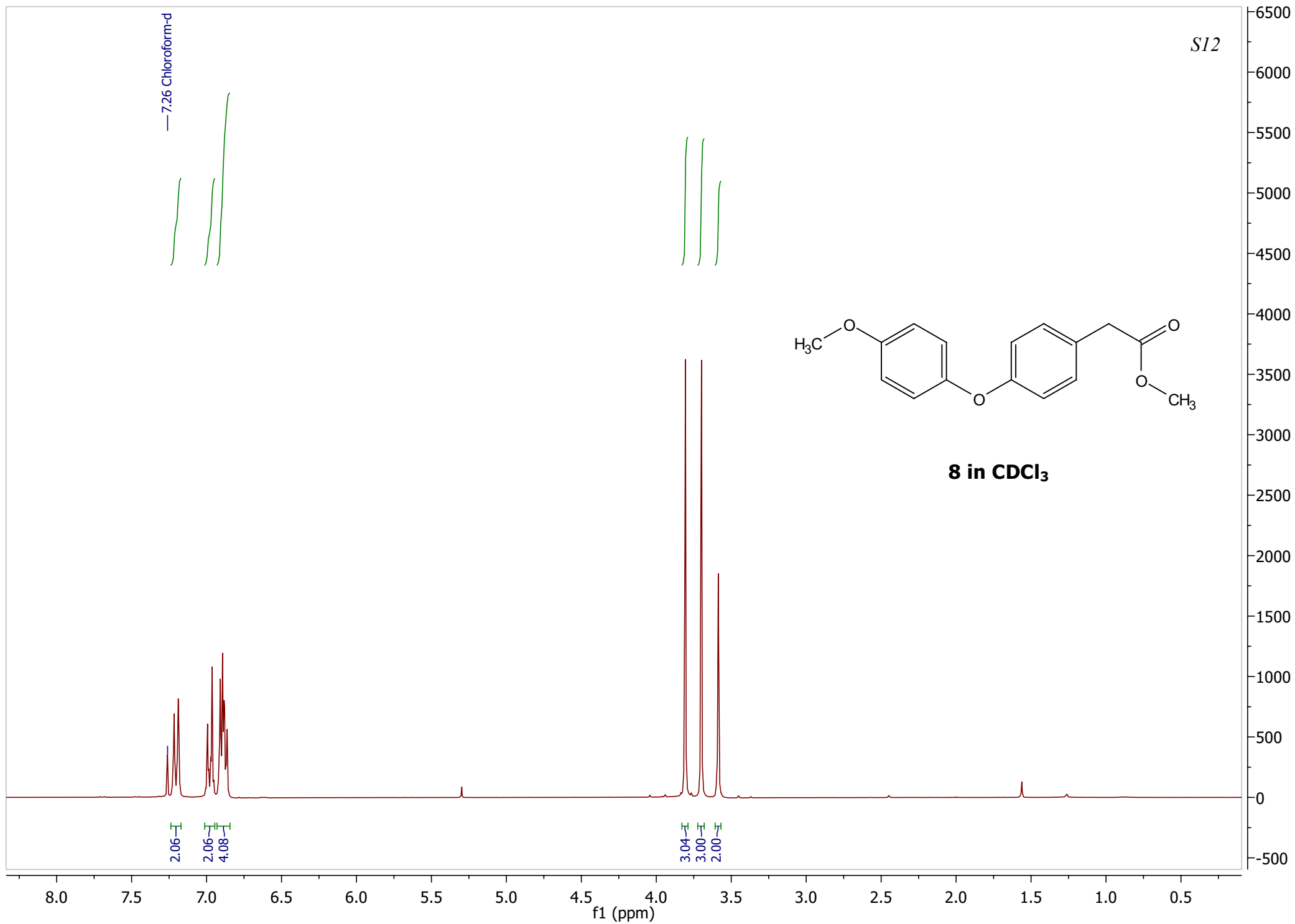


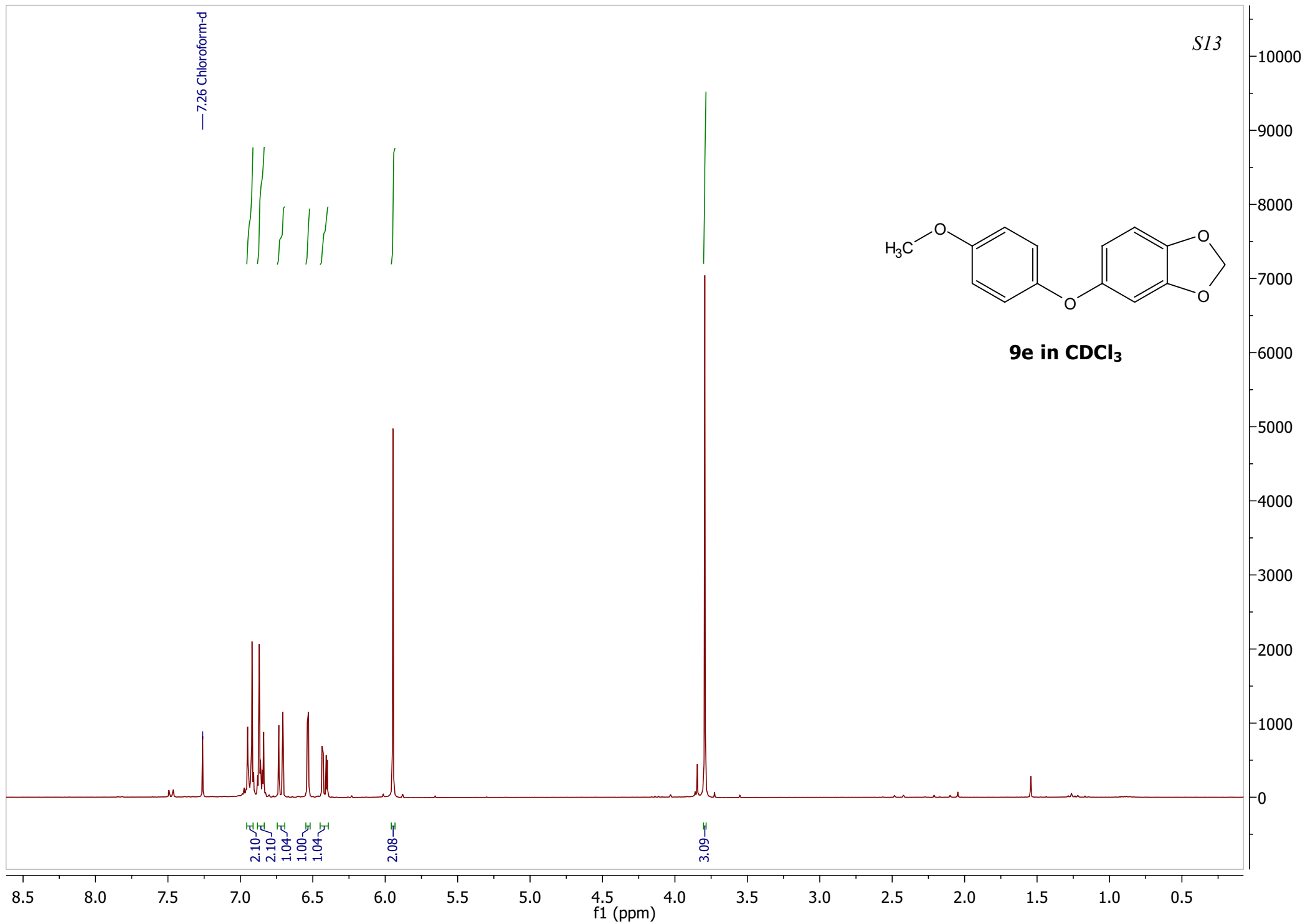
7e in CDCl<sub>3</sub>

—7.26 Chloroform-d

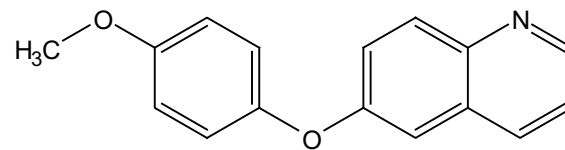


— 7.26 Chloroform-d

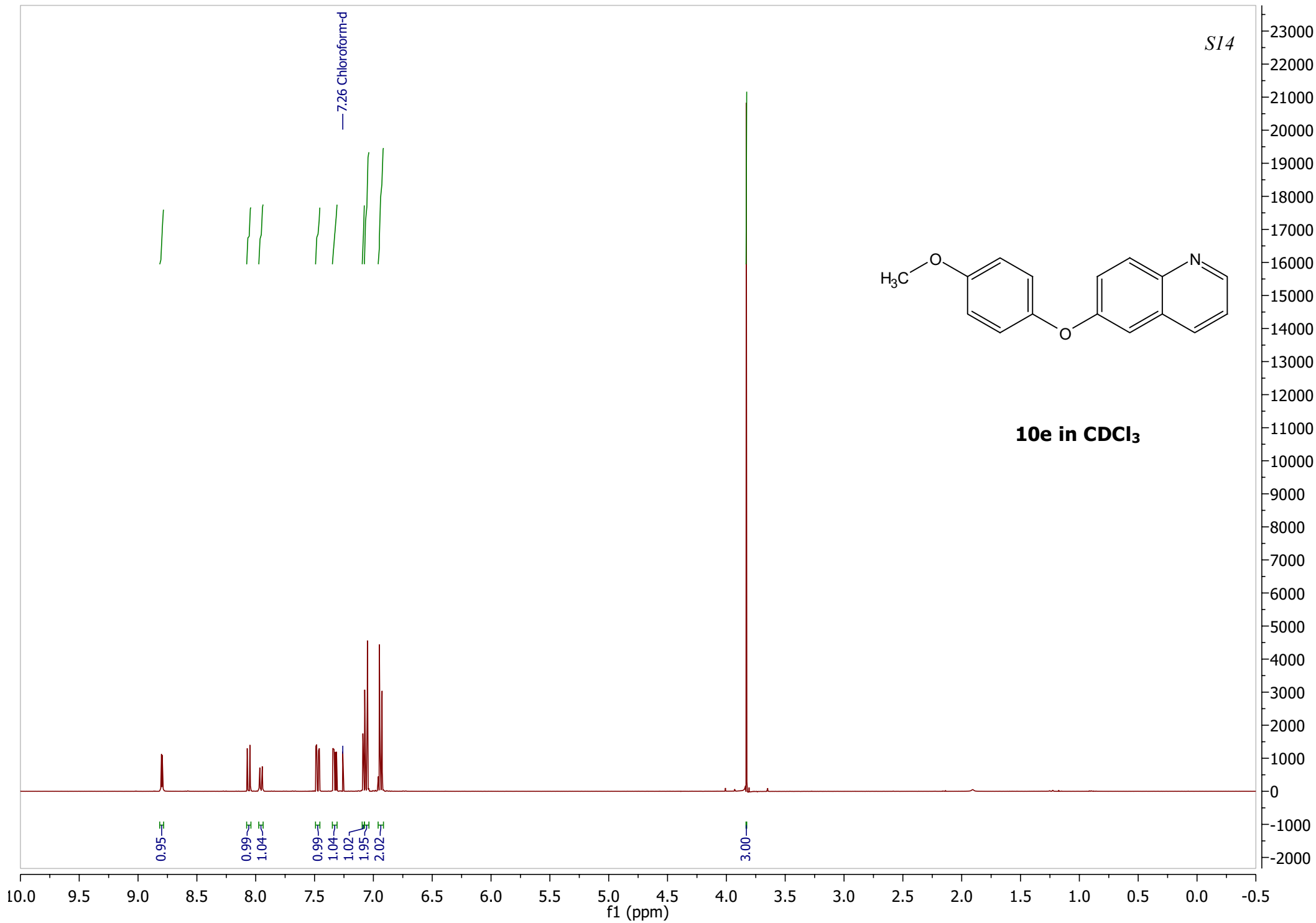




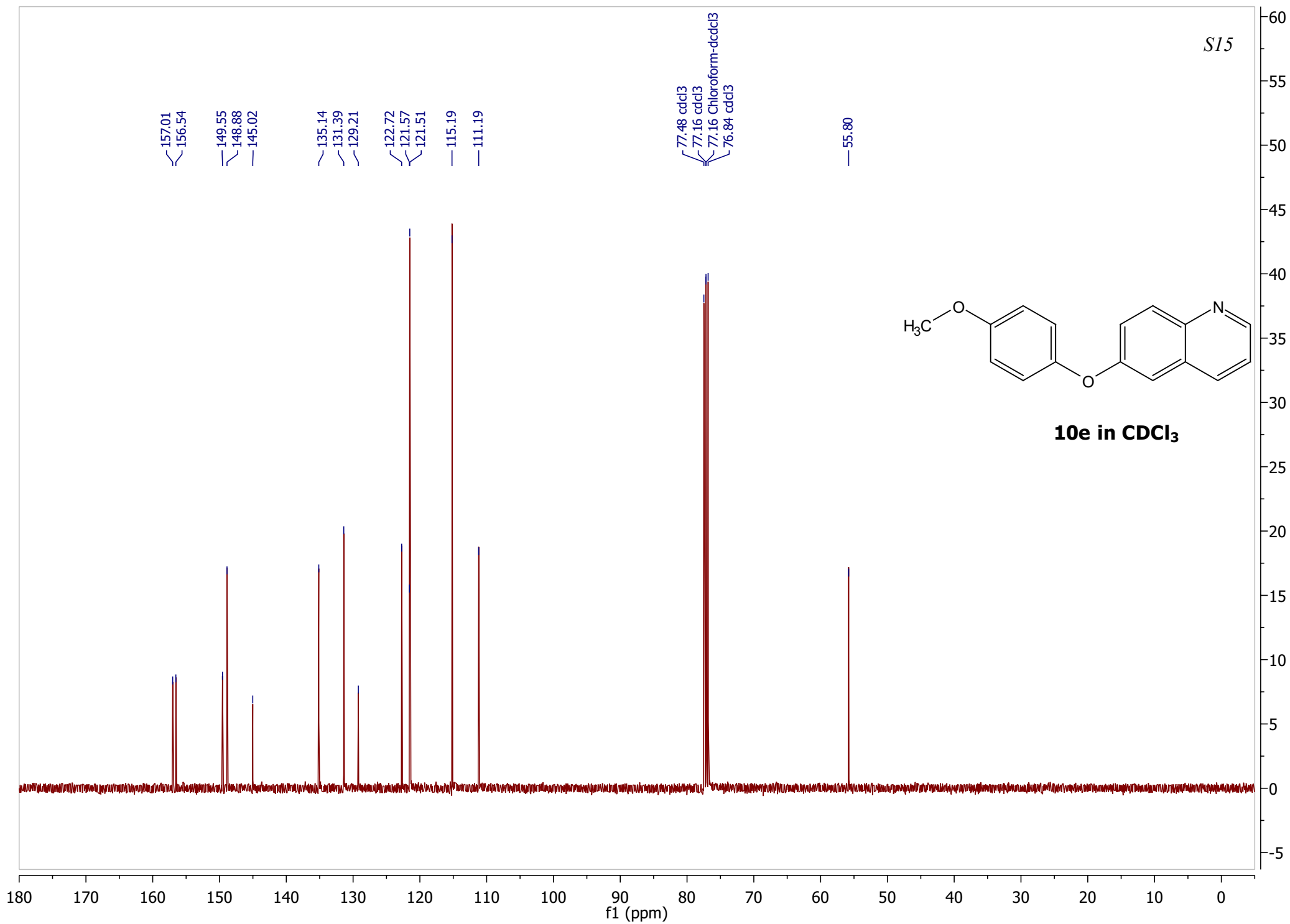
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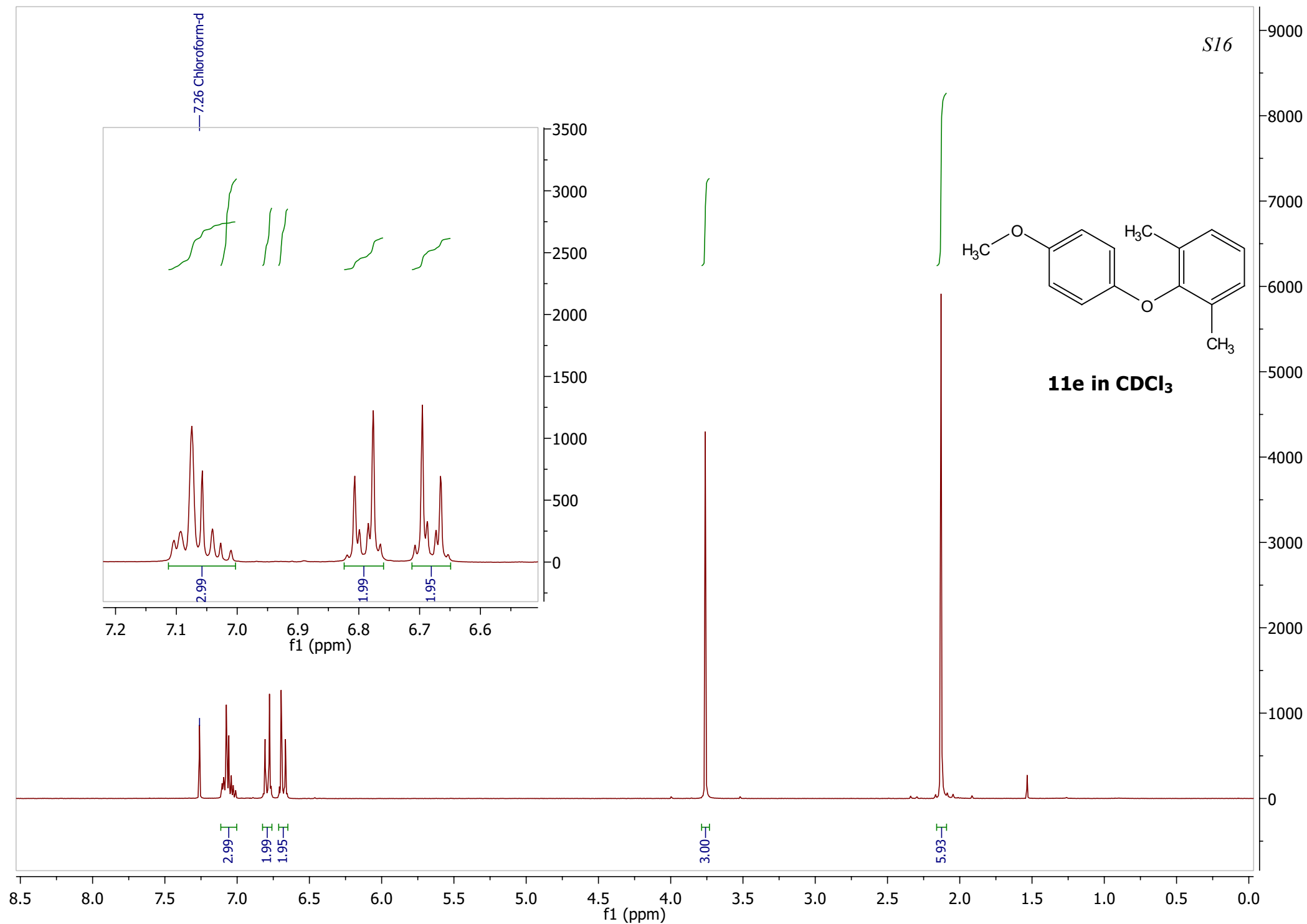
**10e in CDCl<sub>3</sub>**

