

# Supporting Information

## Divergent synthesis of 3,4-dihydro-2*H*-benzo[*h*]chromen-2-one and fluorenone derivatives from *ortho*-alkynylarylketones

Jantra Jantrapirom,<sup>a,‡</sup> Nitwaree Palavong,<sup>a,‡</sup> Jumreang Tummatorn,<sup>\*, a, b</sup>

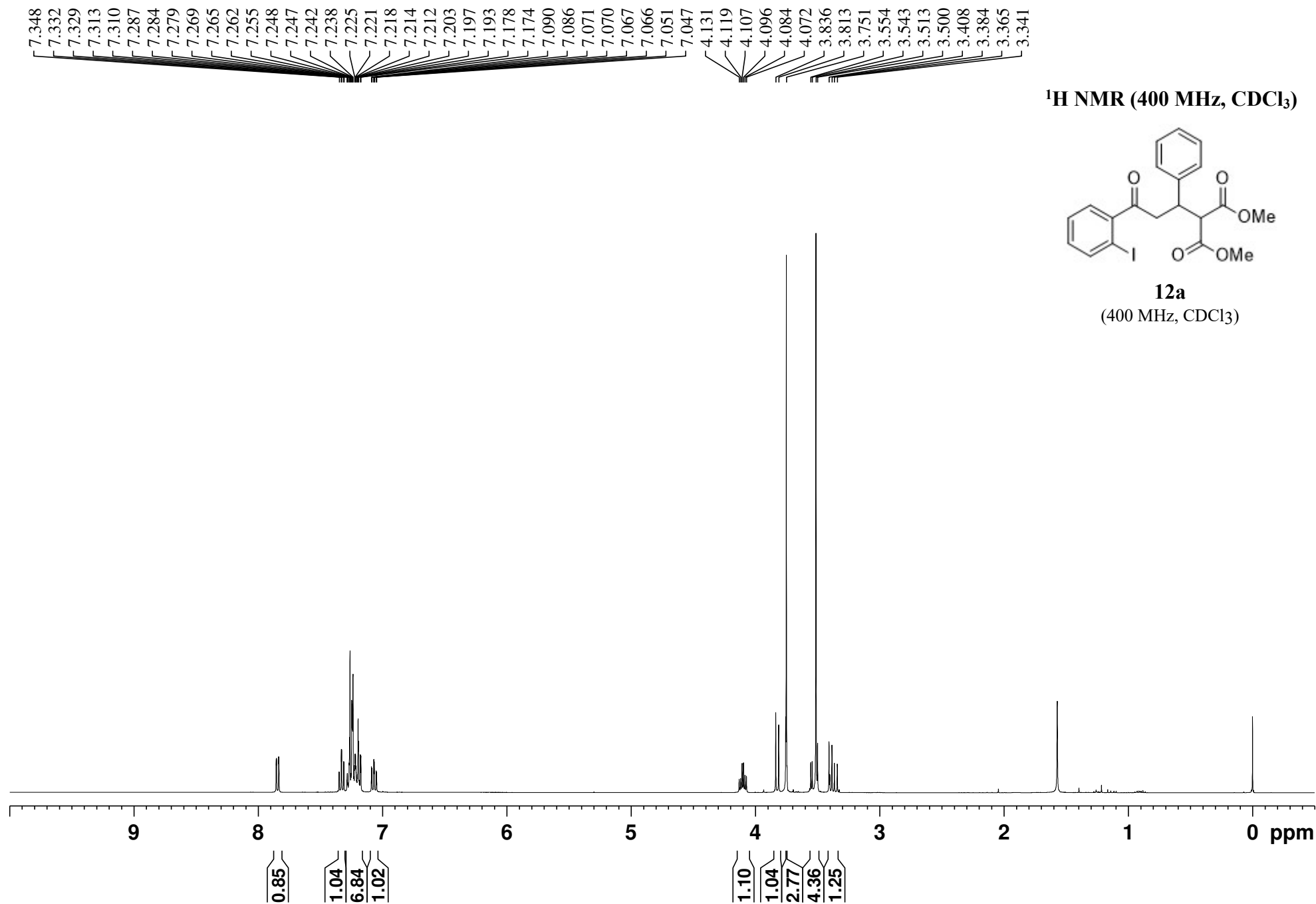
Charnsak Thongsornkleeb,<sup>a, b</sup> and Somsak Ruchirawat<sup>a, b</sup>

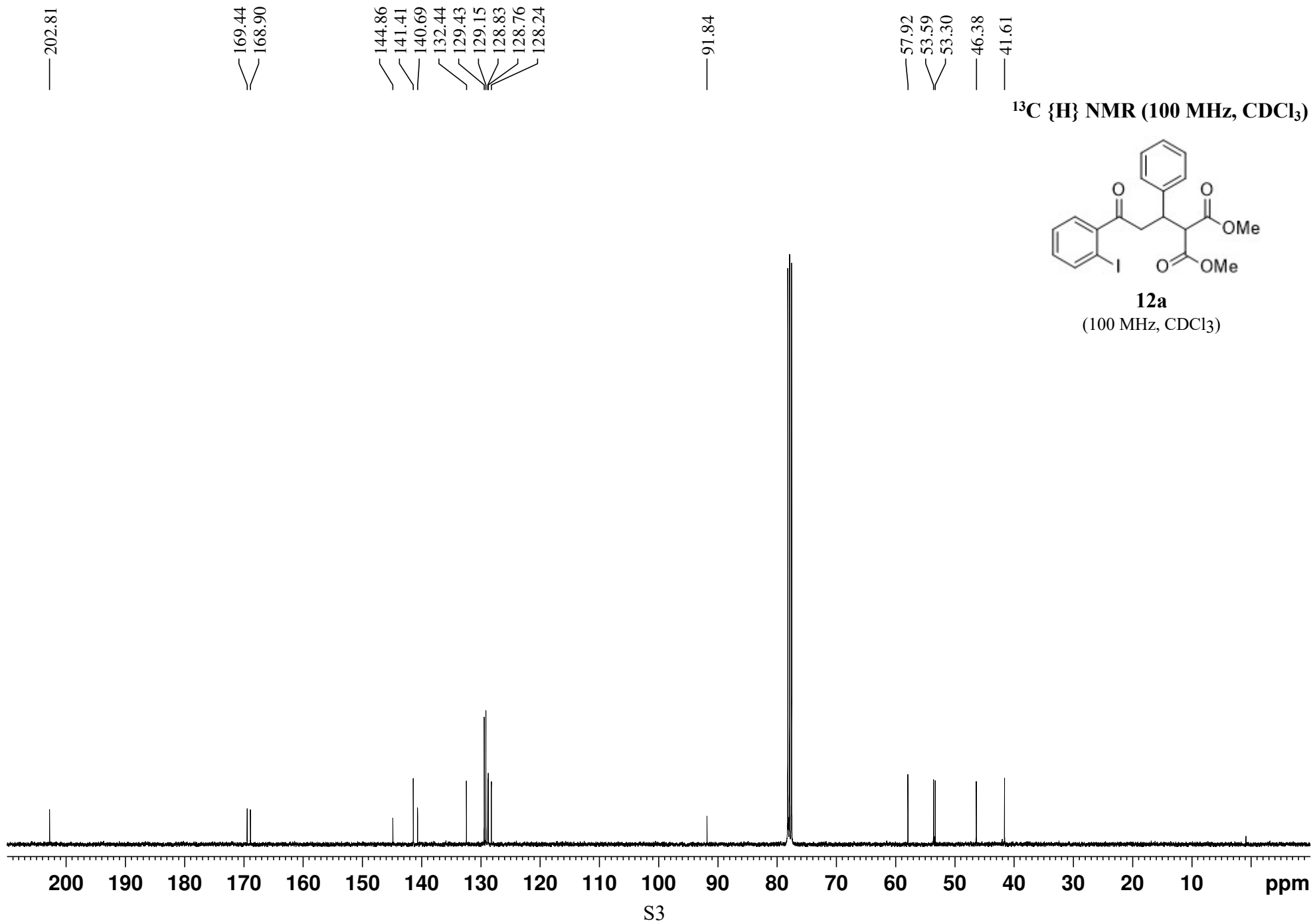
<sup>a</sup>Laboratory of Medicinal Chemistry, Chulabhorn Research Institute, 54 Kamphaeng Phet 6, Laksi, Bangkok 10210, Thailand

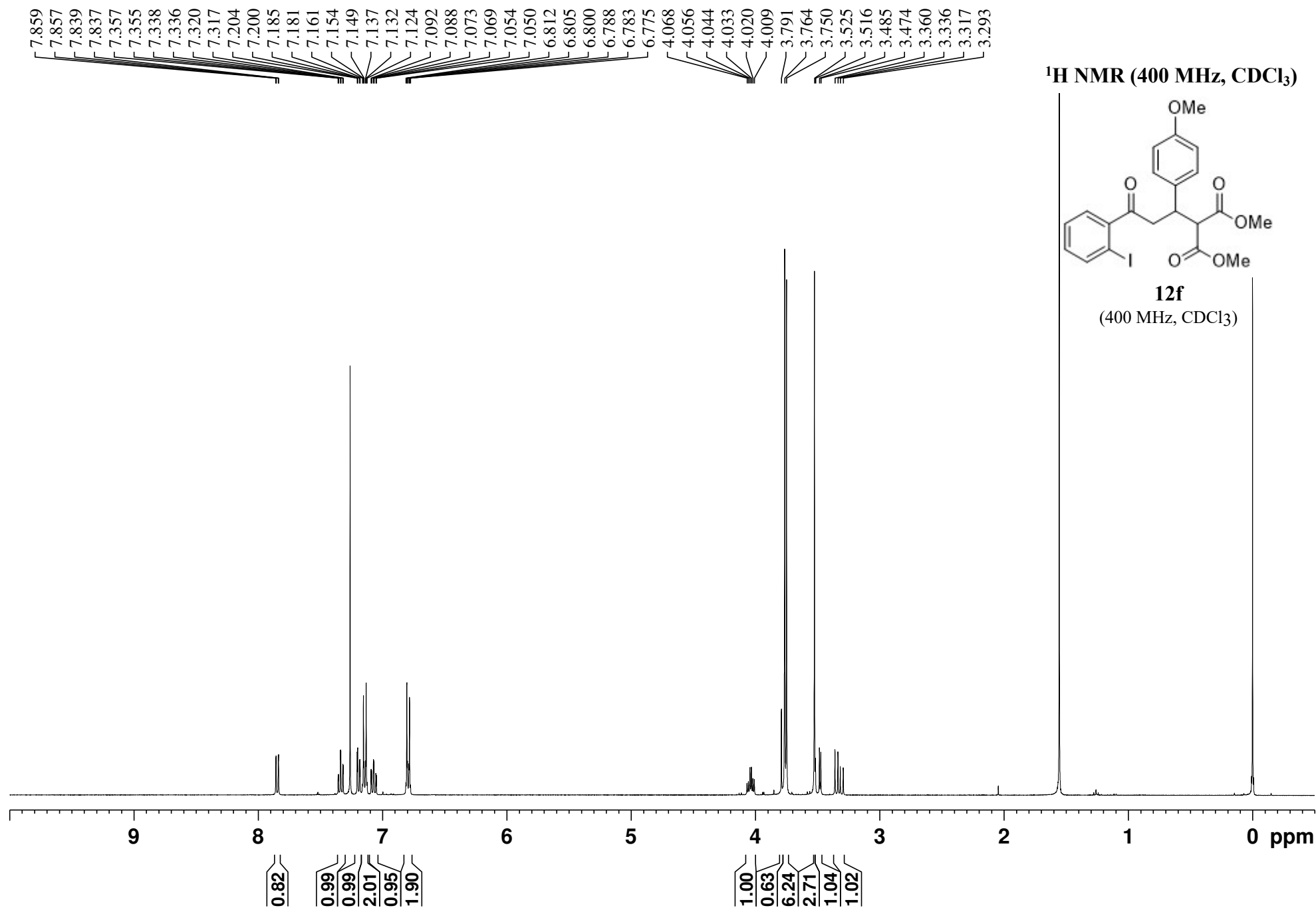
<sup>b</sup>Program on Chemical Sciences, Chulabhorn Graduate Institute, Center of Excellence on Environmental Health and Toxicology (EHT), Ministry of Education, 54 Kamphaeng Phet 6, Laksi, Bangkok 10210, Thailand

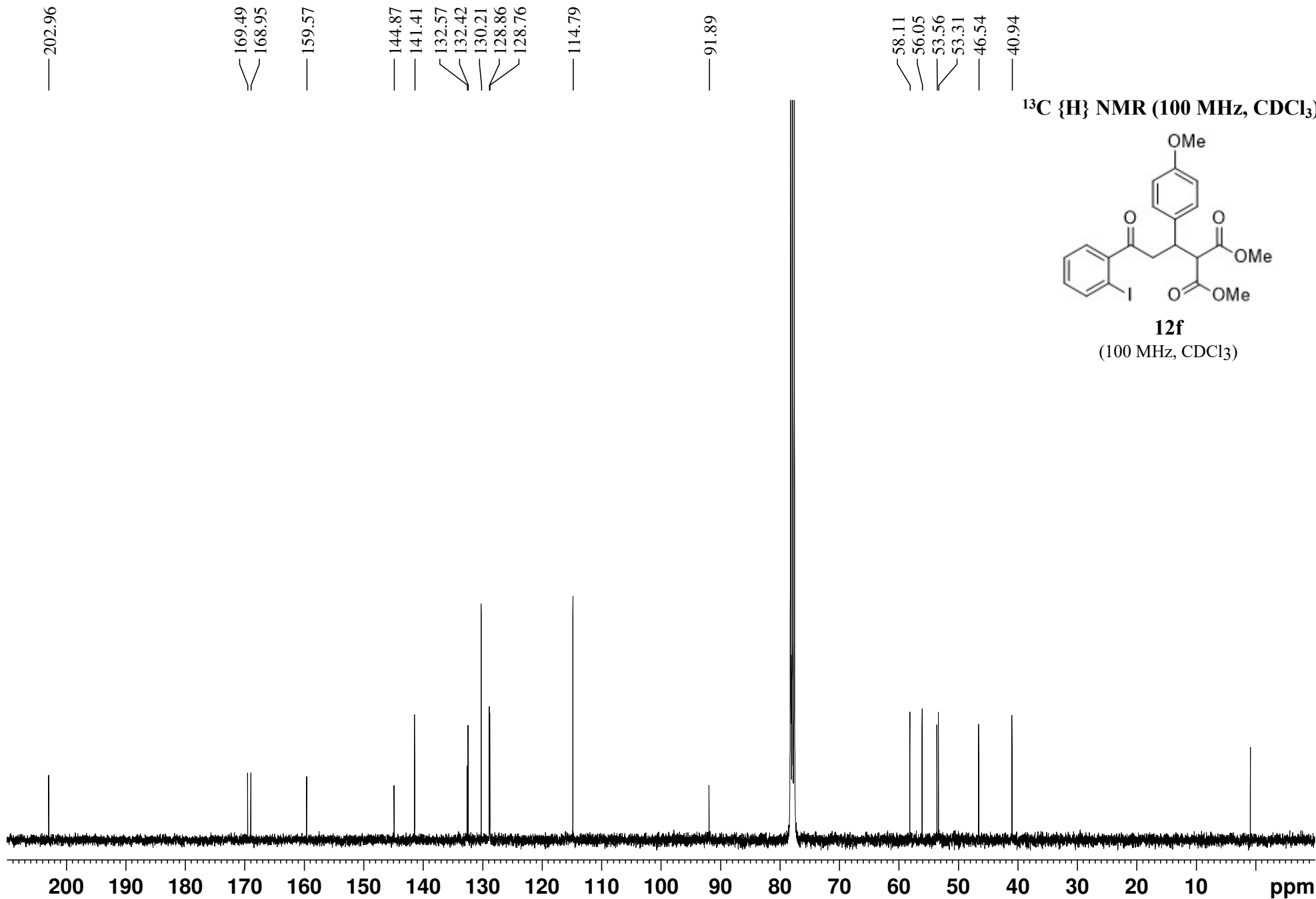
<sup>‡</sup> equal contribution

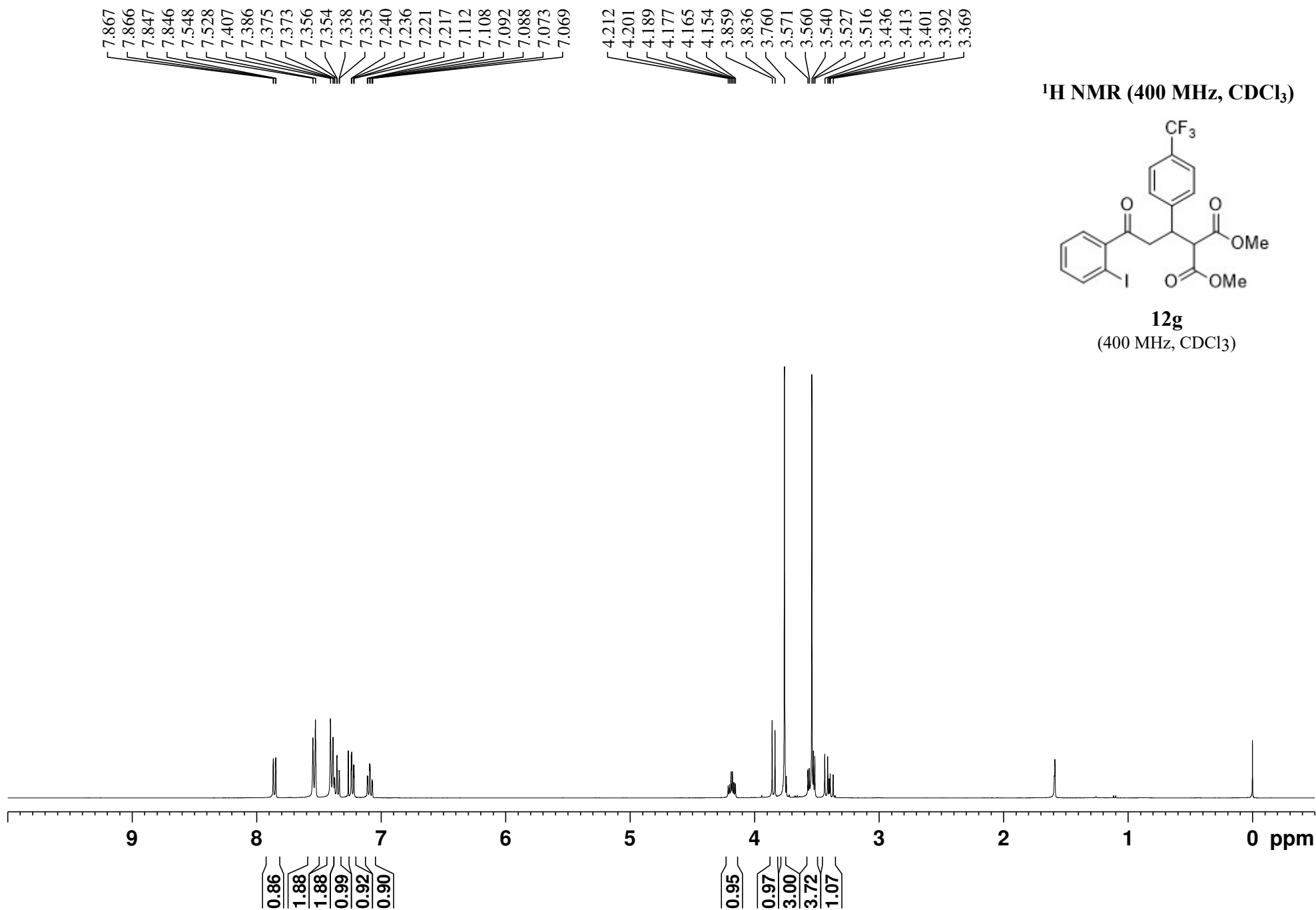
| Contents:                                                                                                                                                                                                                                             | Pages |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------|
| 1. Copies of <sup>1</sup> H and <sup>13</sup> C {1H} NMR spectra for Compound <b>12a</b> and <b>12f-12m</b><br><sup>19</sup> F NMR spectra for <b>12g</b> , <b>12h</b> , <b>12j</b> , and <b>12l</b>                                                  | S2    |
| 2. Copies of <sup>1</sup> H and <sup>13</sup> C {1H} NMR spectra for Compound <b>10</b> and<br><sup>19</sup> F NMR spectra for <b>10c</b> , <b>10d</b> , <b>10g</b> , <b>10h</b> , <b>10j</b> , <b>10l</b> , <b>10m</b> , <b>10s</b> , and <b>10u</b> | S24   |
| 3. Copies of <sup>1</sup> H and <sup>13</sup> C {1H} NMR spectra for Compound <b>3</b> and<br><sup>19</sup> F NMR spectra for <b>3c</b> , <b>3d</b> , <b>3g</b> , and <b>3h</b>                                                                       | S77   |
| 4. Copies of <sup>1</sup> H and <sup>13</sup> C {1H} NMR spectra for Compound <b>9f</b> , <b>9k-9v</b> , and <b>11e</b><br><sup>19</sup> F NMR spectra for <b>9l</b> , <b>9m</b> , <b>9s</b> , and <b>9u</b>                                          | S99   |

