

## Supporting Information

### **Synthesis and biological evaluation of paeoveitol D derivatives as new melatonin receptor agonists with antidepressant activities**

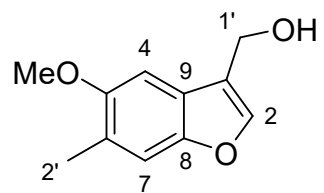
Tian-Ze Li<sup>a, 1</sup>, Jing Hu<sup>a, 1</sup>, Jin-Jin Sun<sup>a</sup>, Xiao-Yan Huang<sup>a</sup>, Chang-An Geng<sup>a</sup>, Shu-Bai Liu<sup>a</sup>, Xue-Mei Zhang<sup>a</sup>, Ji-Jun Chen<sup>a,b\*</sup>

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<sup>b</sup> *University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China*

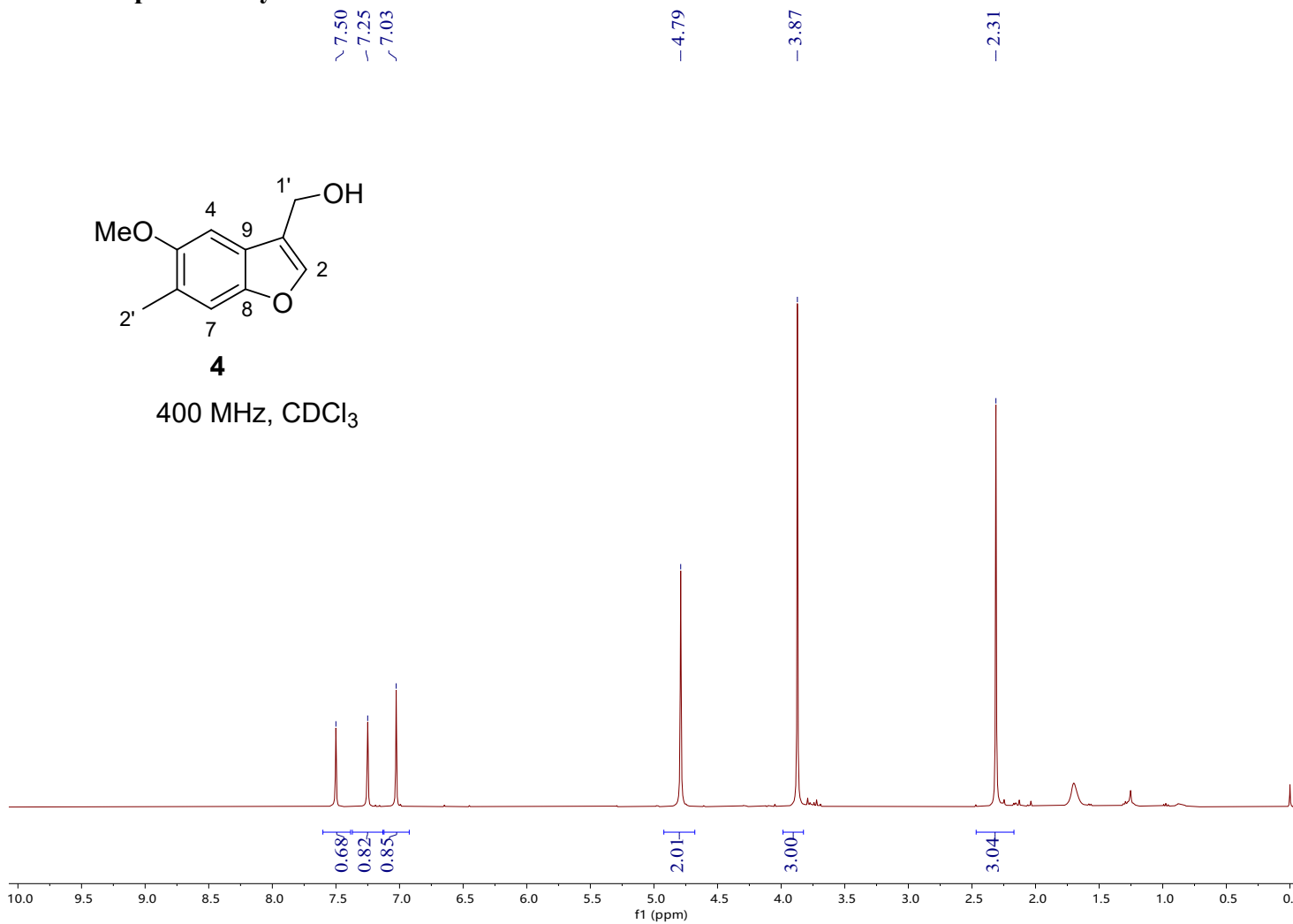
<sup>1</sup> *These authors contributed equally to this work.*

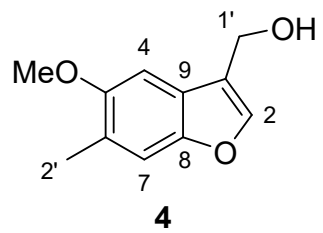
# $^1\text{H}$ NMR and $^{13}\text{C}$ NMR spectra of synthetic derivatives



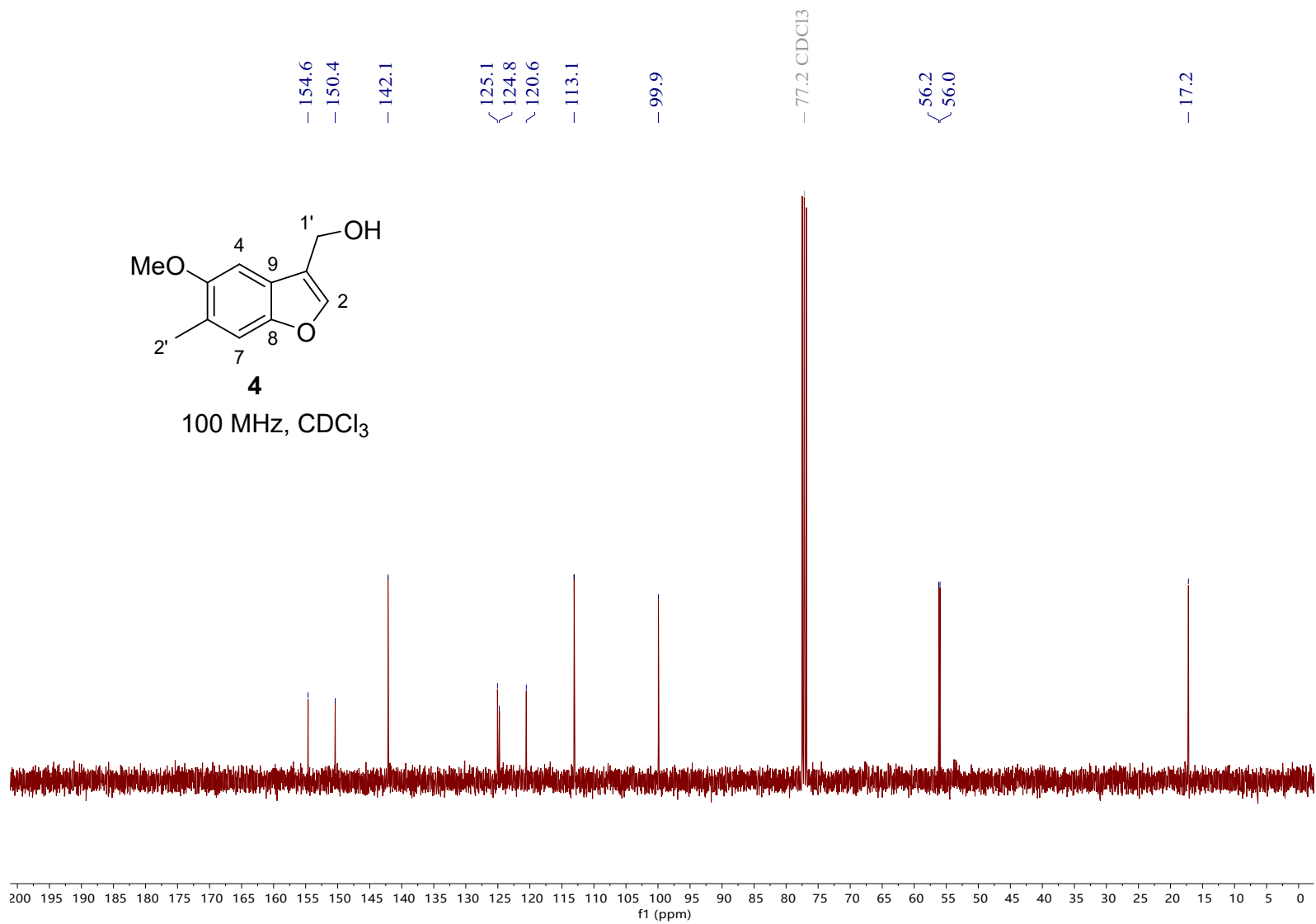
**4**

400 MHz, CDCl<sub>3</sub>





100 MHz, CDCl<sub>3</sub>



jltz53.21.fid  
jltz53 H

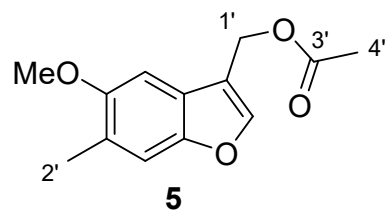
~ 7.59  
~ 7.26  
~ 7.00

— 5.23

— 3.89

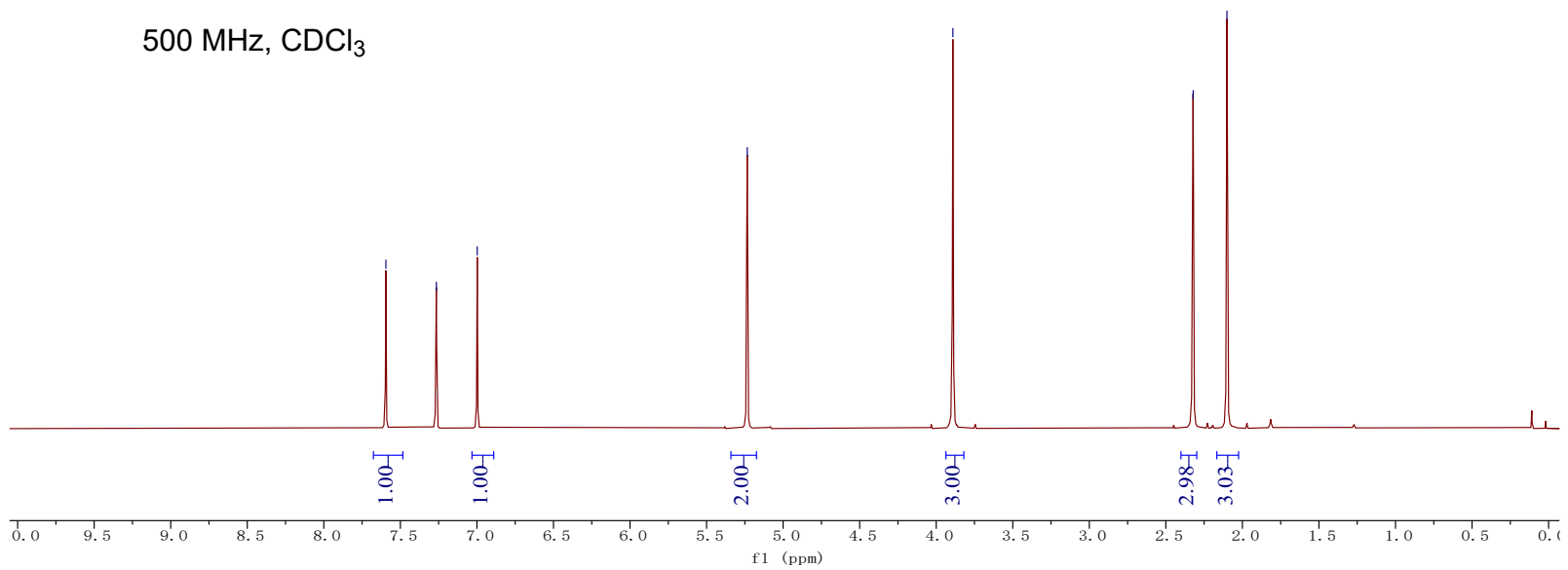
— 2.32

— 2.10

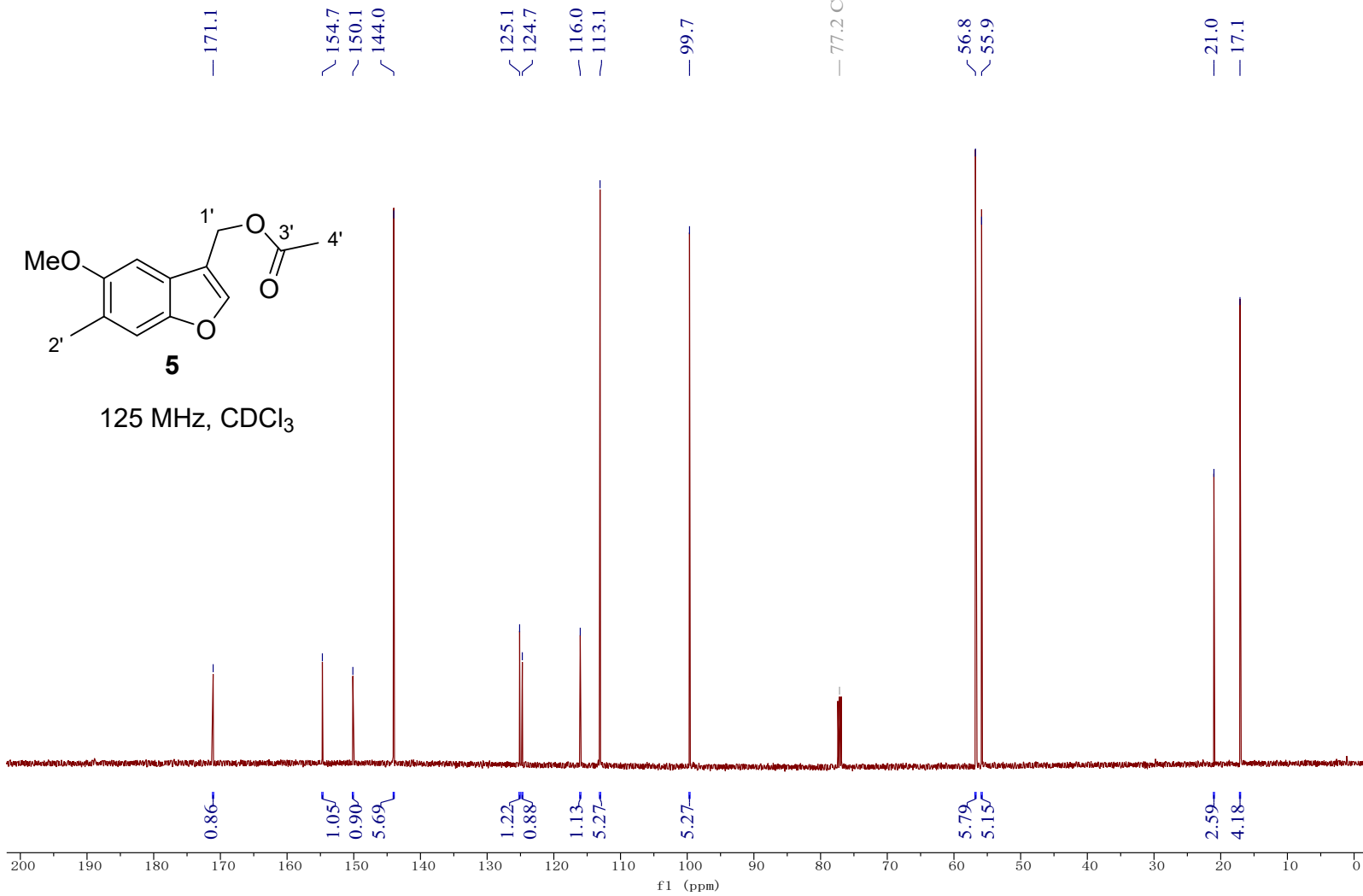


**5**

500 MHz, CDCl<sub>3</sub>



jltz53. 22. fid  
jltz53 c13

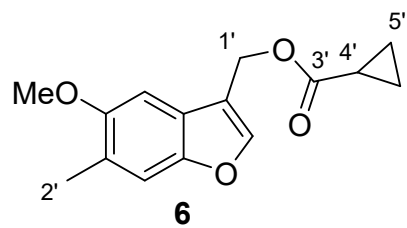


jlz54.21.fid  
jlz54 H

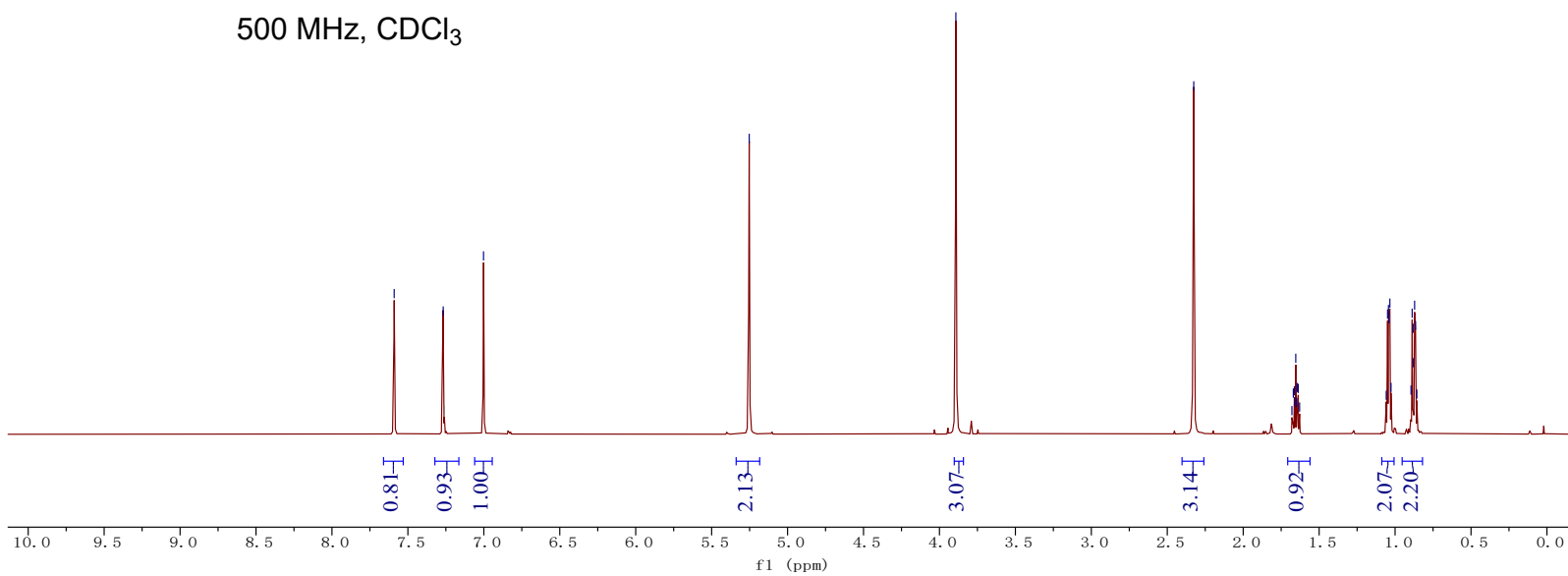
7.59  
7.27  
7.26  
7.00

5.25

3.89  
2.33  
1.68  
1.67  
1.66  
1.66  
1.65  
1.65  
1.64  
1.64  
1.63  
1.06  
1.05  
1.04  
1.04  
1.03  
1.03  
0.90  
0.89  
0.88  
0.88  
0.87  
0.87  
0.86



500 MHz, CDCl<sub>3</sub>



jltz54.22.fid  
jltz54 c13

— 175.0

— 154.7  
— 150.2  
— 143.8

— 125.1  
— 124.8

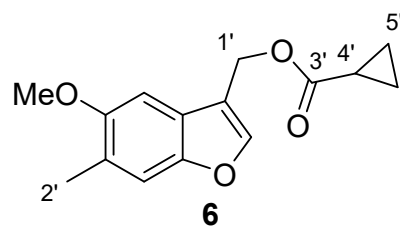
— 116.2  
— 113.0

— 99.7

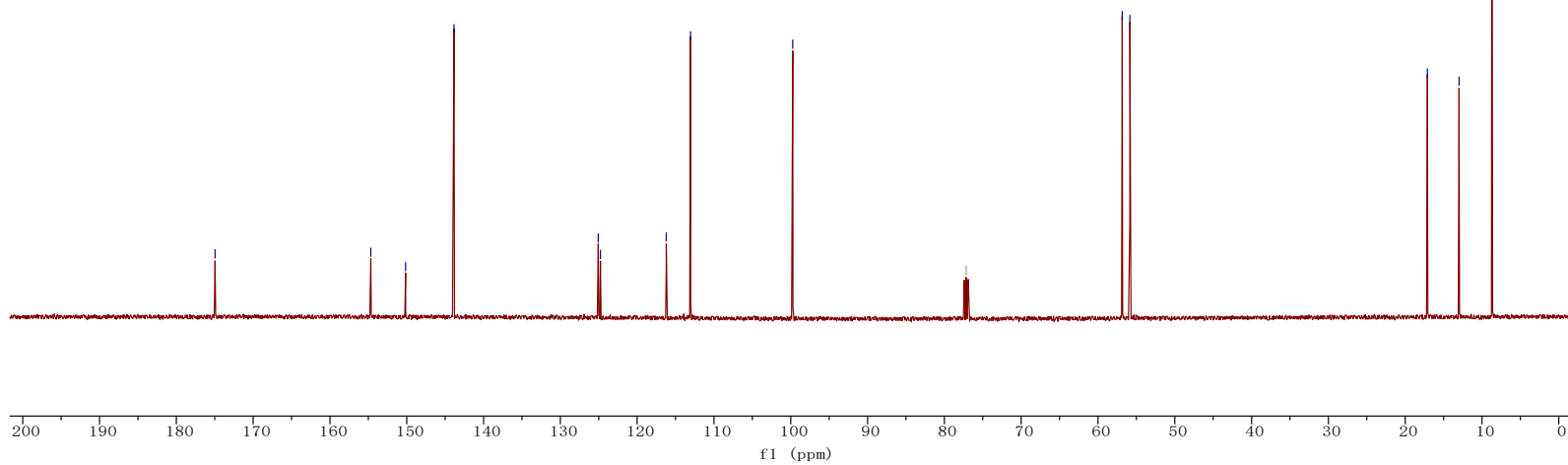
— 77.2 CDCl<sub>3</sub>

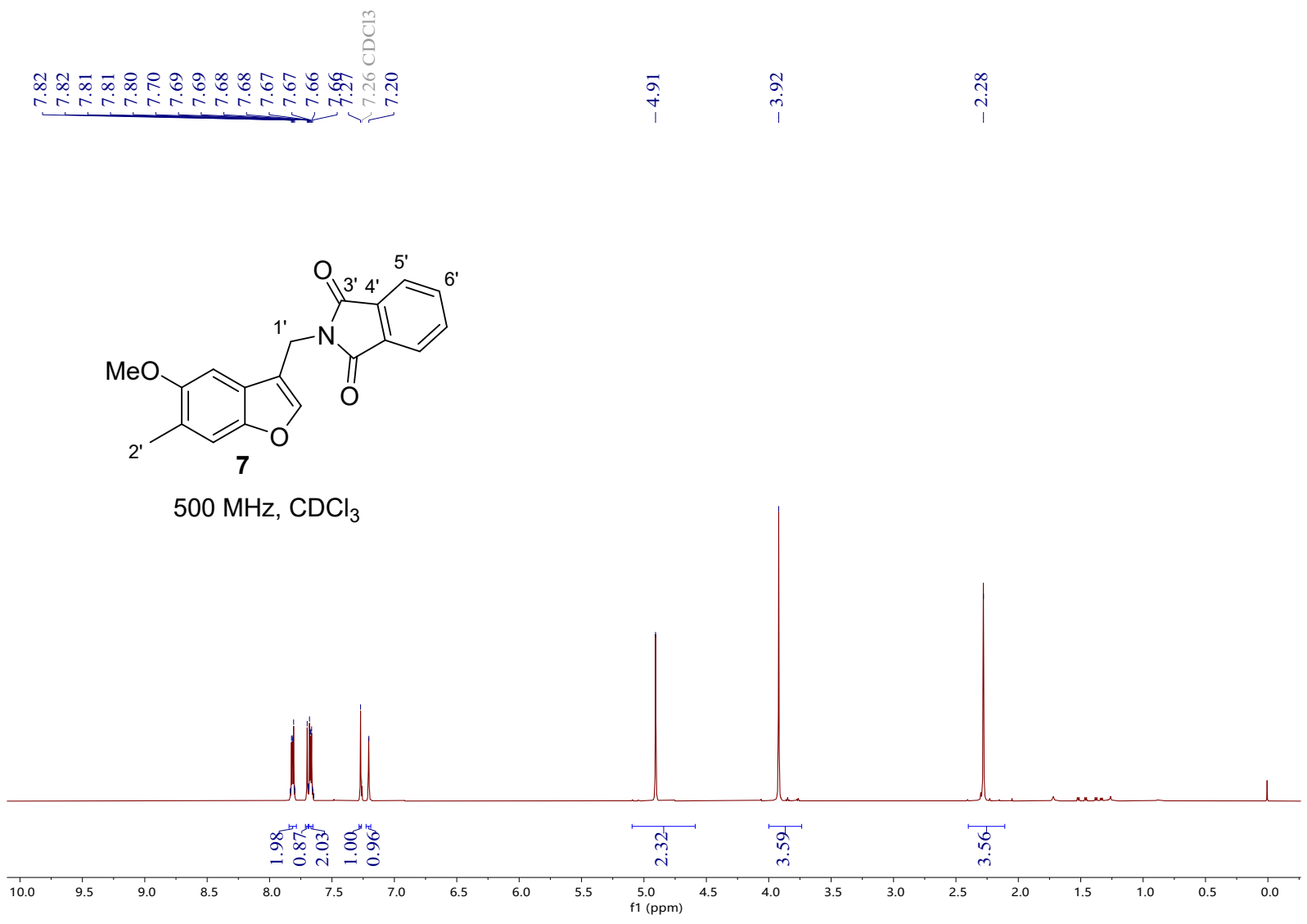
— 56.8  
— 55.8

— 17.1  
— 13.0  
— 8.7

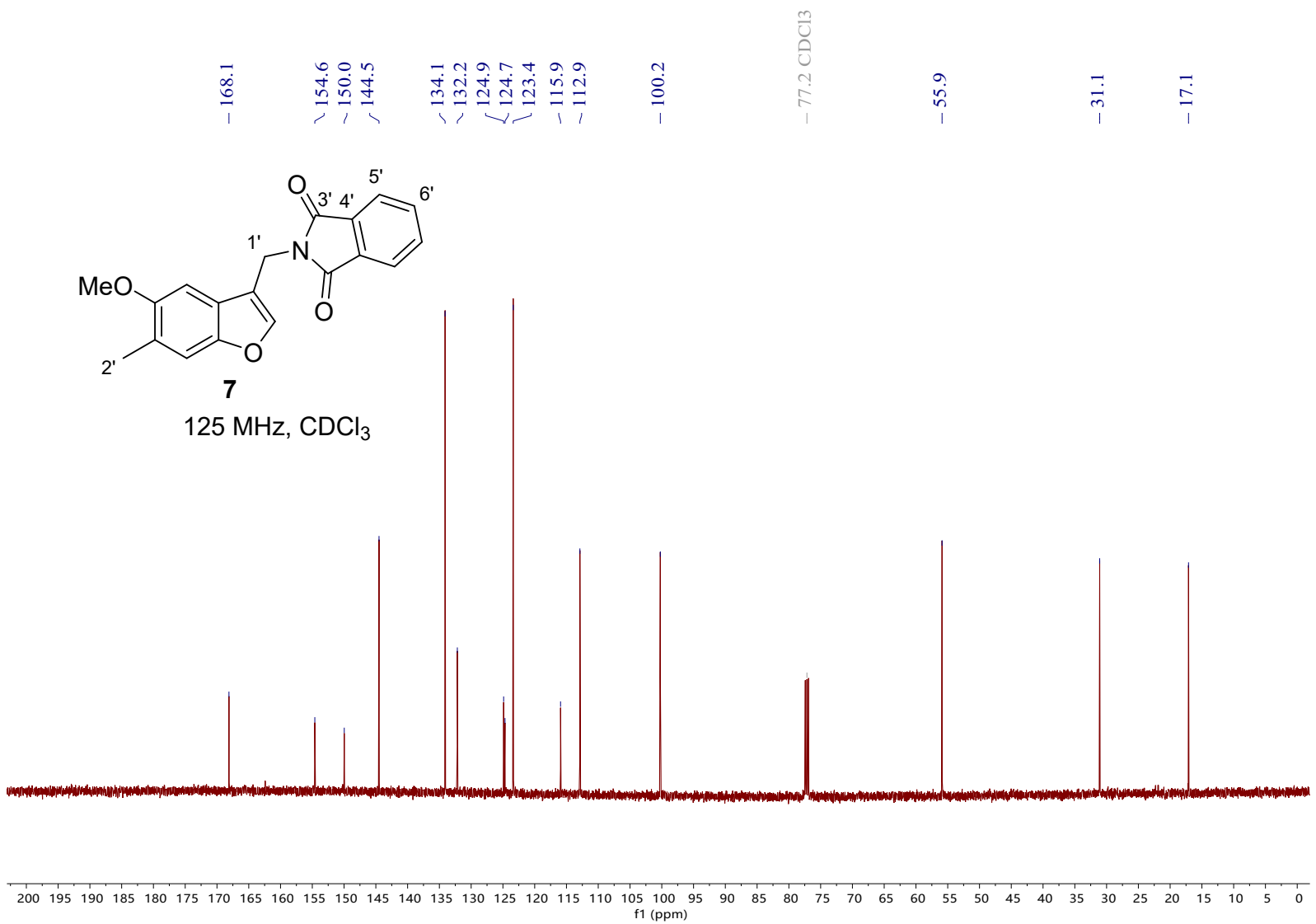


125 MHz, CDCl<sub>3</sub>







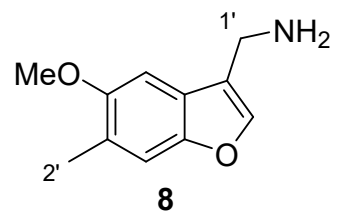


jltz069.21.fid  
jltz069 H

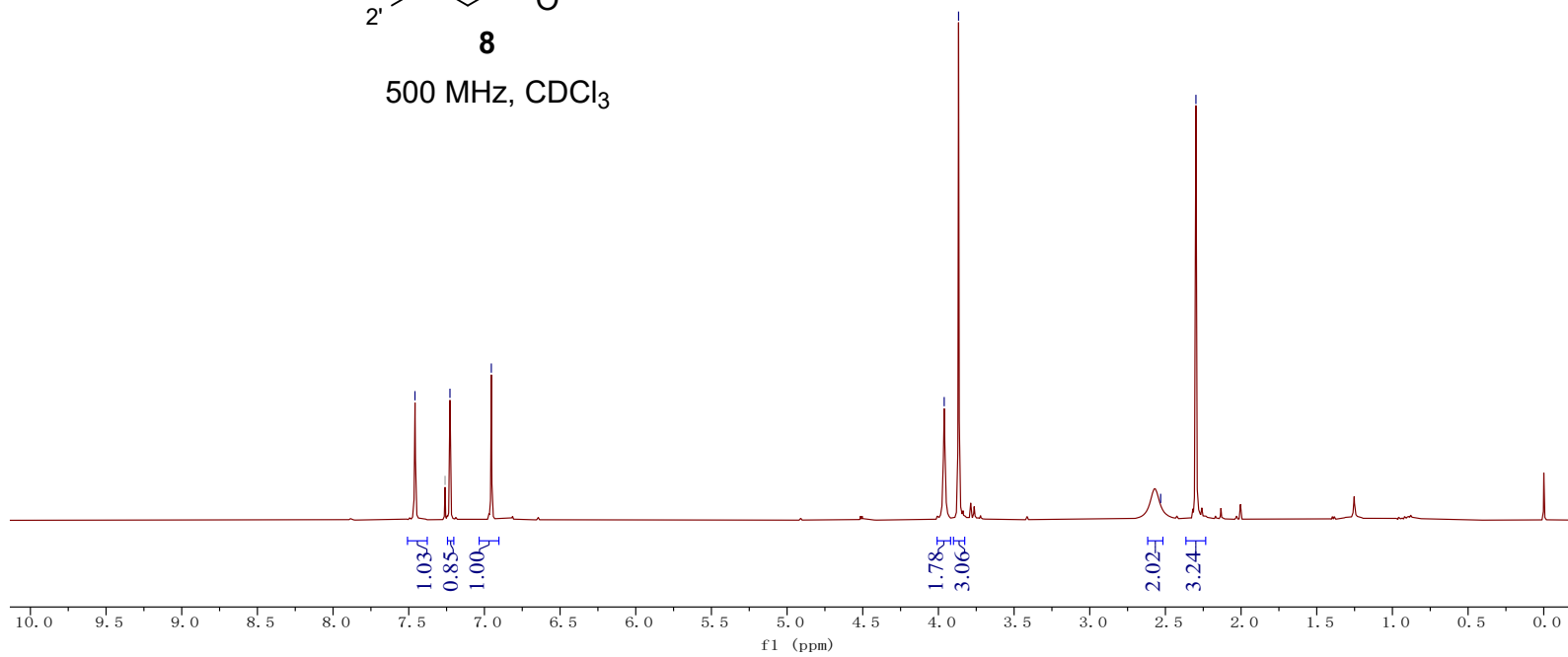
7.46  
7.26 CDCl<sub>3</sub>  
7.23  
6.95