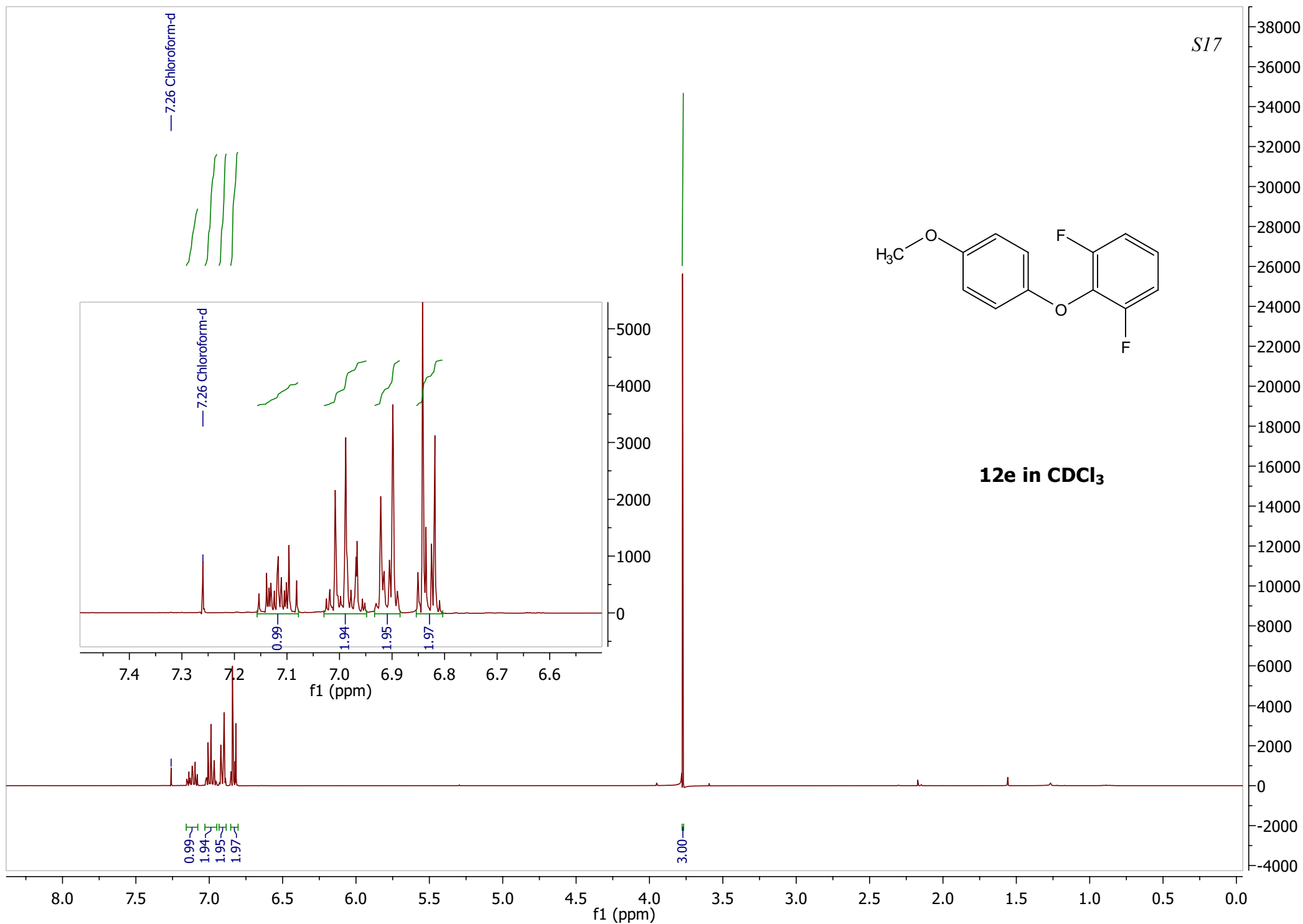


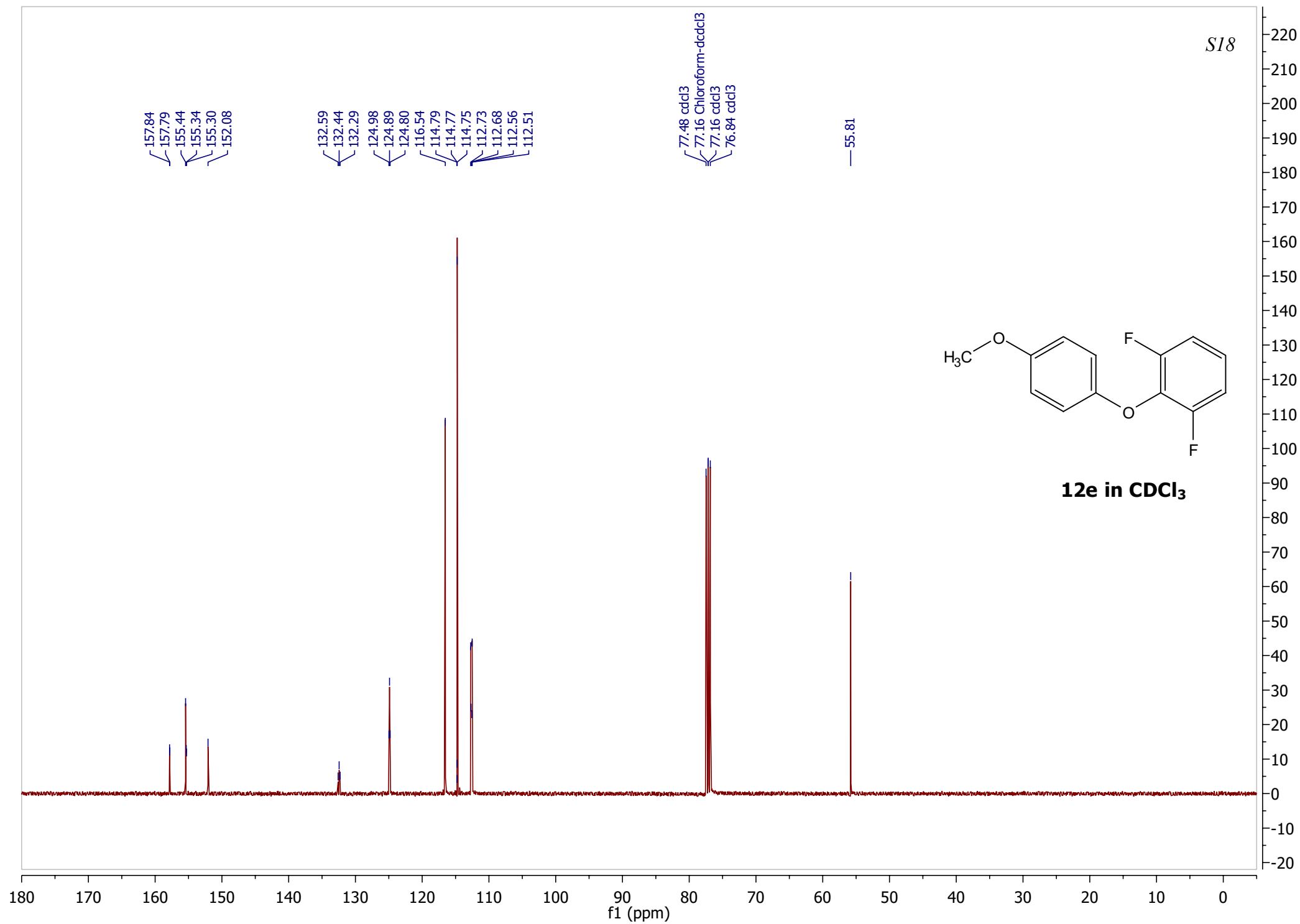
S15



S16





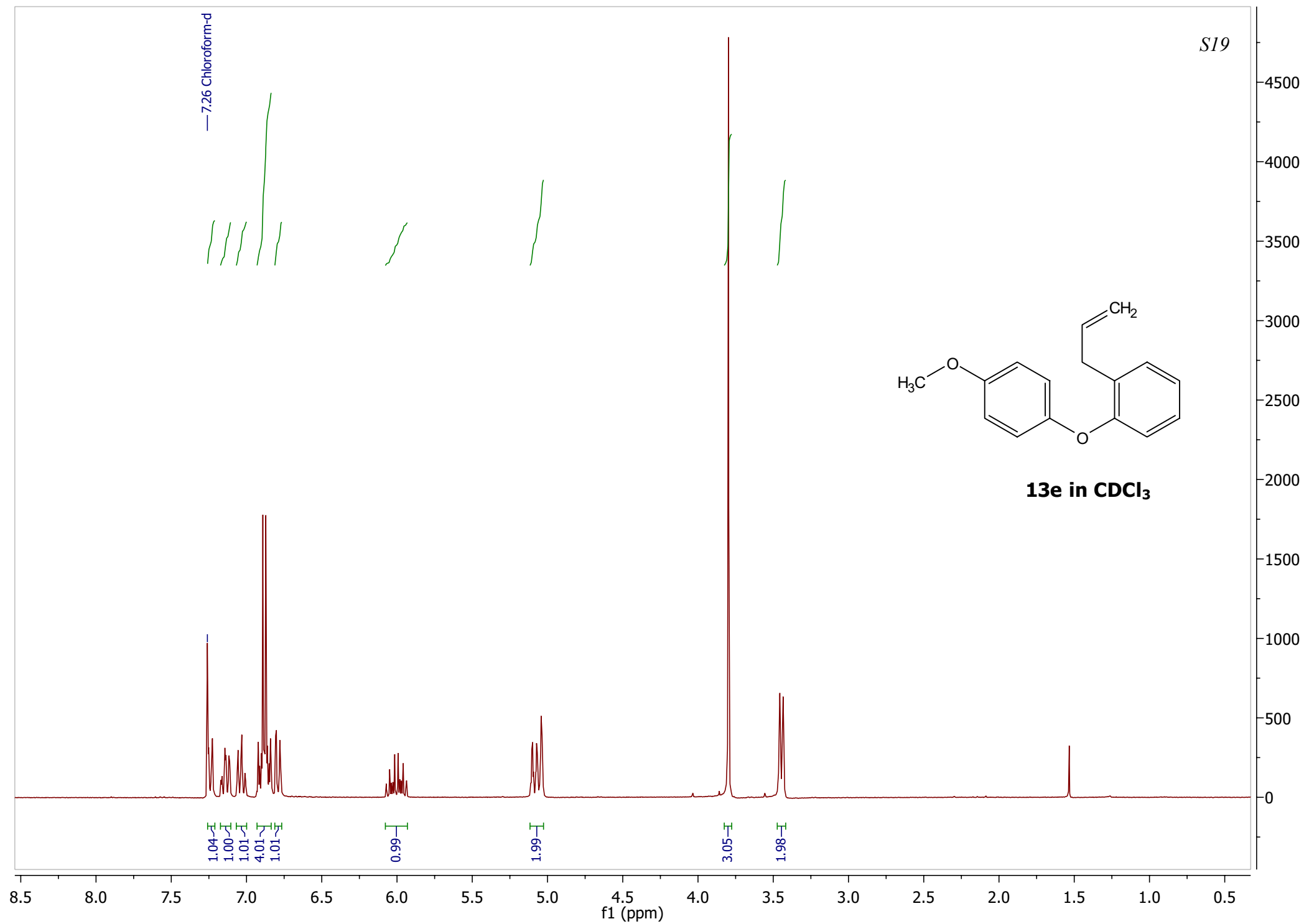


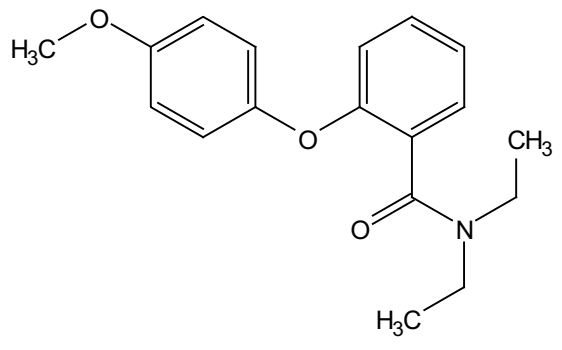
157.84  
157.79  
155.44  
155.34  
155.30  
152.08

132.59  
132.44  
132.29  
124.98  
124.89  
124.80  
116.54  
114.79  
114.77  
114.75  
112.73  
112.68  
112.56  
112.51

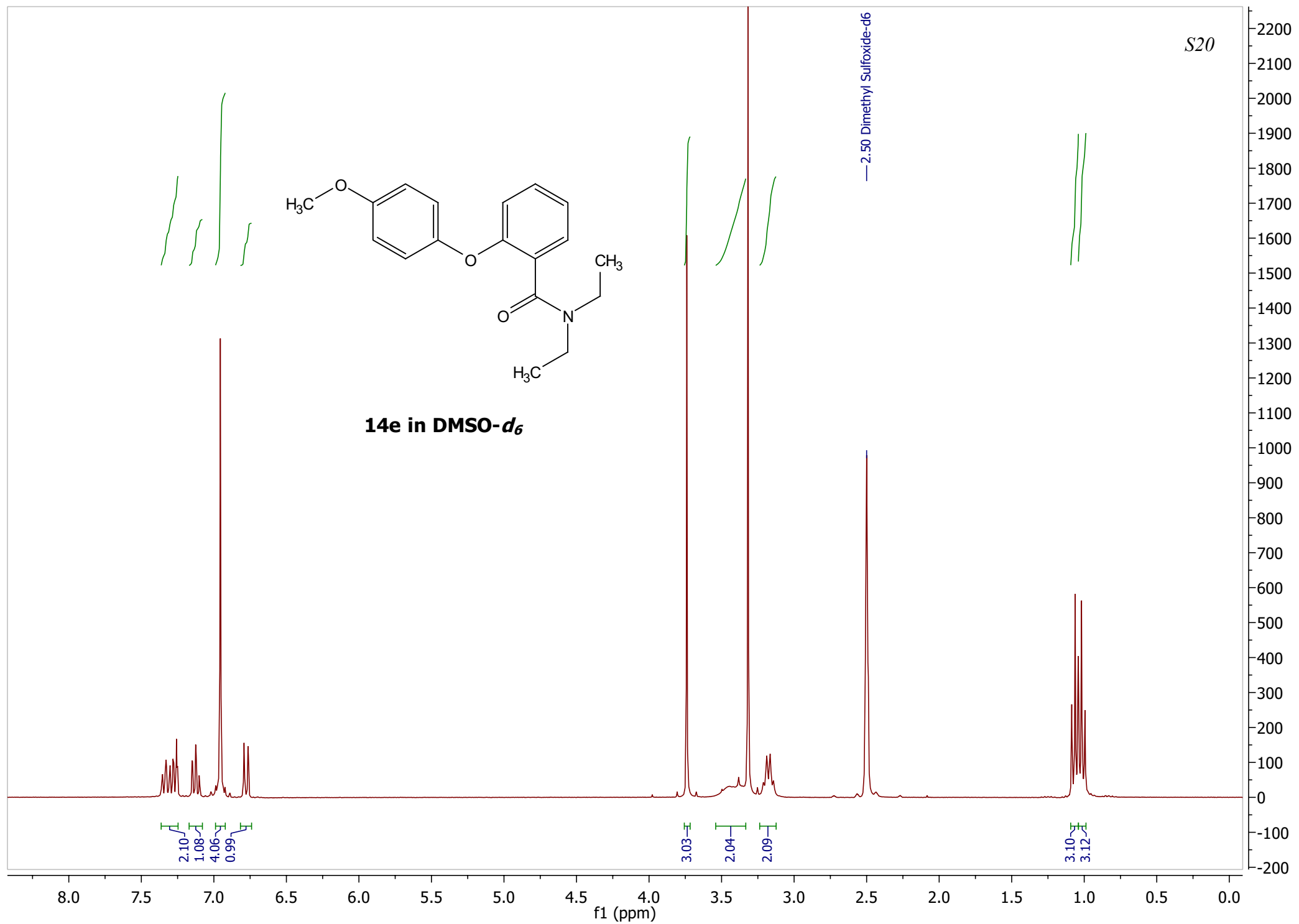
77.48 cdc13  
77.16 Chloroform-dcd13  
77.16 cdc13  
76.84 cdc13

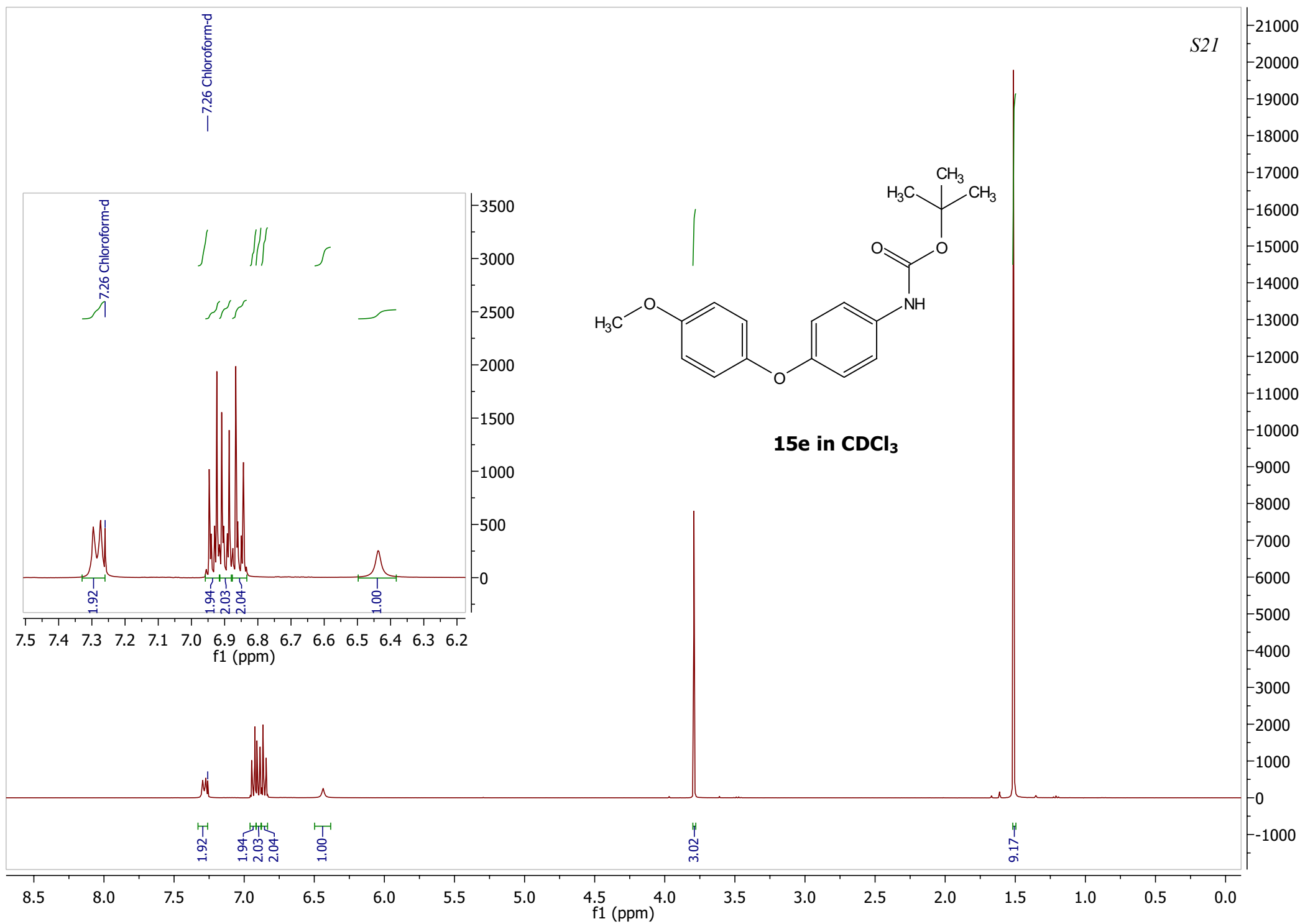
55.81

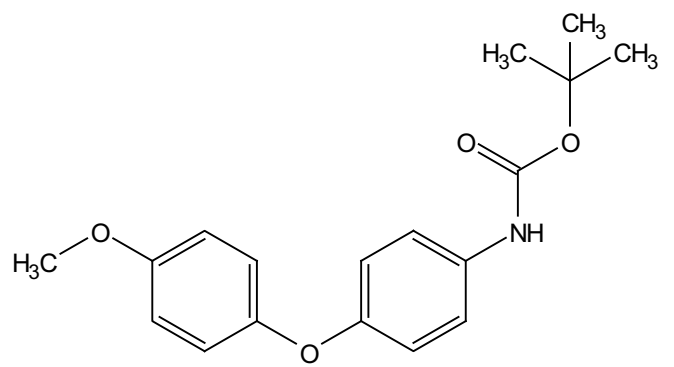




**14e in DMSO-d<sub>6</sub>**







15e in CDCl<sub>3</sub>

155.72  
153.97  
153.14  
151.01

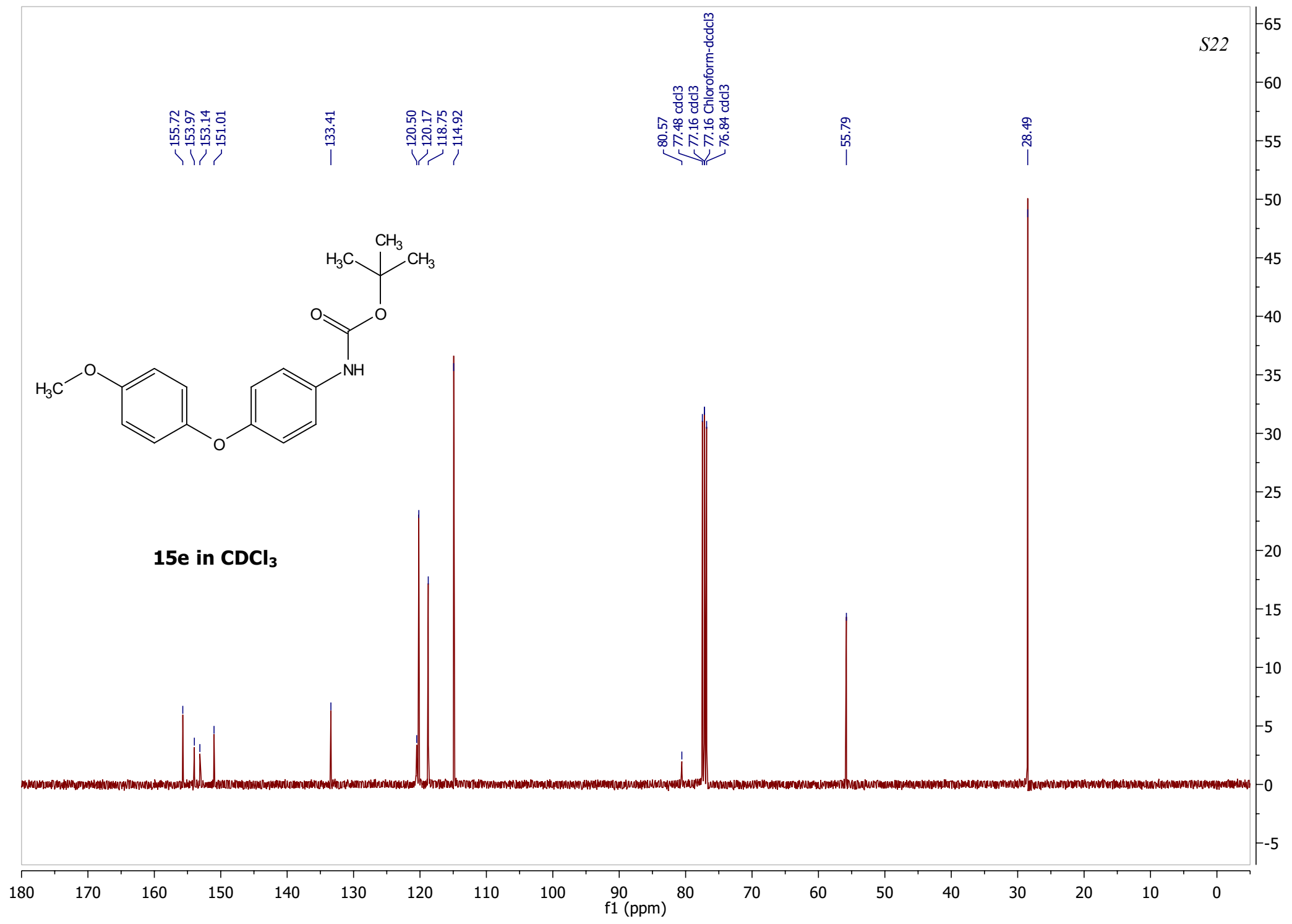
133.41

120.50  
120.17  
118.75  
114.92

80.57  
77.48 cdd3  
77.16 cdd3  
77.16 Chloroform-dcd3  
76.84 cdd3

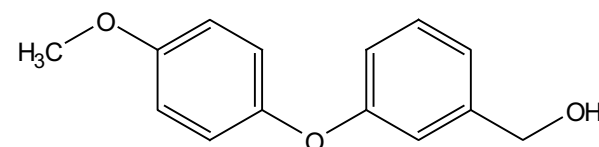
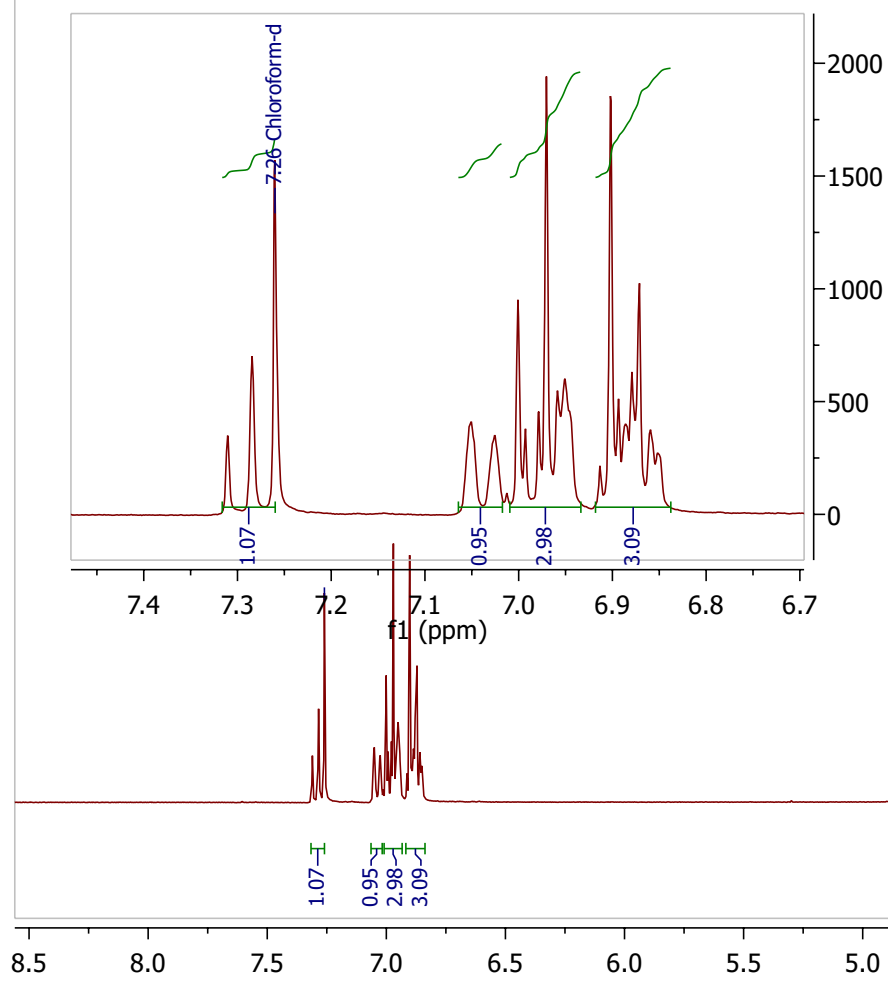
55.79