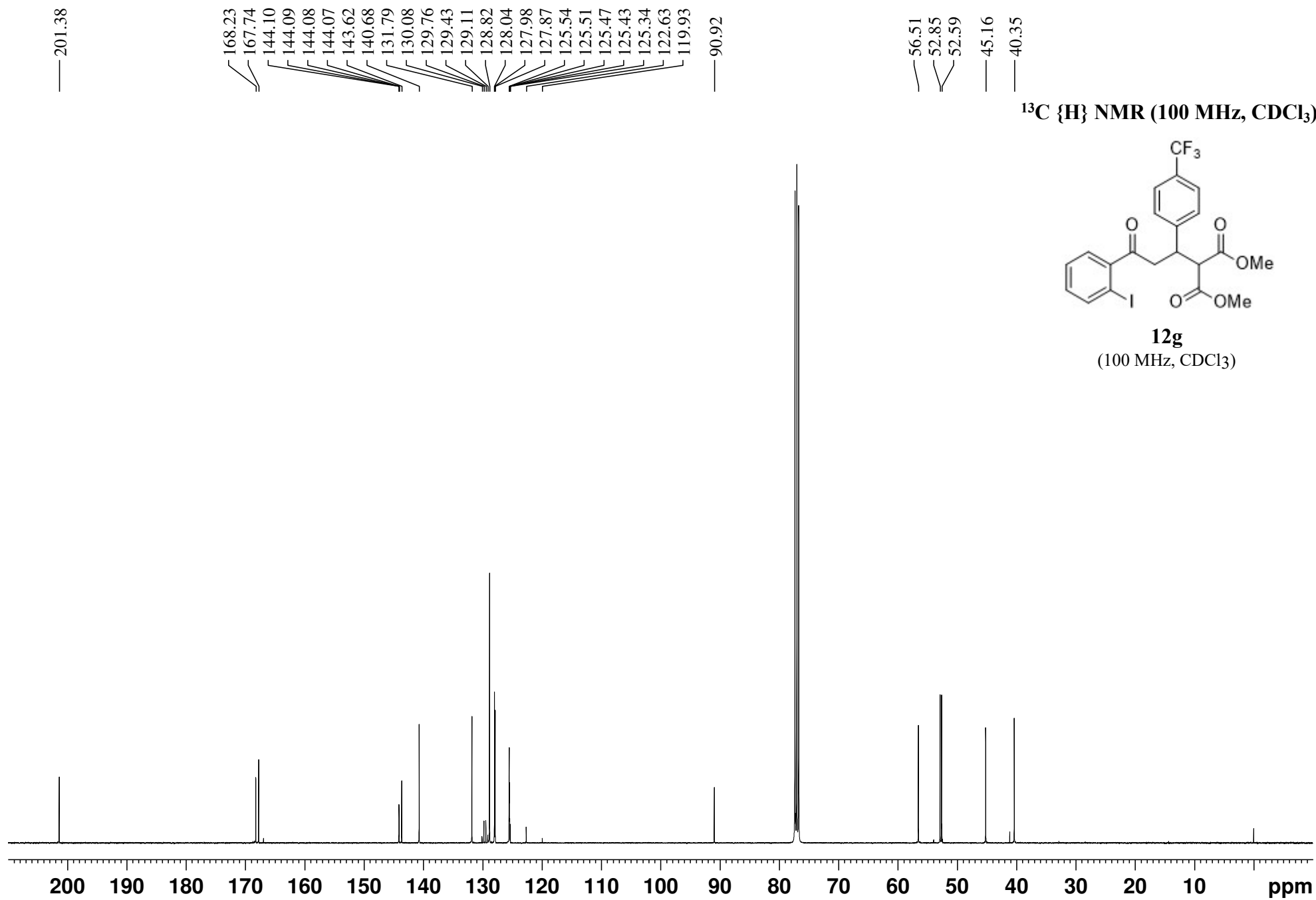


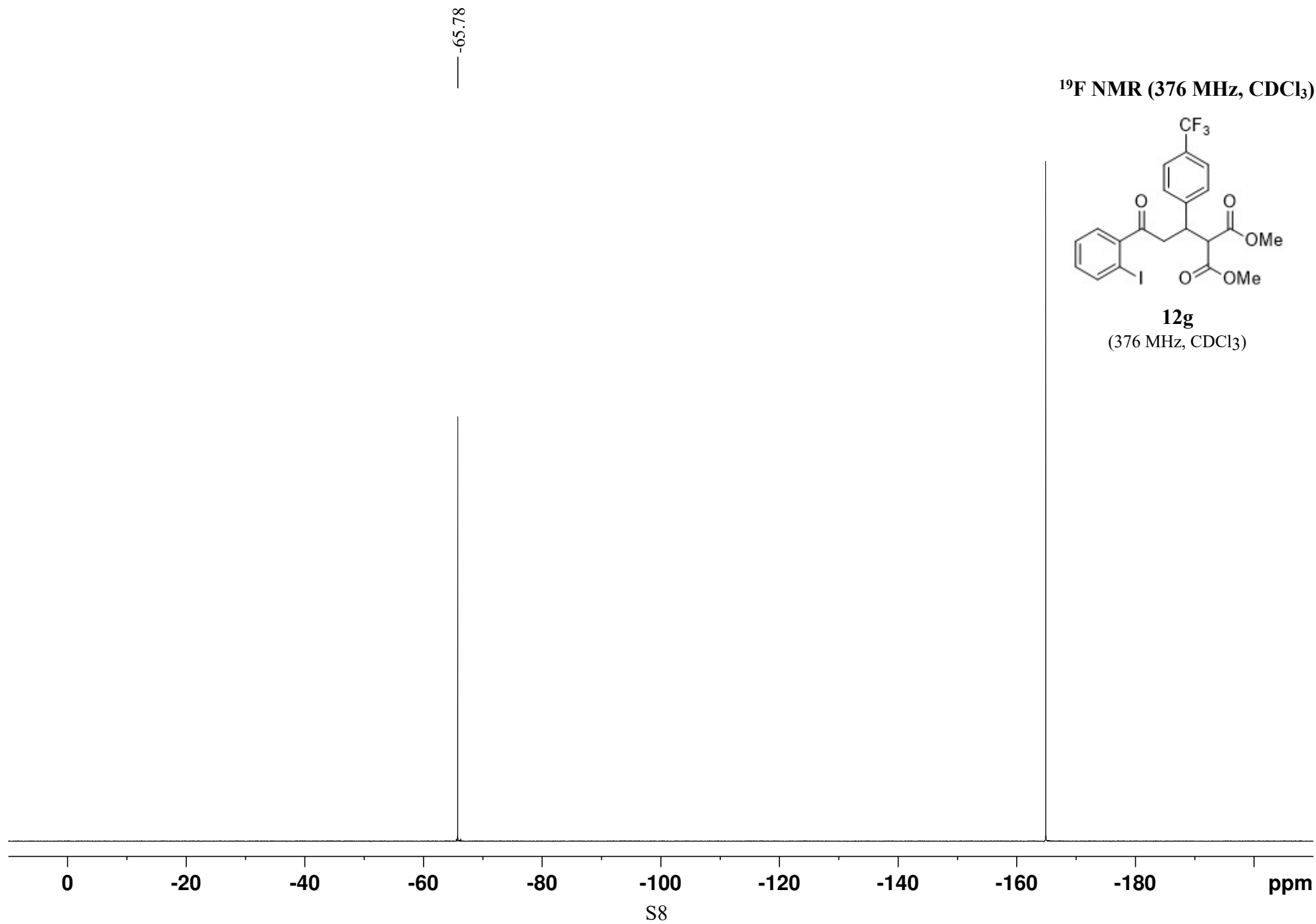


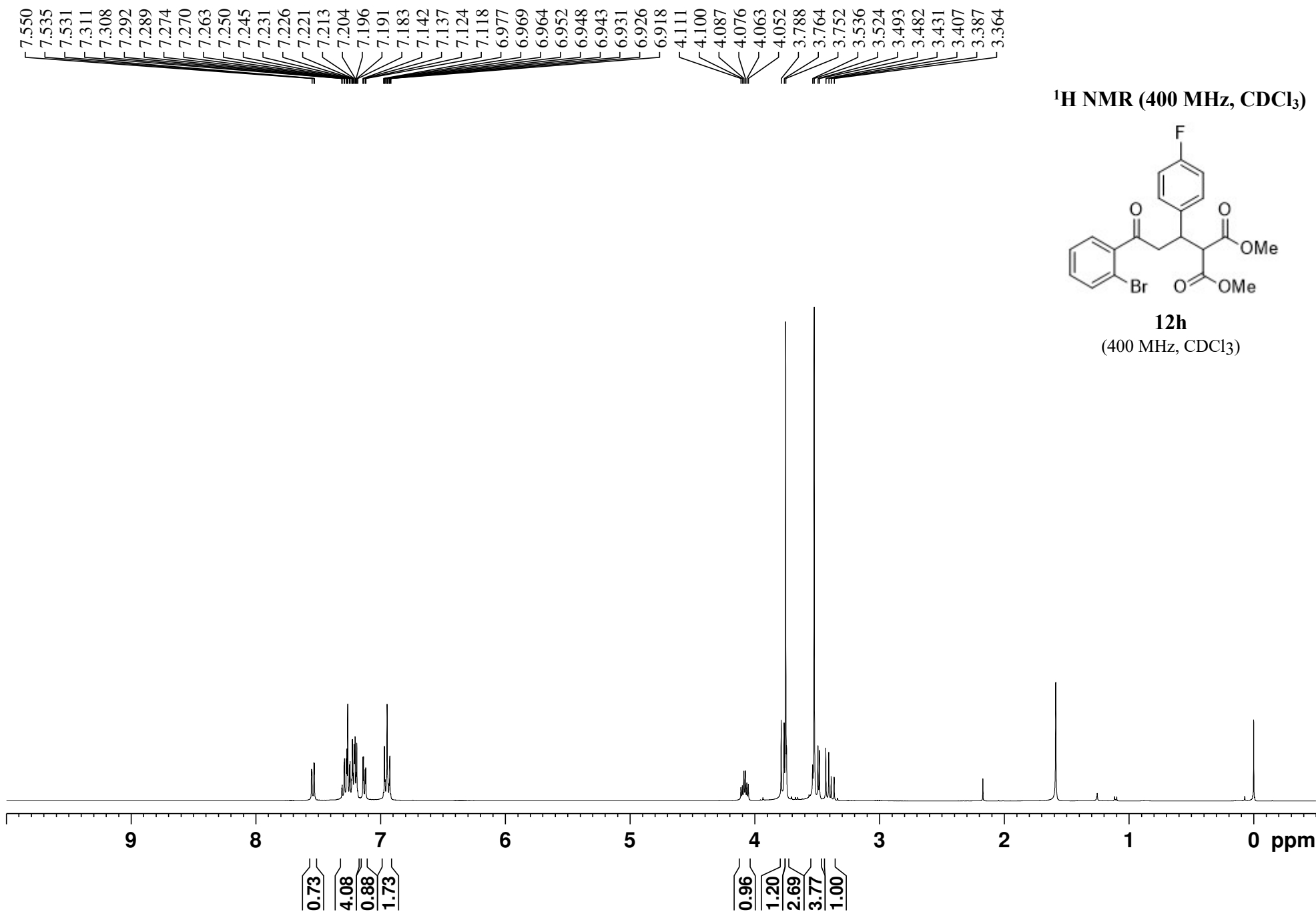


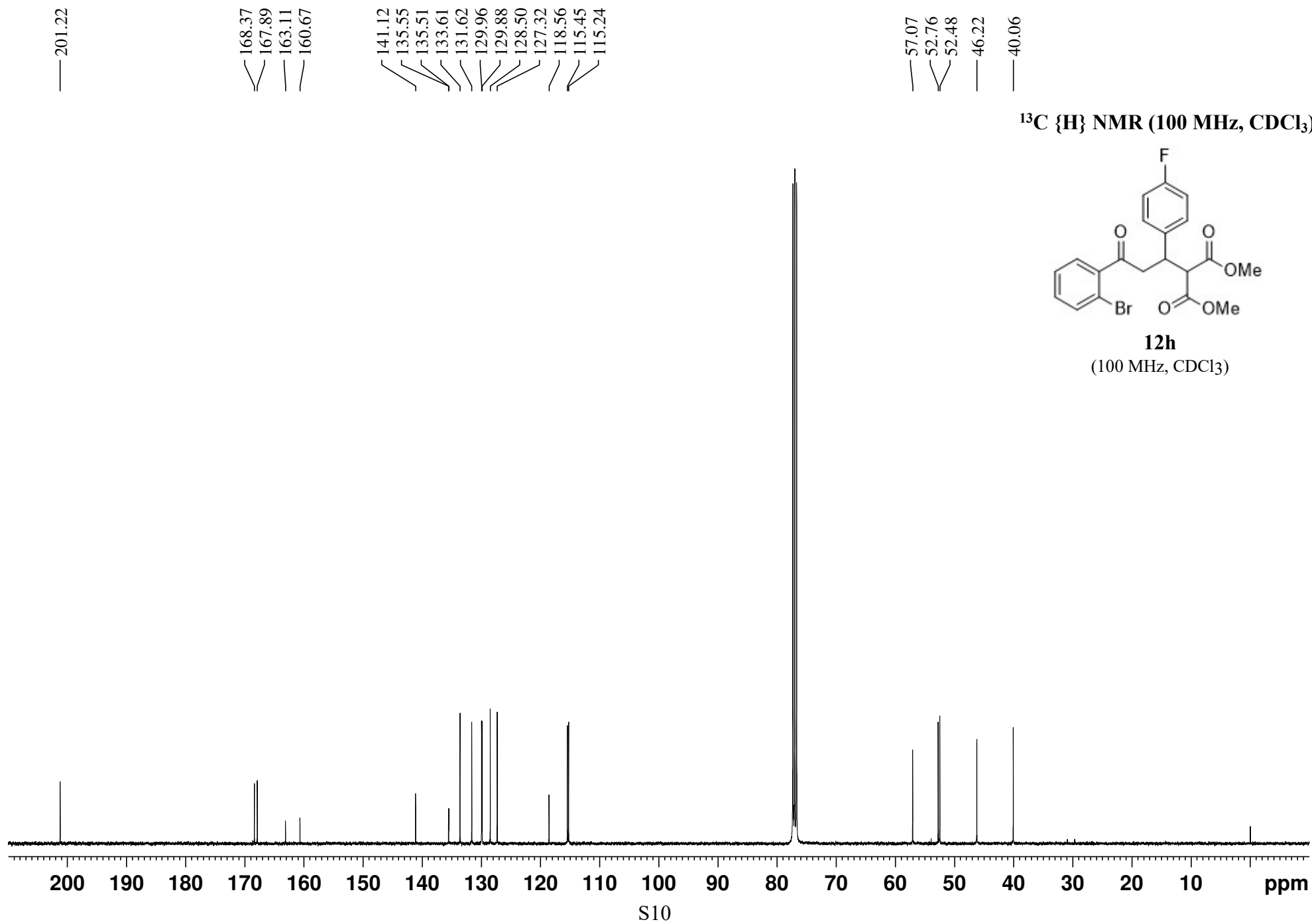


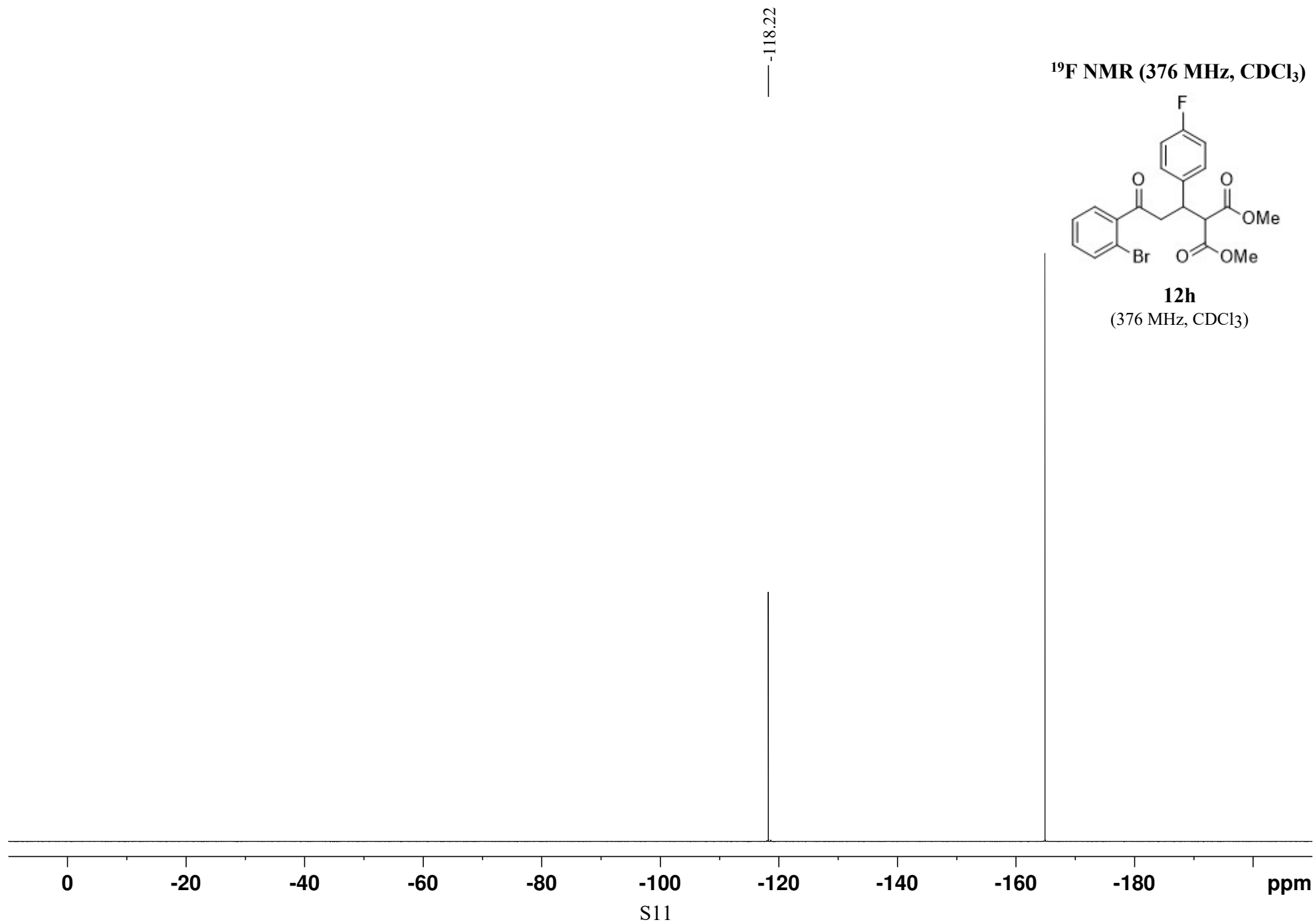


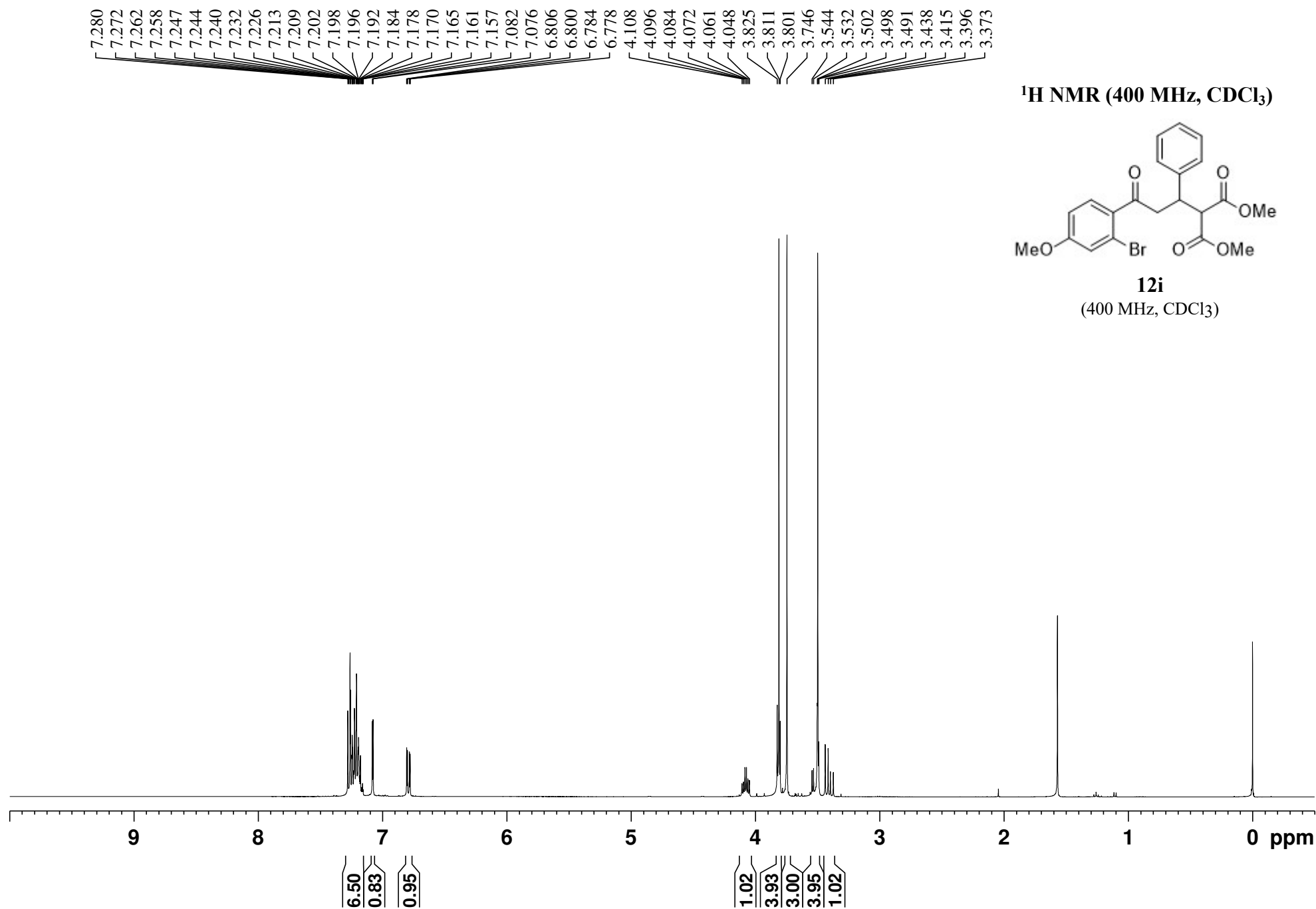


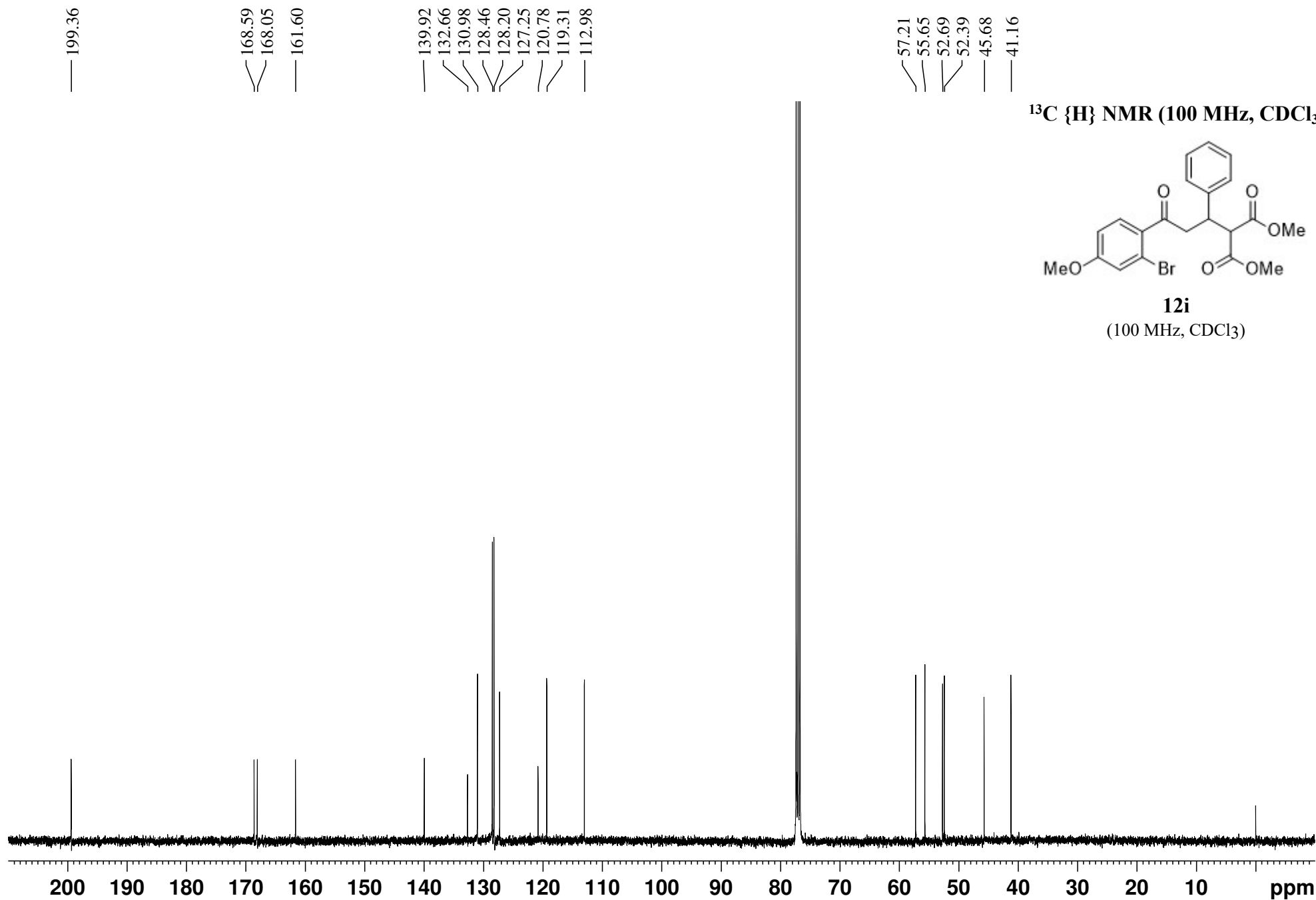


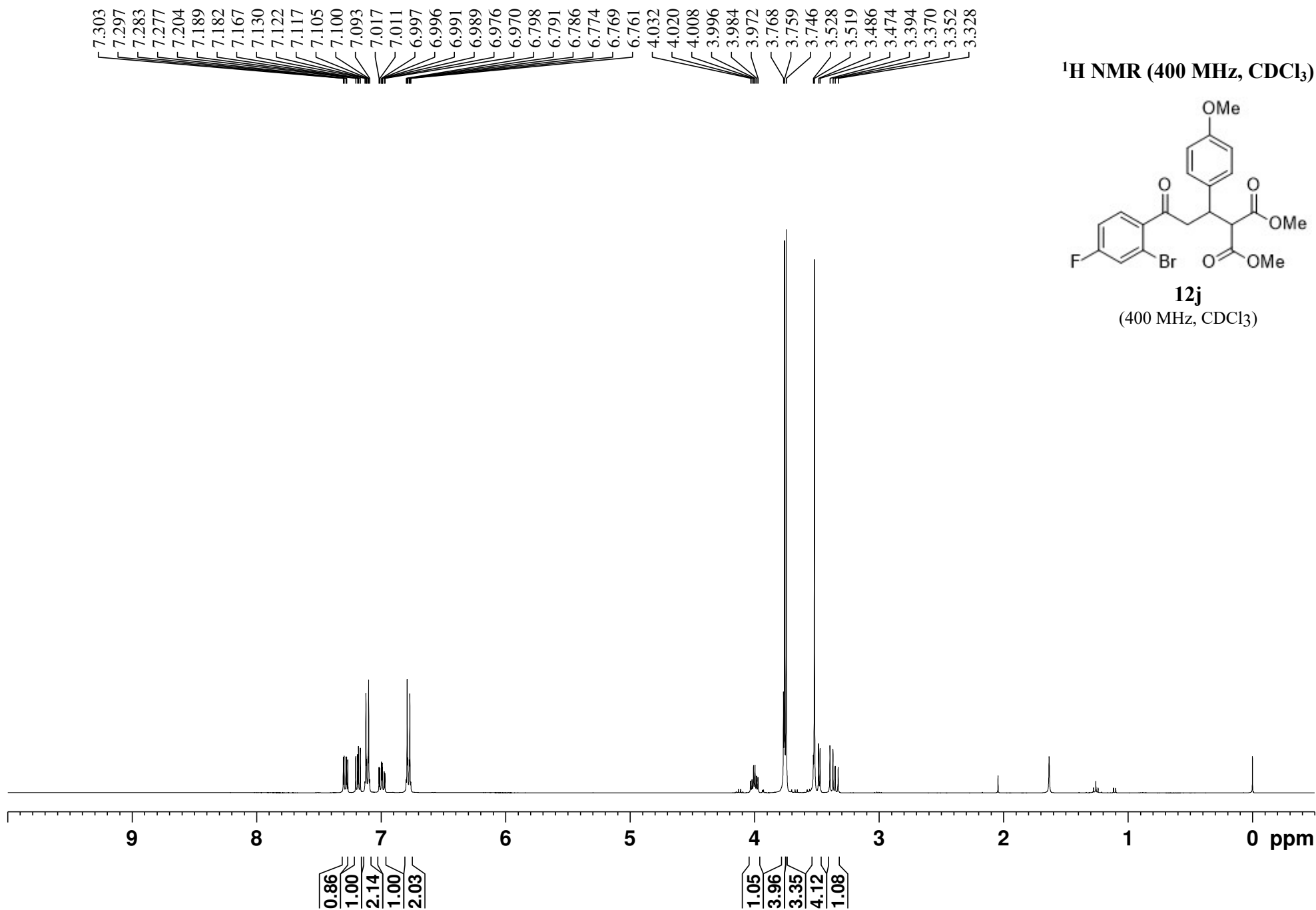


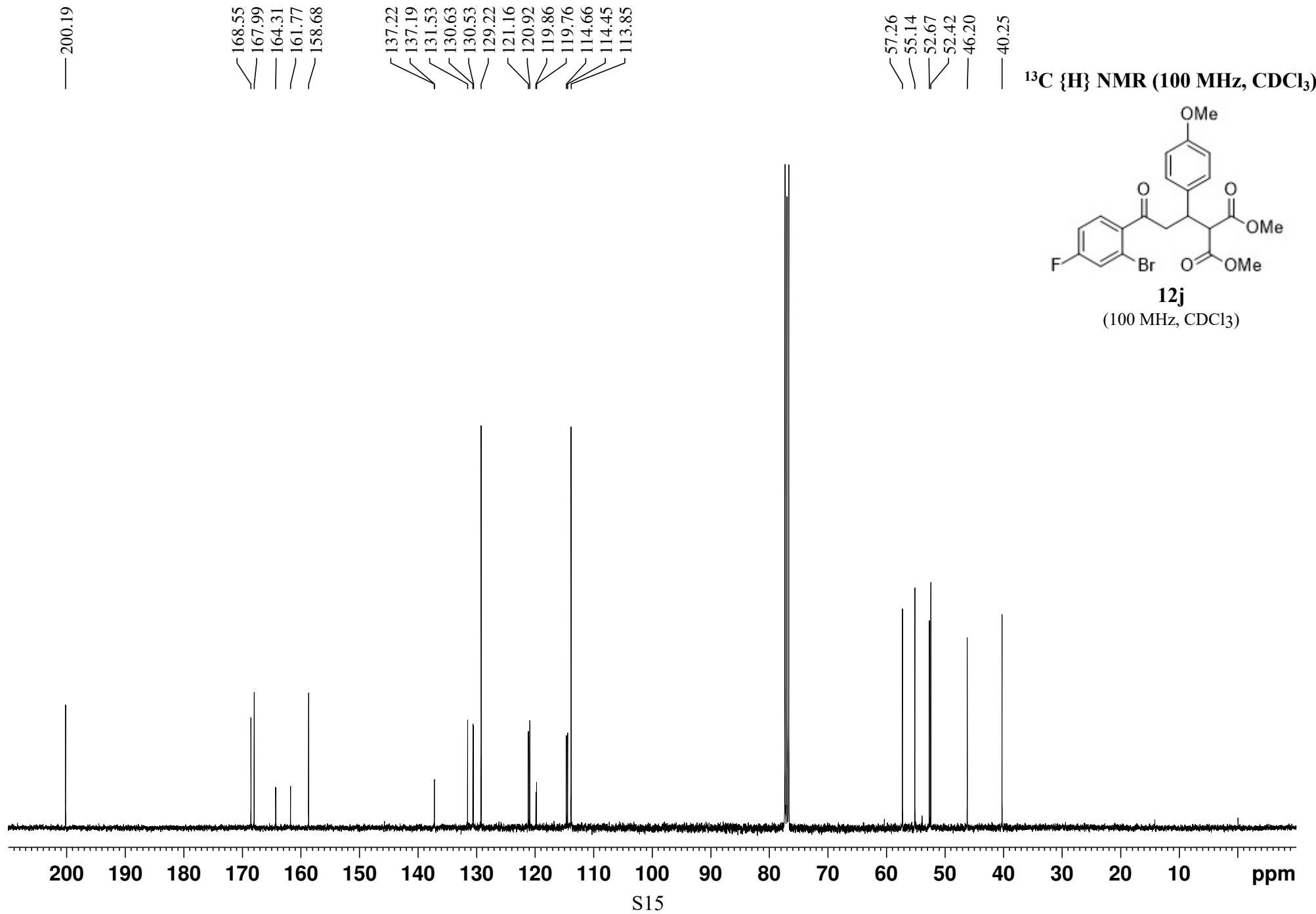


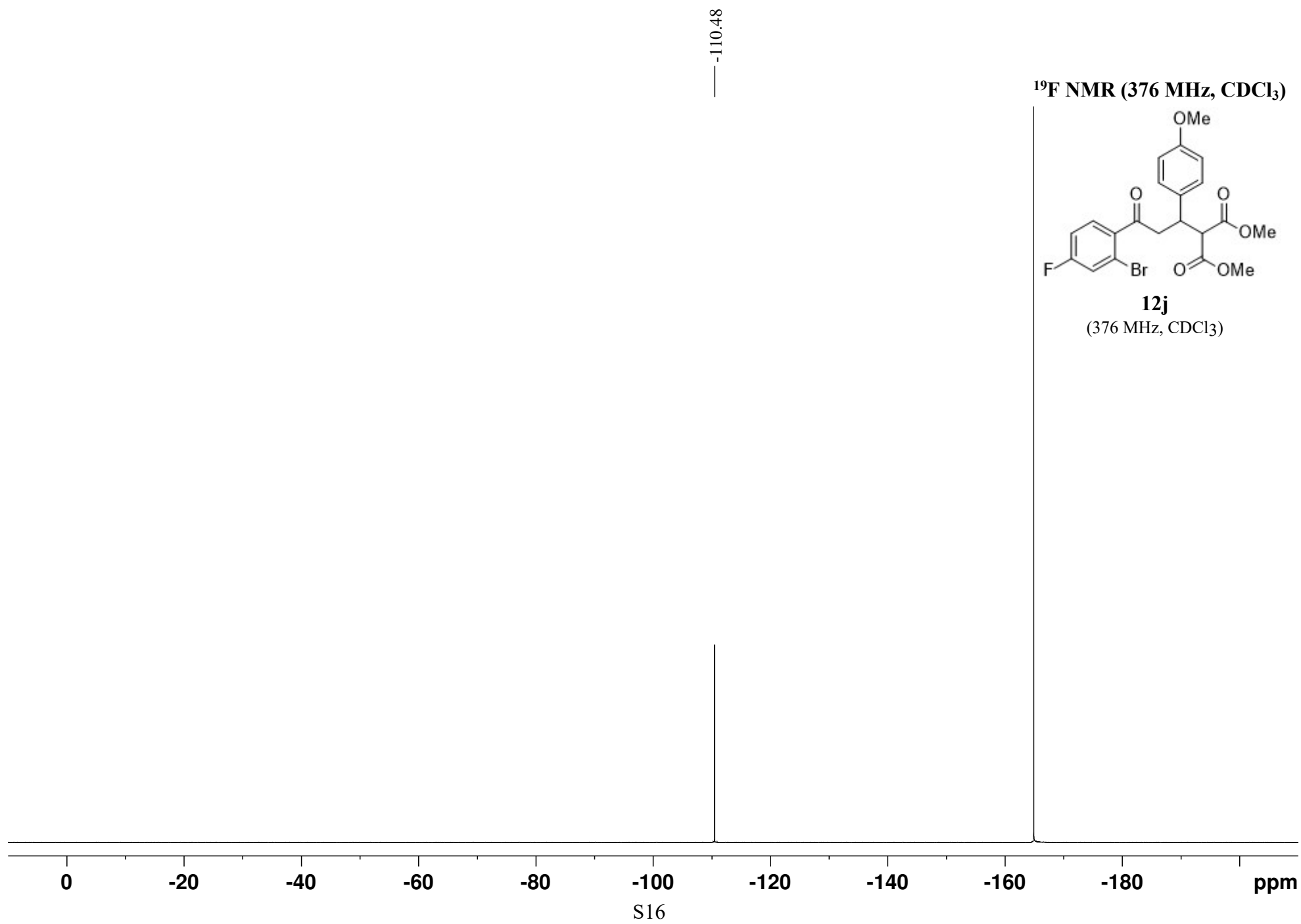


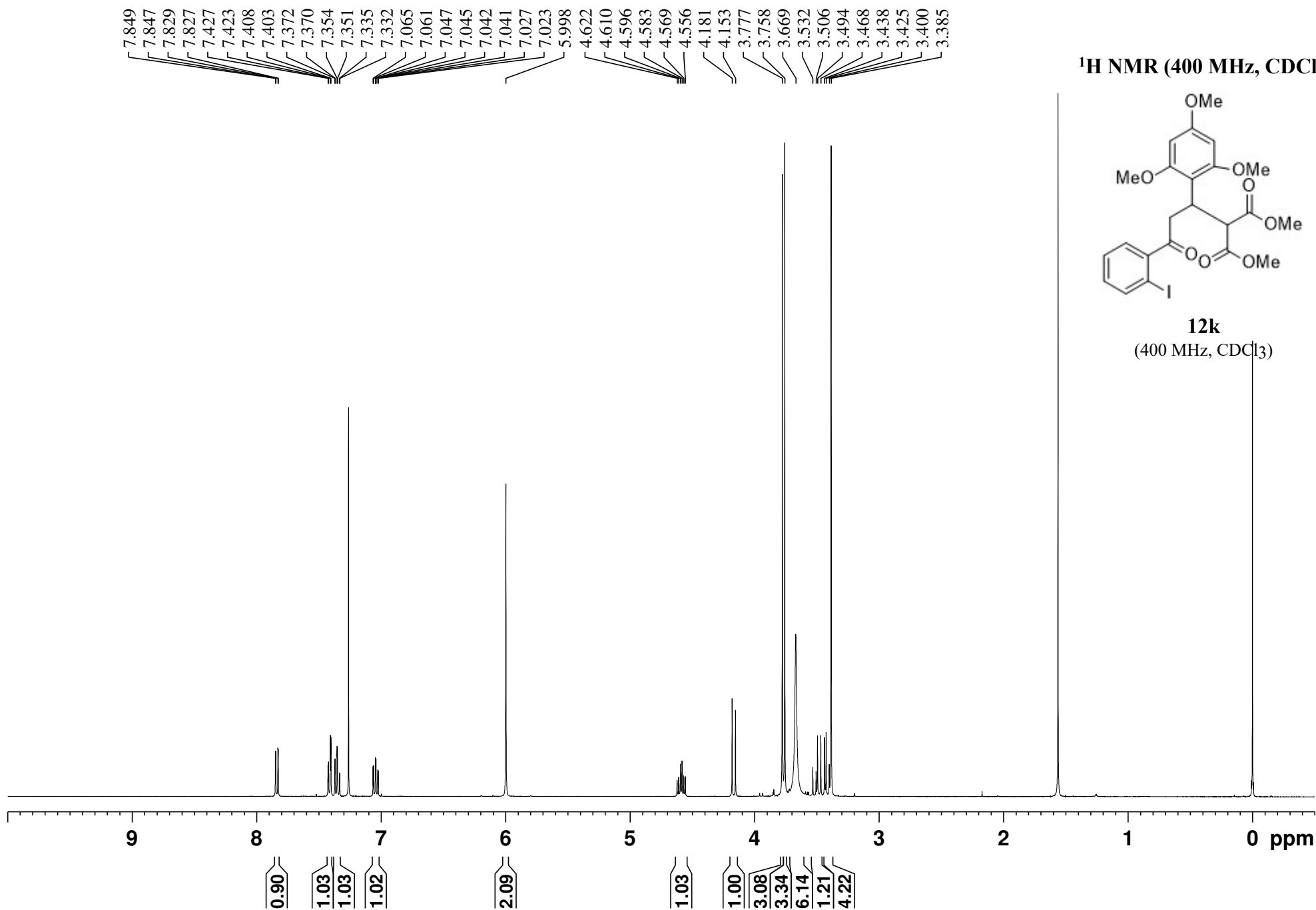


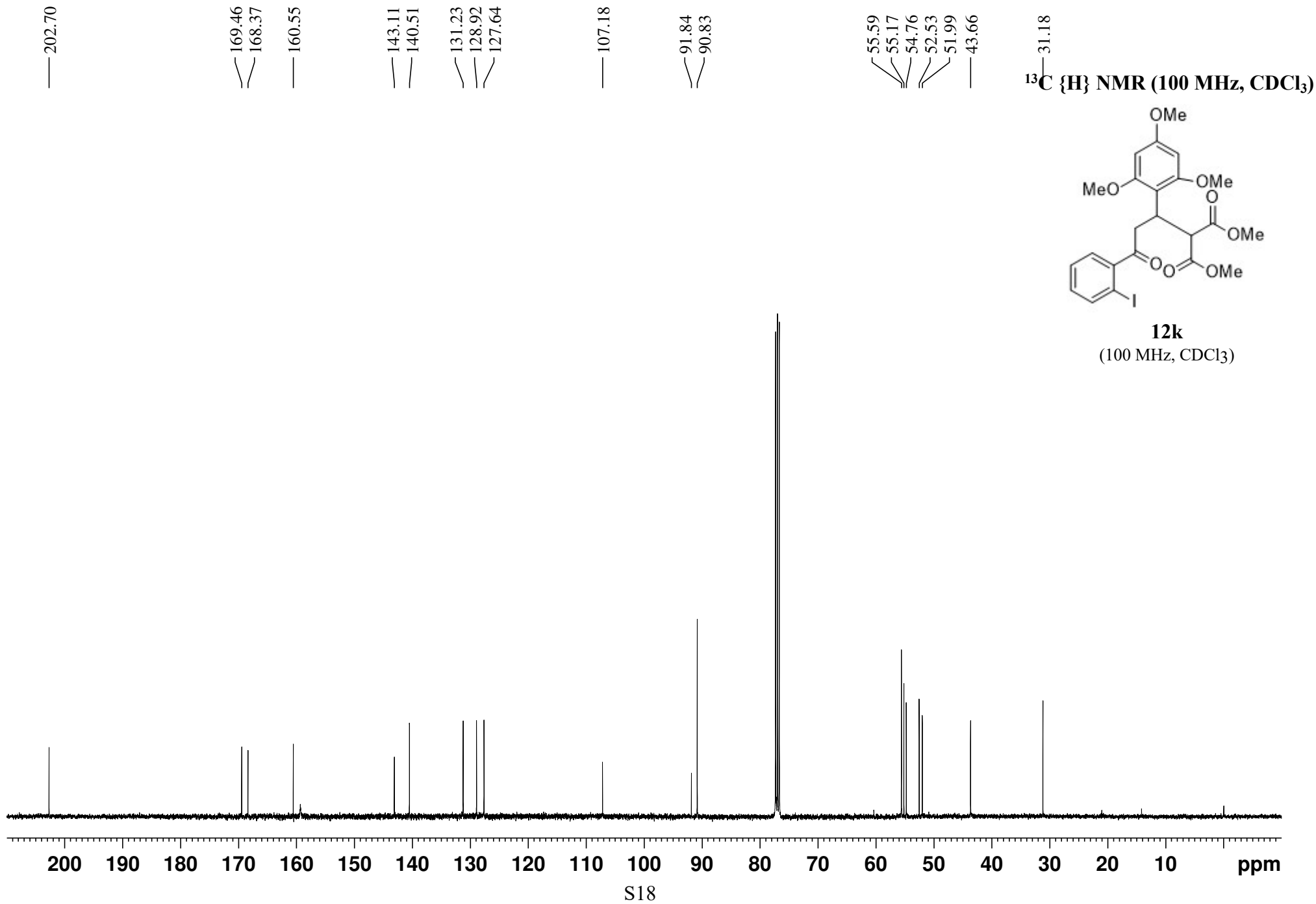


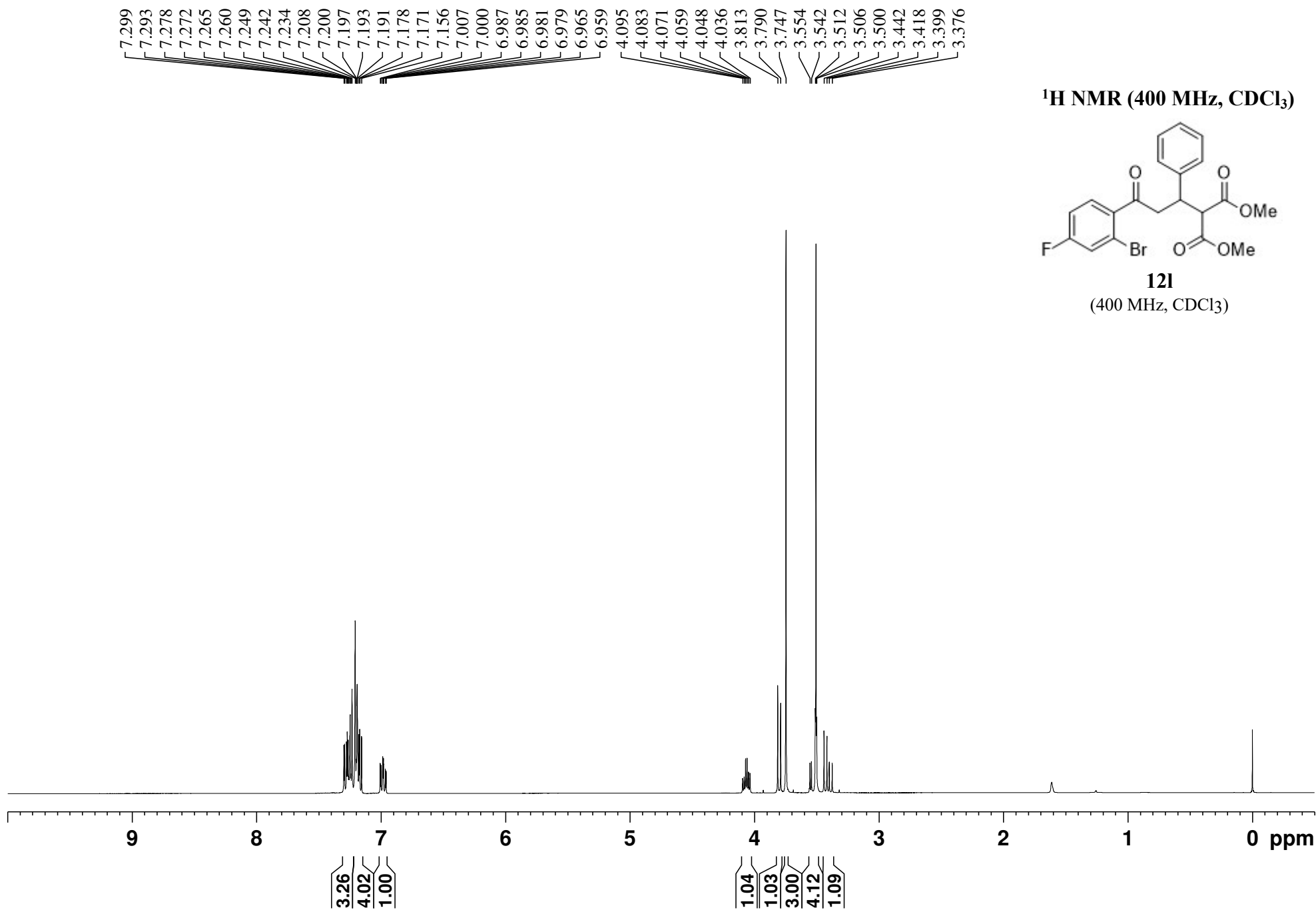


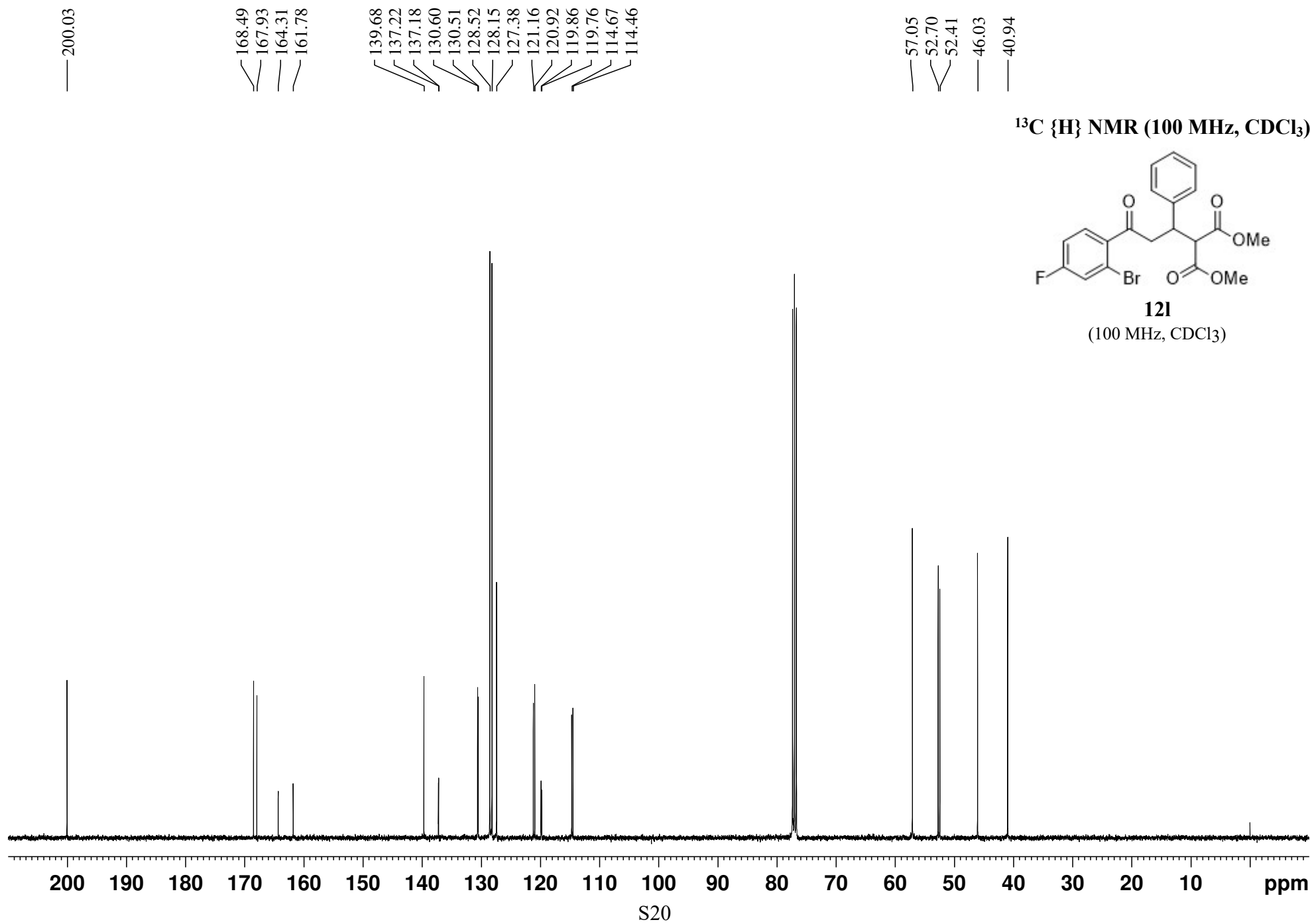


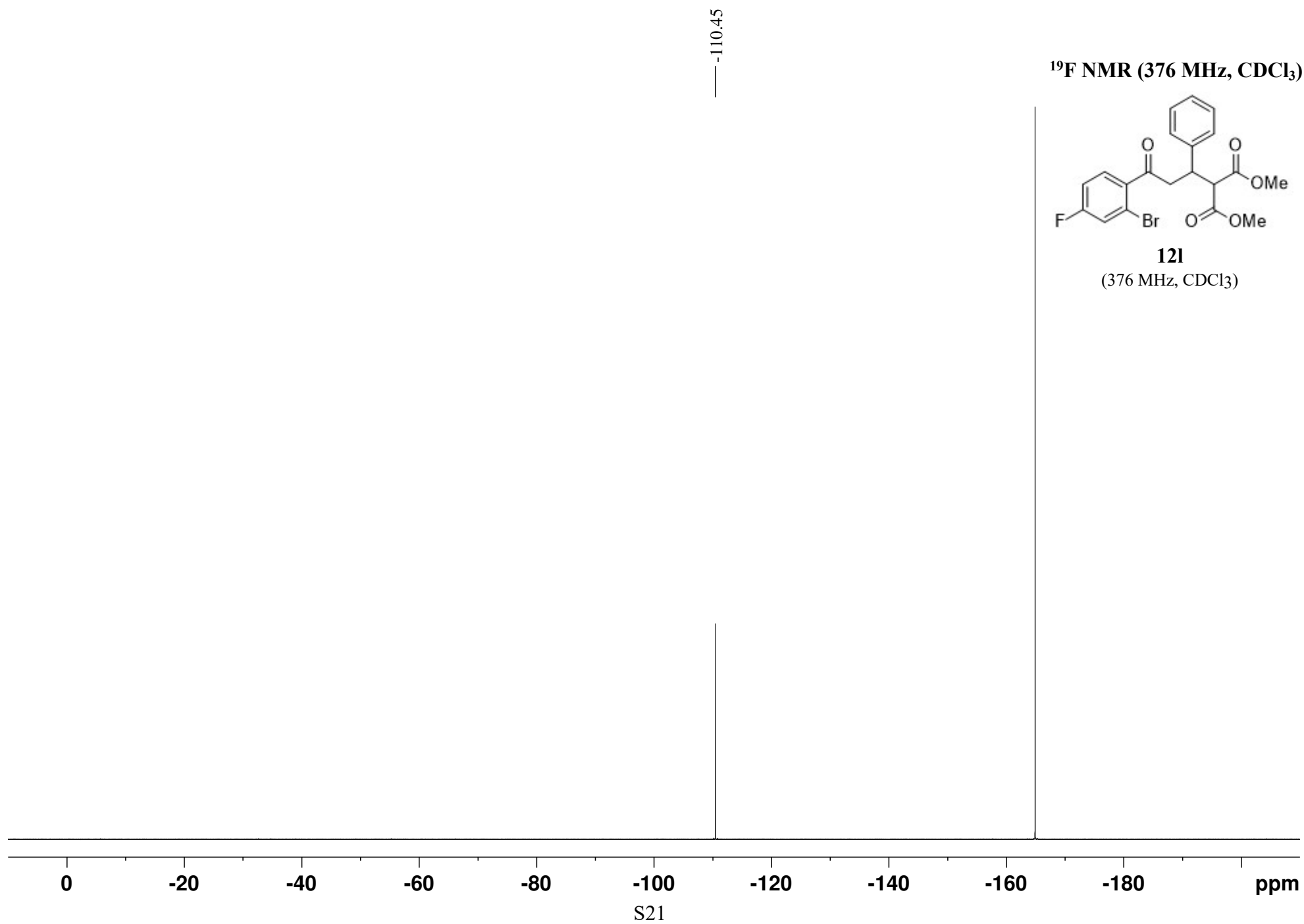








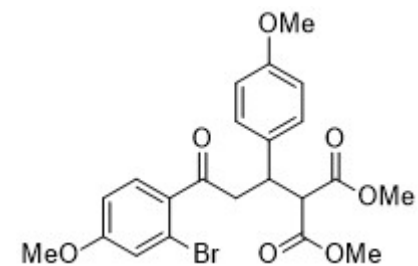




7.285  
7.264  
7.134  
7.126  
7.121  
7.109  
7.104  
7.097  
7.084  
7.078  
6.812  
6.806  
6.791  
6.784  
6.778  
6.767  
6.762  
6.754

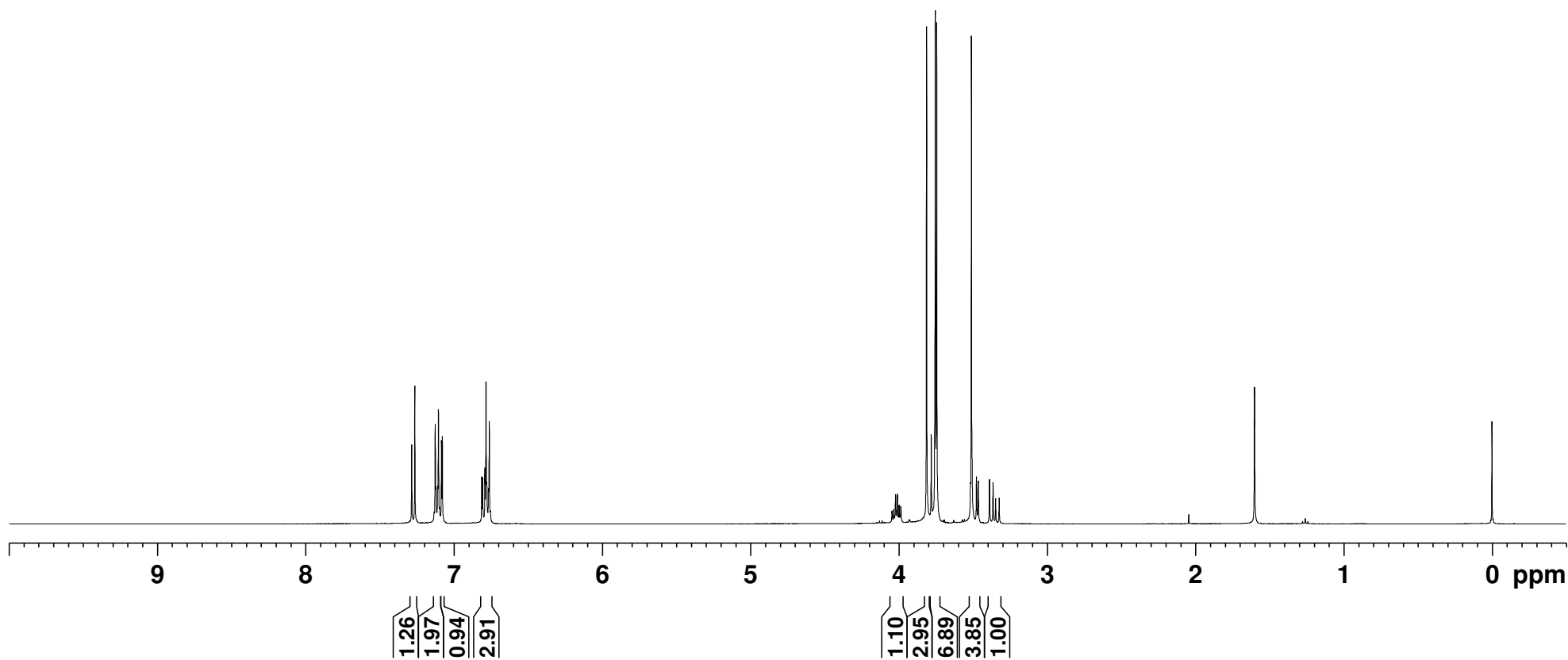
4.046  
4.034  
4.022  
4.010  
3.998  
3.986  
3.813  
3.781  
3.754  
3.744  
3.517  
3.510  
3.476  
3.464  
3.388  
3.364  
3.347  
3.323

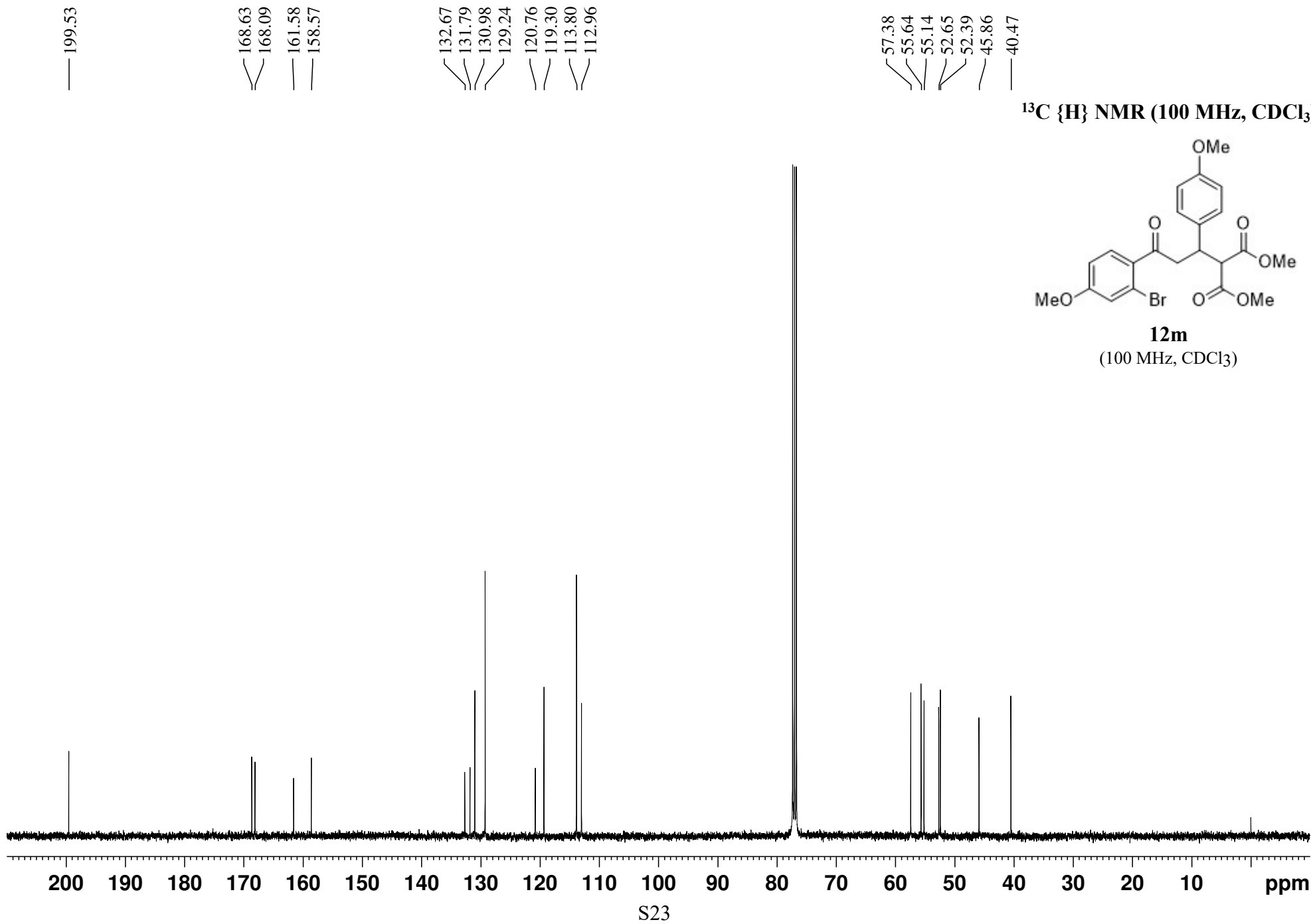
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



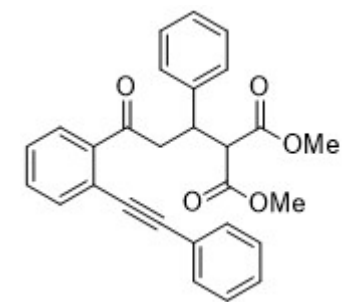
**12m**

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



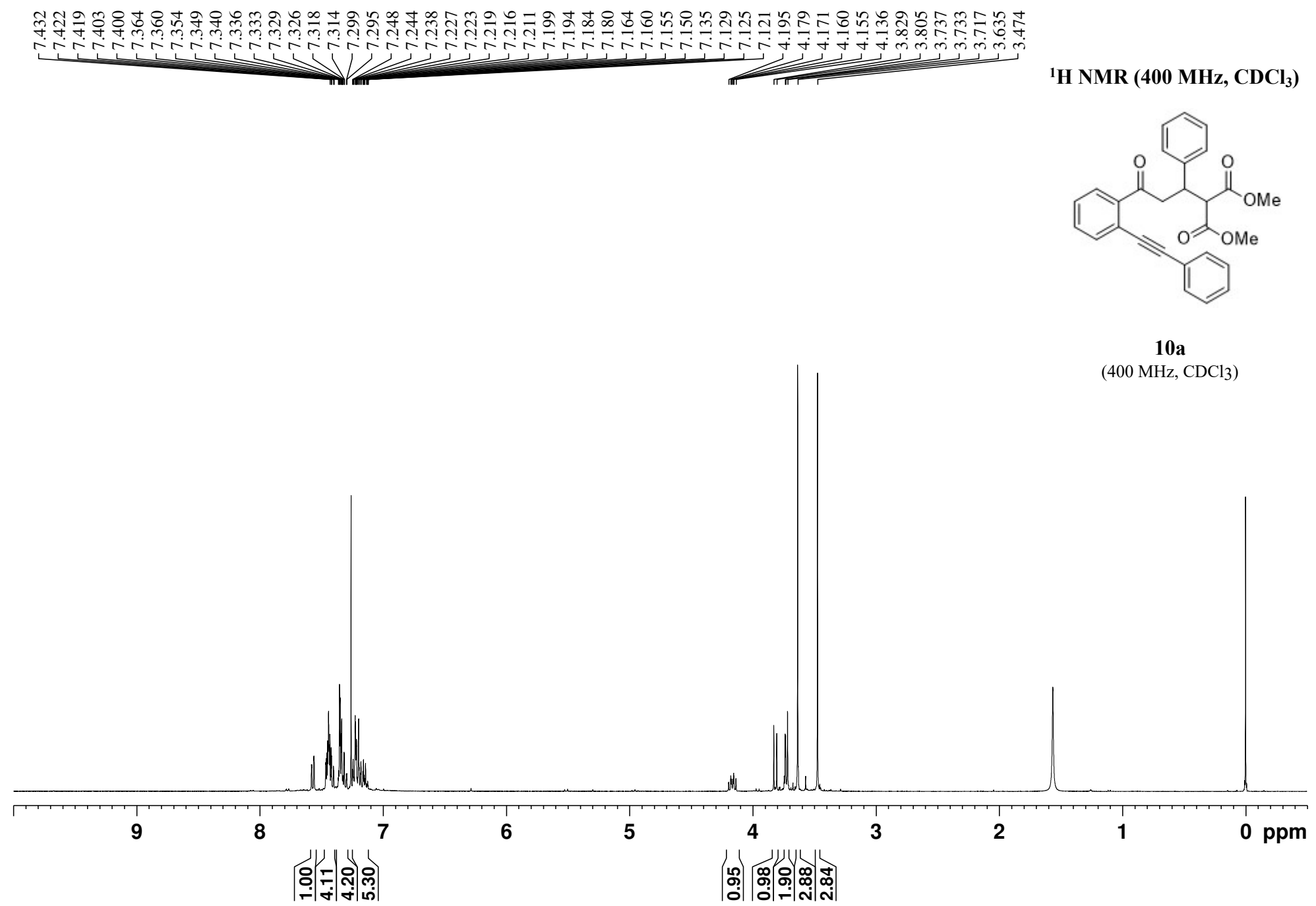


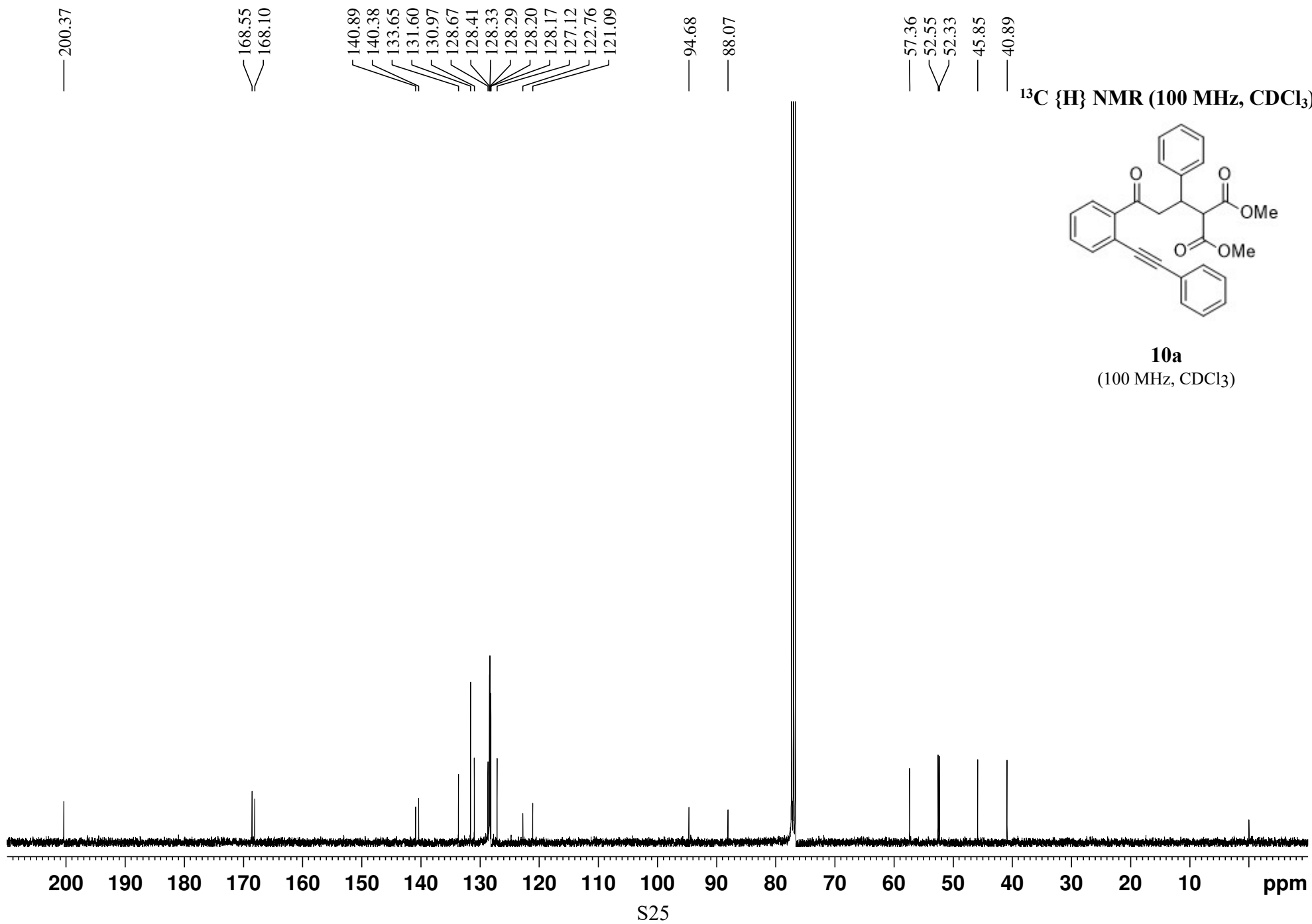
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