3.96  
3.87

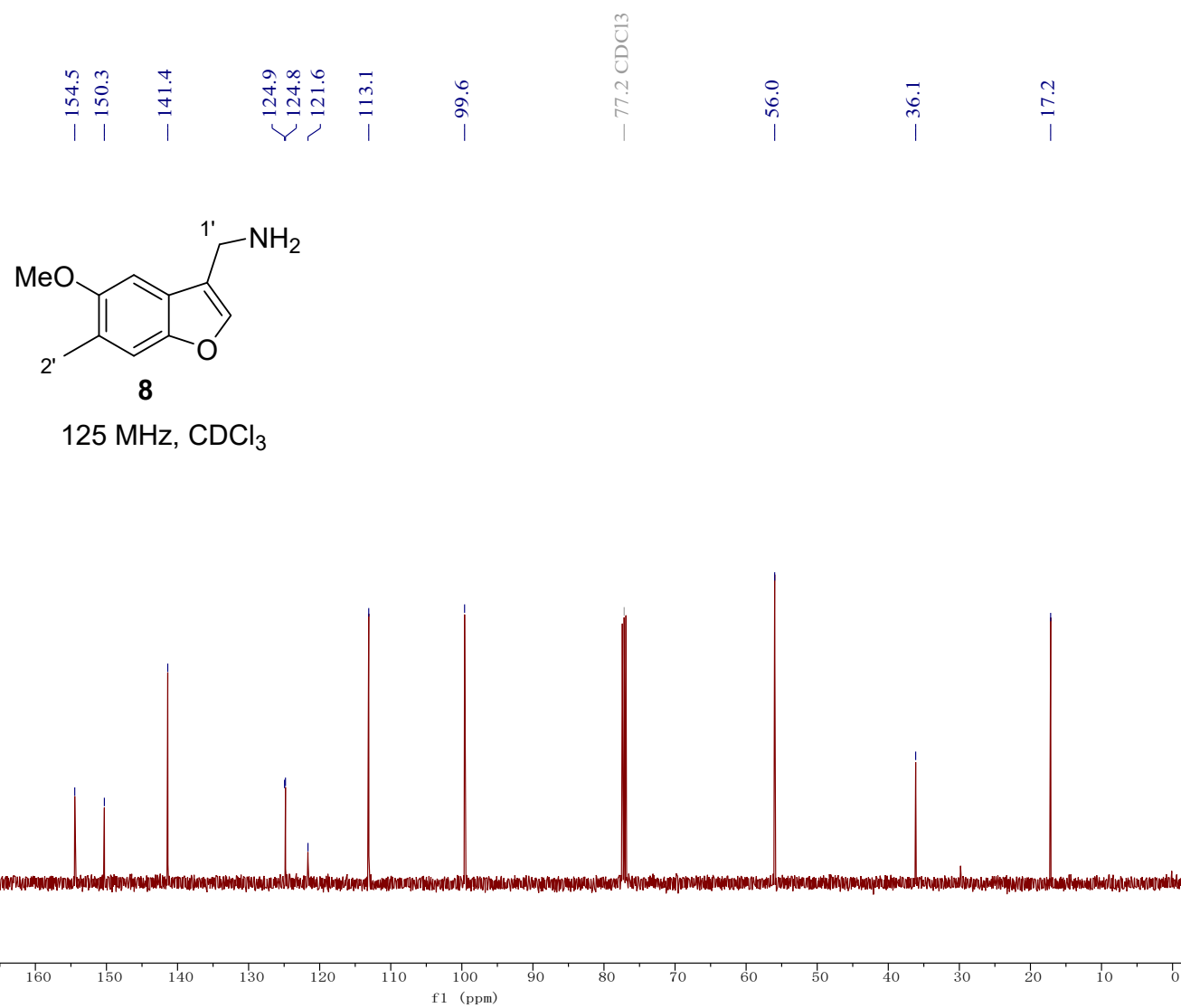
2.53  
2.30



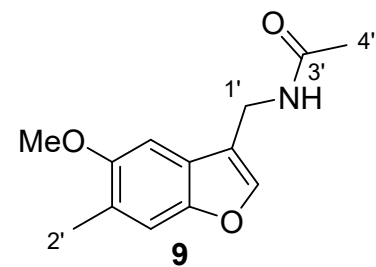
500 MHz, CDCl<sub>3</sub>



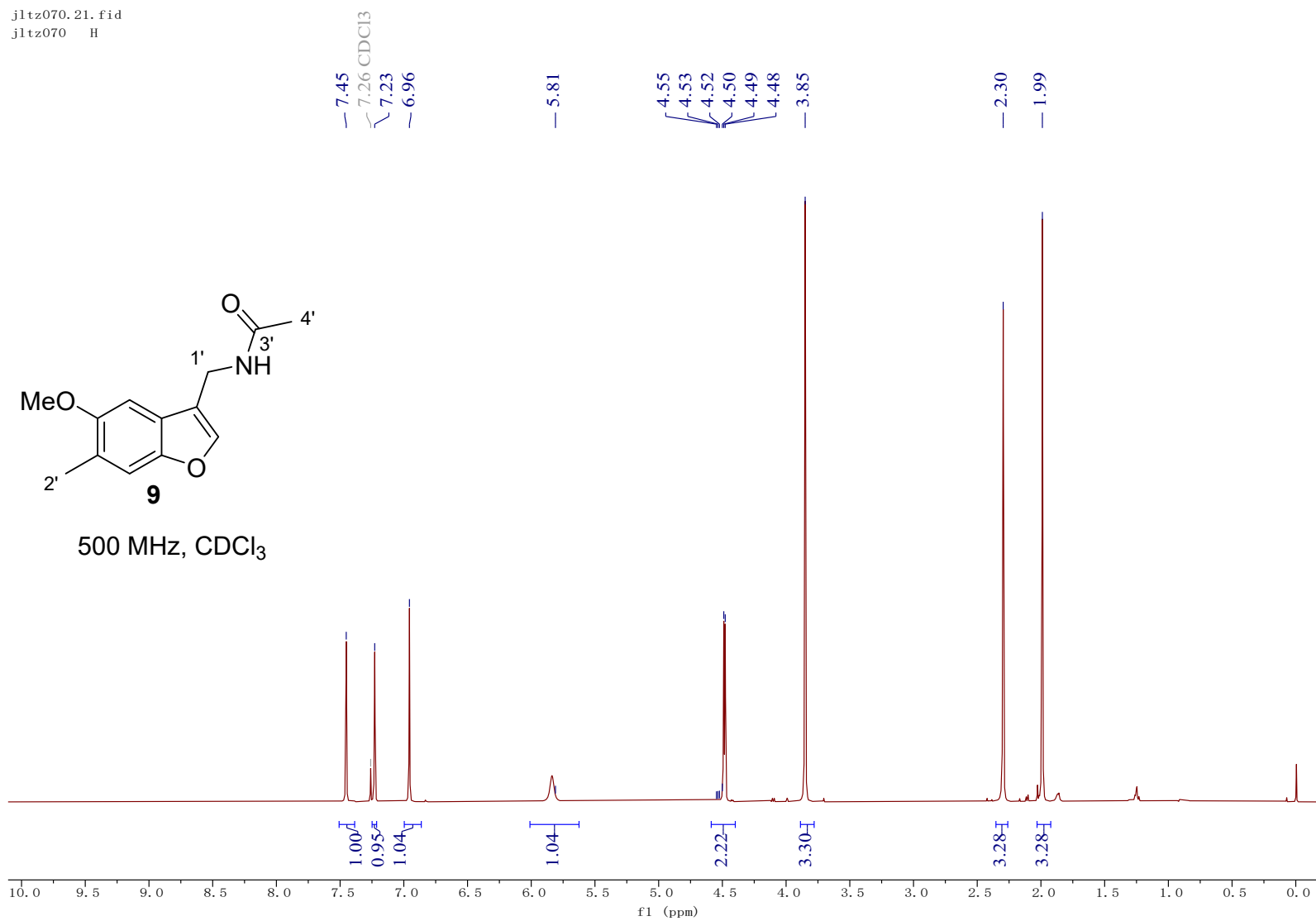
jltz069.22.fid  
jltz069 c13



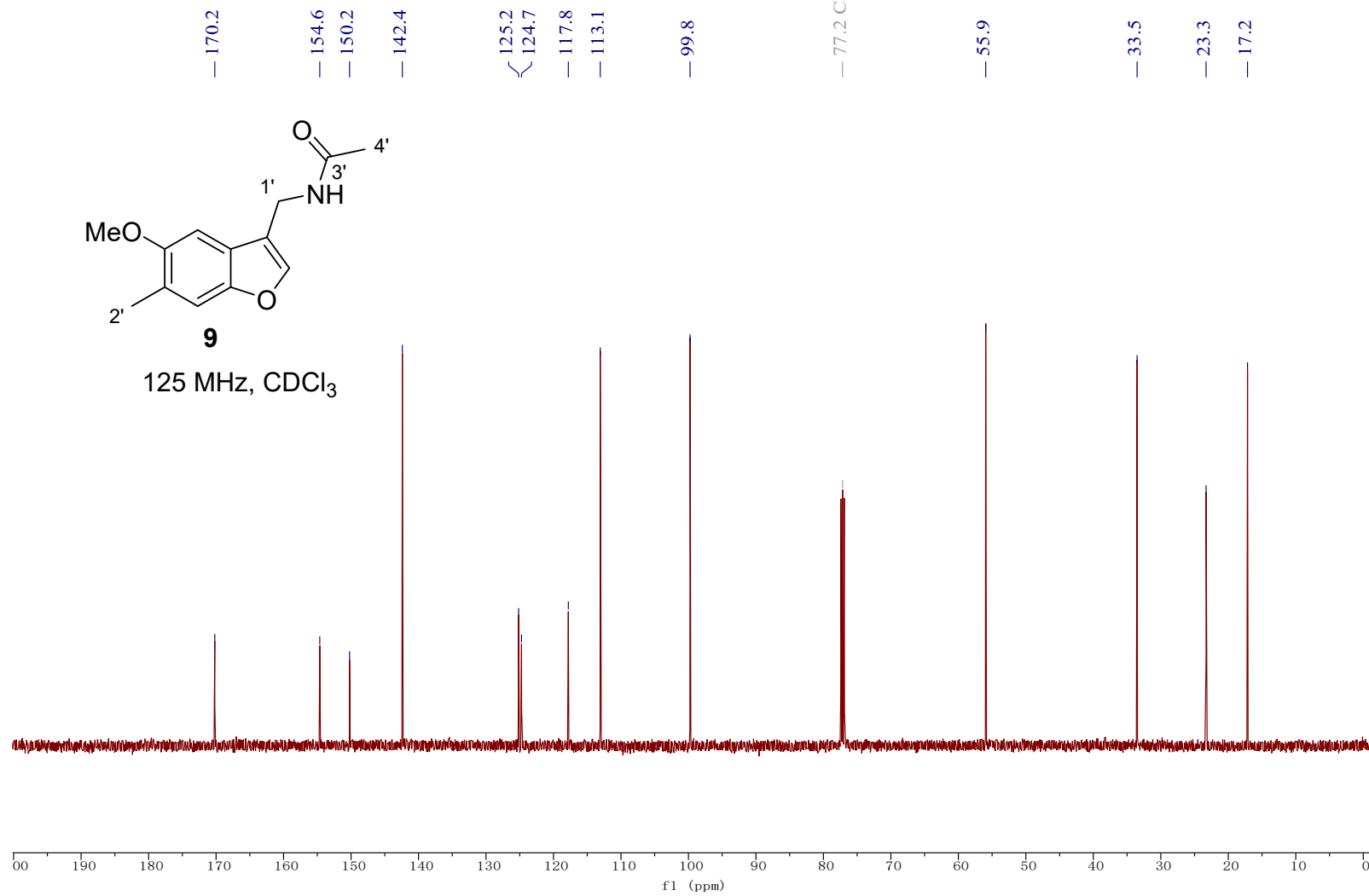
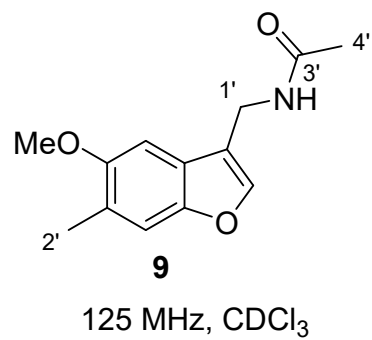
jltz070.21.fid  
jltz070 H



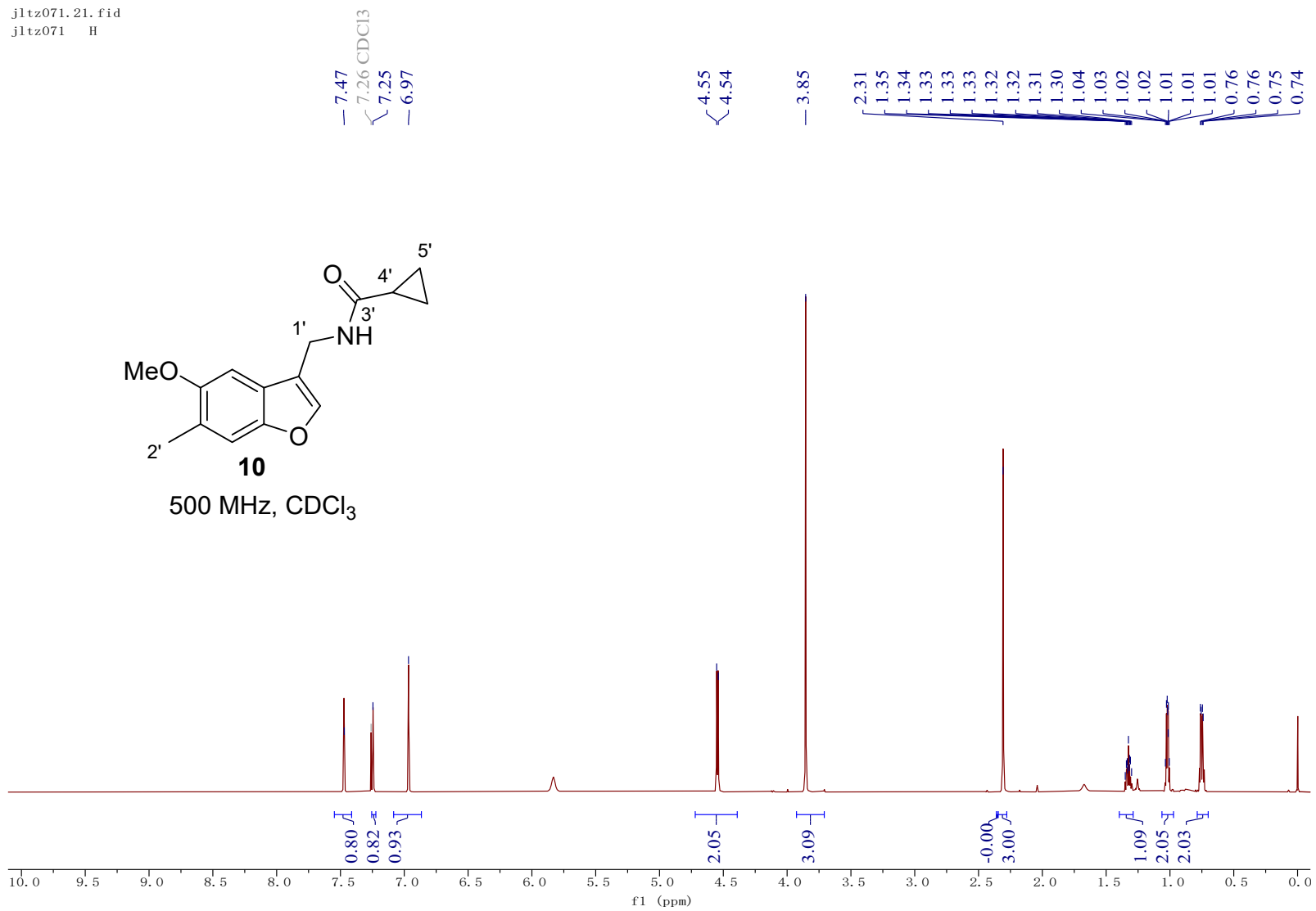
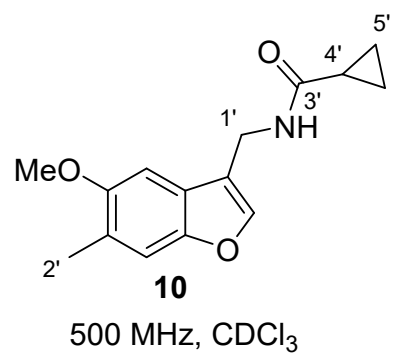
500 MHz, CDCl<sub>3</sub>



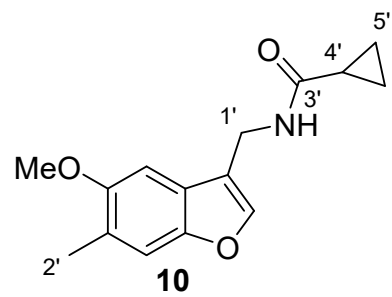
jltz070.22.fid  
jltz070



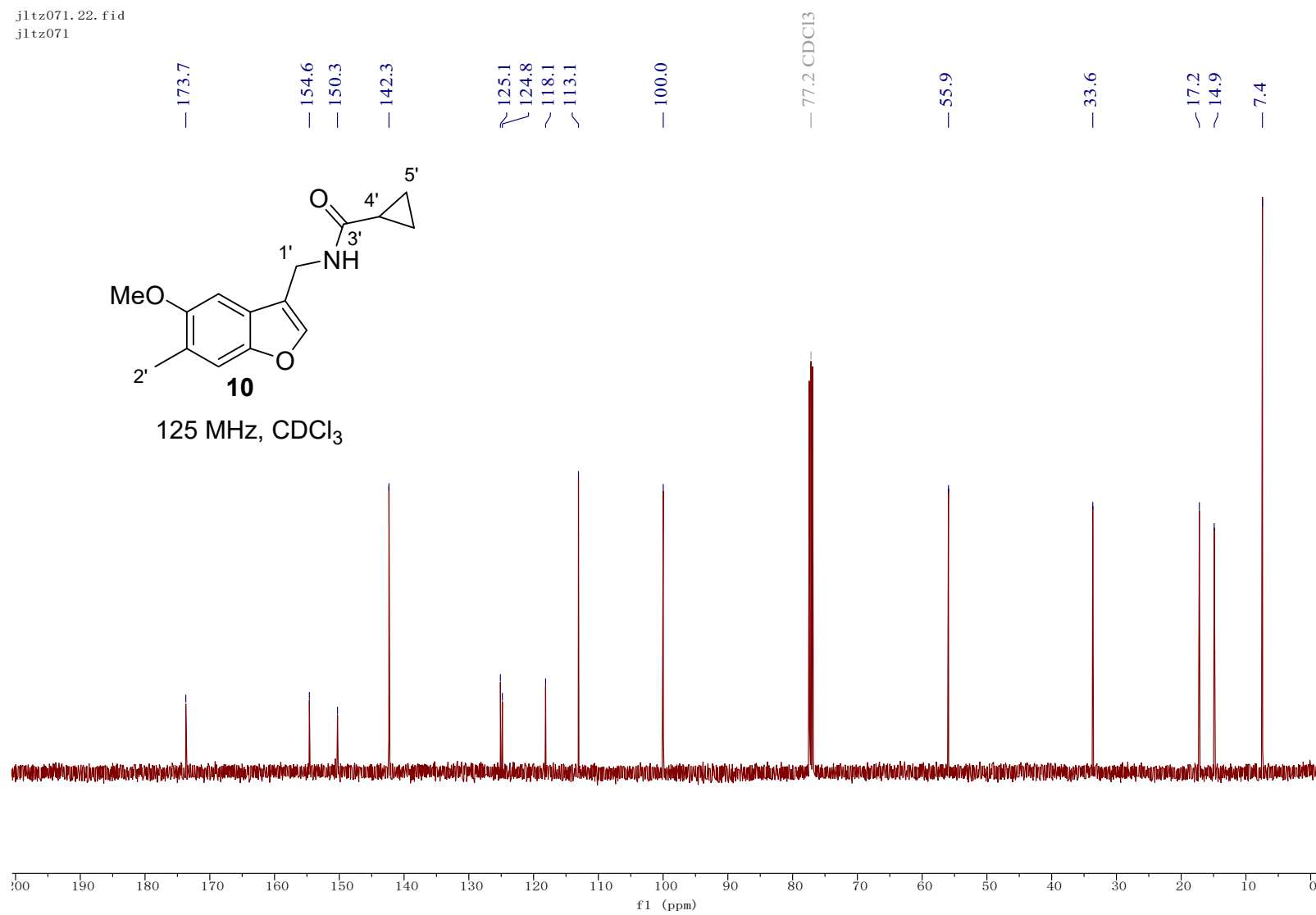
jltz071.21.fid  
jltz071 H



jl1tz071.22.fid  
jl1tz071



125 MHz, CDCl<sub>3</sub>



jltz47.21.fid  
jltz47 H

— 10.11

— 8.16

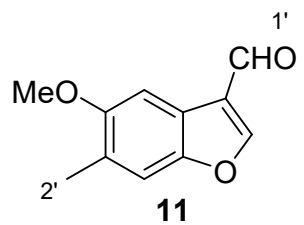
7.53

7.30

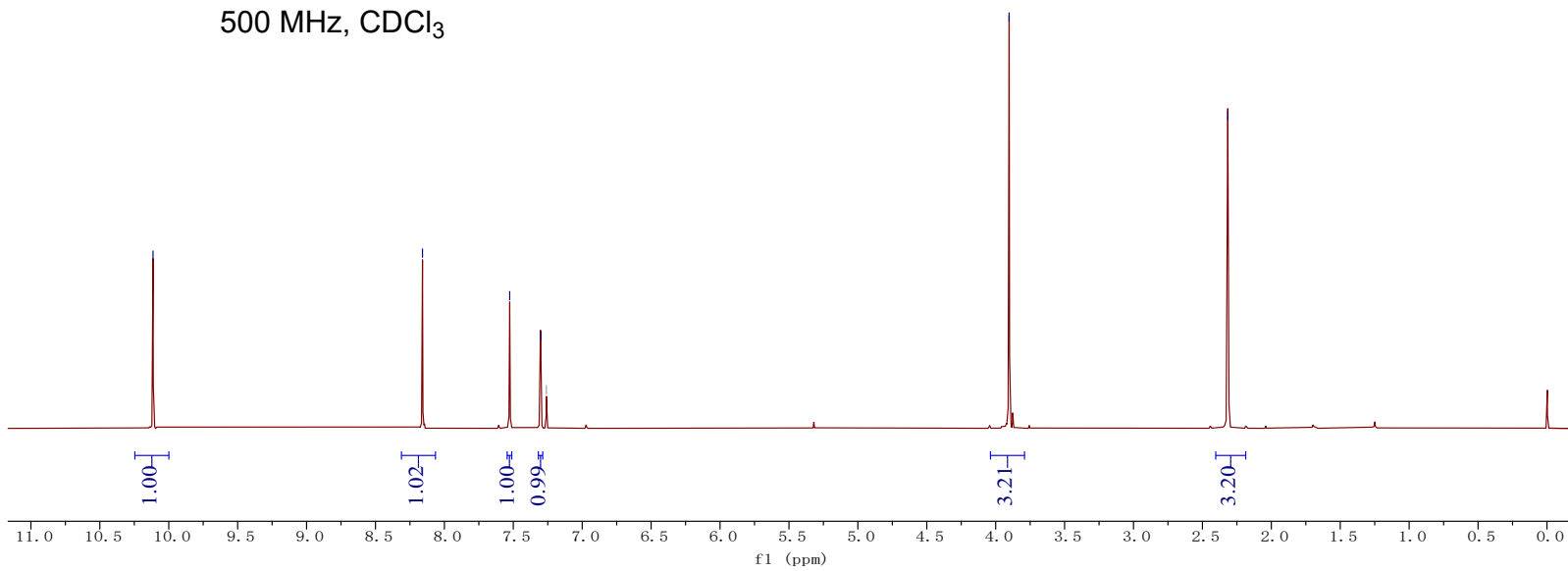
7.26 CDCl<sub>3</sub>

— 3.90

— 2.32



500 MHz, CDCl<sub>3</sub>





jlz47.22.fid  
jlz47 c13

— 185.2

— 156.0

— 155.3

— 150.7

— 126.9

— 124.1

— 121.1

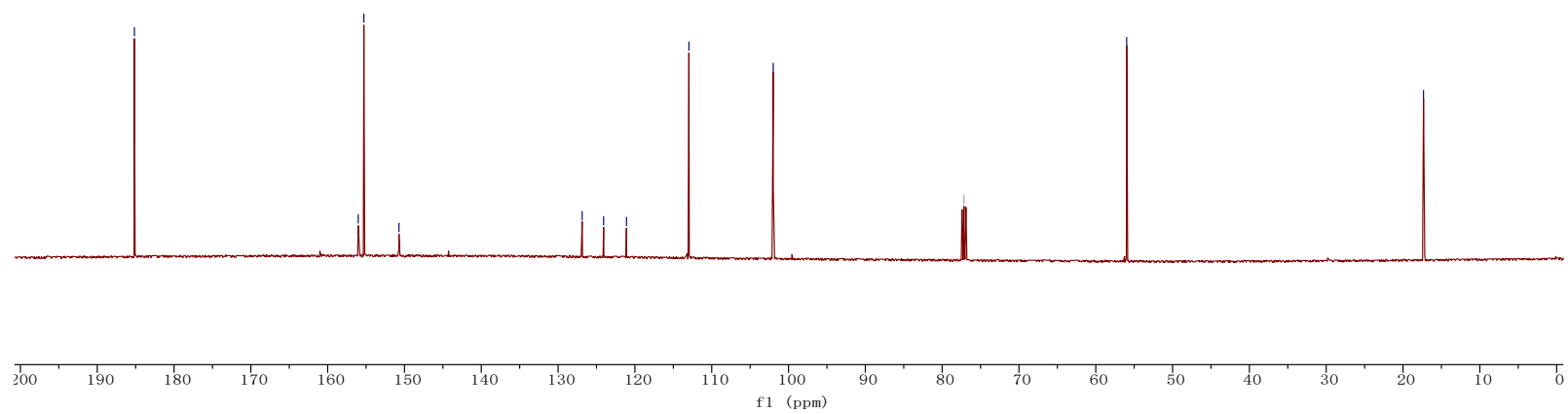
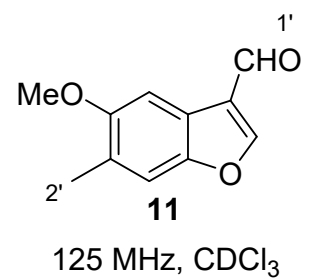
— 113.0

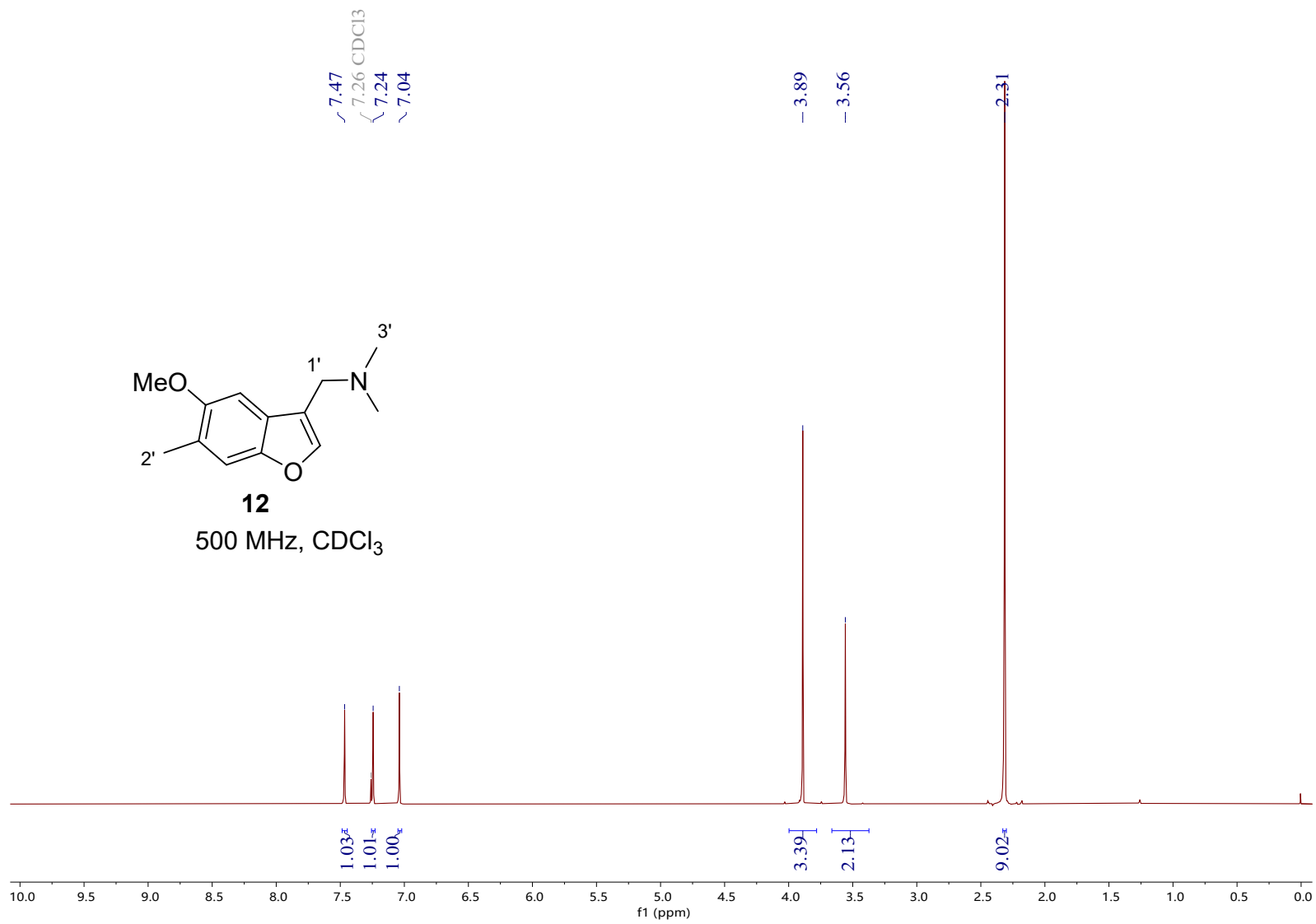
— 102.0

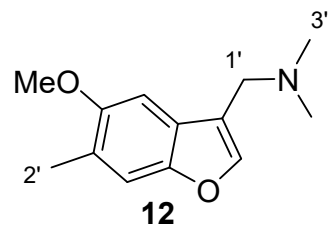
— 77.2 CDCl<sub>3</sub>

— 56.0

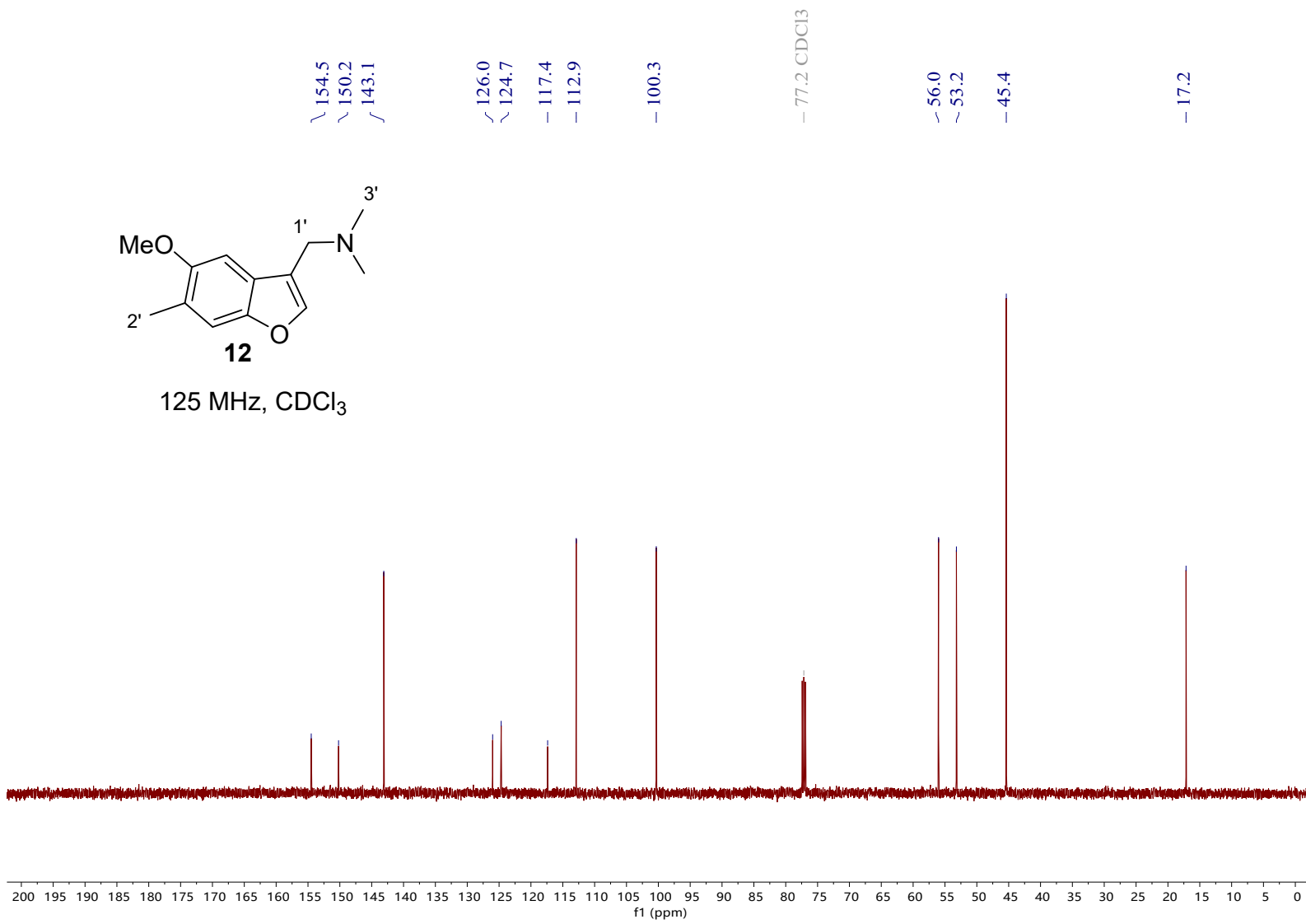
— 17.3







125 MHz, CDCl<sub>3</sub>



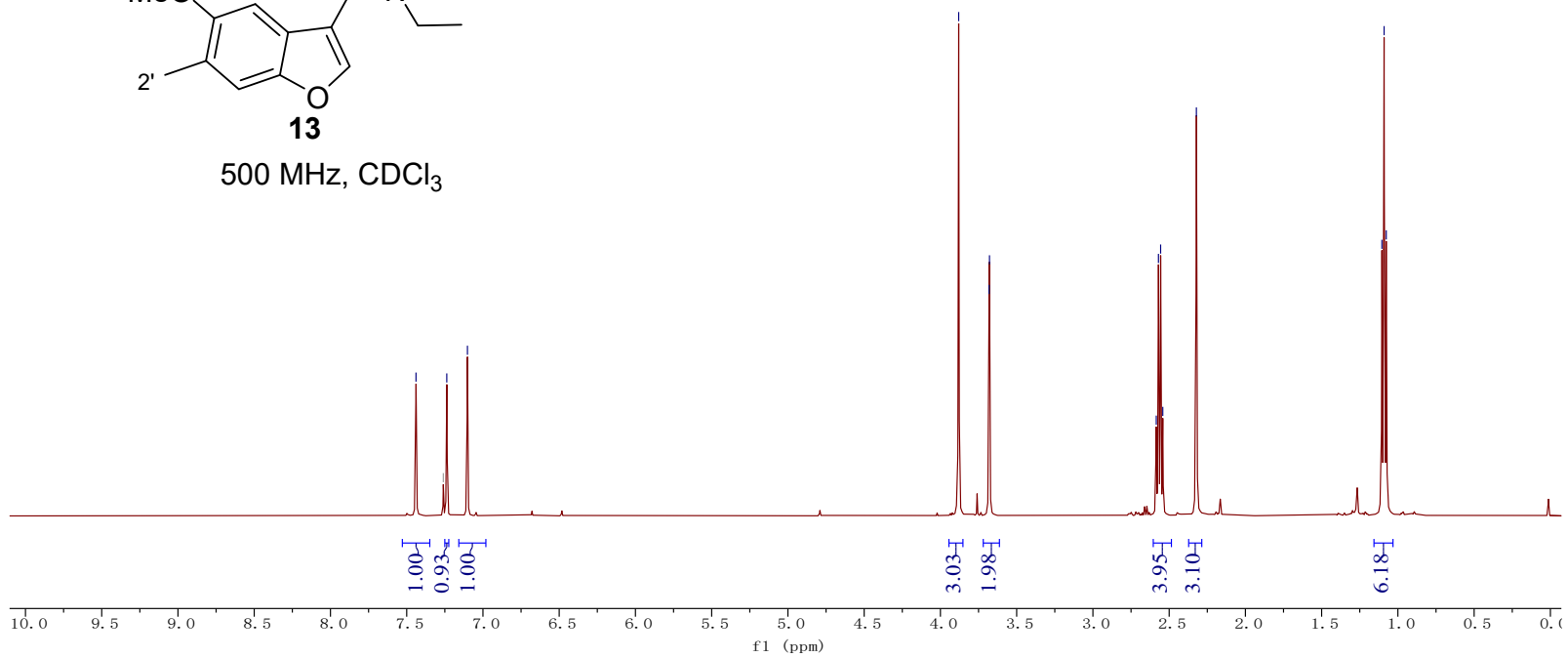
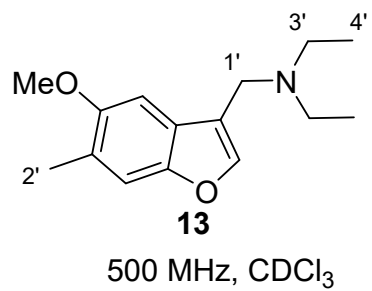
jltz45.21.fid  
jltz45 H

7.44  
7.26 CDCl<sub>3</sub>  
7.24  
7.10

3.88  
3.68  
3.68

2.58  
2.57  
2.56  
2.54  
2.32

1.10  
1.09  
1.08



jltz45.22.fid  
jltz45 c13

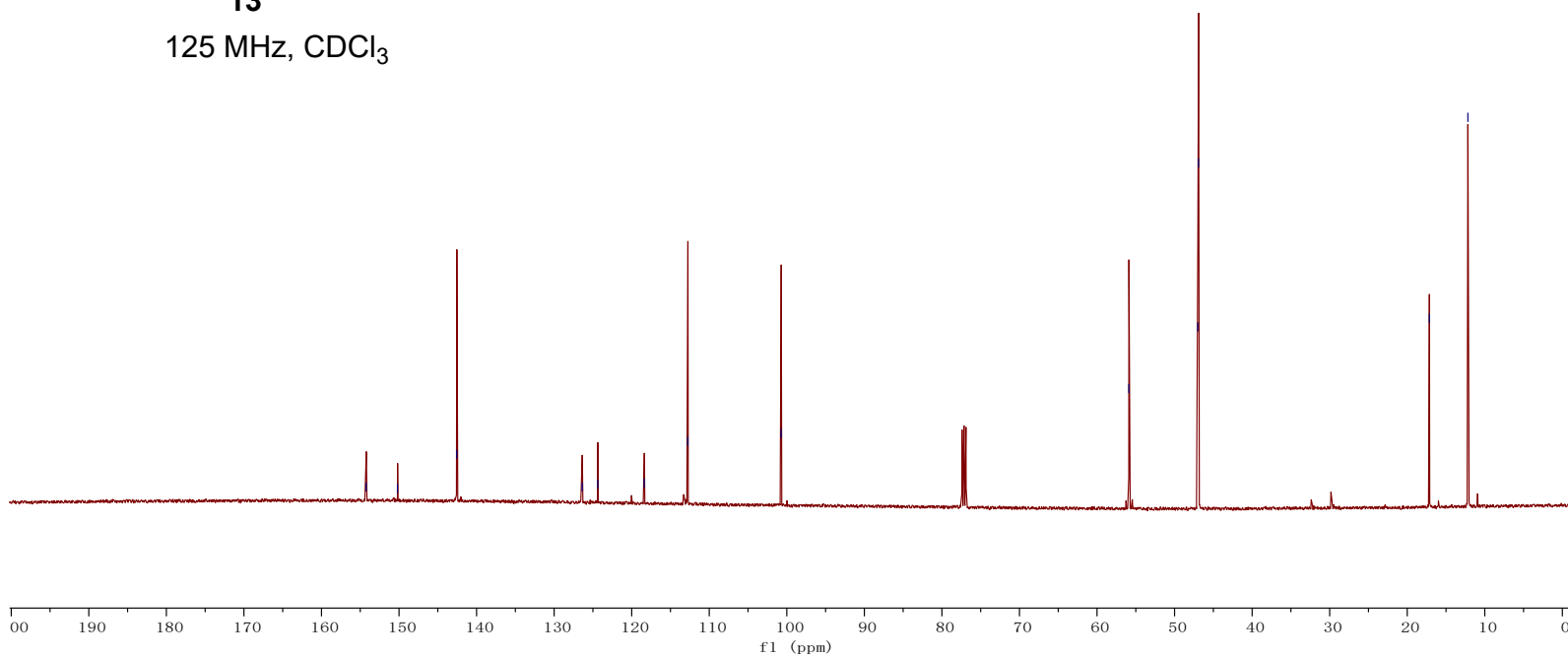
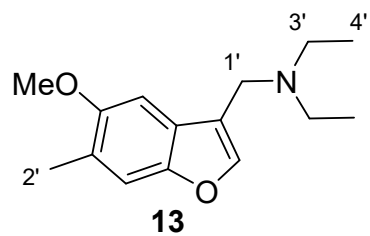
— 154.2  
— 150.2  
— 142.6