28.49



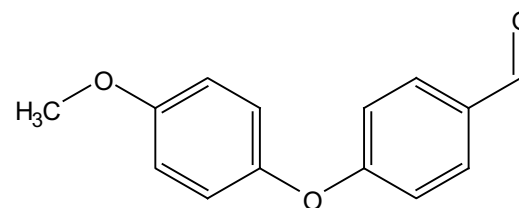
— 7.26 Chloroform-d

7.26 Chloroform-d

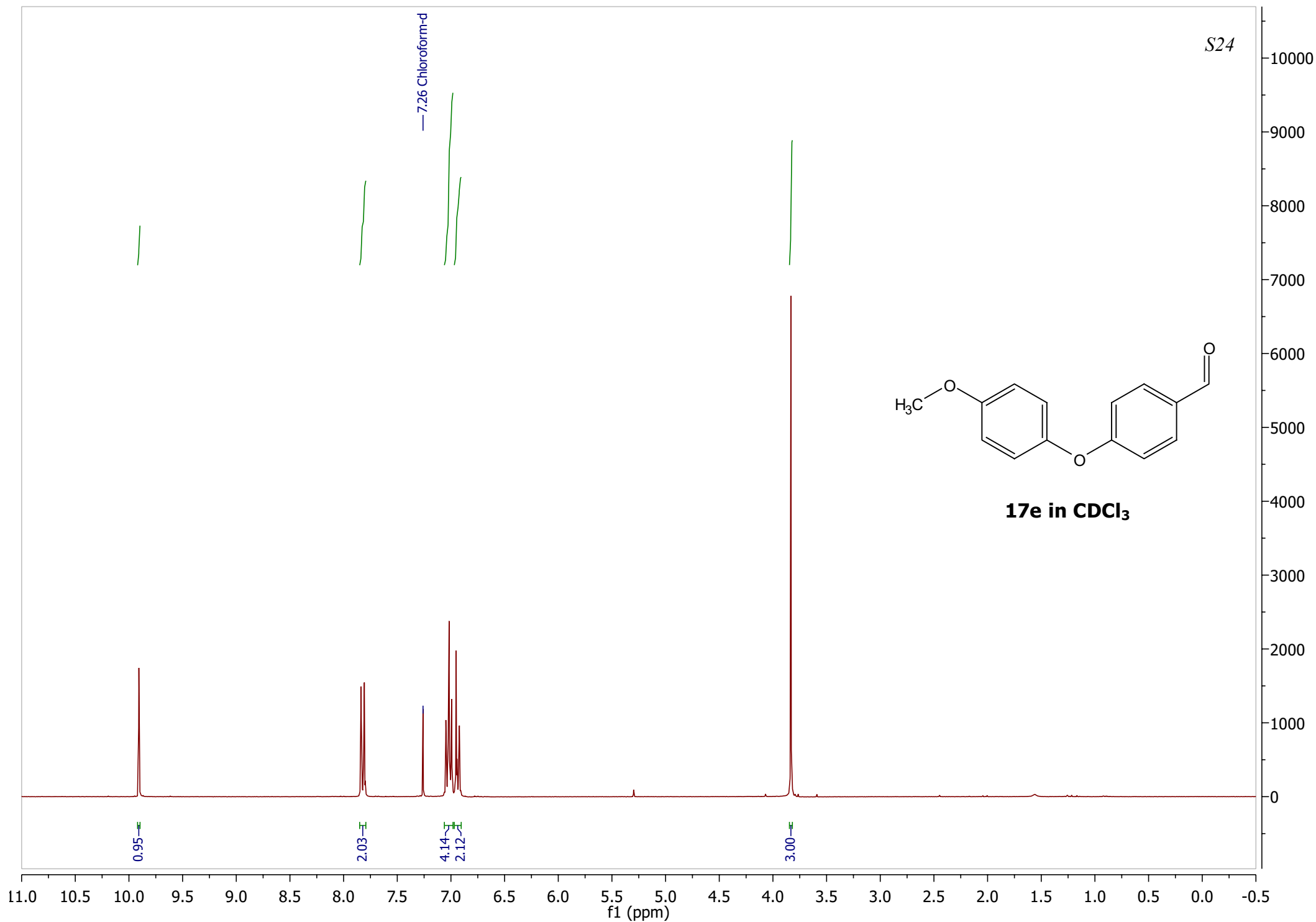
**16e in CDCl<sub>3</sub>**

f1 (ppm)