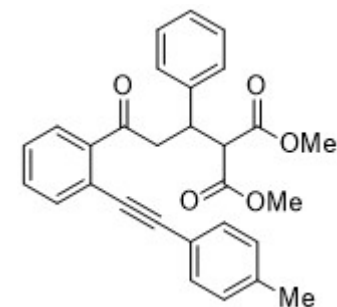
**10a**

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



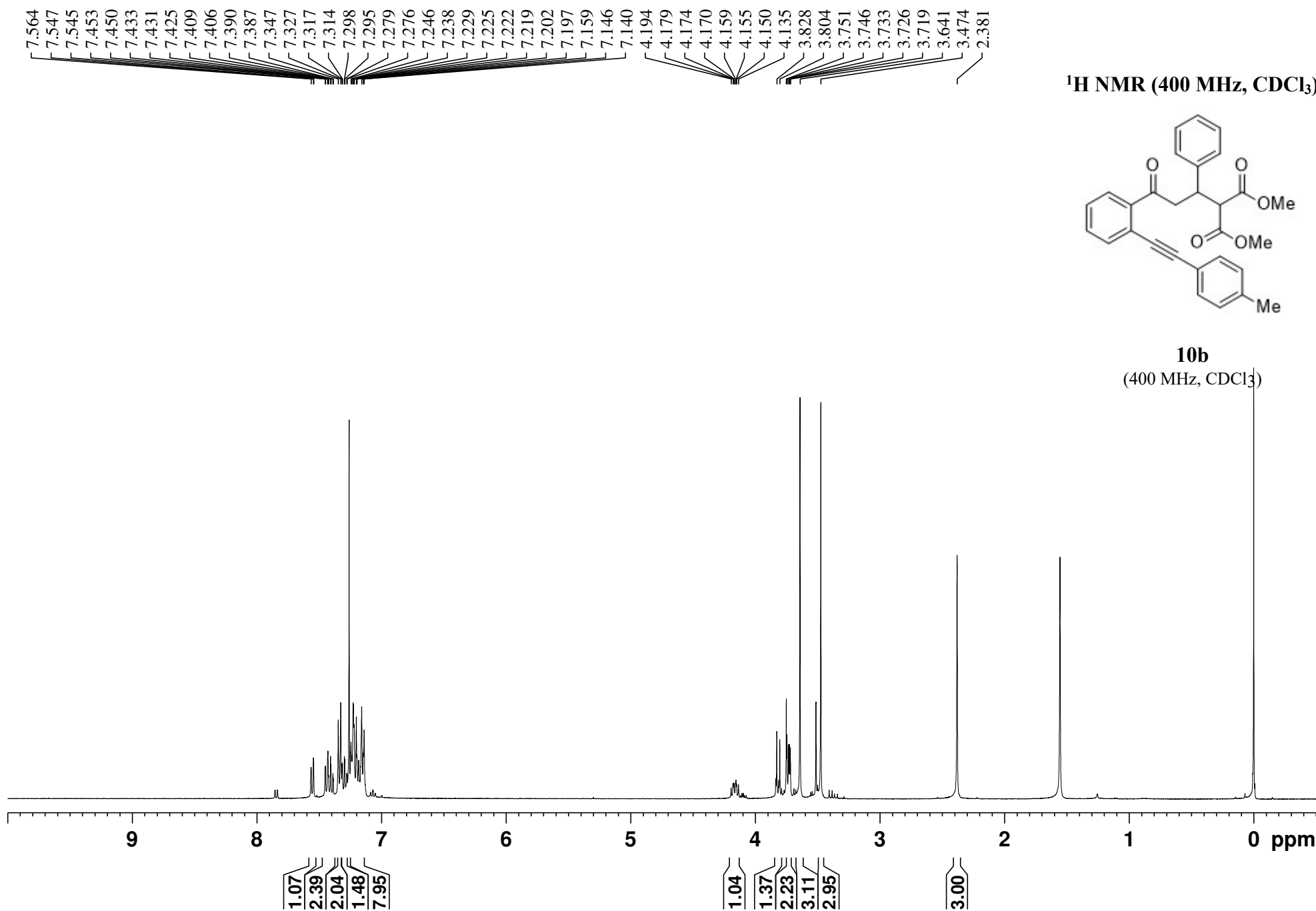


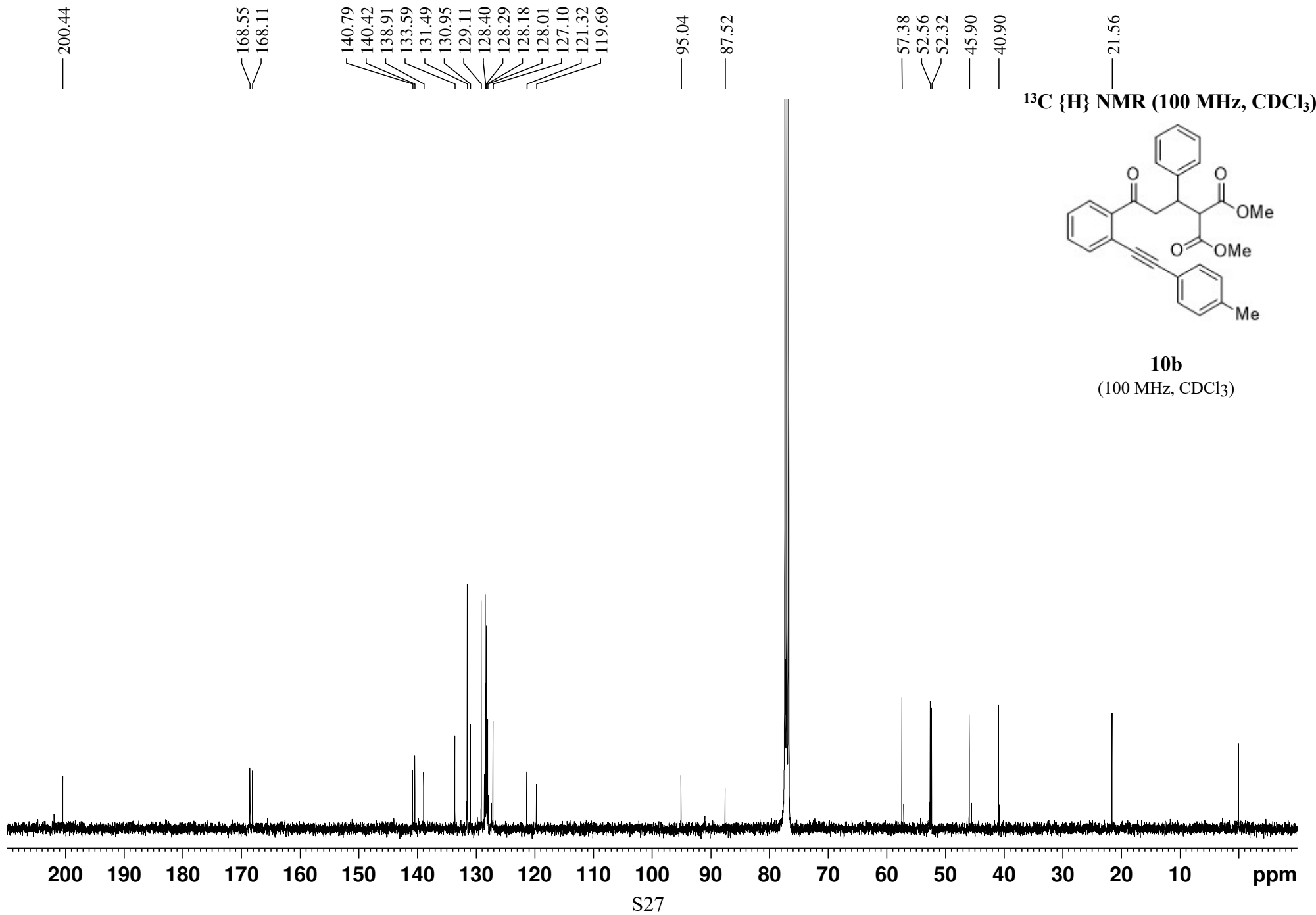
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**

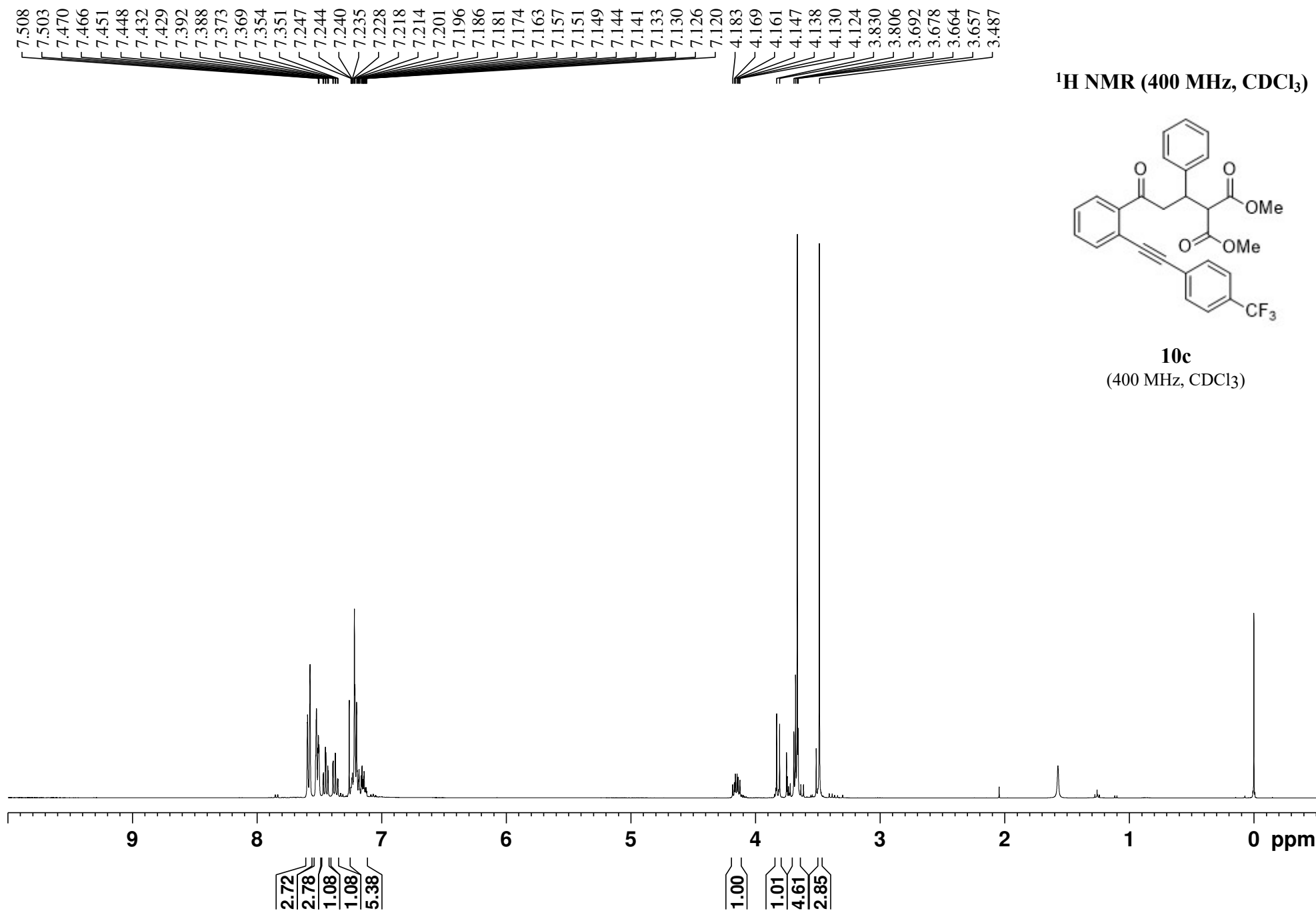


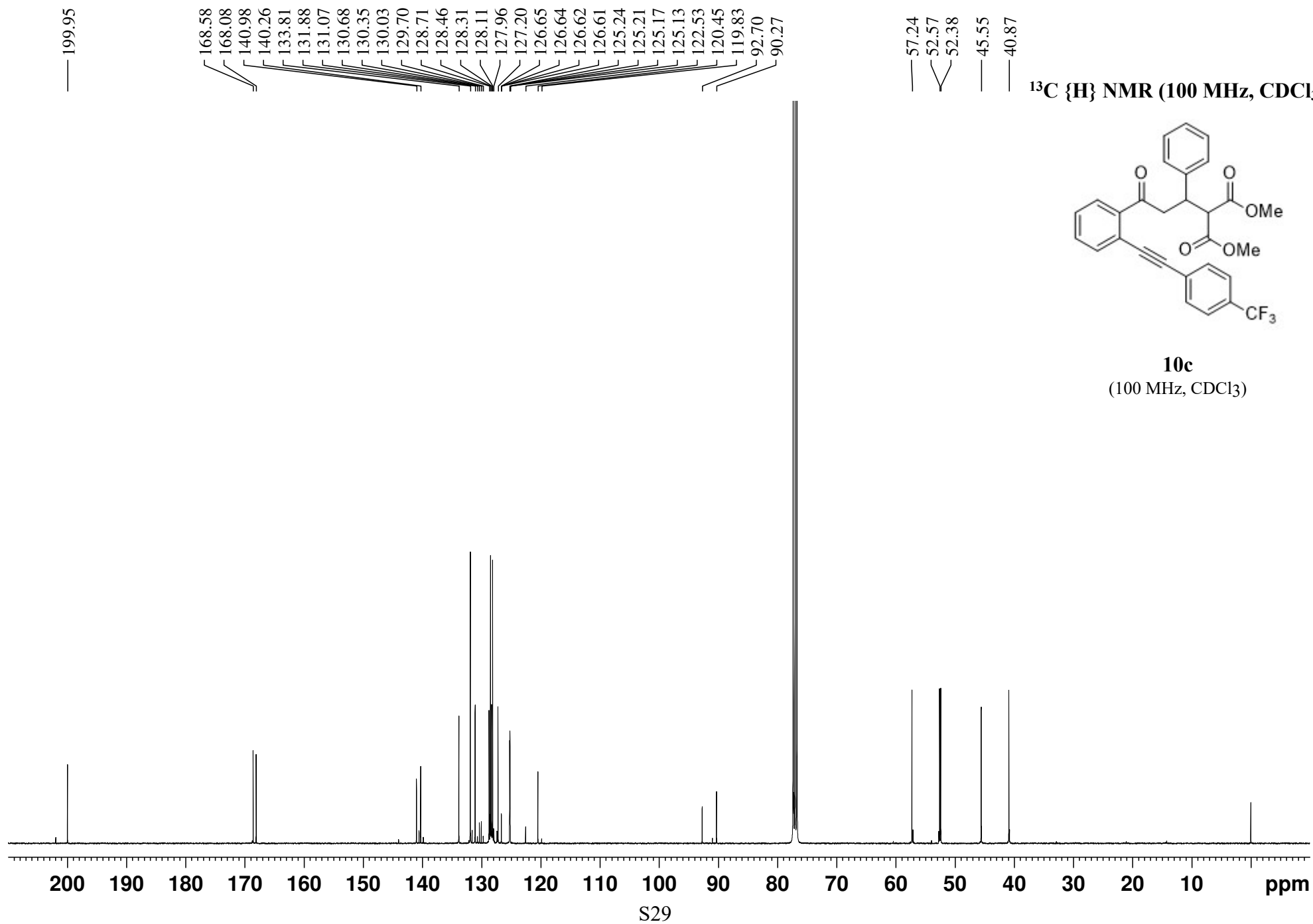
**10b**

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

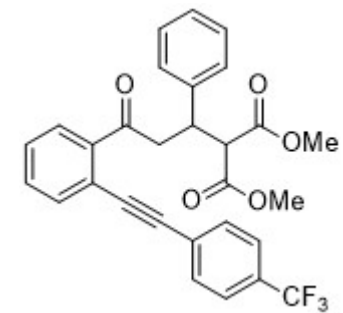




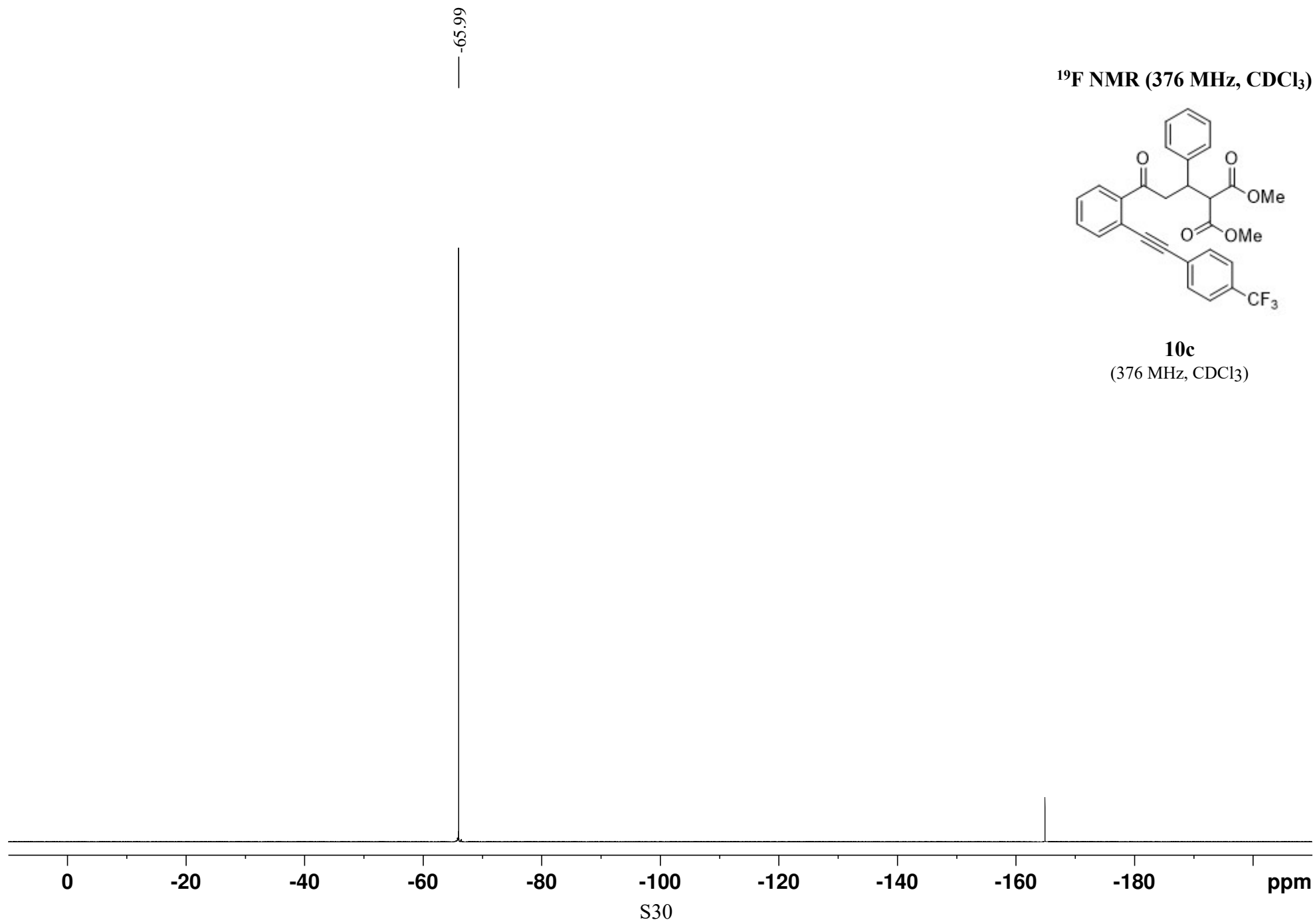


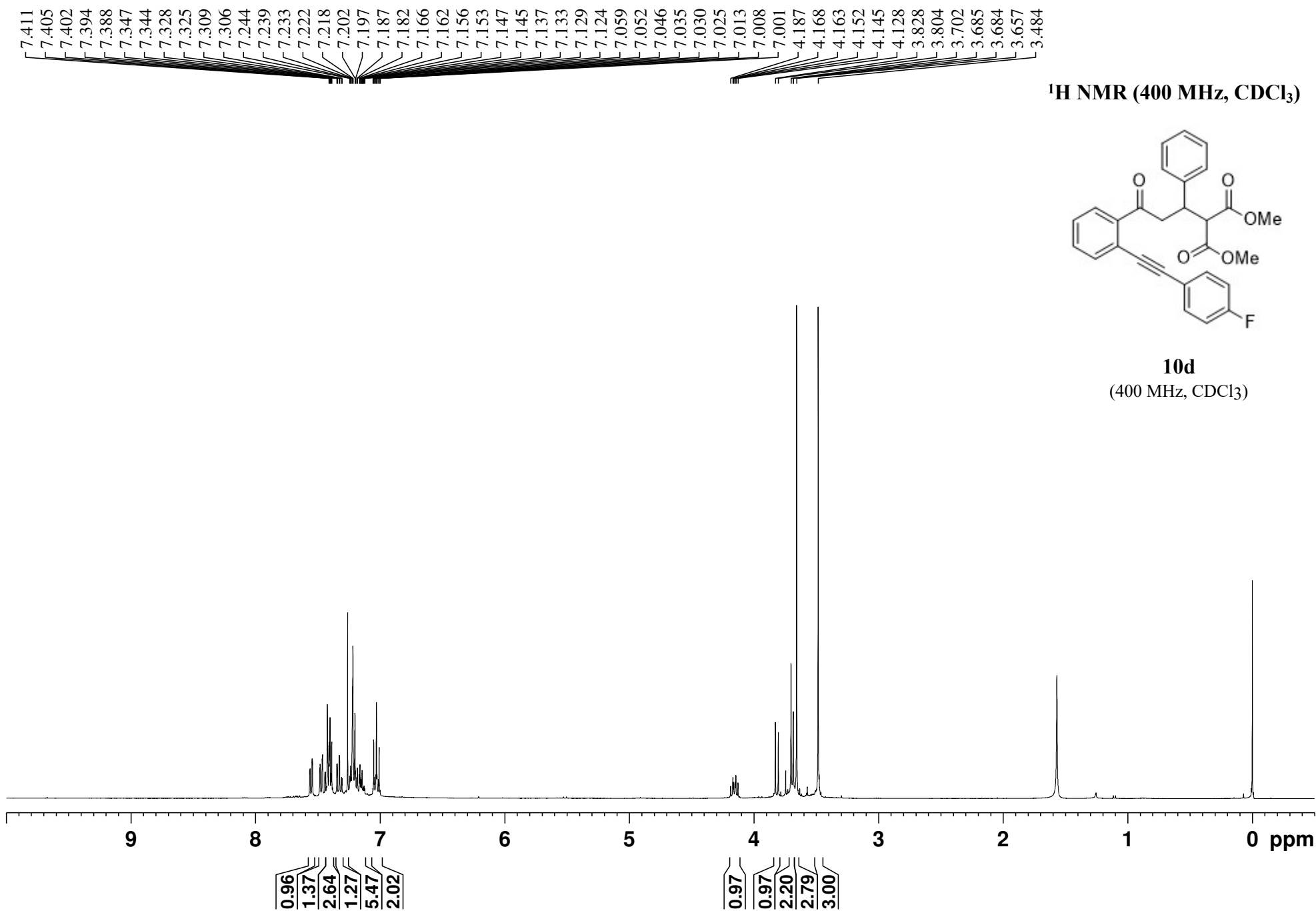


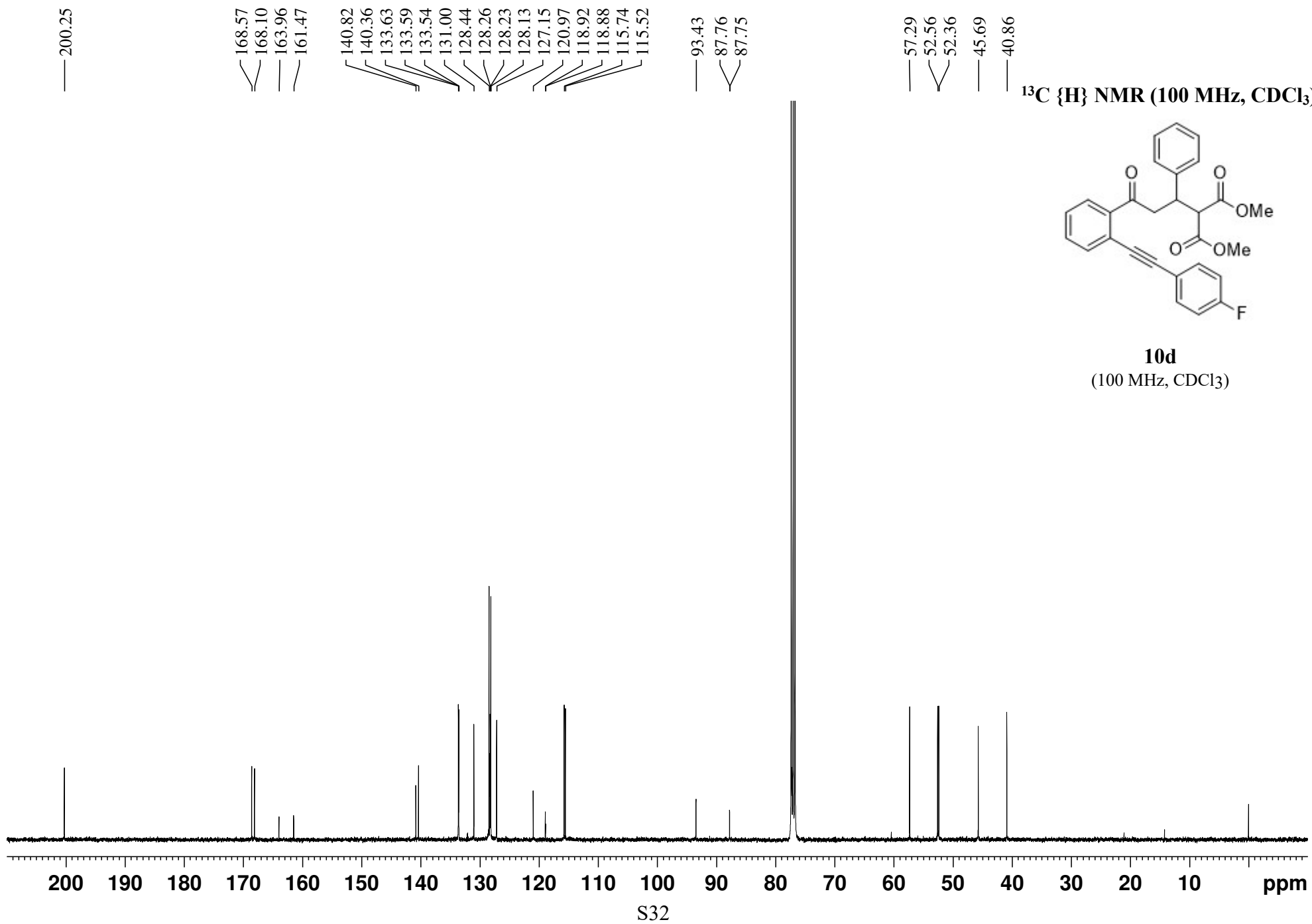
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**



**10c**  
(376 MHz,  $\text{CDCl}_3$ )

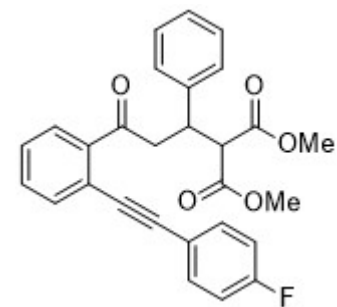






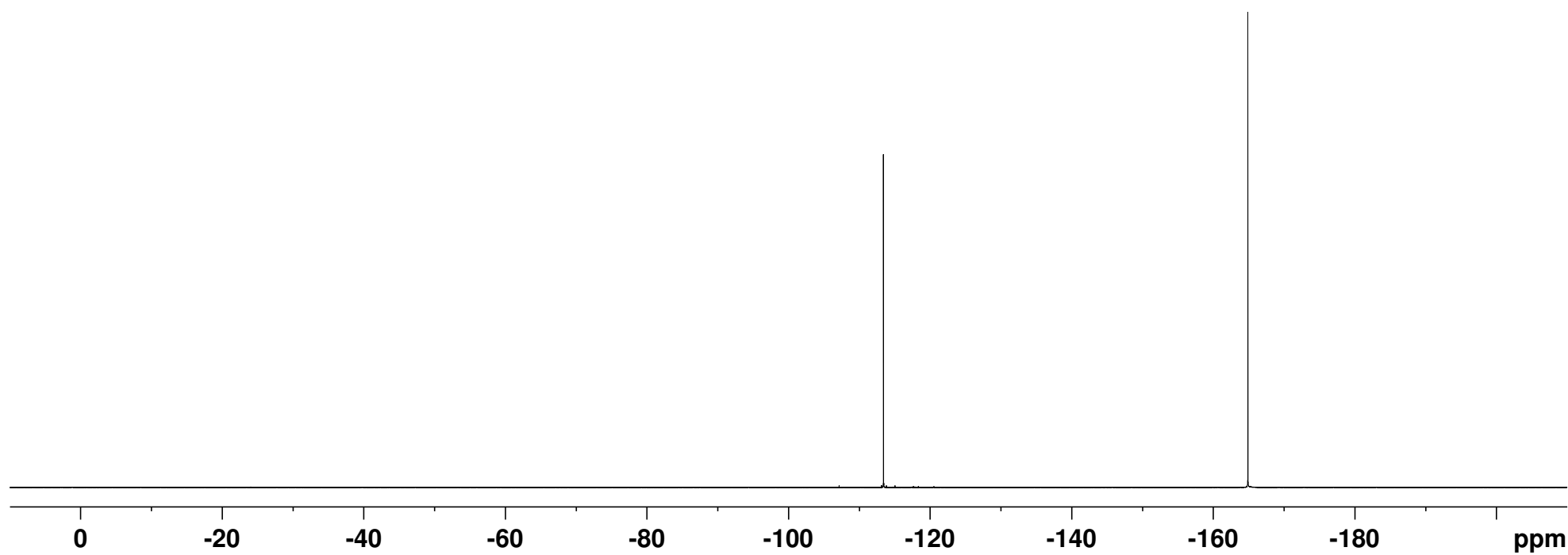
— -113.40

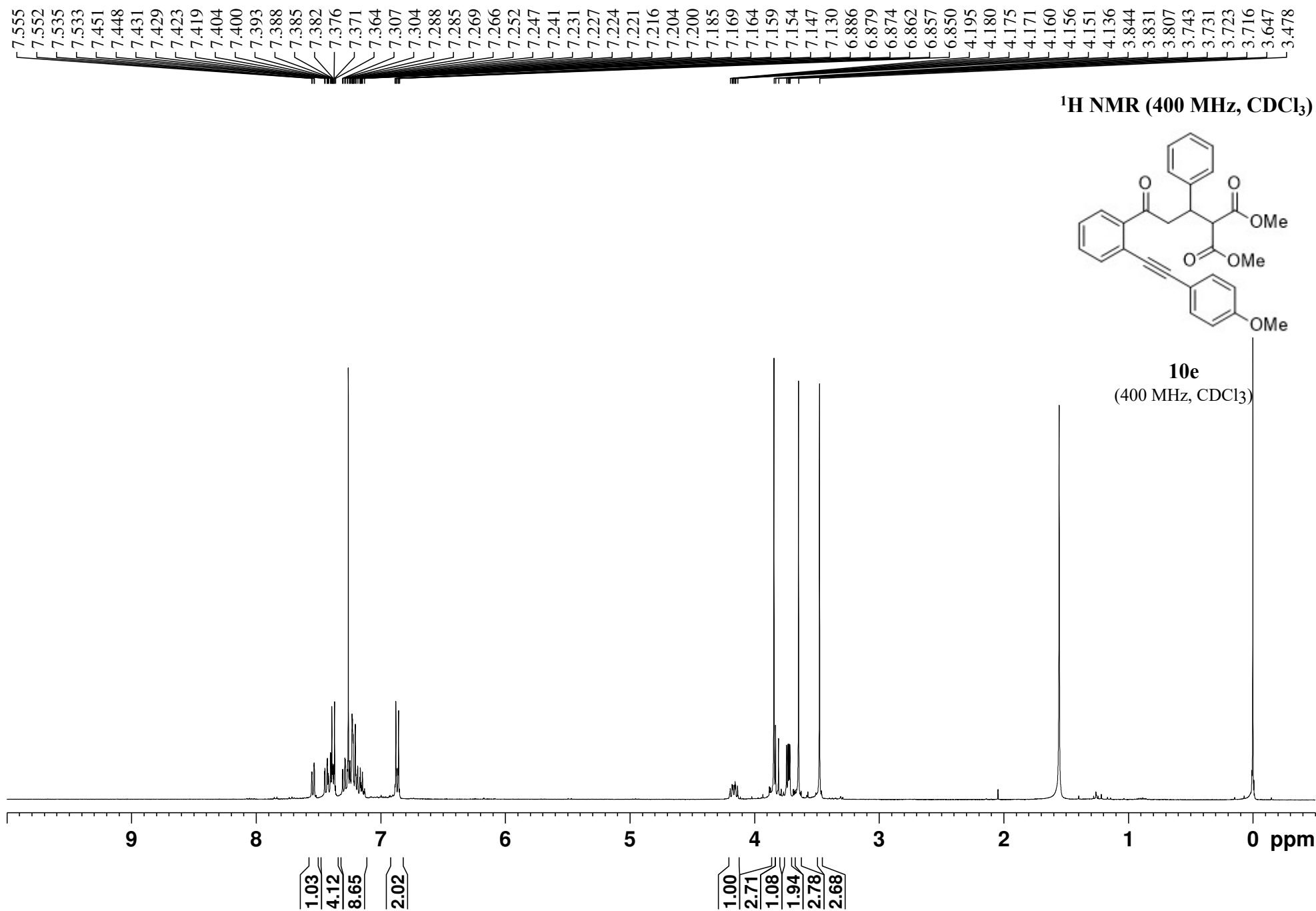
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**

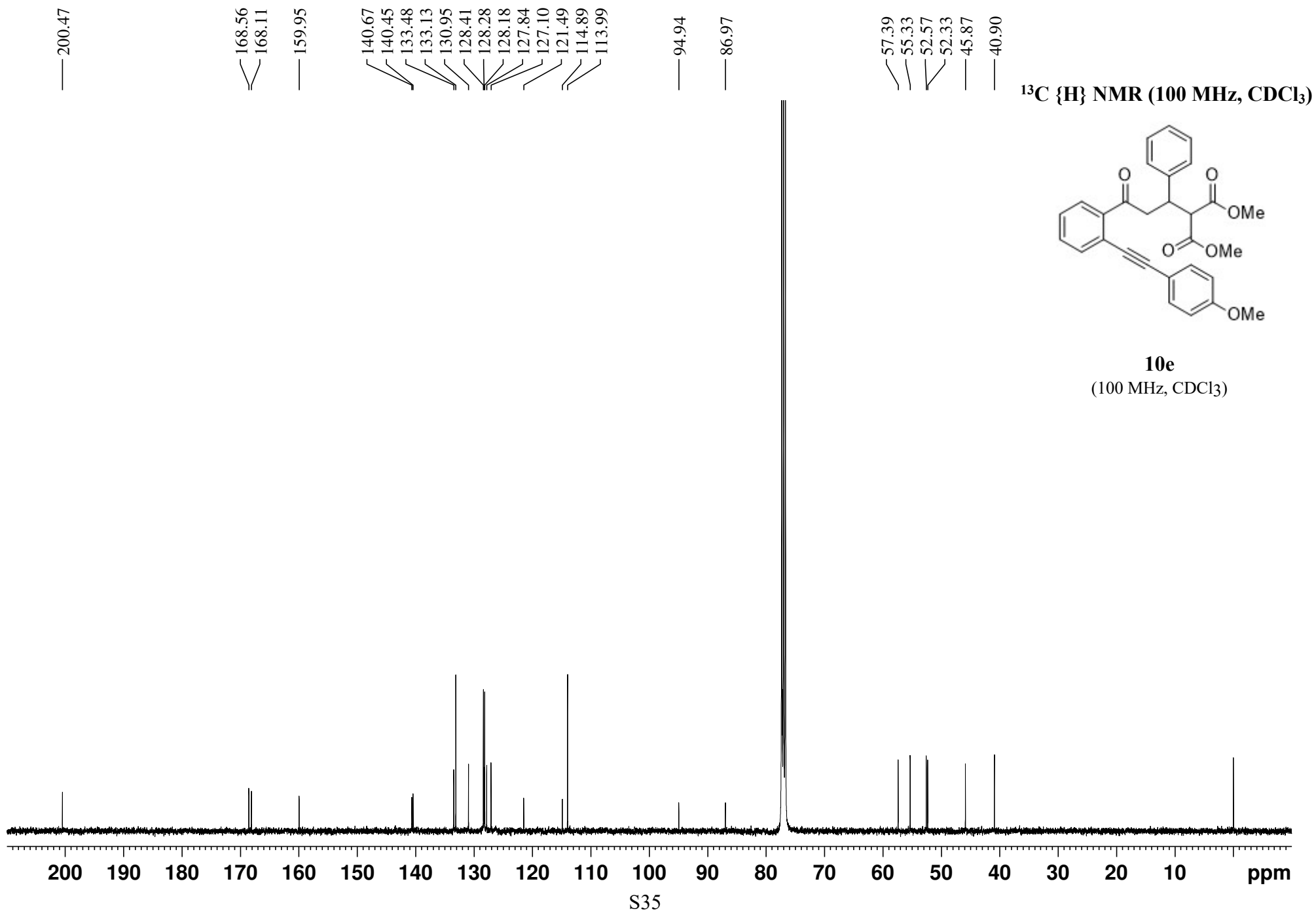


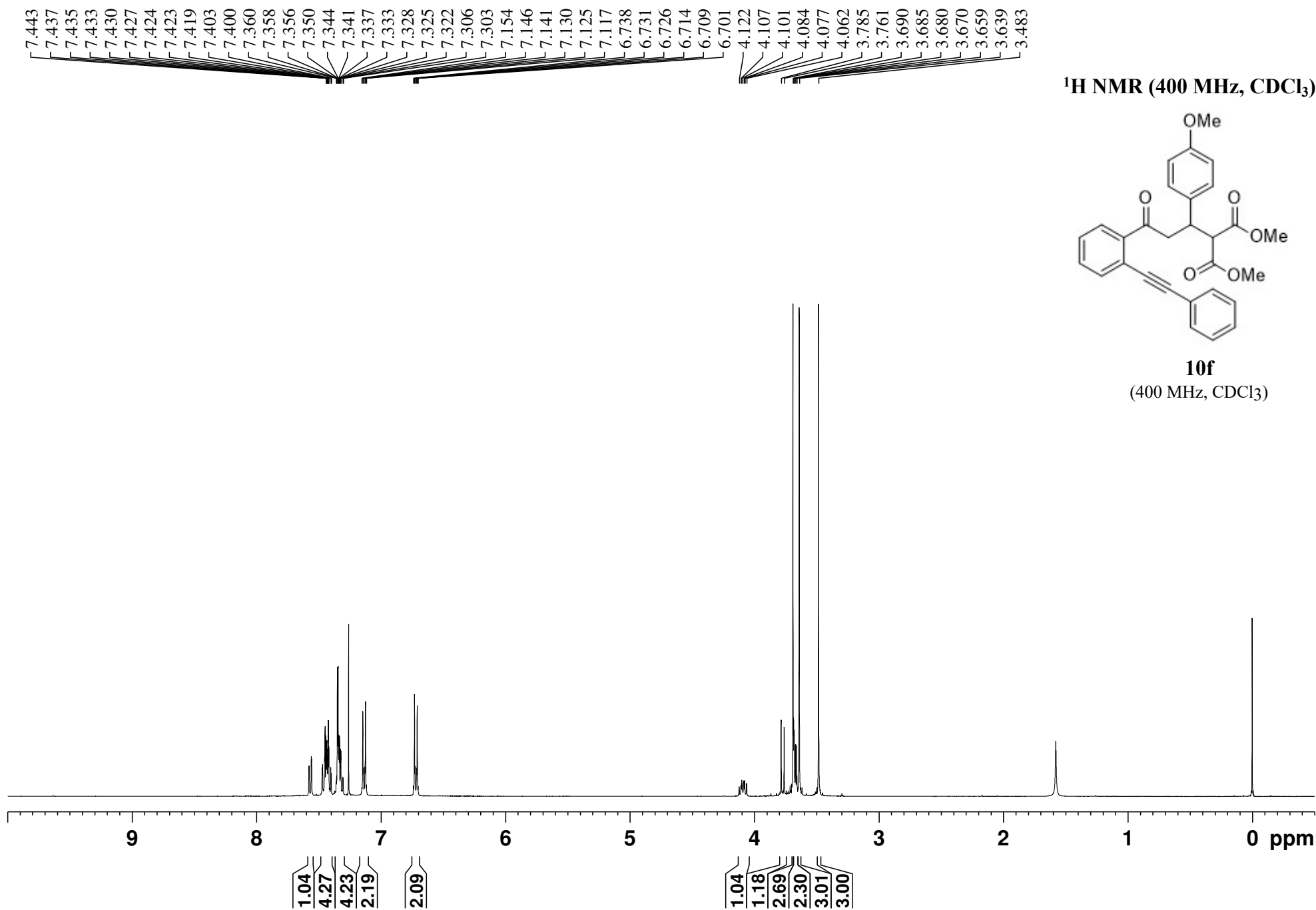
**10d**

(376 MHz,  $\text{CDCl}_3$ )









— 200.53

168.58  
168.12

— 158.45

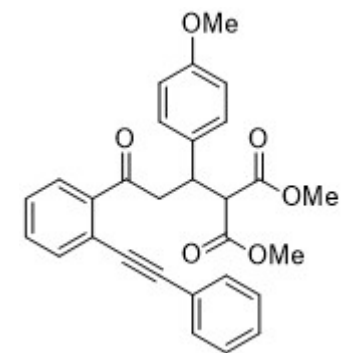
140.94  
133.60  
132.16  
131.59  
130.90  
129.20  
128.62  
128.29  
128.22  
128.16  
122.77  
121.07  
113.73

— 94.53

— 88.02

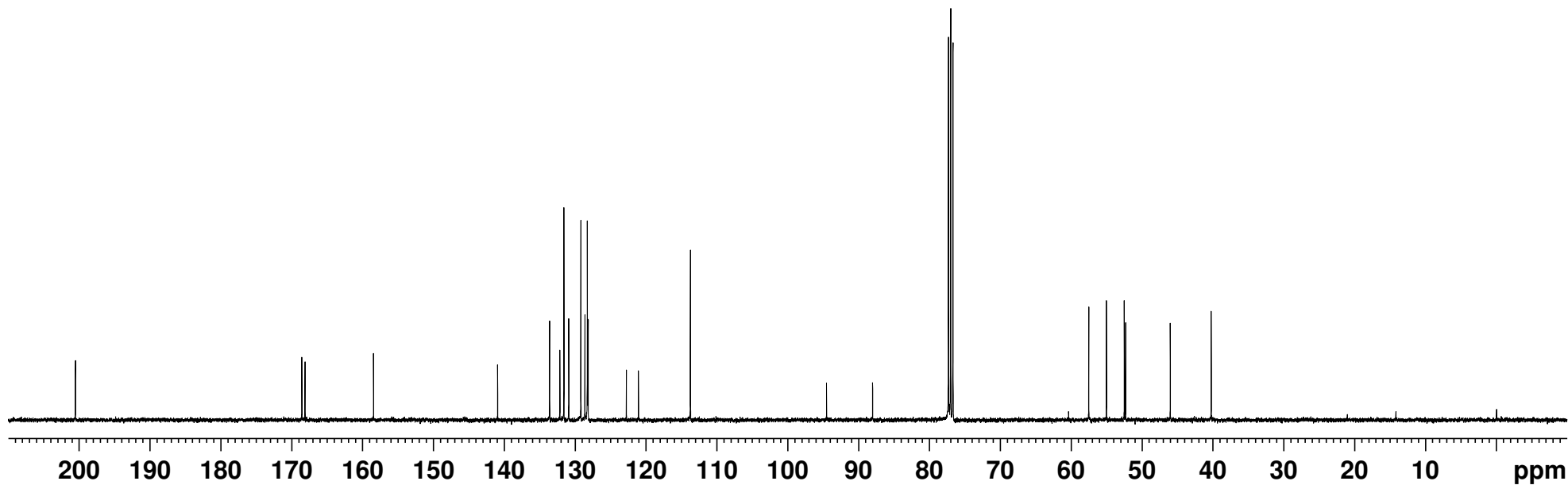
57.51  
55.02  
52.50  
52.31  
46.01  
40.23

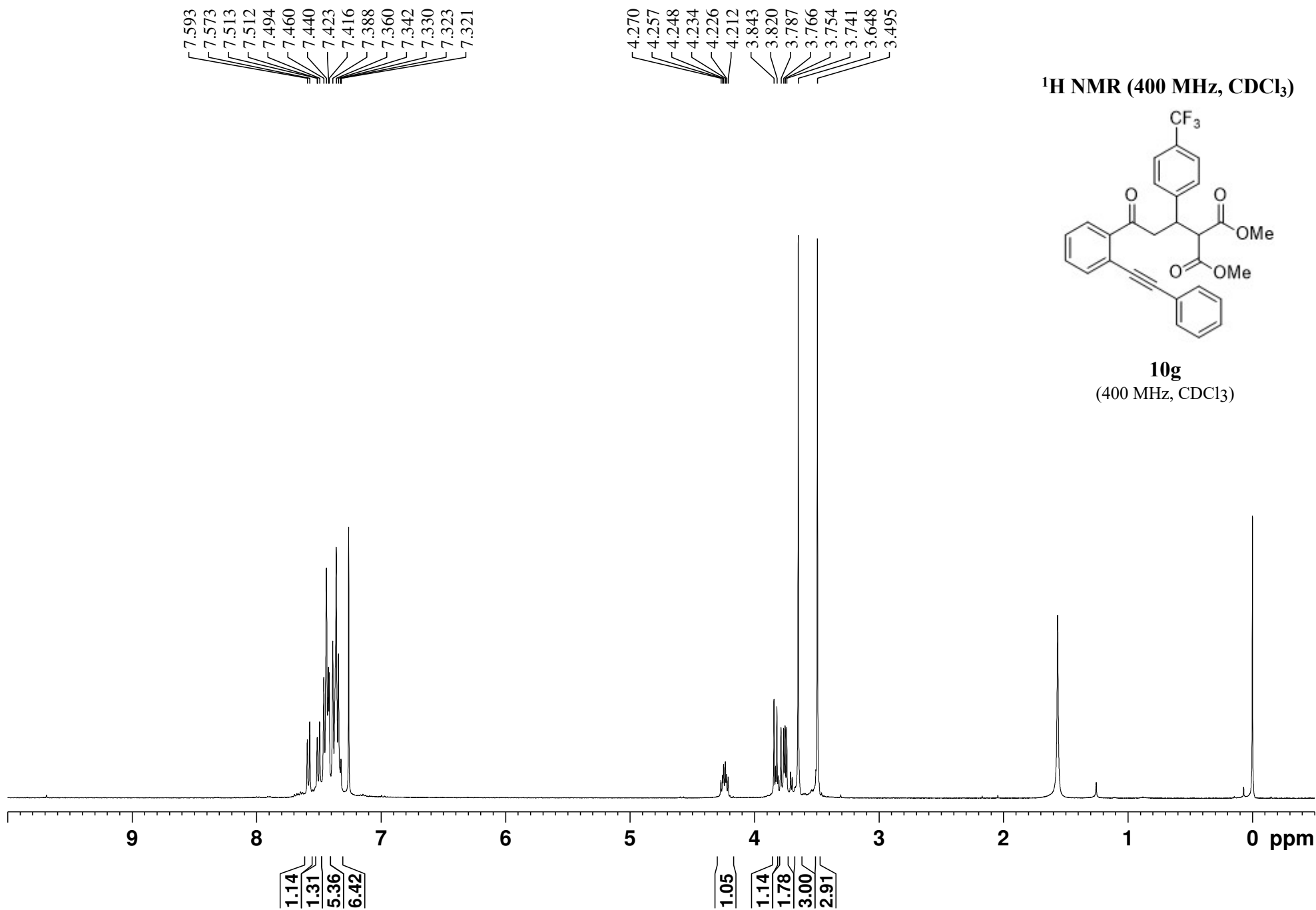
<sup>13</sup>C {<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>)

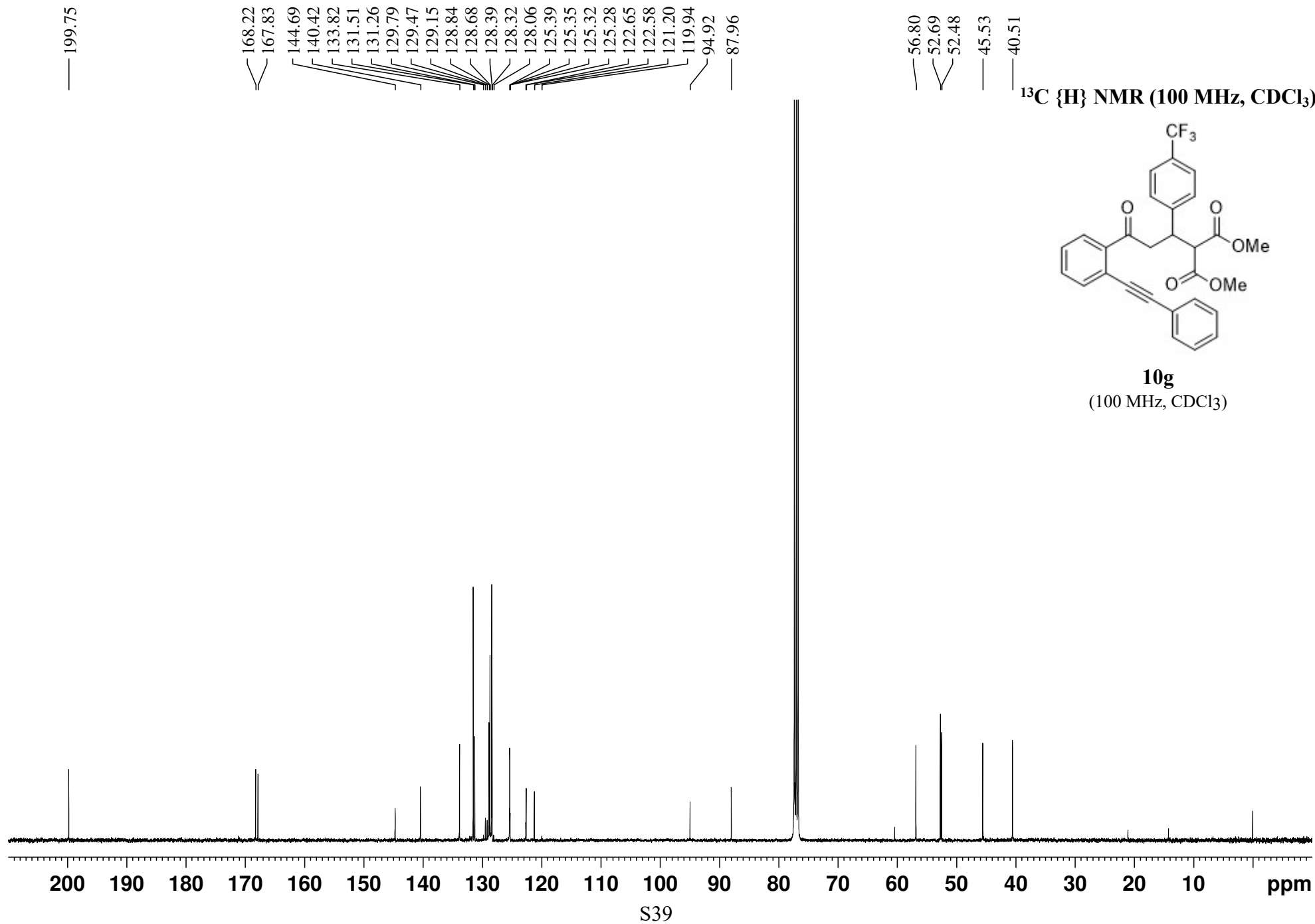


**10f**

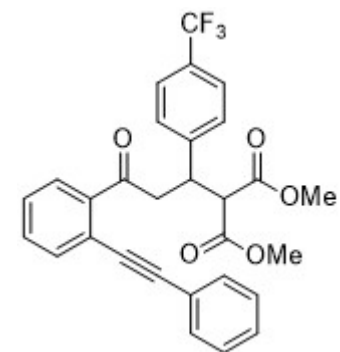
(100 MHz, CDCl<sub>3</sub>)