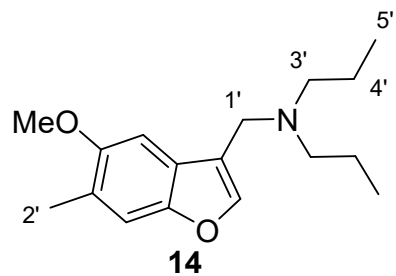
— 126.4  
— 124.4  
— 118.4  
— 112.8

— 100.7

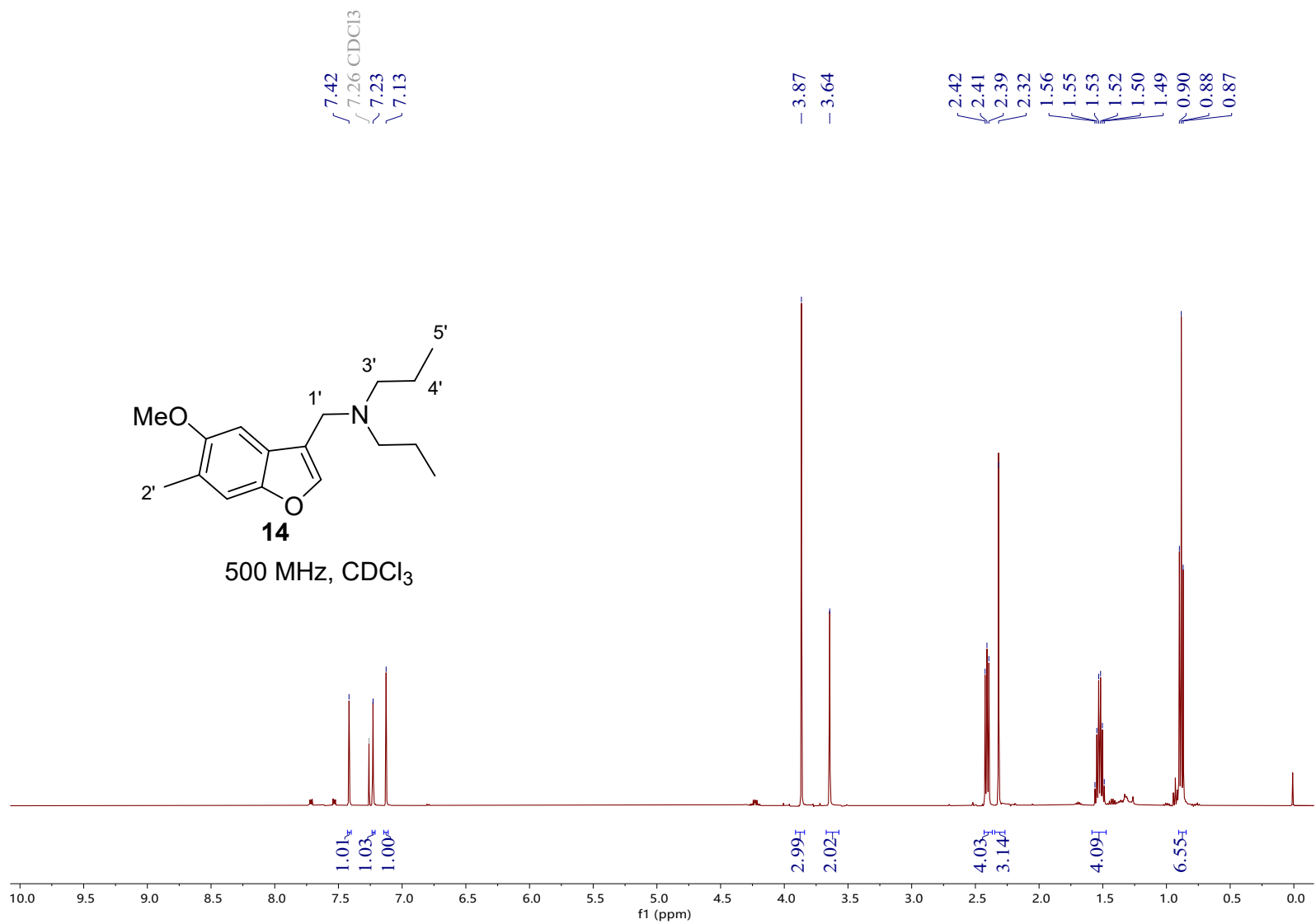
— 55.9  
— 47.0  
— 46.9

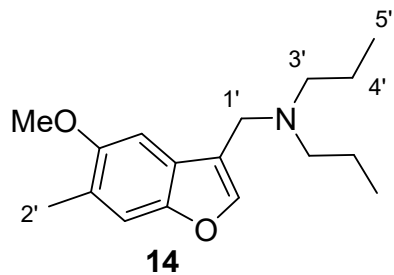
— 17.1  
— 12.2



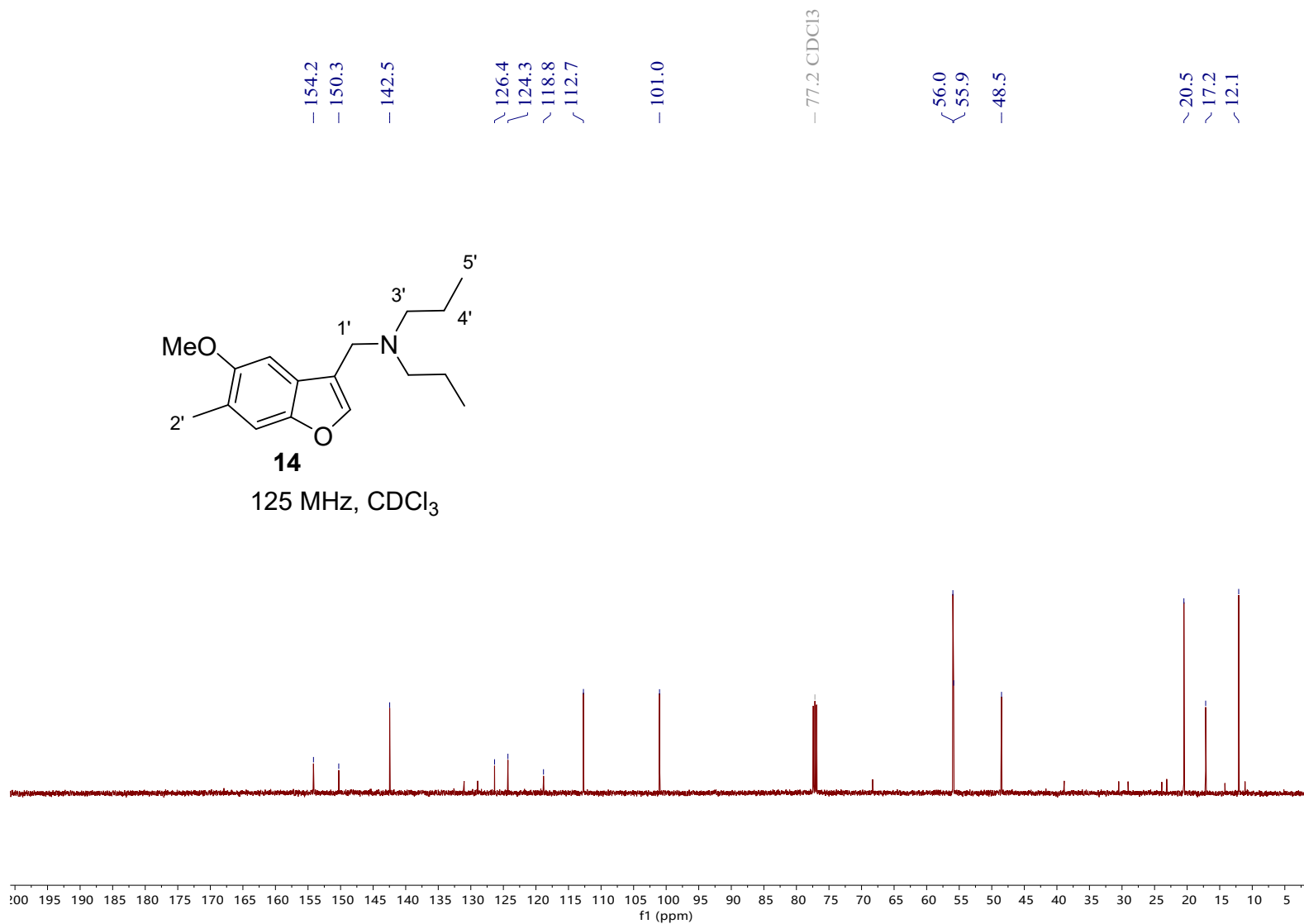


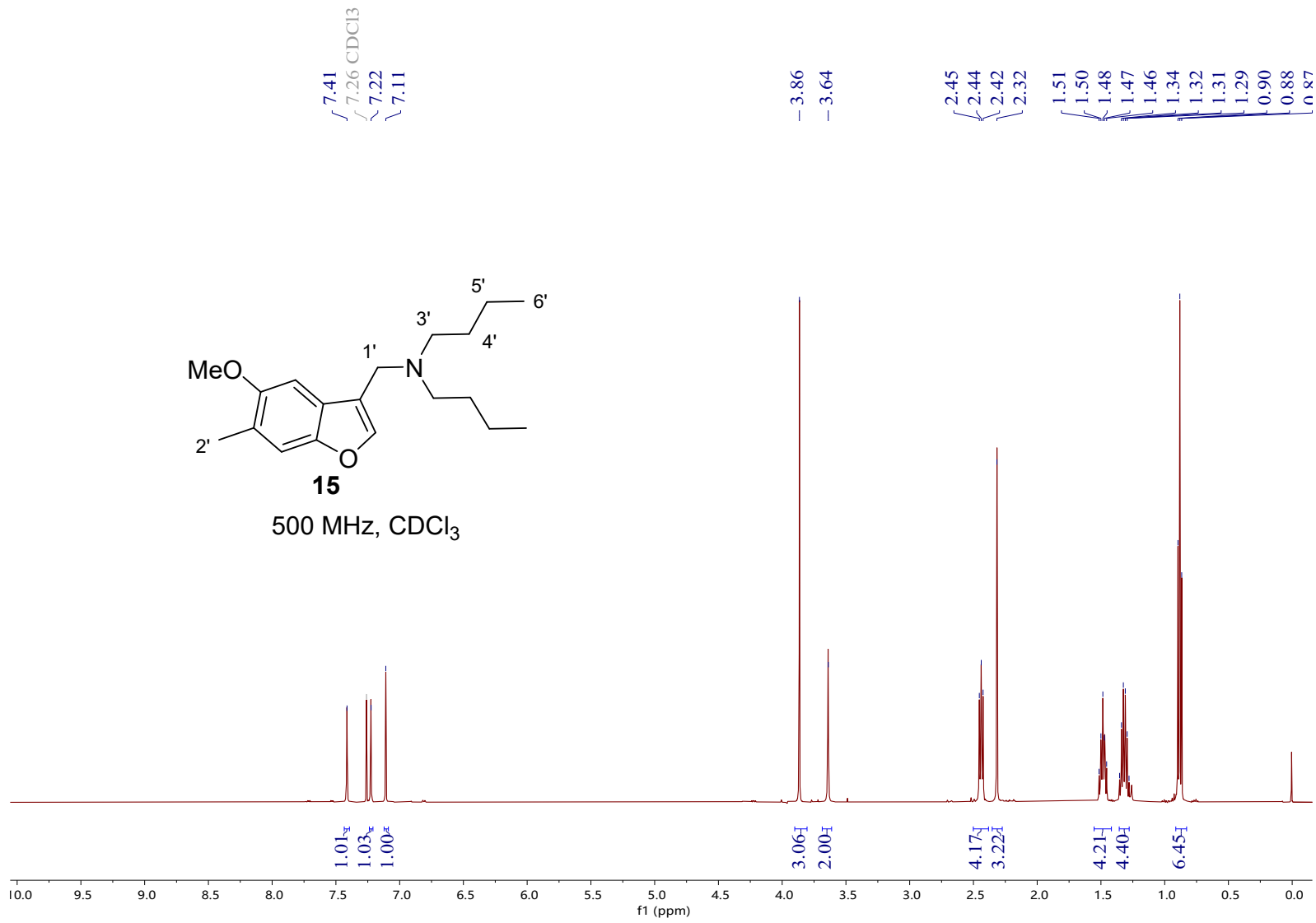
500 MHz, CDCl<sub>3</sub>



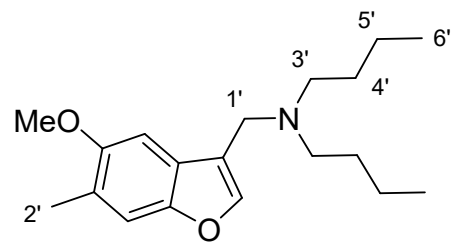


125 MHz, CDCl<sub>3</sub>



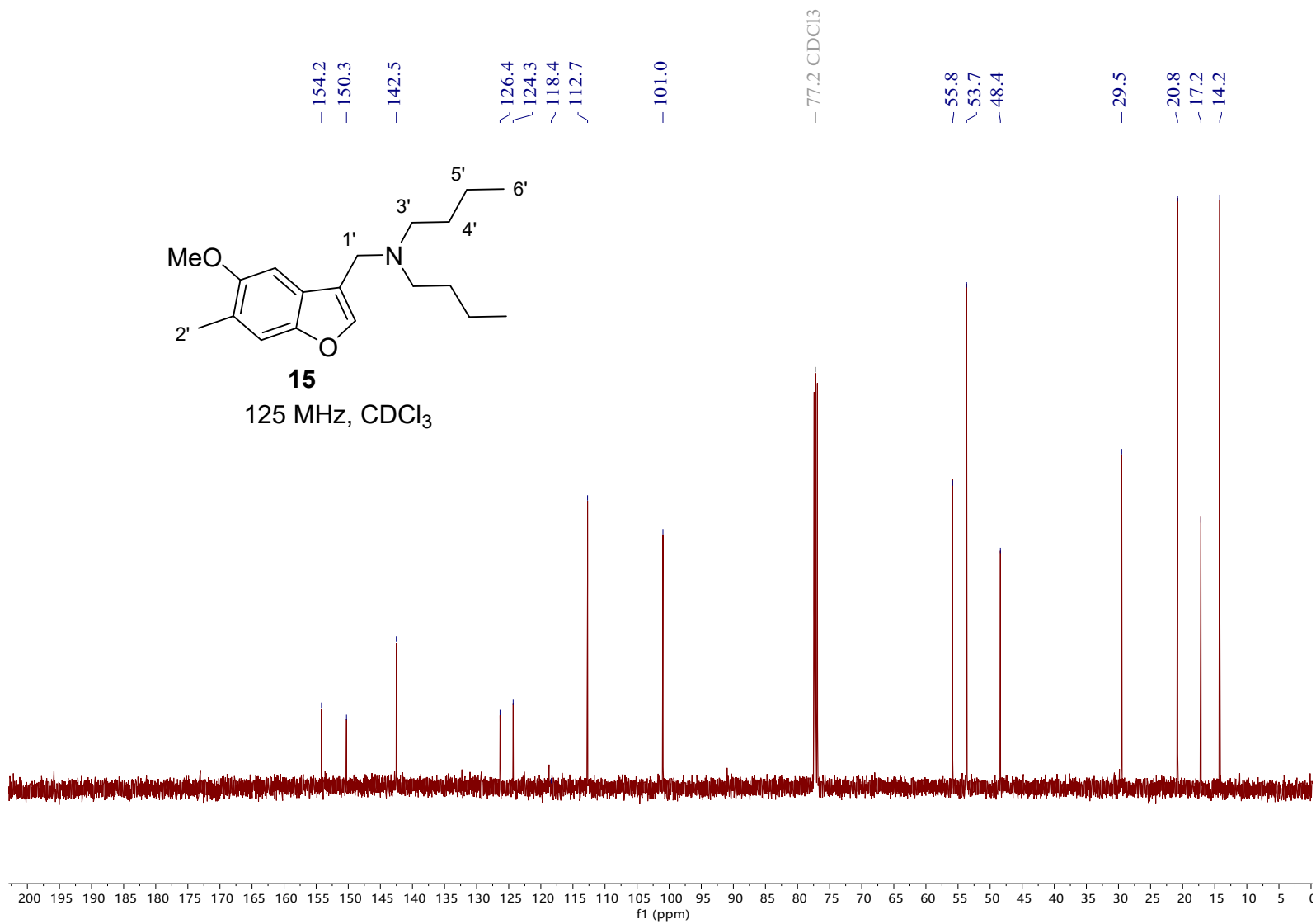






**15**

125 MHz, CDCl<sub>3</sub>

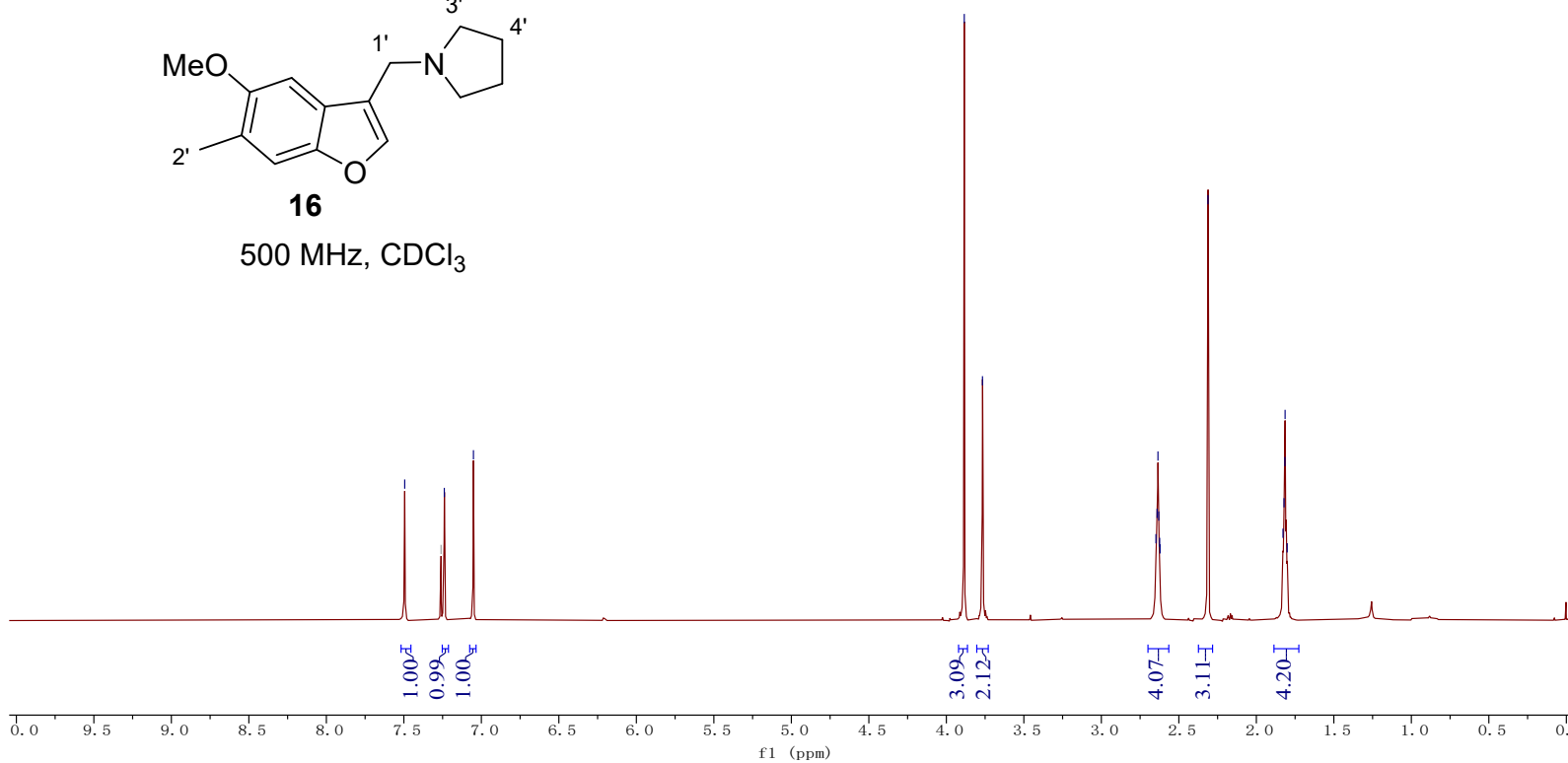
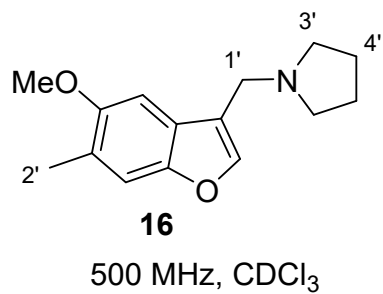


ltz87i.21.fid  
Ltz87i H

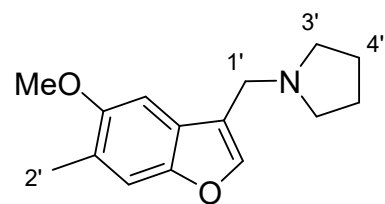
7.495  
7.260 CDCl<sub>3</sub>  
7.239  
7.051

3.884  
3.767

2.648  
2.640  
2.635  
2.630  
2.624  
2.621  
2.312  
1.828  
1.821  
1.816  
1.814  
1.801

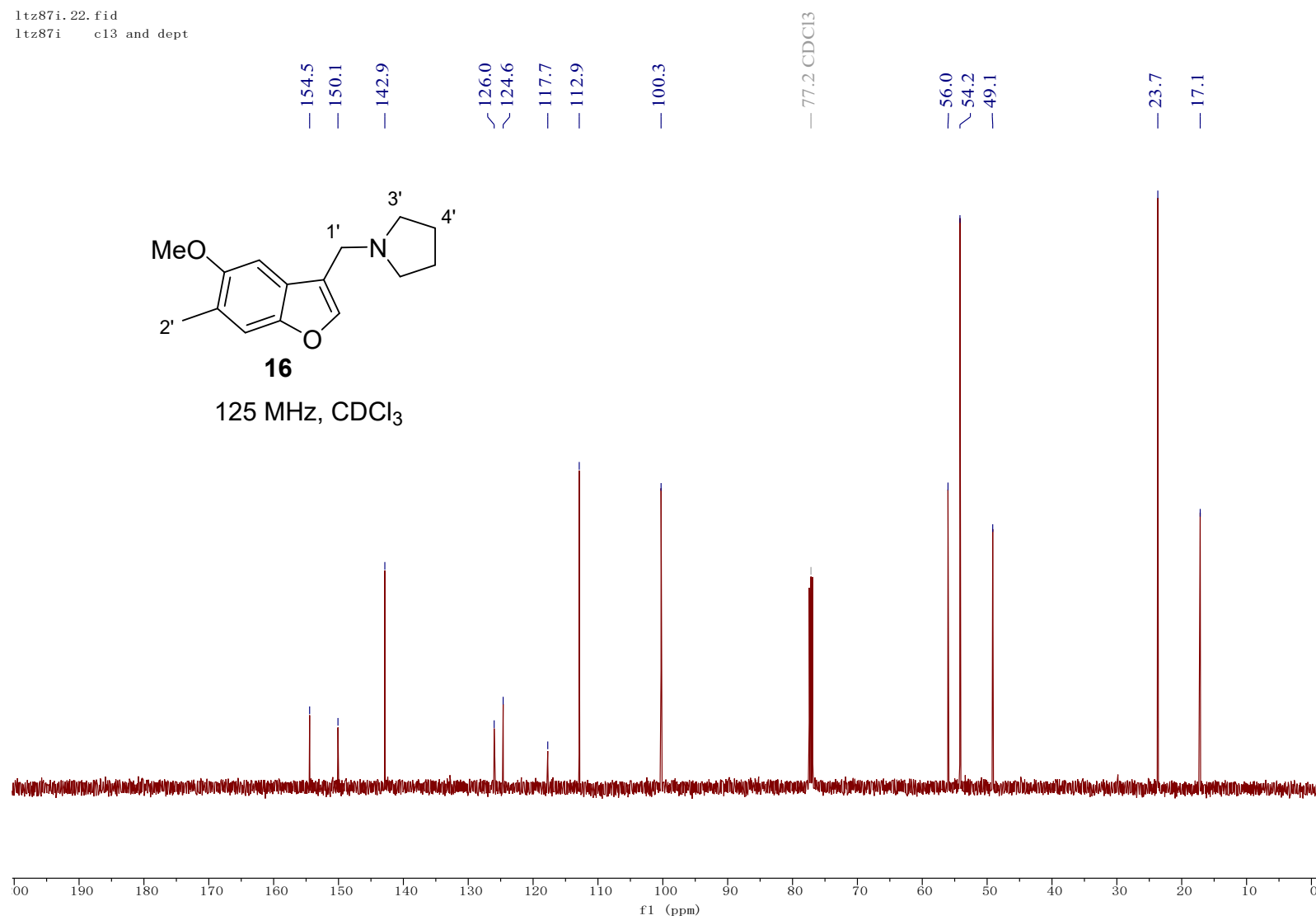


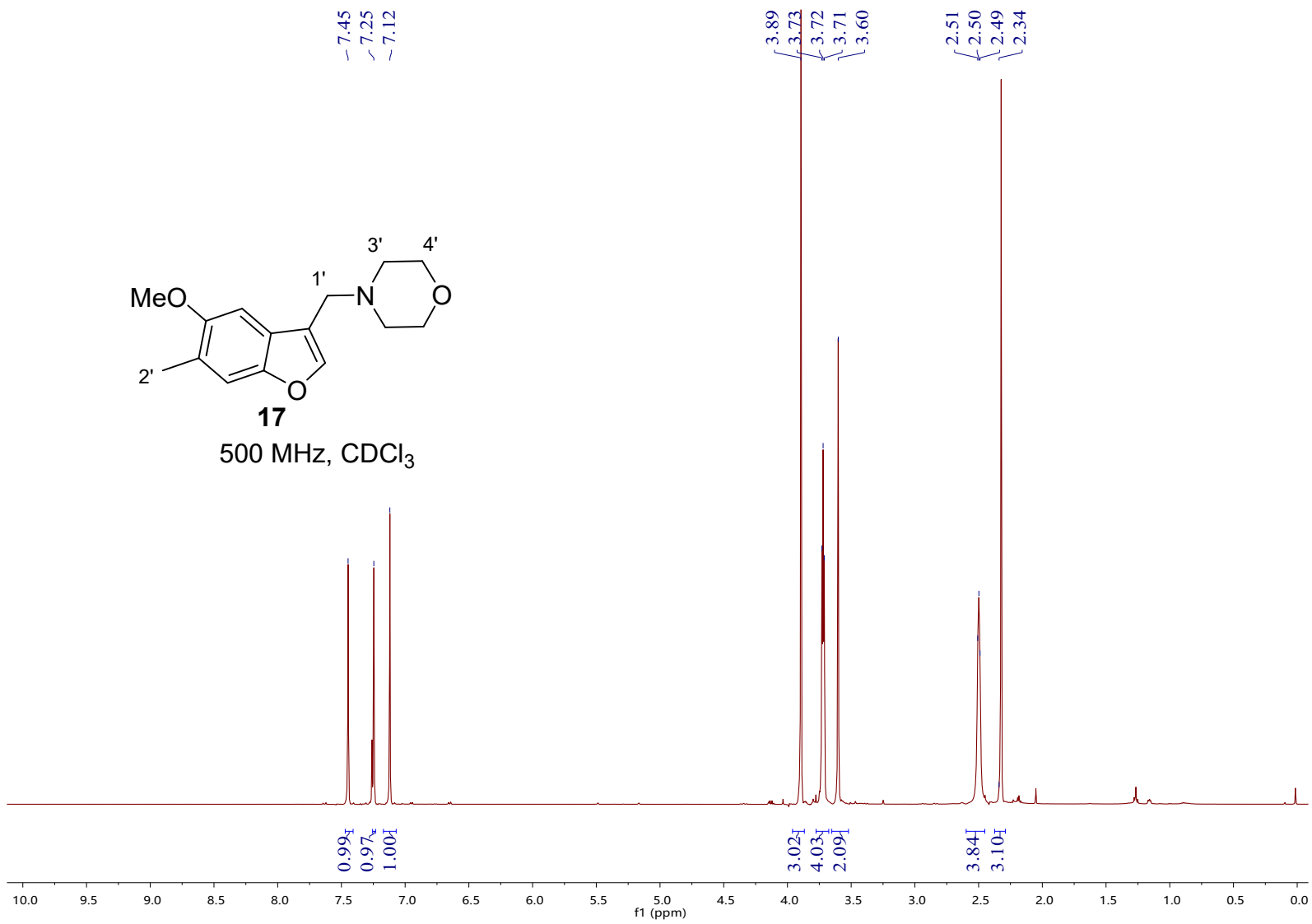
ltz87i.22.fid  
ltz87i c13 and dept

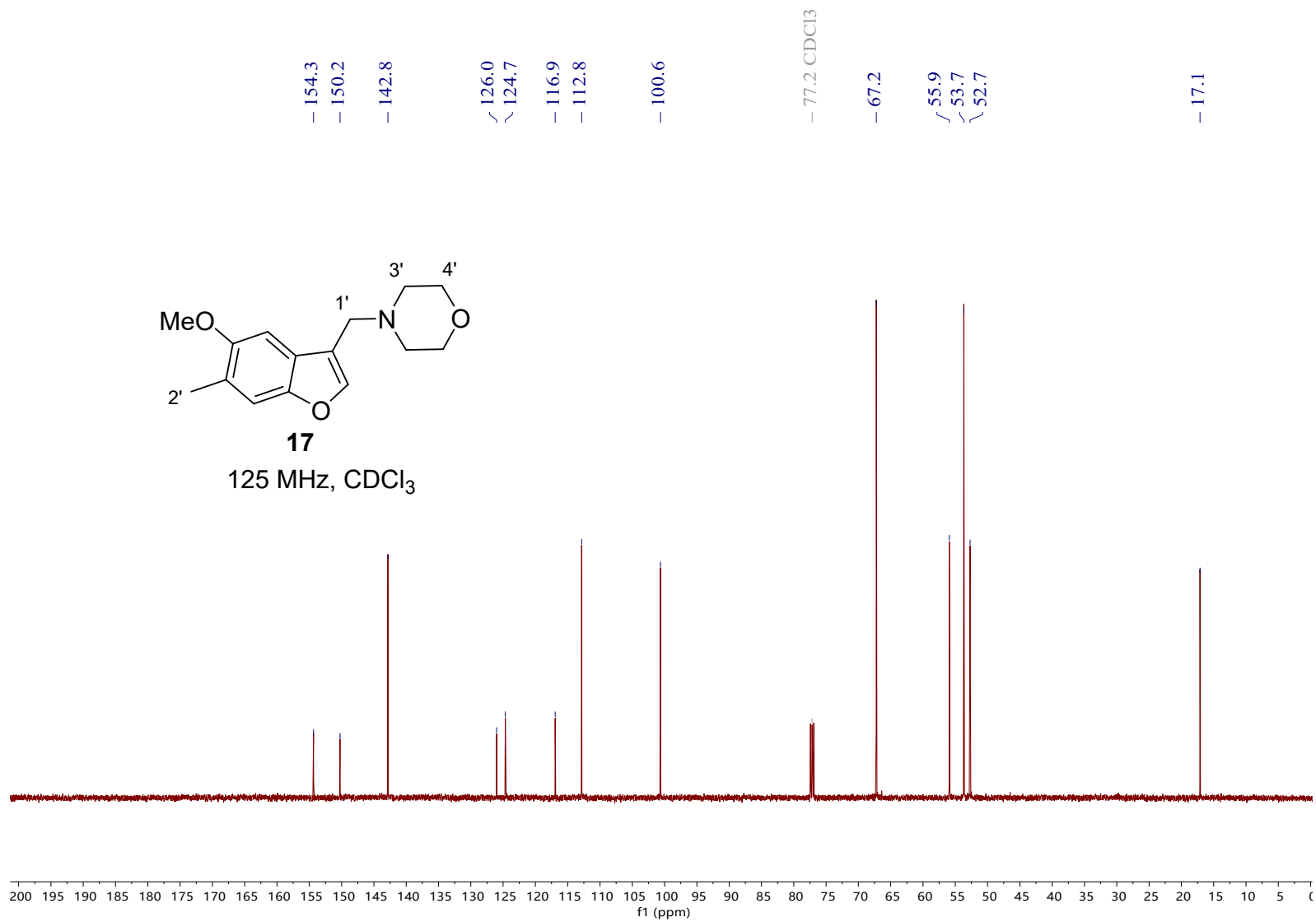


**16**

125 MHz, CDCl<sub>3</sub>



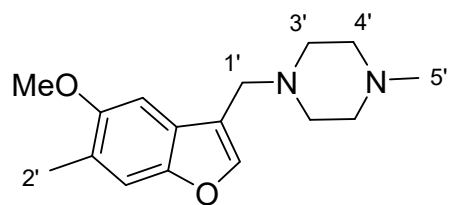




jltz49.21.fid  
jltz49 H

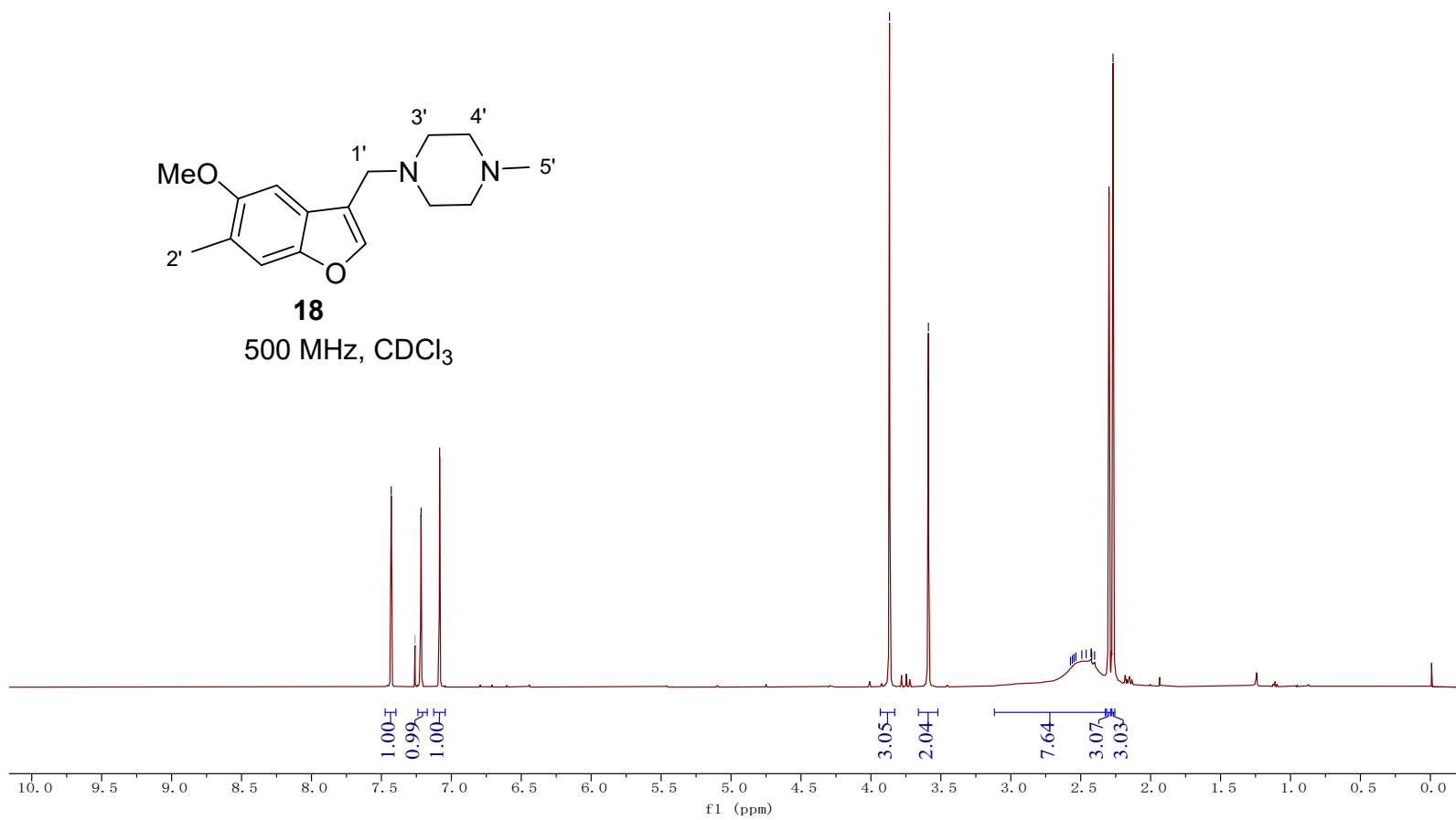
7.43  
7.26 CDCl<sub>3</sub>  
7.22  
7.08