S24



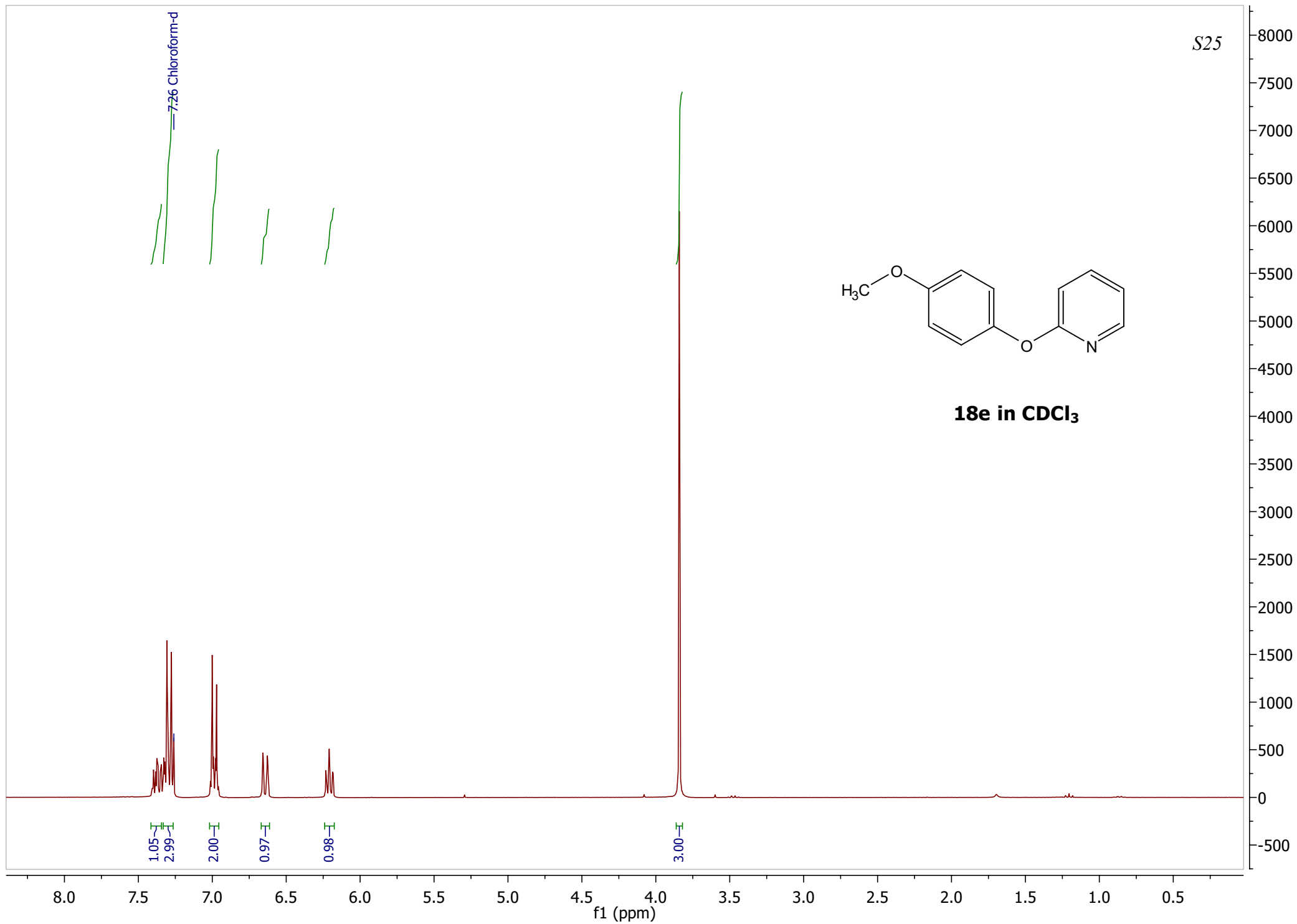
**17e** in CDCl<sub>3</sub>

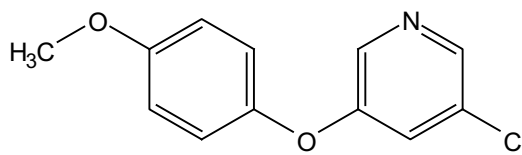


S25

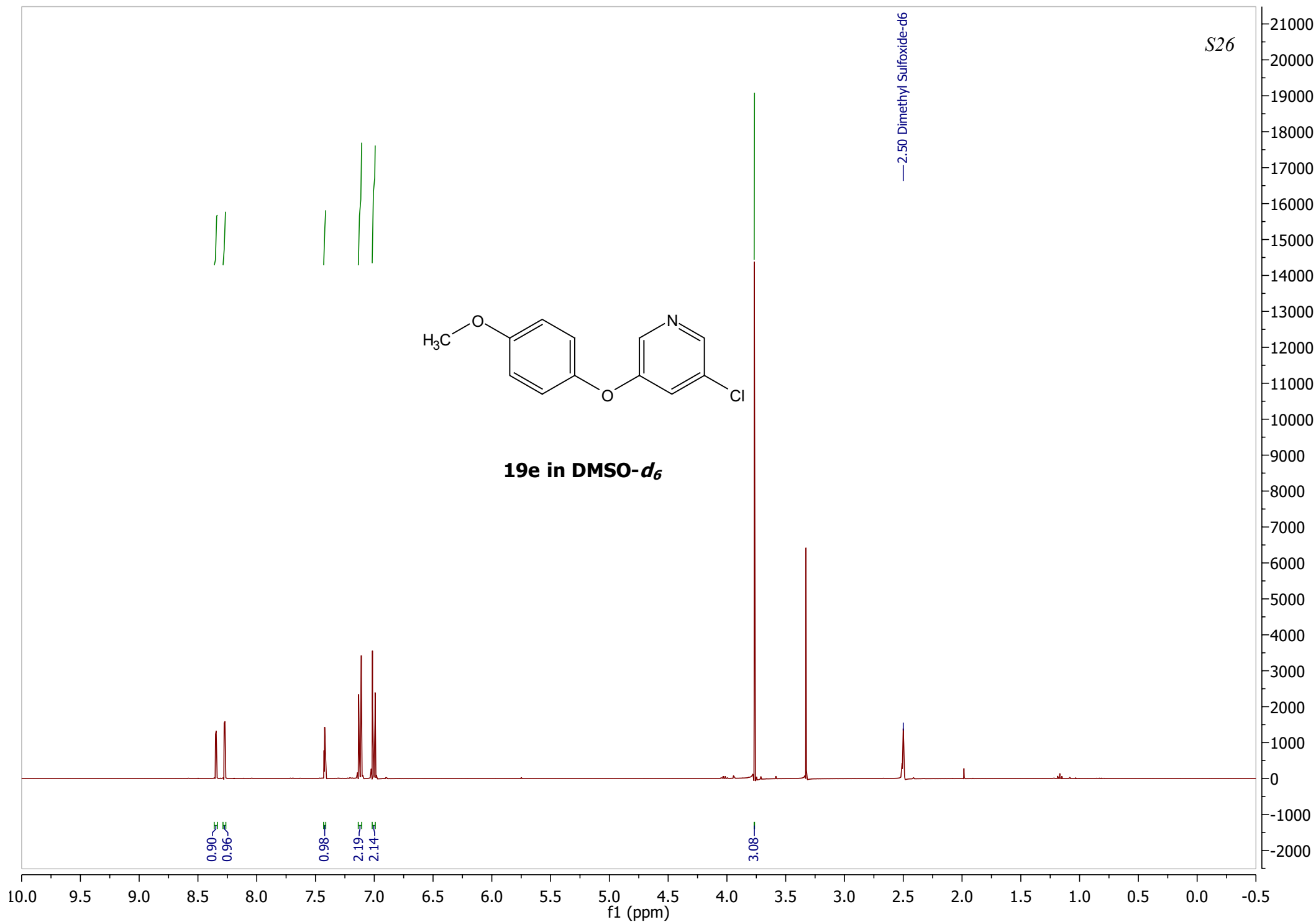


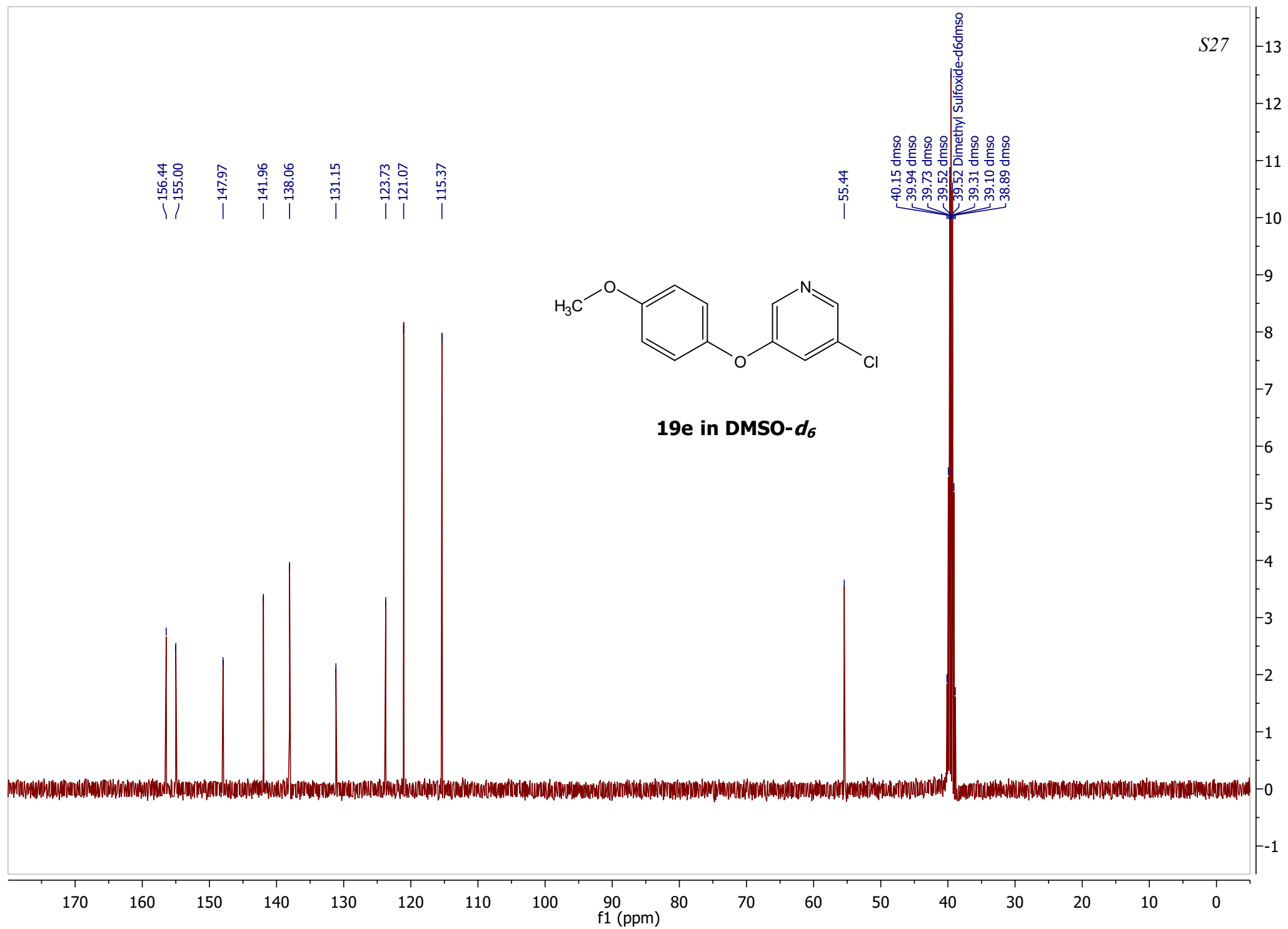
**18e in CDCl<sub>3</sub>**

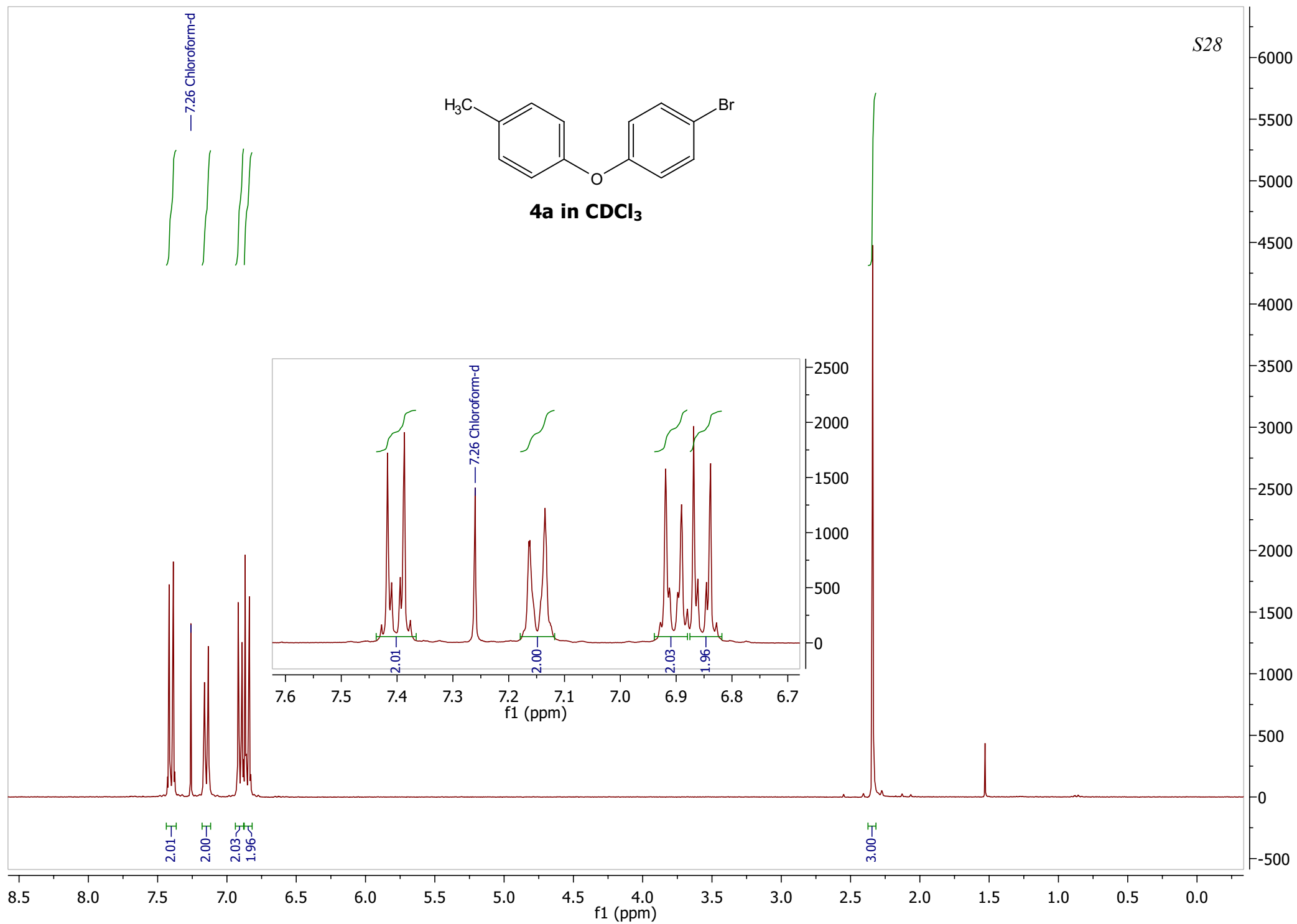


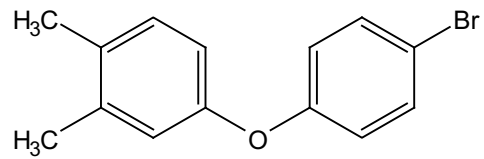


**19e in DMSO-*d*<sub>6</sub>**

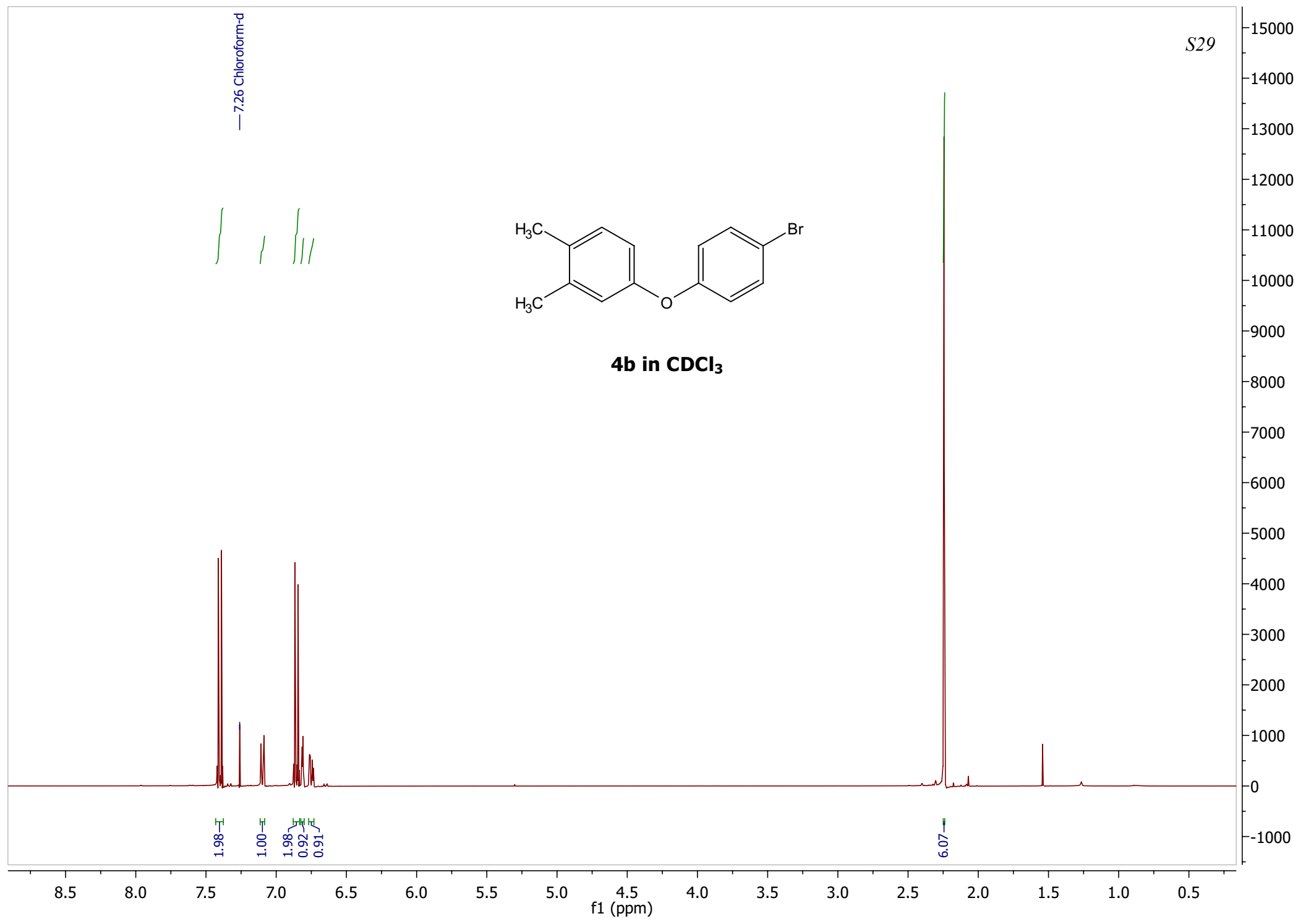




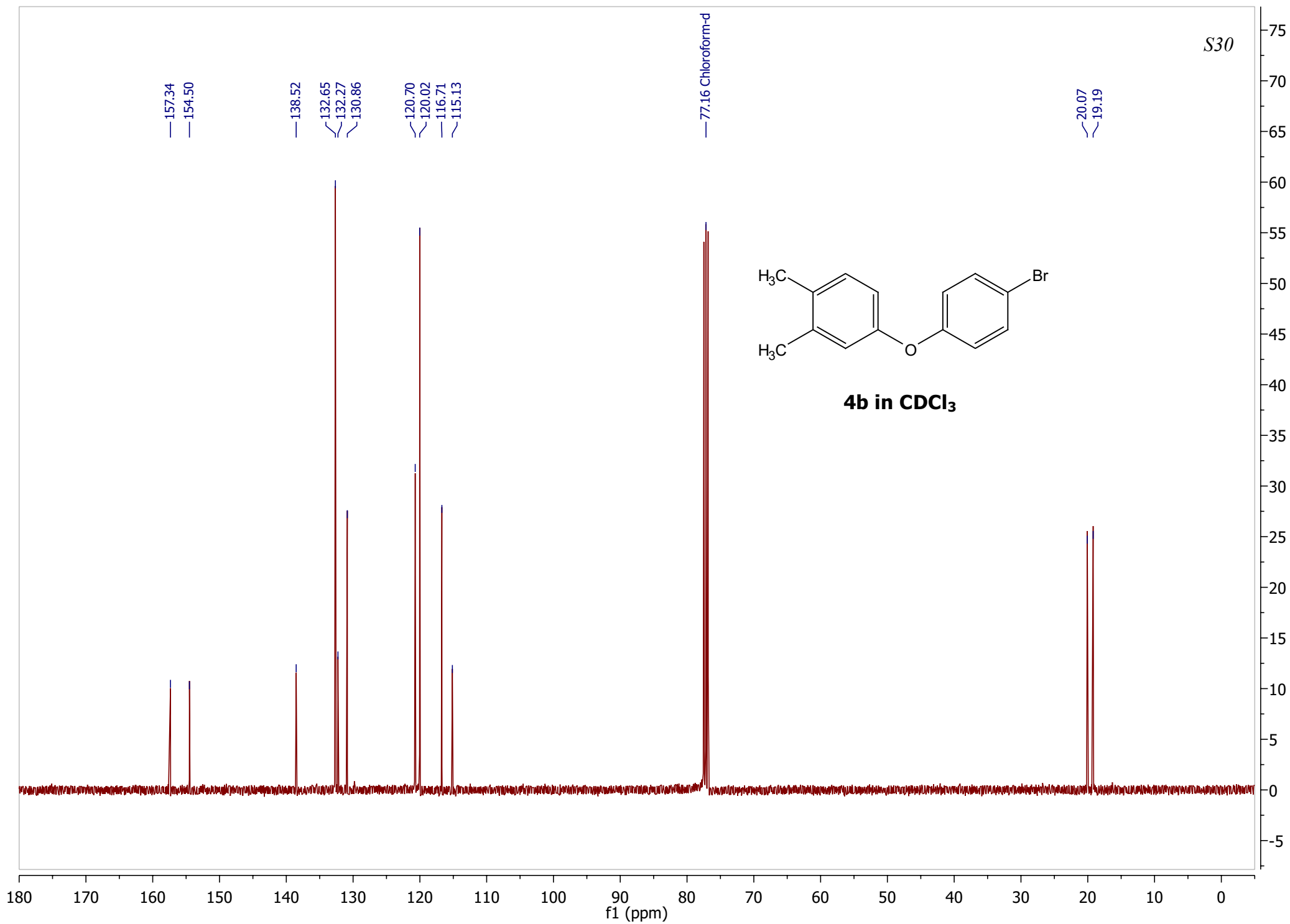


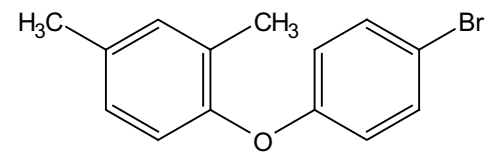


4b in CDCl<sub>3</sub>

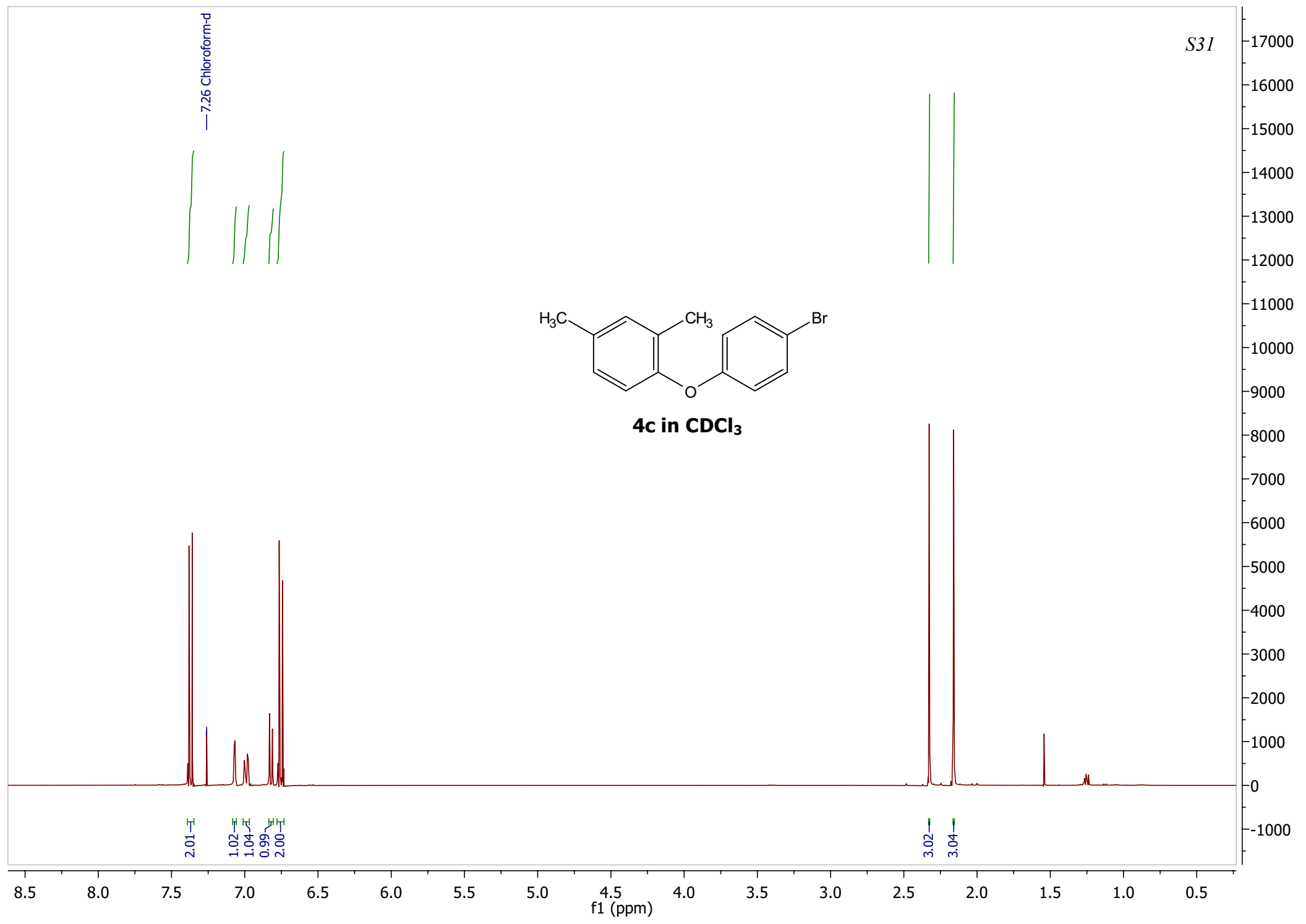


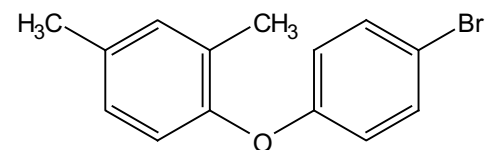