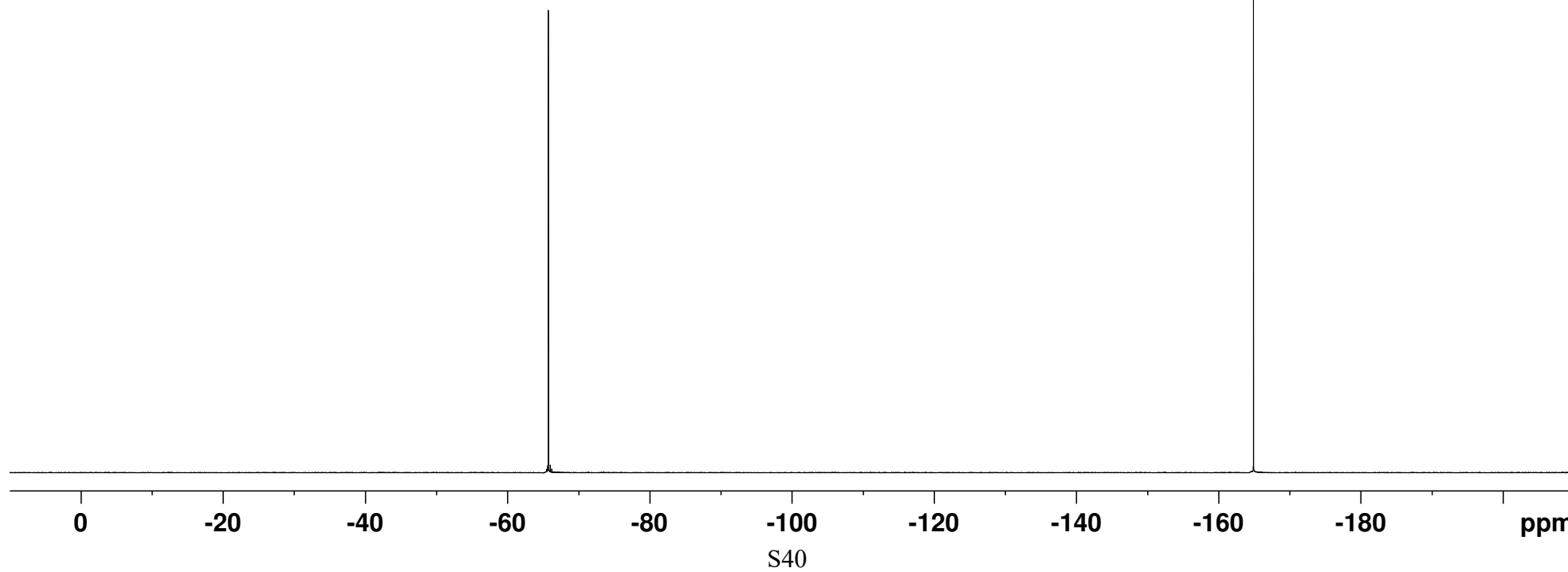
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**

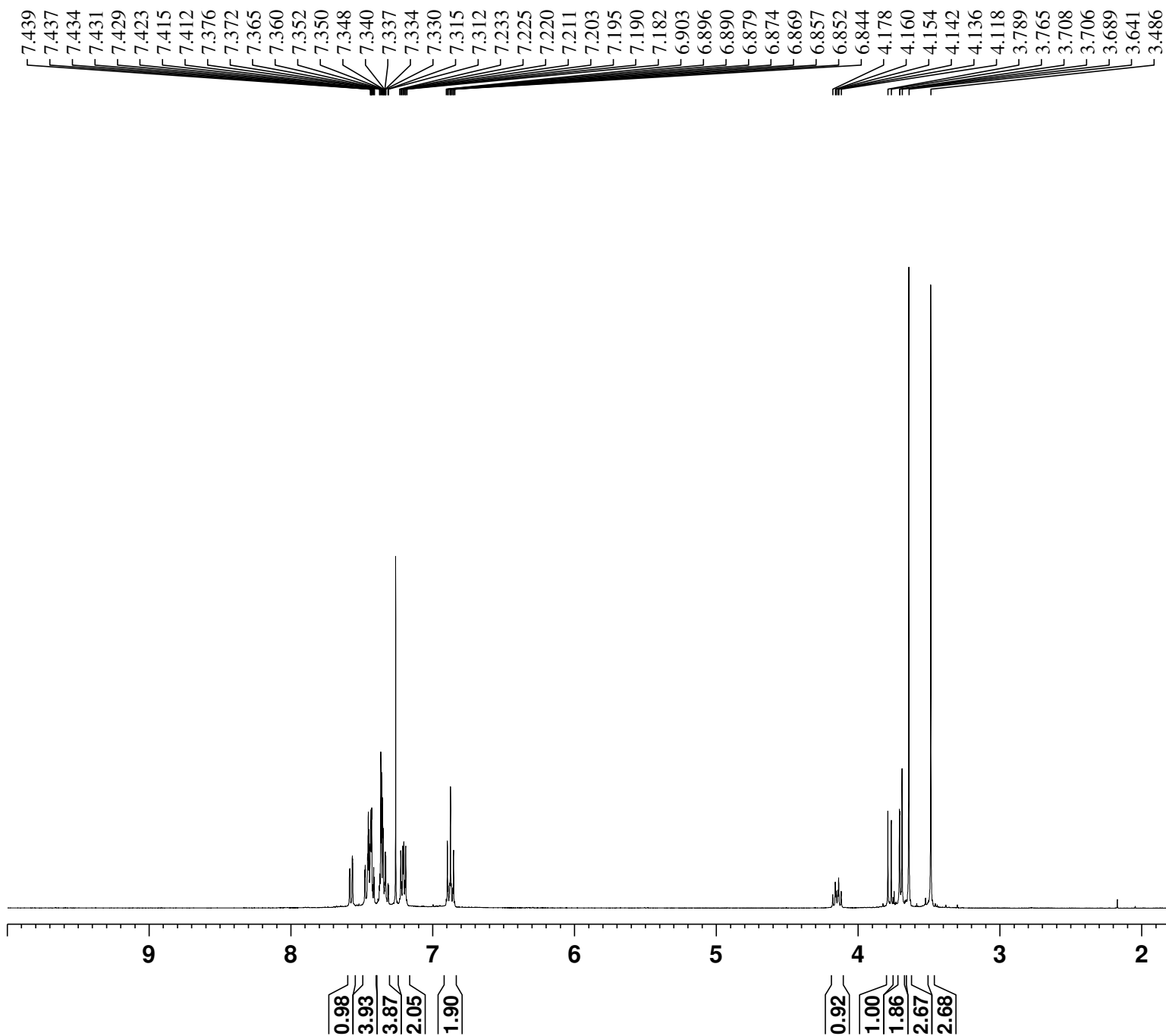


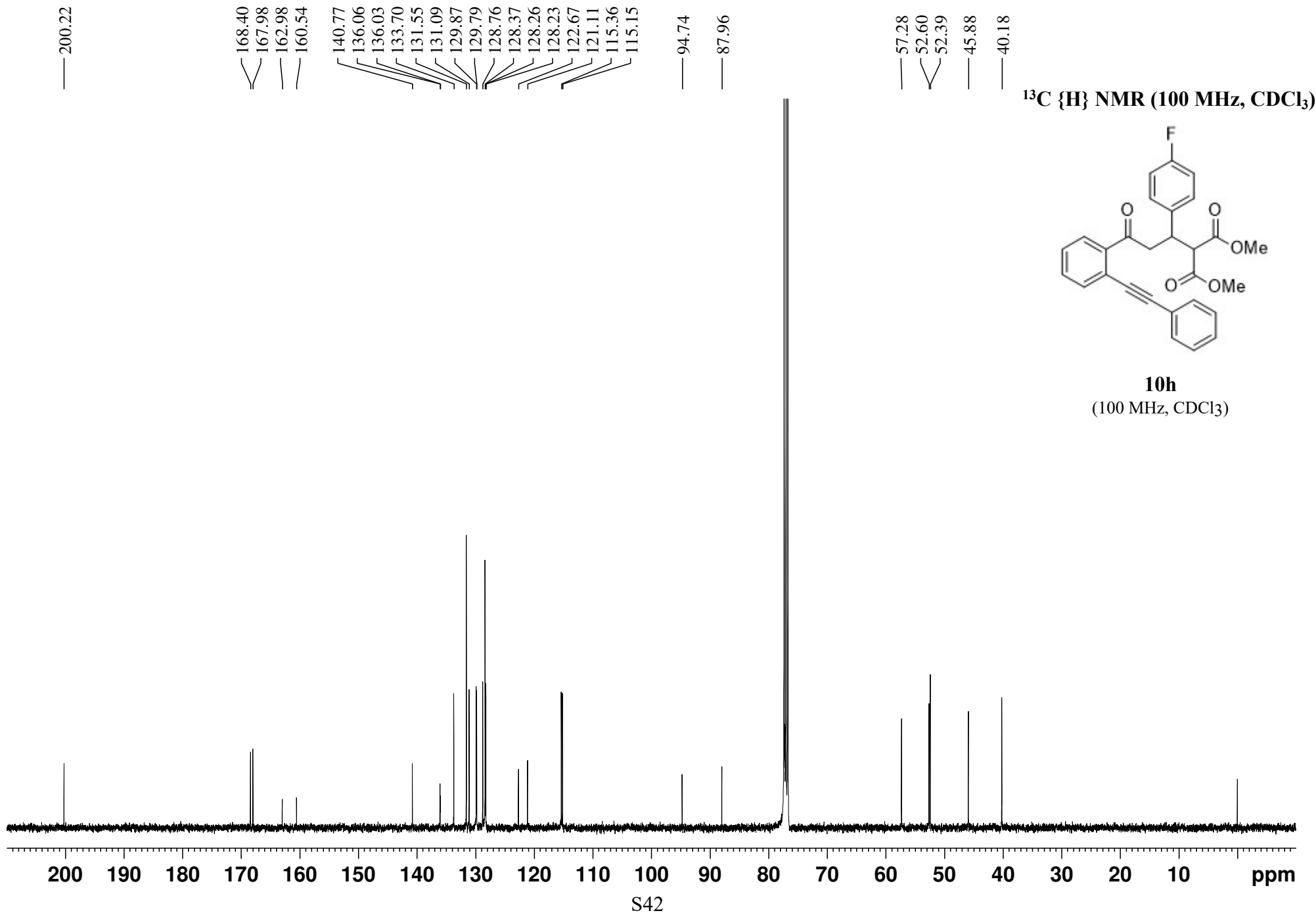
**10g**

(376 MHz,  $\text{CDCl}_3$ )

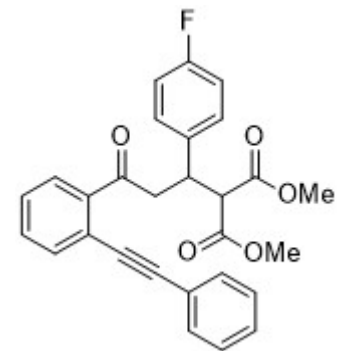
— -65.75







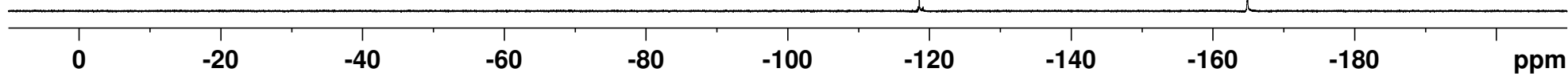
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**



**10h**

(376 MHz,  $\text{CDCl}_3$ )

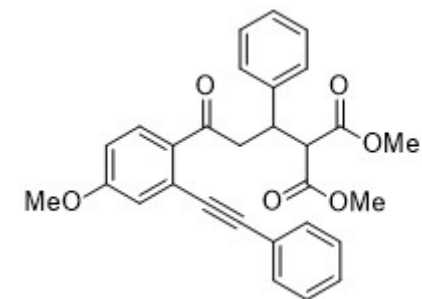
— -118.56



S43

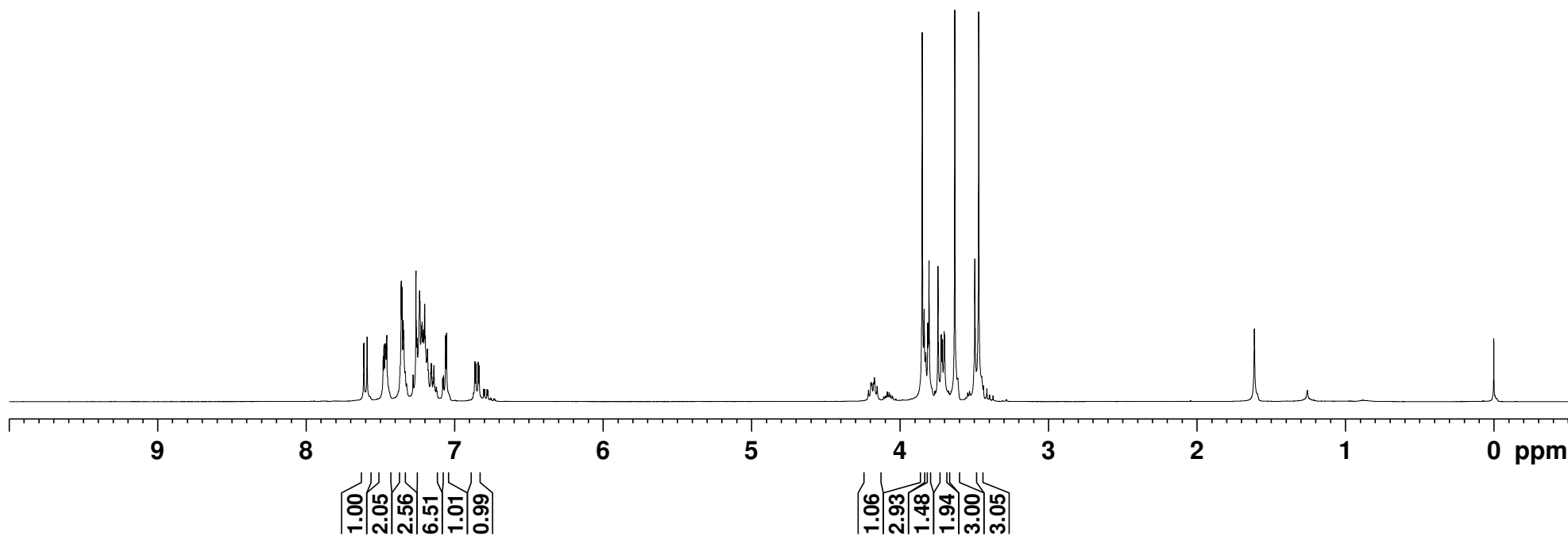
7.459  
7.456  
7.359  
7.354  
7.346  
7.342  
7.253  
7.246  
7.236  
7.233  
7.226  
7.221  
7.219  
7.214  
7.210  
7.201  
7.197  
7.186  
7.183  
7.177  
7.160  
7.157  
7.152  
7.146  
7.139  
7.132  
7.125  
7.122  
7.118  
7.060  
7.054  
6.863  
6.856  
6.841  
6.834  
4.212  
4.196  
4.193  
4.188  
4.177  
4.172  
4.153  
3.850  
3.813  
3.809  
3.804  
3.722  
3.715  
3.703  
3.699  
3.631  
3.469

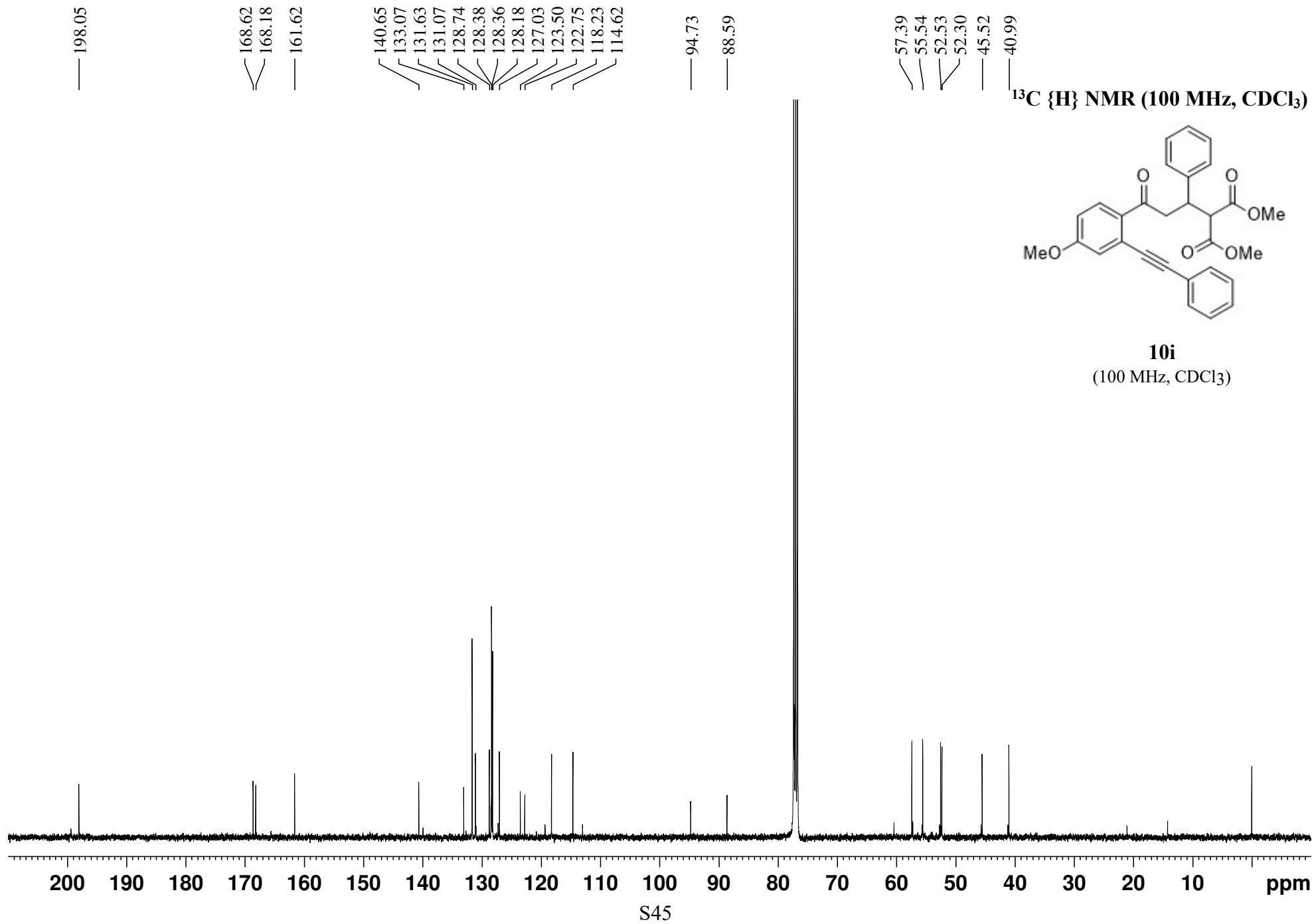
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



**10i**

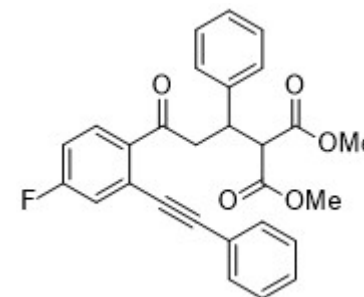
(400 MHz, CDCl<sub>3</sub>)





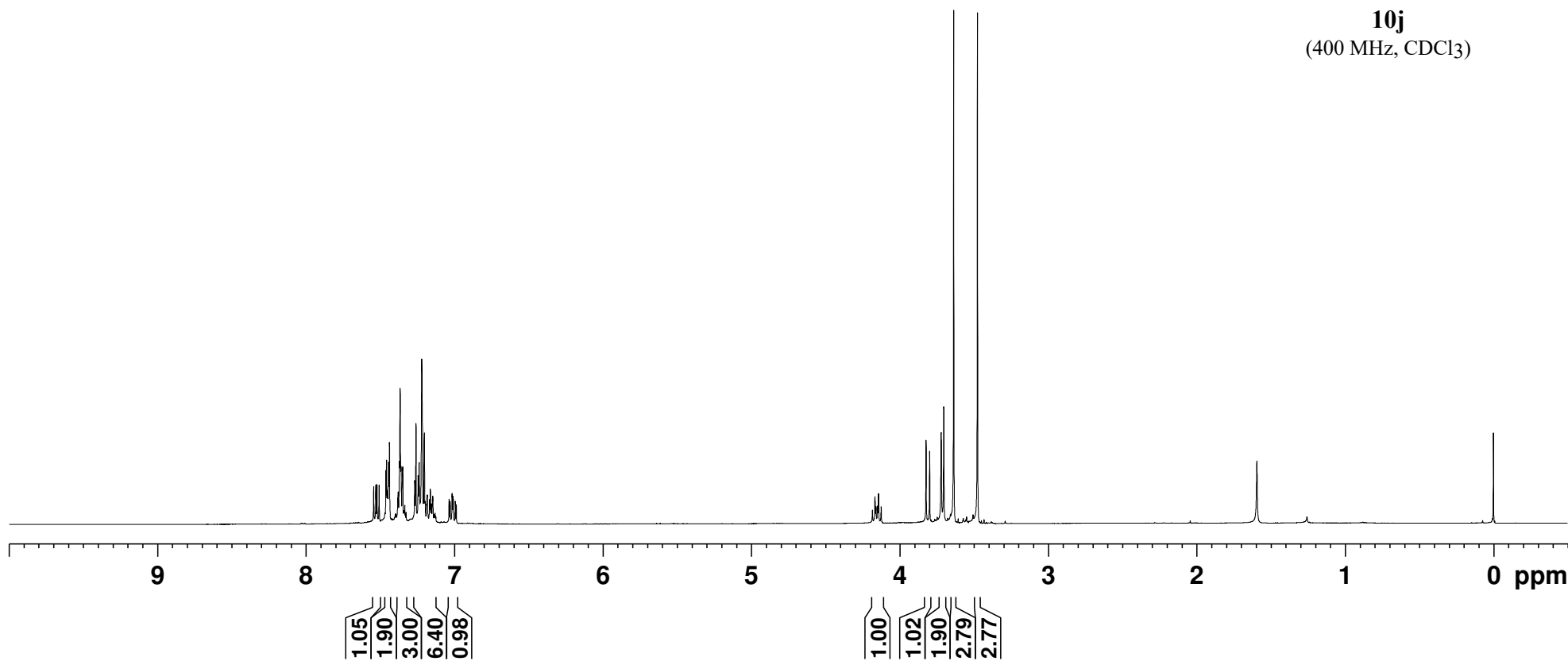
7.544  
7.529  
7.522  
7.507  
7.468  
7.461  
7.457  
7.453  
7.451  
7.448  
7.444  
7.437  
7.382  
7.379  
7.370  
7.366  
7.361  
7.359  
7.352  
7.350  
7.348  
7.342  
7.338  
7.334  
7.330  
7.326  
7.267  
7.258  
7.244  
7.238  
7.230  
7.220  
7.202  
7.197  
7.187  
7.183  
7.167  
7.162  
7.156  
7.154  
7.148  
7.146  
7.138  
7.135  
7.130  
7.035  
7.029  
7.016  
7.014  
7.009  
7.007  
6.994  
6.987  
4.184  
4.166  
4.160  
4.149  
4.143  
4.125  
3.822  
3.798  
3.721  
3.703  
3.636  
3.476

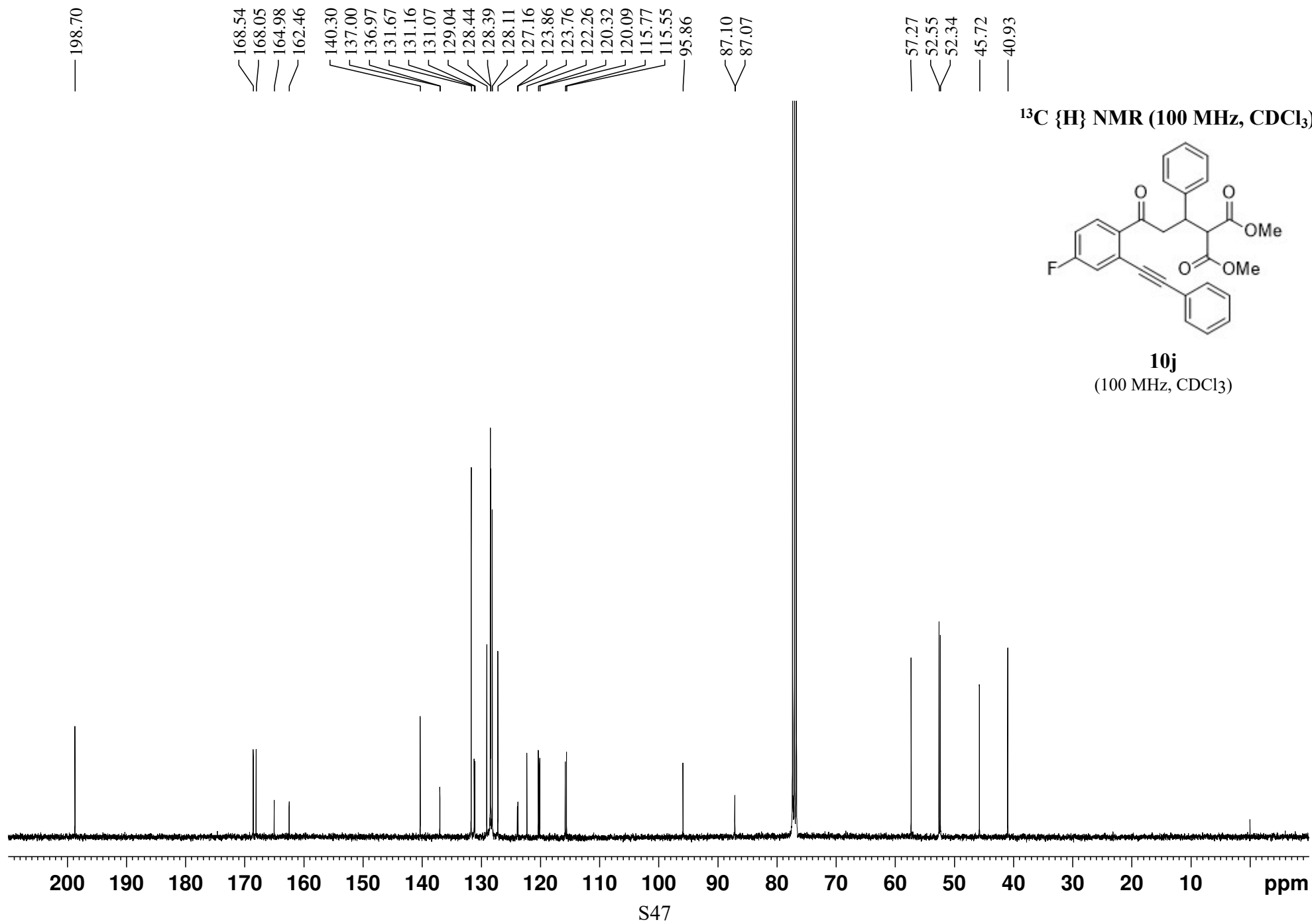
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



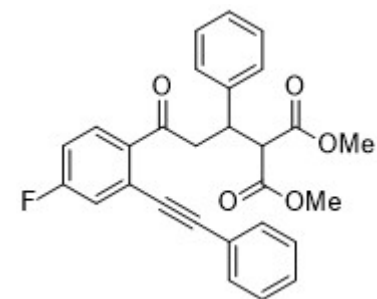
**10j**

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



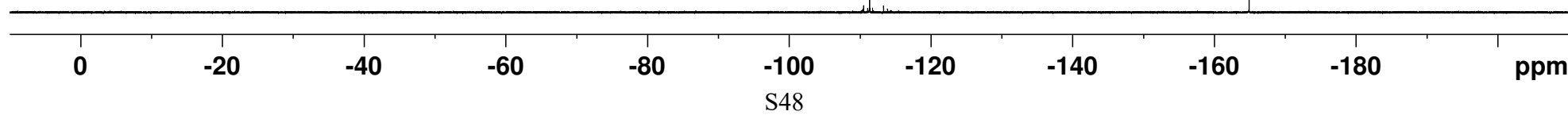


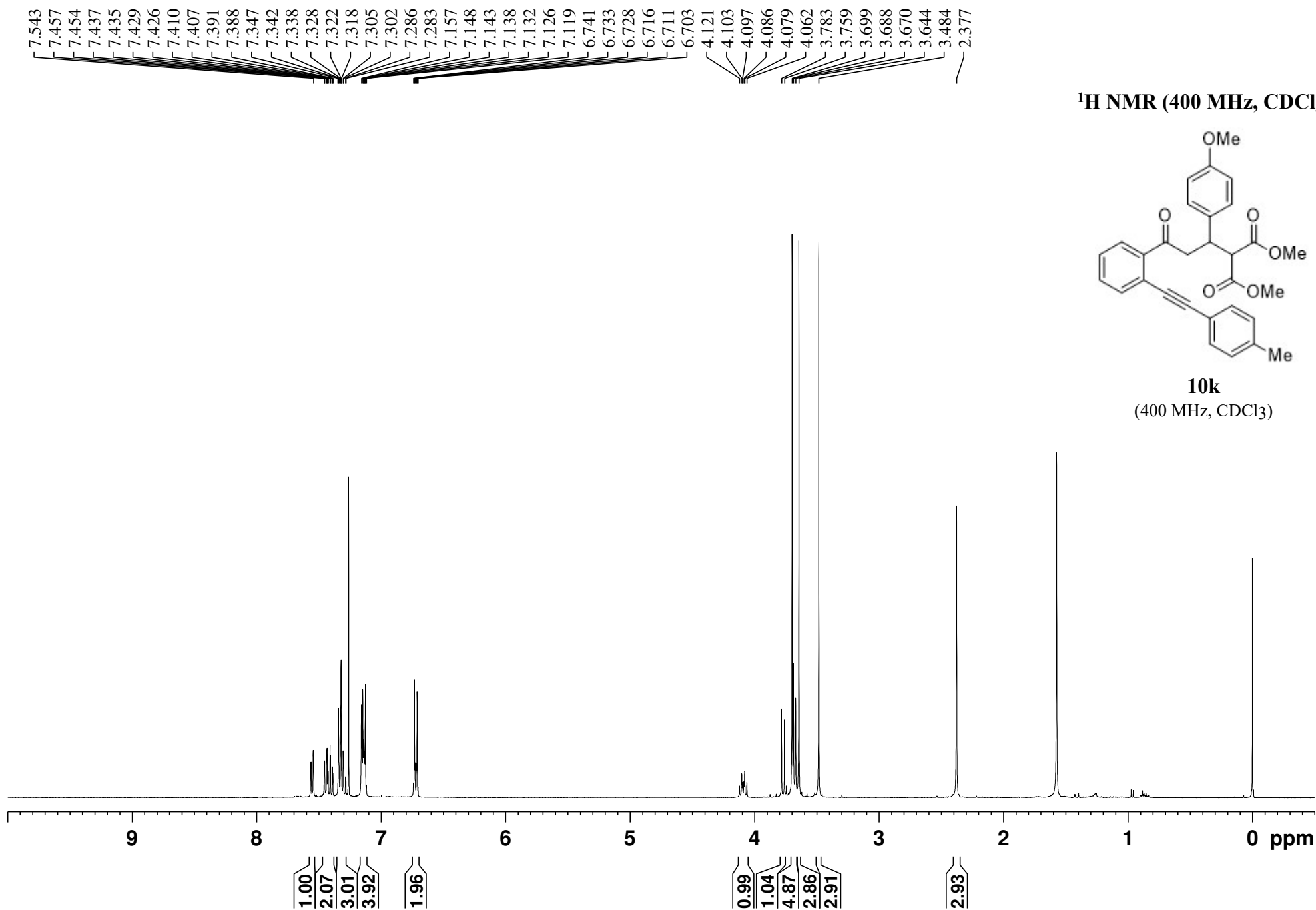
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**

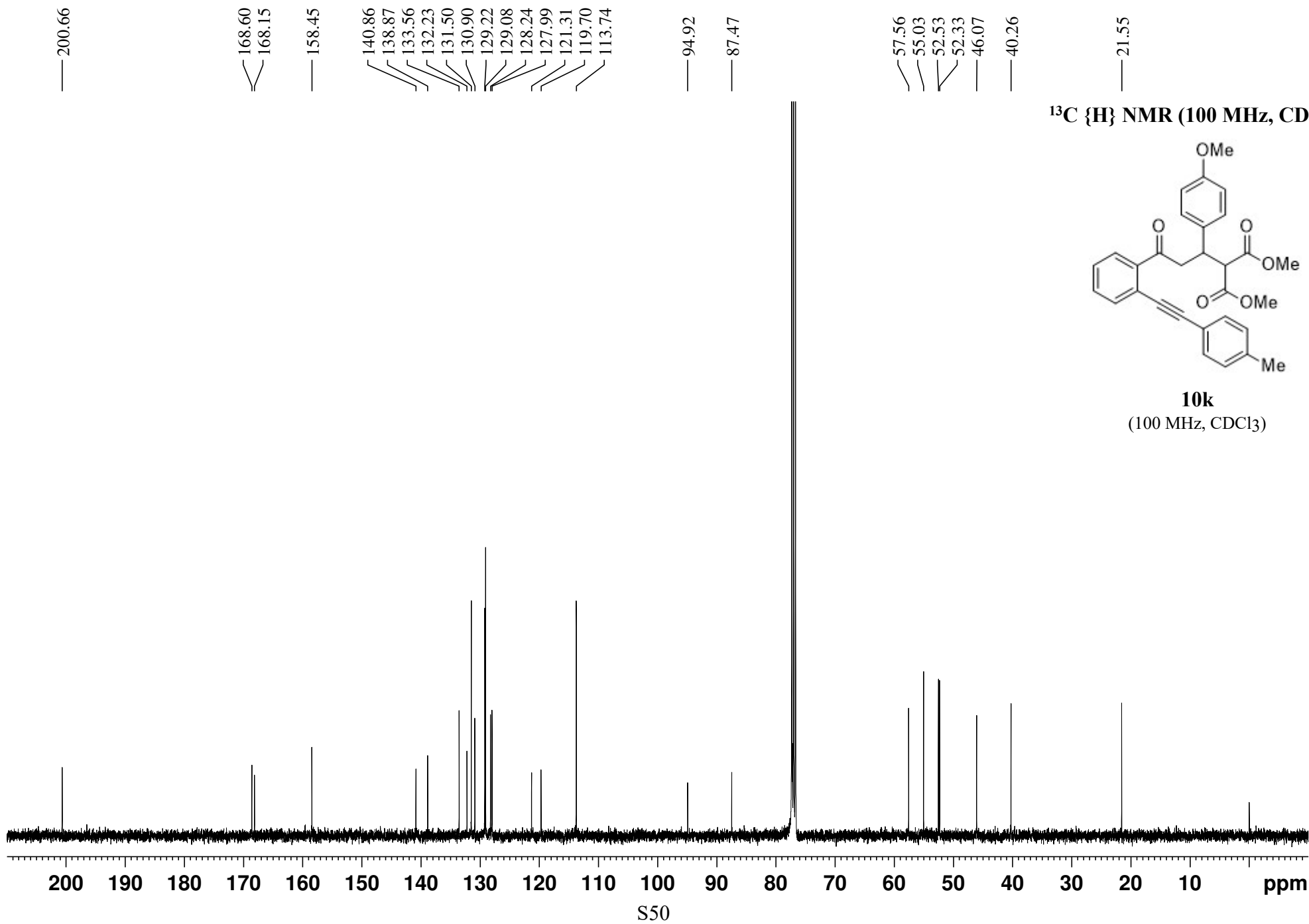


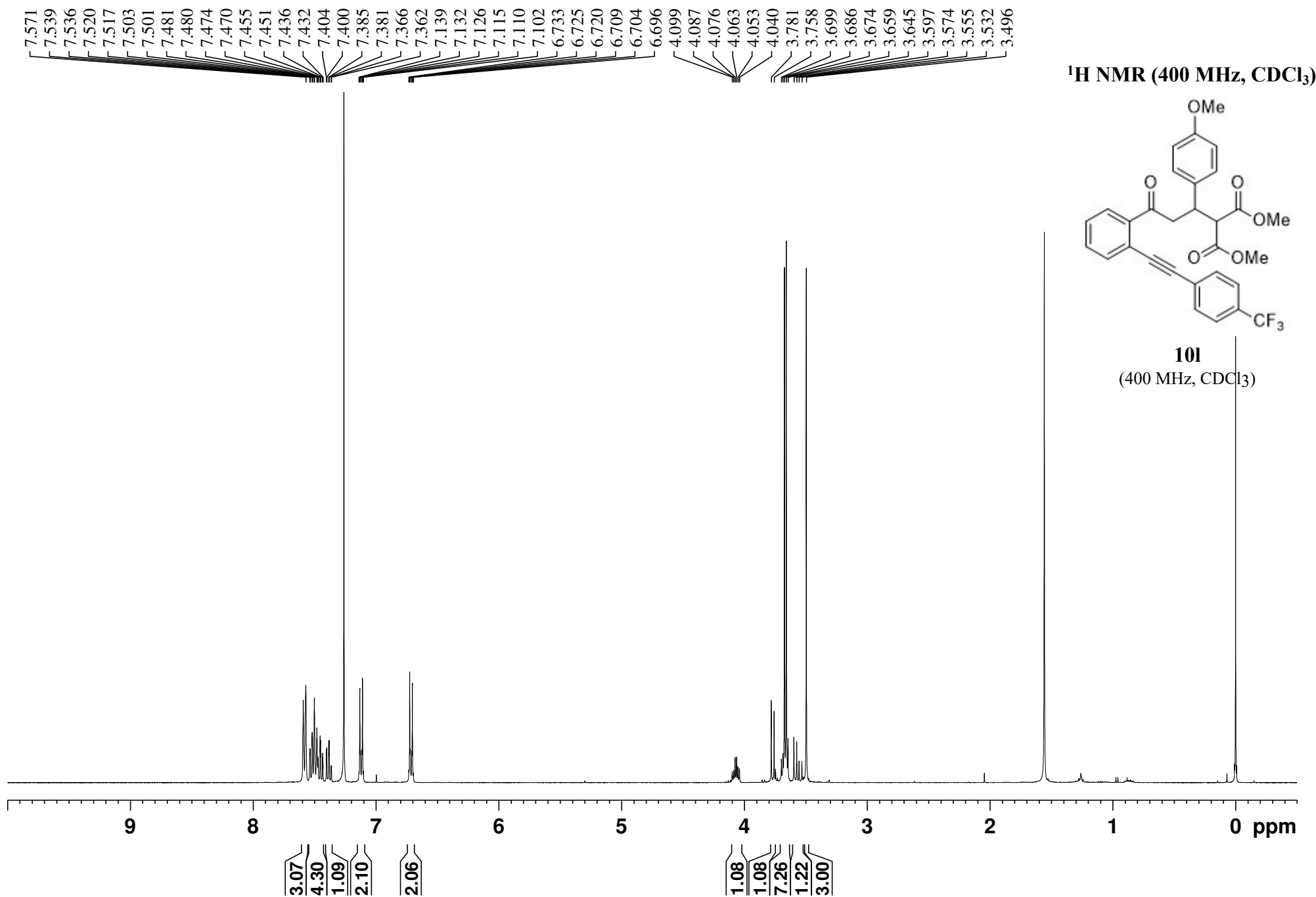
**10j**  
(376 MHz,  $\text{CDCl}_3$ )

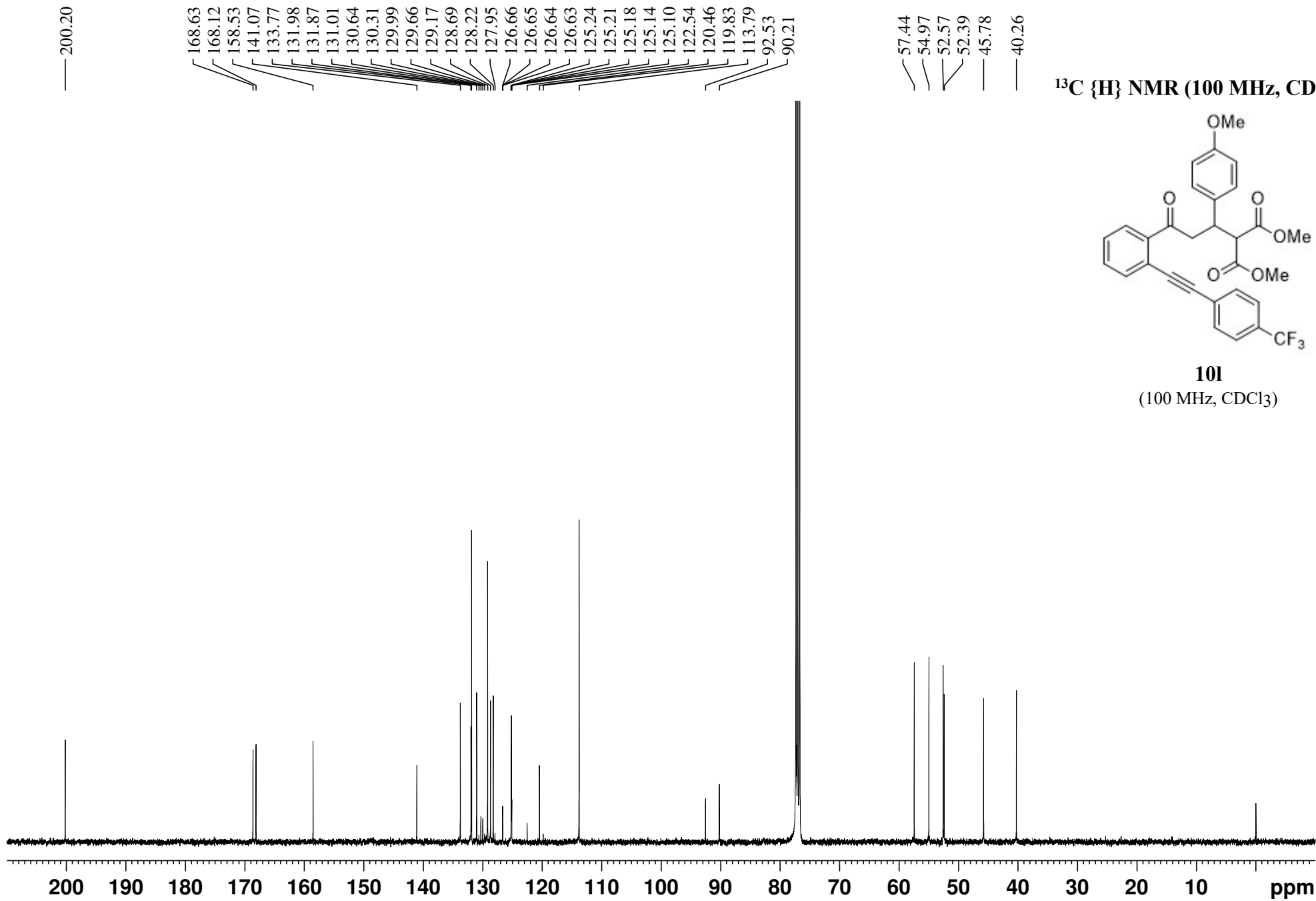
— -111.35



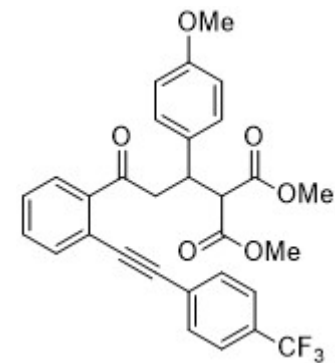








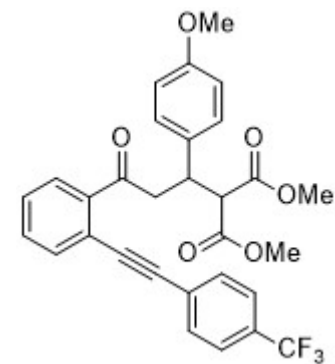
$^{13}\text{C}$  {H} NMR (100 MHz,  $\text{CDCl}_3$ )



**10l**

(100 MHz,  $\text{CDCl}_3$ )

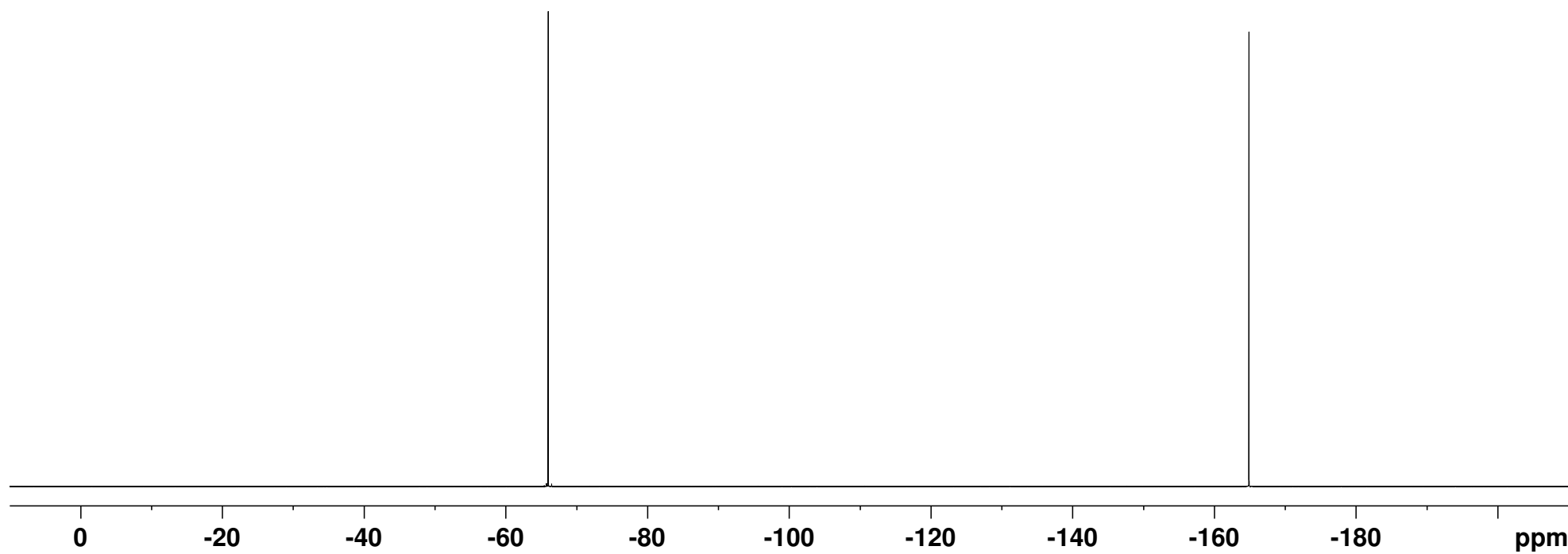
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**