3.87  
3.59  
3.59  
2.57  
2.56  
2.55  
2.53  
2.49  
2.46  
2.43  
2.42  
2.42  
2.40  
2.30  
2.27



**18**

500 MHz, CDCl<sub>3</sub>



jltz49.22.fid  
jltz49 c13

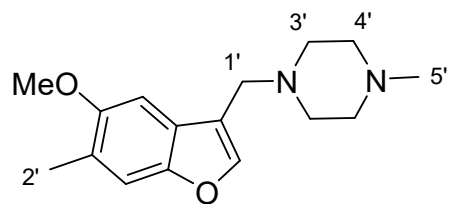
— 154.3  
— 150.1  
— 142.8

— 126.1  
— 124.5  
— 117.2  
— 112.8

— 100.6

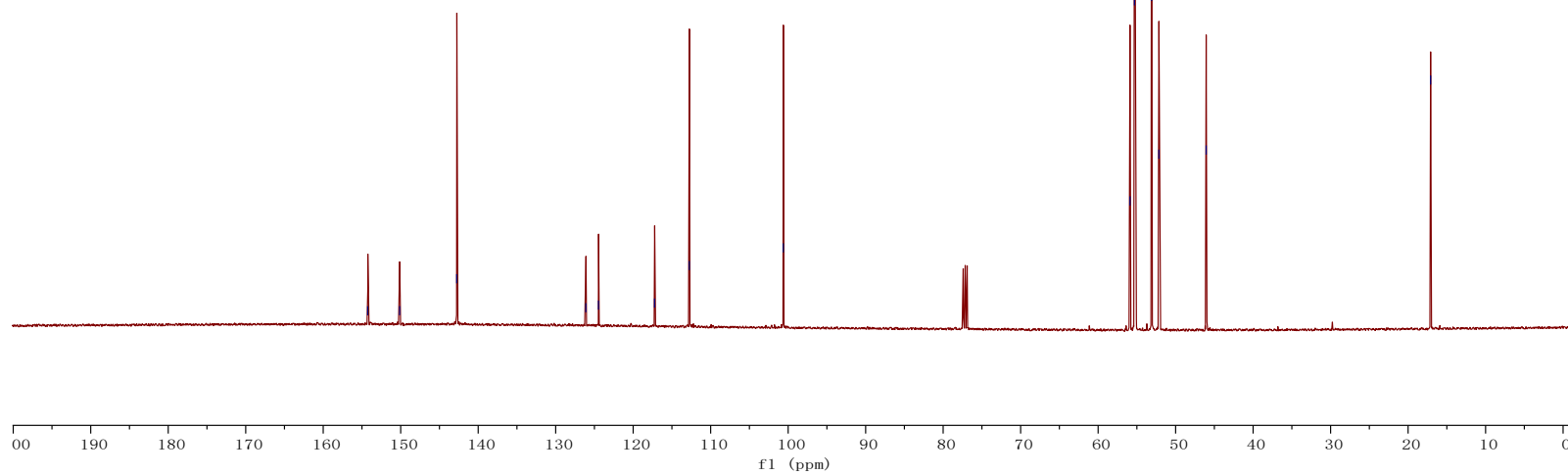
— 55.9  
— 55.3  
— 53.1  
— 52.2  
— 46.1

— 17.1



**18**

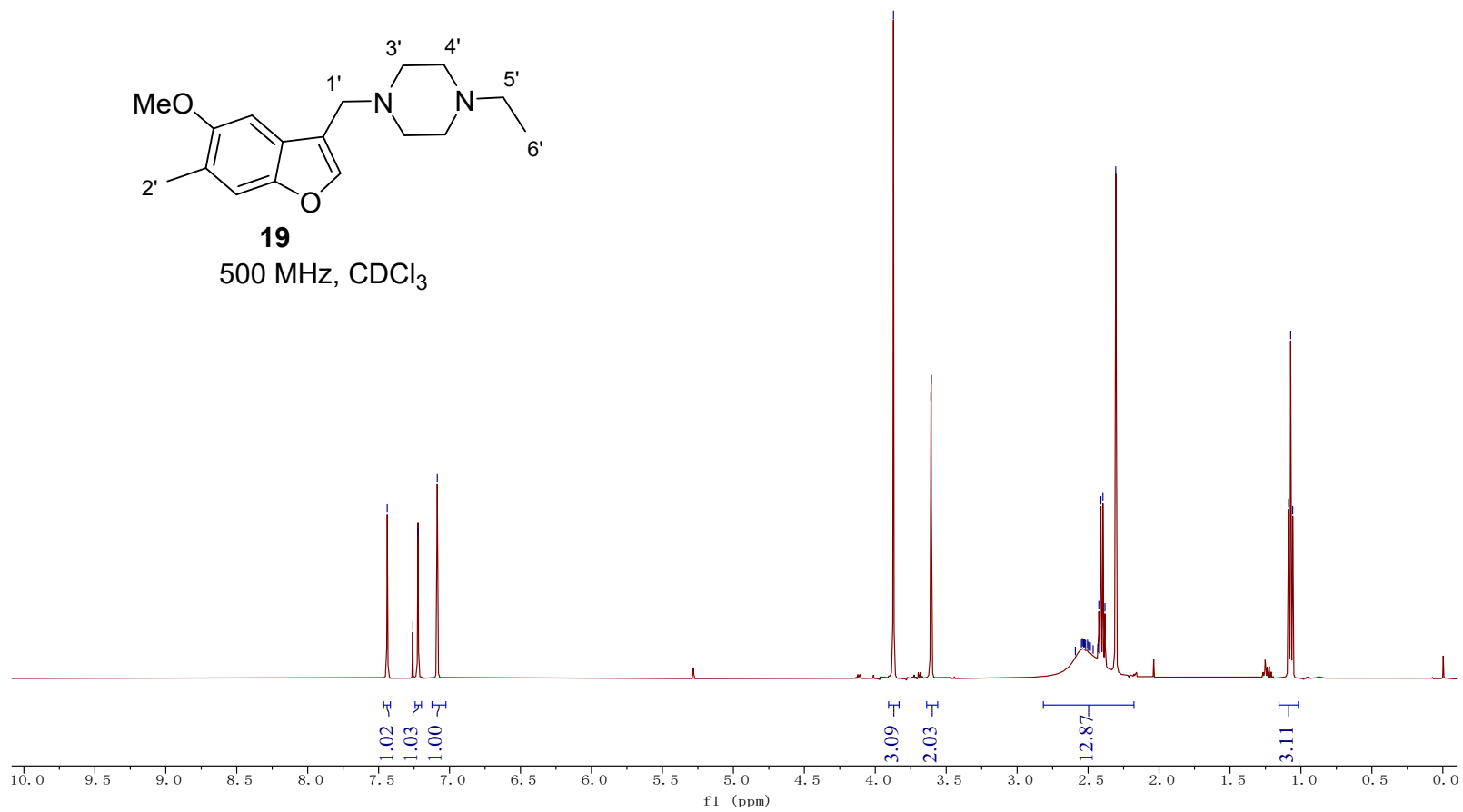
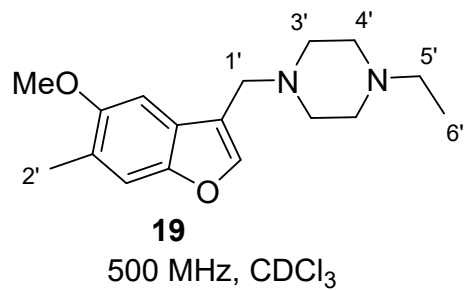
500 MHz, CDCl<sub>3</sub>



ltz4087c.21.fid  
ltz4087c H

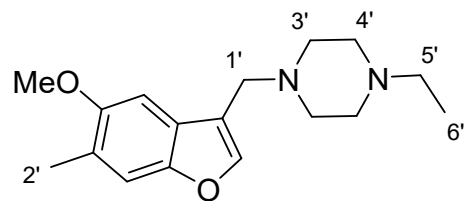
7.44  
7.26 CDCl<sub>3</sub>  
7.22  
7.09

3.87  
3.61  
3.61  
2.59  
2.56  
2.55  
2.54  
2.53  
2.52  
2.52  
2.50  
2.50  
2.49  
2.49  
2.48  
2.46  
2.43  
2.42  
2.41  
2.40  
2.38  
2.30  
1.09  
1.07  
1.06

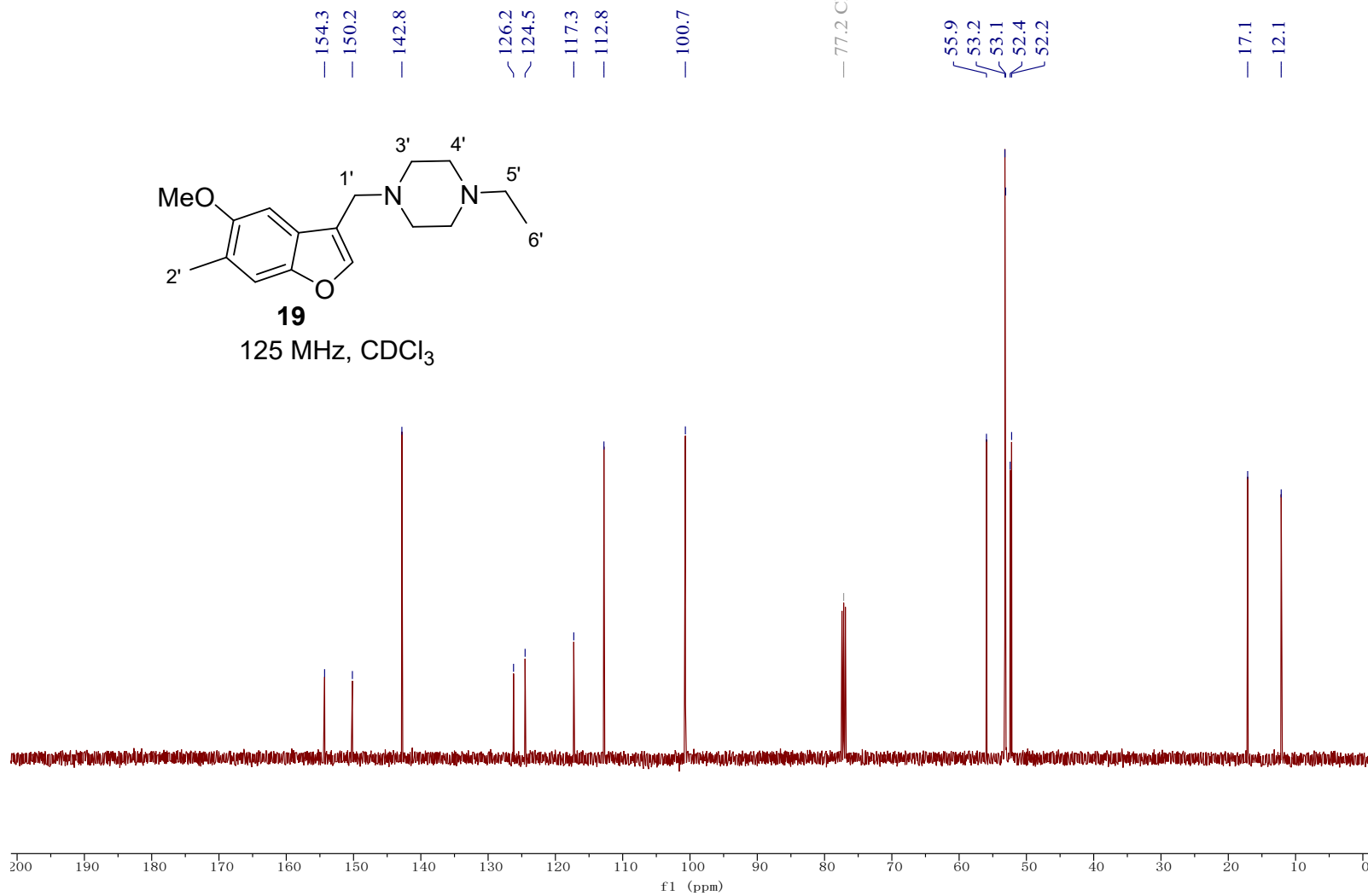




ltz4087c.22.fid  
ltz4087c c13 and dept



**19**  
125 MHz, CDCl<sub>3</sub>

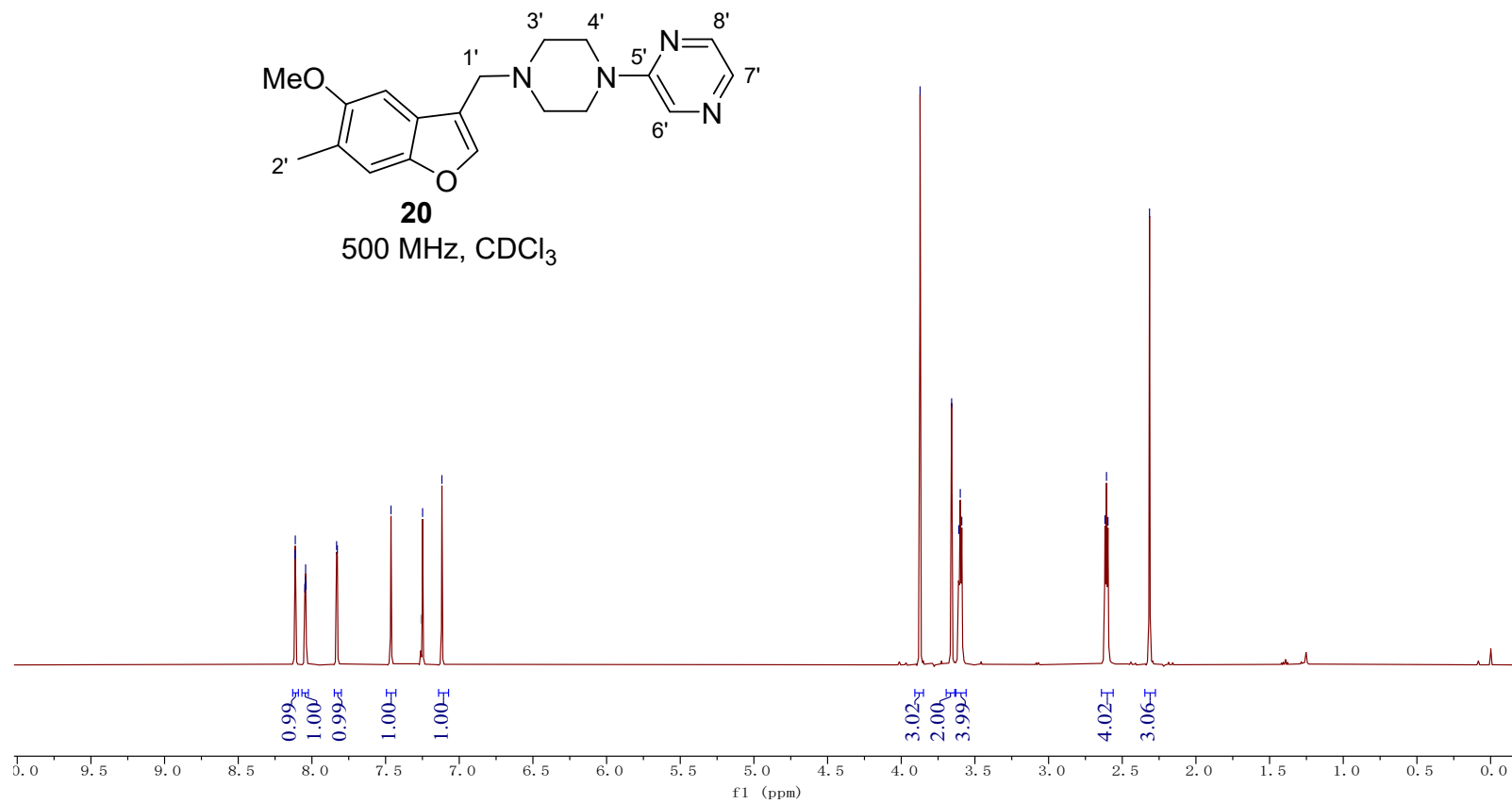
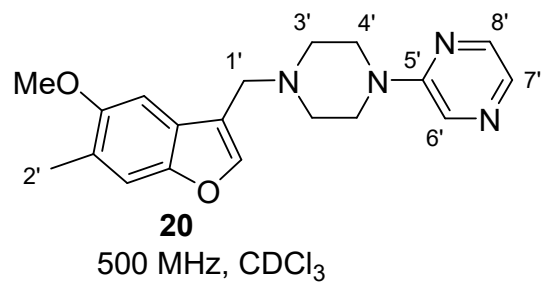


ltz87f. 21. fid  
Ltz87f H

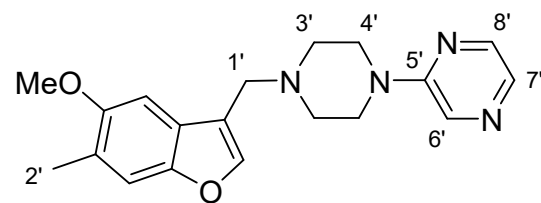
8.12  
8.11  
8.05  
8.05  
8.04  
8.04  
7.83  
7.83  
7.46  
7.26 CDCl<sub>3</sub>  
7.25  
7.12