S30



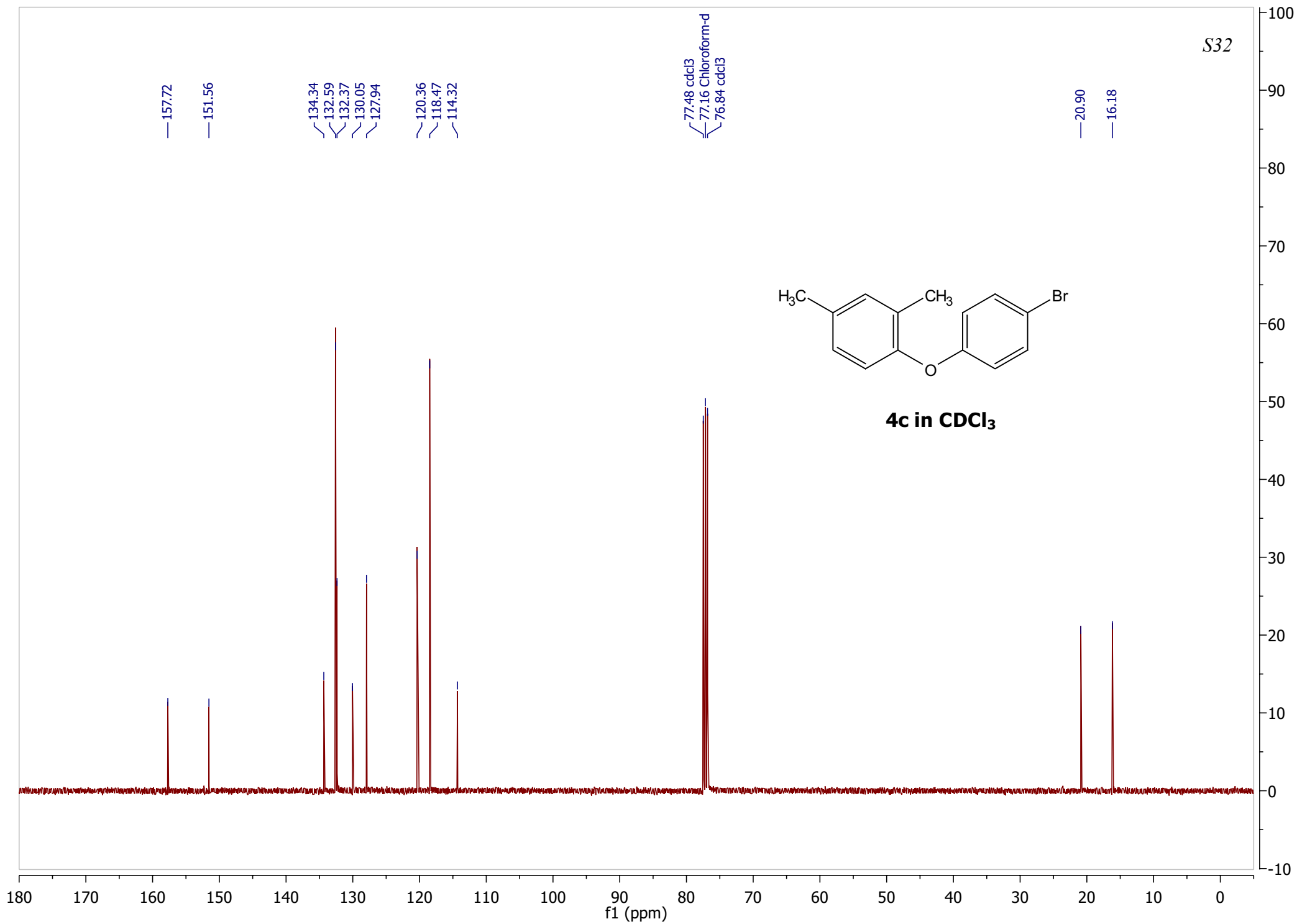


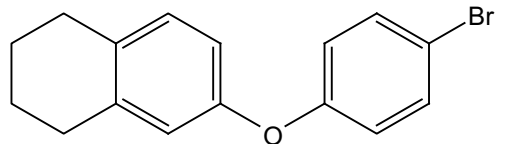
4c in CDCl<sub>3</sub>



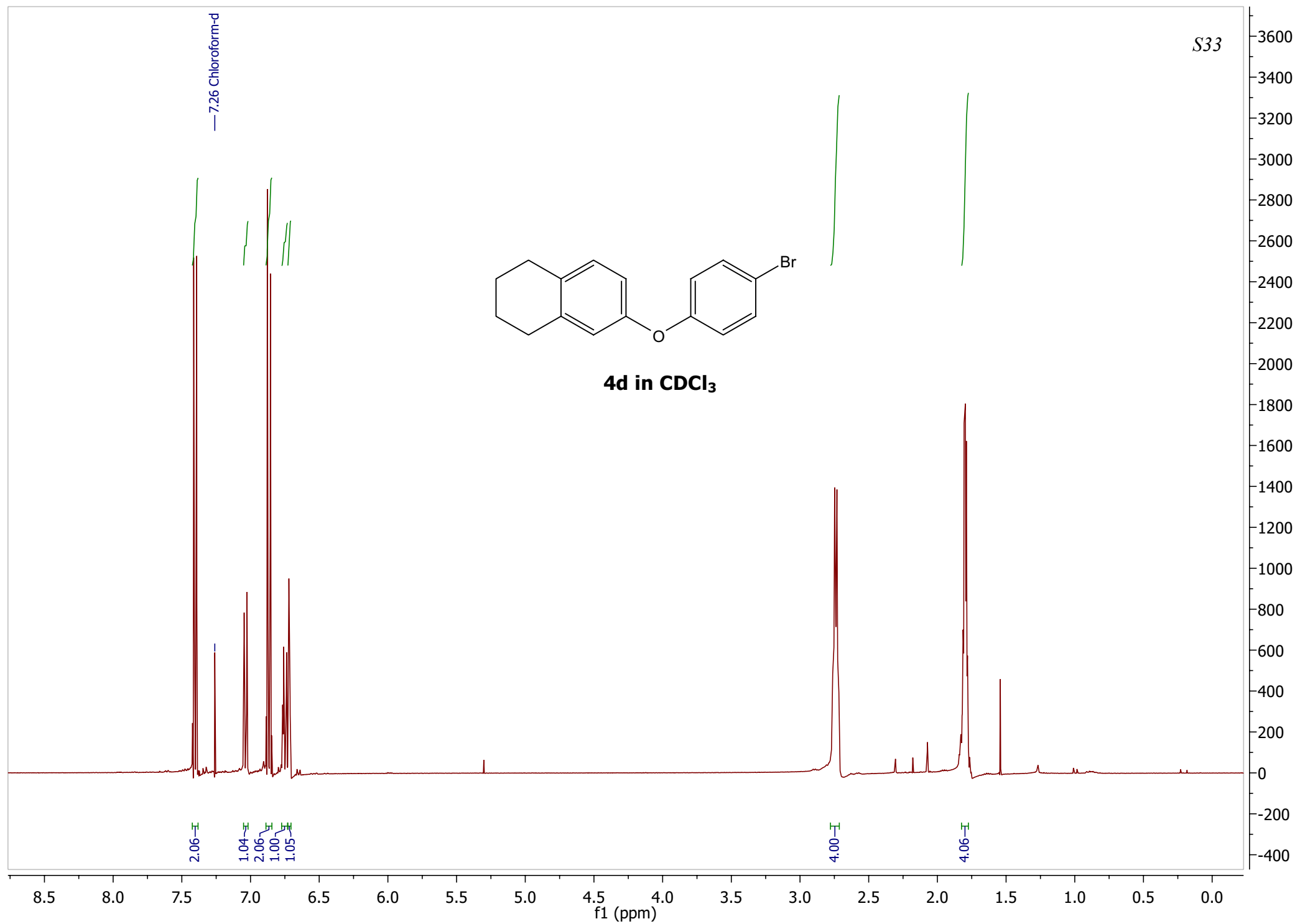


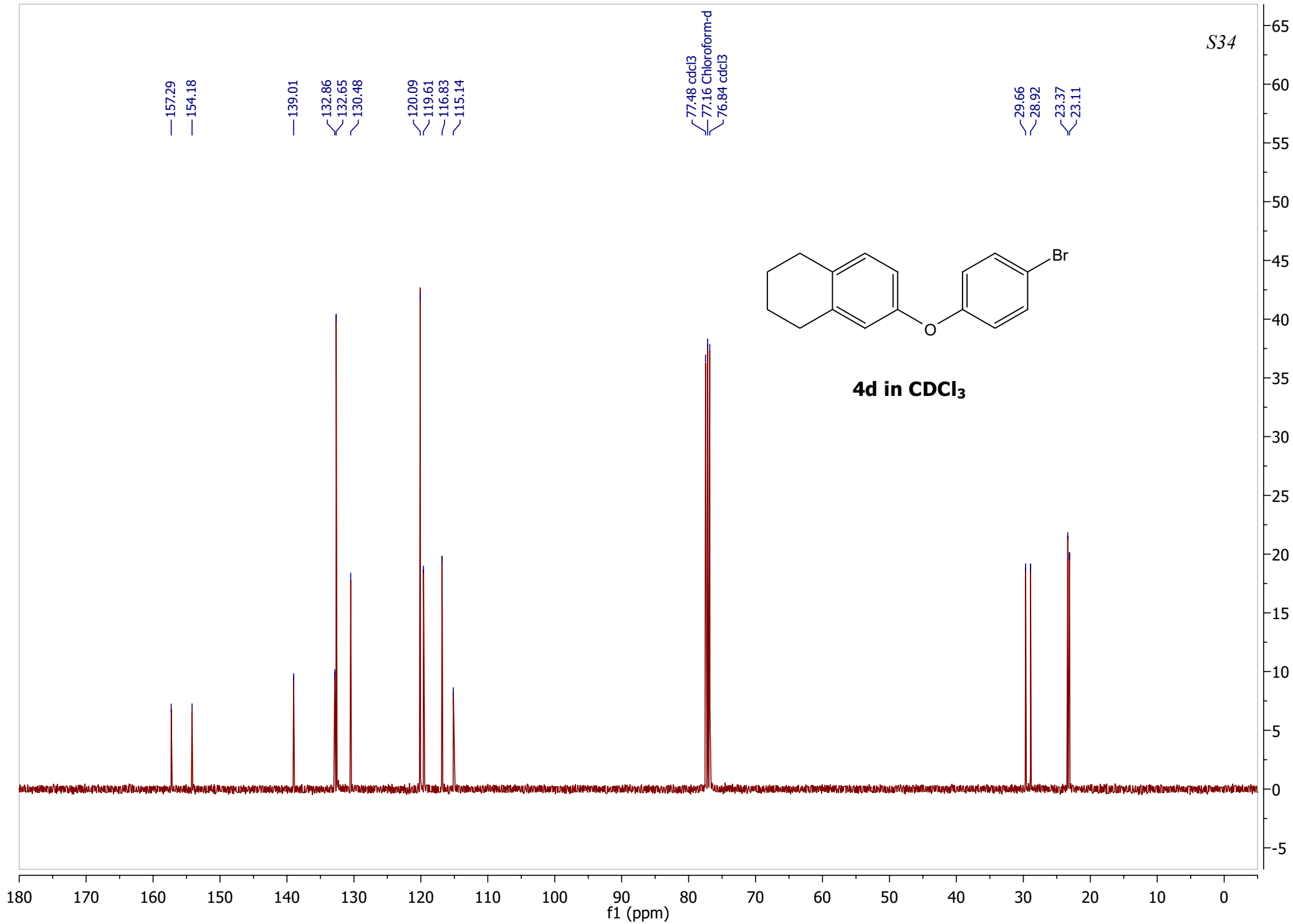
**4c in CDCl<sub>3</sub>**



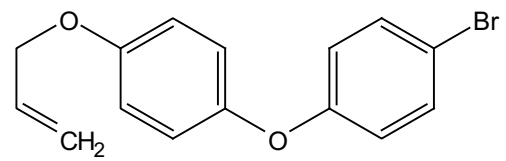


4d in CDCl<sub>3</sub>

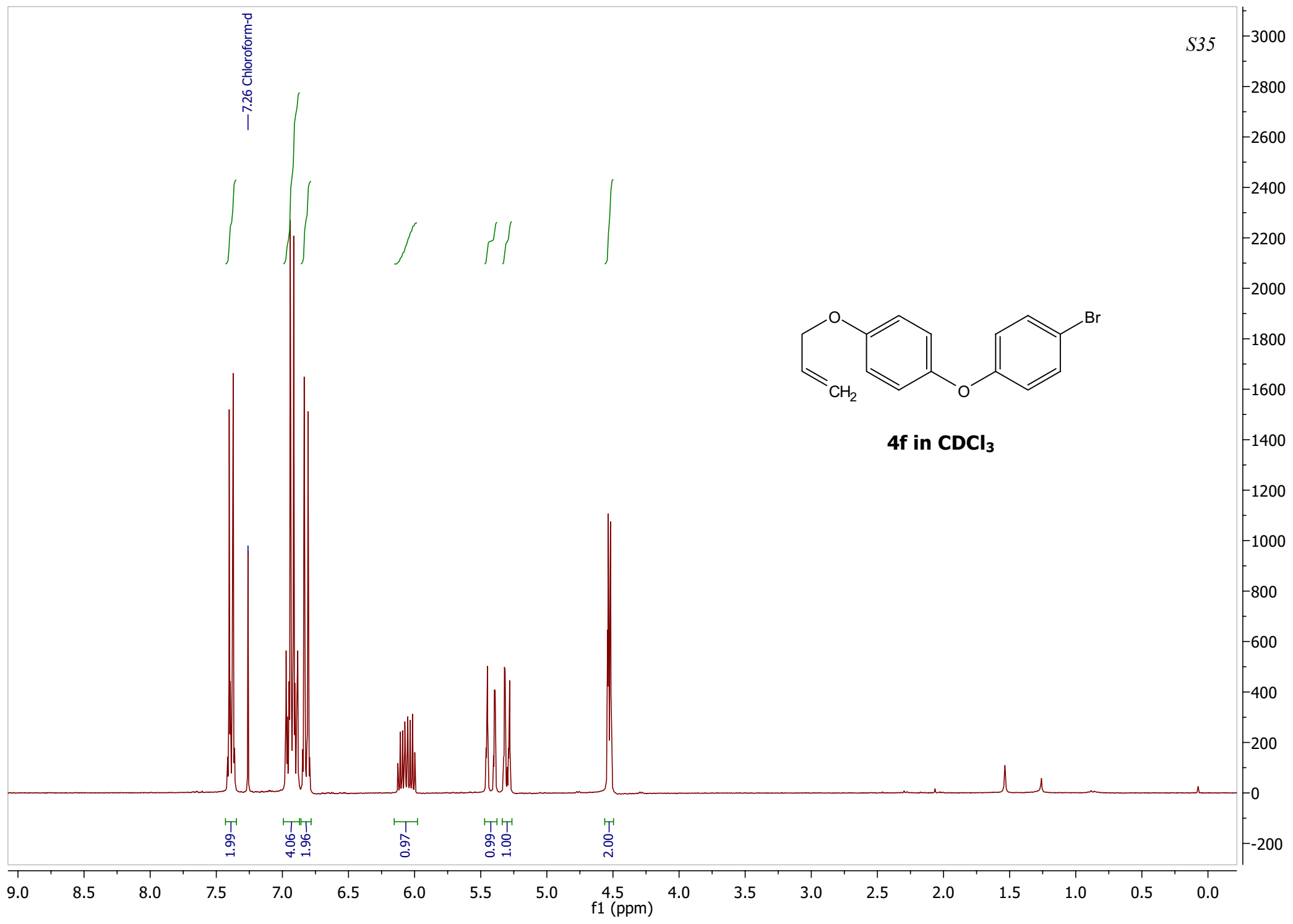


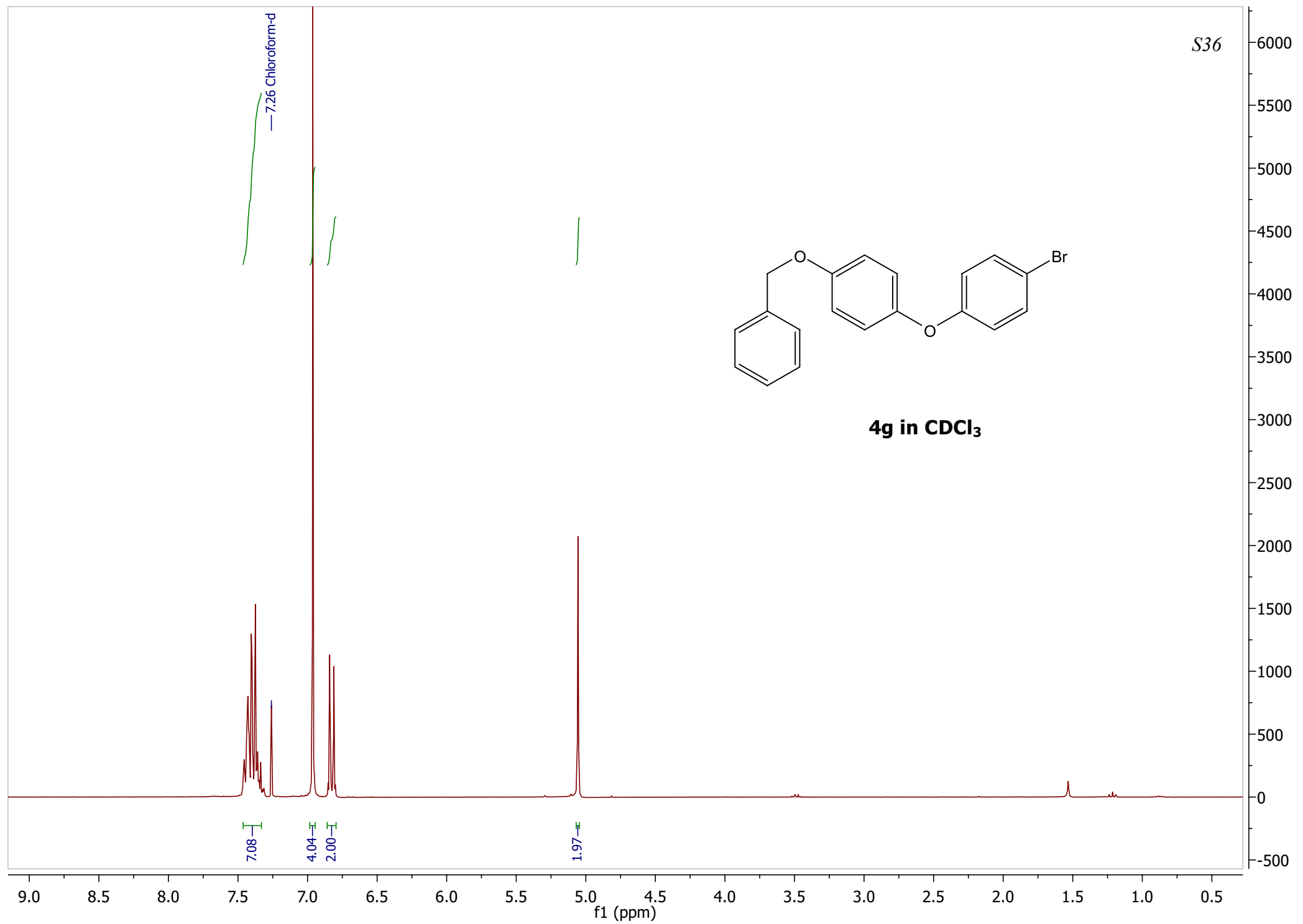


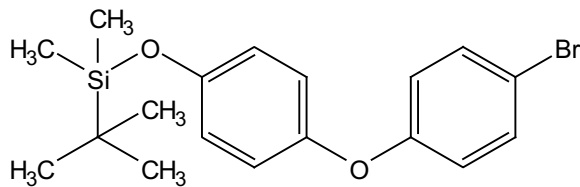
— 7.26 Chloroform-d



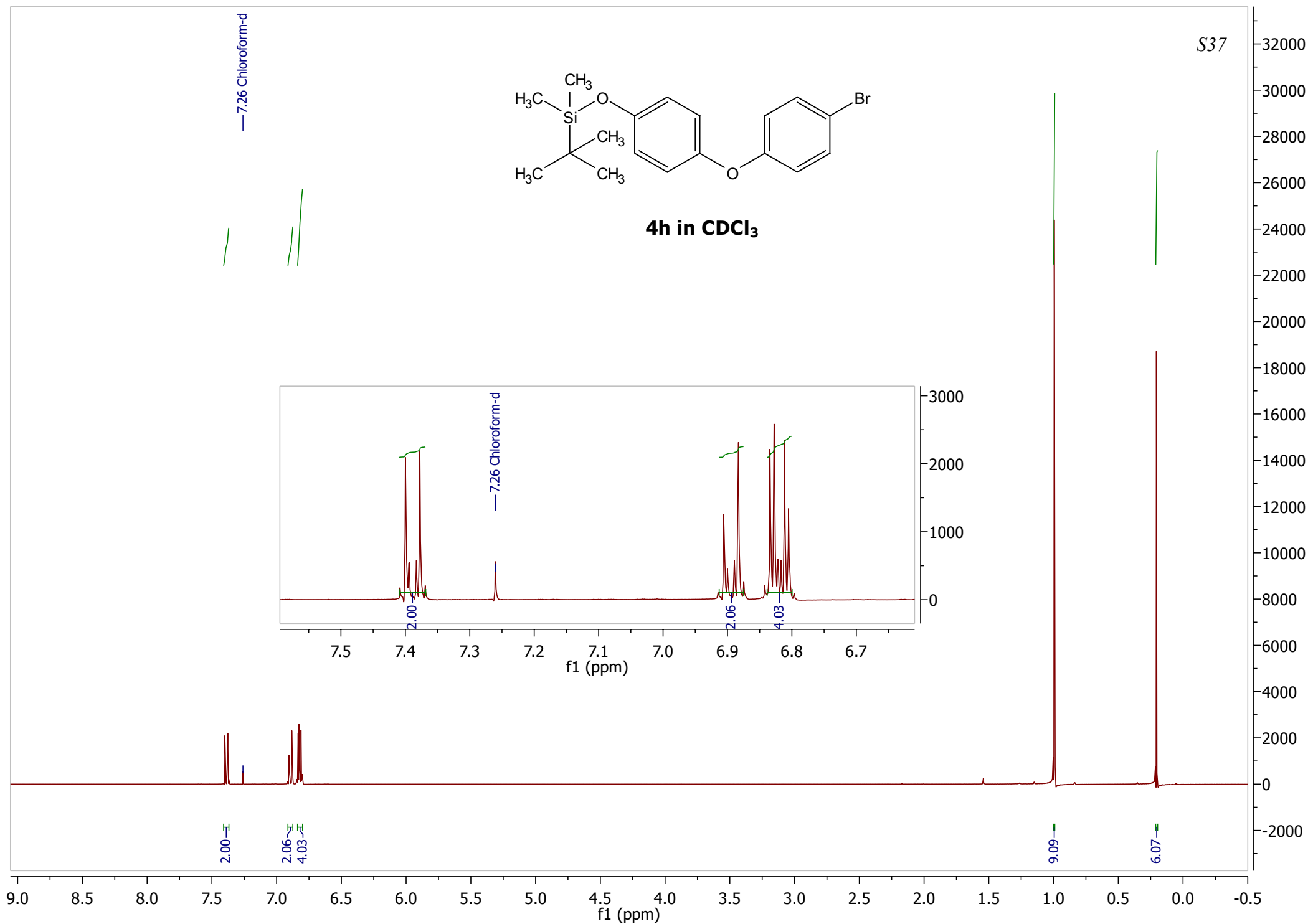
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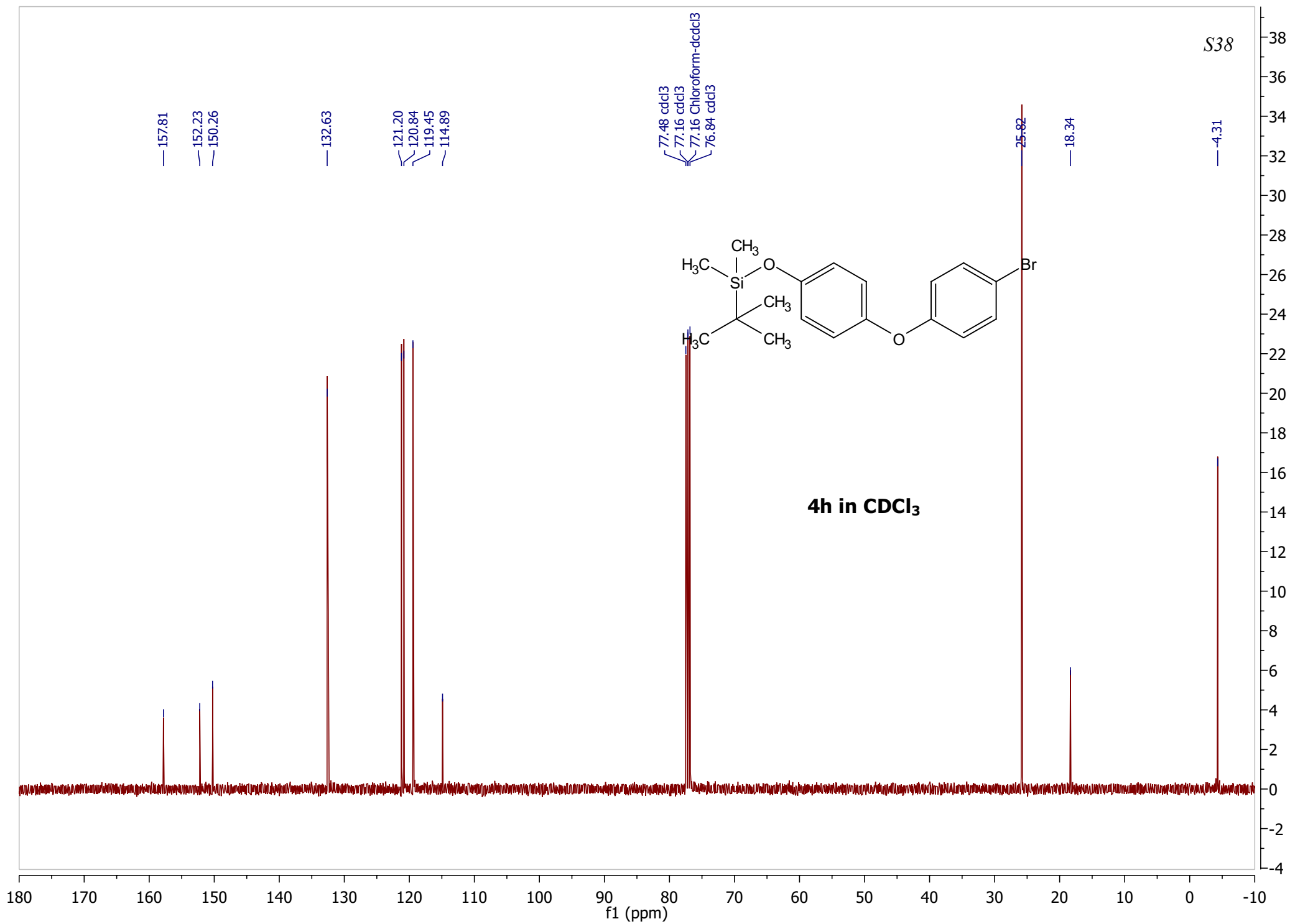