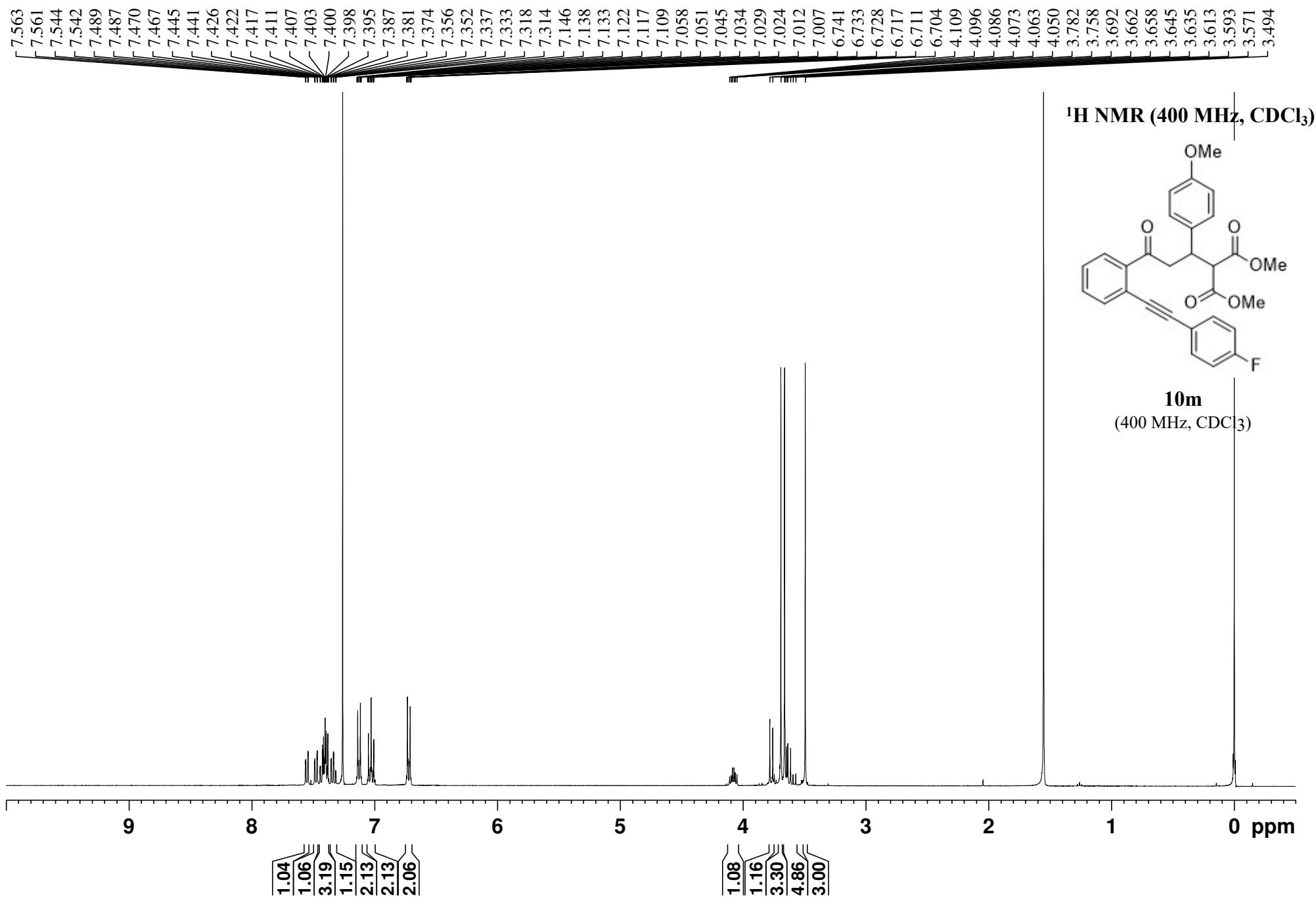
**10l**

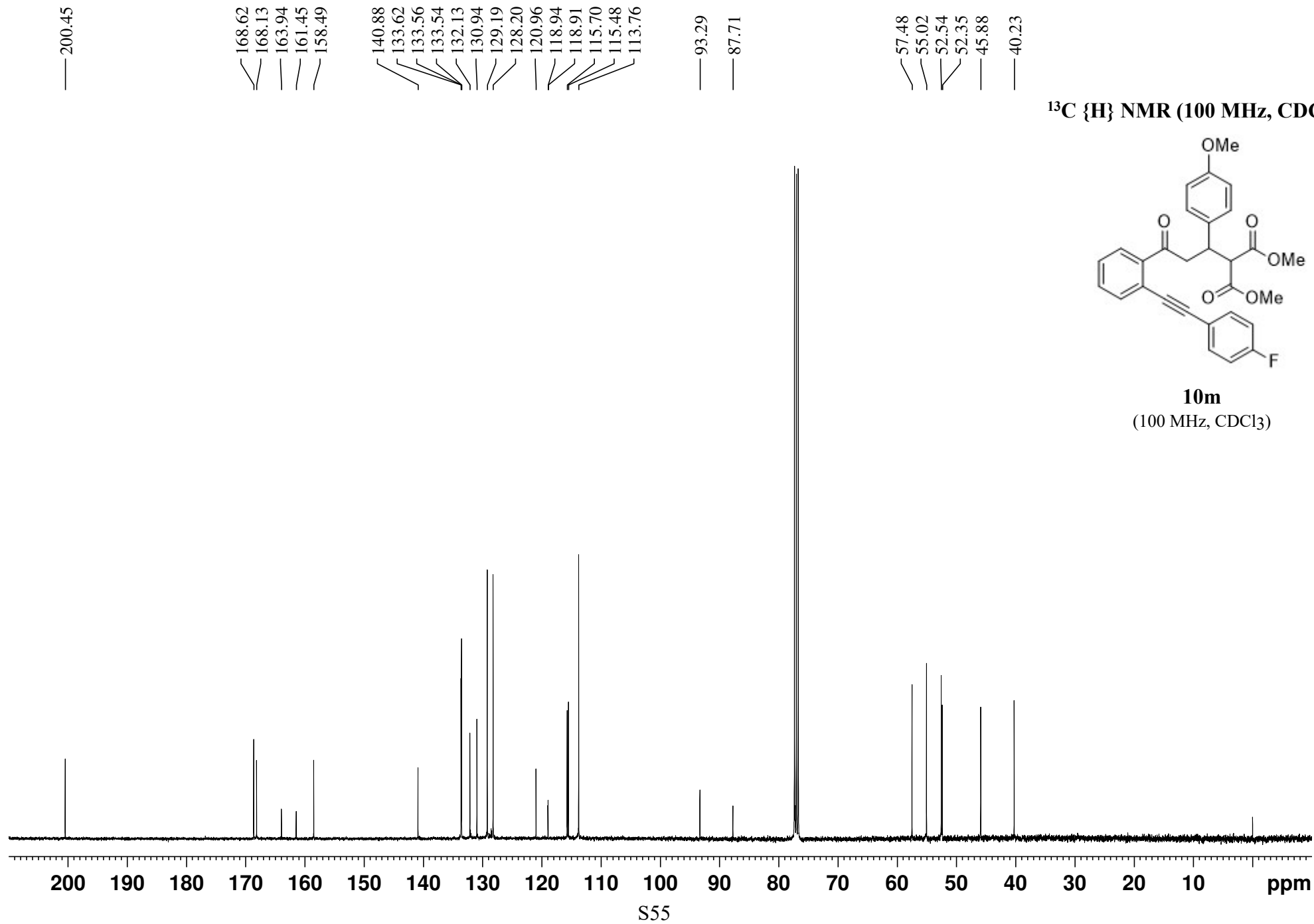
(376 MHz,  $\text{CDCl}_3$ )

— -66.00



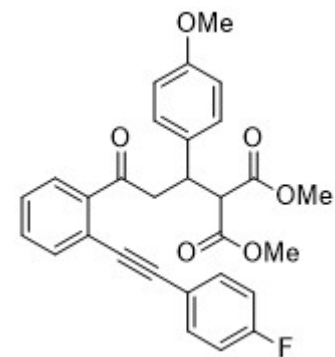
S53





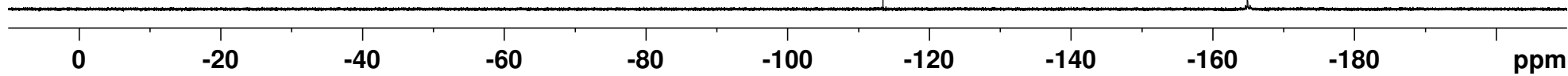
— -113.47

**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**

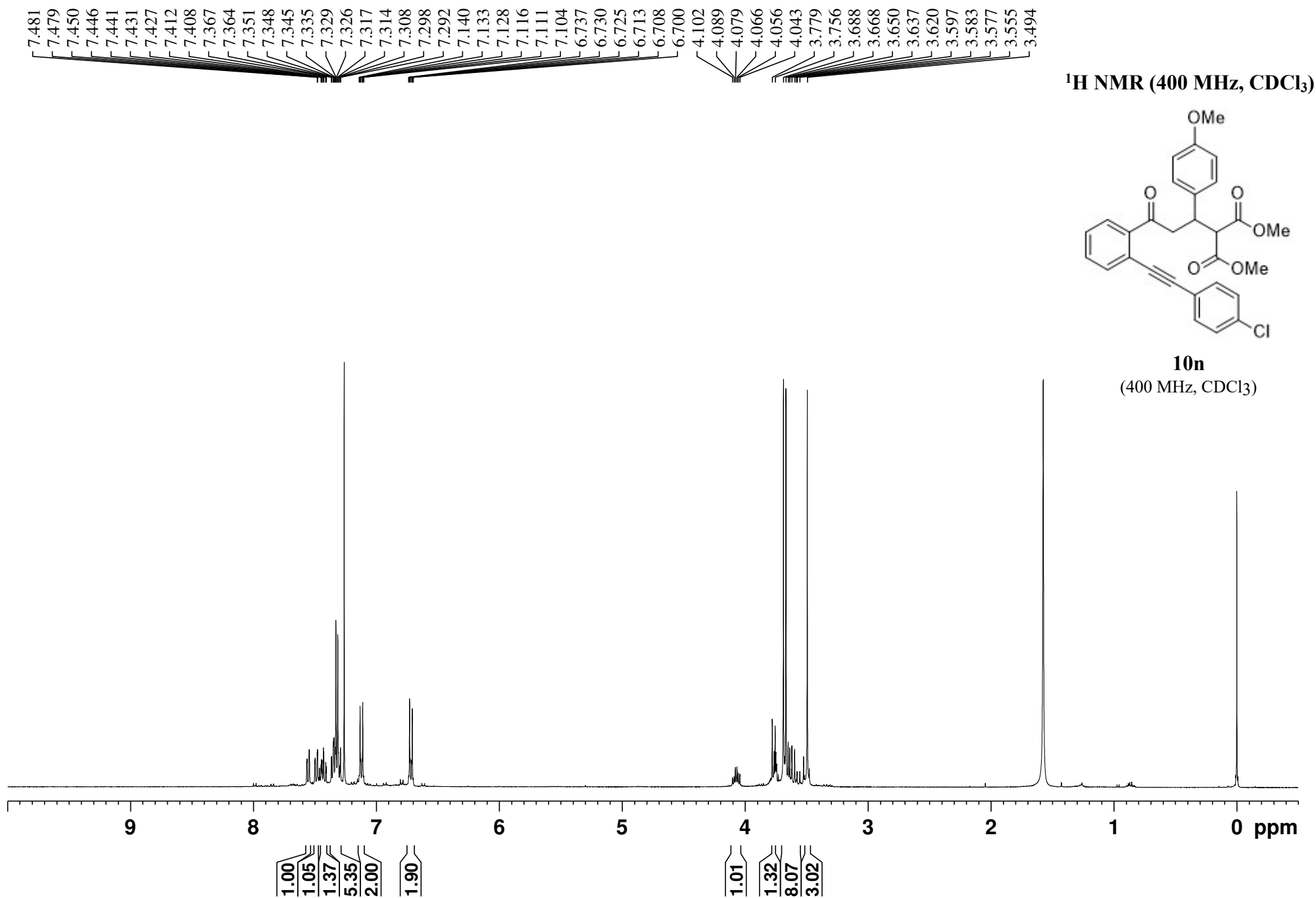


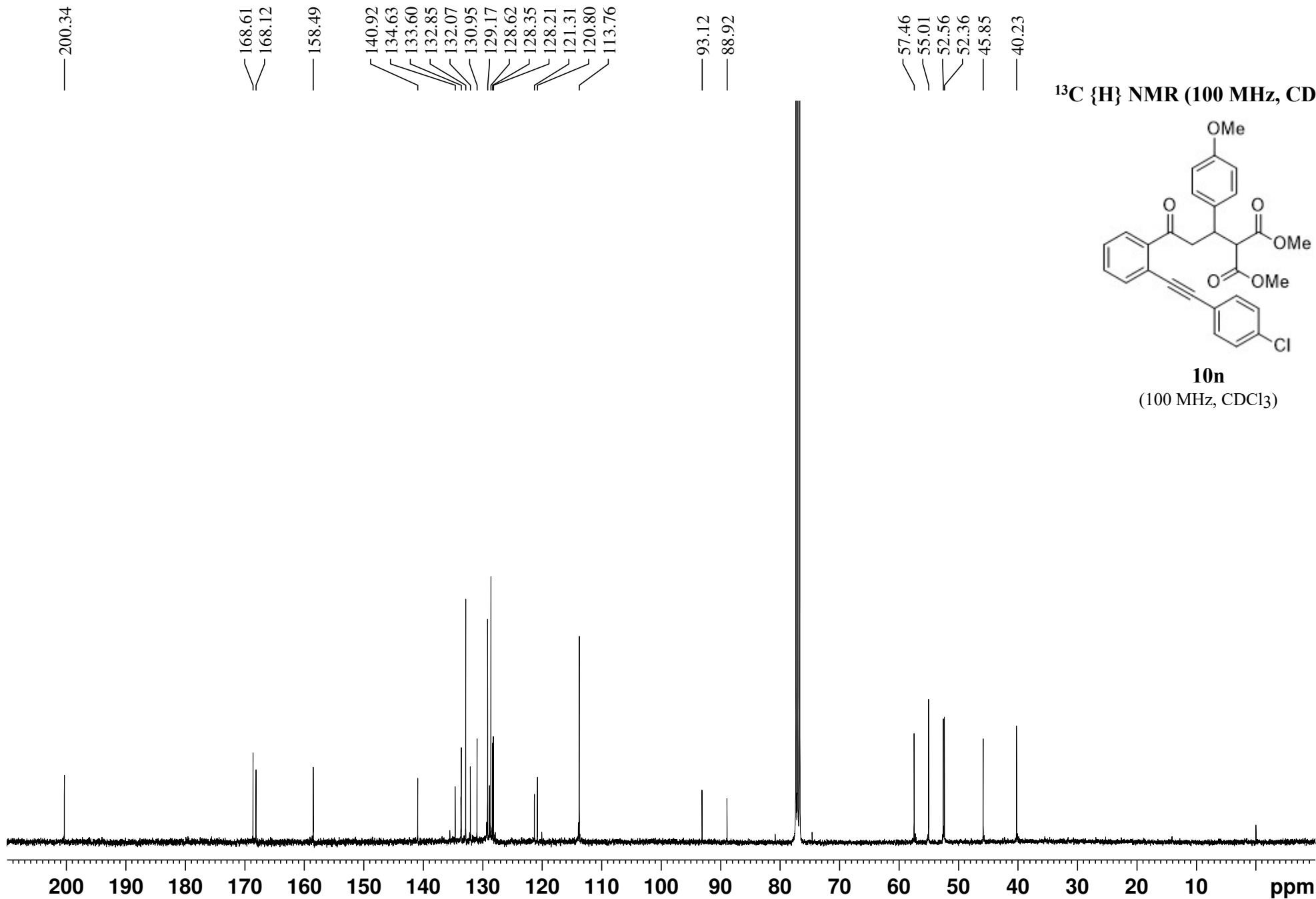
**10m**

(376 MHz,  $\text{CDCl}_3$ )



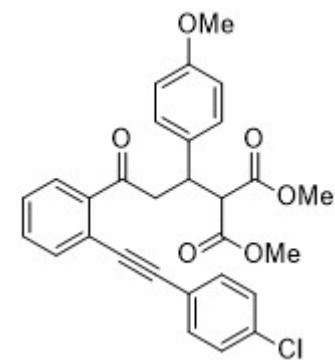
S56



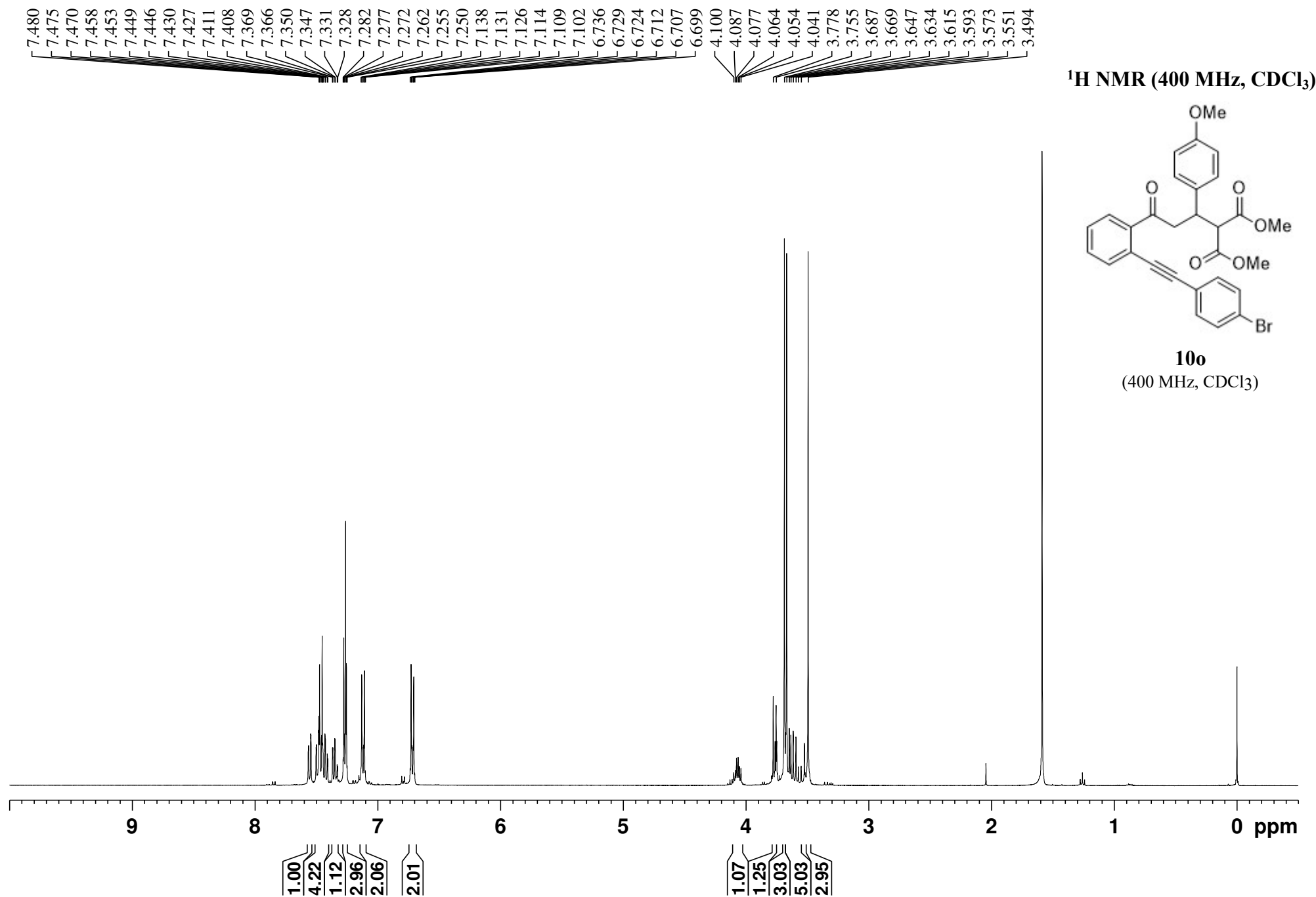


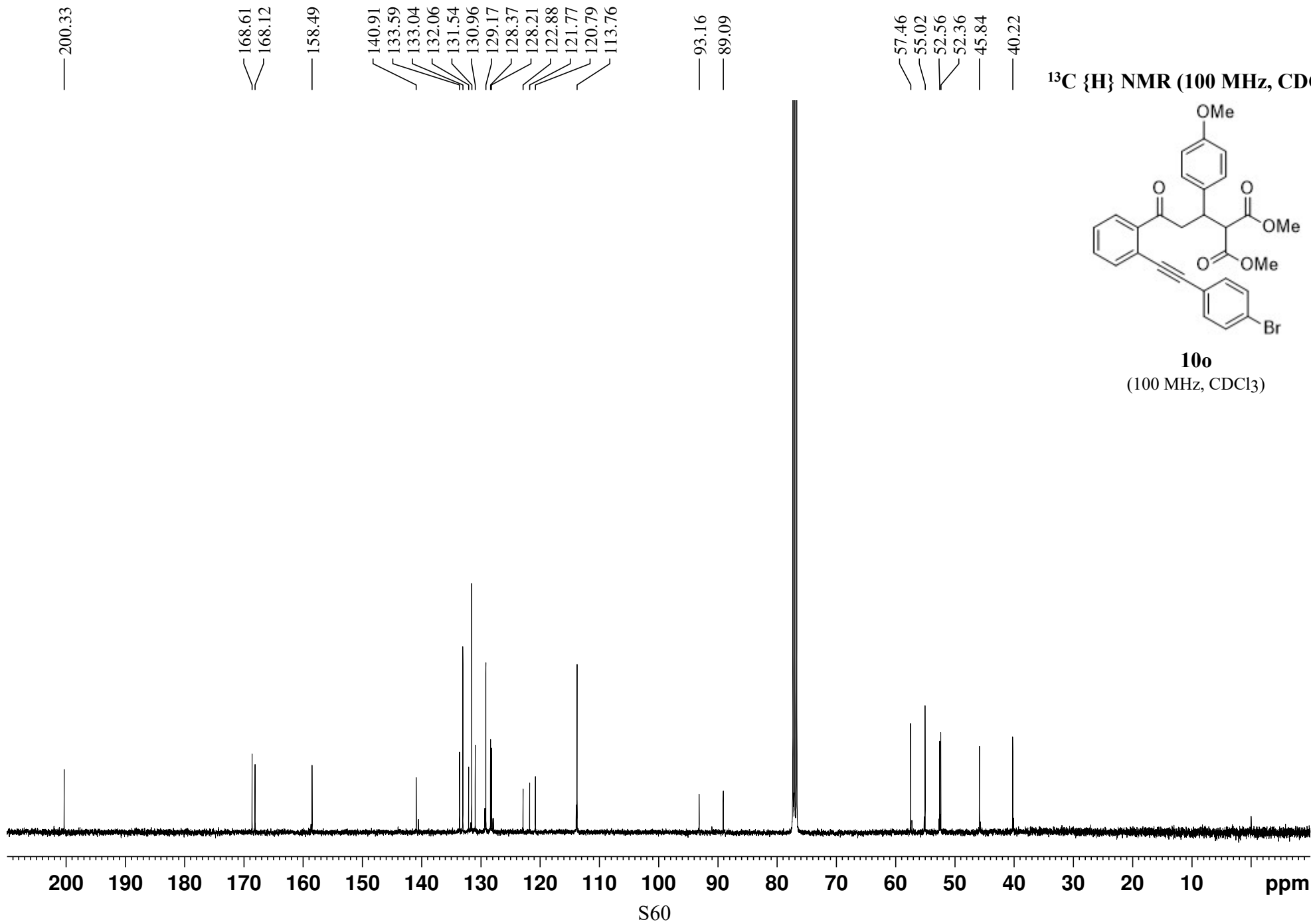
S58

$^{13}\text{C}$  {H} NMR (100 MHz,  $\text{CDCl}_3$ )



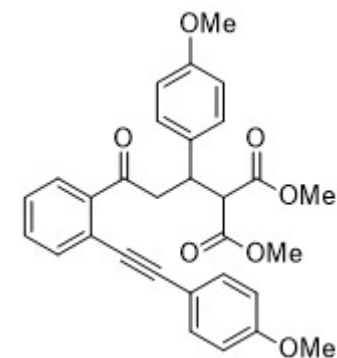
**10n**  
(100 MHz,  $\text{CDCl}_3$ )



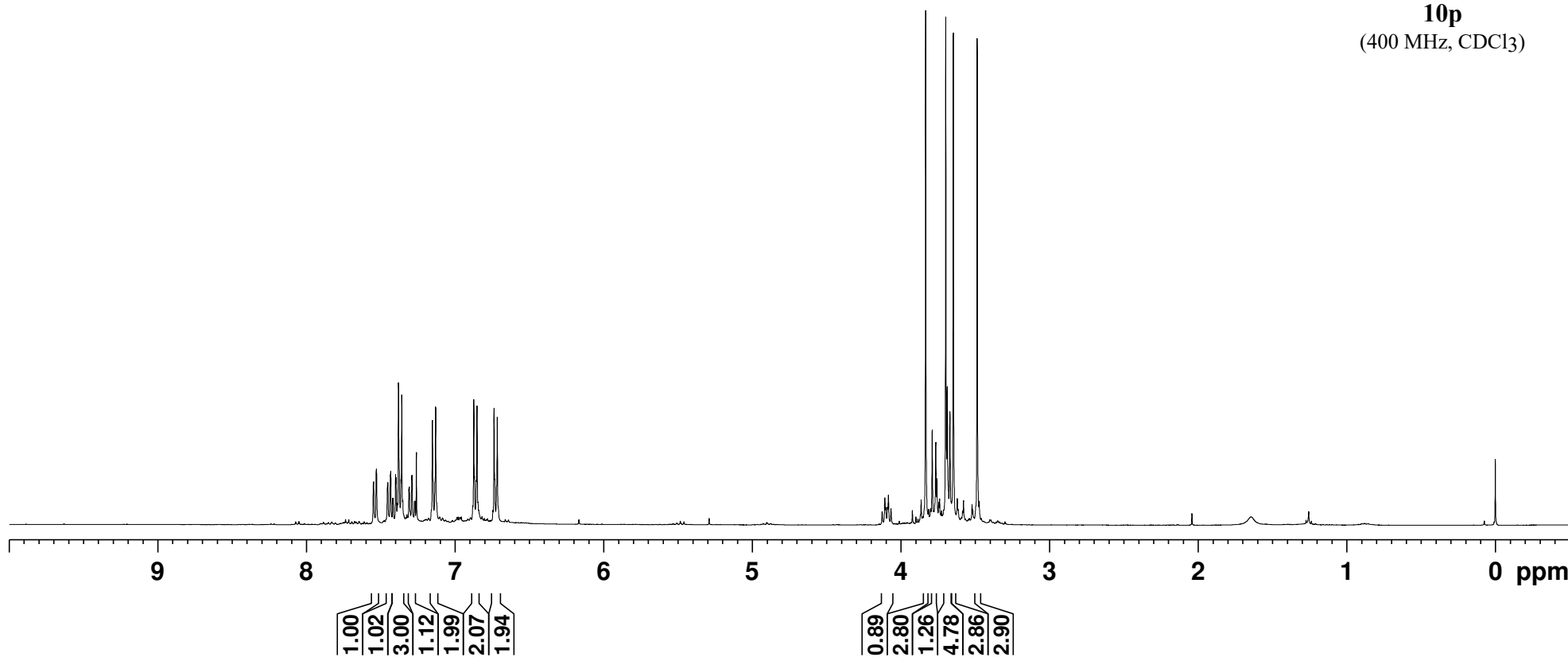


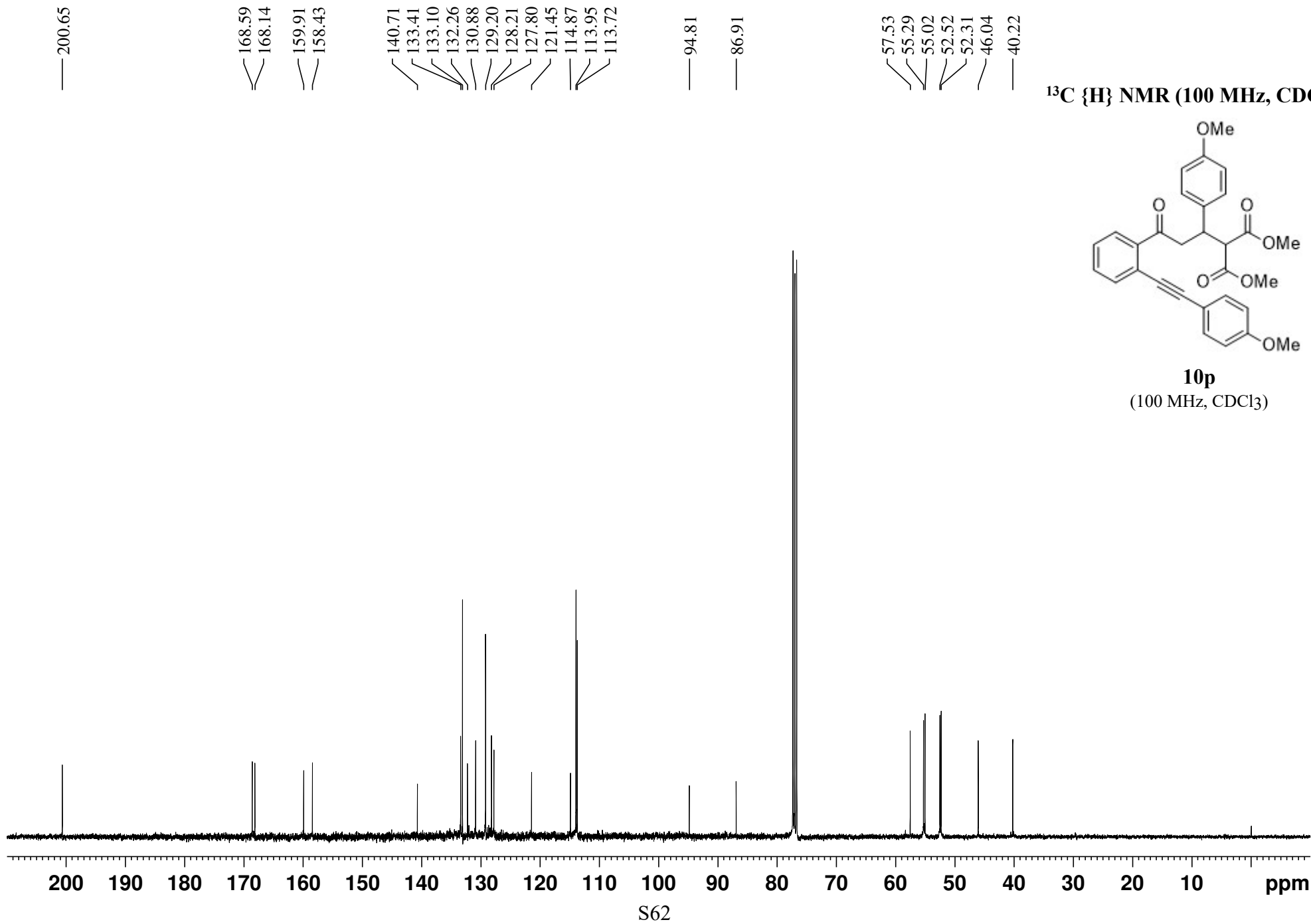
7.435  
7.433  
7.419  
7.416  
7.400  
7.397  
7.387  
7.381  
7.376  
7.364  
7.358  
7.352  
7.311  
7.308  
7.291  
7.289  
7.273  
7.270  
7.159  
7.152  
7.148  
7.136  
7.131  
7.125  
6.881  
6.874  
6.869  
6.857  
6.852  
6.845  
6.841  
6.745  
6.737  
6.733  
6.721  
6.716  
6.709  
4.126  
4.108  
4.102  
4.090  
4.084  
4.066  
3.833  
3.789  
3.765  
3.698  
3.688  
3.670  
3.647  
3.486

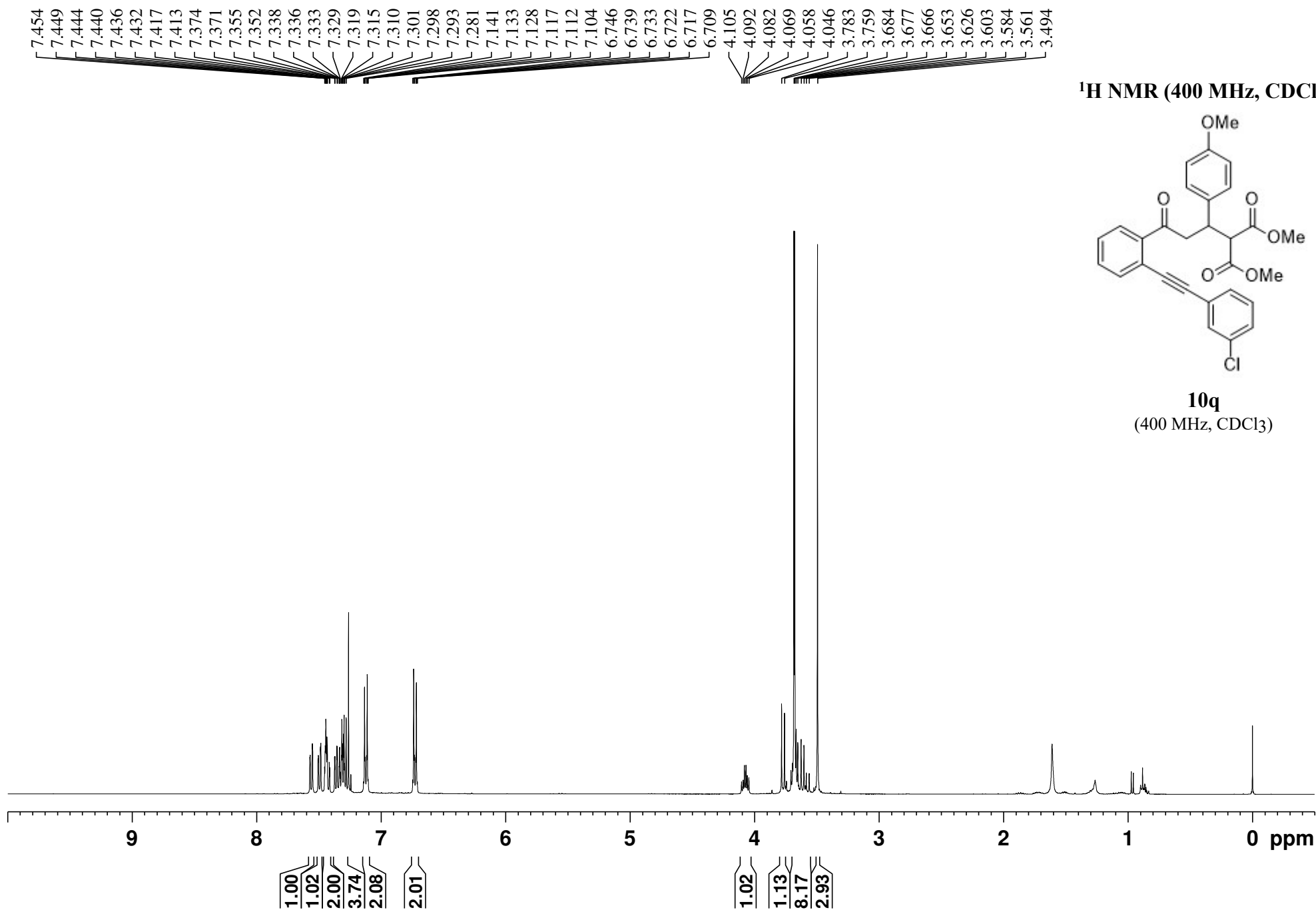
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

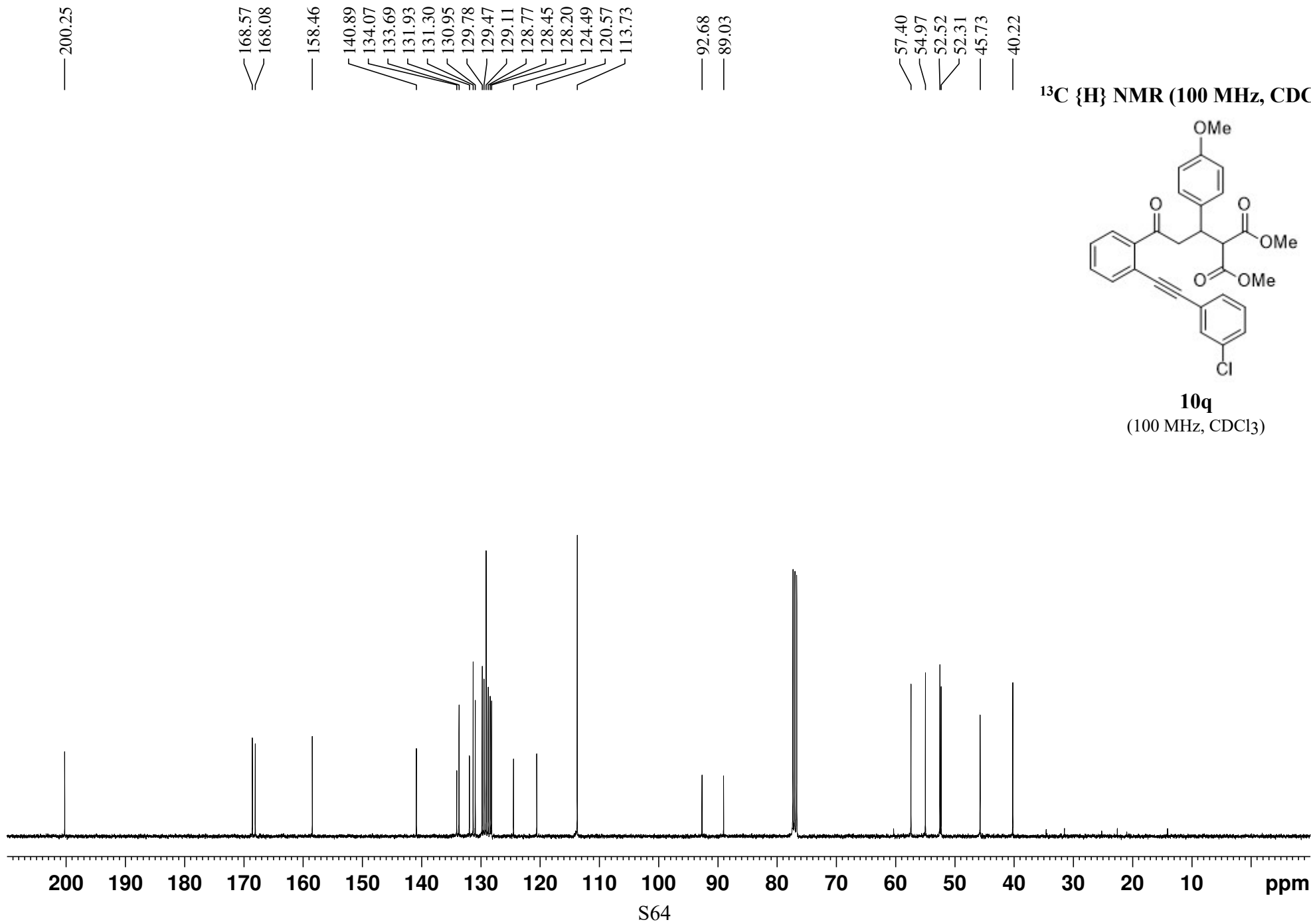


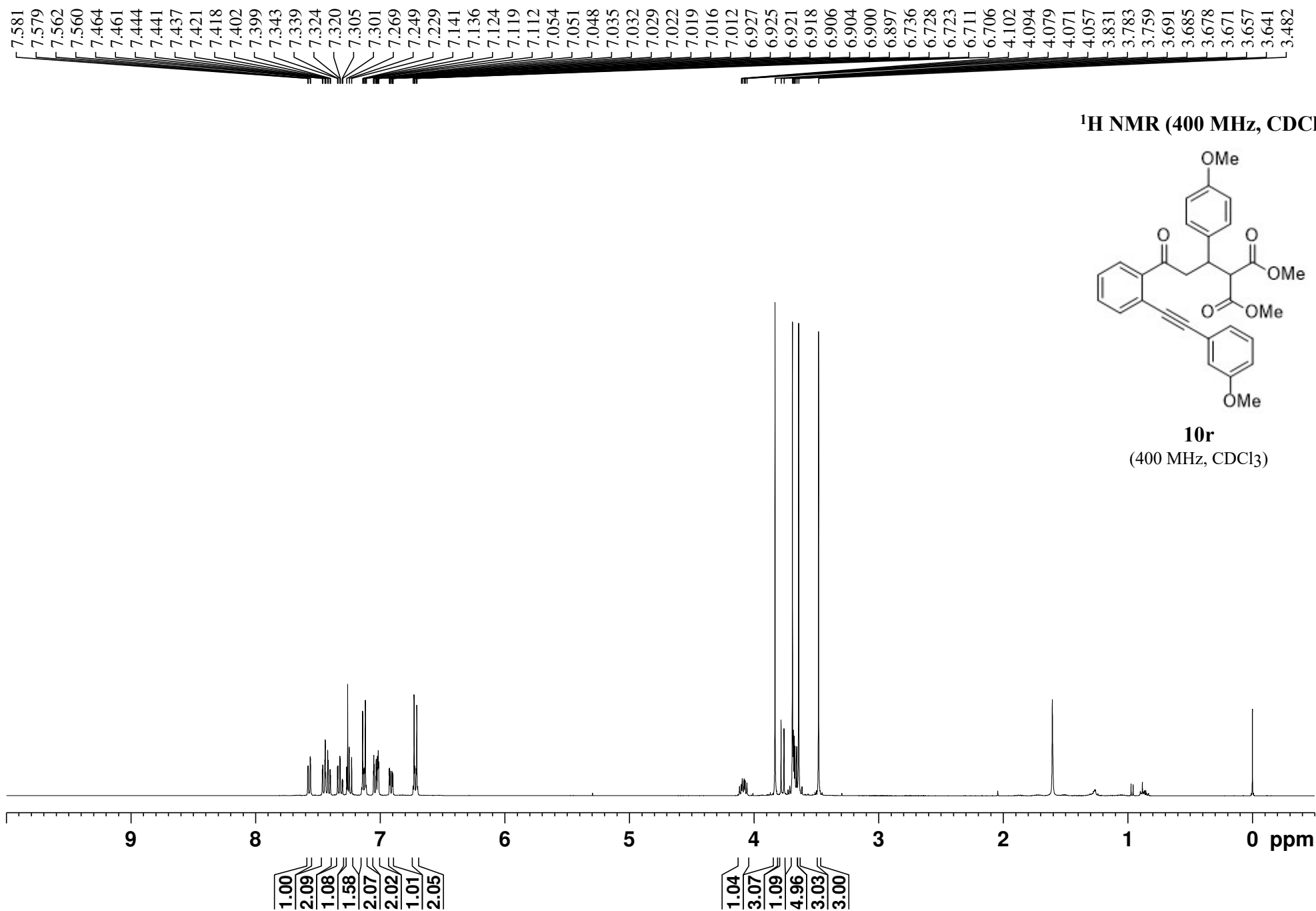
**10p**  
(400 MHz, CDCl<sub>3</sub>)