3.87  
3.66  
3.61  
3.60  
3.59

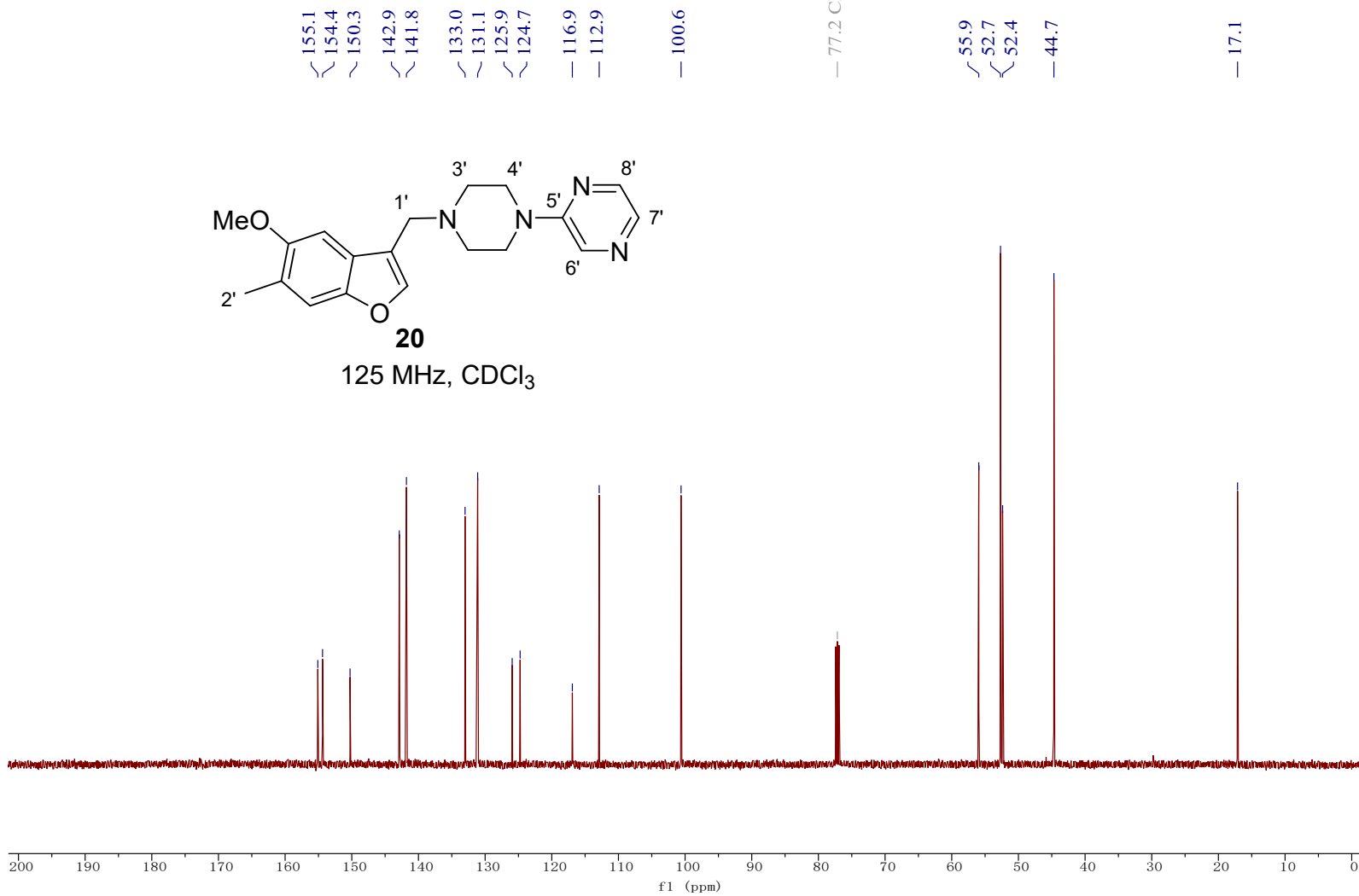
2.62  
2.61  
2.60  
2.32

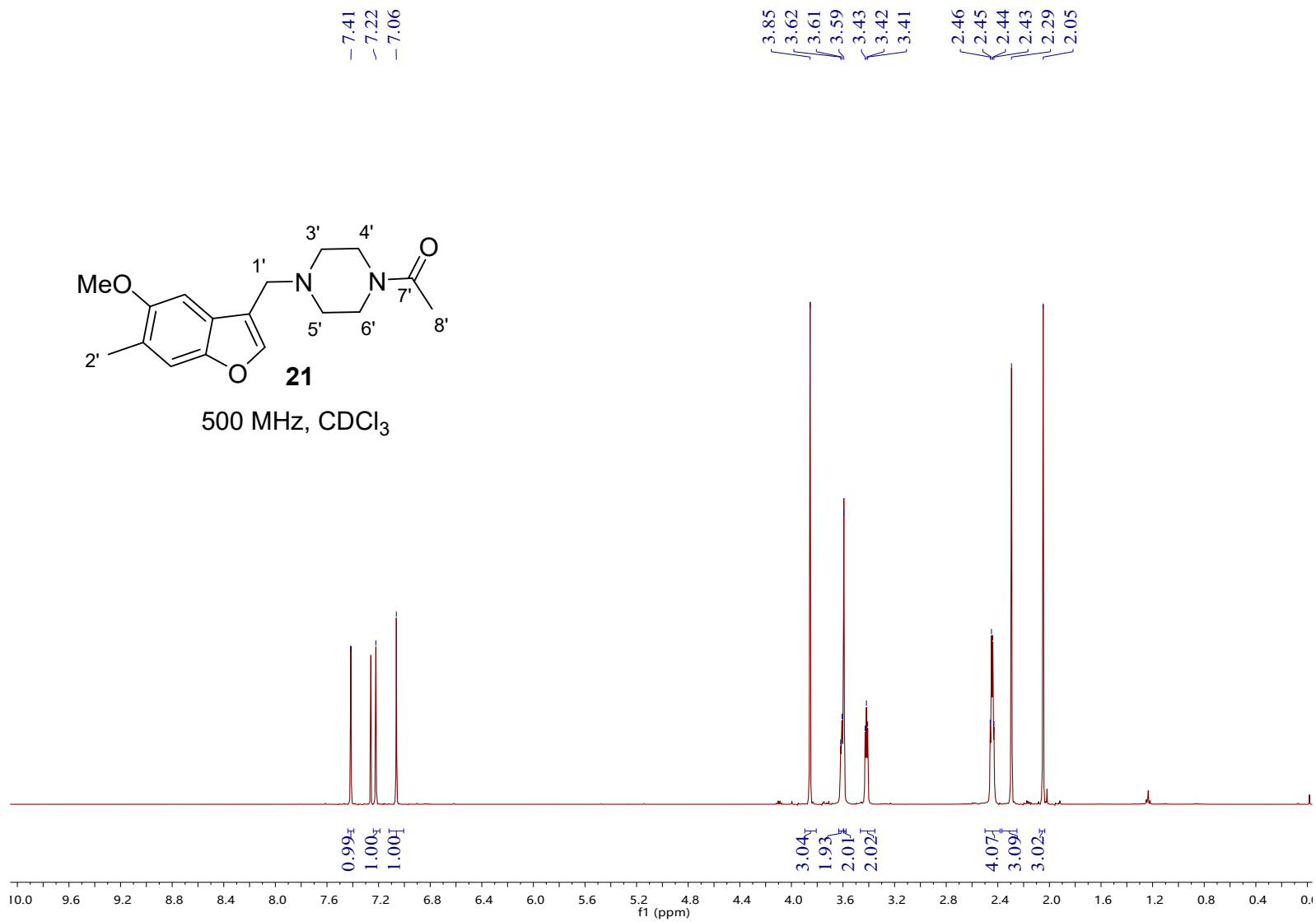


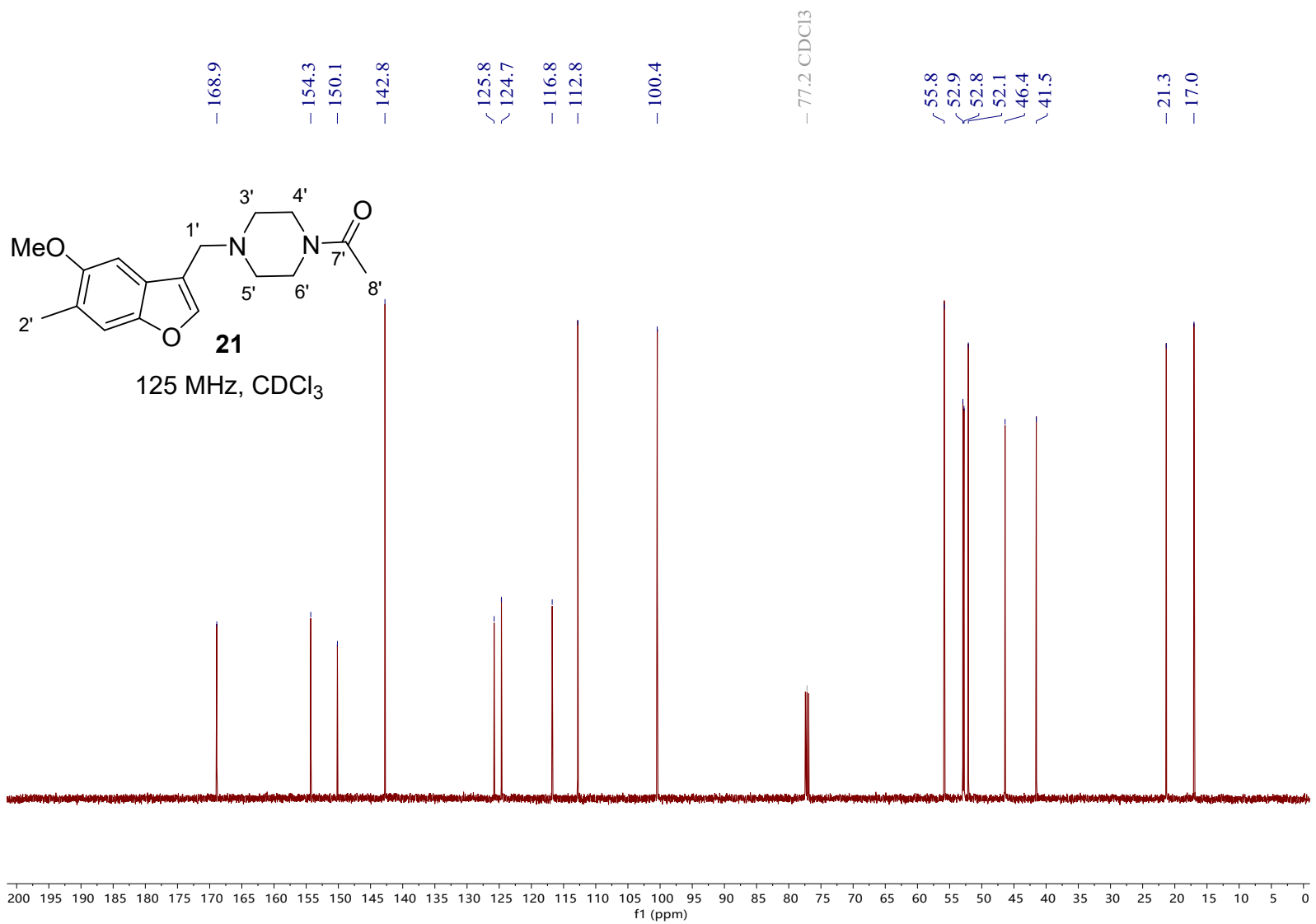
ltz87f.22.fid  
ltz87f c13 and dept

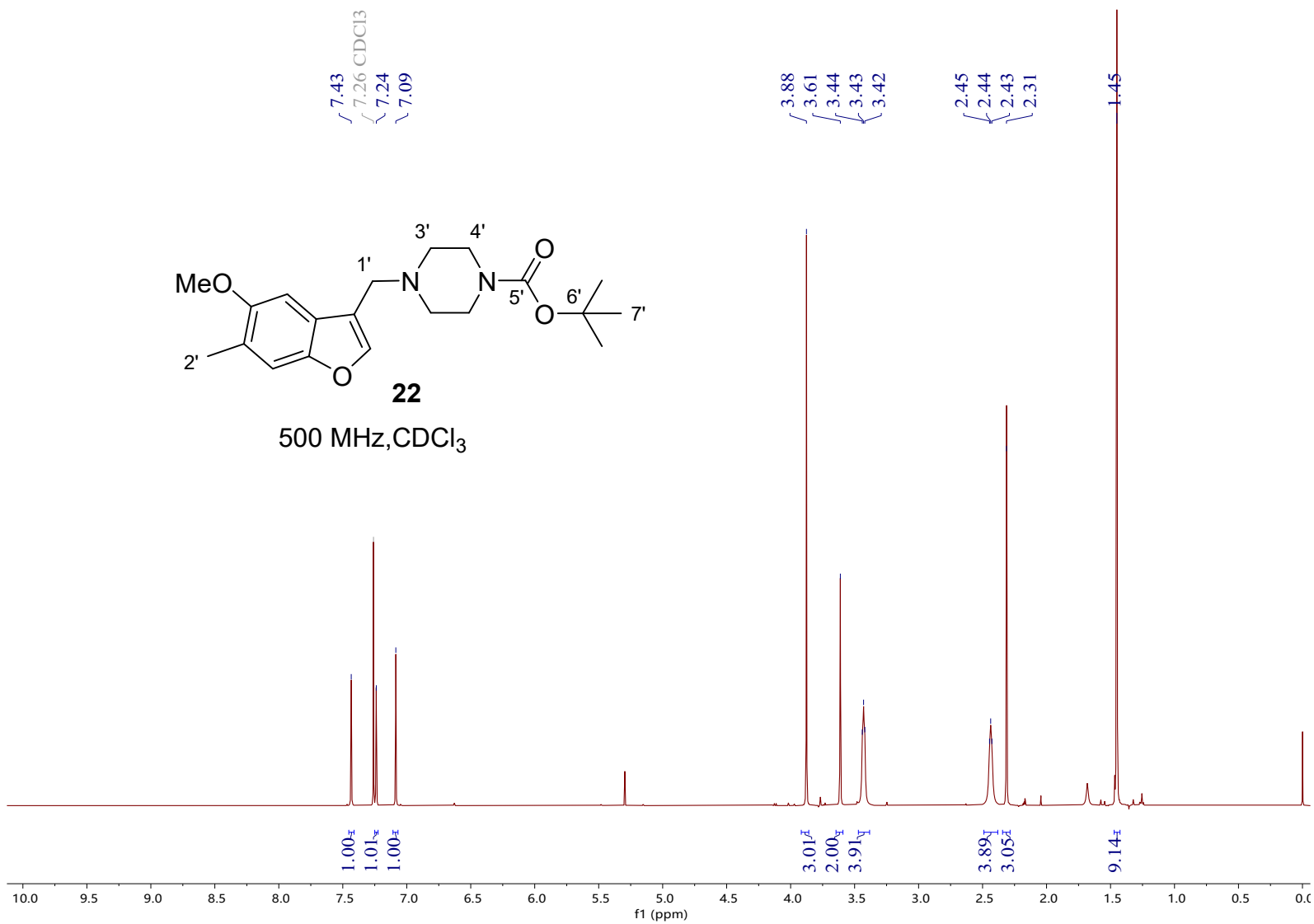


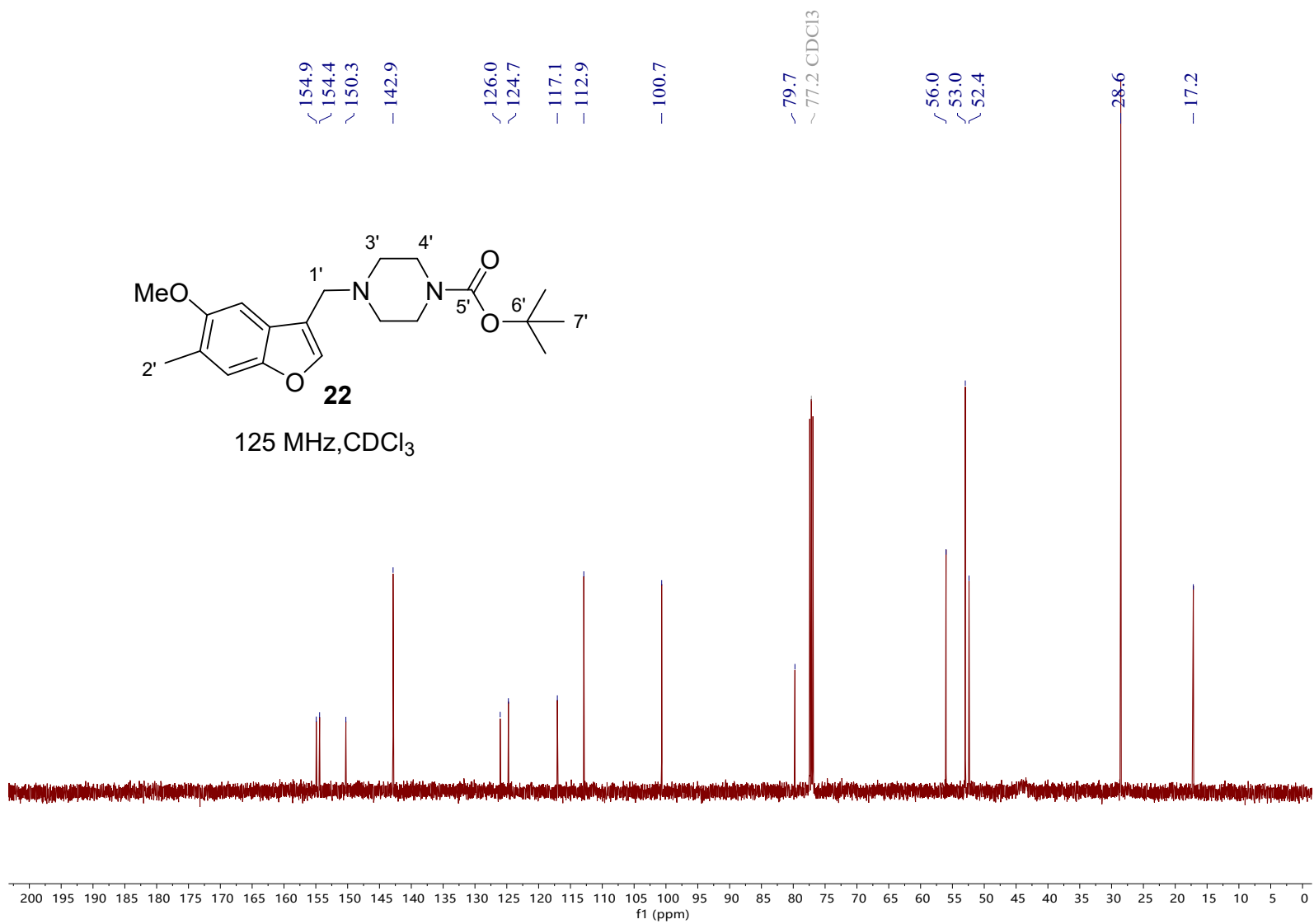
125 MHz, CDCl<sub>3</sub>

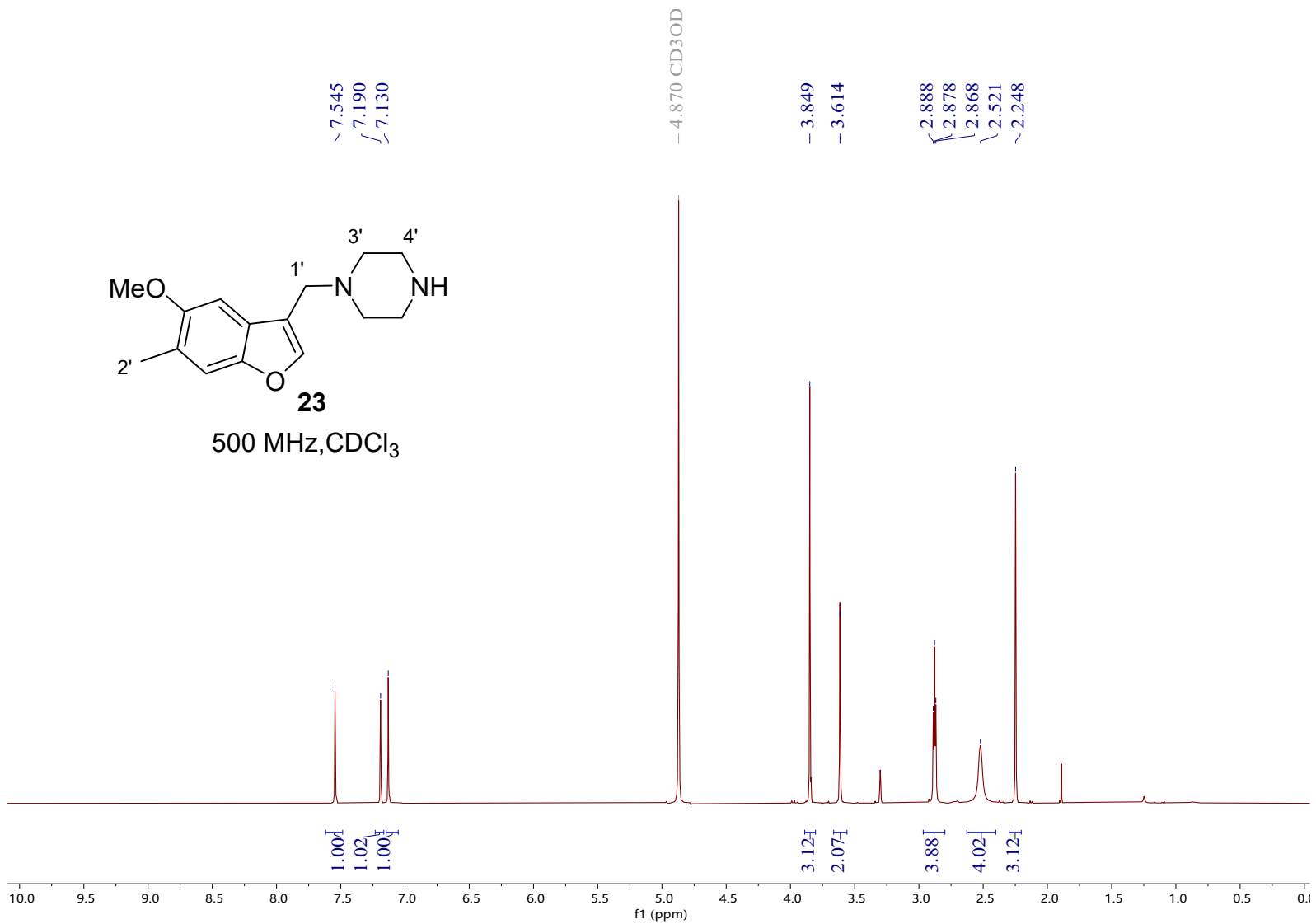




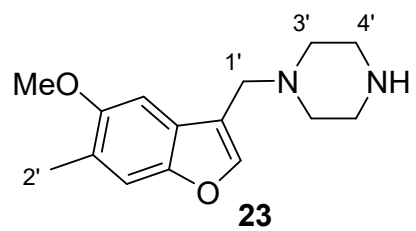




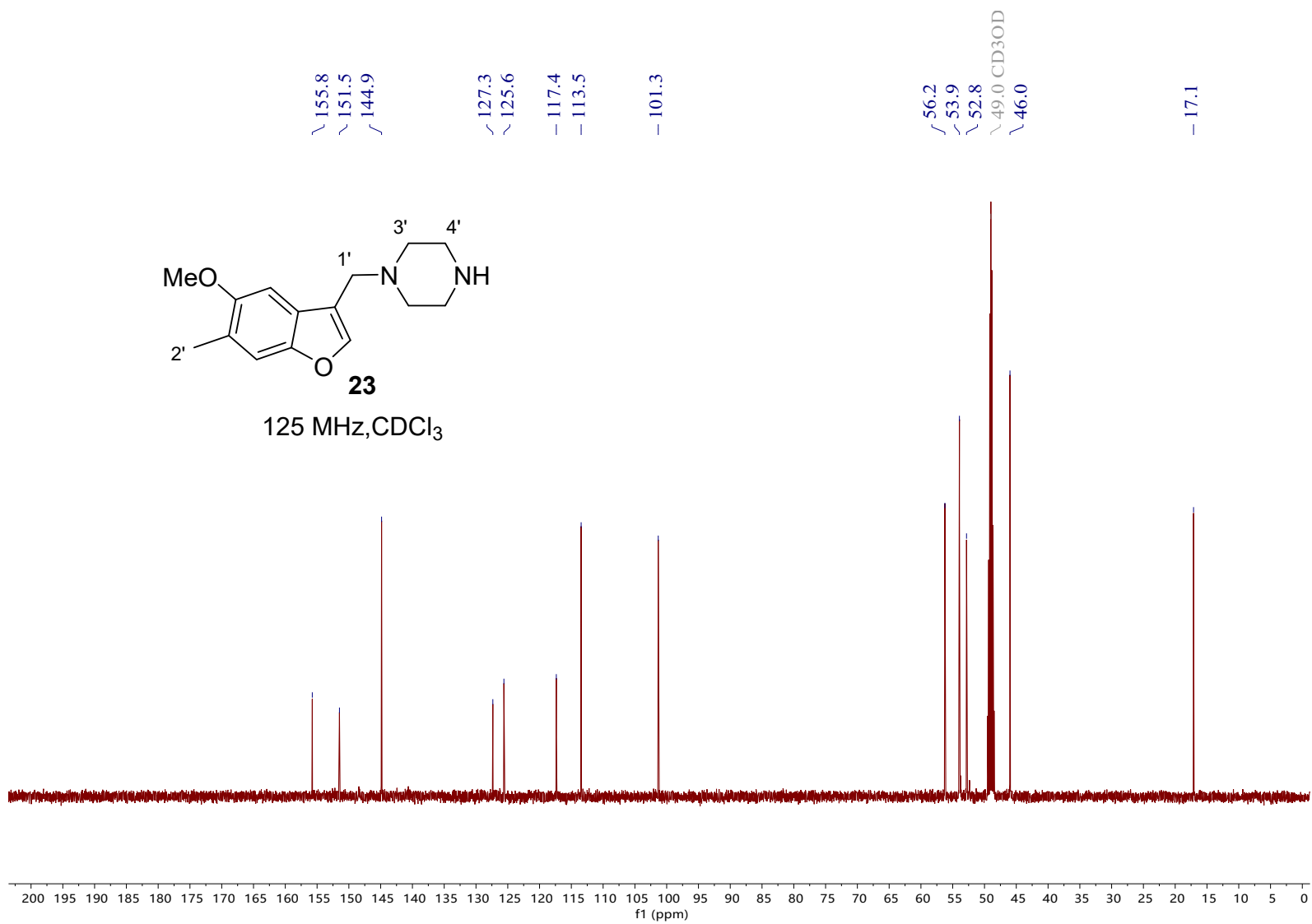








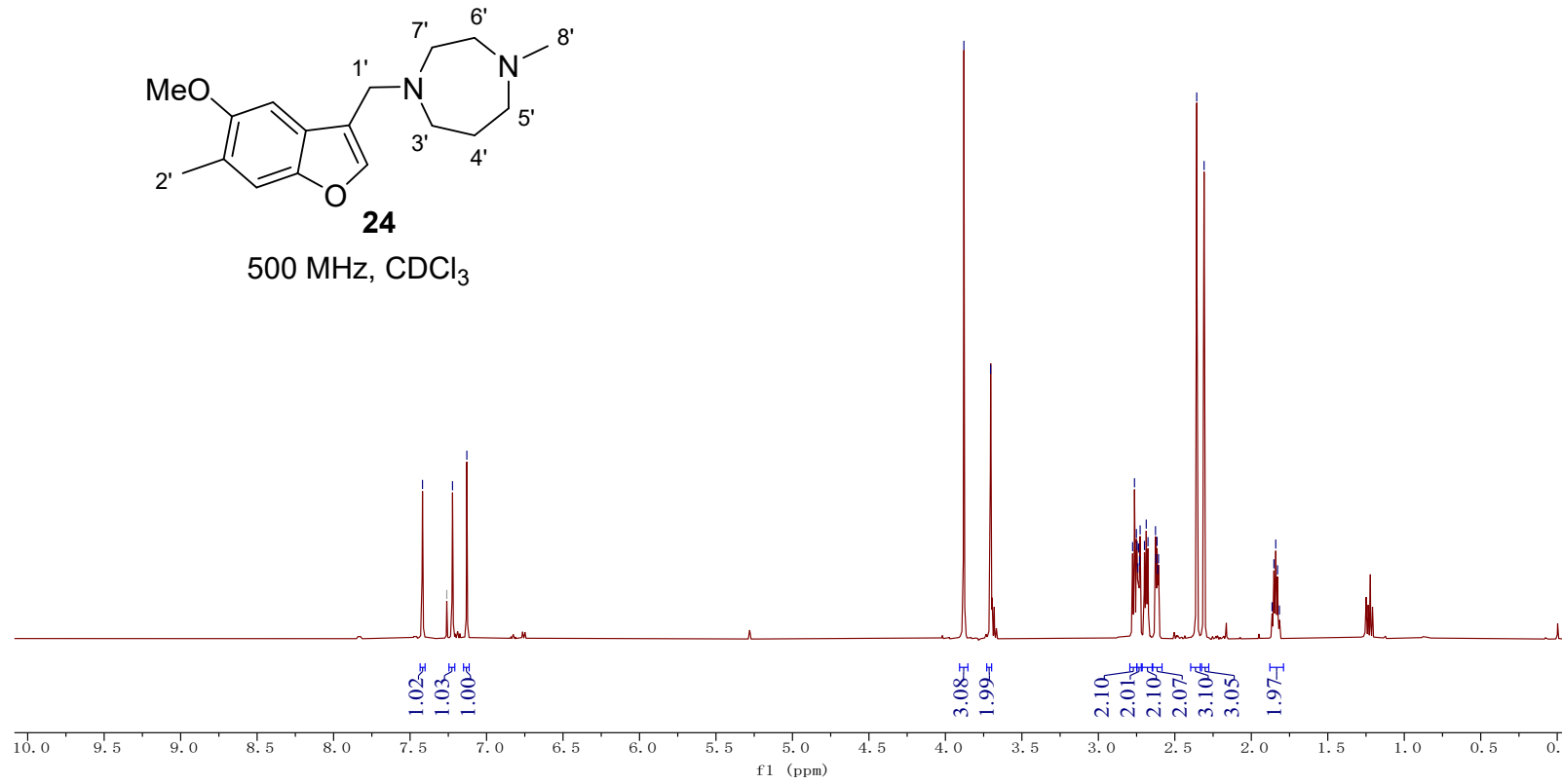
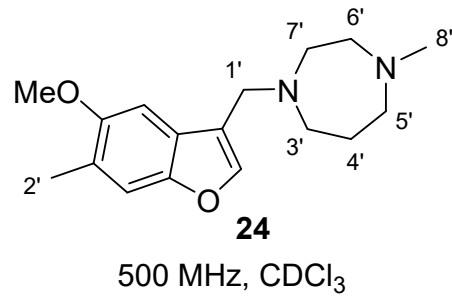
125 MHz, CDCl<sub>3</sub>



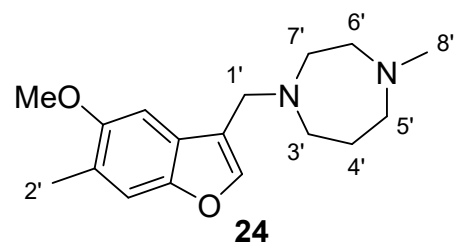
ltz4087d.21.fid  
ltz4087d H

7.42  
7.26 CDCl<sub>3</sub>  
7.22  
7.13

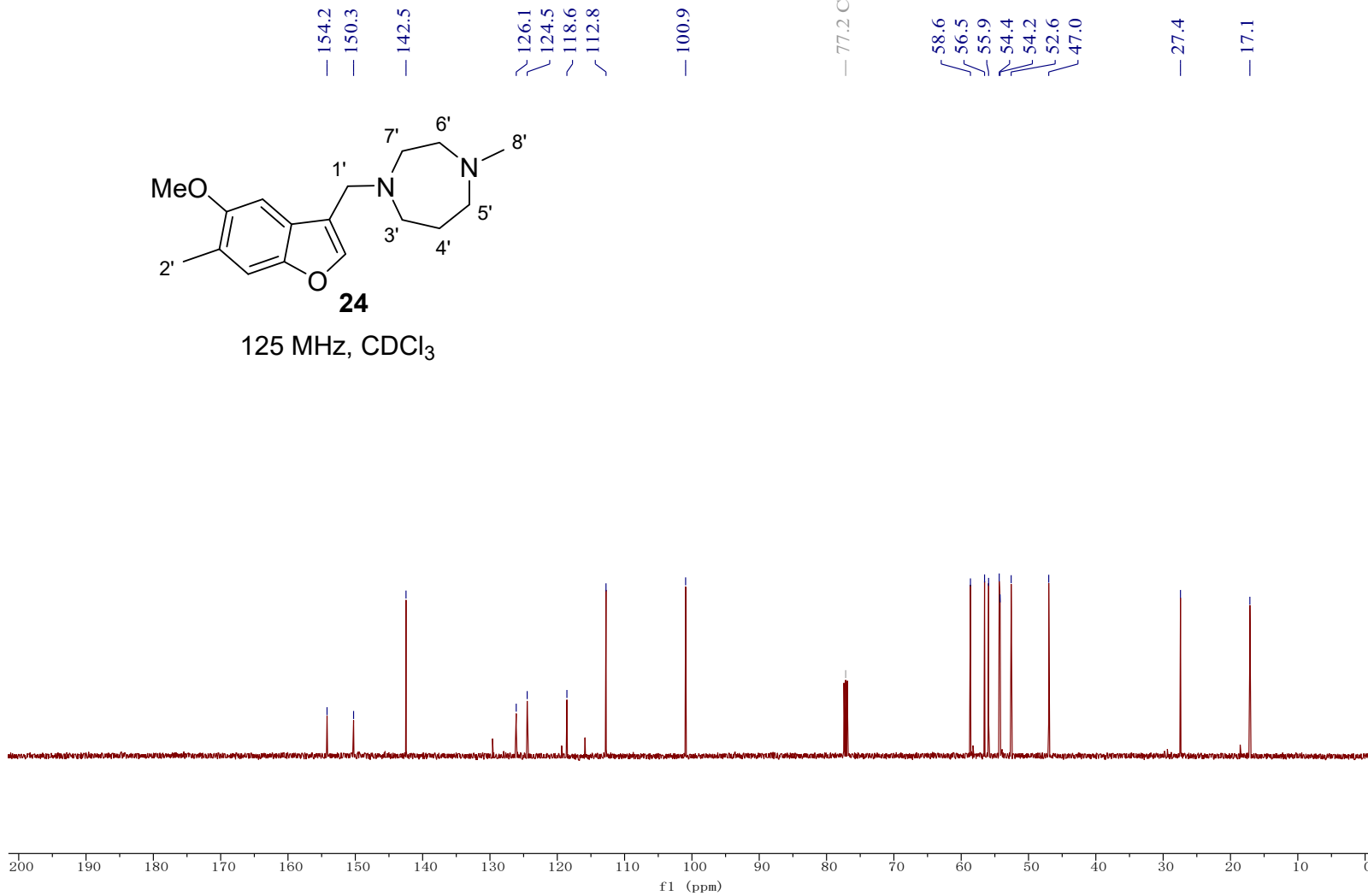
3.88  
3.70  
2.78  
2.76  
2.75  
2.75  
2.74  
2.74  
2.73  
2.73  
2.70  
2.69  
2.68  
2.63  
2.62  
2.62  
2.61  
2.61  
2.36  
2.31  
1.86  
1.85  
1.84  
1.83  
1.82



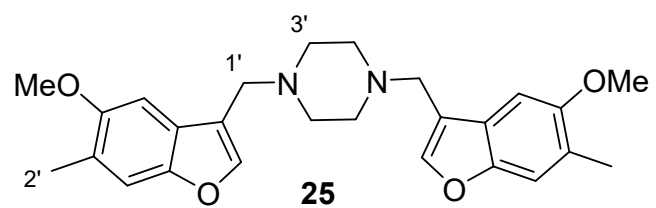
ltz4087d.22.fid  
ltz4087d c13 and dept



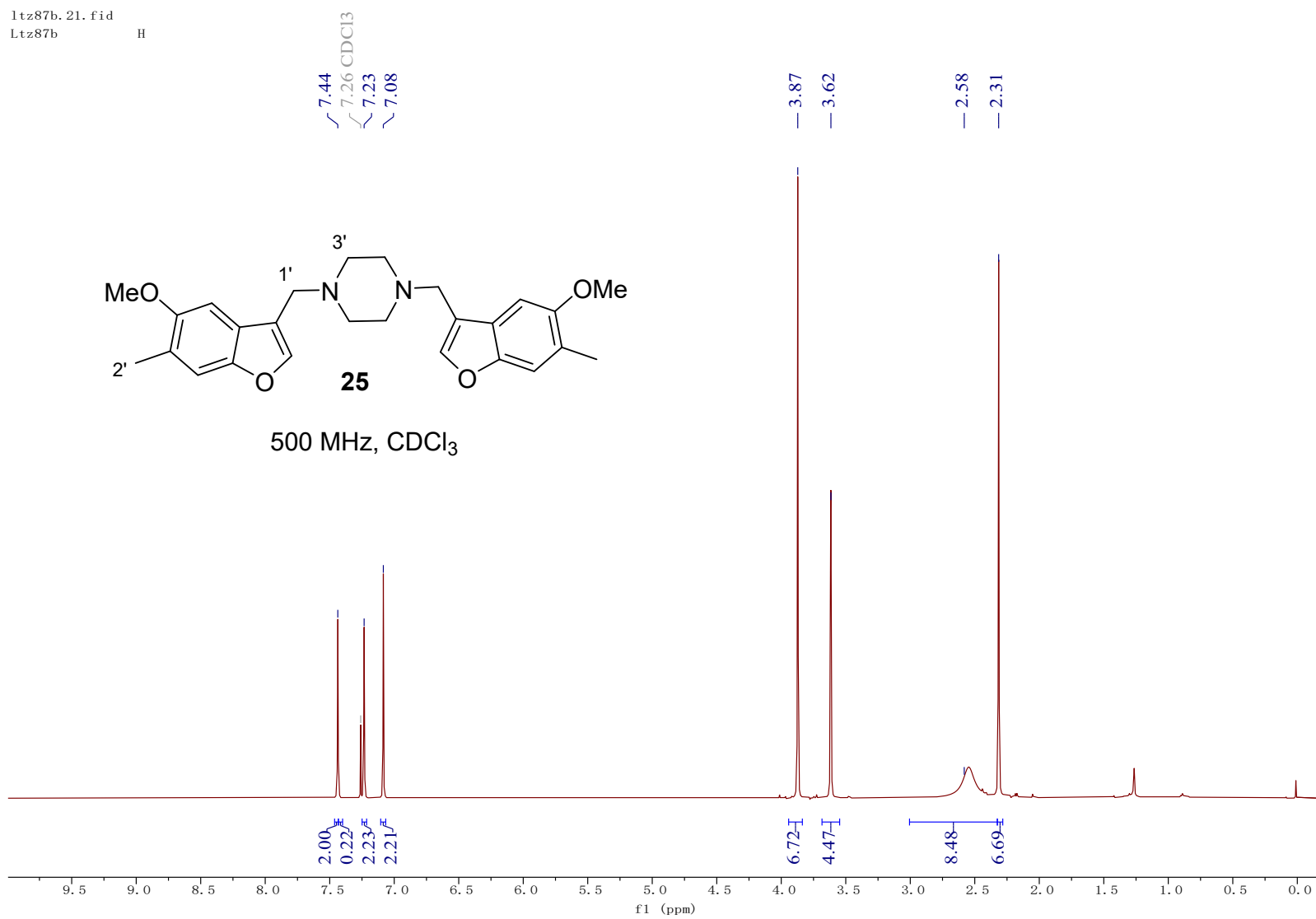
125 MHz, CDCl<sub>3</sub>



ltz87b. 21. fid  
Ltz87b H

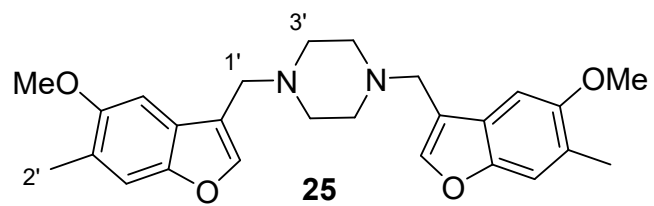


500 MHz, CDCl<sub>3</sub>

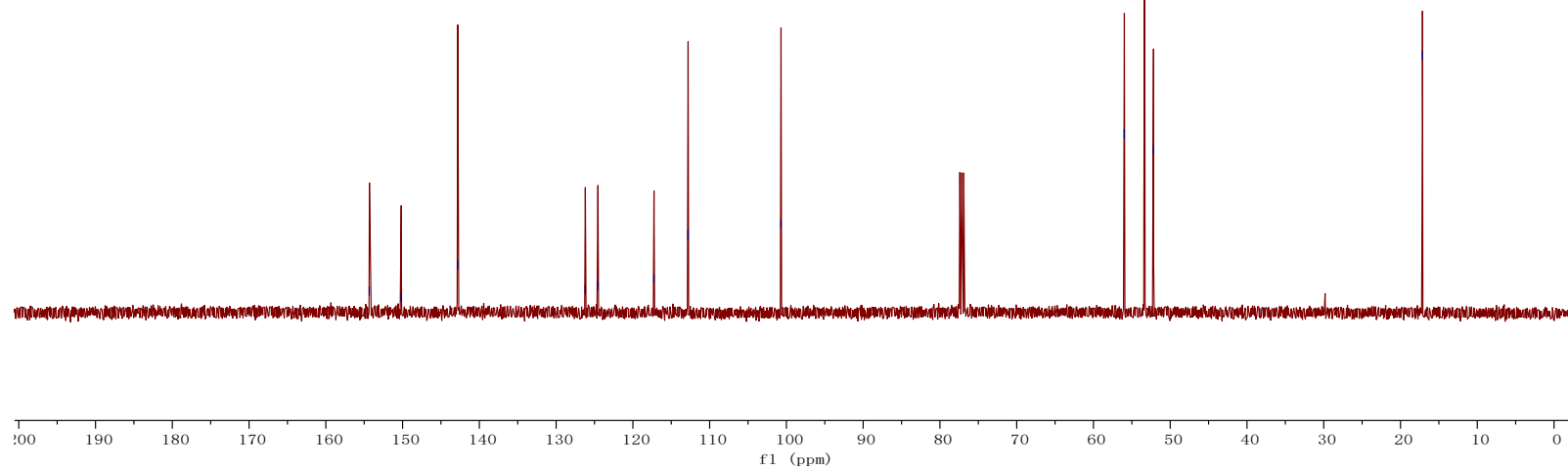


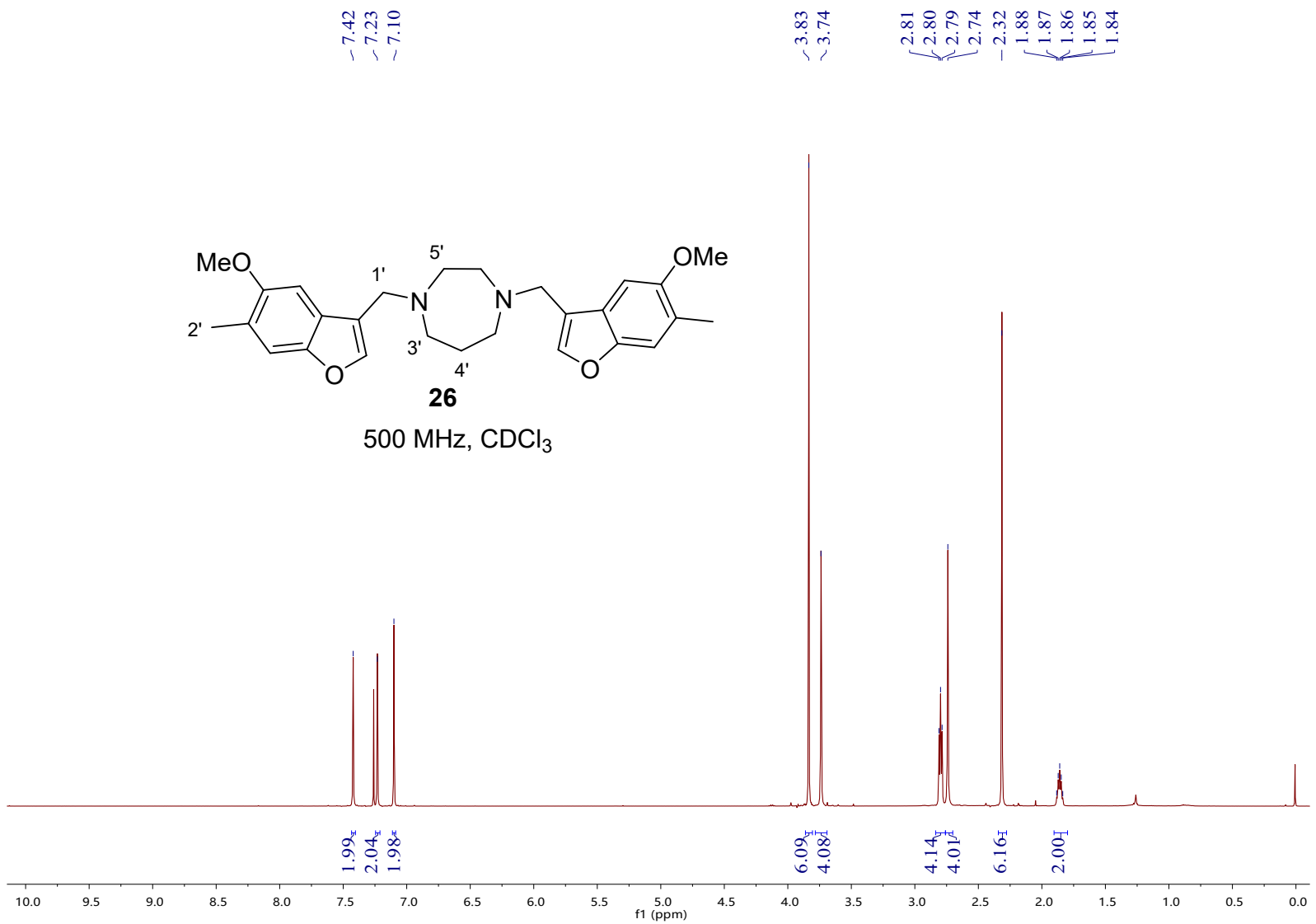
ltz87b.22.fid  
ltz87b c13 and dept

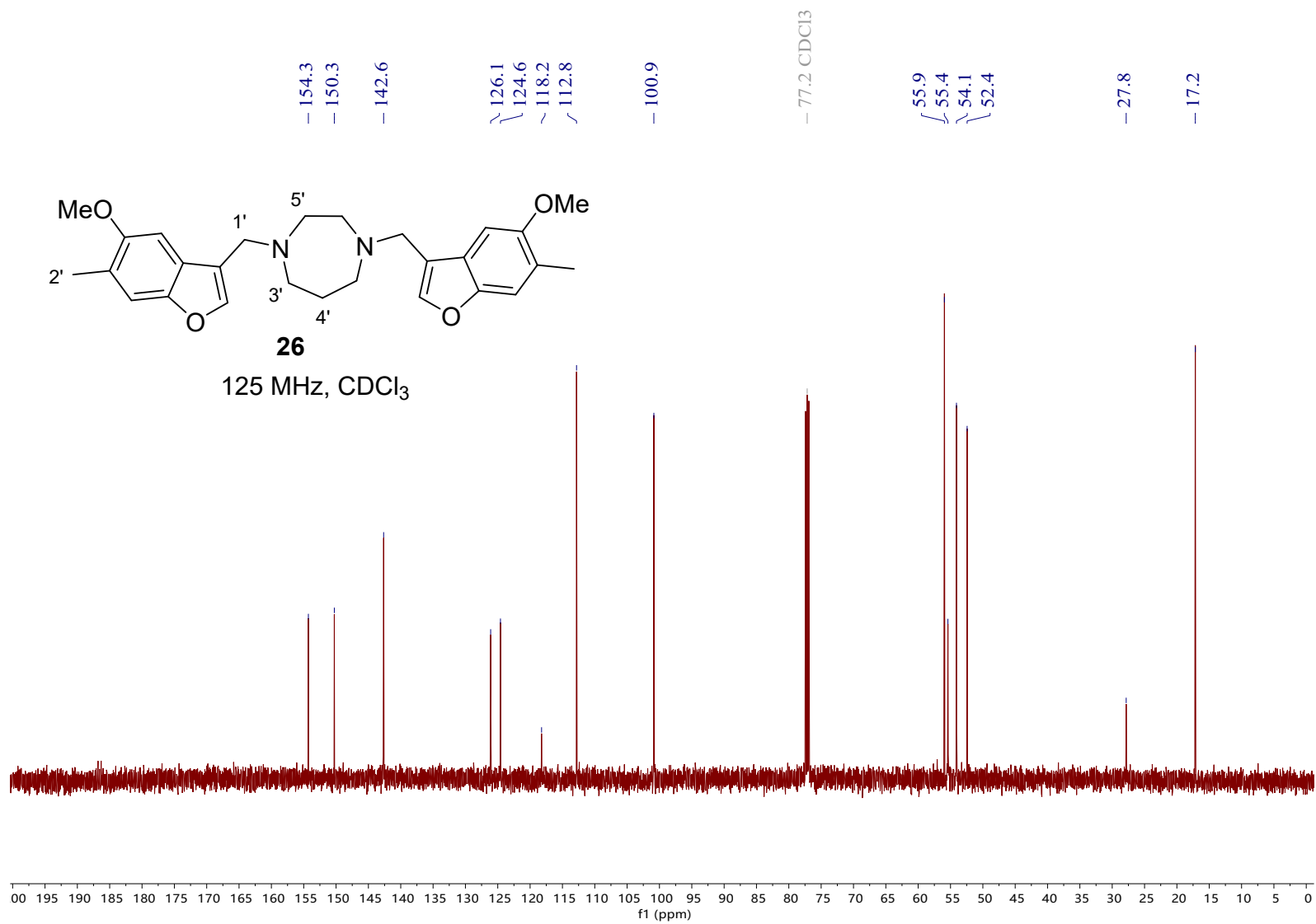
— 154.3  
— 150.2  
— 142.8  
~ 126.2  
~ 124.6  
— 117.3  
— 112.8  
— 100.7  
  