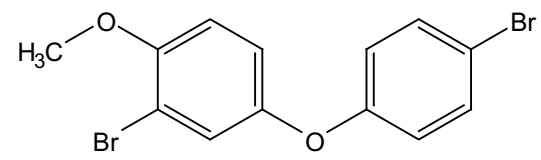


4h in CDCl<sub>3</sub>

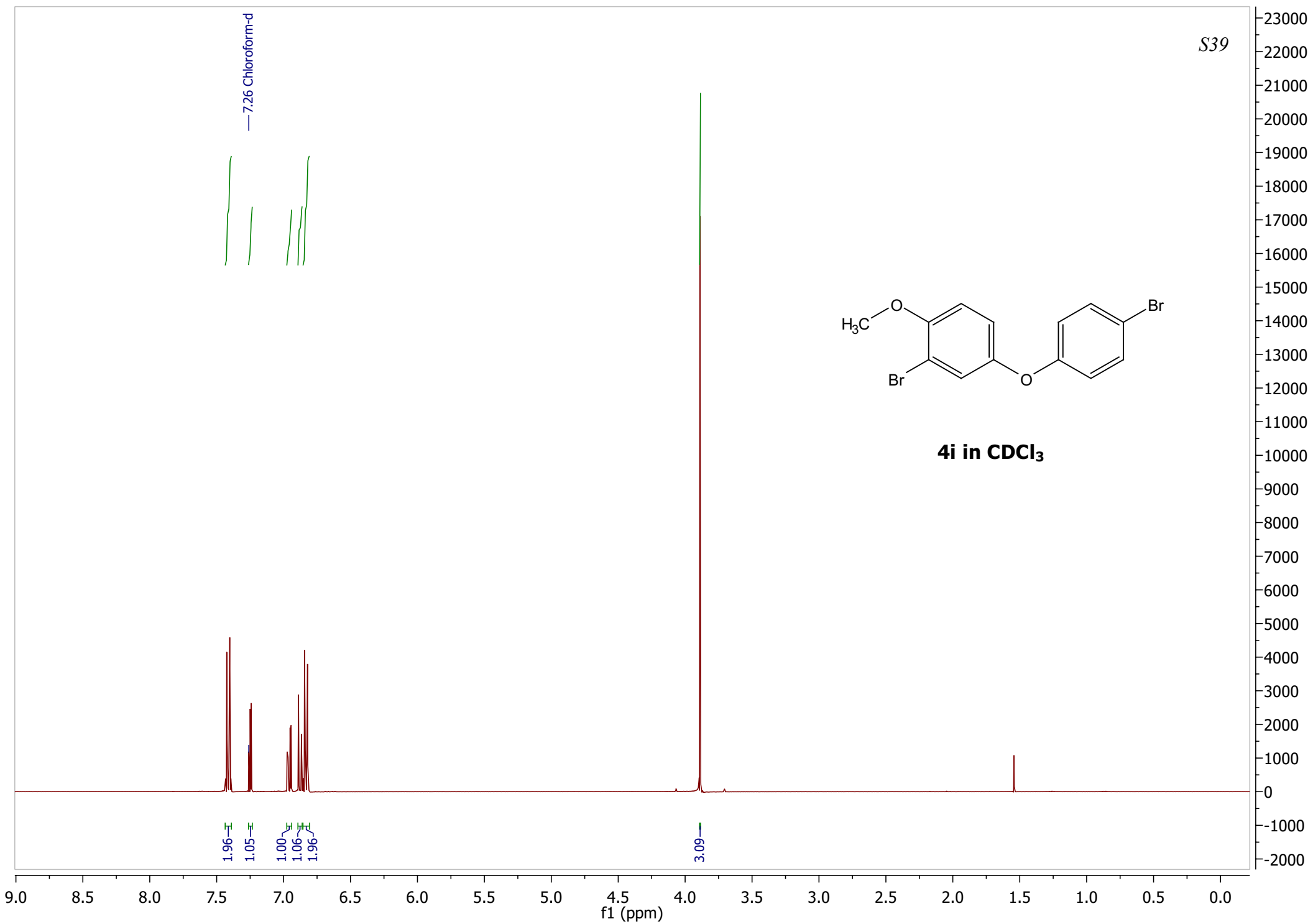


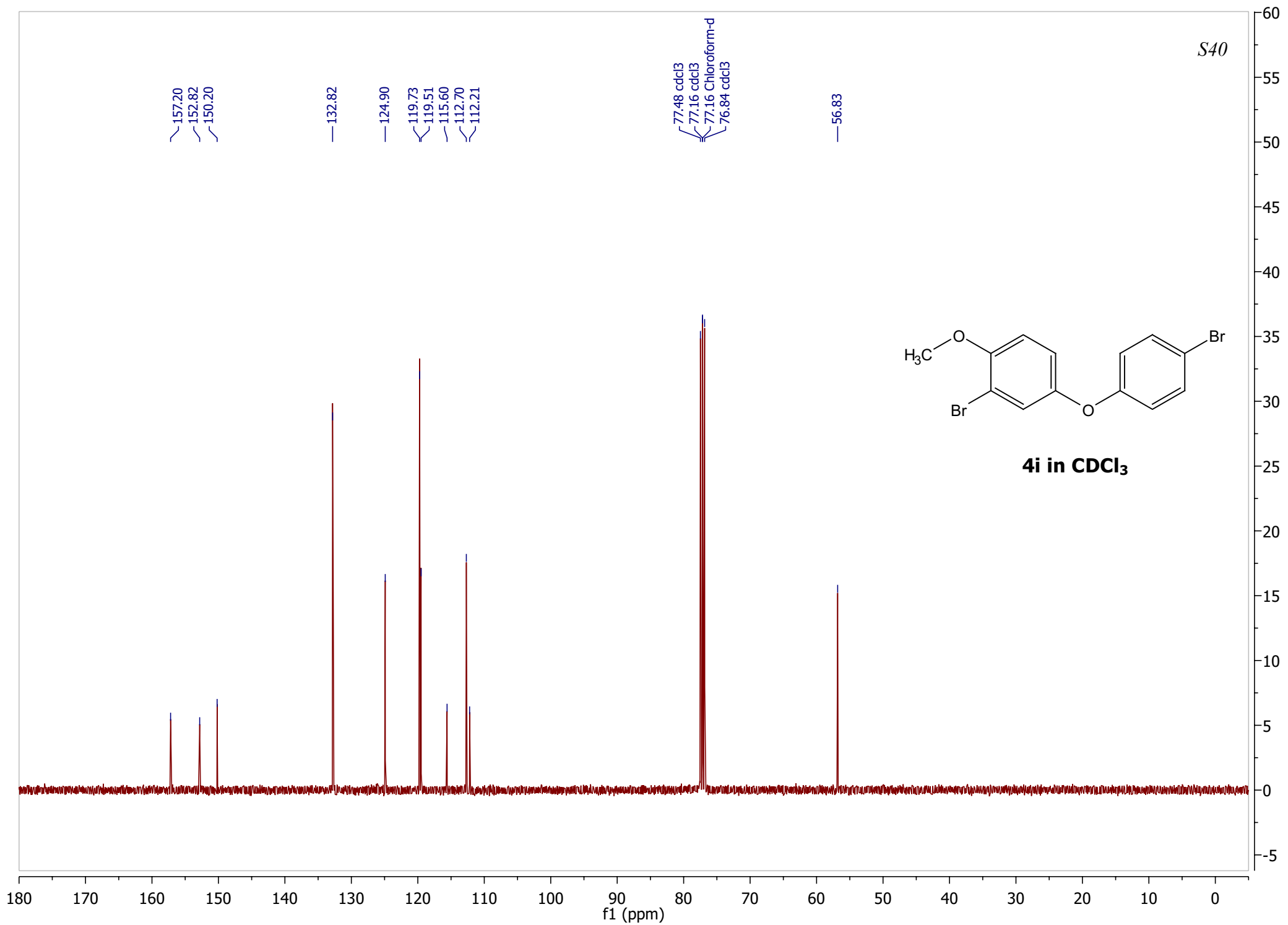


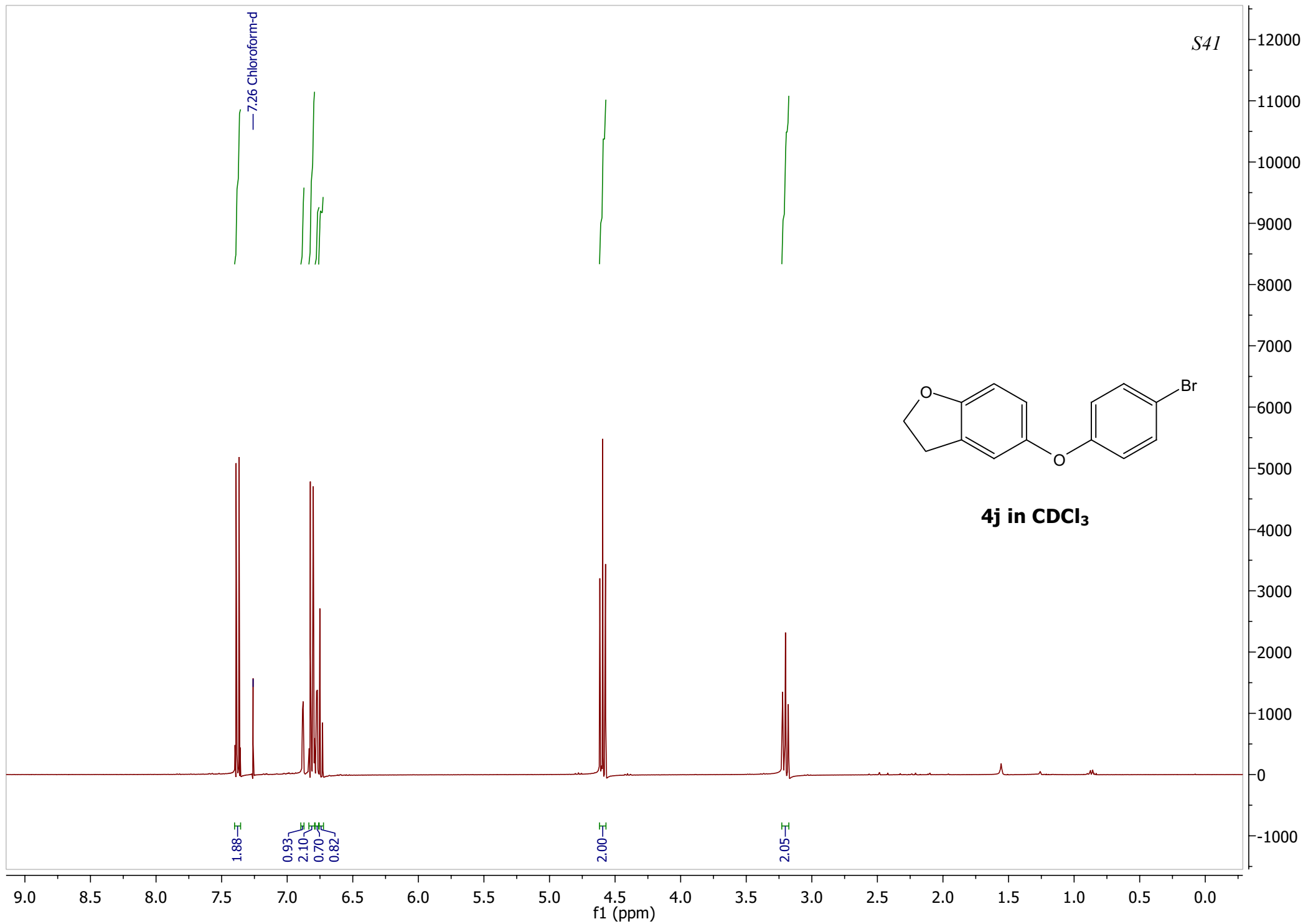
7.26 Chloroform-d

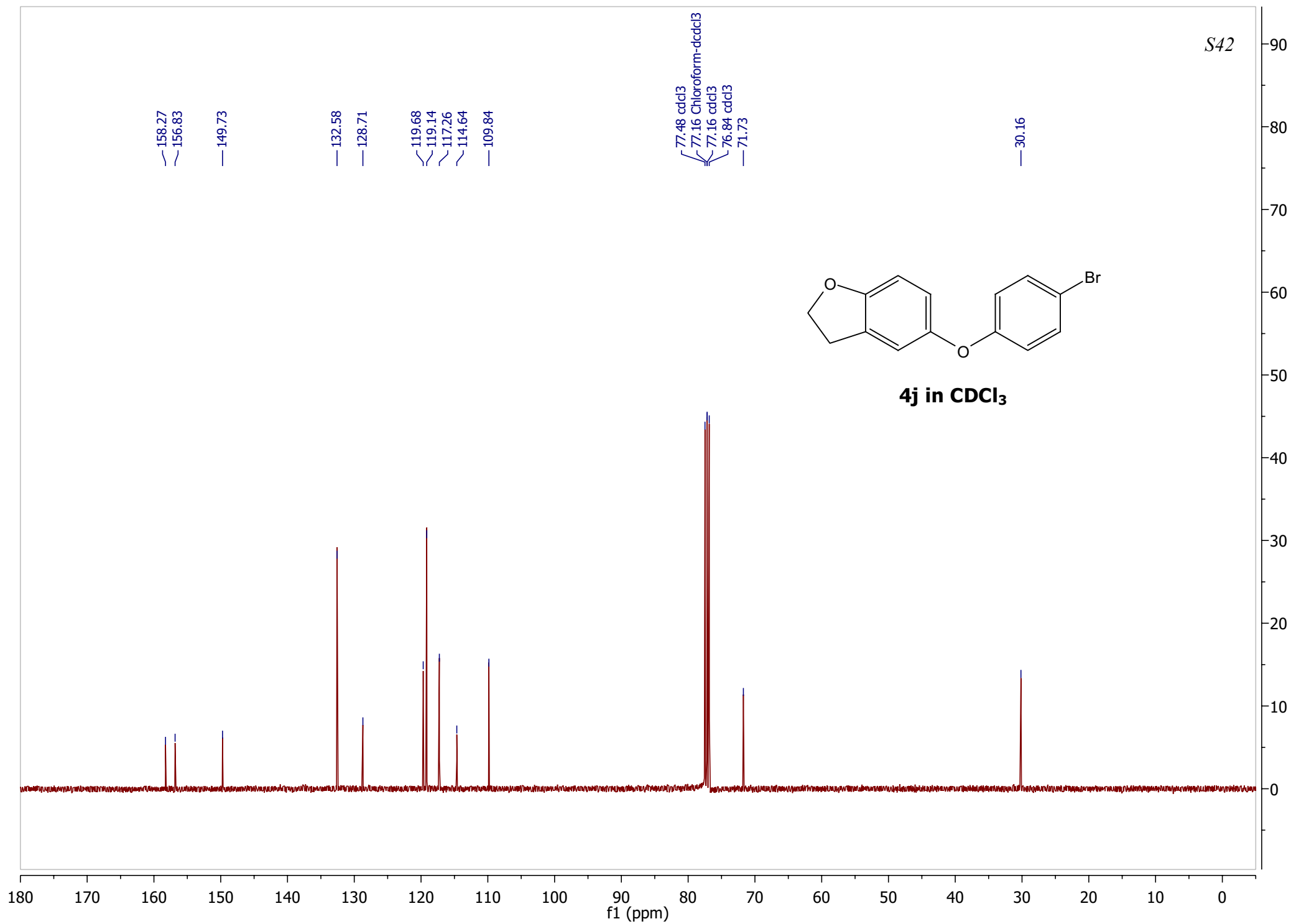


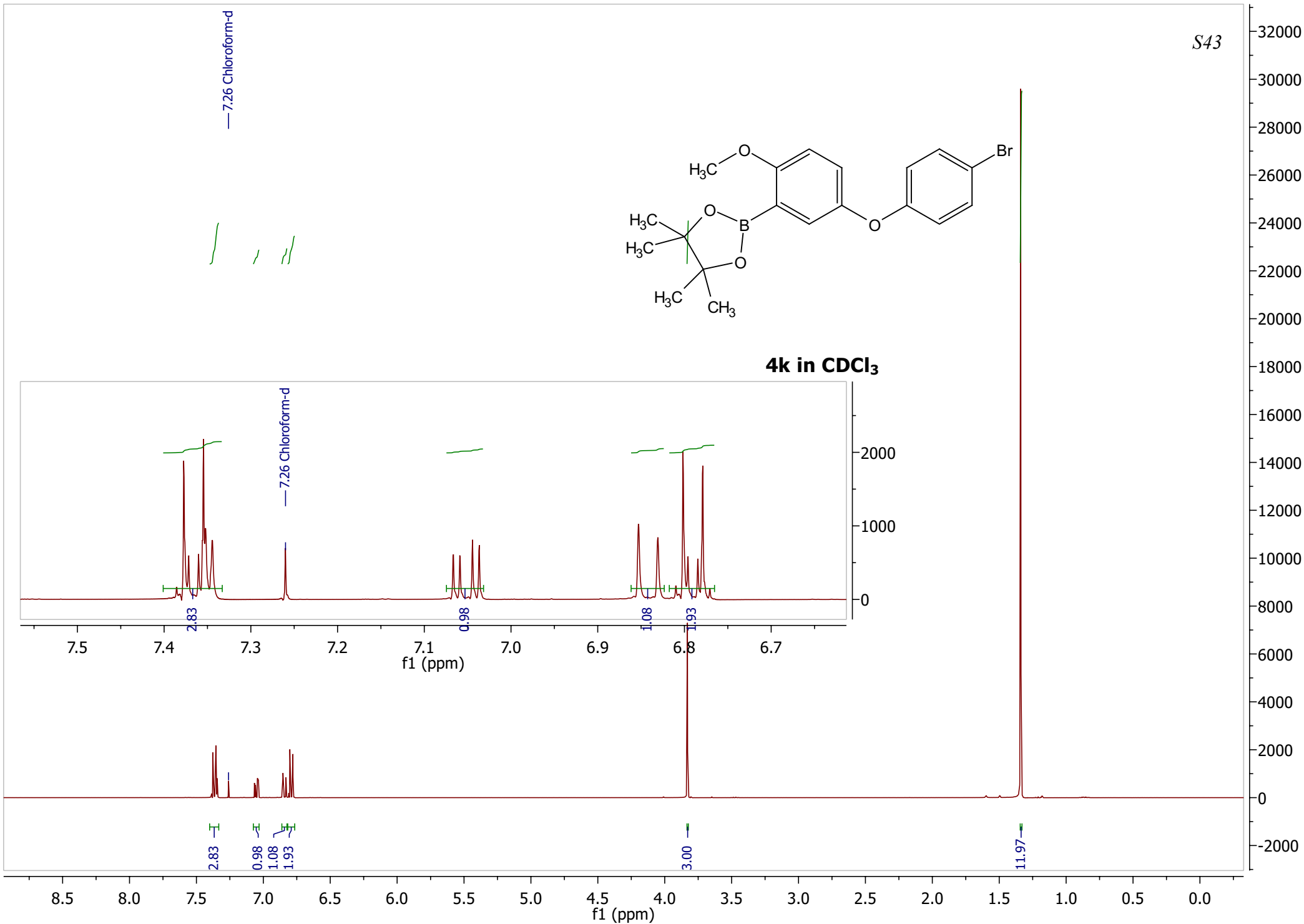
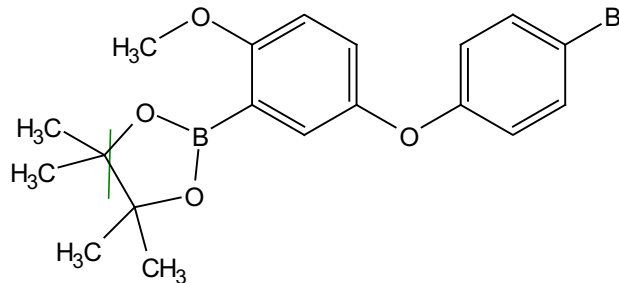
4i in CDCl<sub>3</sub>

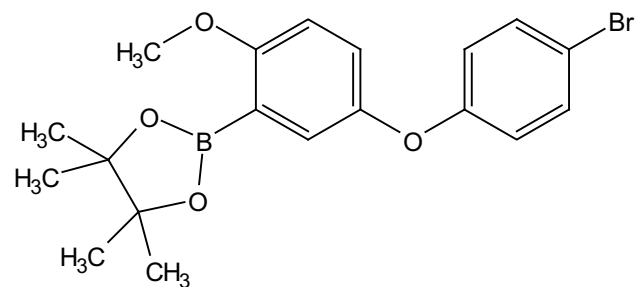




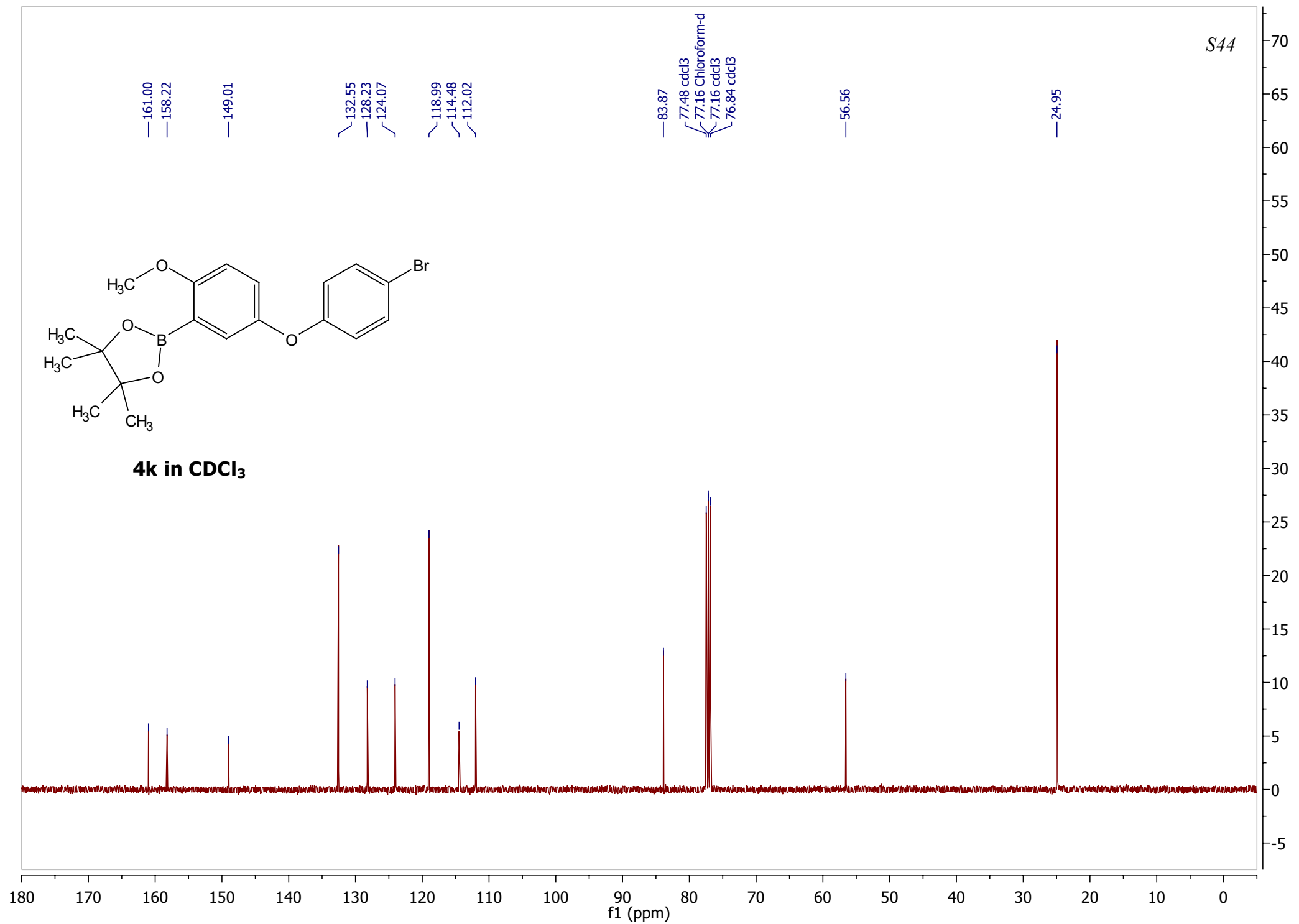




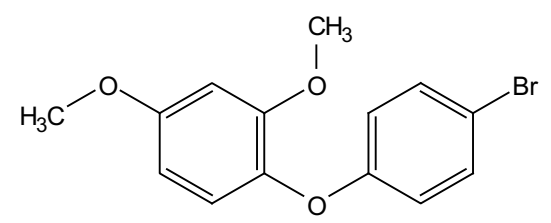




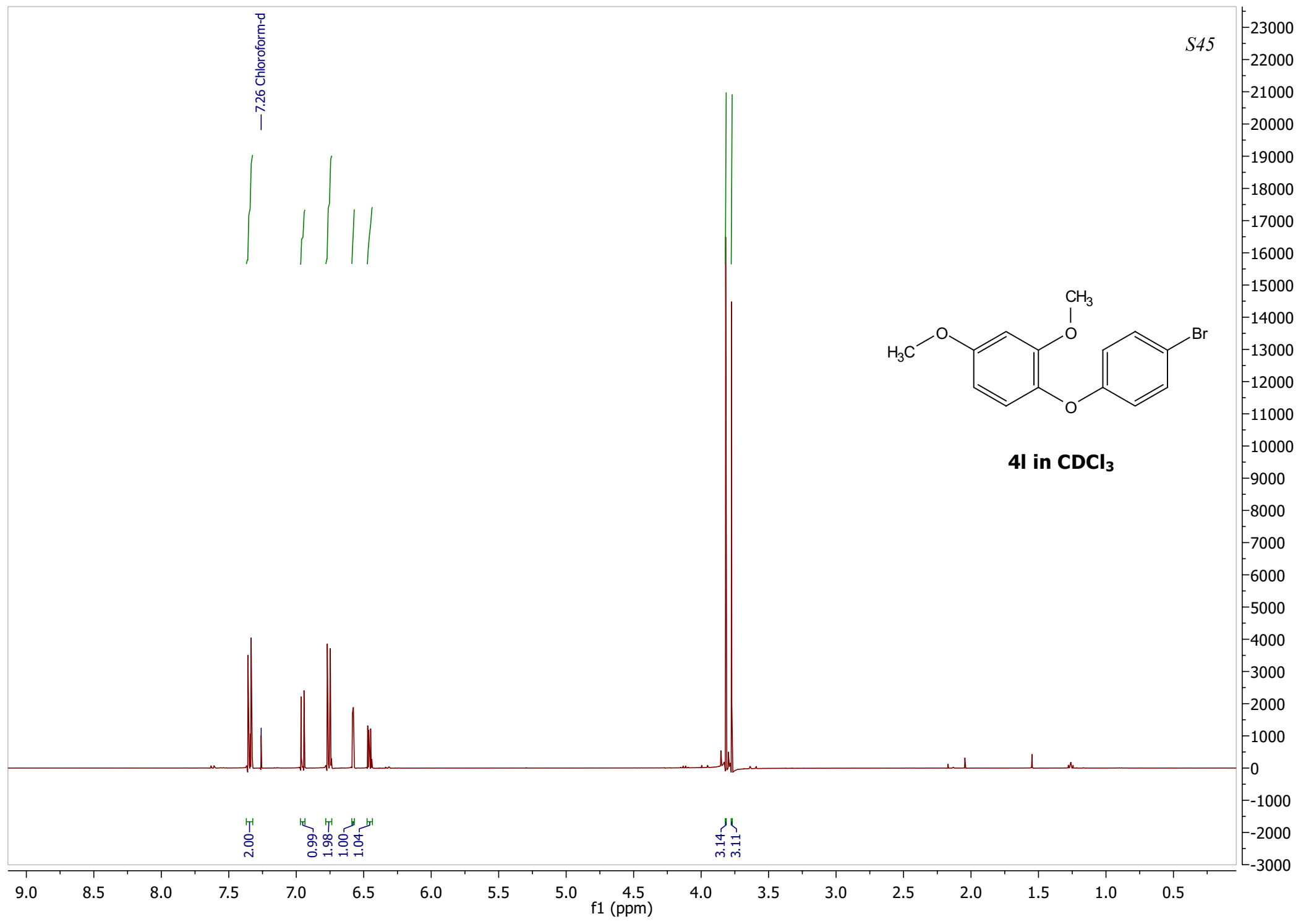
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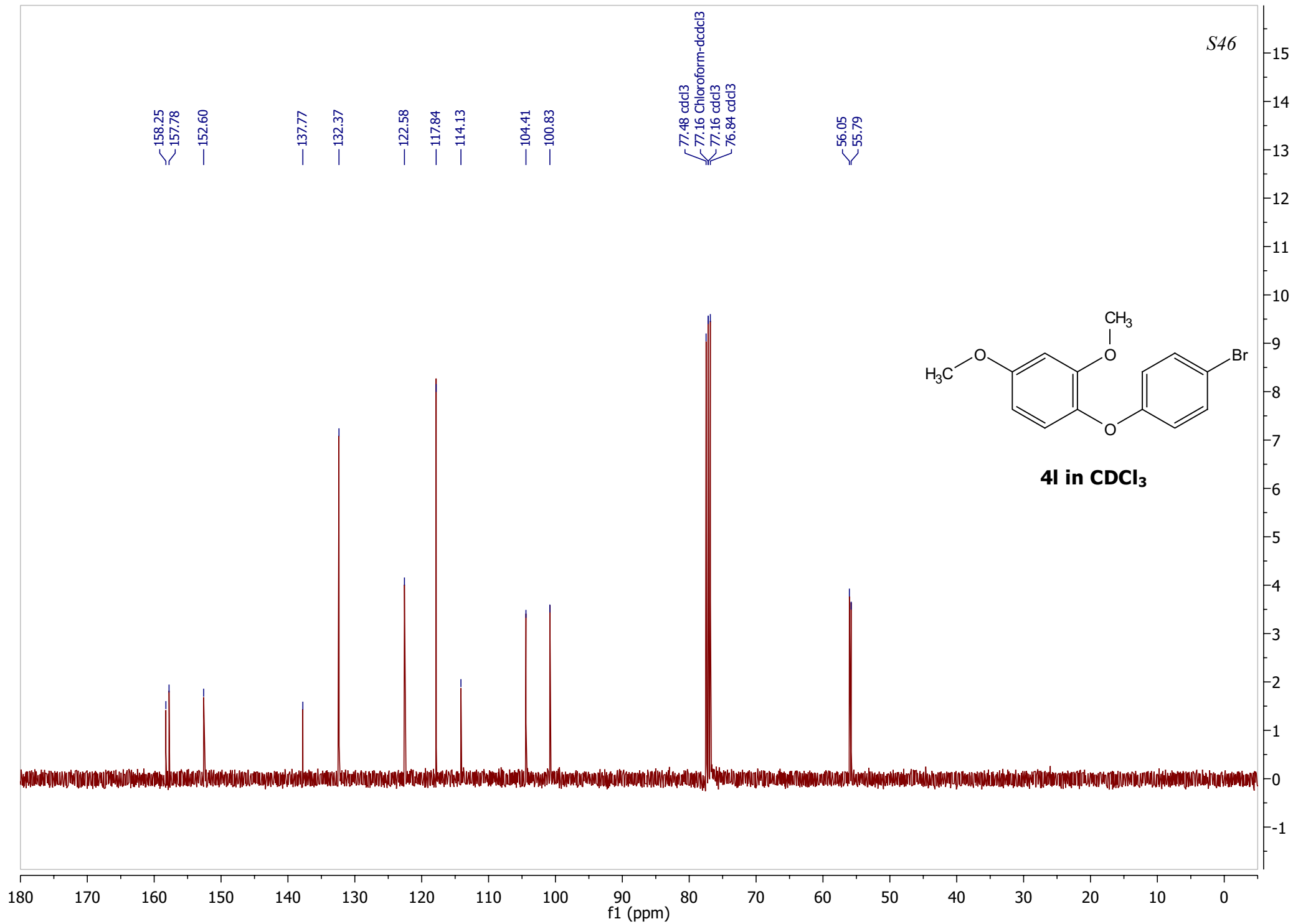