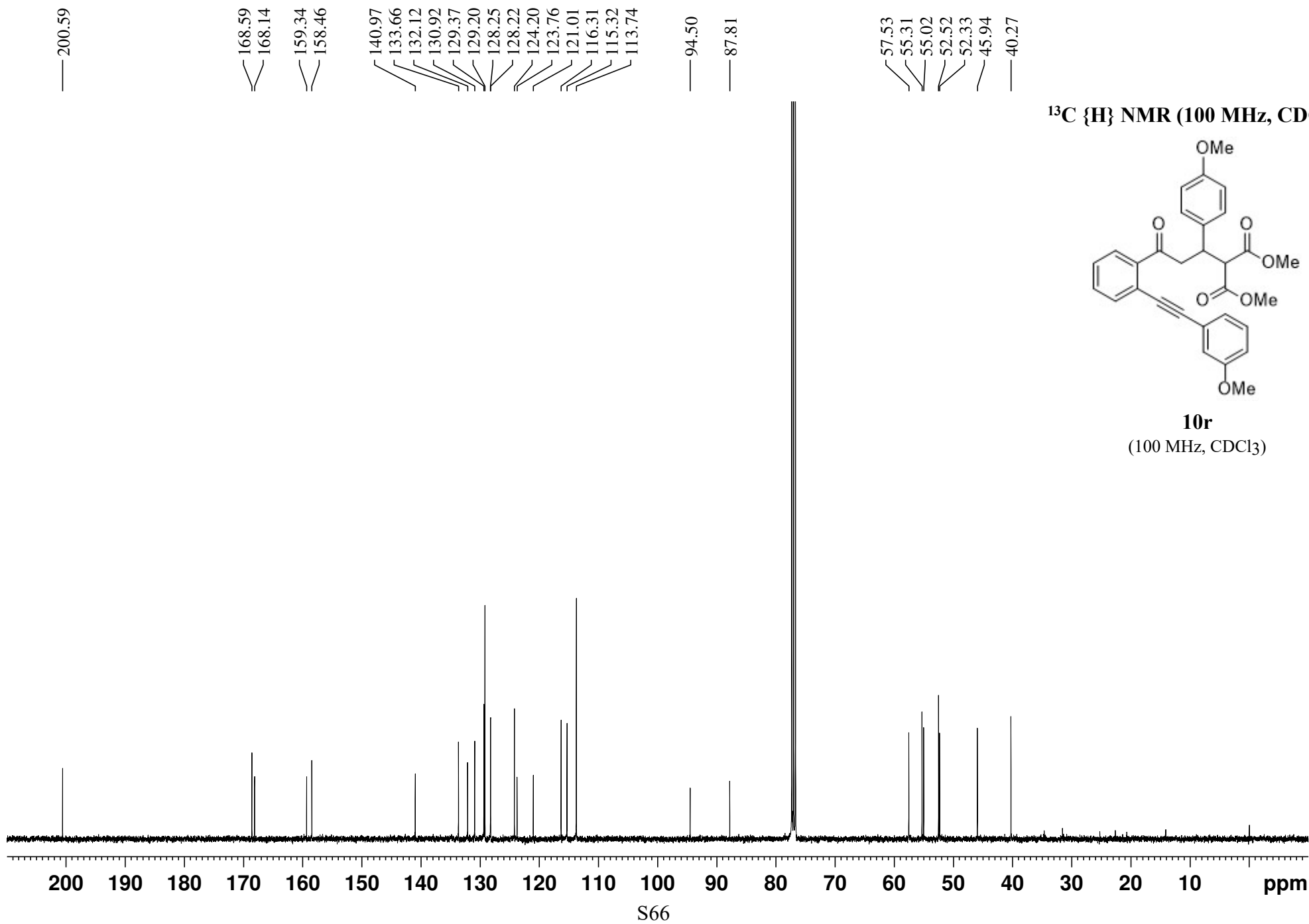


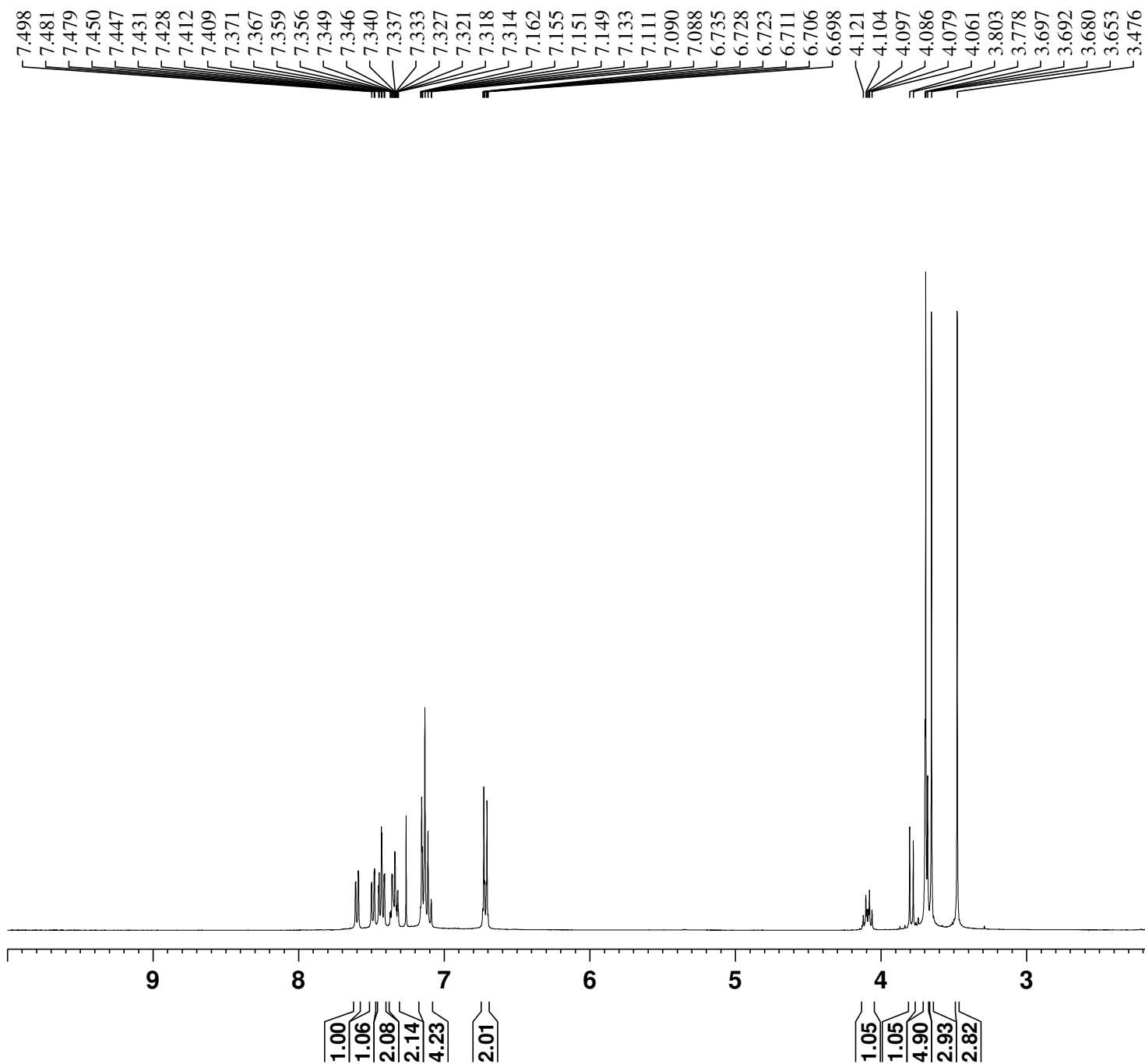




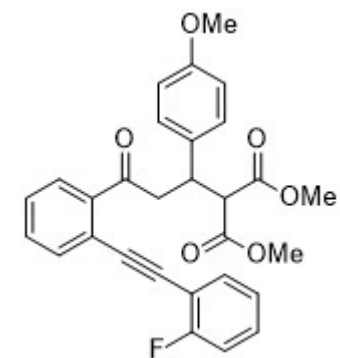






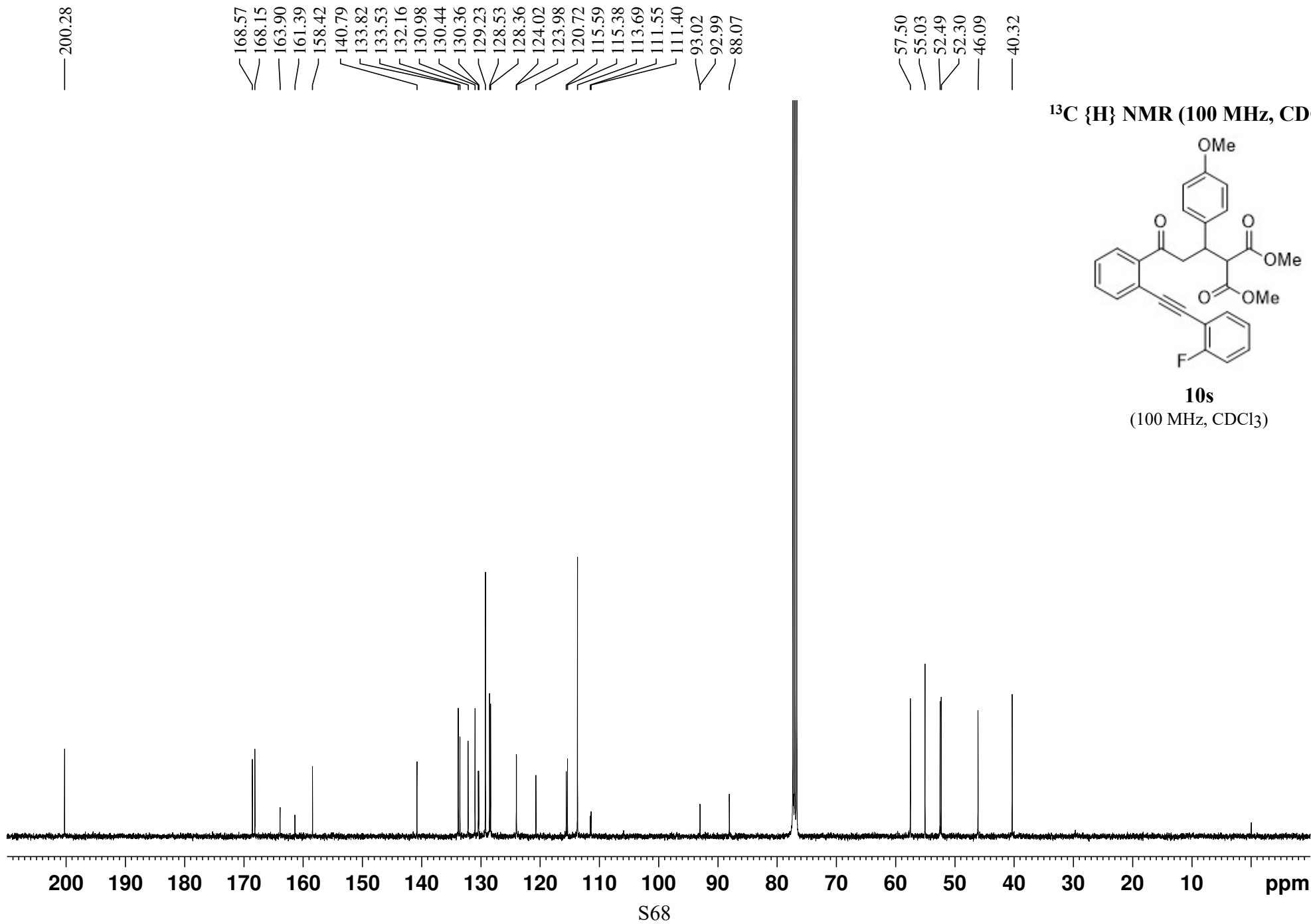


<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



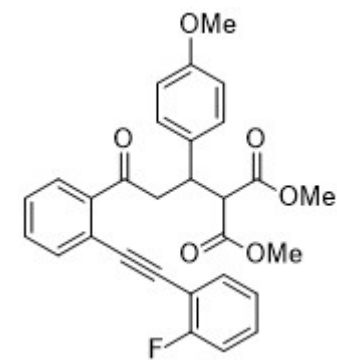
**10s**

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



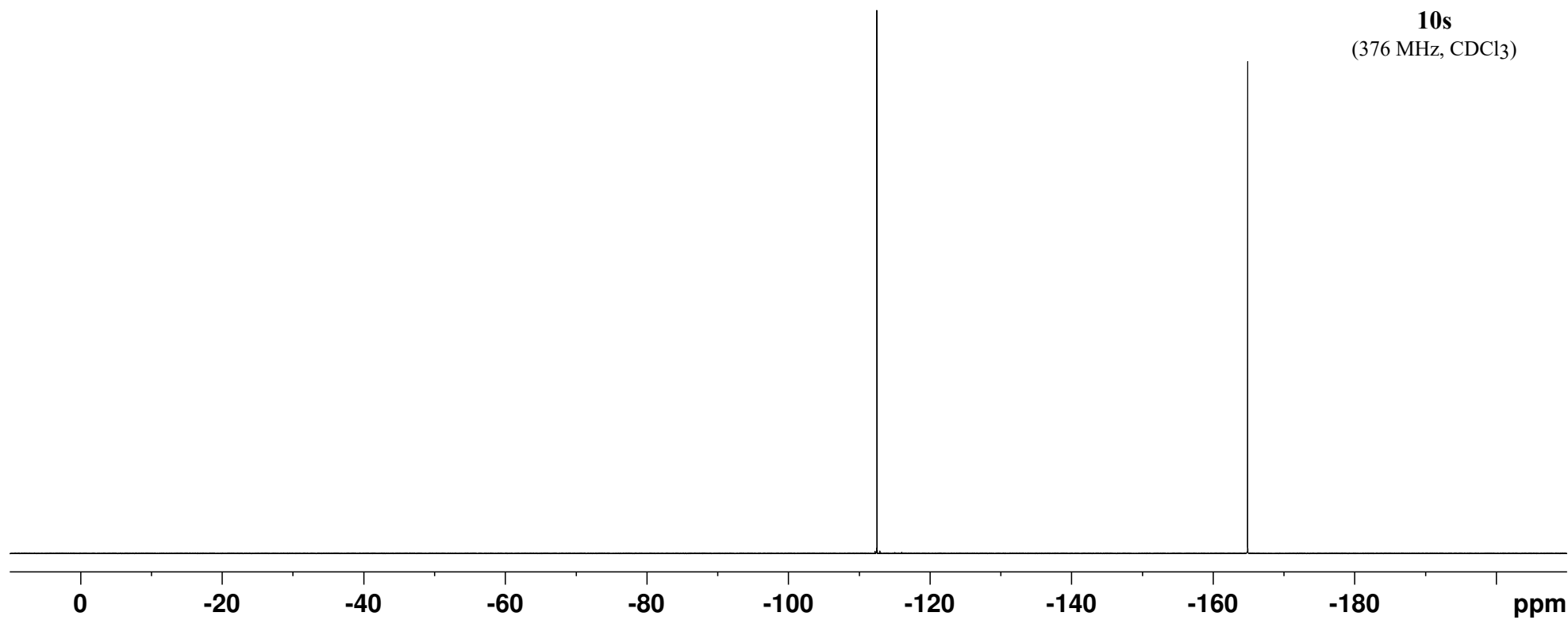
— -112.52

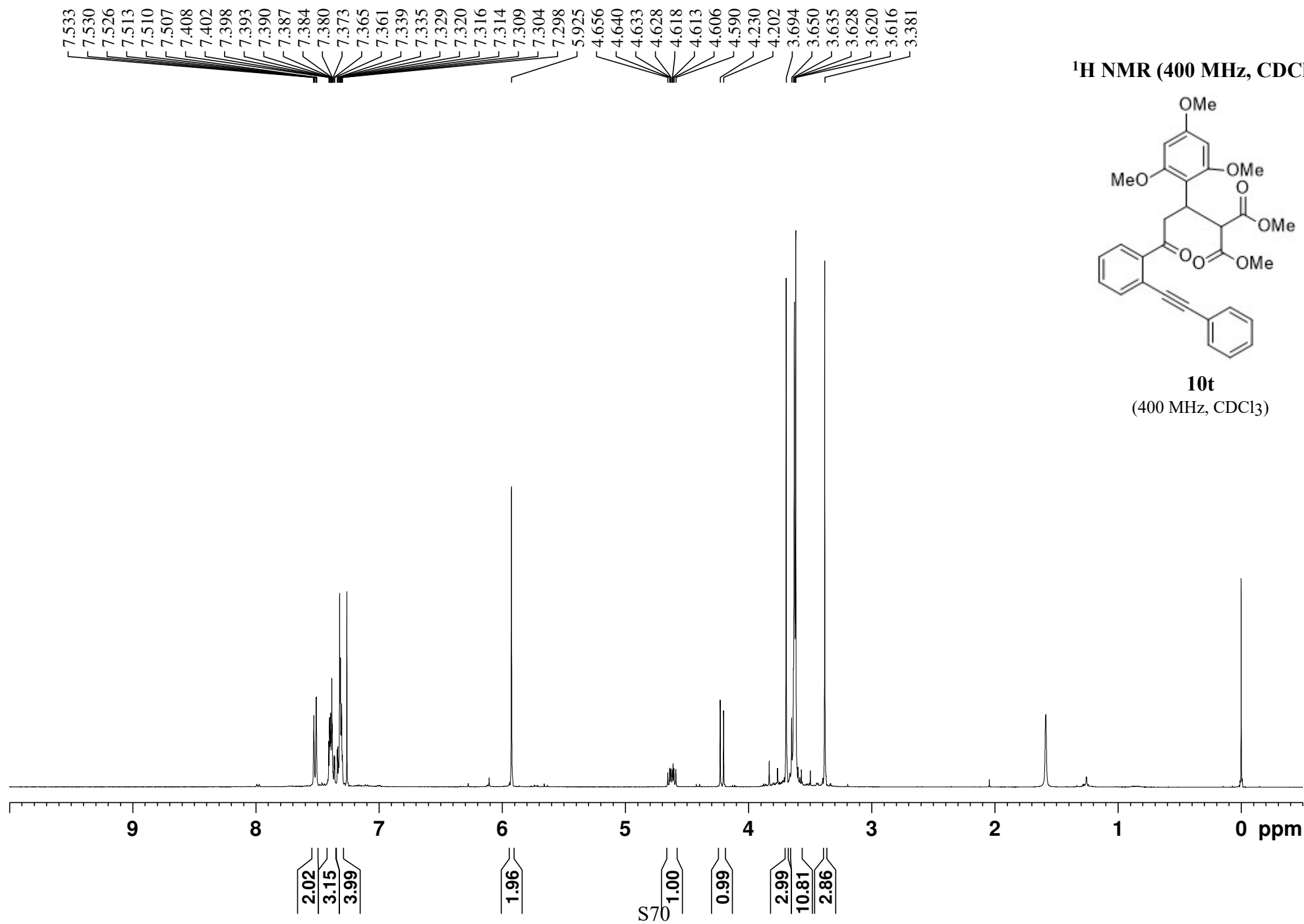
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**

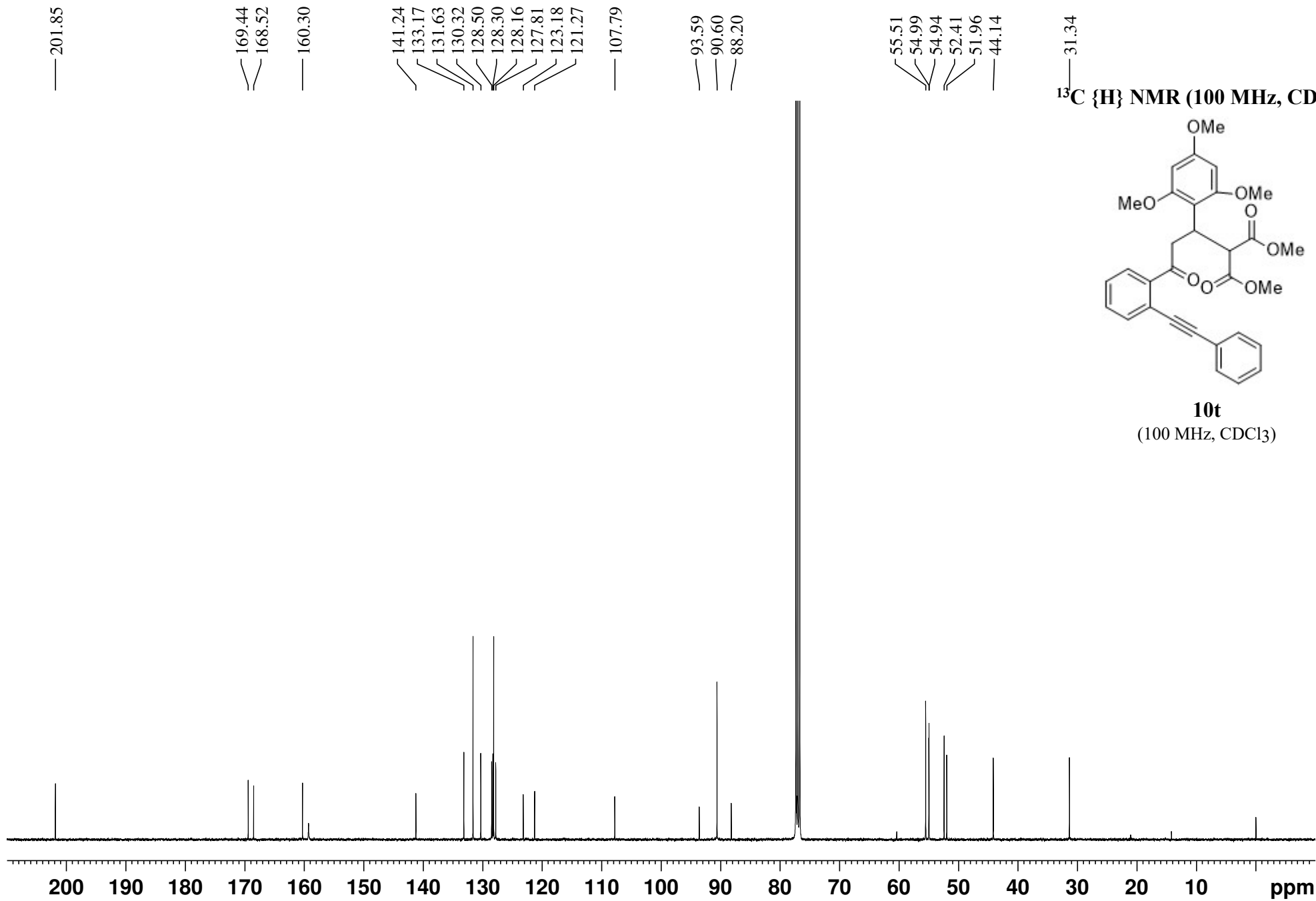


**10s**

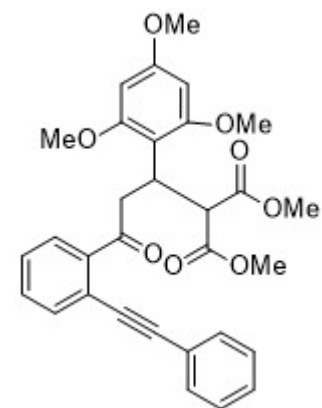
(376 MHz,  $\text{CDCl}_3$ )



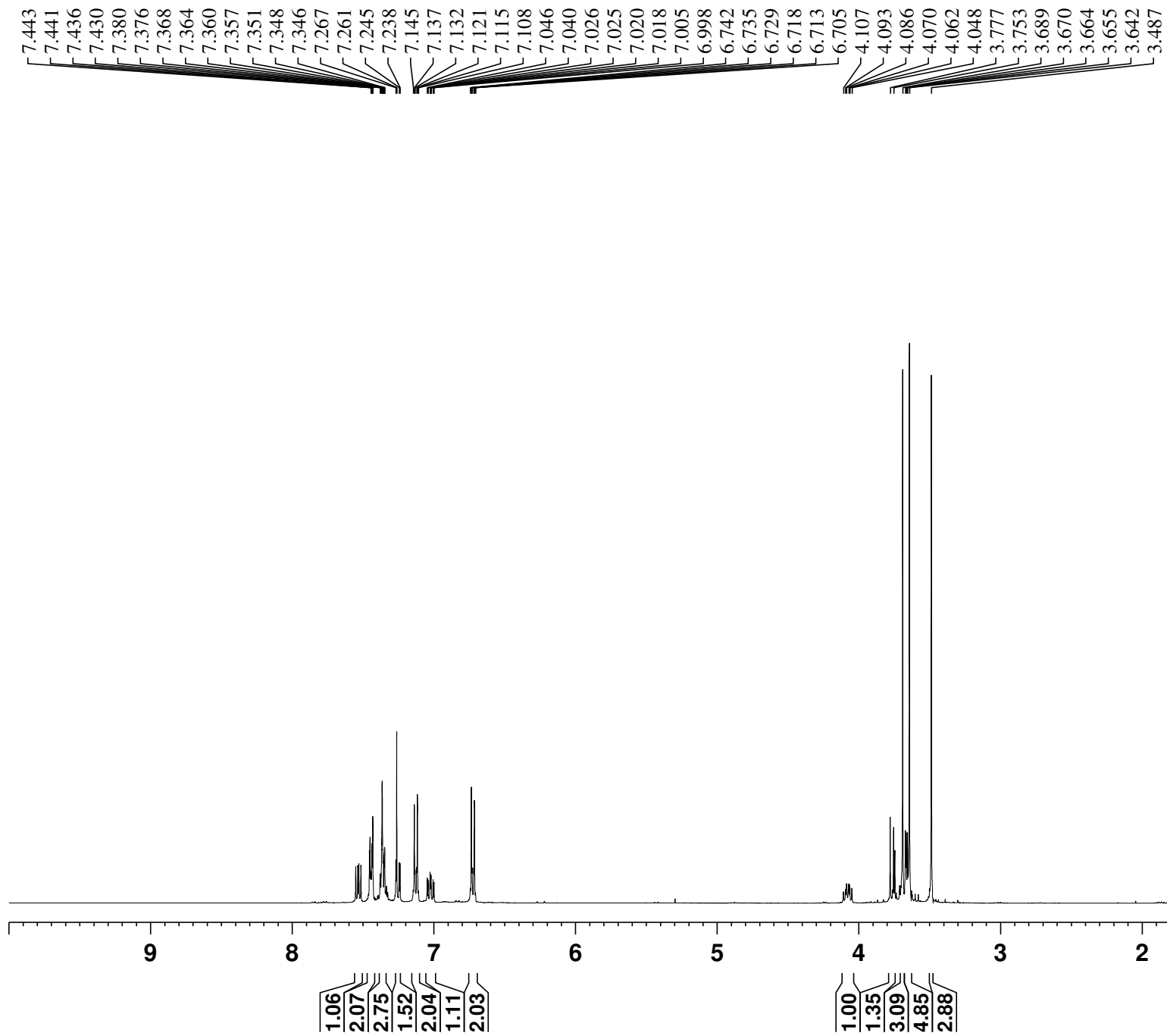




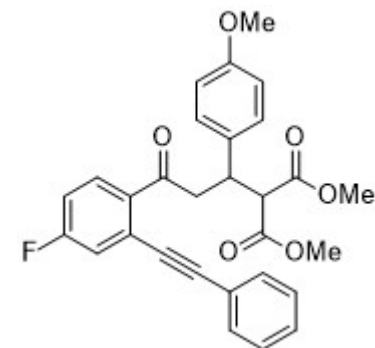
<sup>13</sup>C {H} NMR (100 MHz, CDCl<sub>3</sub>)



**10t**  
(100 MHz, CDCl<sub>3</sub>)

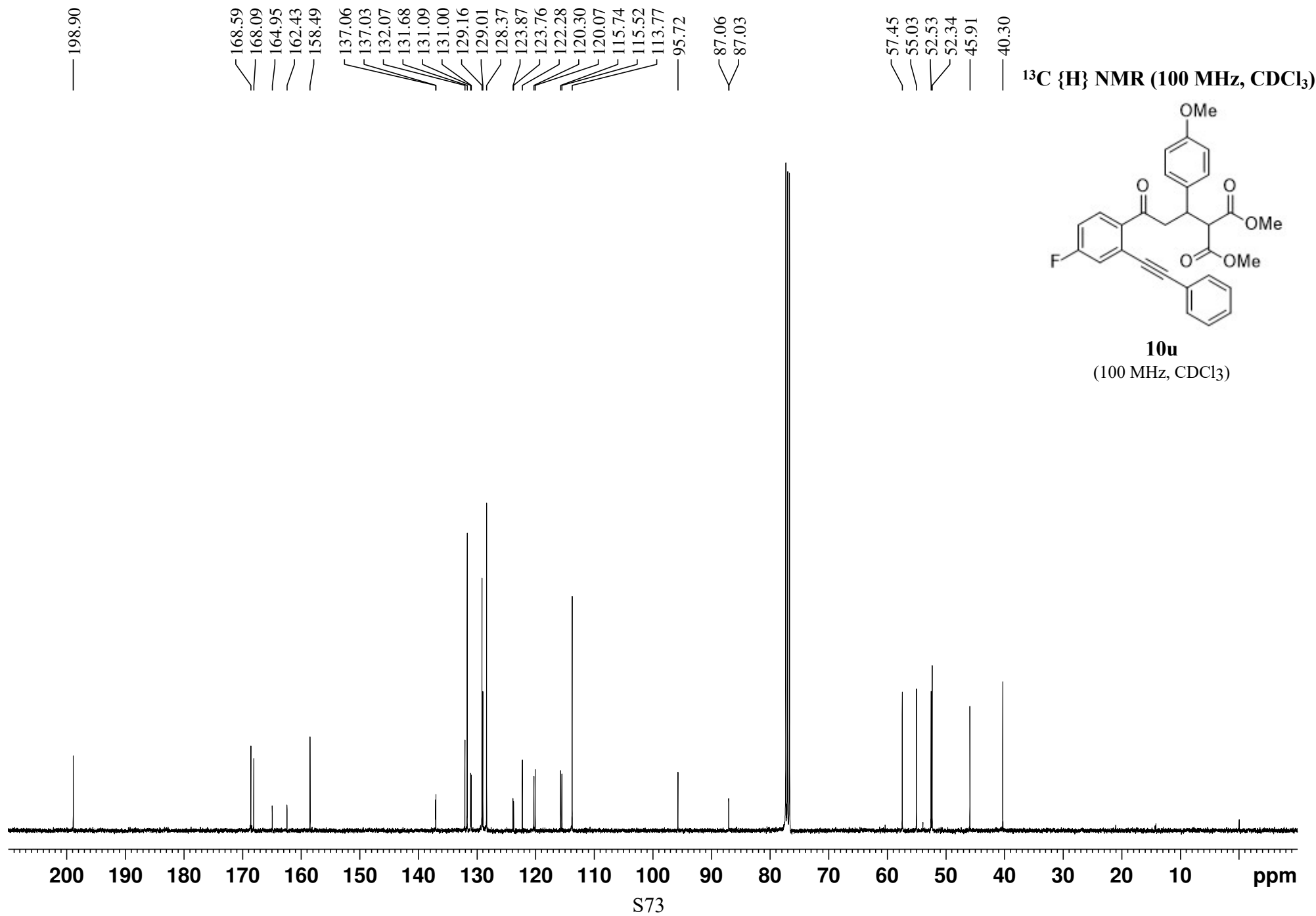


<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



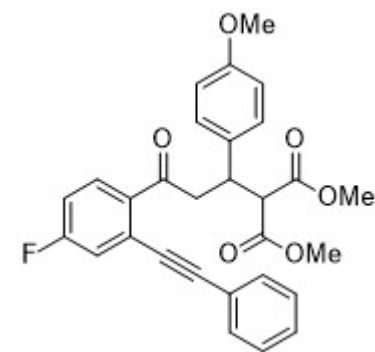
**10u**

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



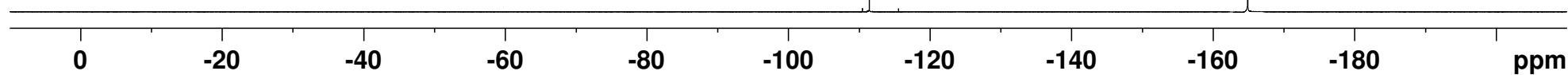
— -111.44

**<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)**



**10u**

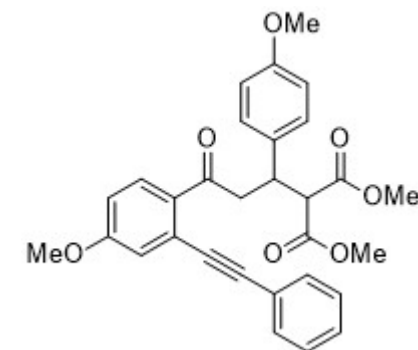
(376 MHz, CDCl<sub>3</sub>)



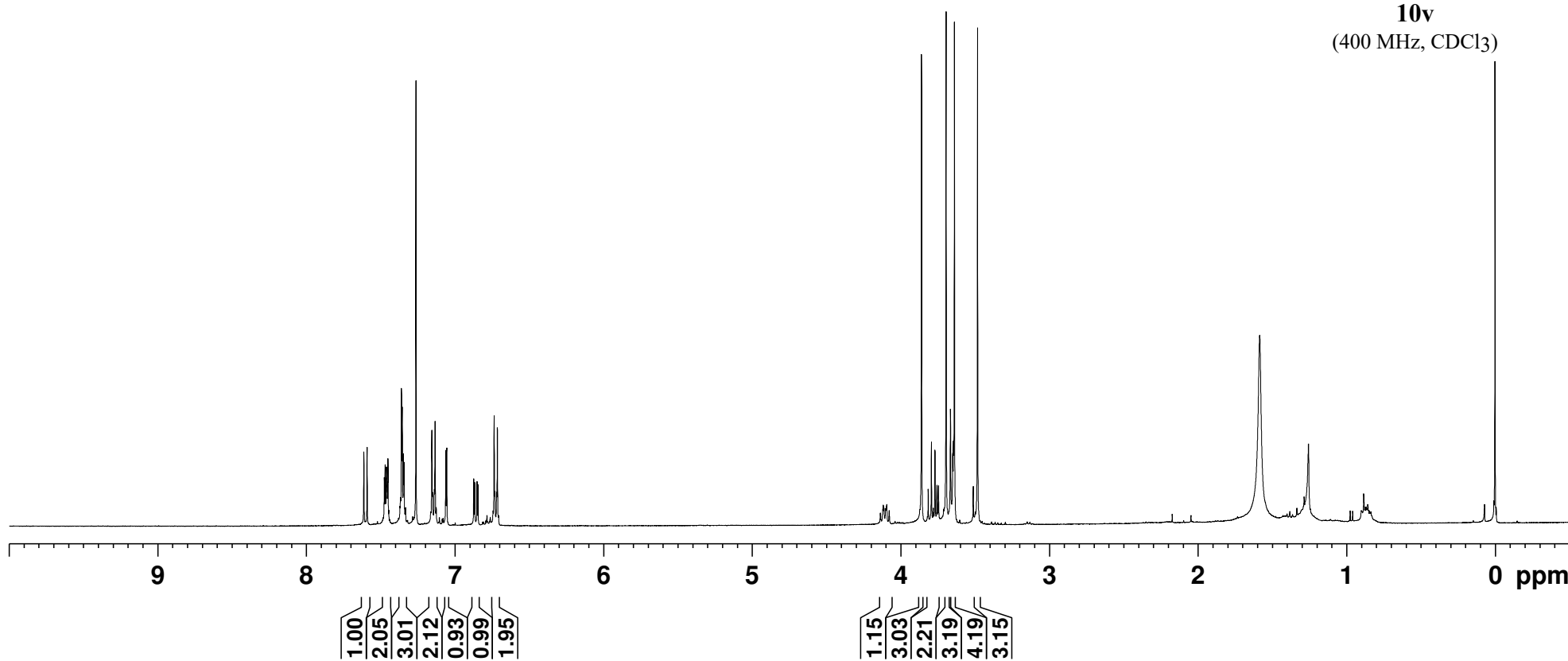
S74

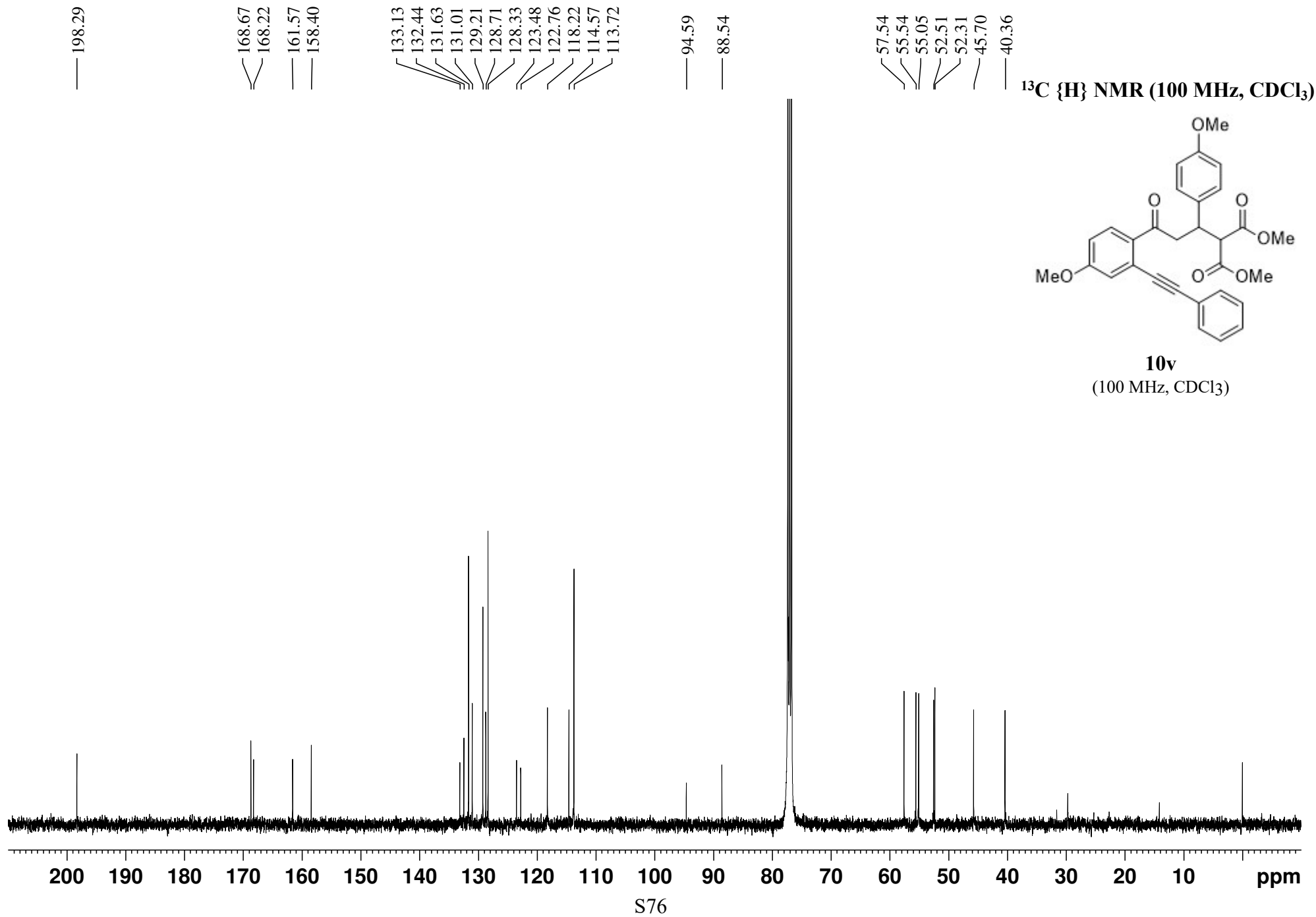
7.466  
7.461  
7.459  
7.456  
7.453  
7.450  
7.445  
7.370  
7.366  
7.359  
7.354  
7.346  
7.342  
7.335  
7.332  
7.162  
7.155  
7.150  
7.138  
7.133  
7.126  
7.061  
7.055  
6.873  
6.866  
6.851  
6.844  
6.743  
6.736  
6.730  
6.719  
6.714  
6.706  
4.136  
4.121  
4.117  
4.112  
4.101  
4.096  
4.093  
4.077  
3.859  
3.814  
3.793  
3.769  
3.755  
3.745  
3.694  
3.664  
3.649  
3.644  
3.638  
3.482

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

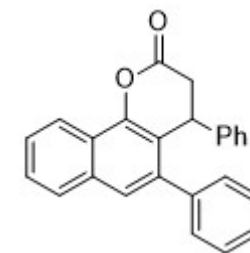


**10v**  
(400 MHz, CDCl<sub>3</sub>)



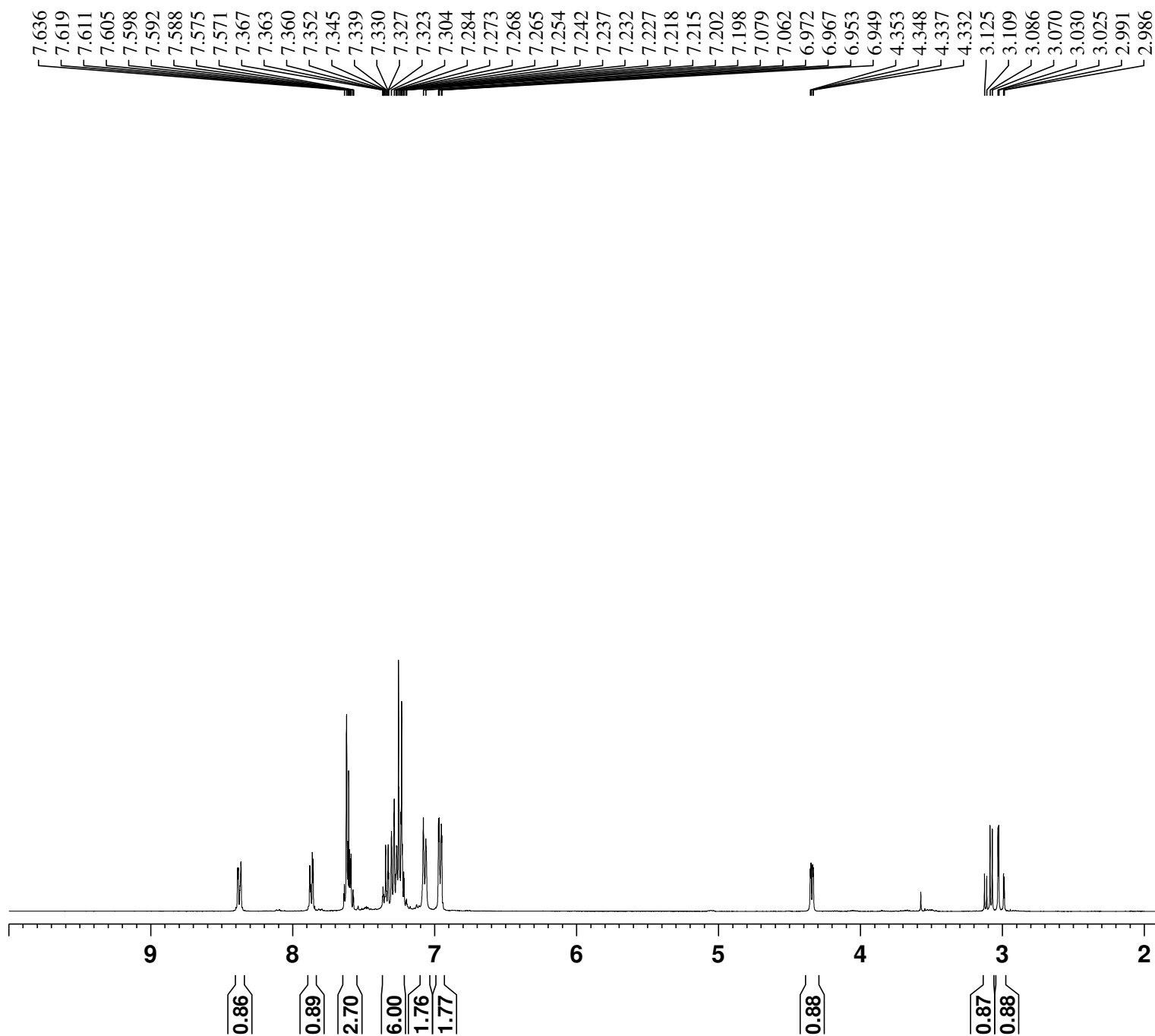


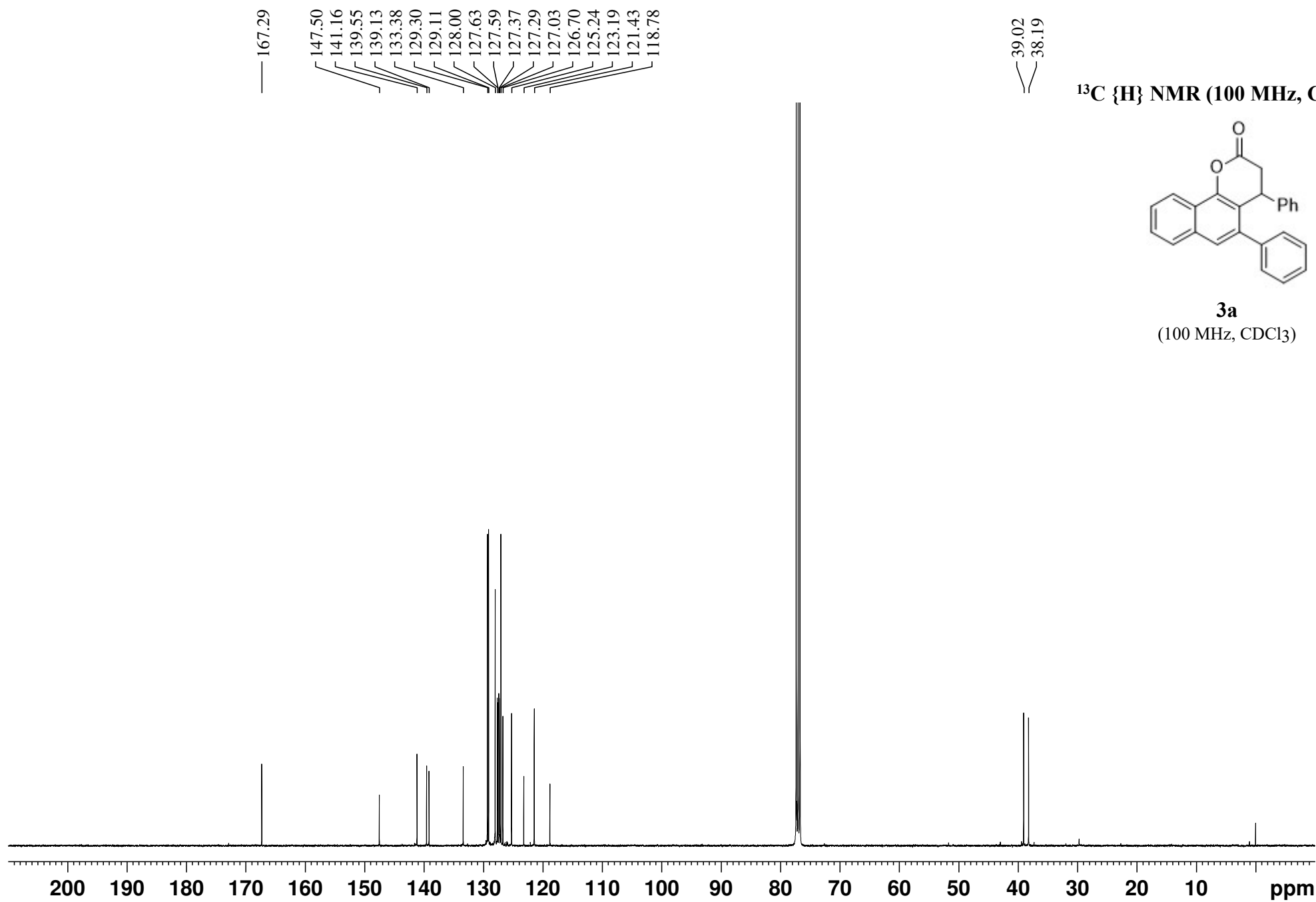
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