/ 56.0  
/ 53.3  
/ 52.2  
  
— 17.1

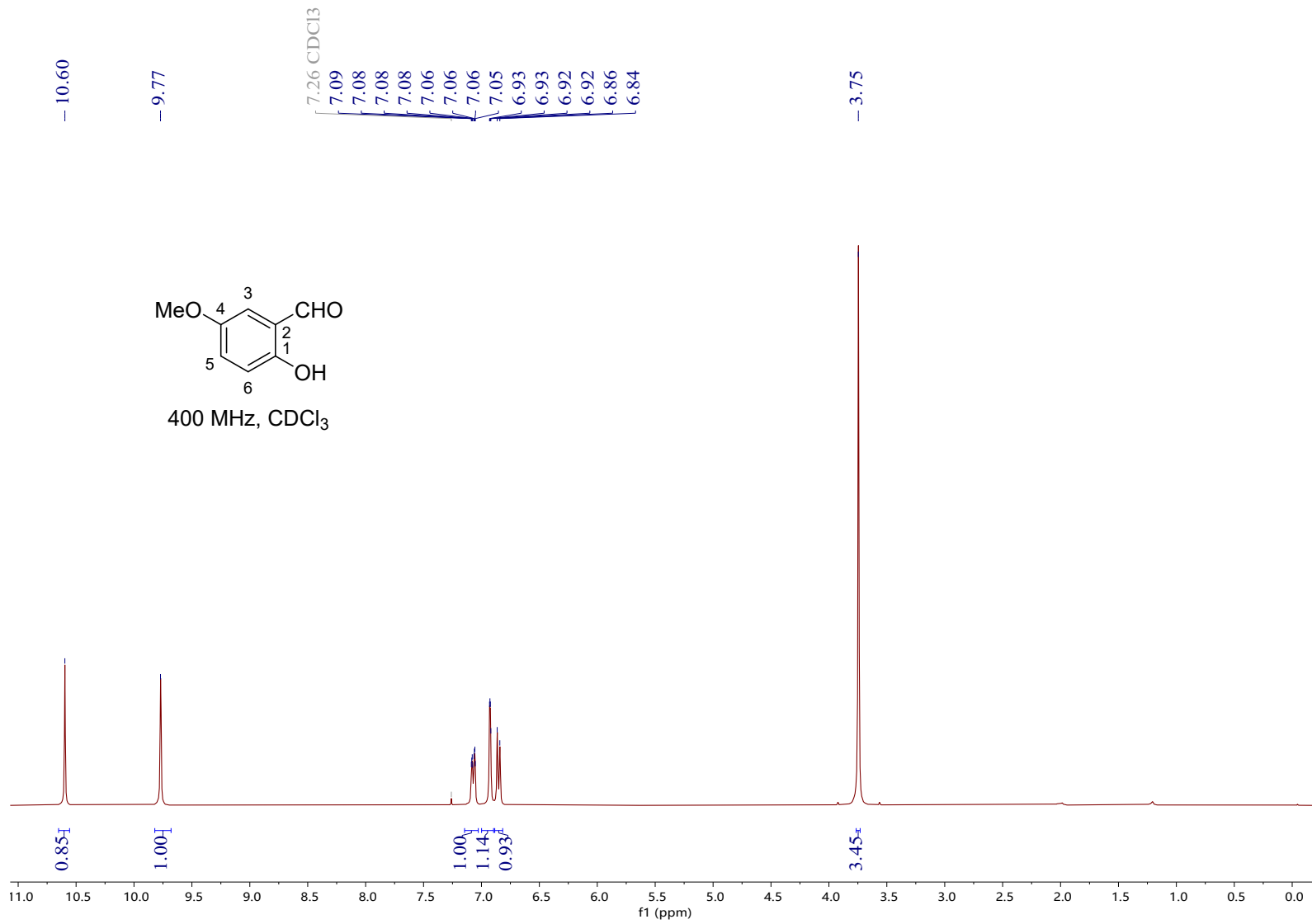


125 MHz, CDCl<sub>3</sub>

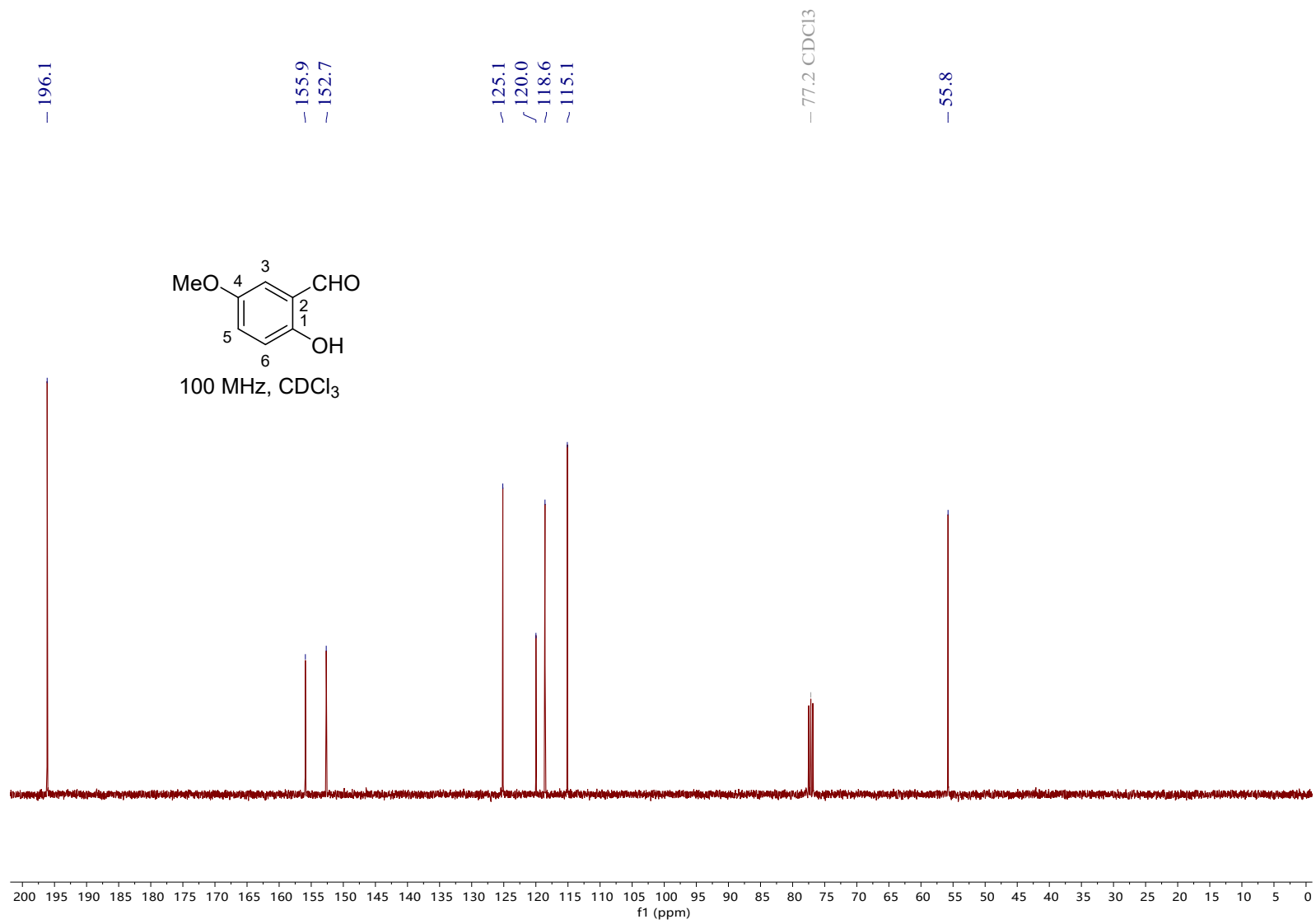


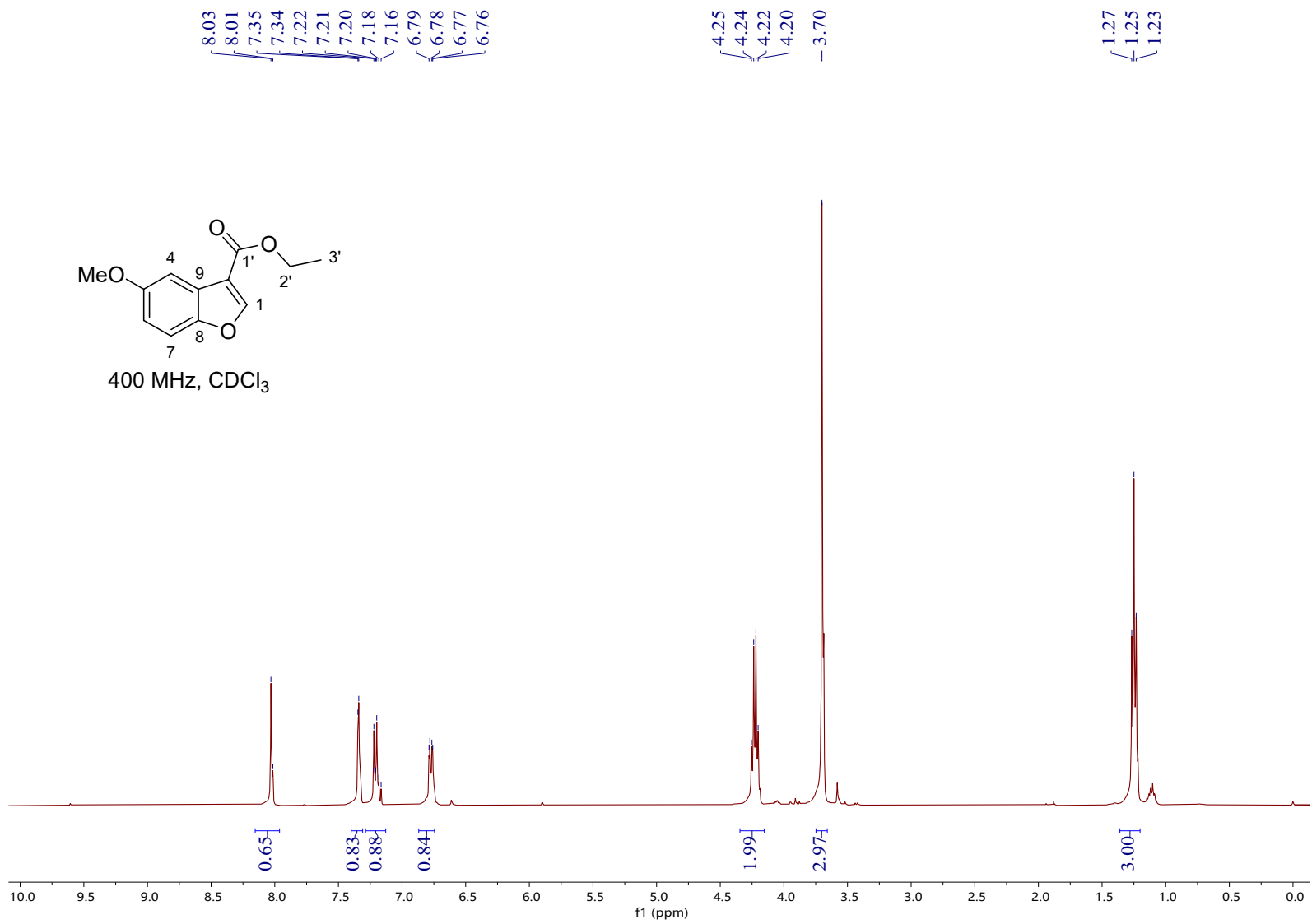


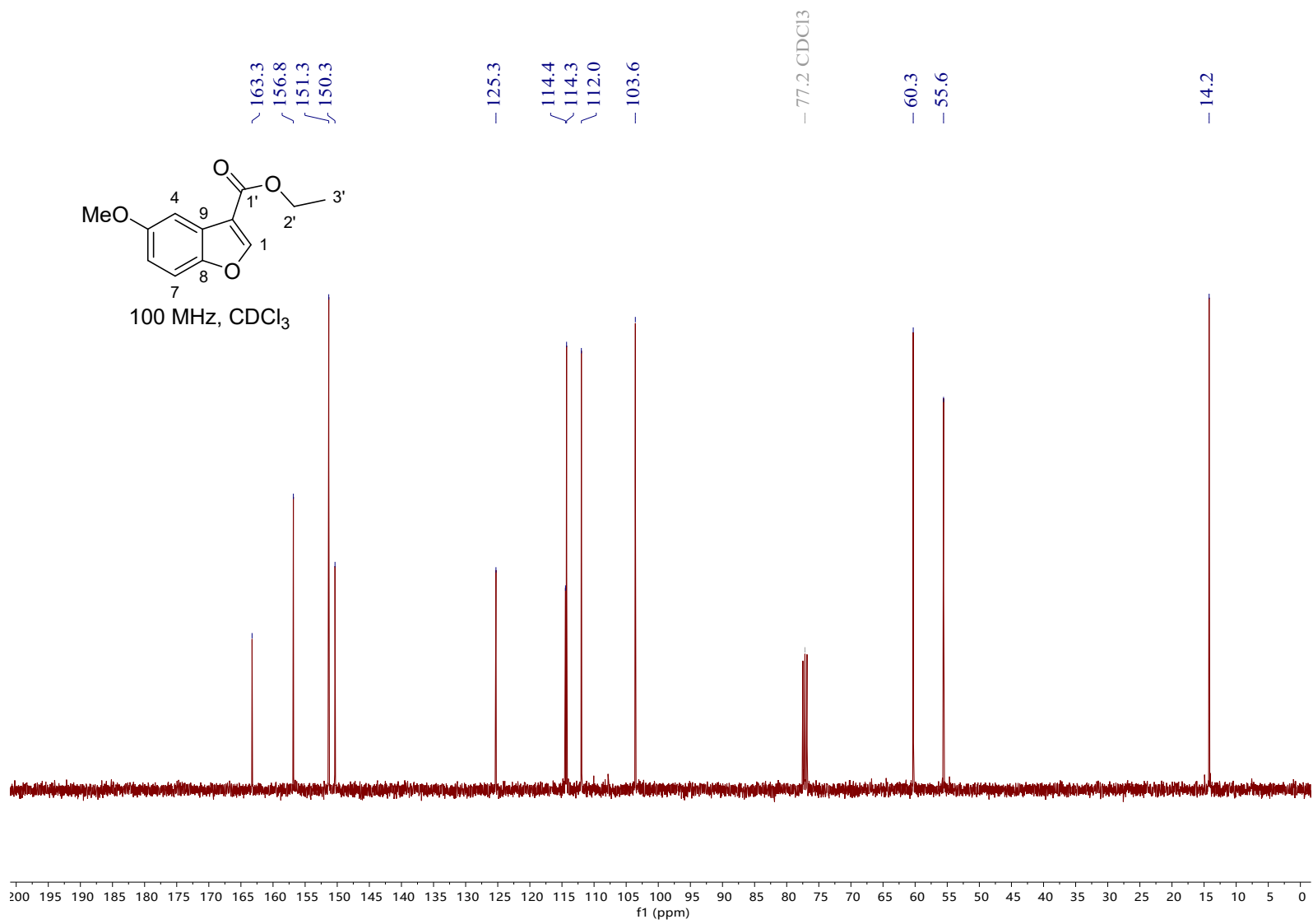


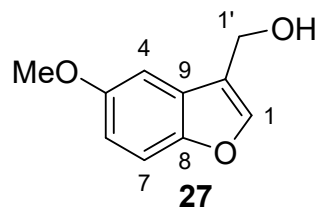




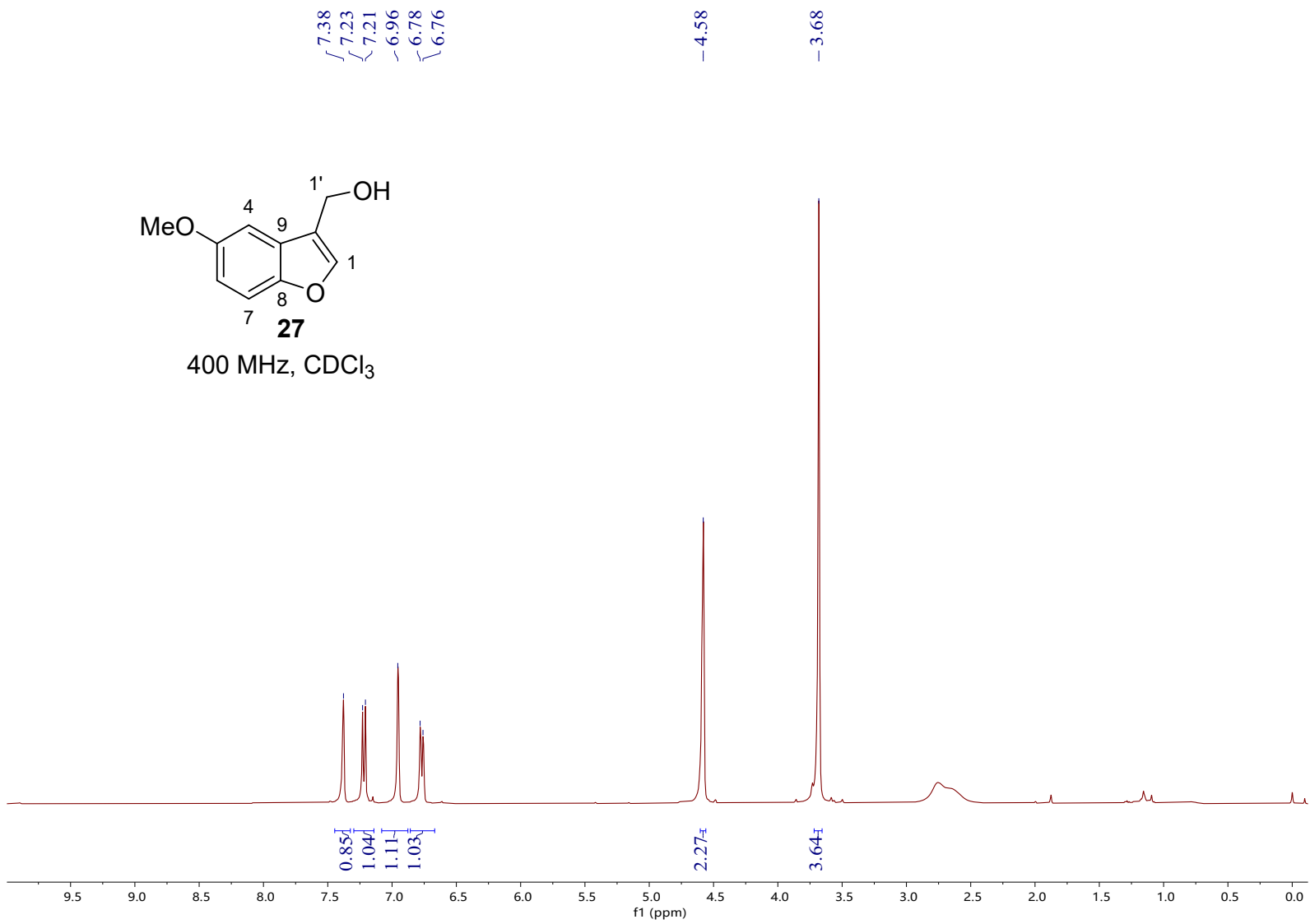


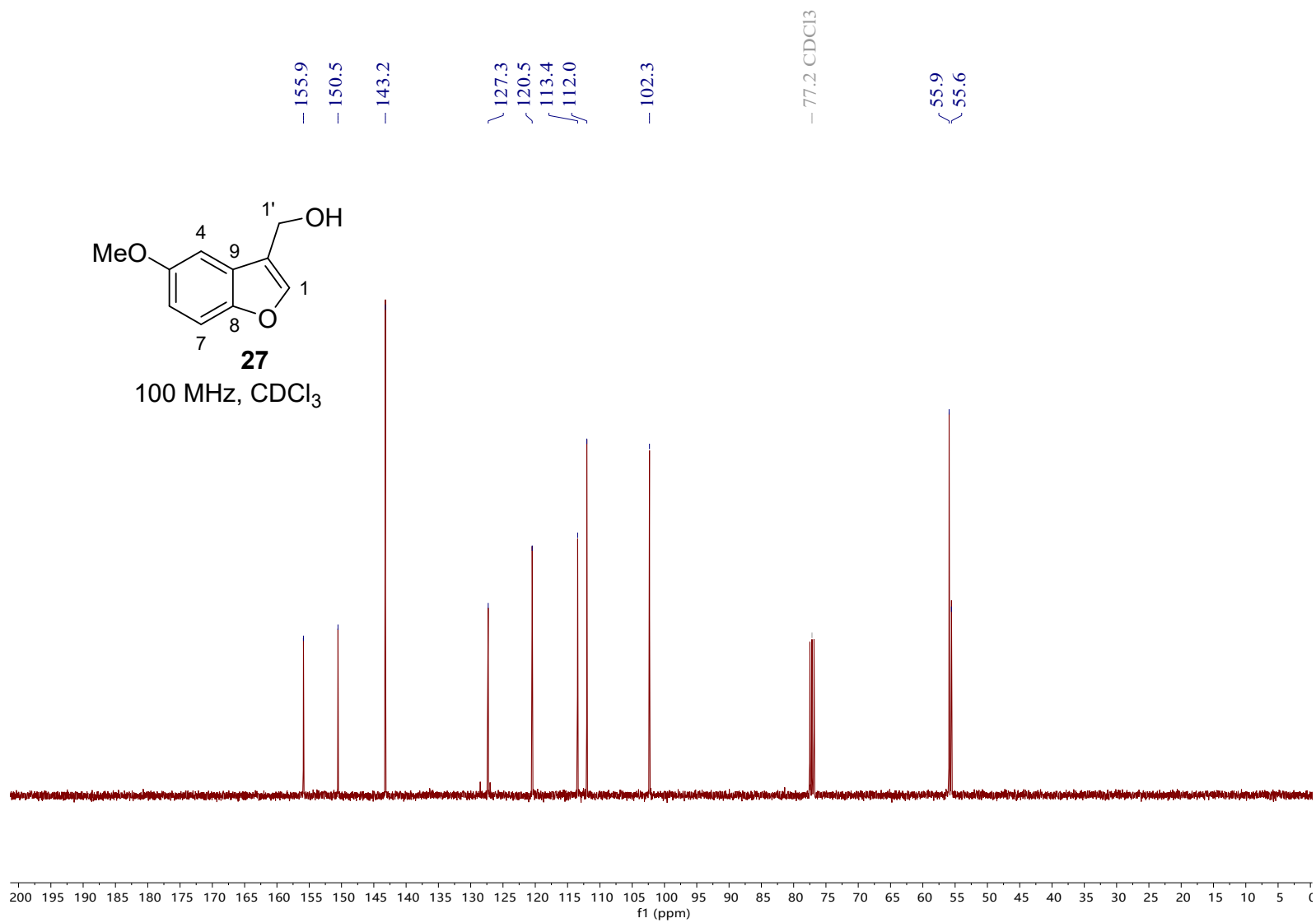


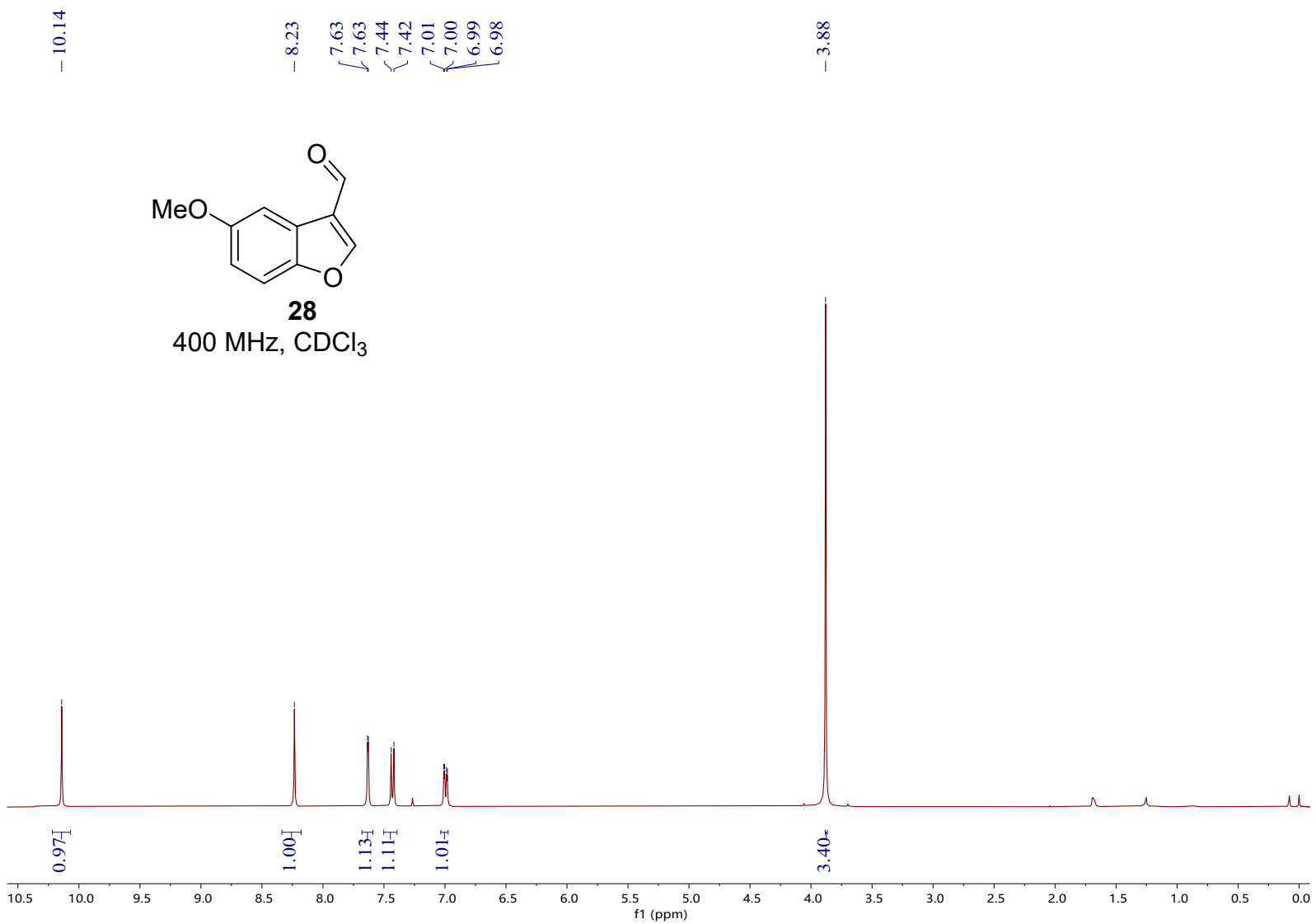


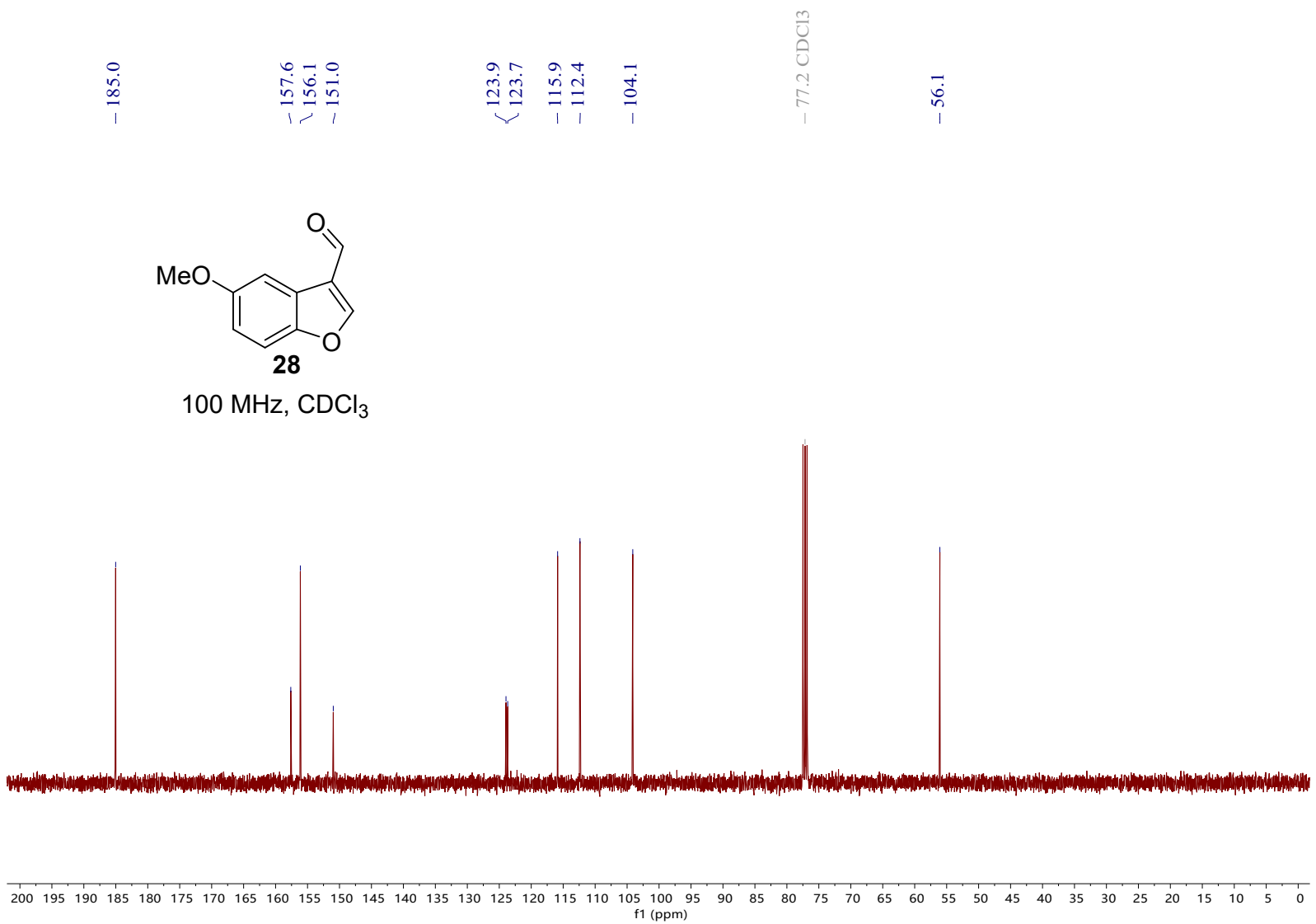


400 MHz, CDCl<sub>3</sub>







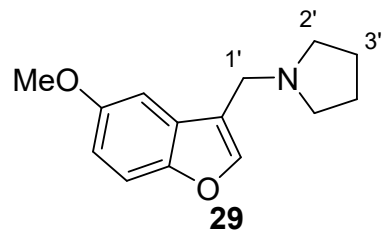


7.50  
7.29  
7.27  
7.05  
7.04  
6.83  
6.83  
6.81  
6.80

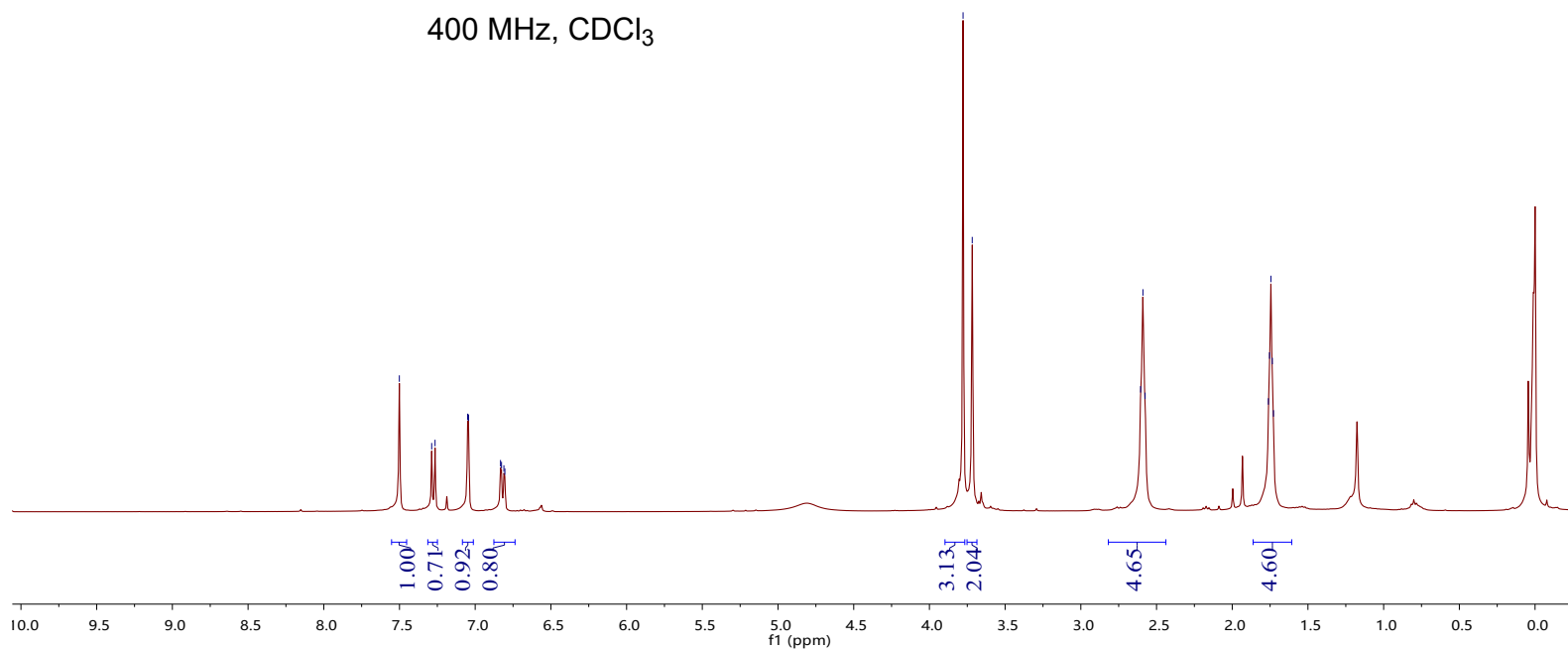
3.78  
3.72

2.61  
2.59  
2.58

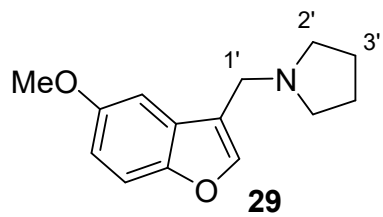
1.76  
1.75  
1.74  
1.74  
1.73



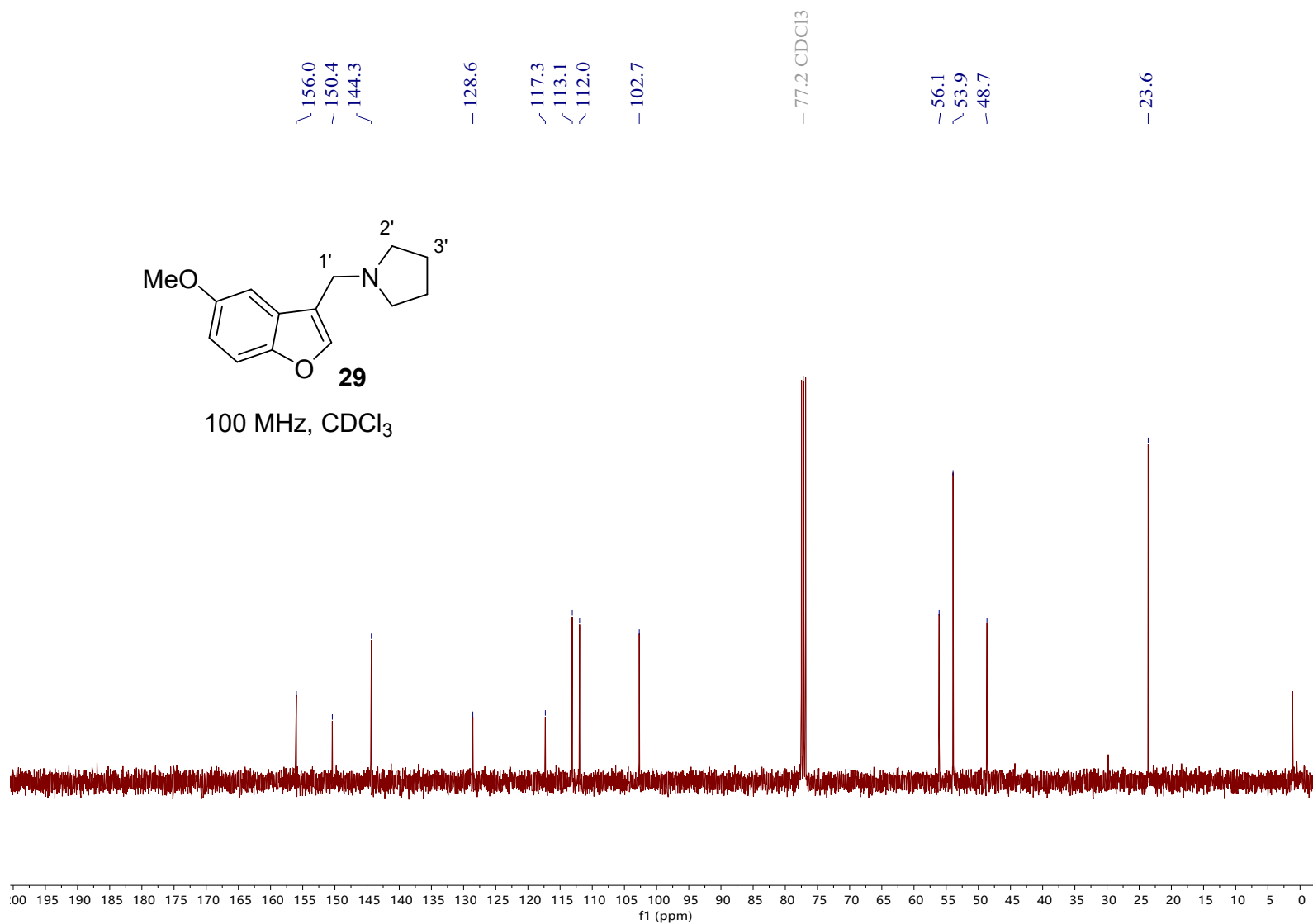
400 MHz, CDCl<sub>3</sub>

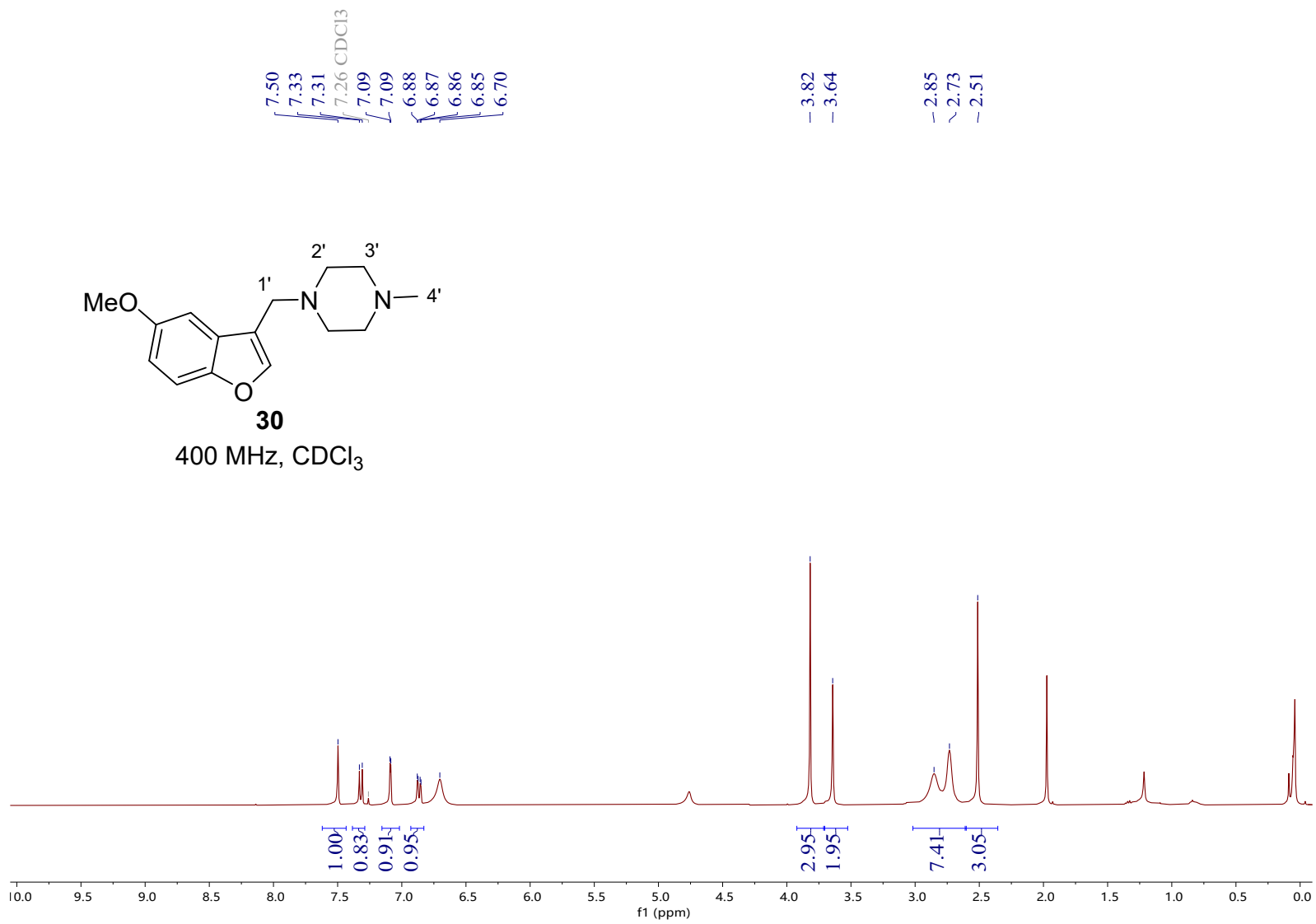