S45

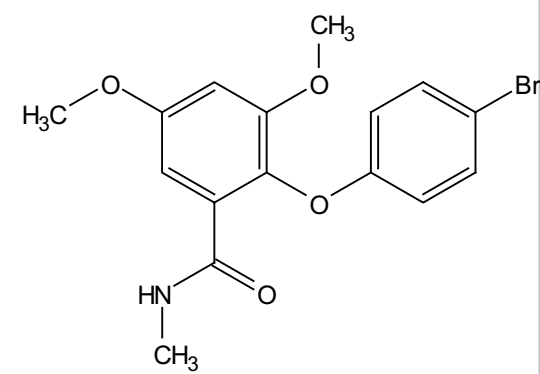


**4I in CDCl<sub>3</sub>**



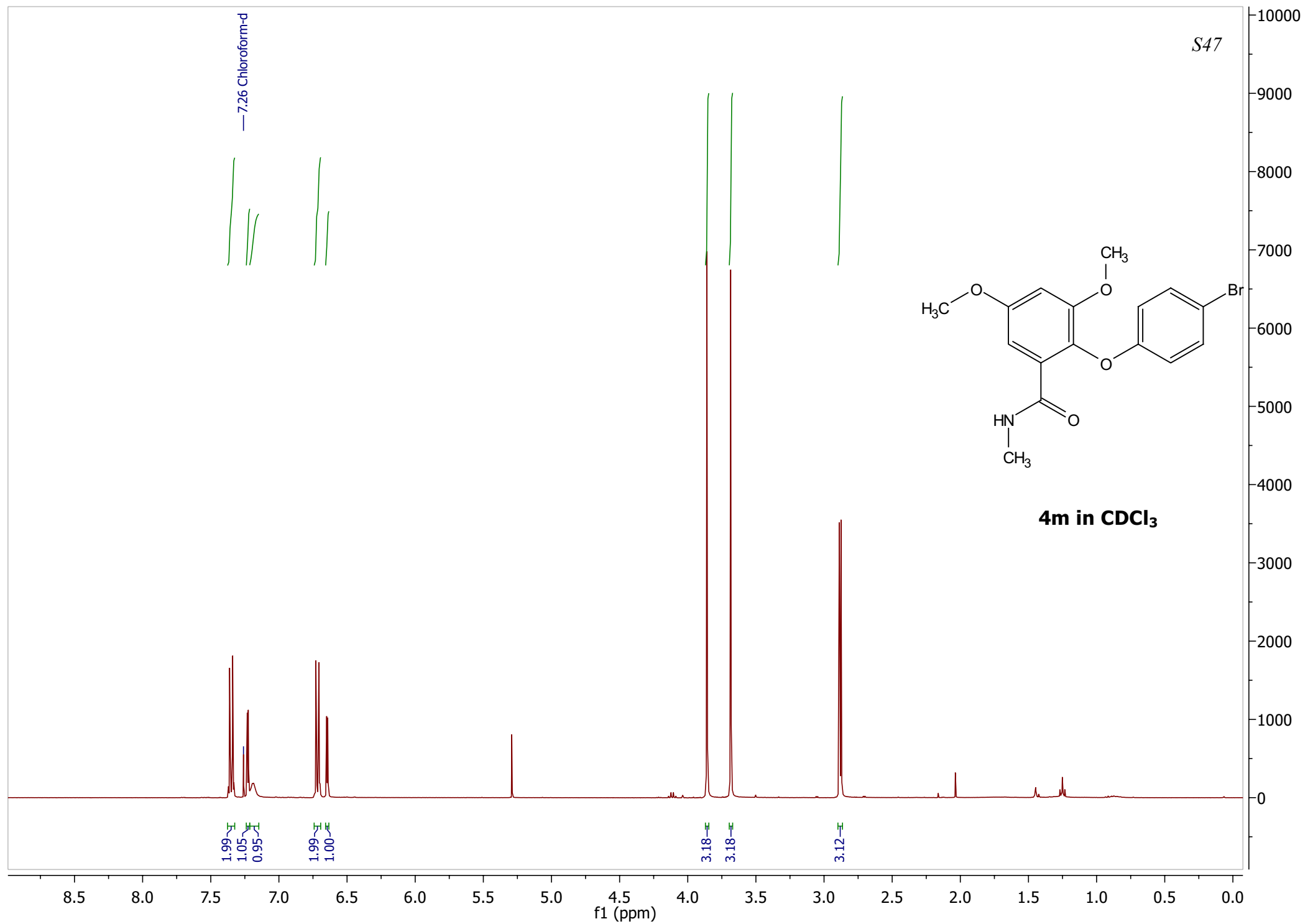


S47

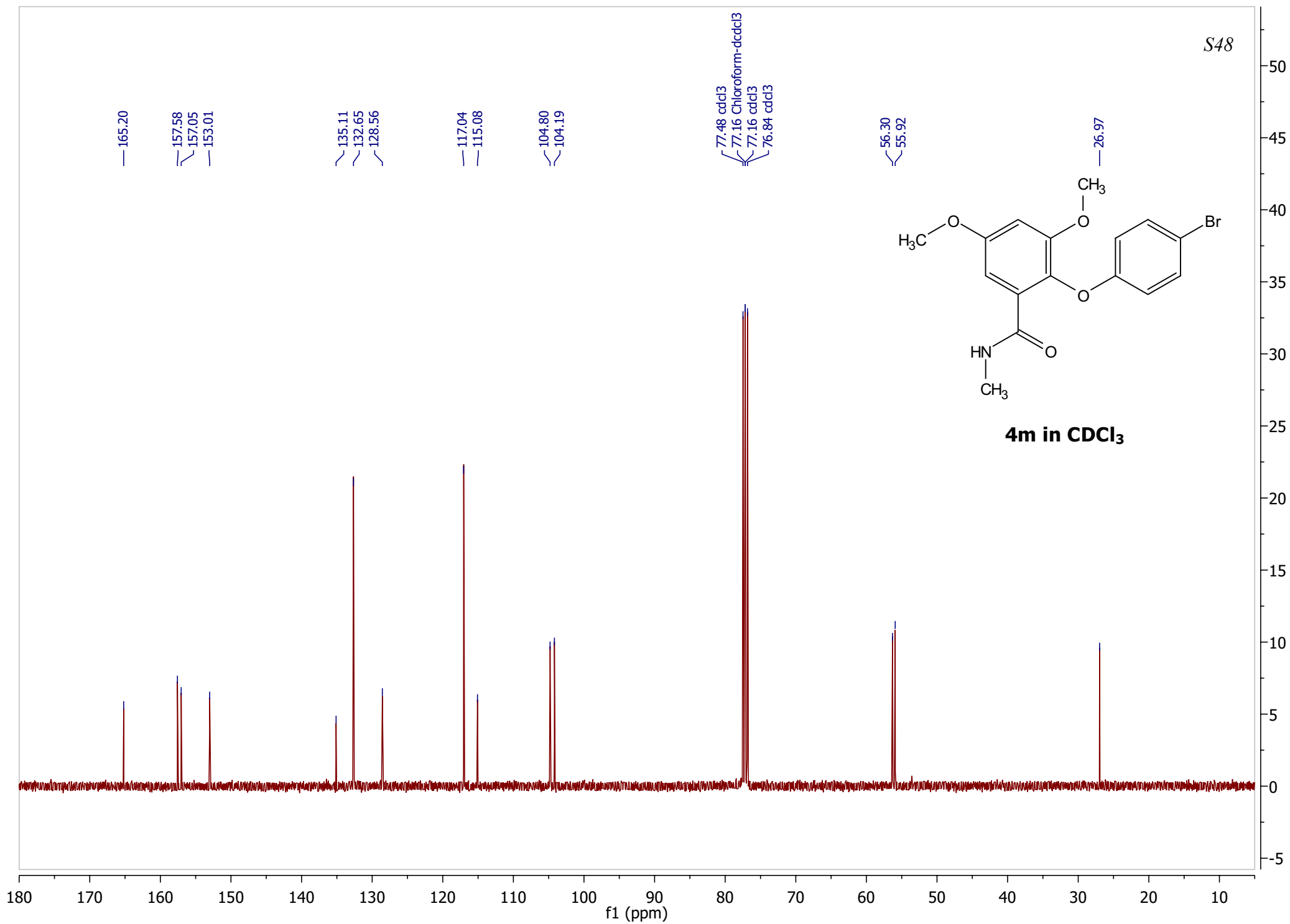


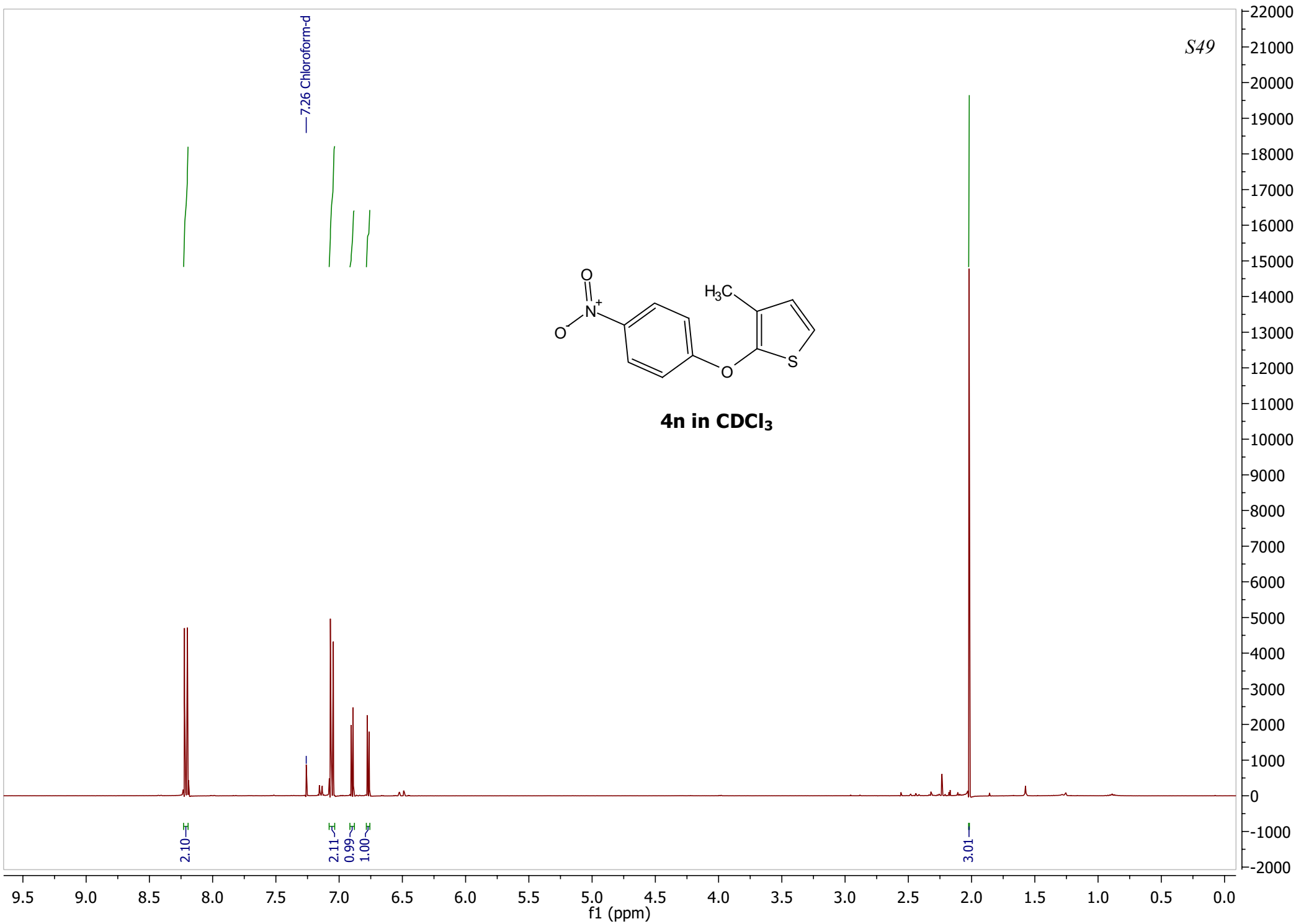
**4m in CDCl<sub>3</sub>**

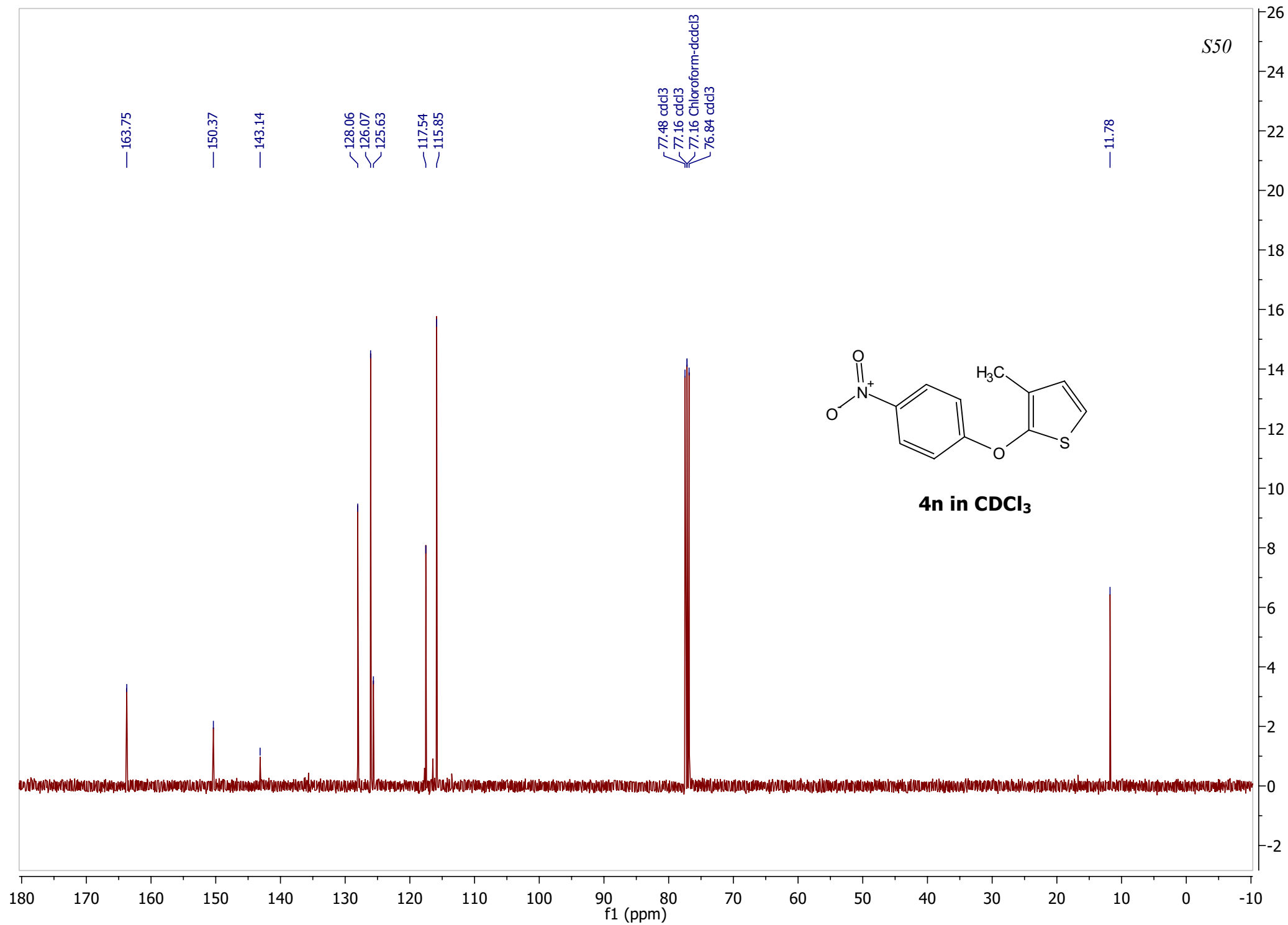
— 7.26 Chloroform-d



S48

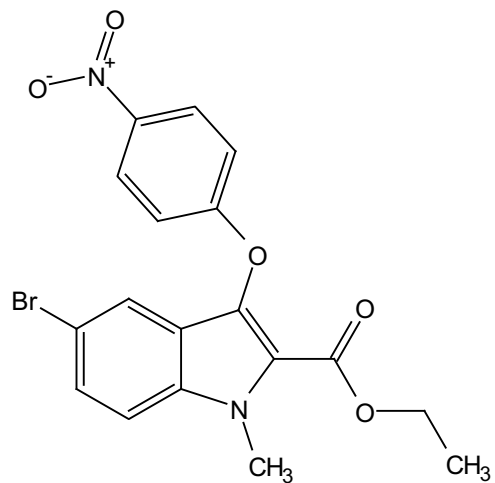




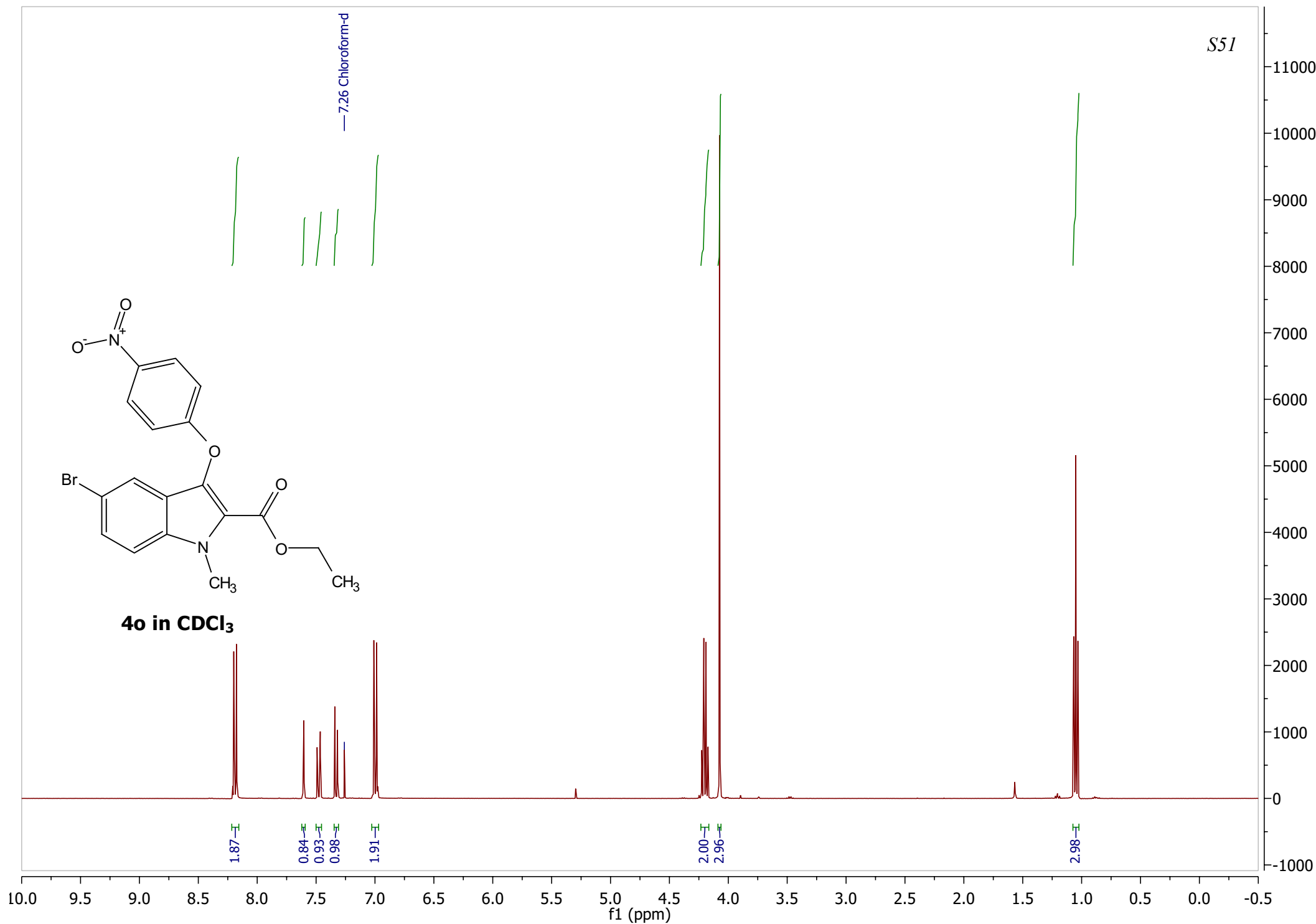


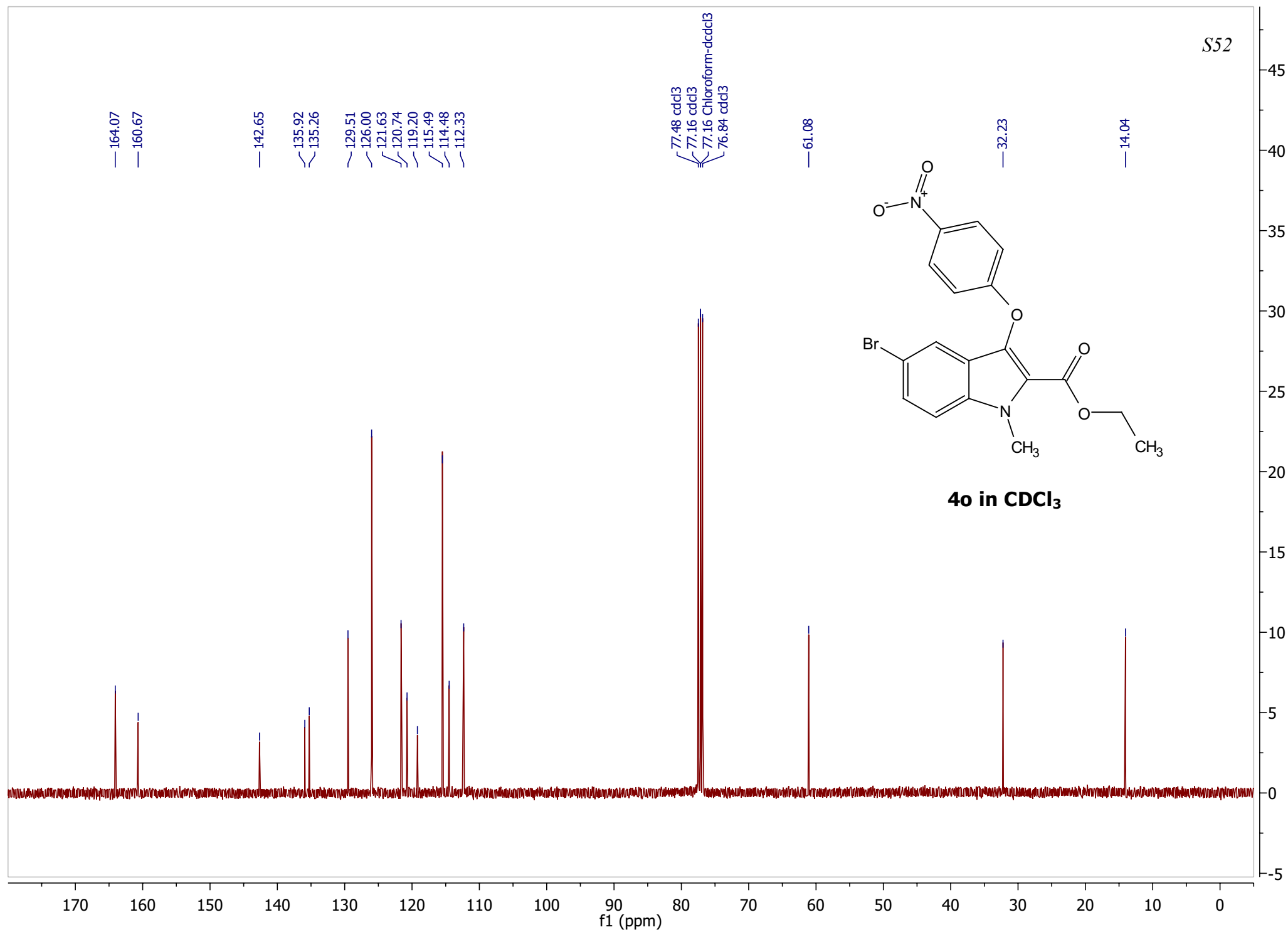