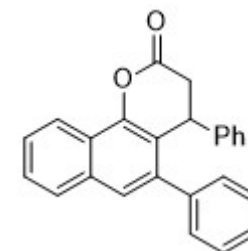
**3a**

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



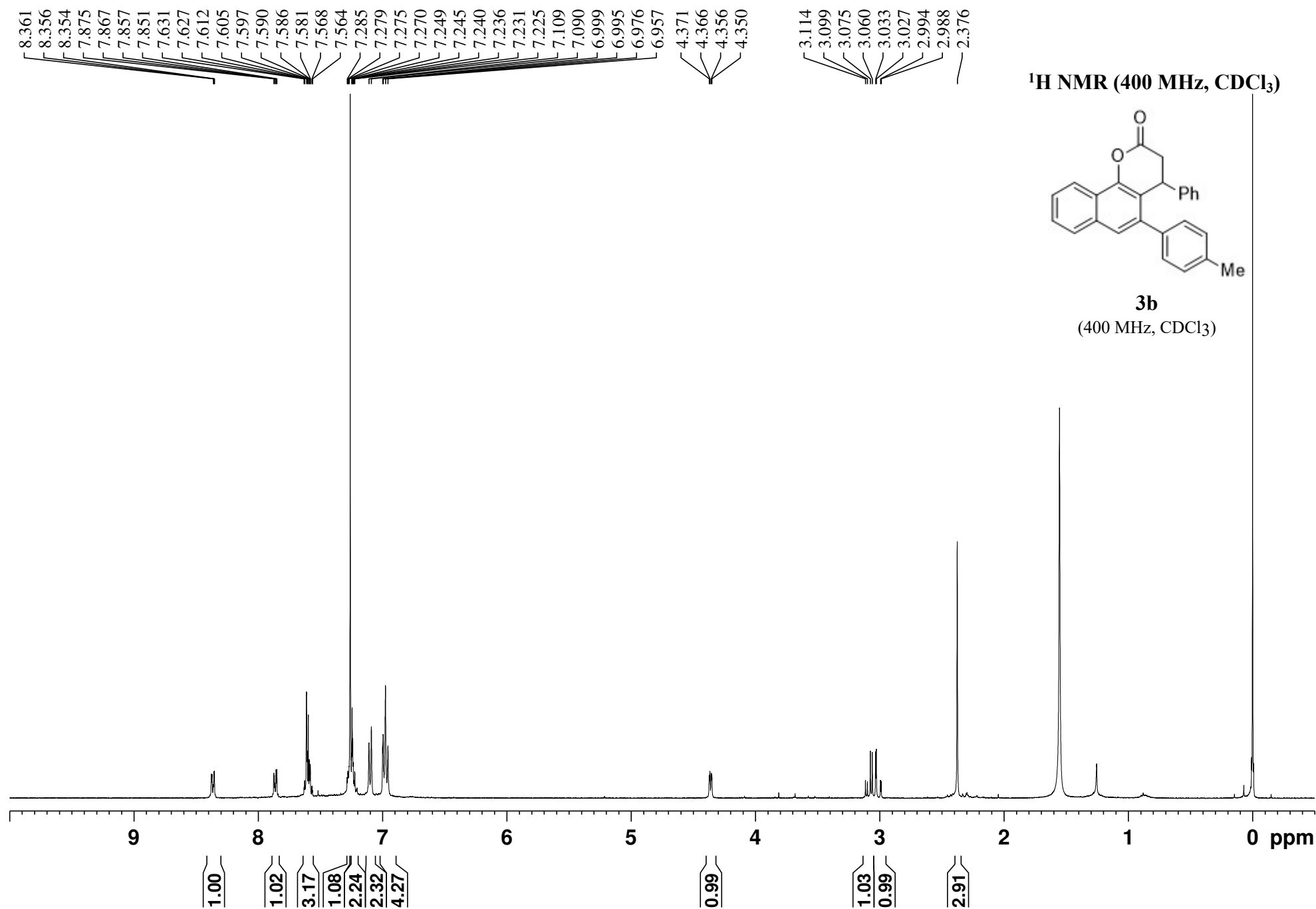


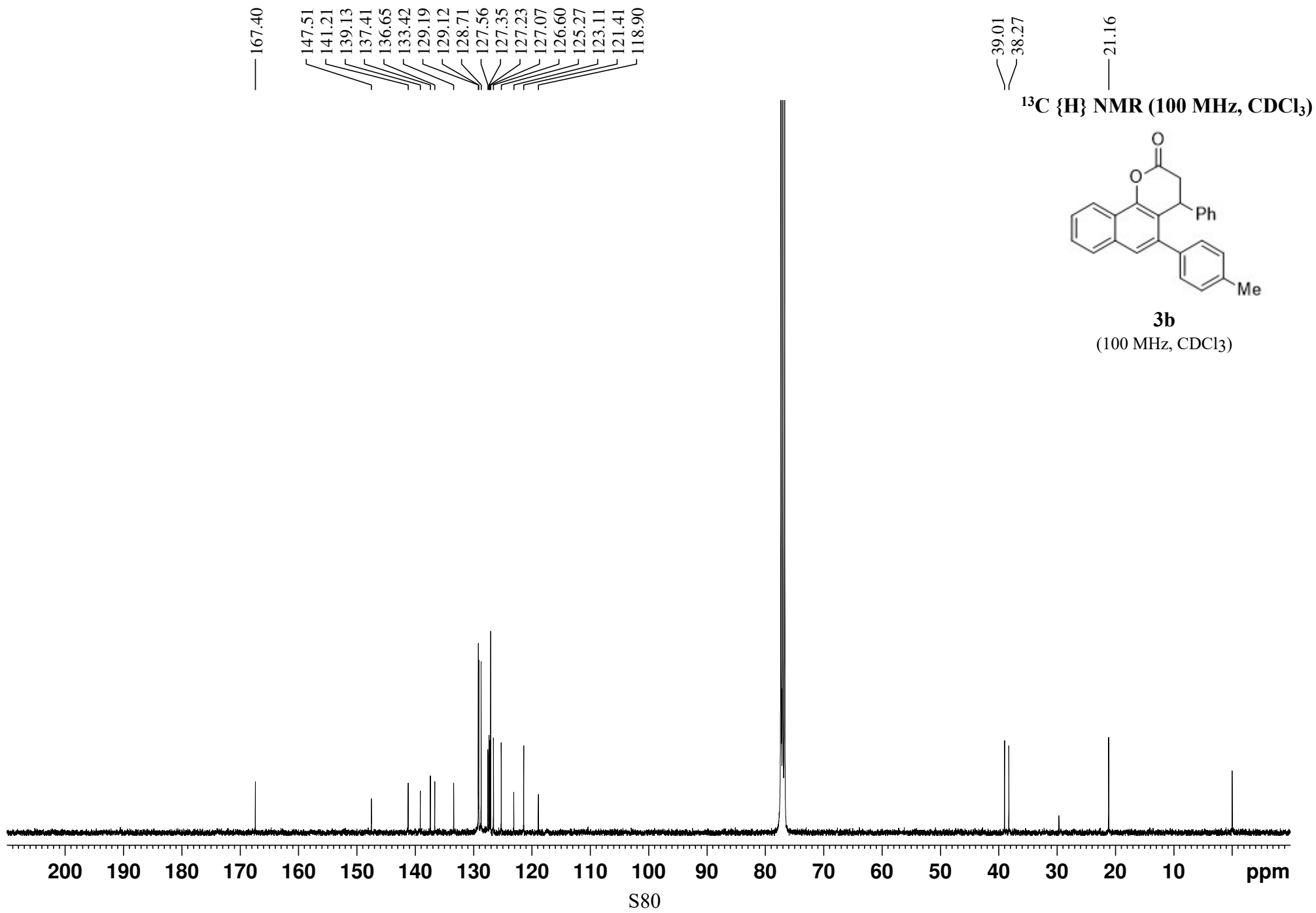
<sup>13</sup>C {<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>)

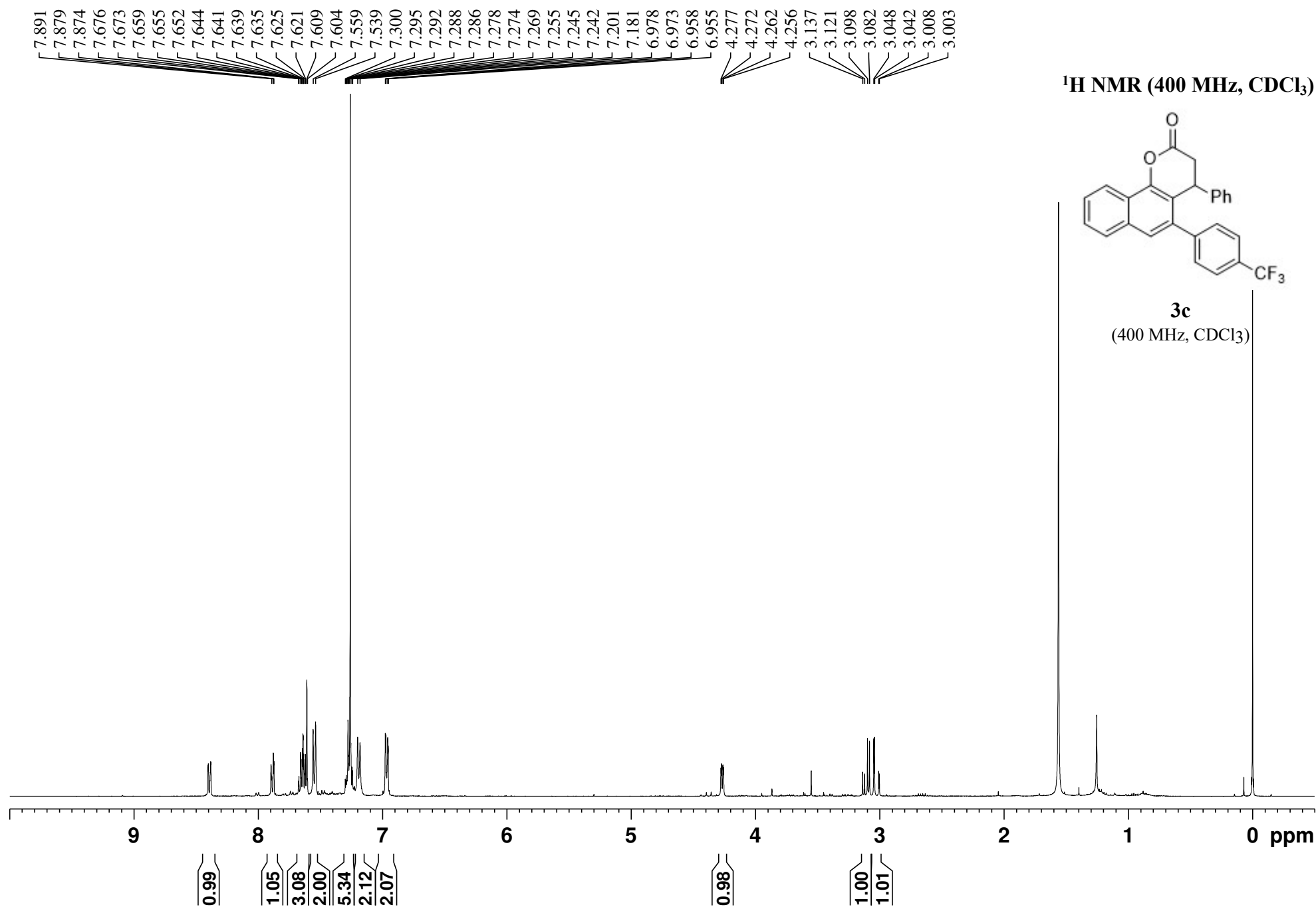


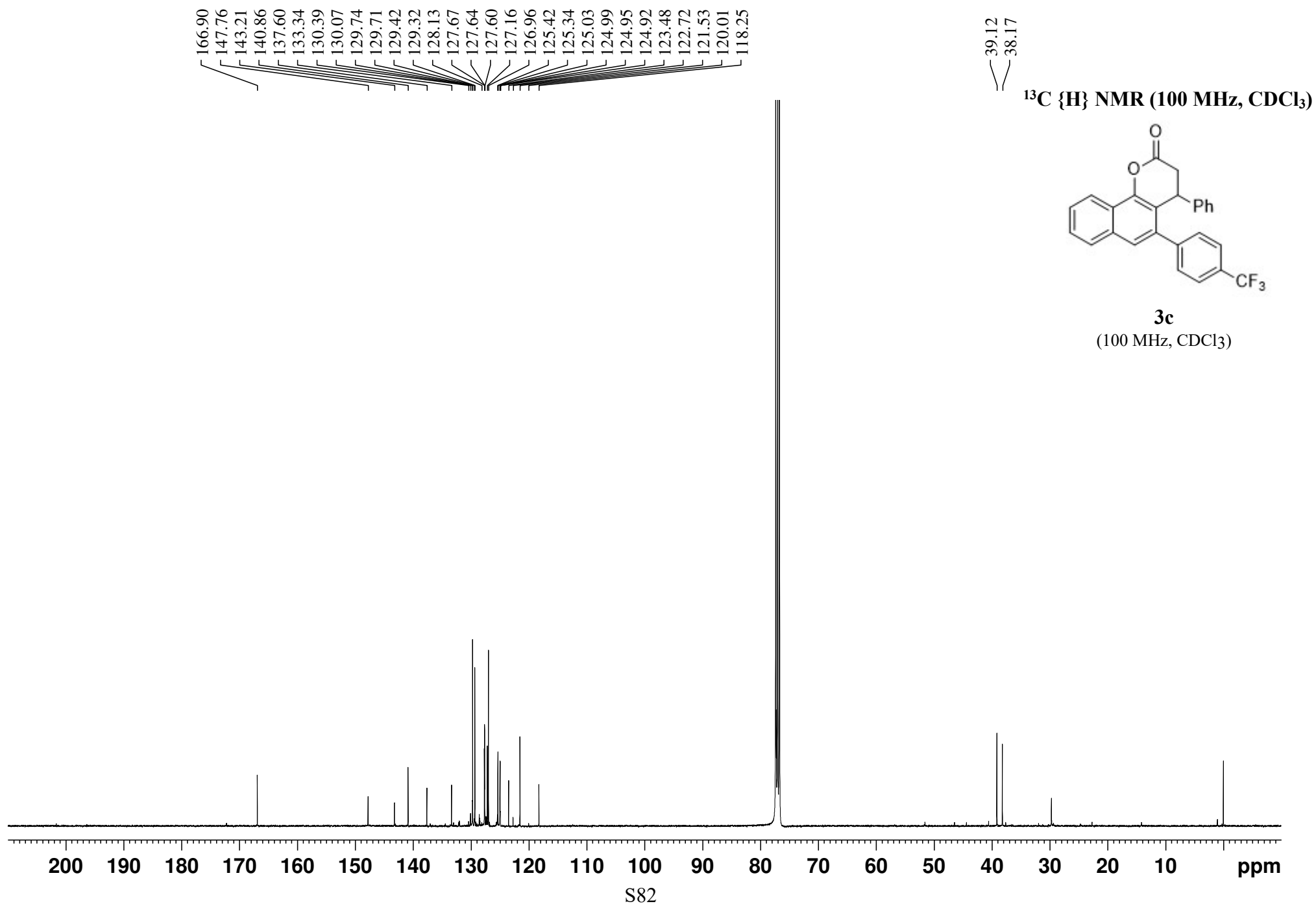
**3a**

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

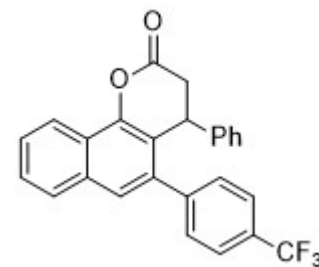






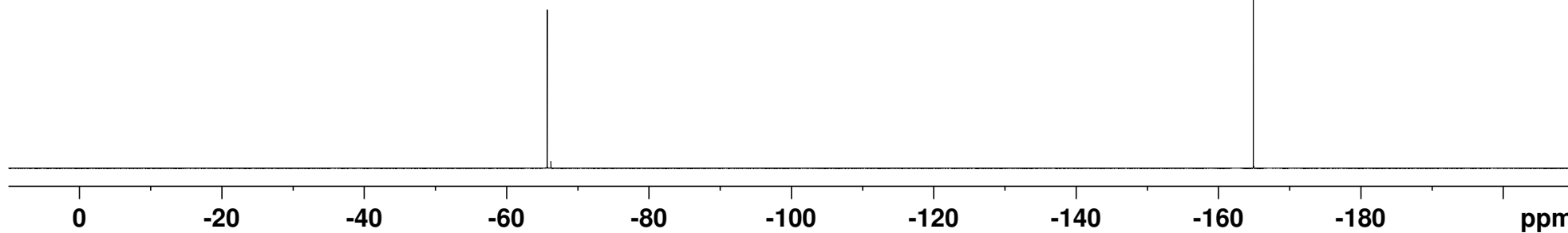


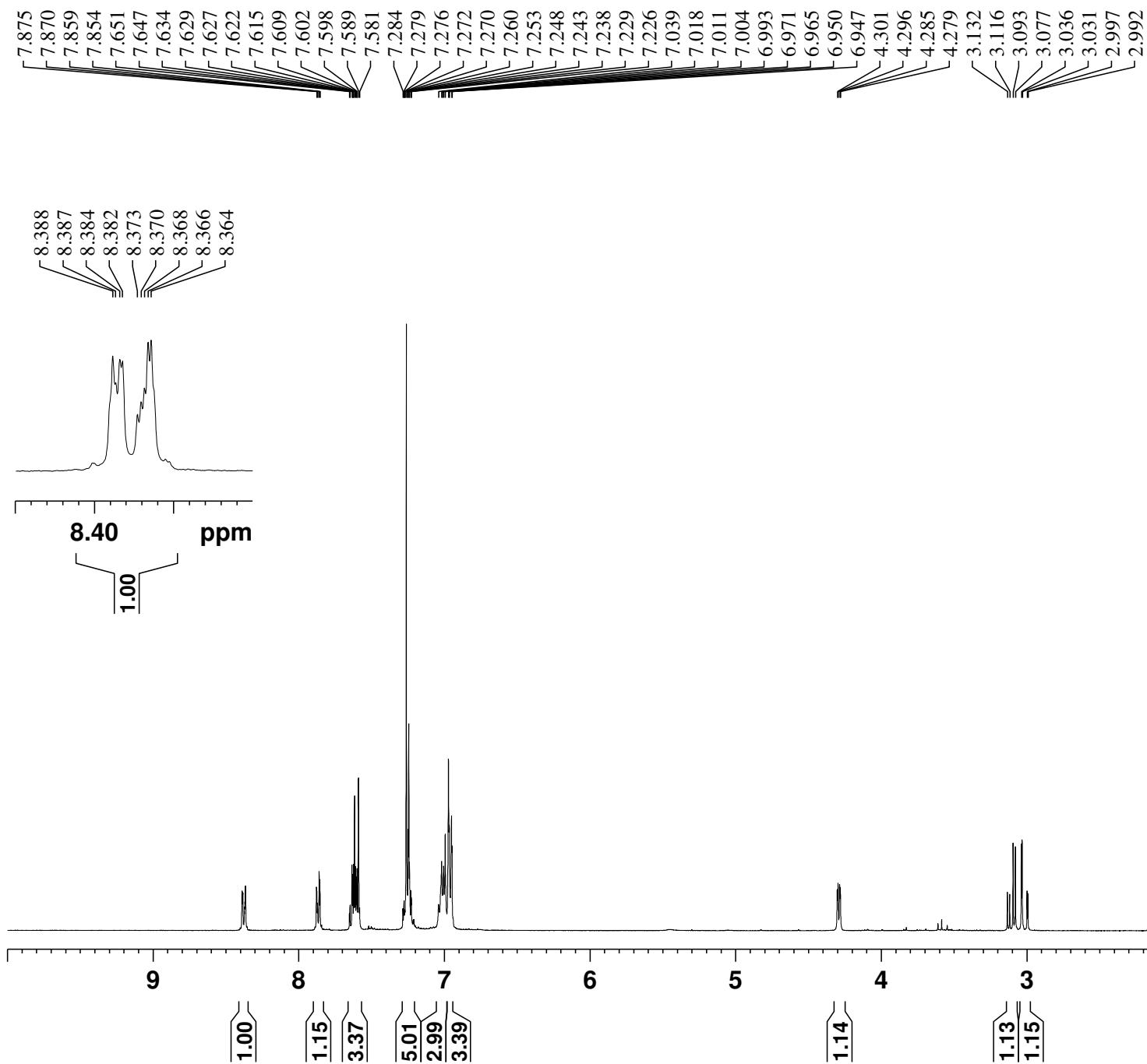
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**



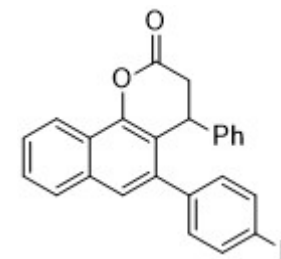
**3c**  
(376 MHz,  $\text{CDCl}_3$ )

— -65.71

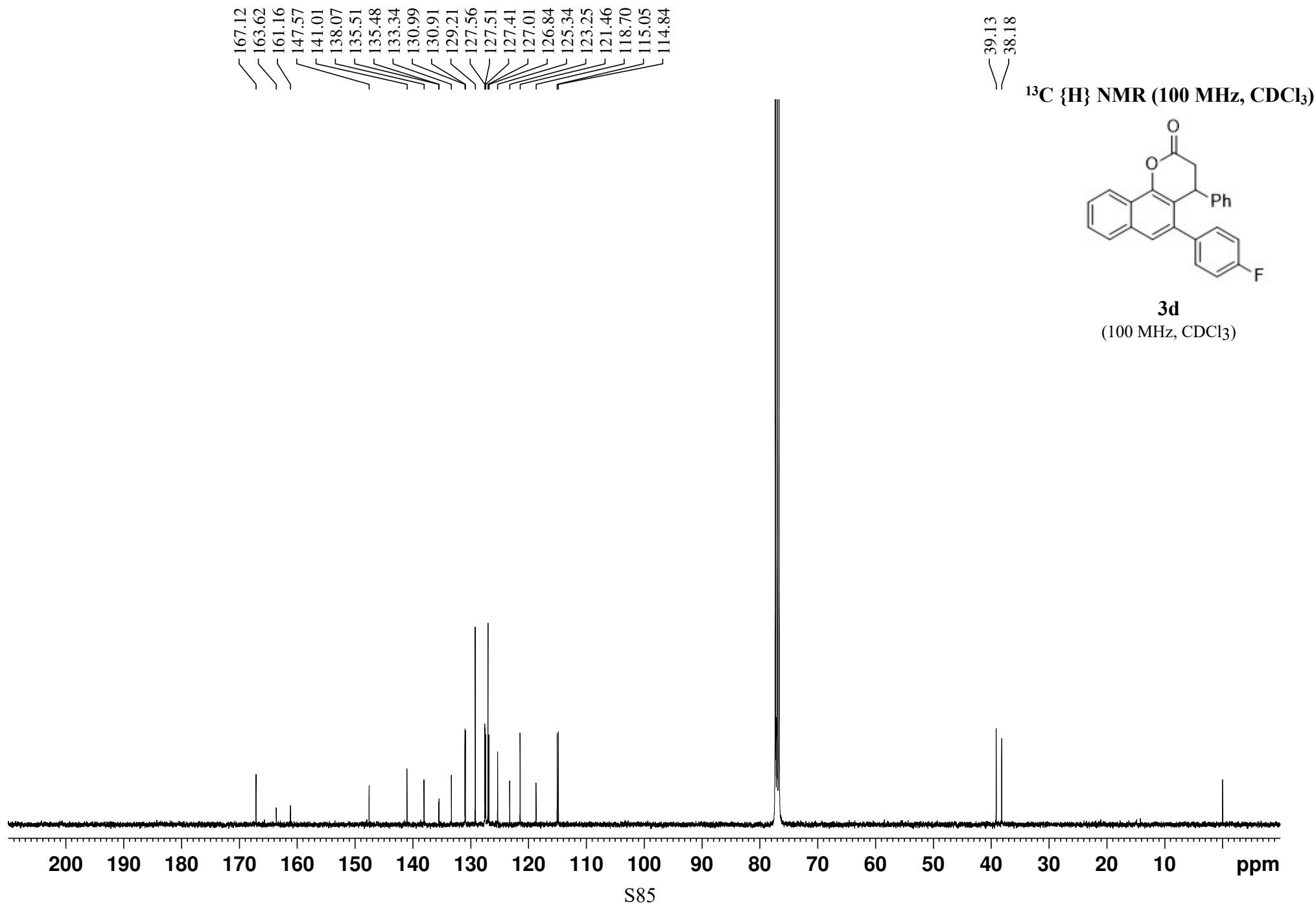




**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**

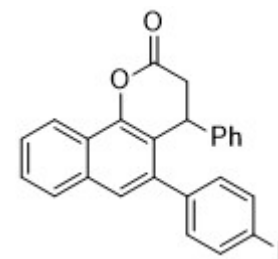


**3d**  
(400 MHz, CDCl<sub>3</sub>)



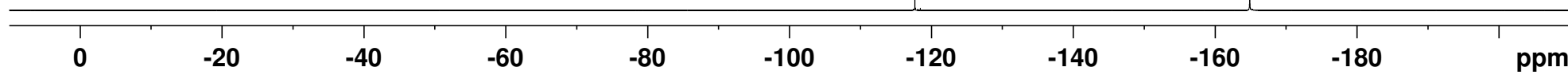
— -117.69

**<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)**



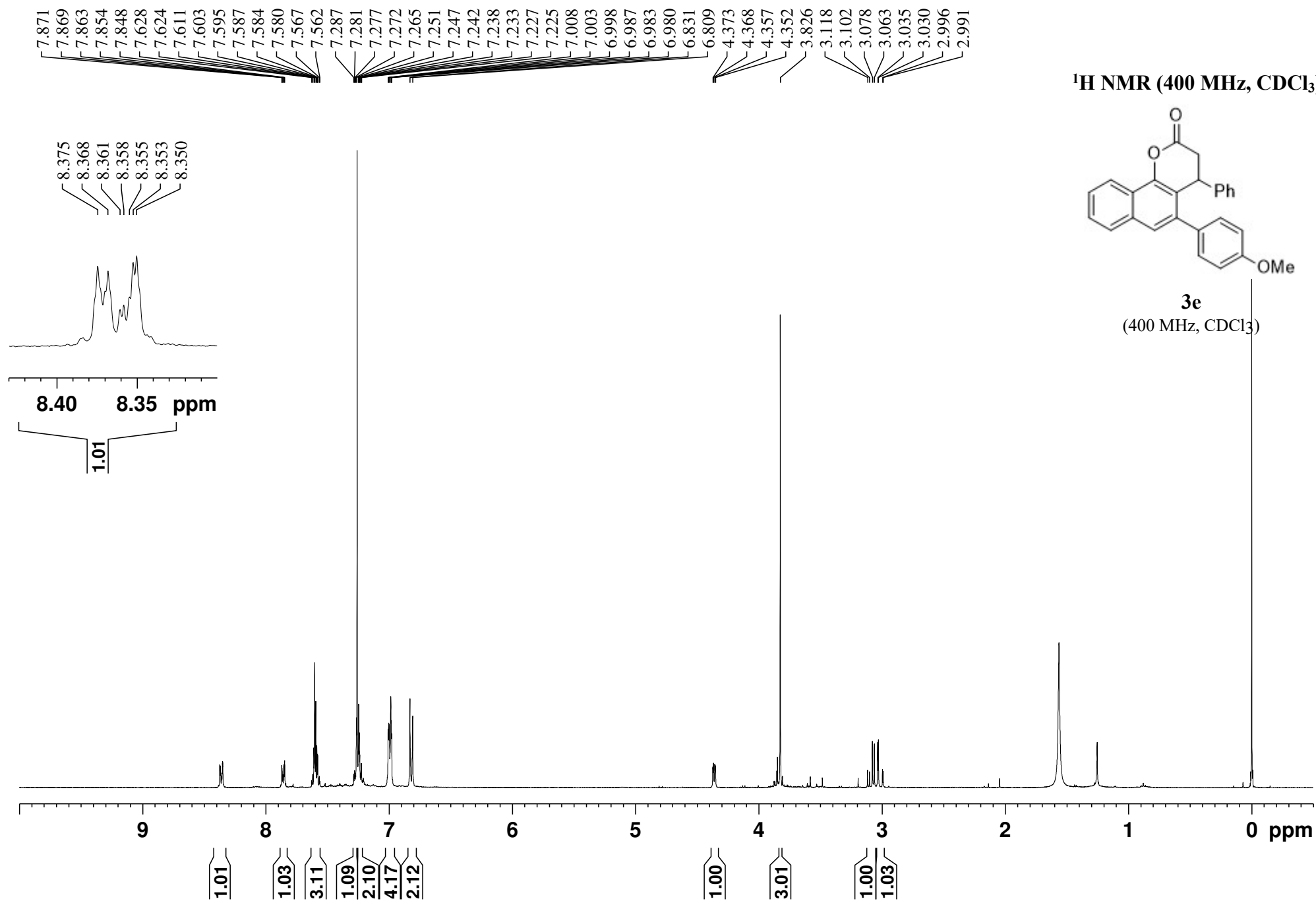
**3d**

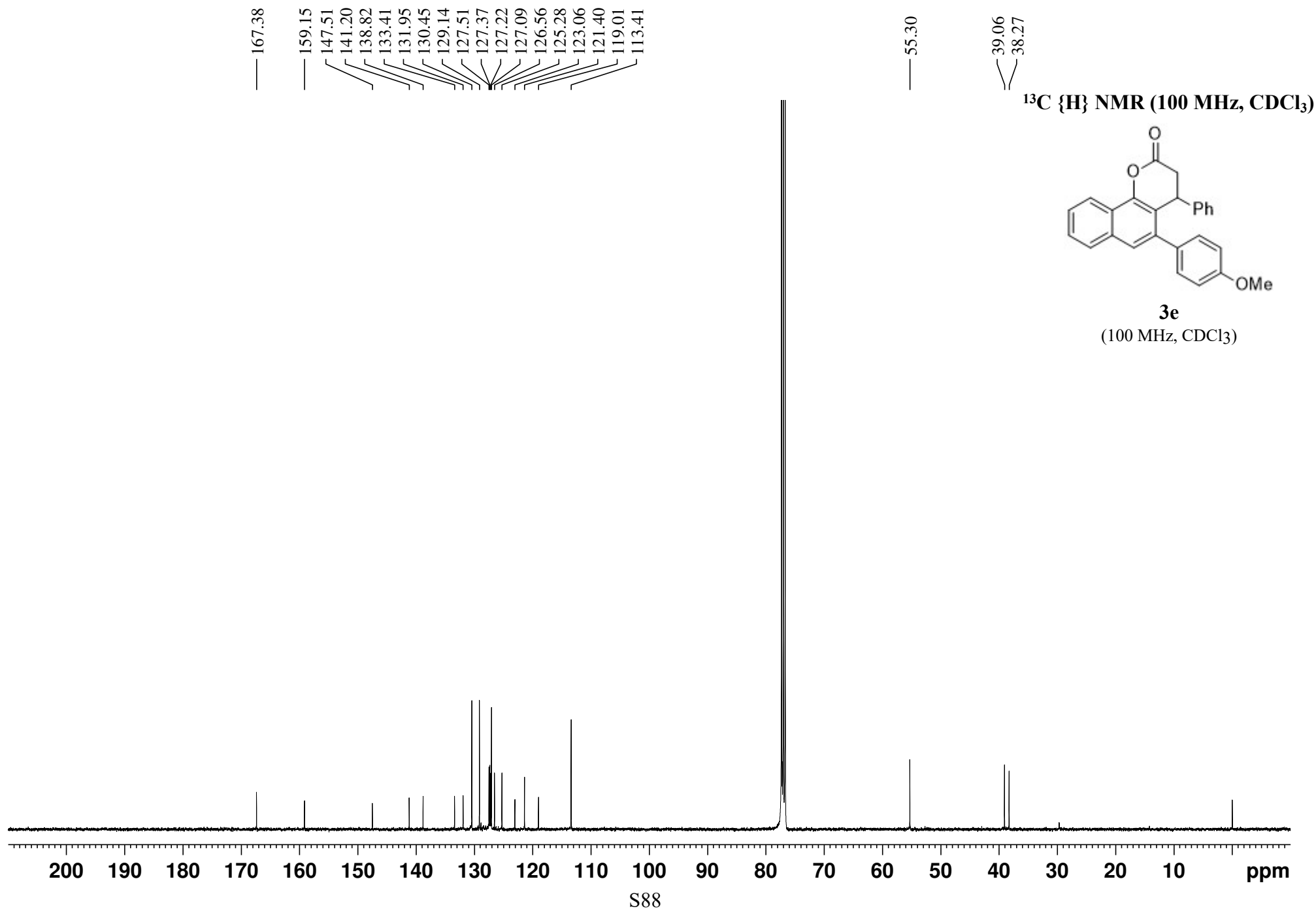
(376 MHz, CDCl<sub>3</sub>)

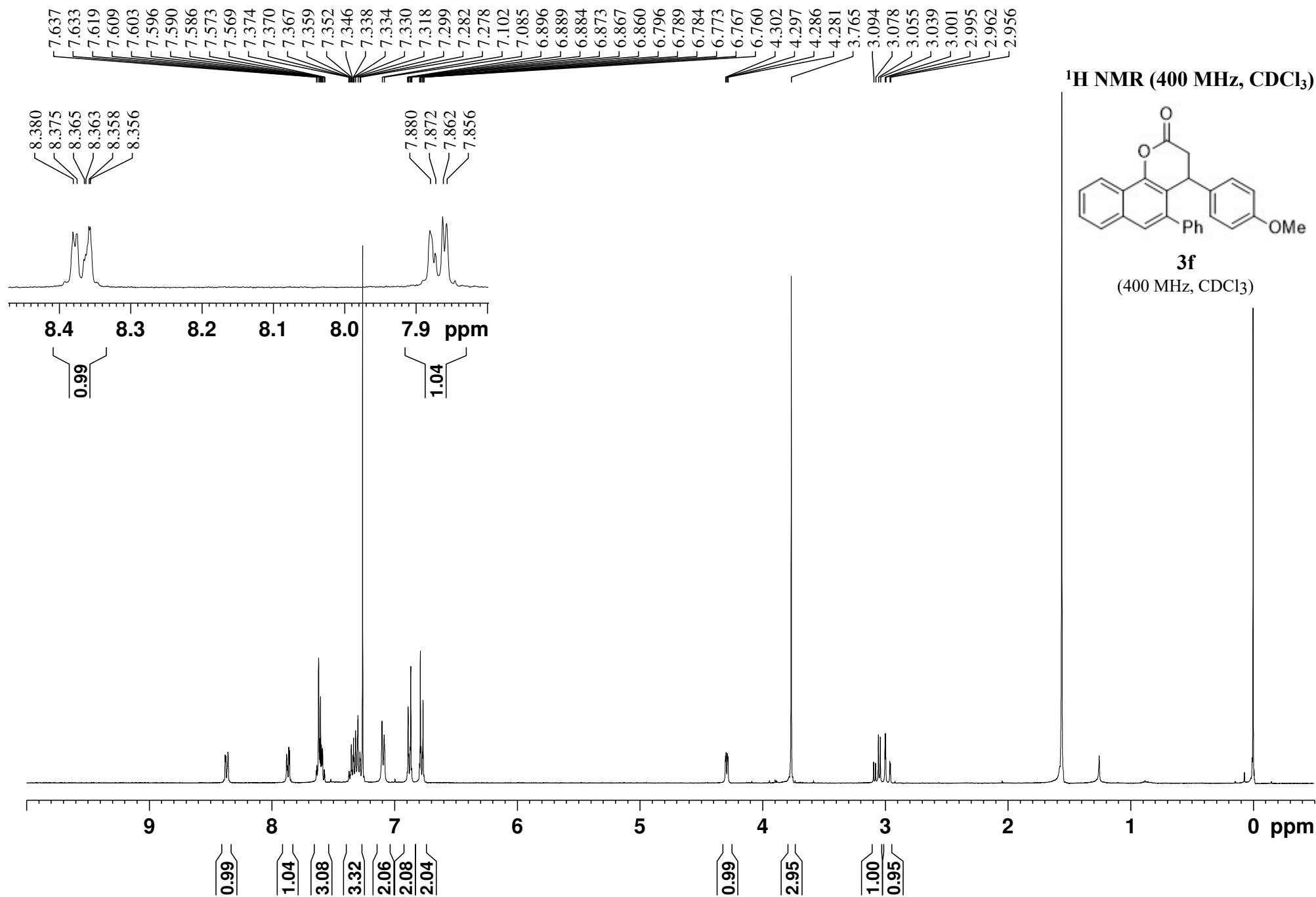


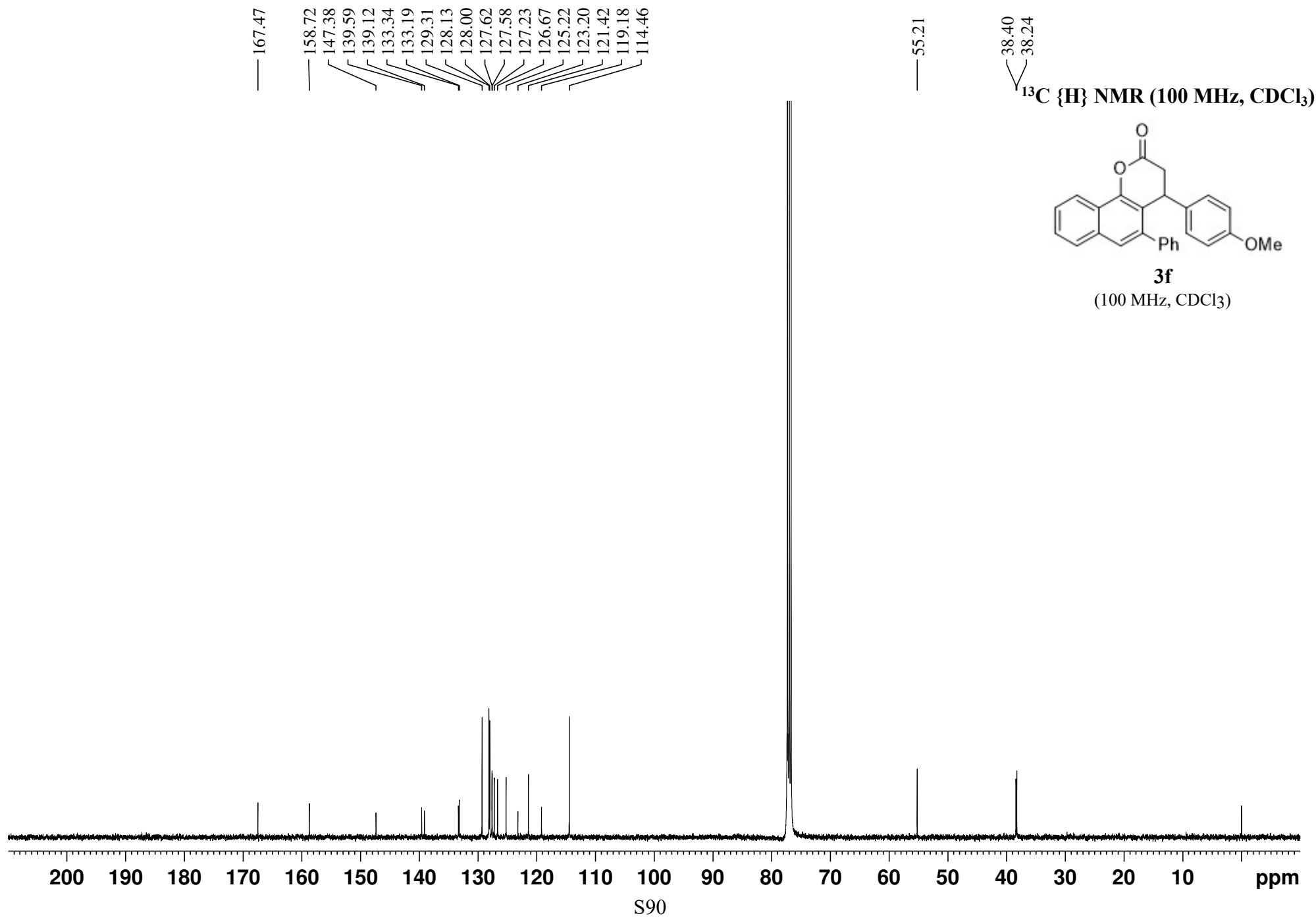
0.16

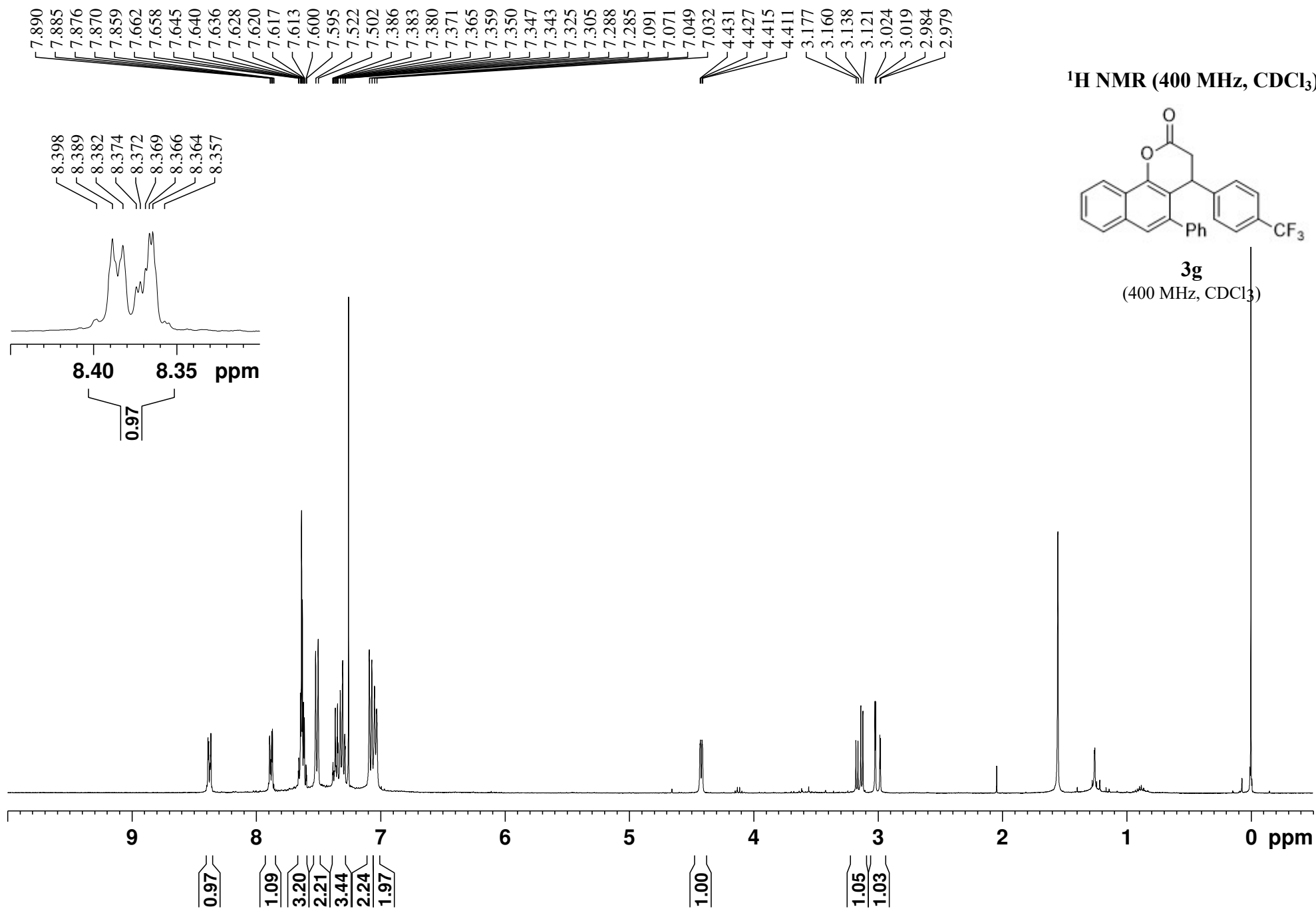
0.62

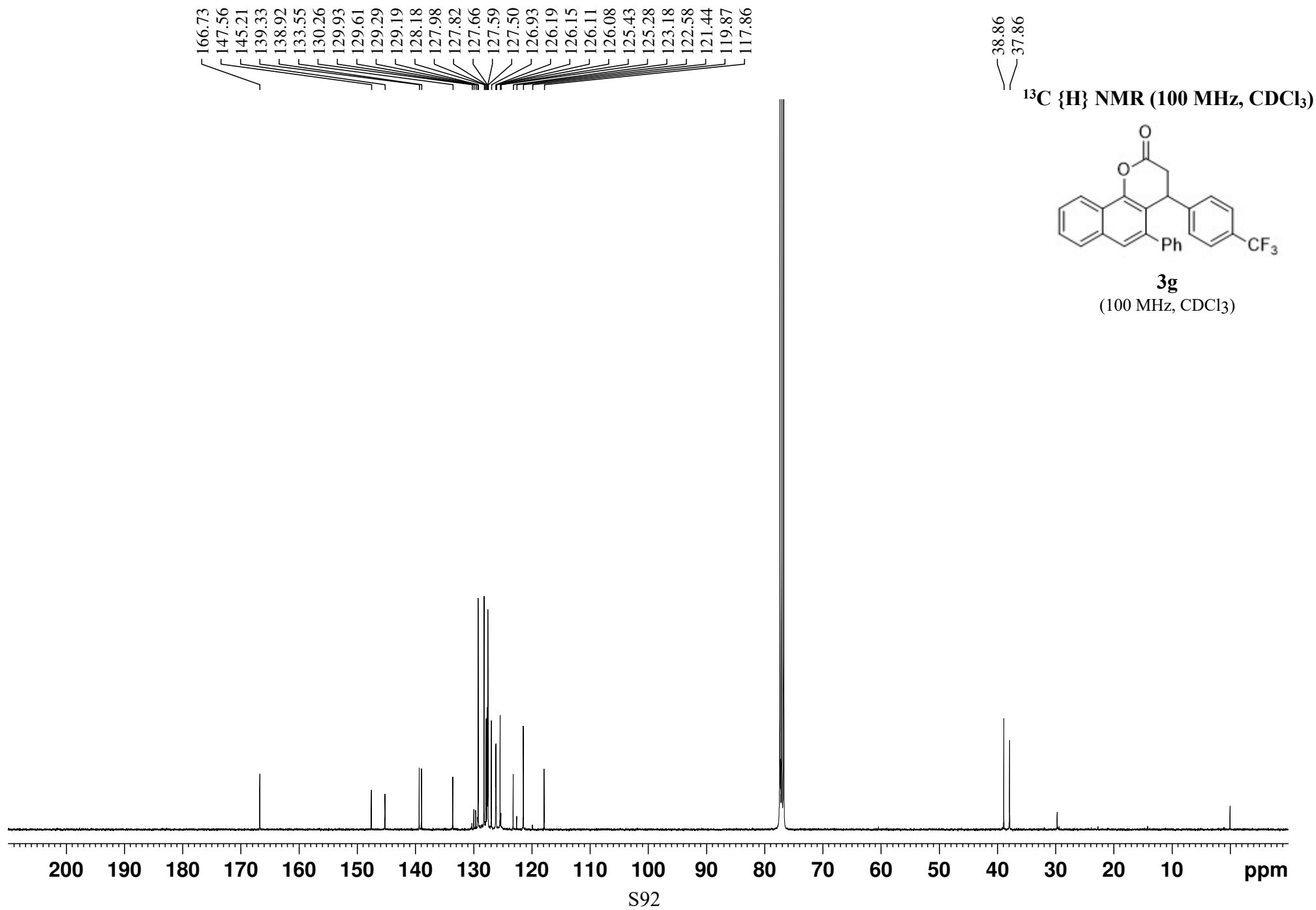




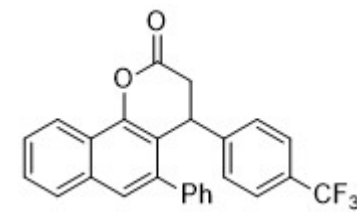






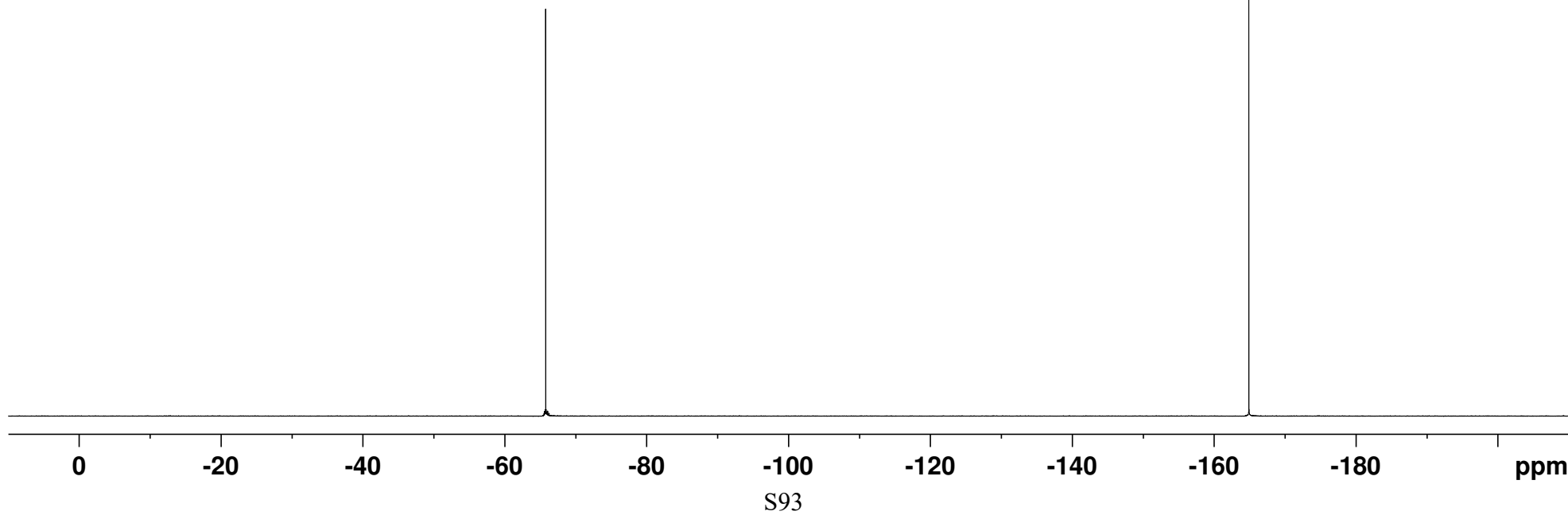


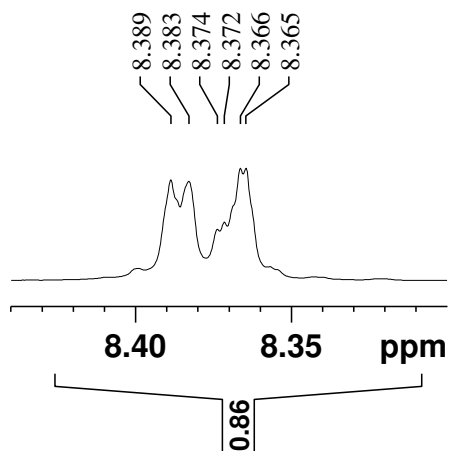
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**