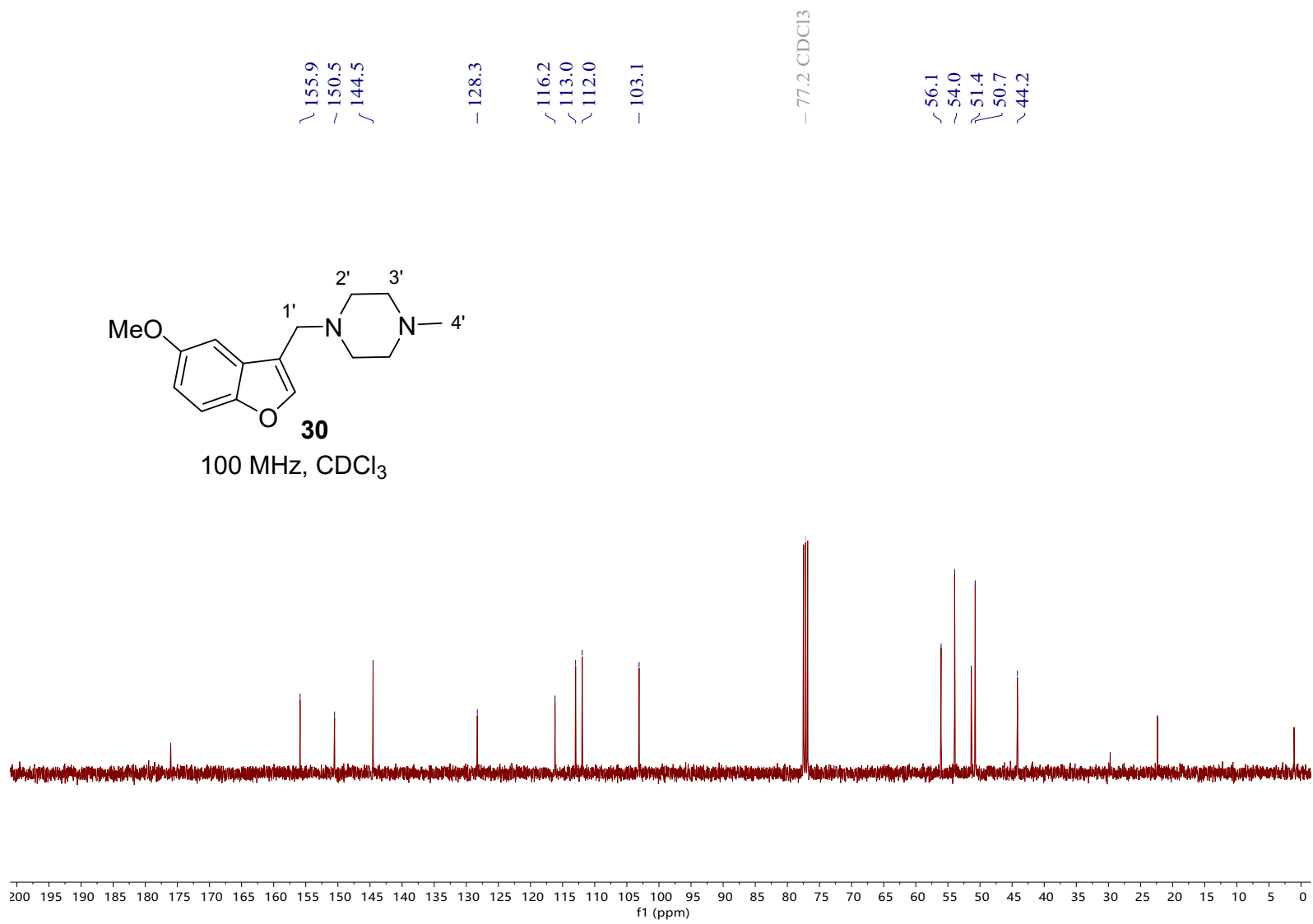


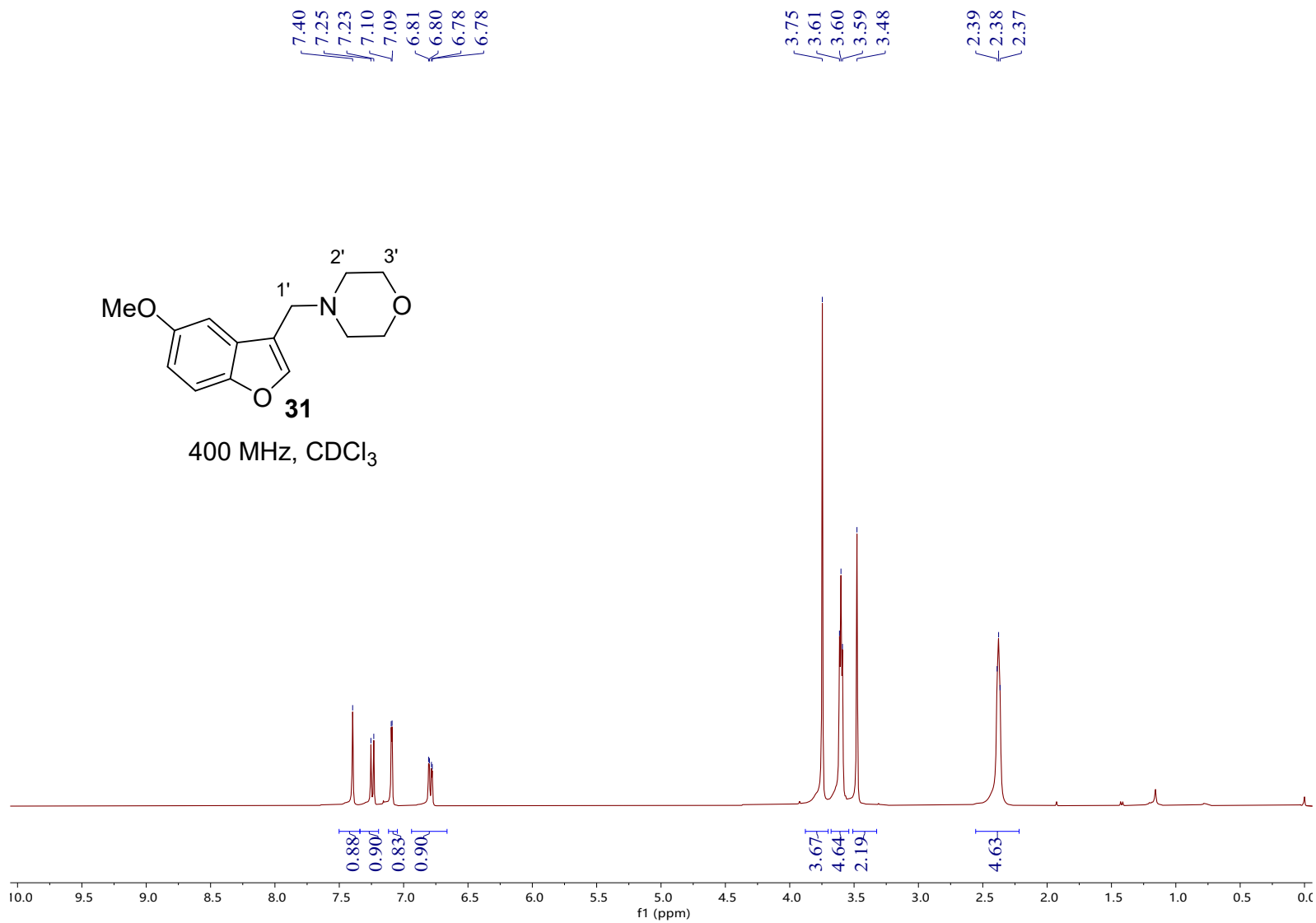


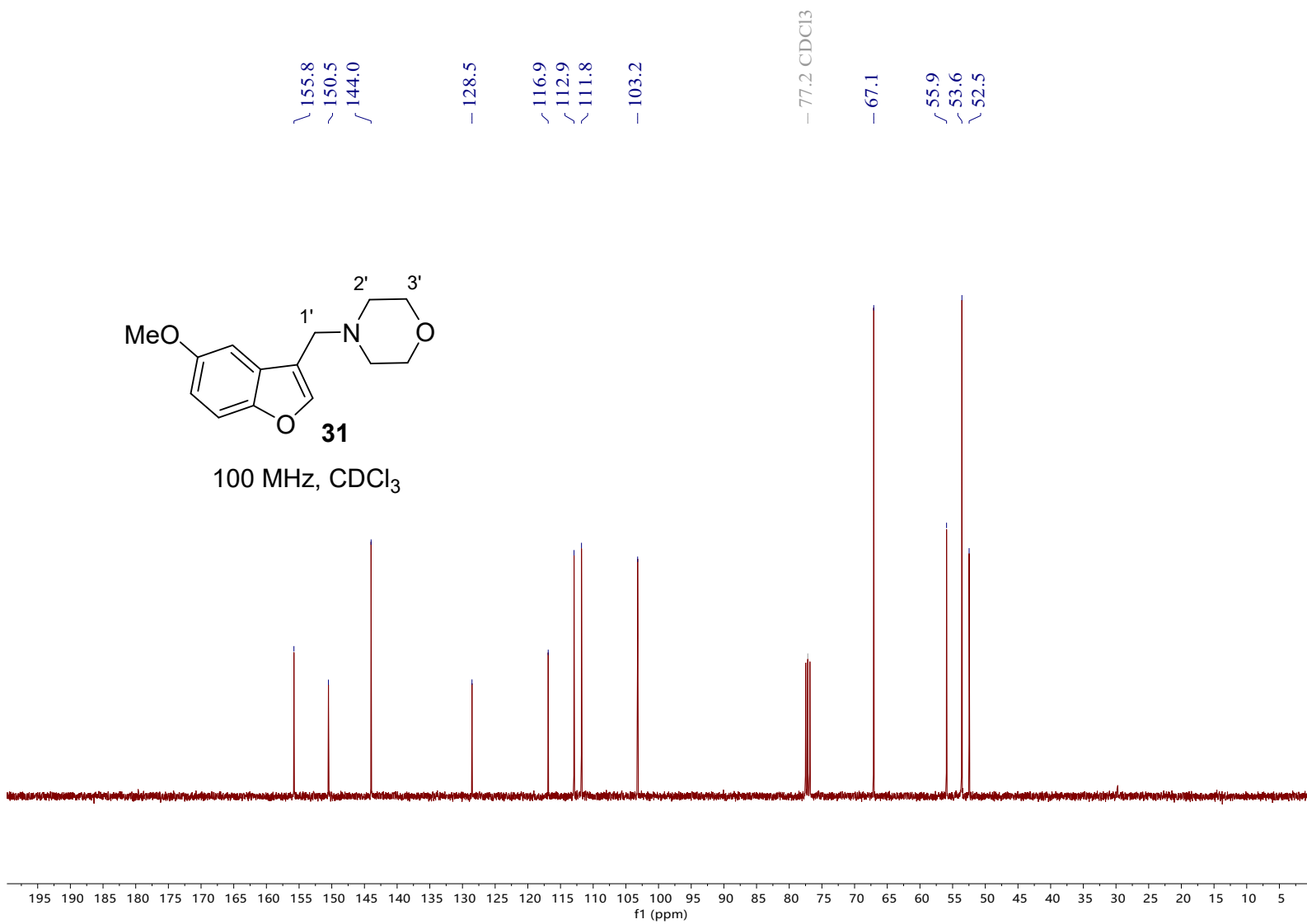
100 MHz, CDCl<sub>3</sub>

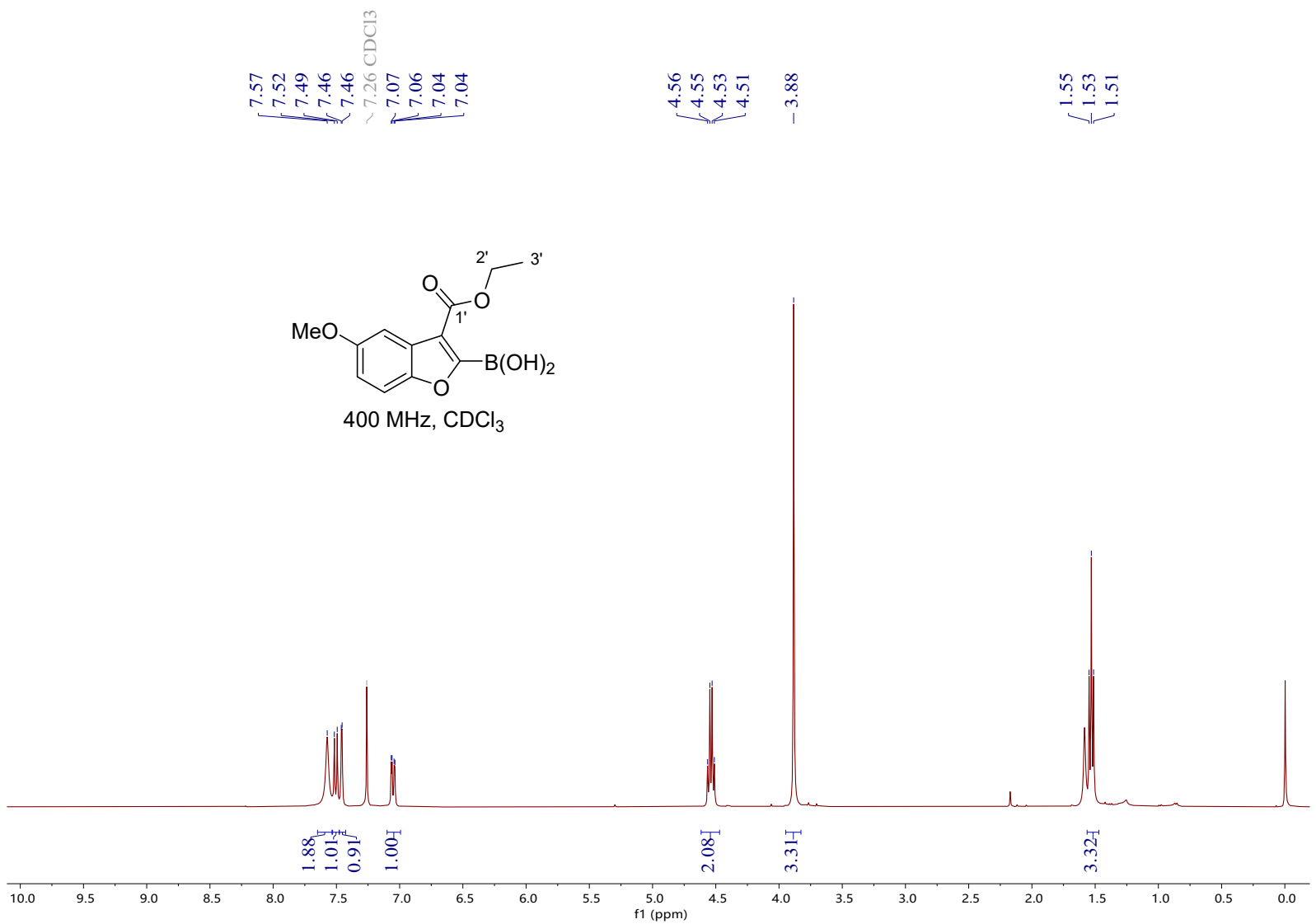


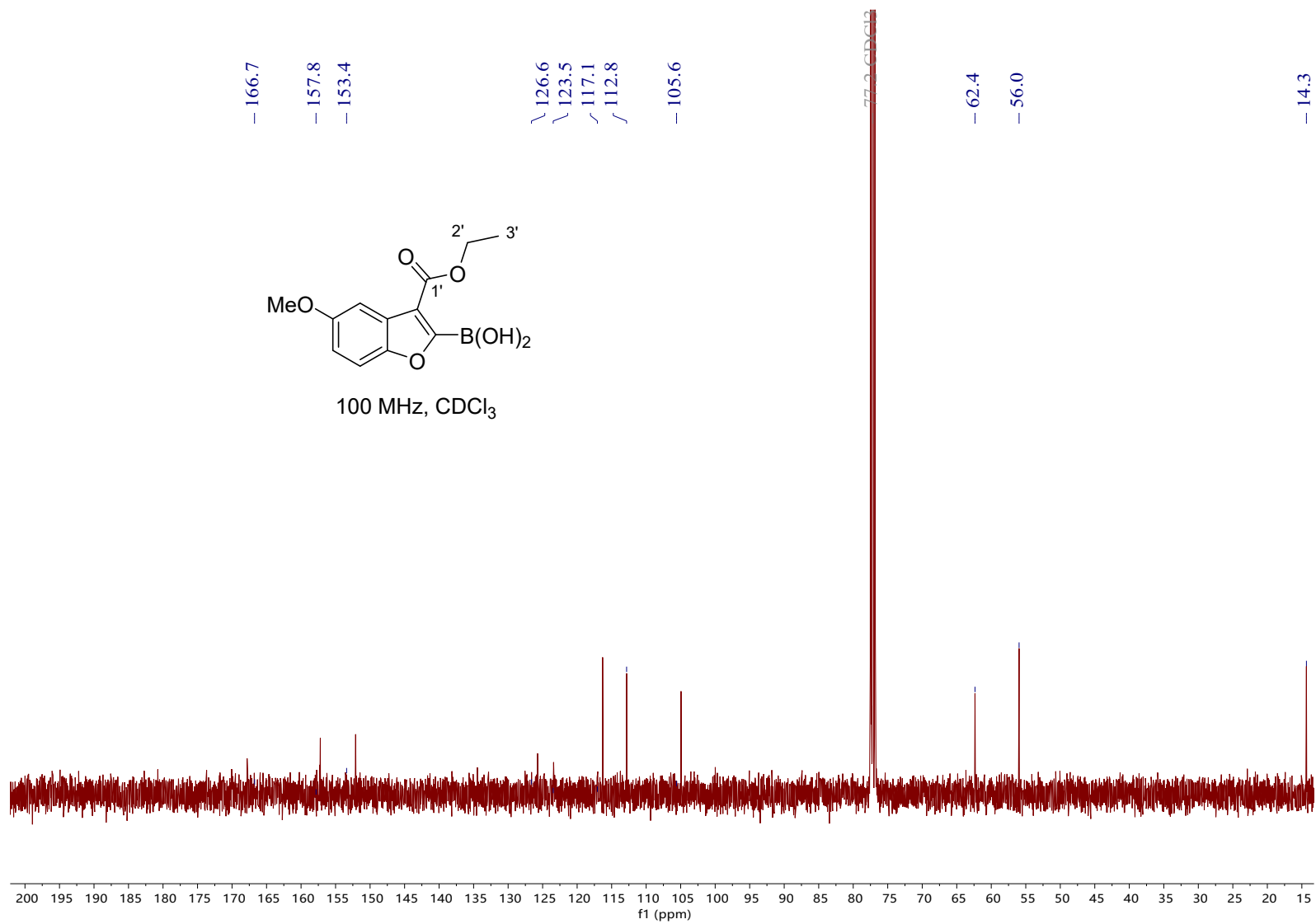


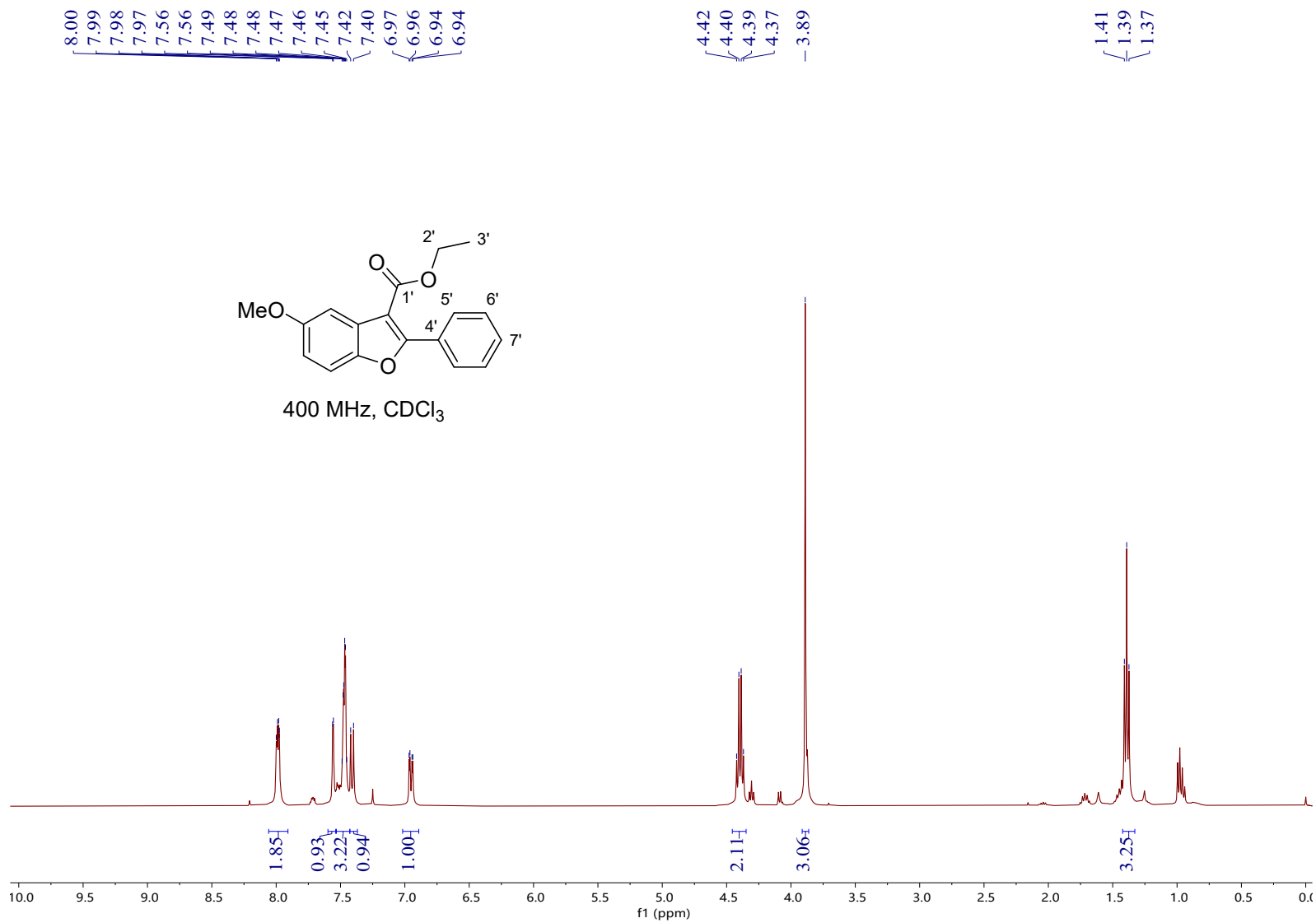














- 164.2  
~ 161.5  
- 157.0  
- 149.0

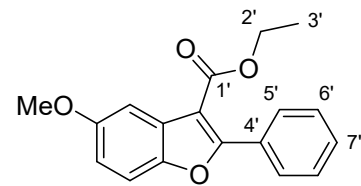
{ 130.3  
129.9  
129.6  
128.1 }

~ 114.3  
~ 111.8  
~ 109.1  
~ 105.0

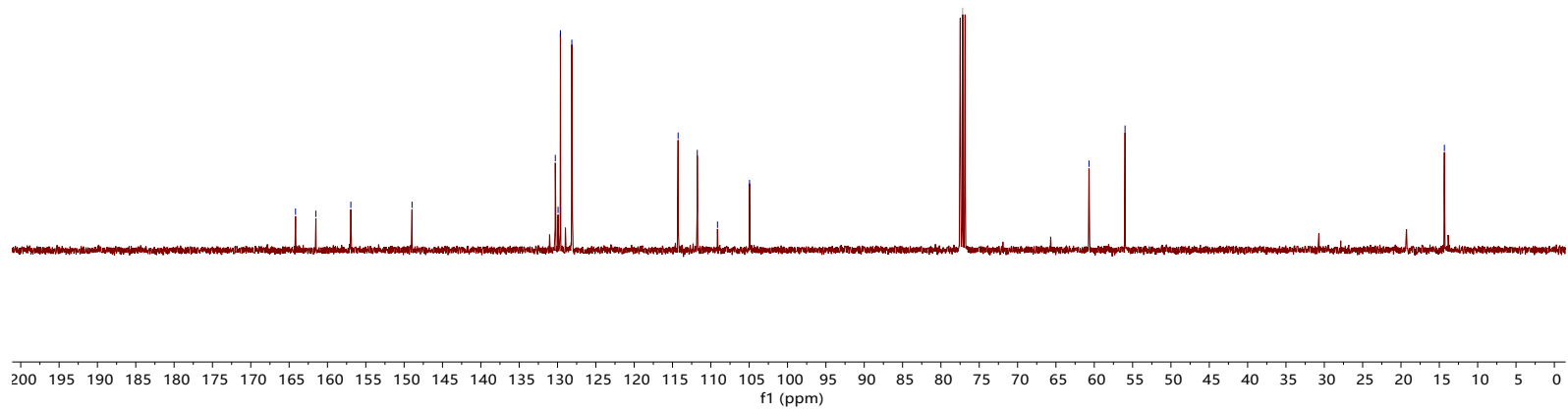
- 77.2 CDCl<sub>3</sub>

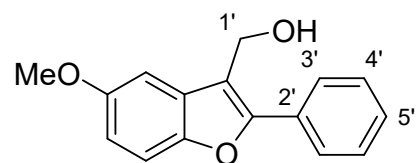
- 60.7  
- 56.0

- 14.3



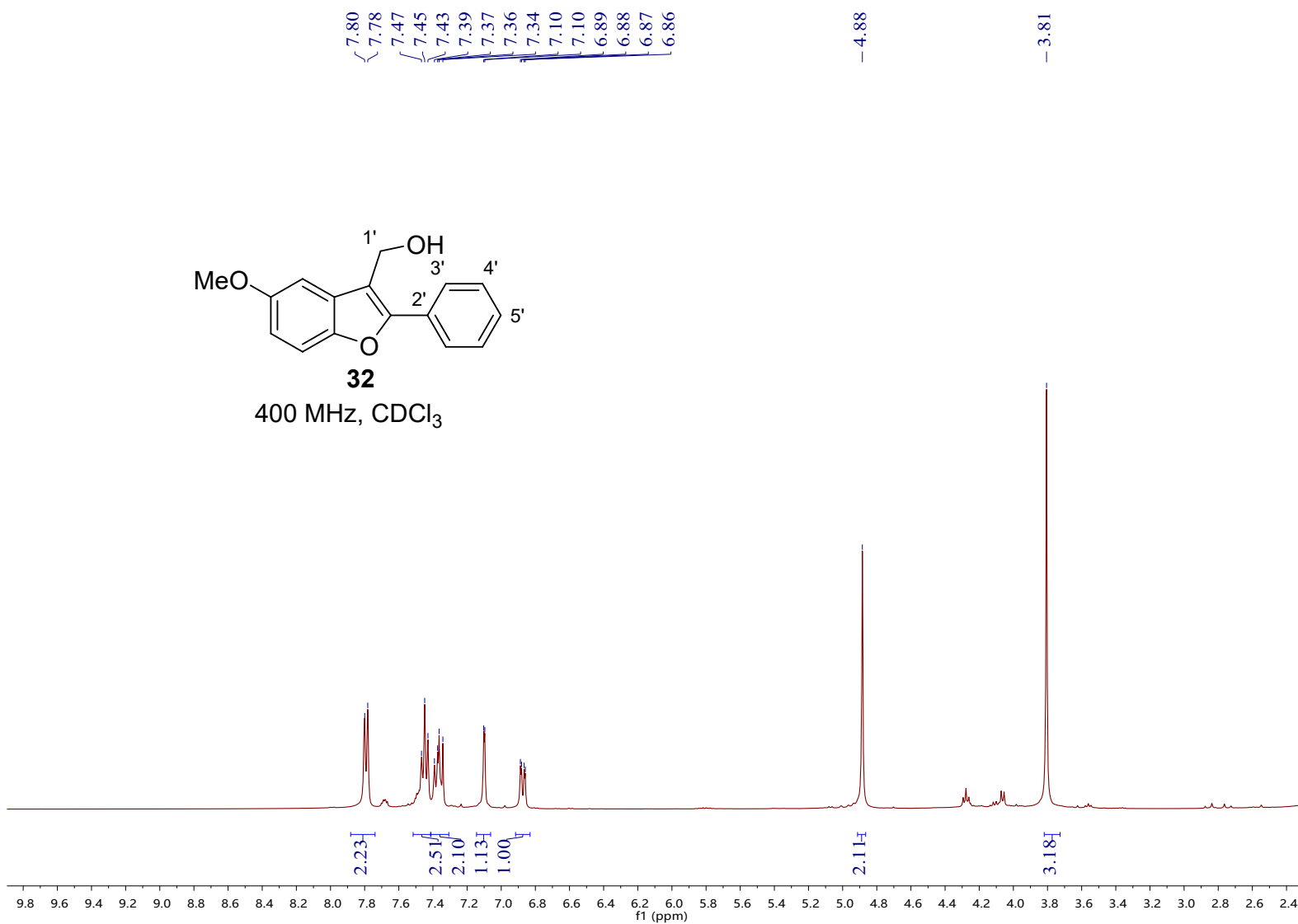
100 MHz, CDCl<sub>3</sub>

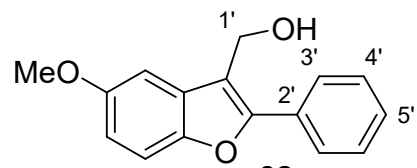




**32**

400 MHz, CDCl<sub>3</sub>





**32**

100 MHz, CDCl<sub>3</sub>

- 156.5  
- 154.3  
- 149.0

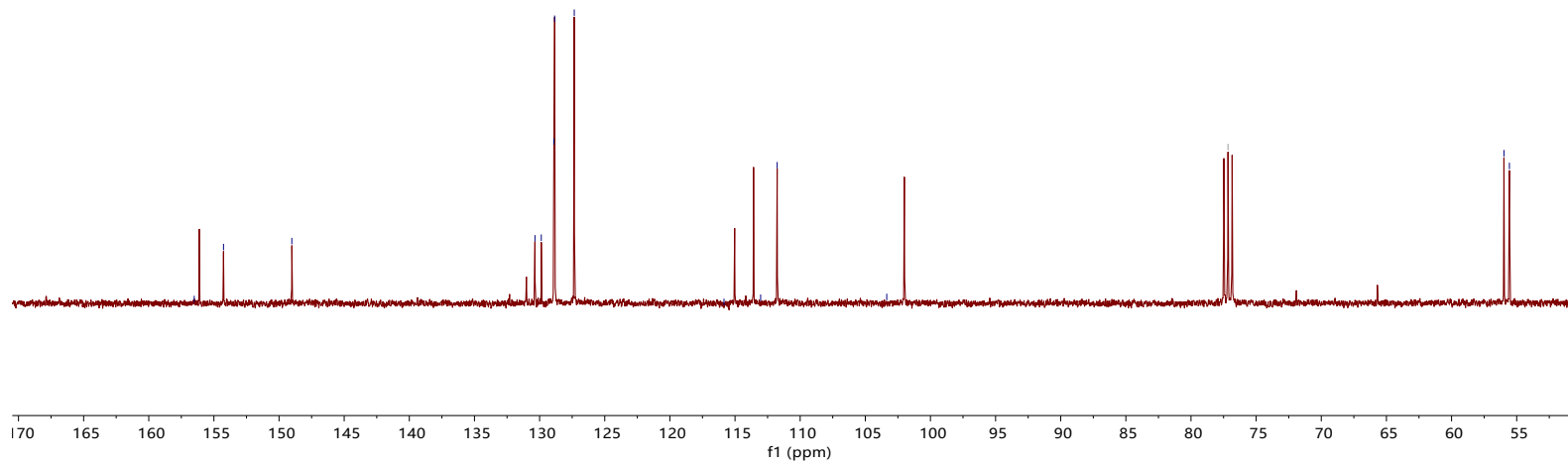
- 130.4  
- 129.9  
- 128.9  
- 128.8  
- 127.3