S51

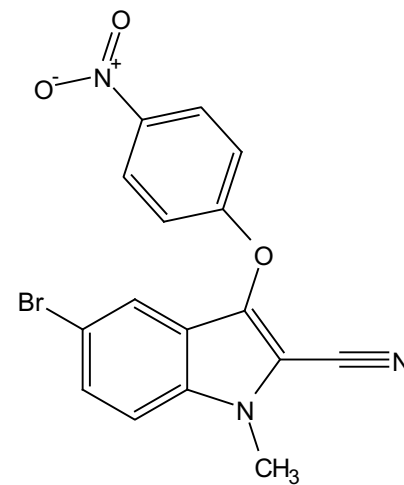
7.26 Chloroform-d



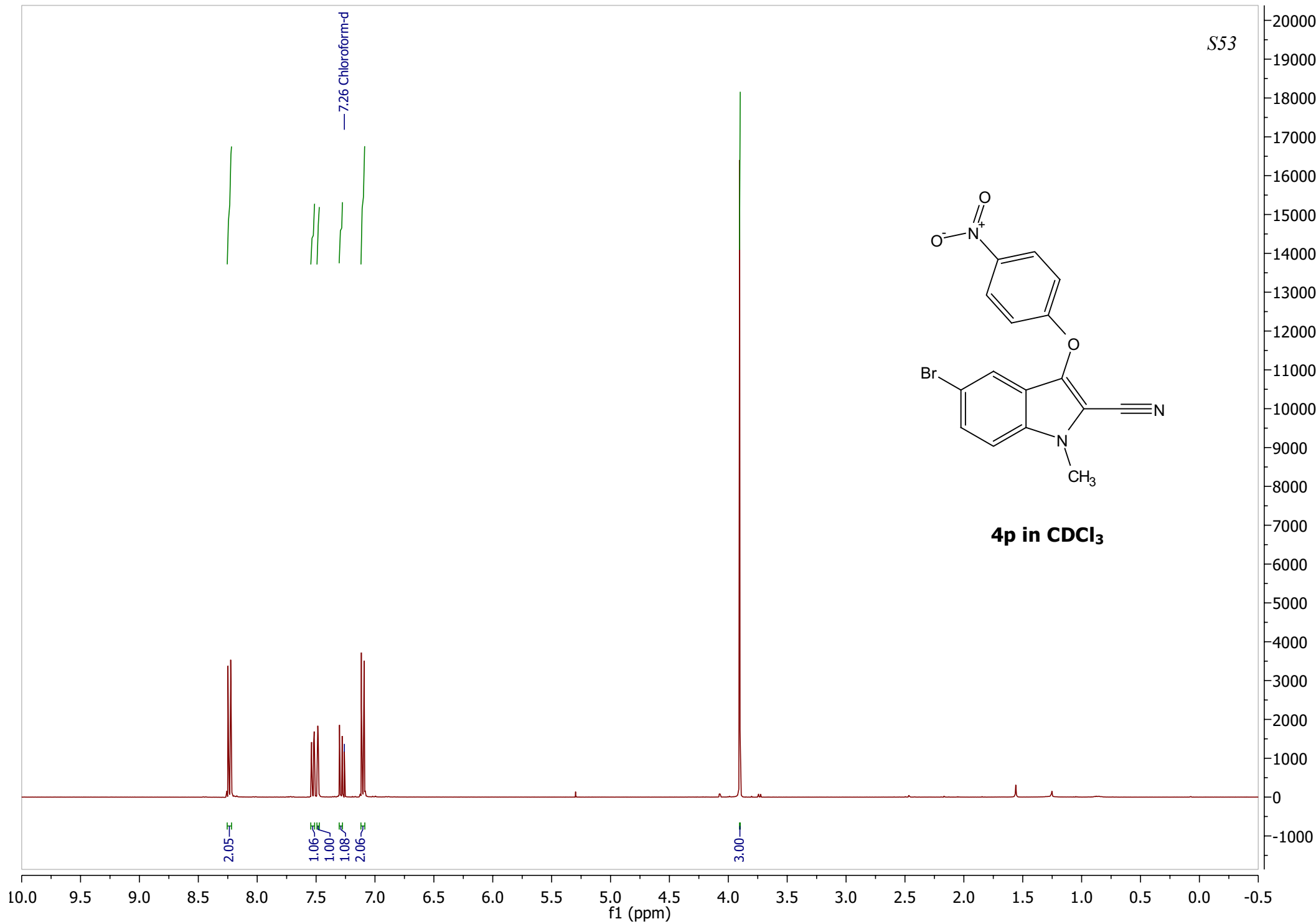
4o in CDCl<sub>3</sub>

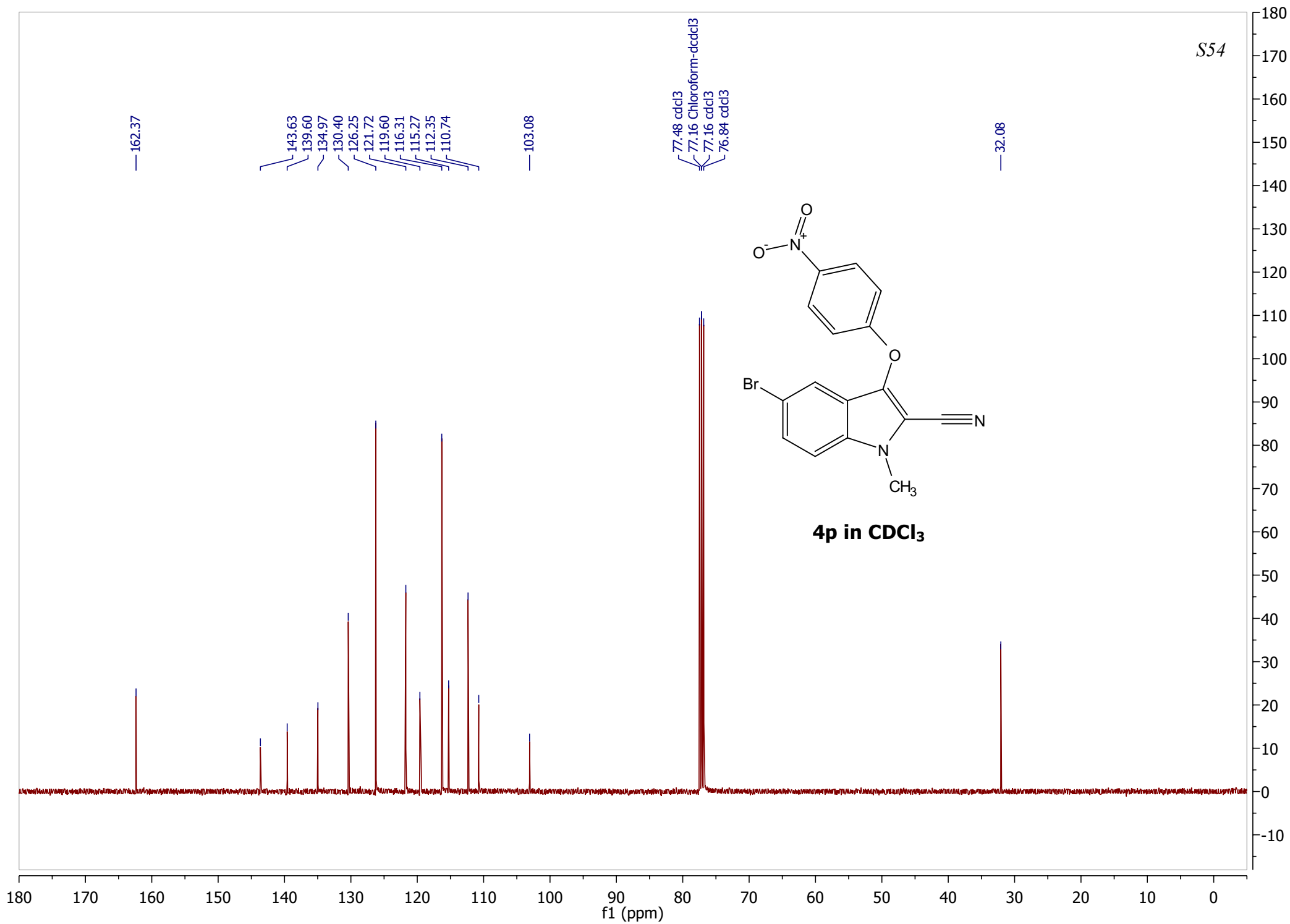


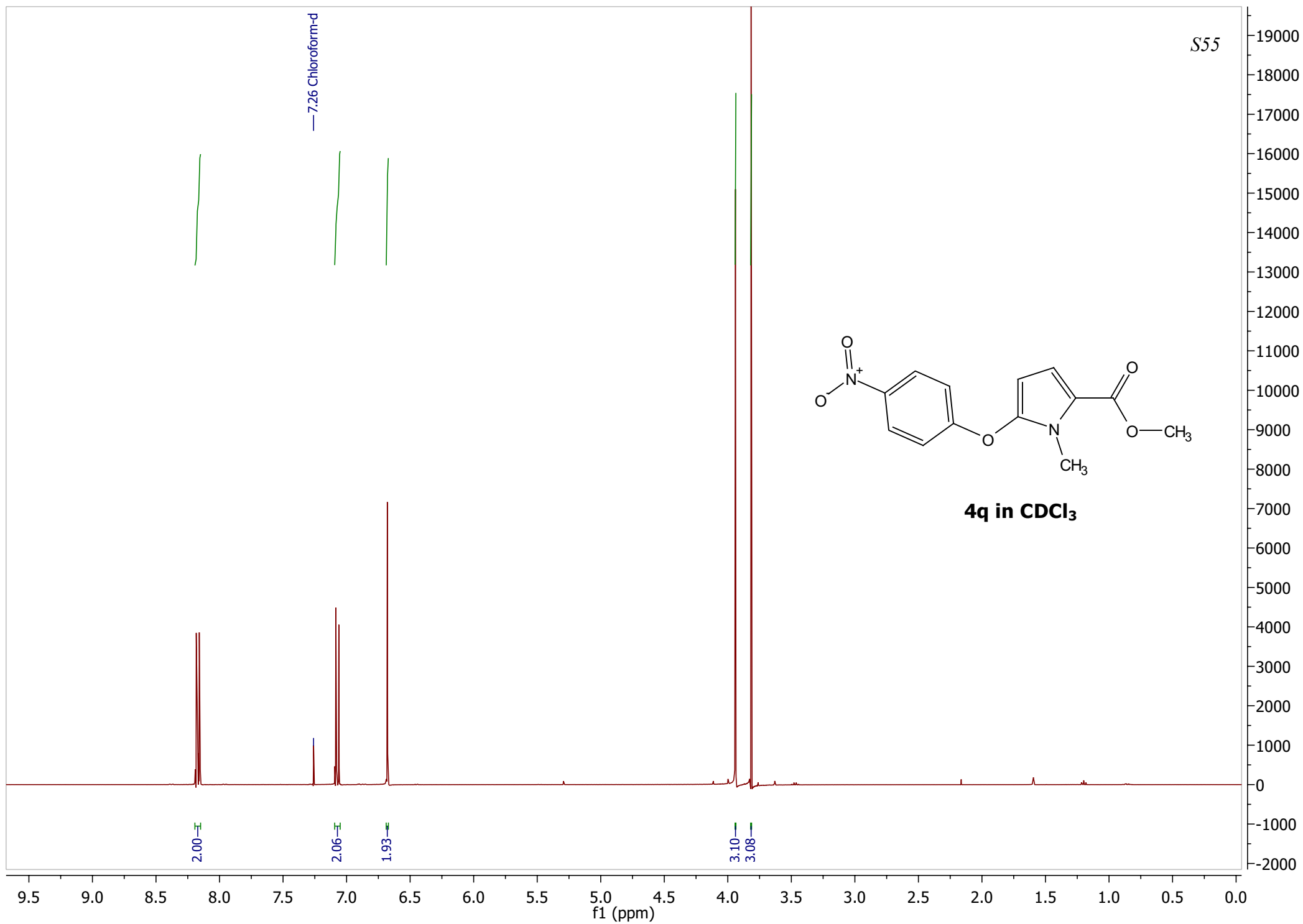




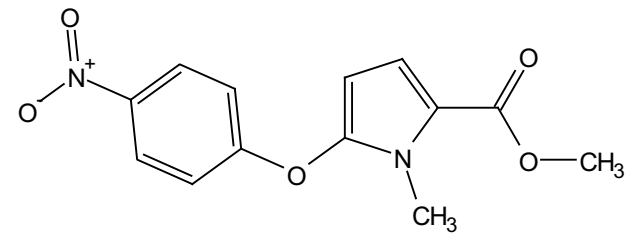
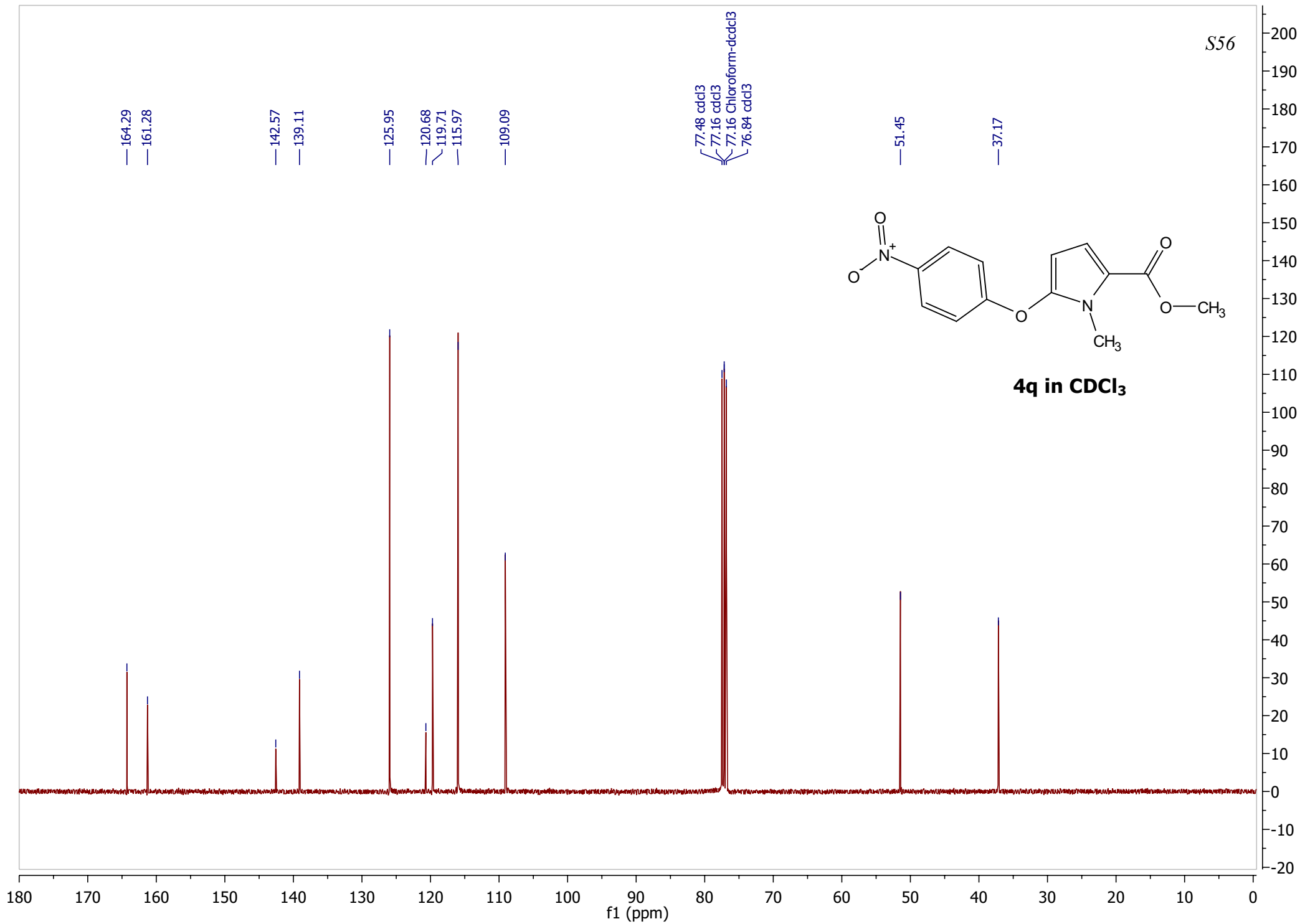
**4p in CDCl<sub>3</sub>**



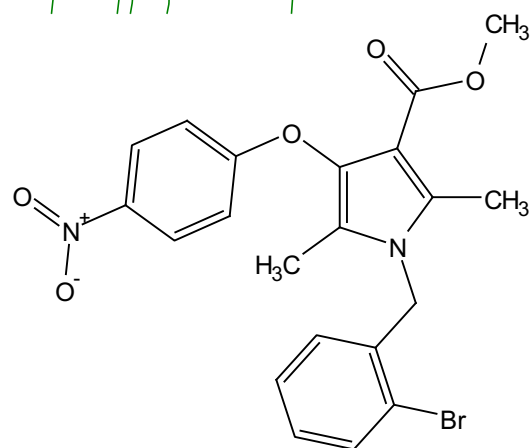




S56



4q in CDCl<sub>3</sub>

**4r in  $\text{CDCl}_3$** 