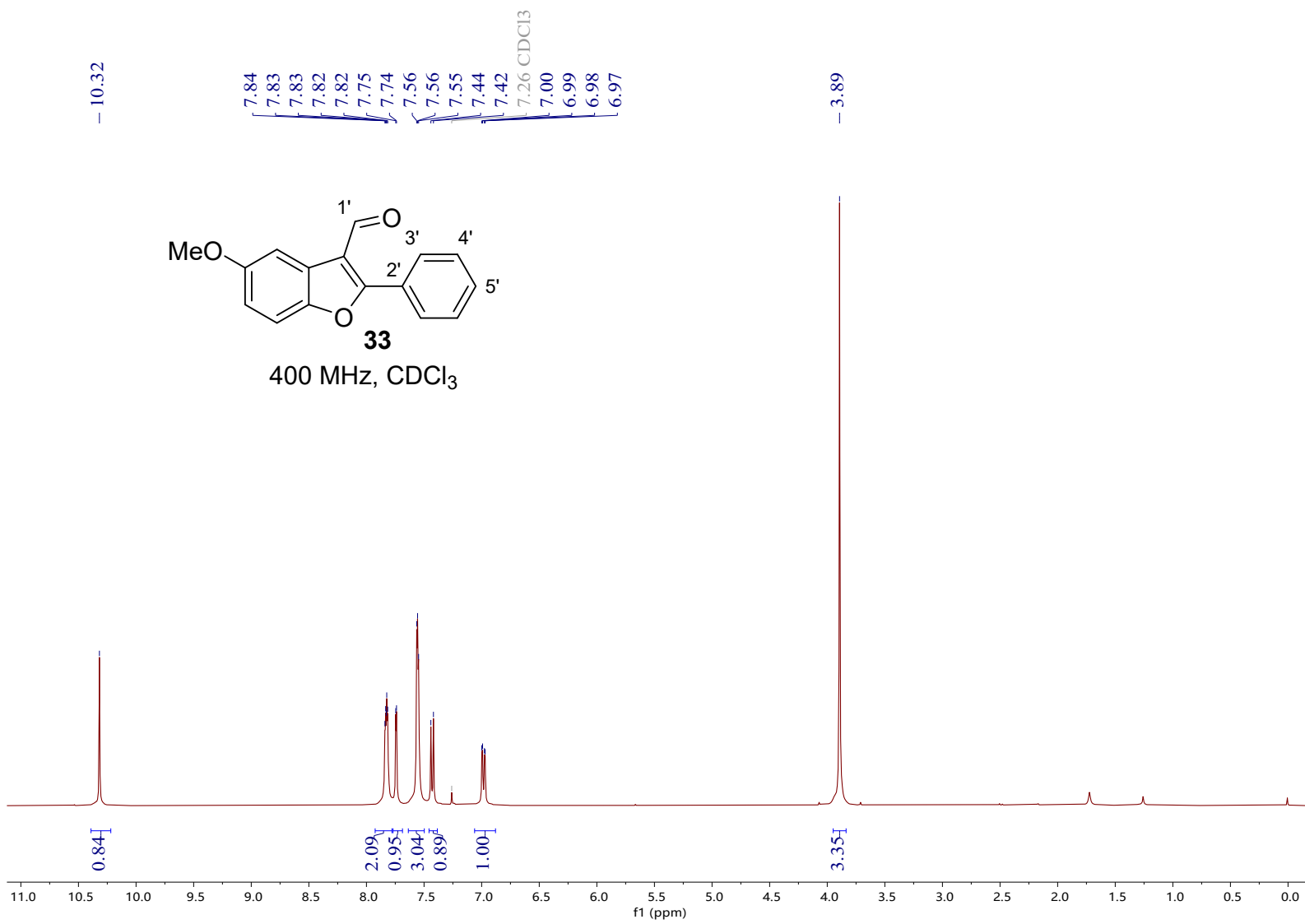
- 115.8  
- 113.0  
- 111.8

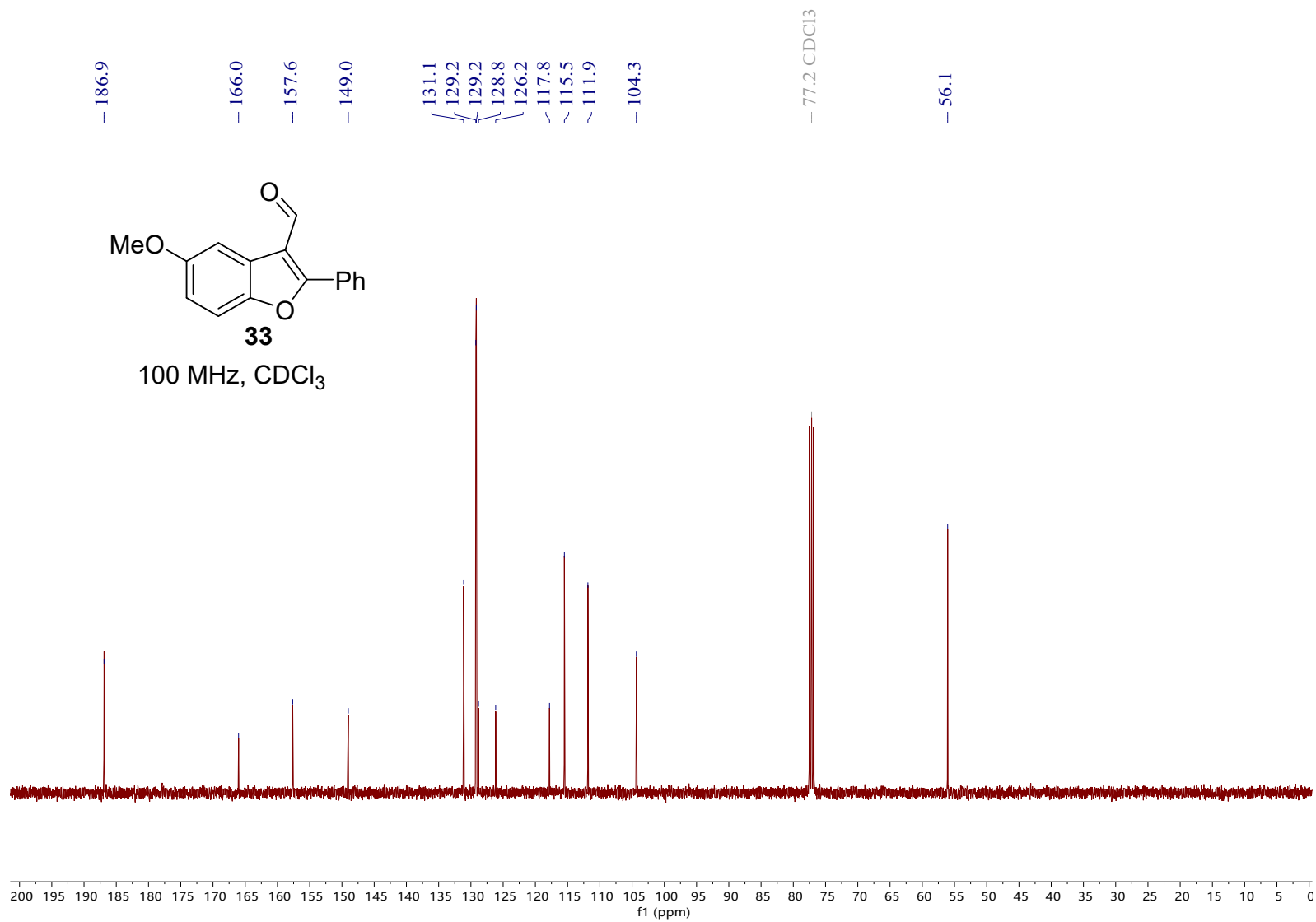
- 103.4

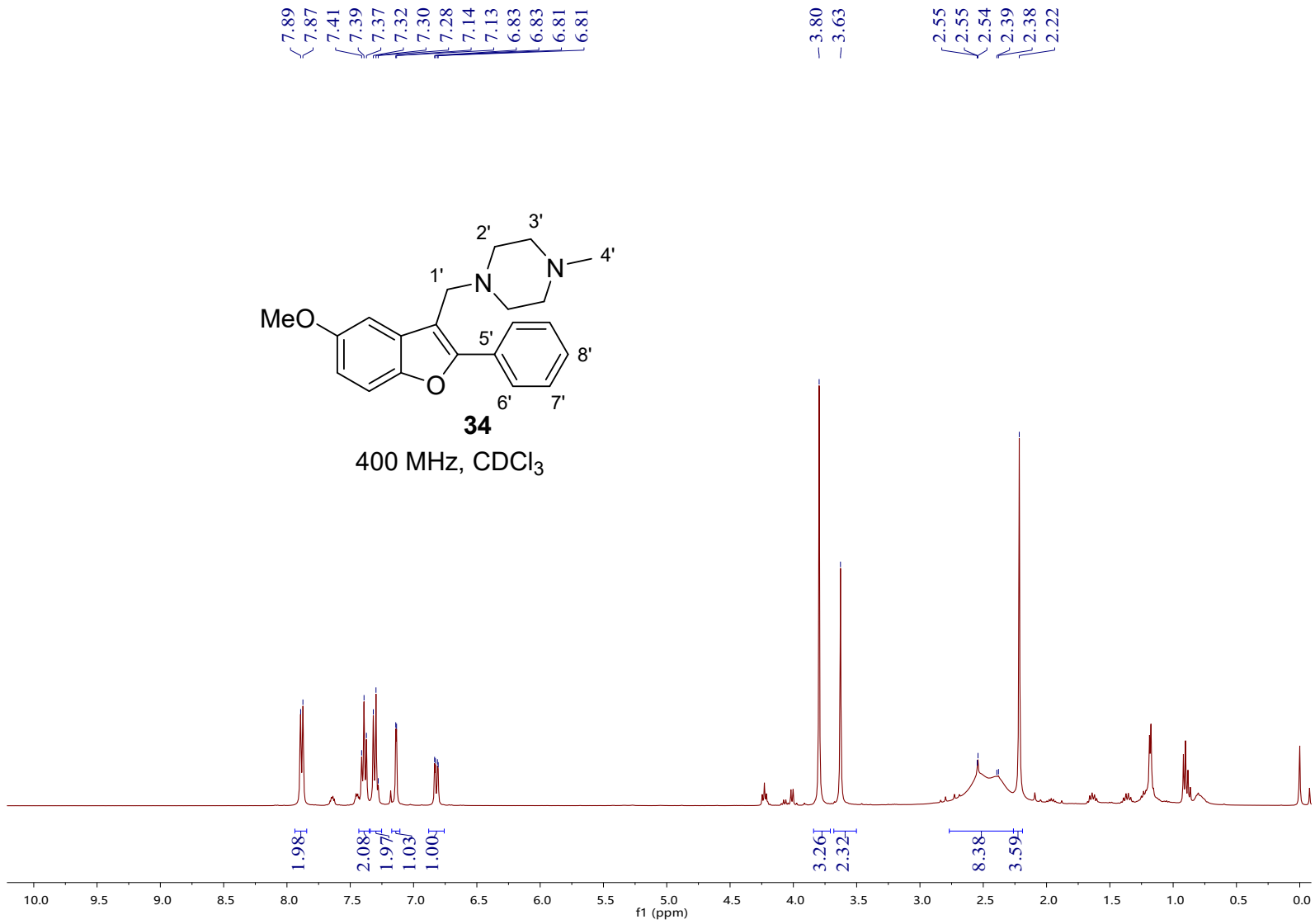
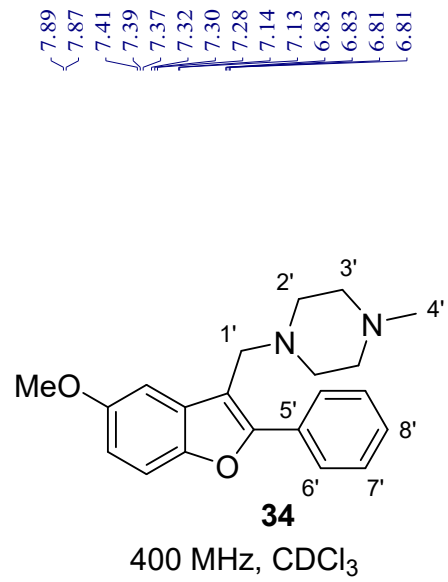
- 77.2 CDCl<sub>3</sub>

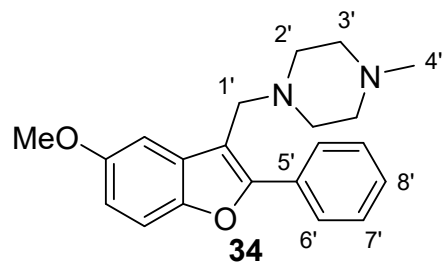
- 56.0  
- 55.6



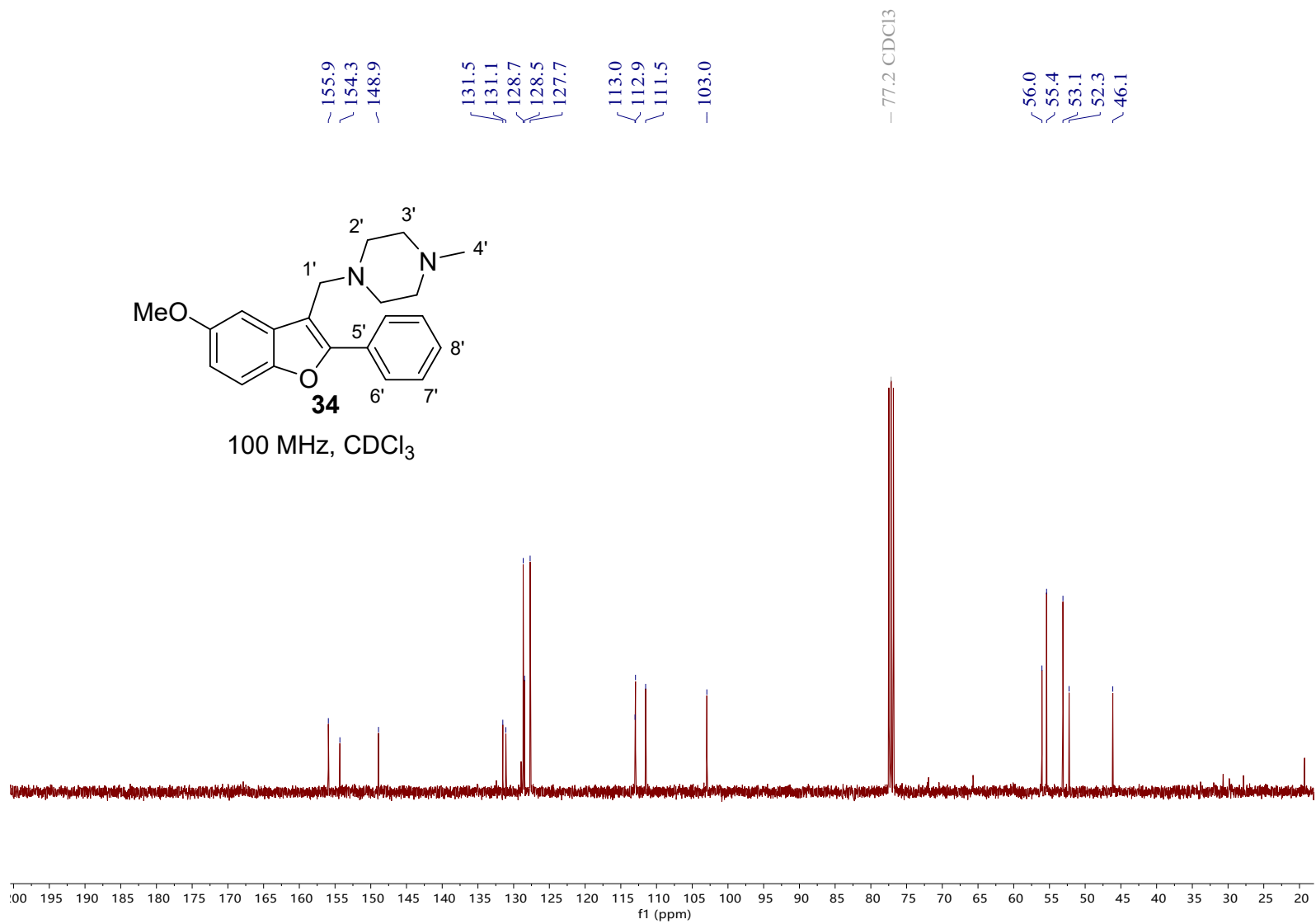


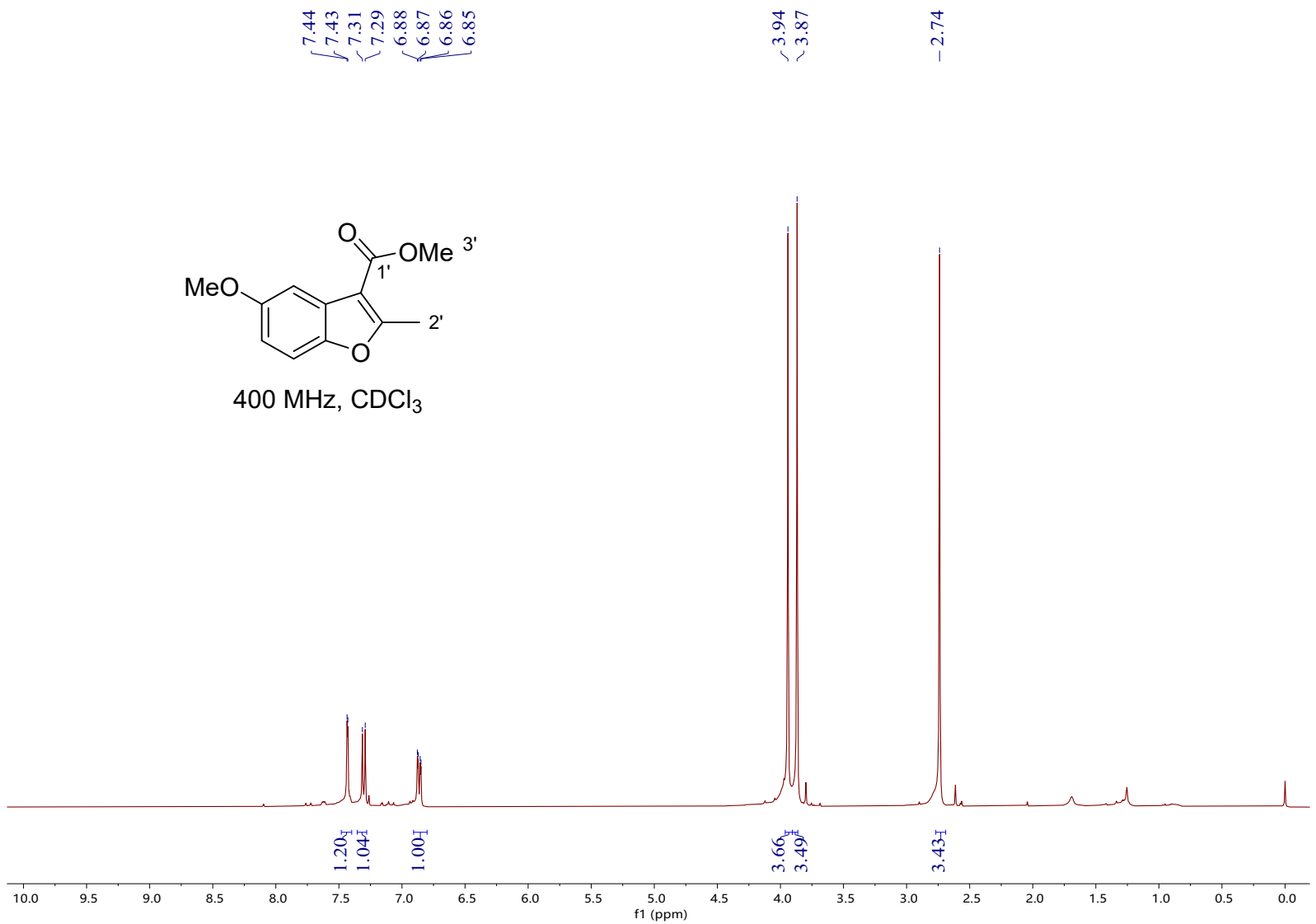




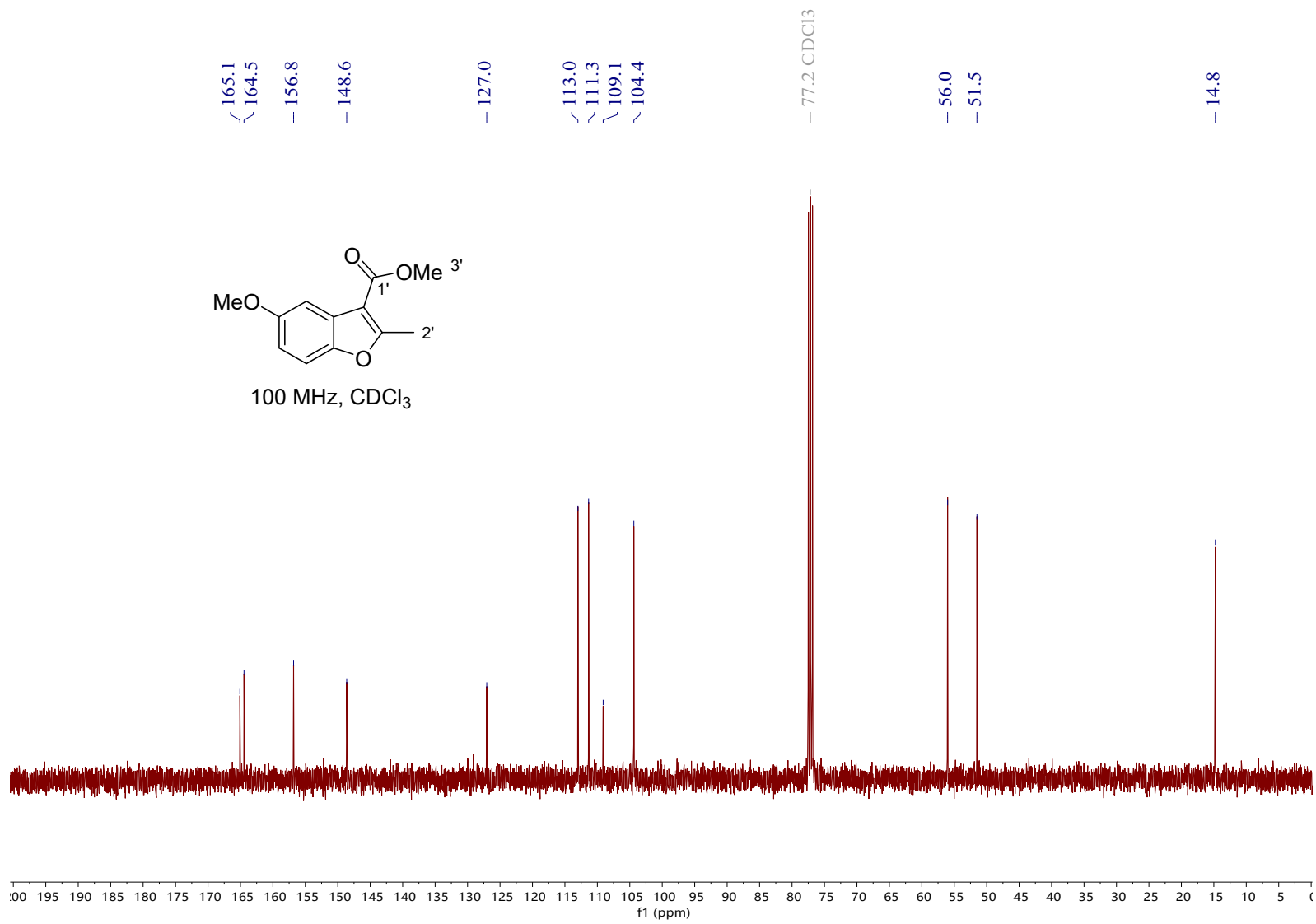


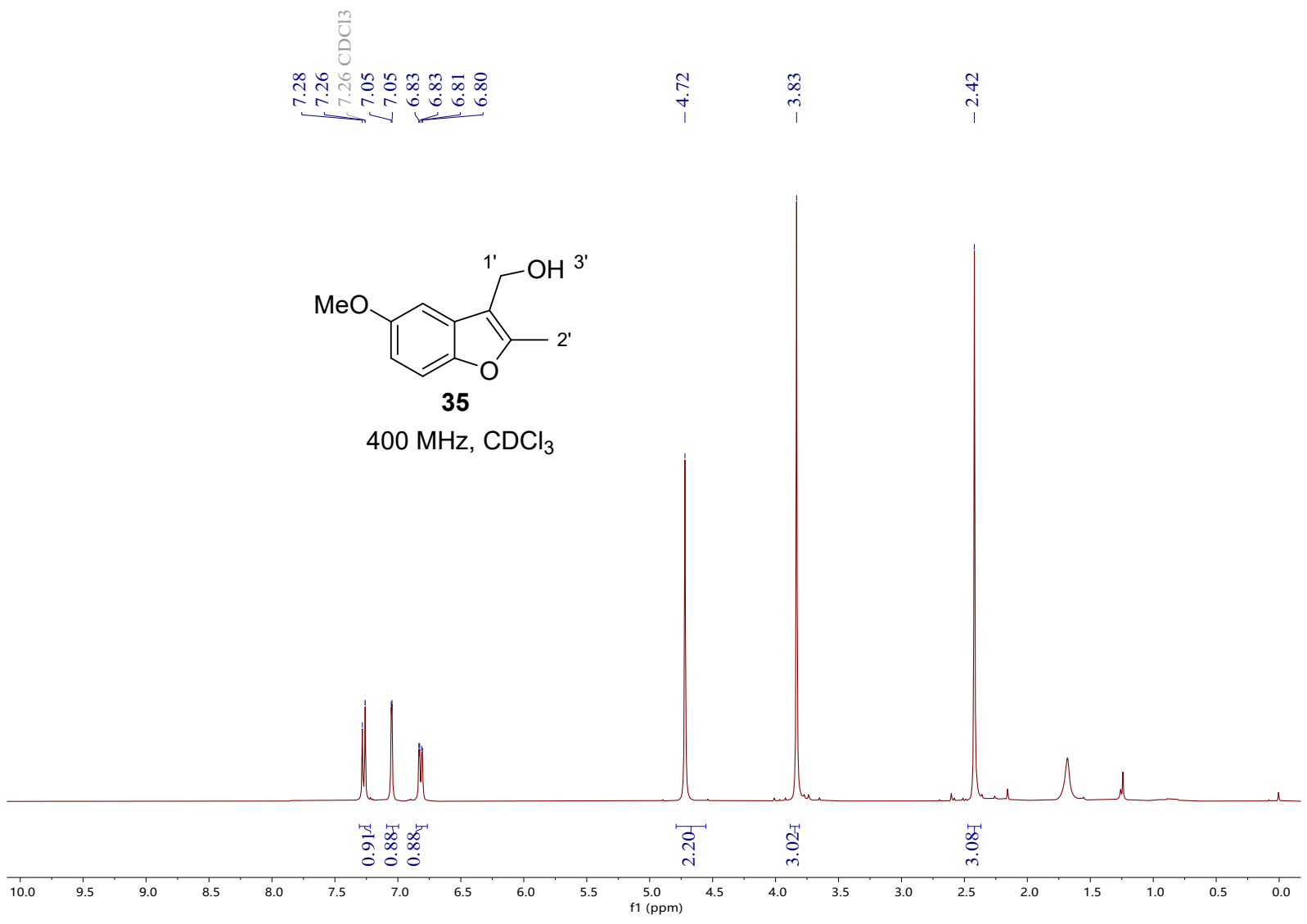
100 MHz, CDCl<sub>3</sub>

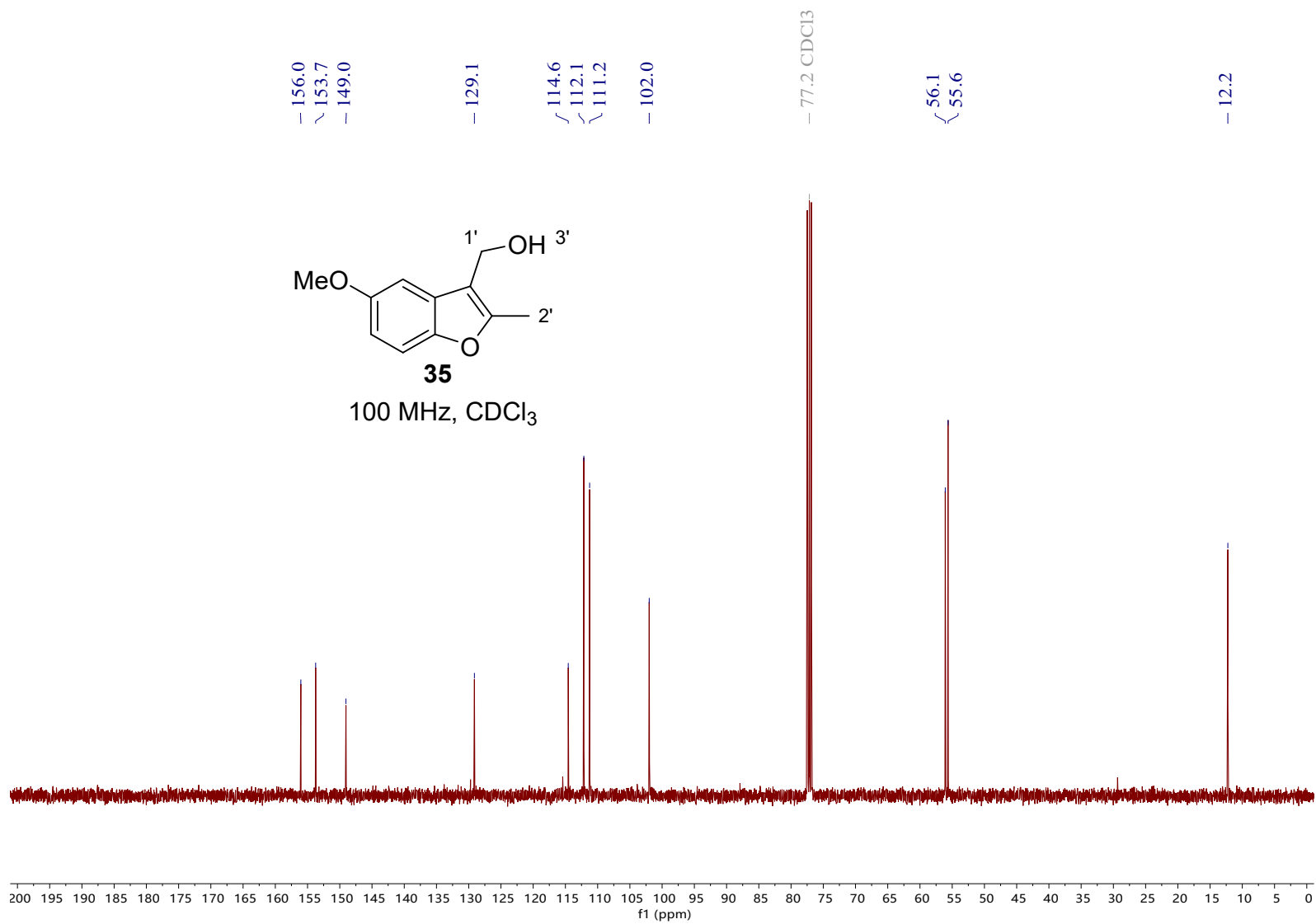


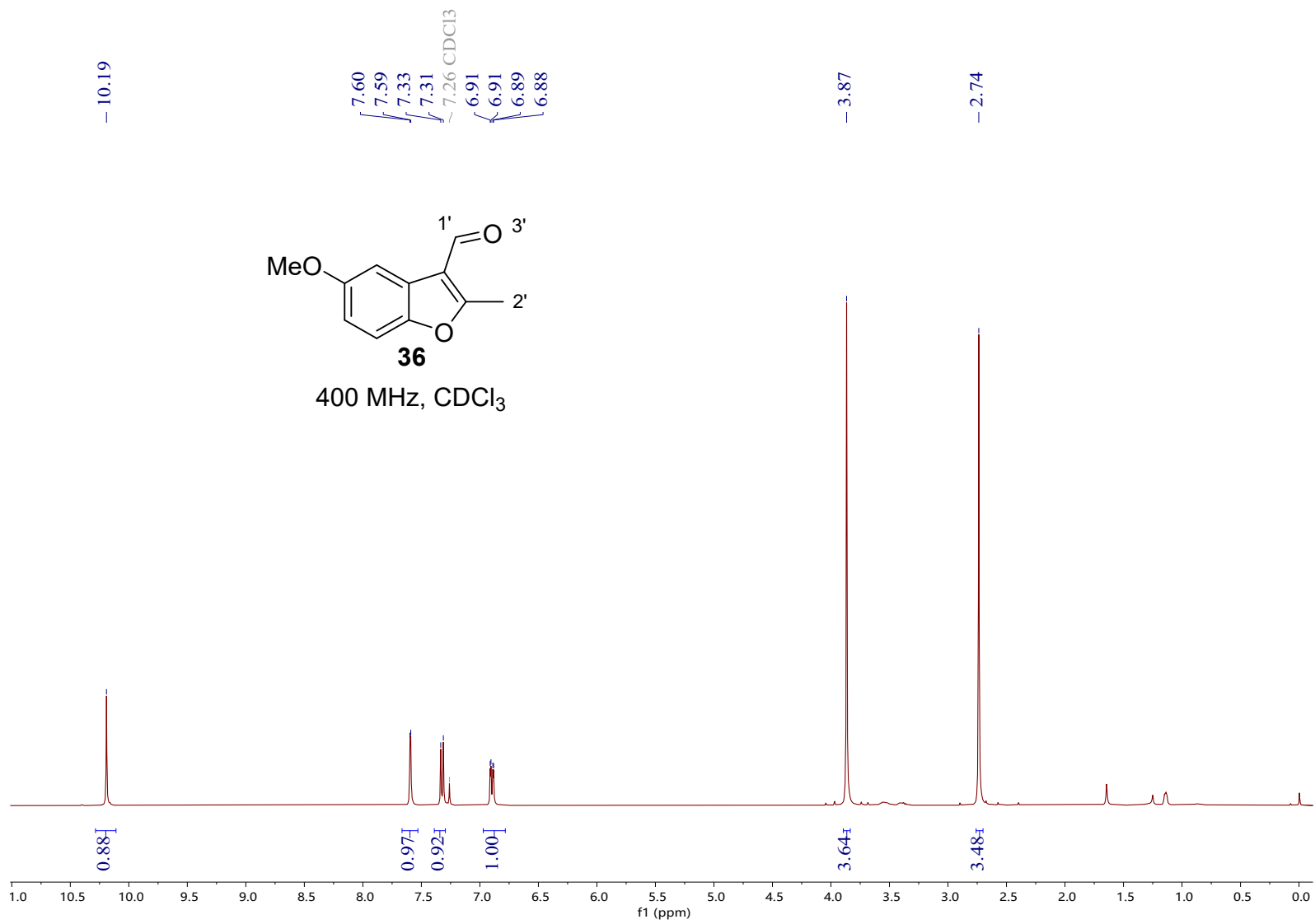


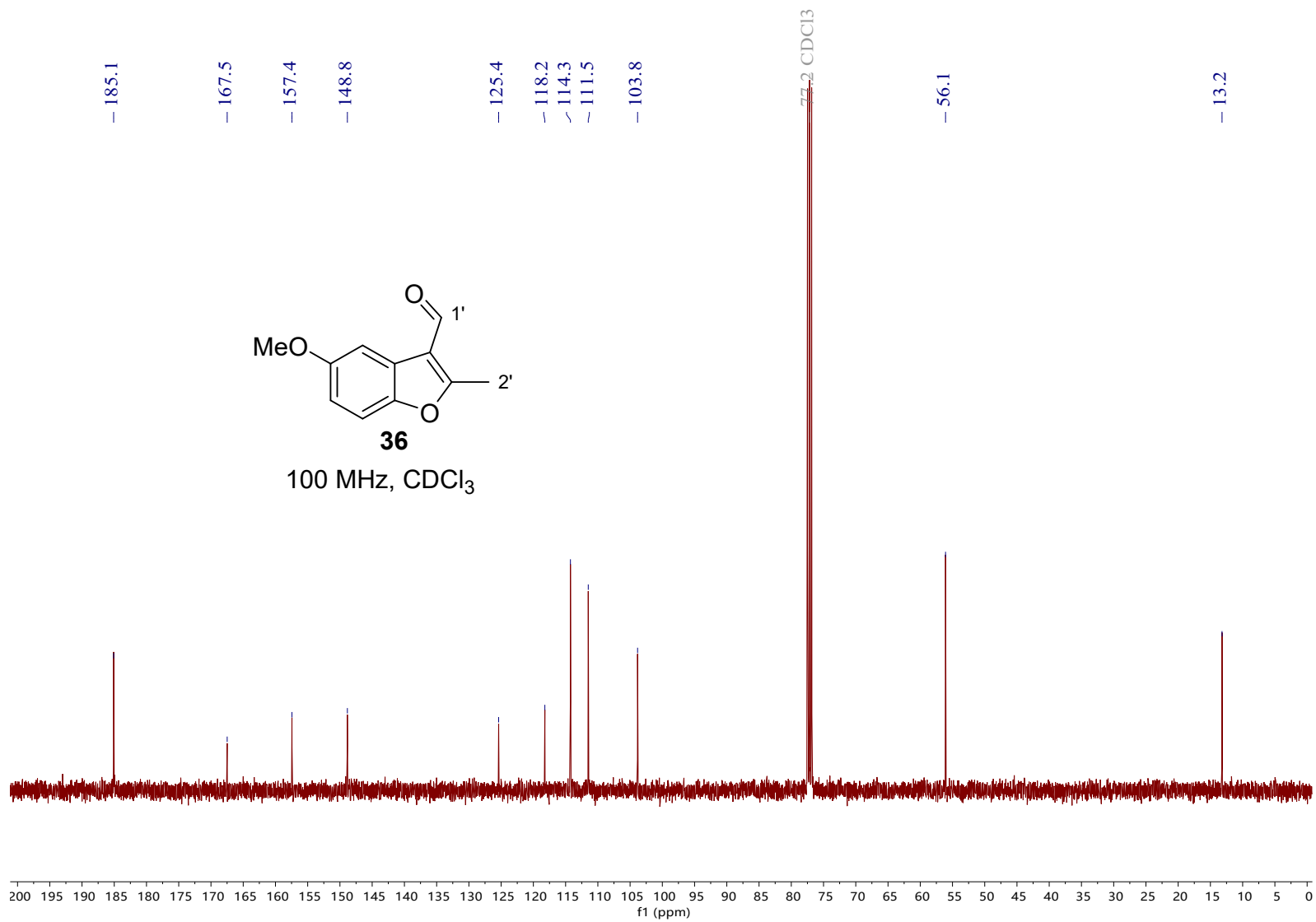


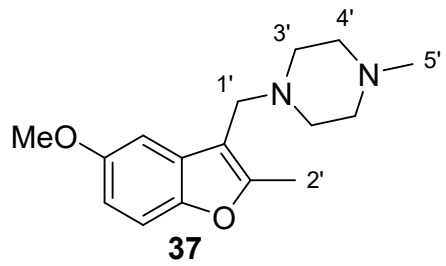




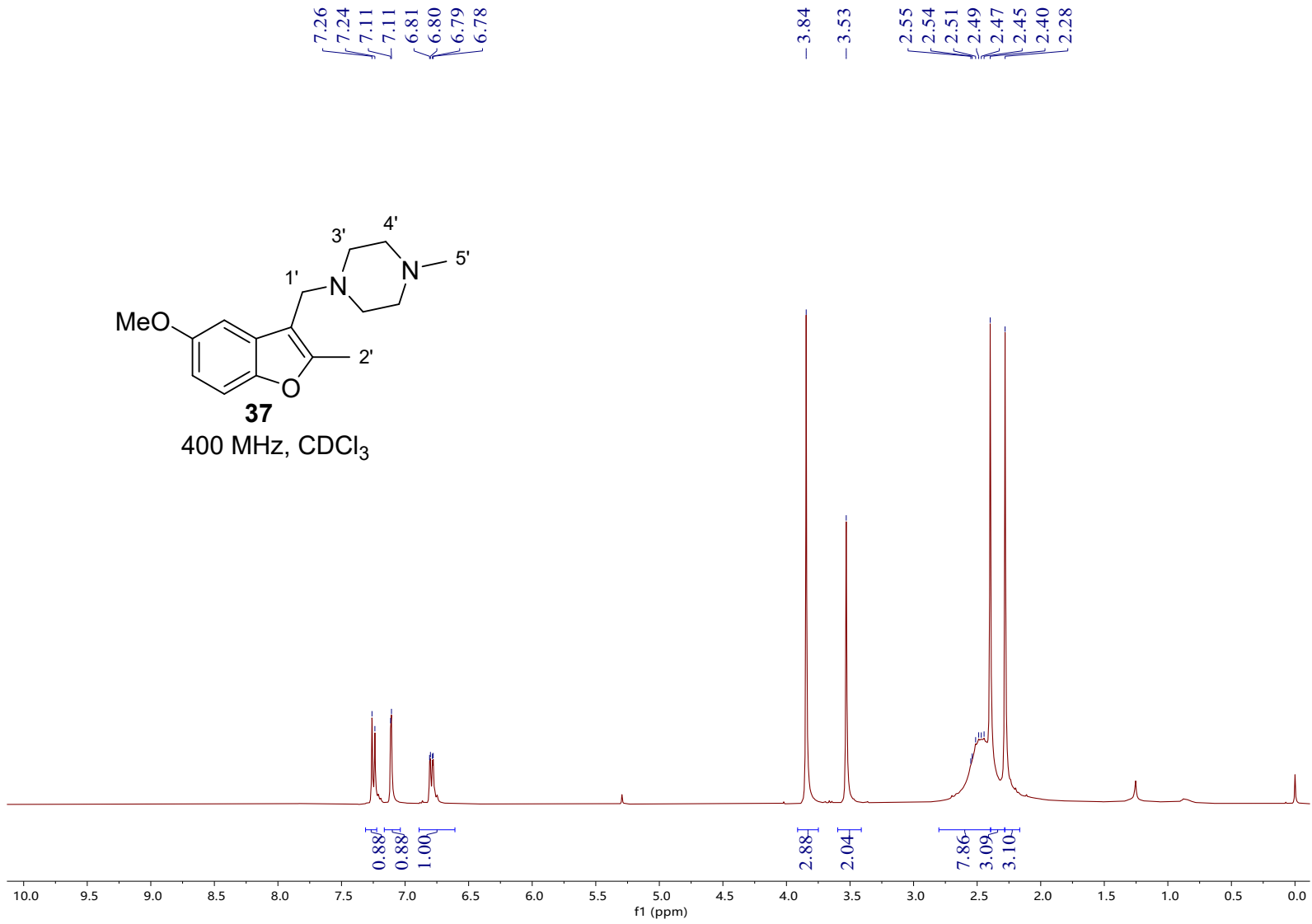


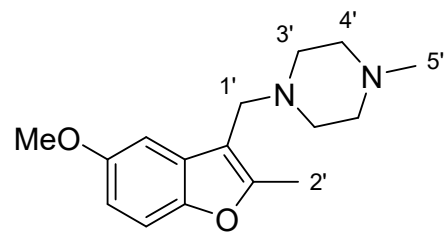






400 MHz, CDCl<sub>3</sub>





**37**  
100 MHz, CDCl<sub>3</sub>