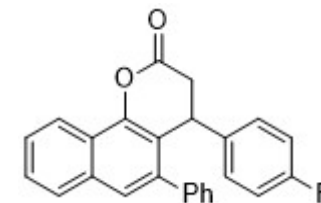
**3g**  
(376 MHz,  $\text{CDCl}_3$ )

— -65.76

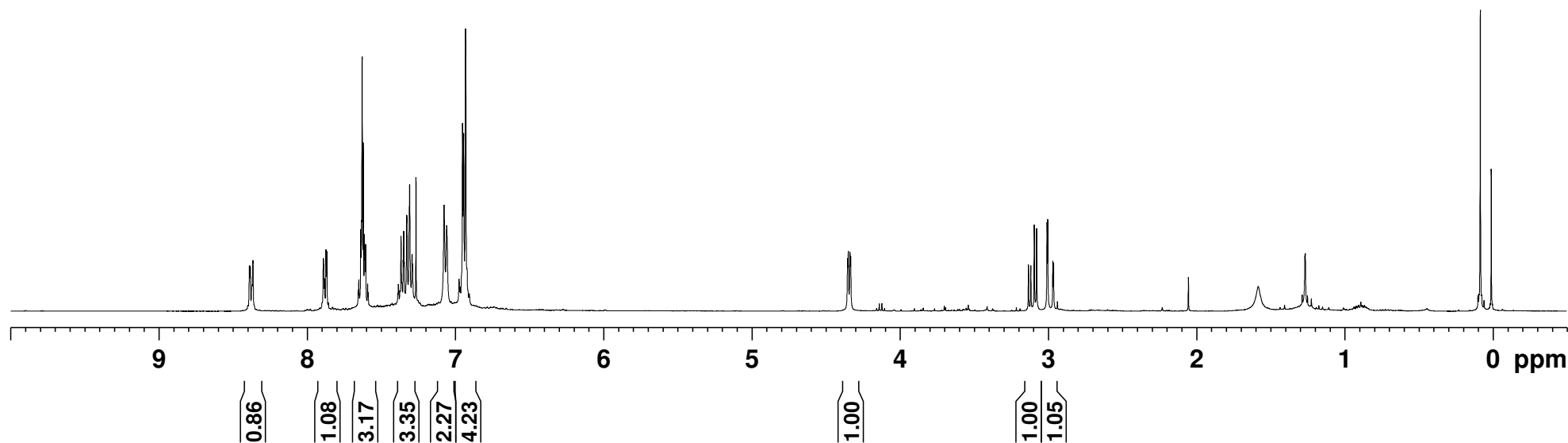


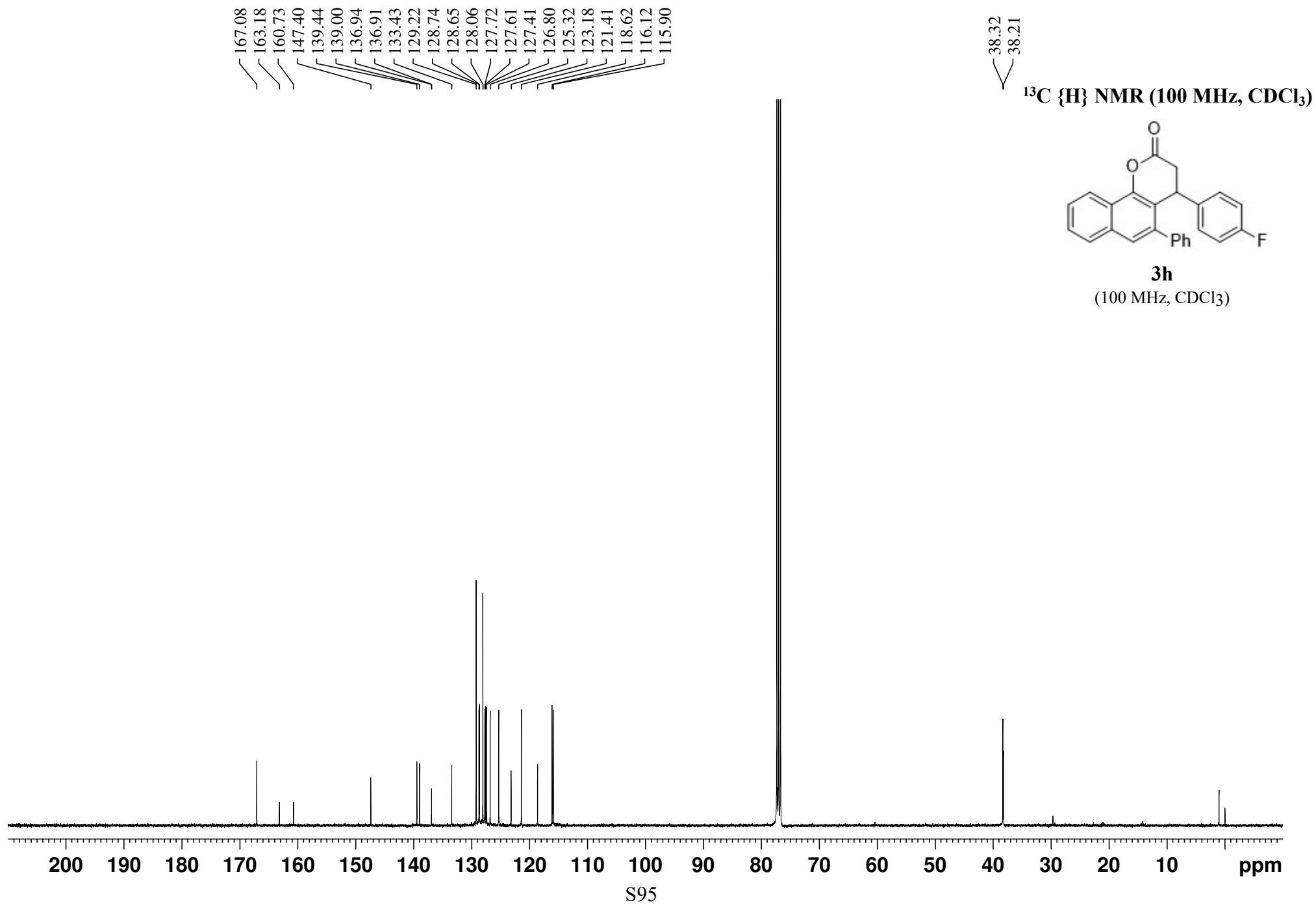


**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**

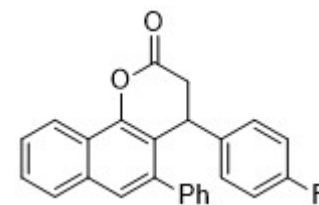


**3h**  
(400 MHz, CDCl<sub>3</sub>)





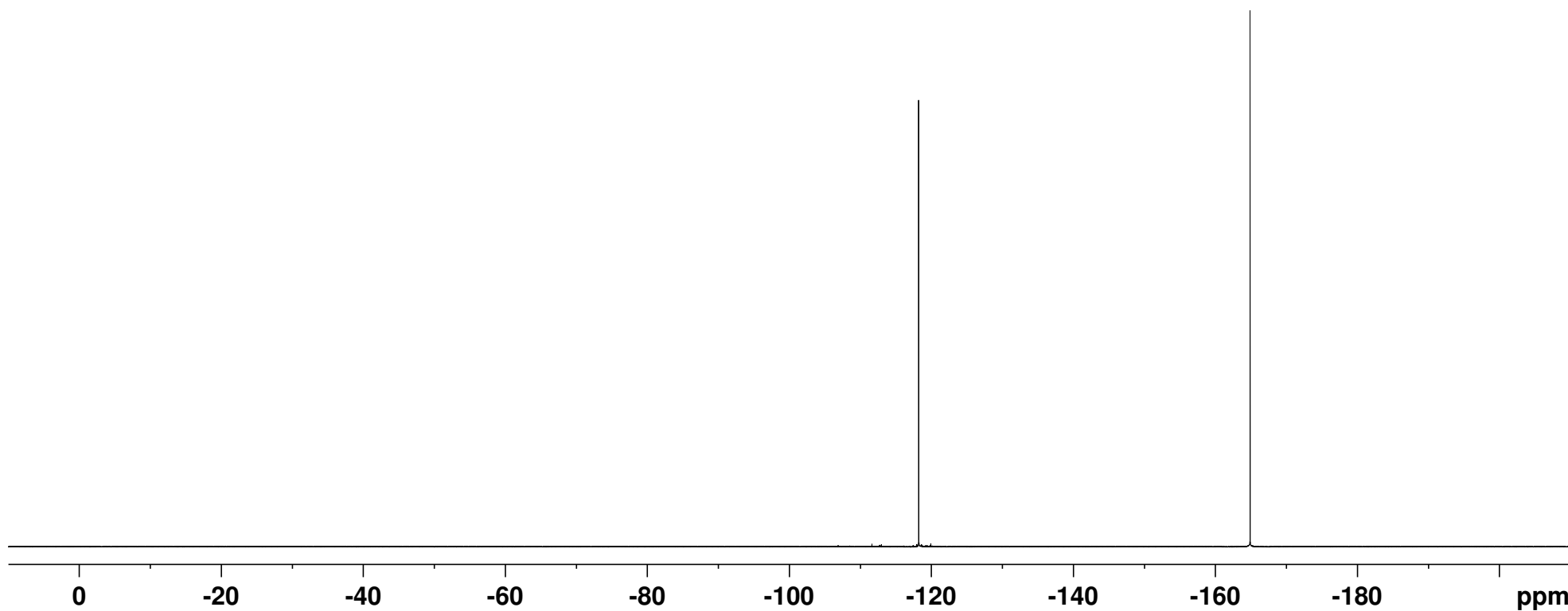
**$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )**



**3h**

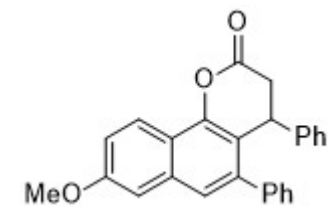
(376 MHz,  $\text{CDCl}_3$ )

— -118.21



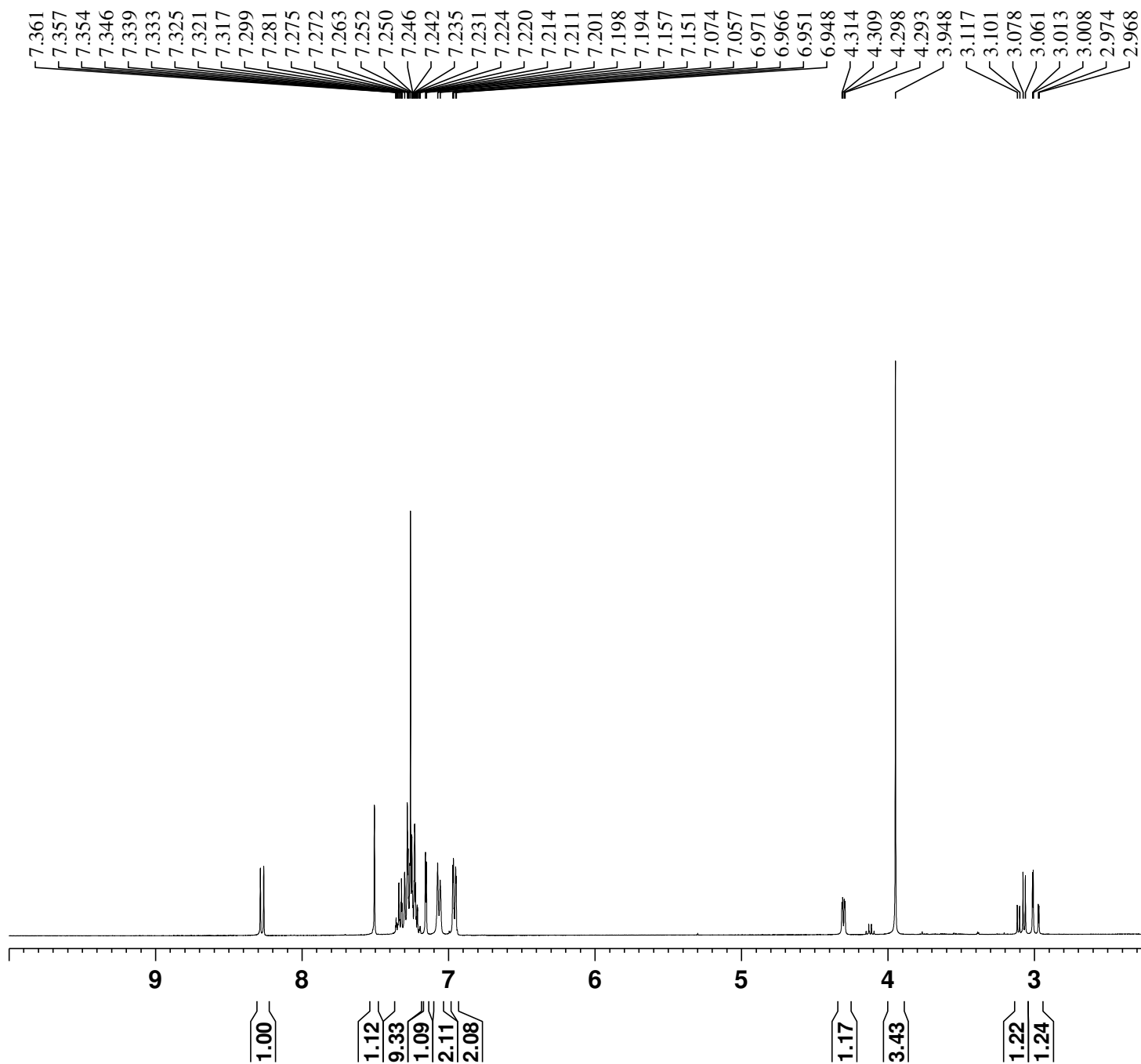
S96

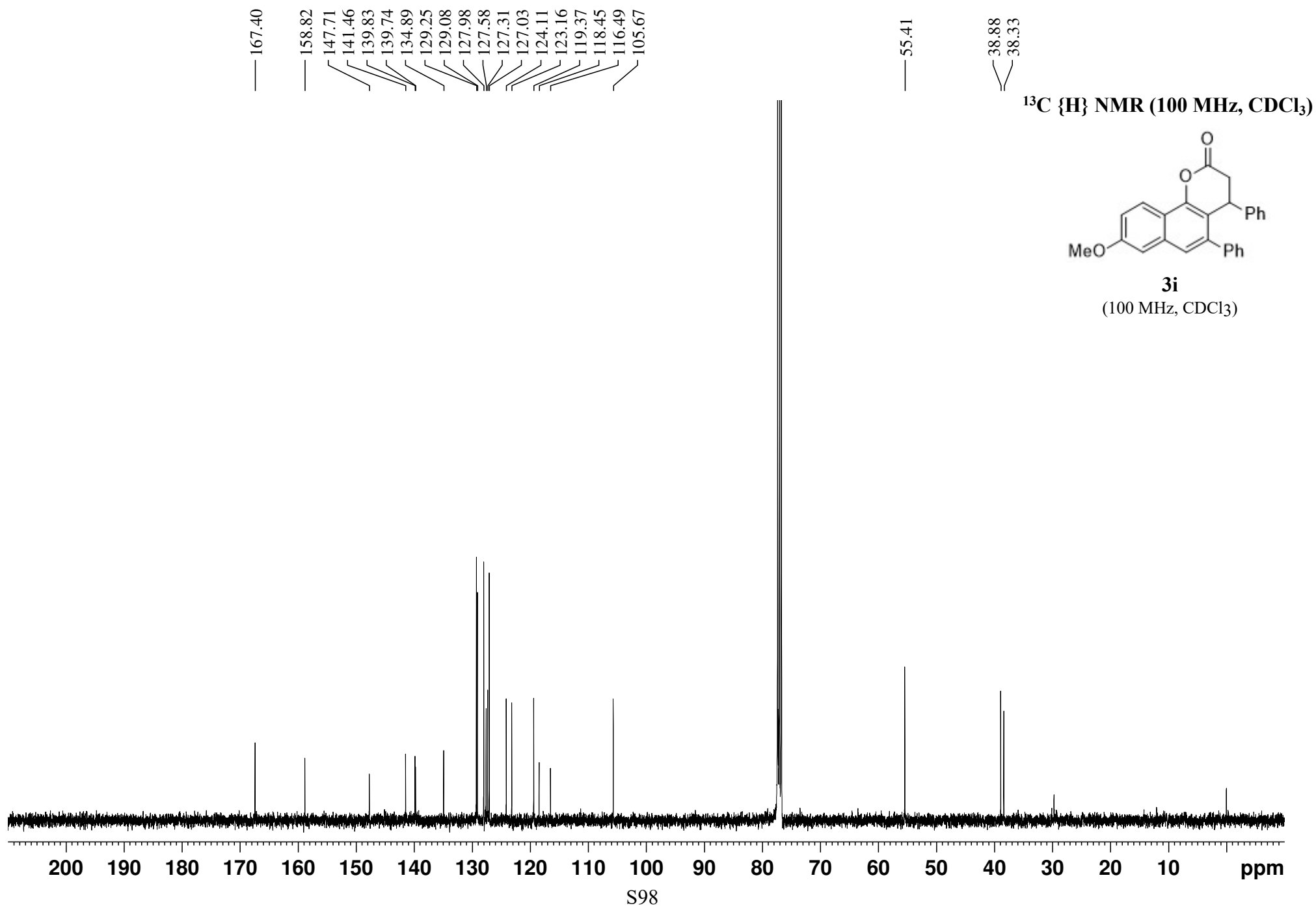
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

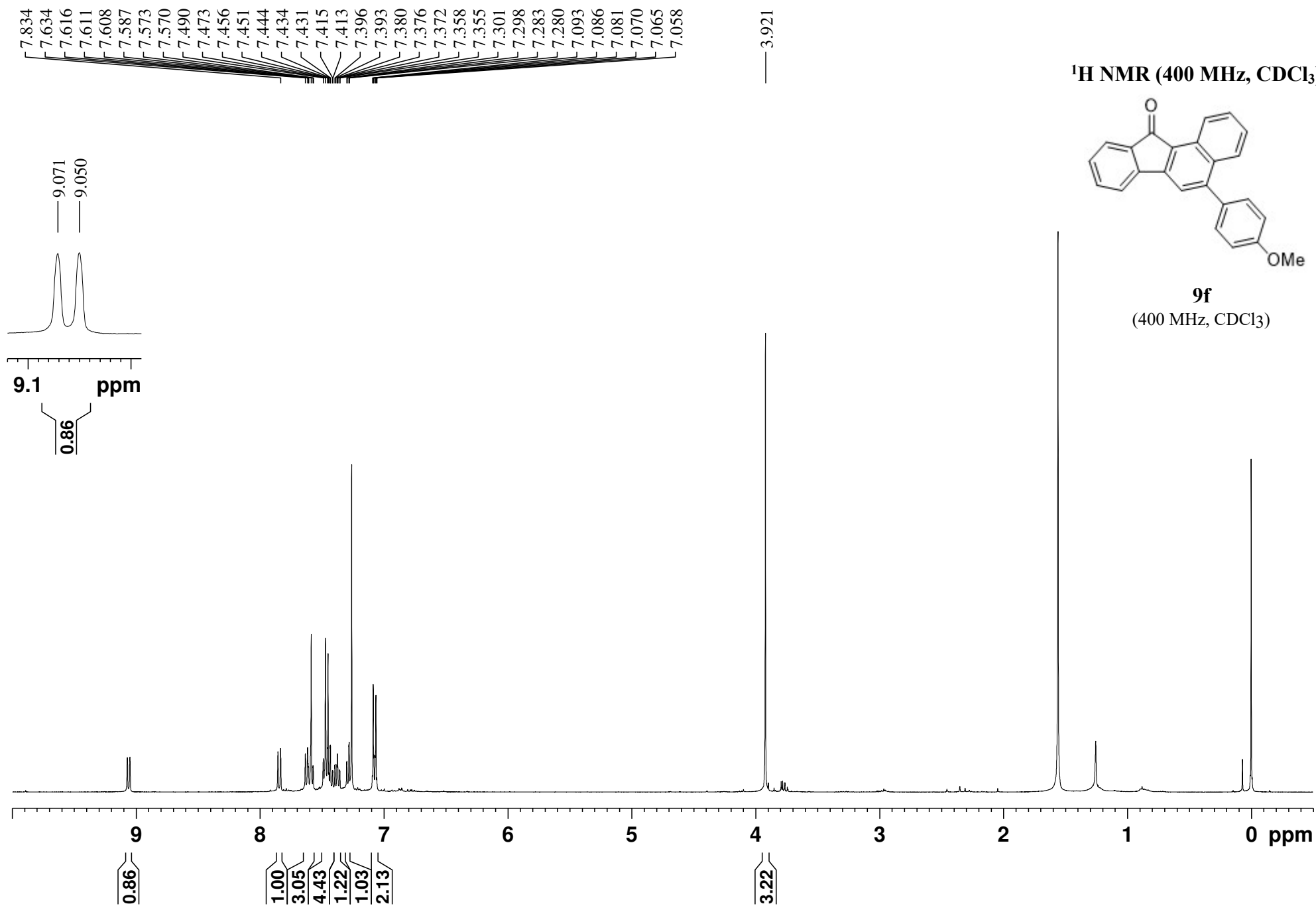


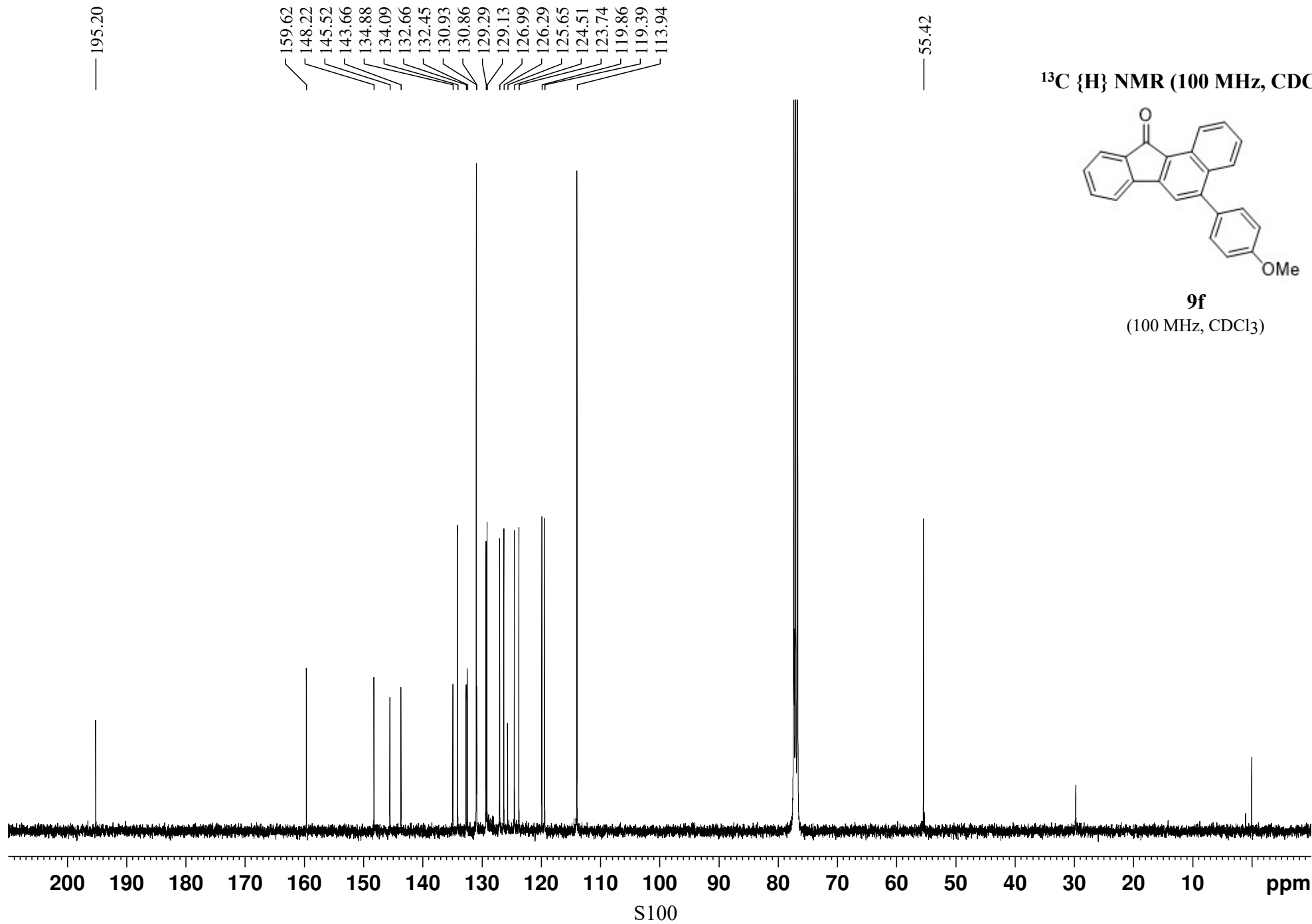
**3i**

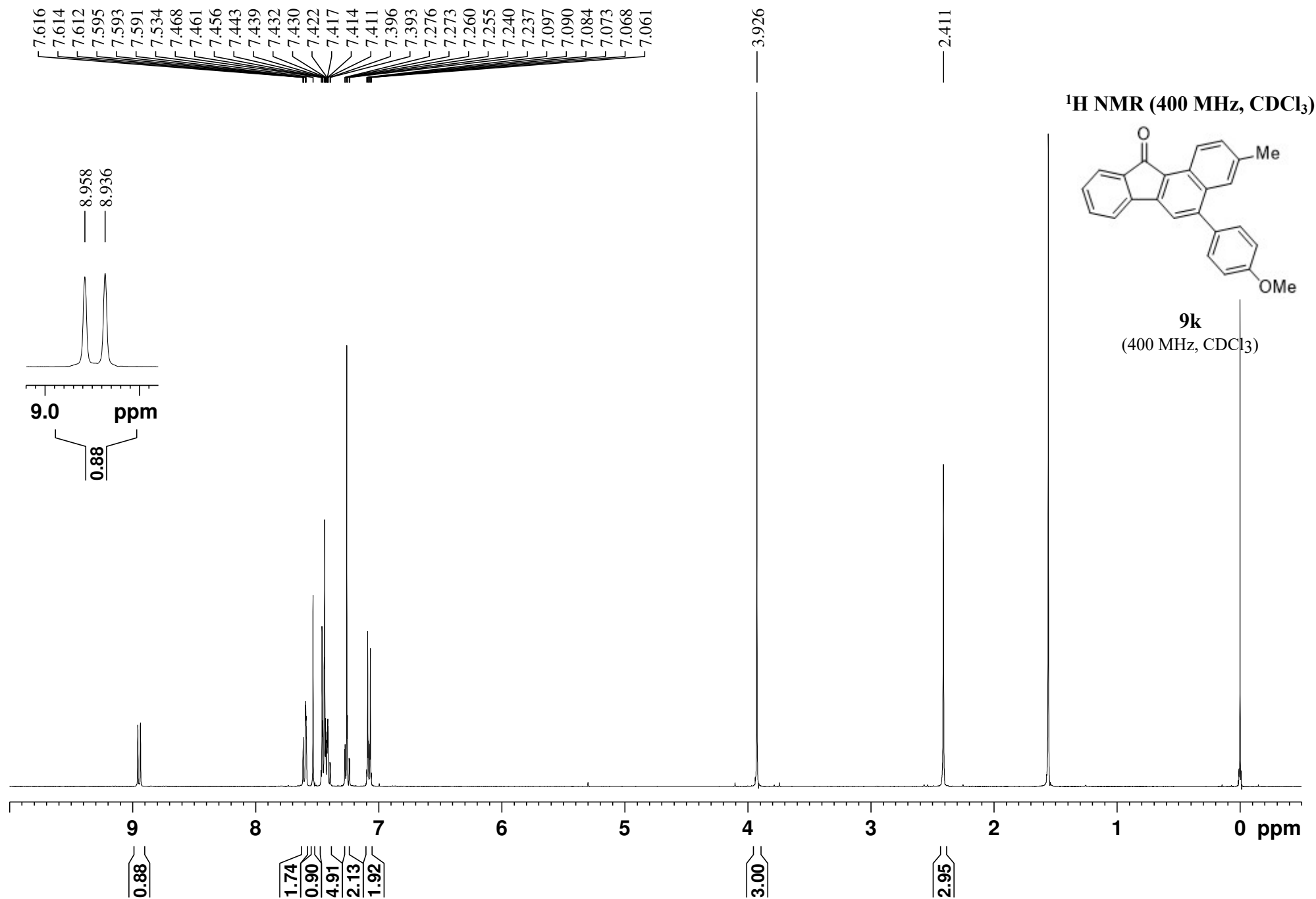
(400 MHz, CDCl<sub>3</sub>)

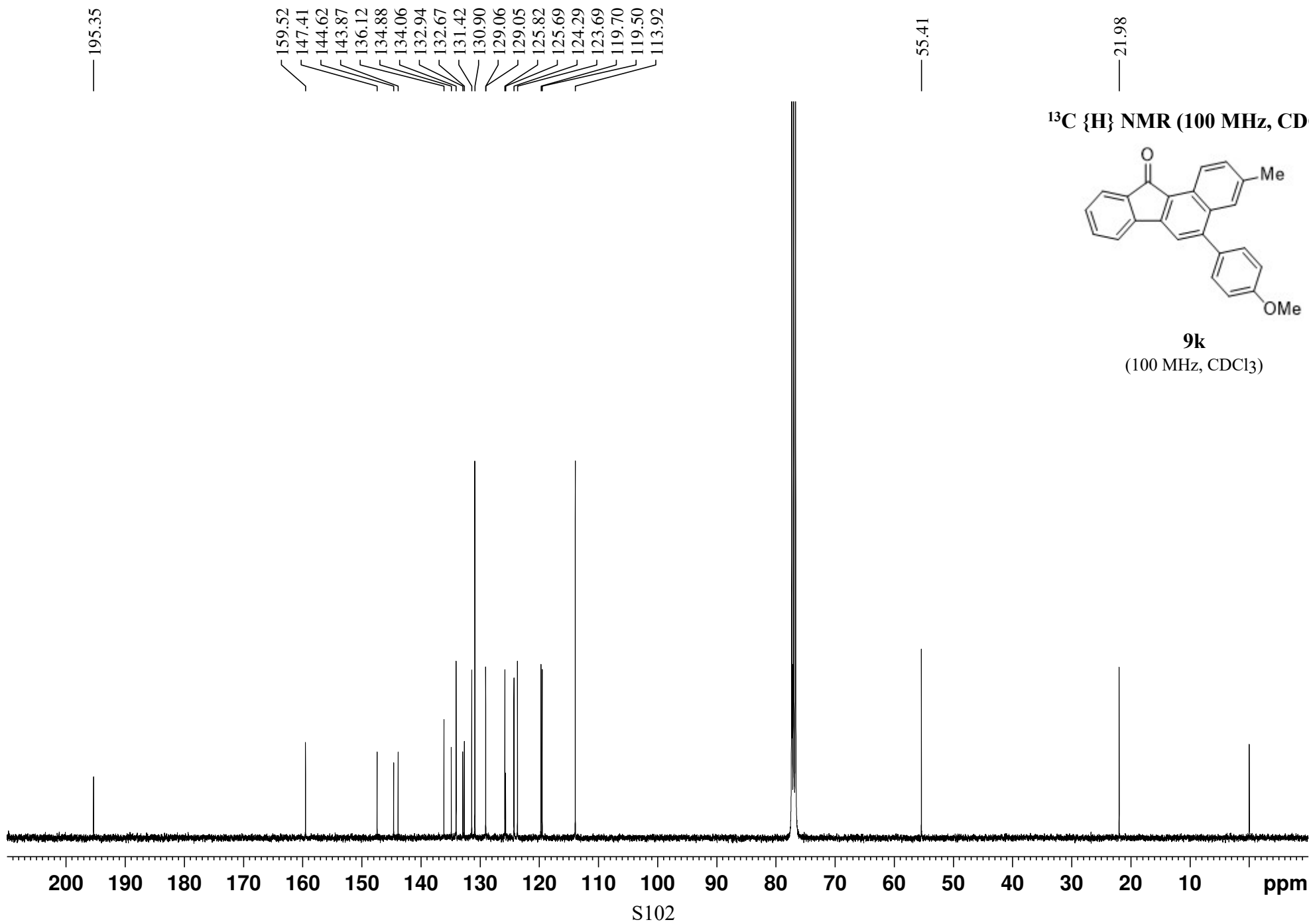


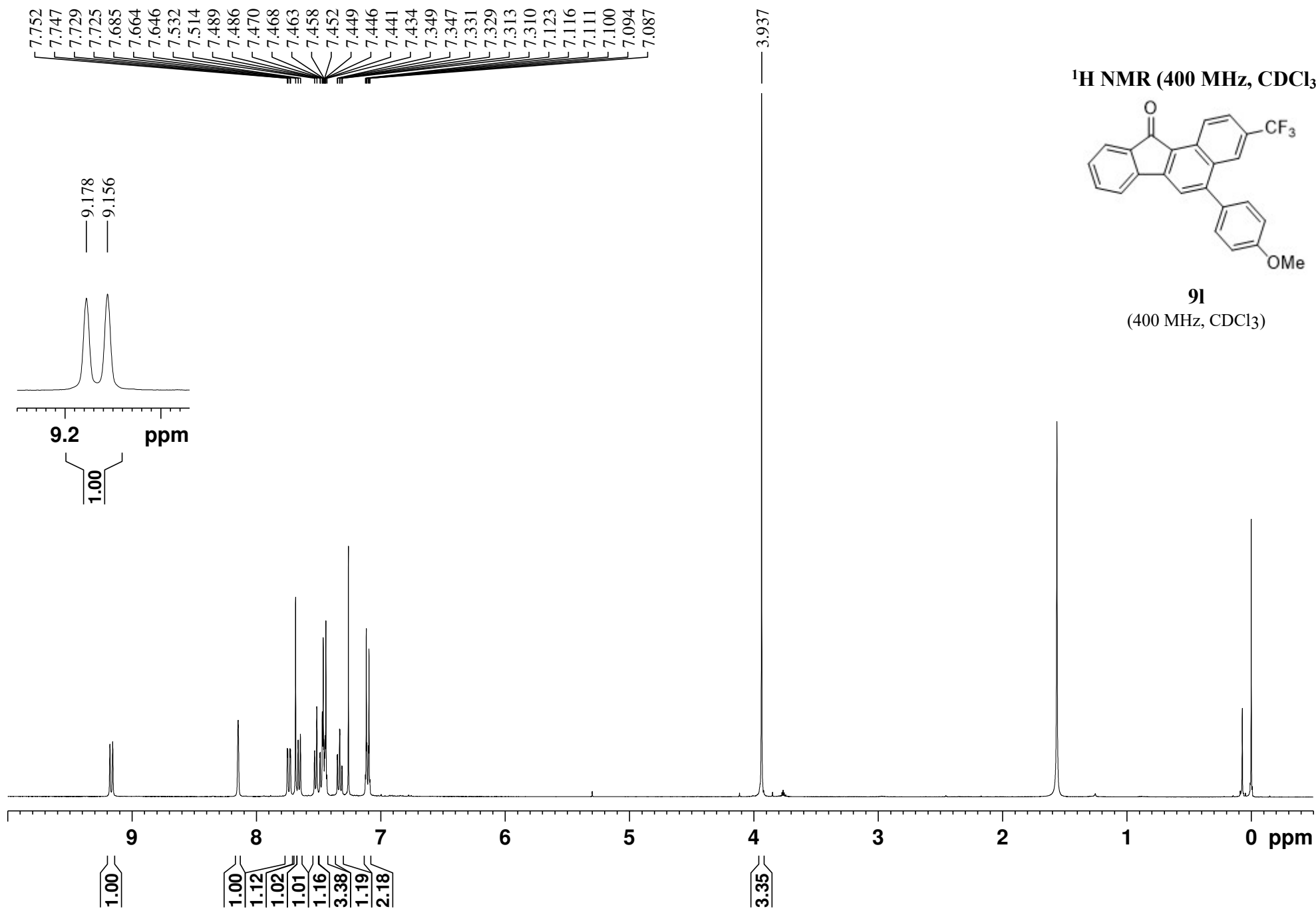


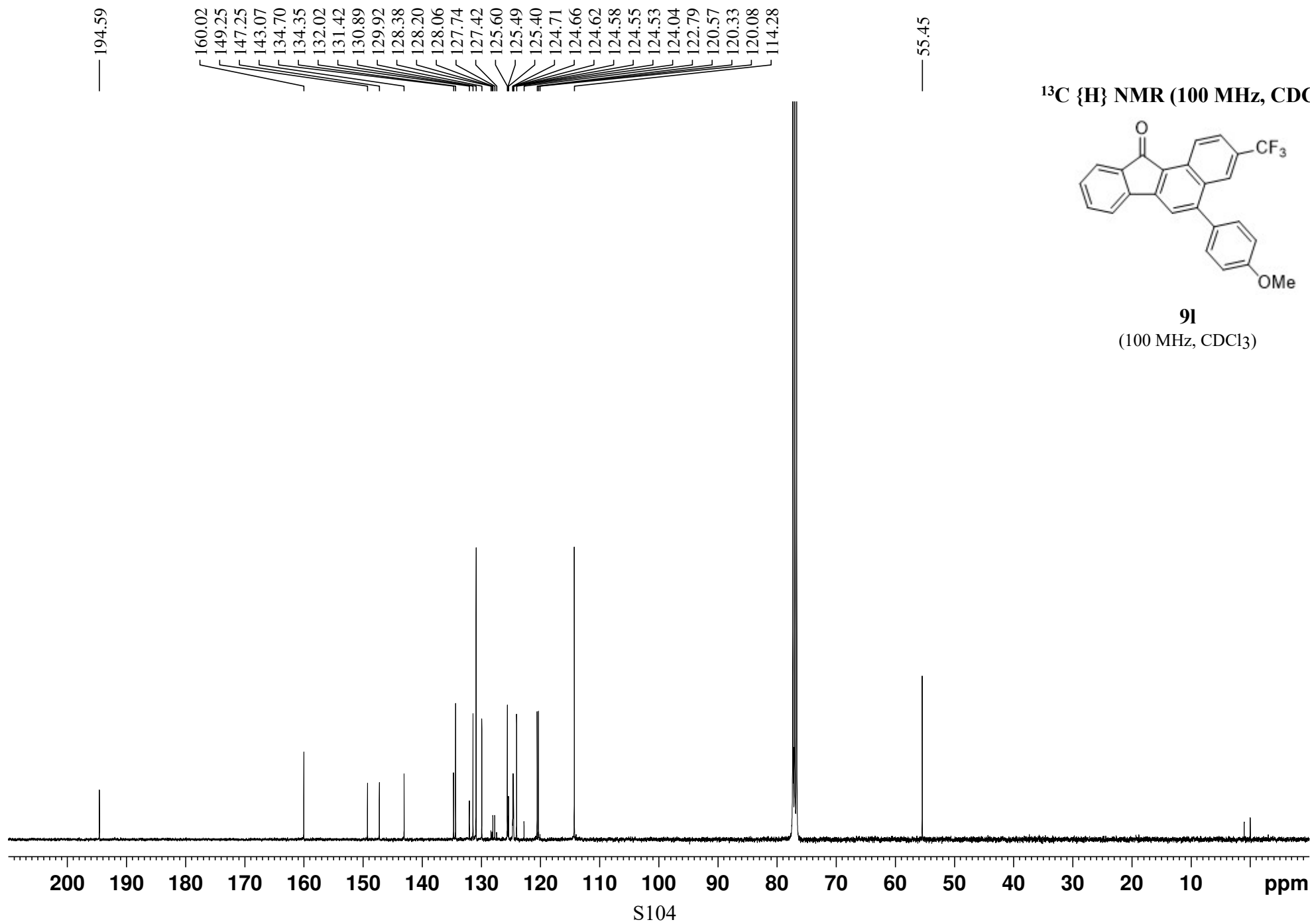


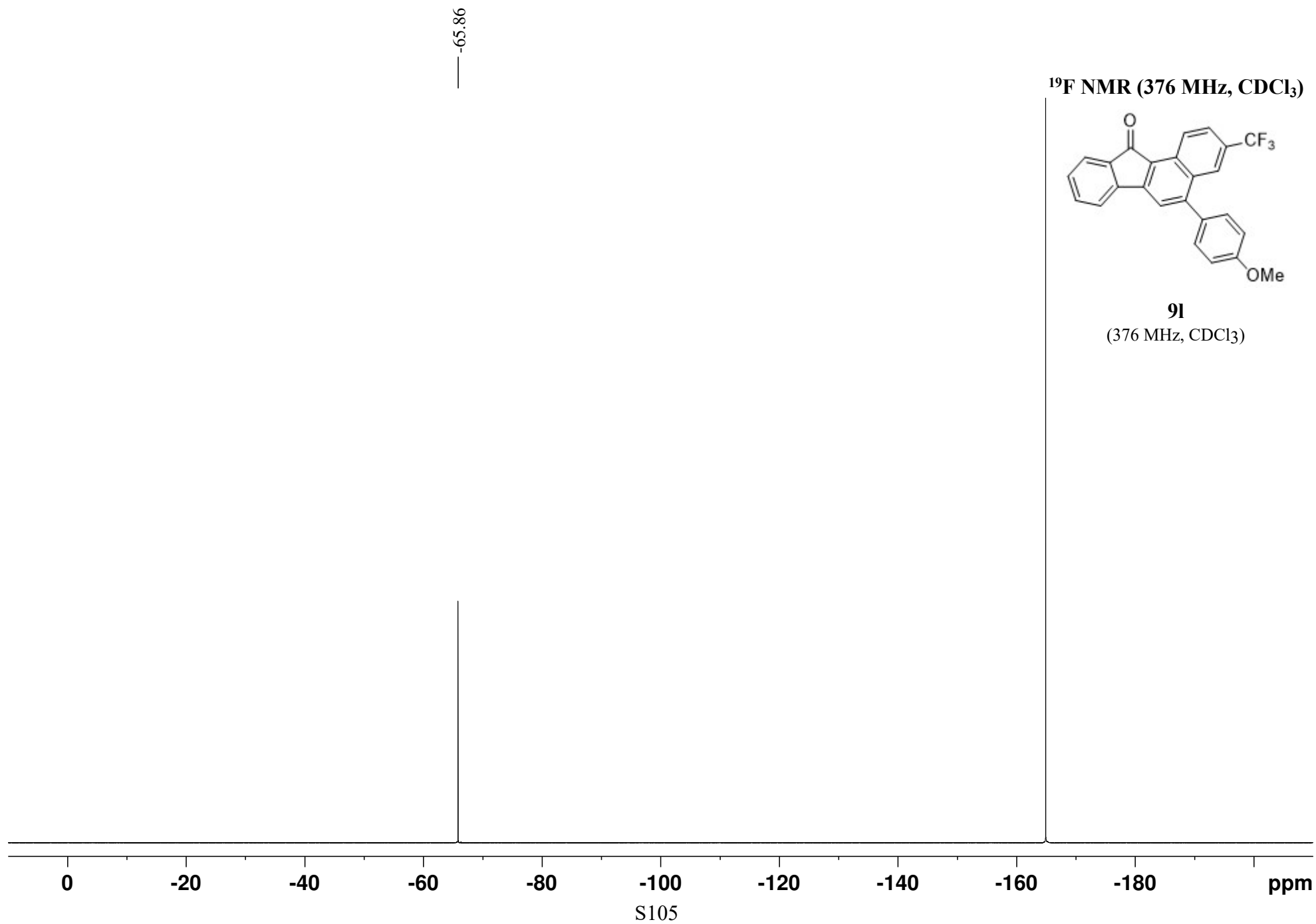


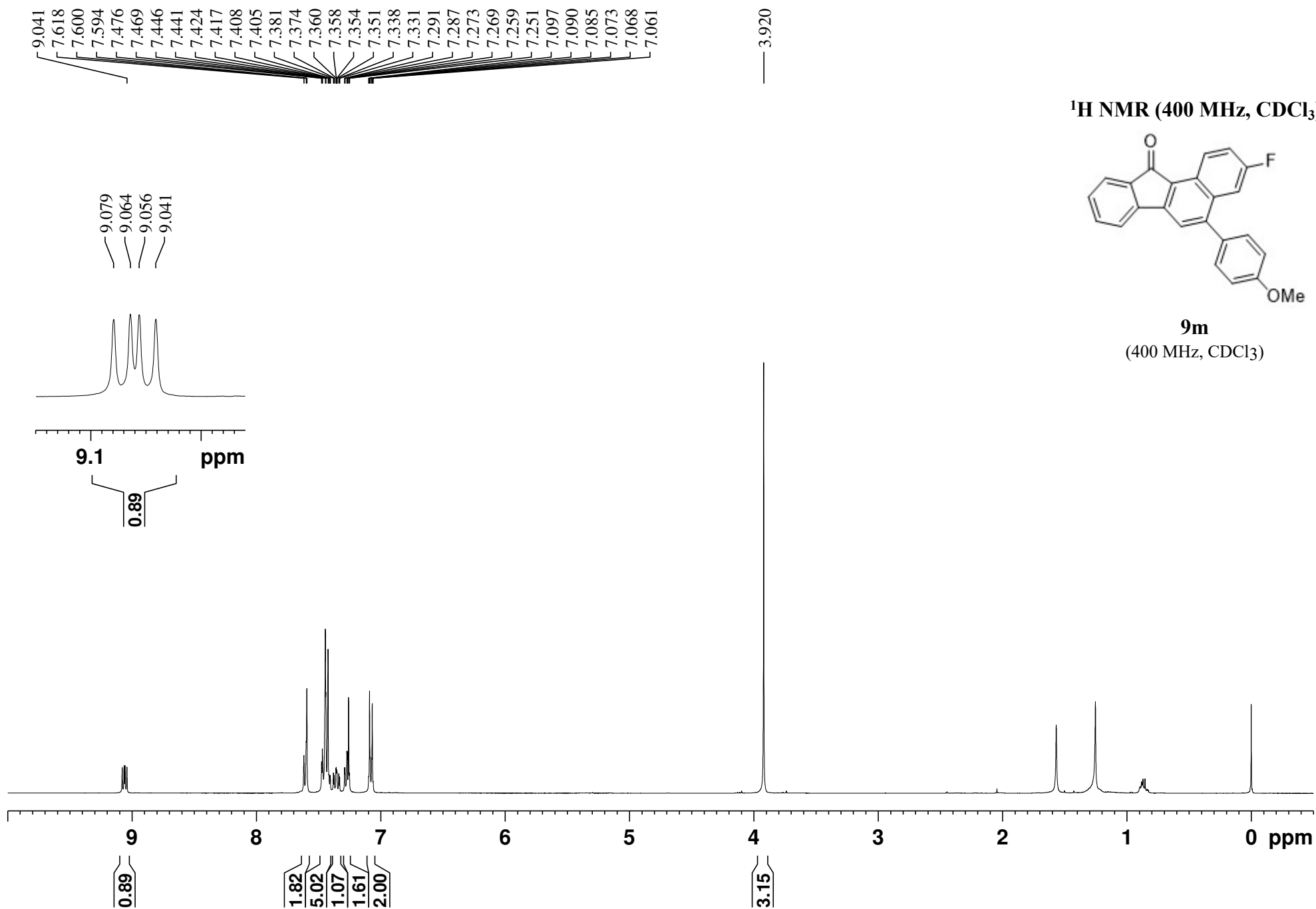


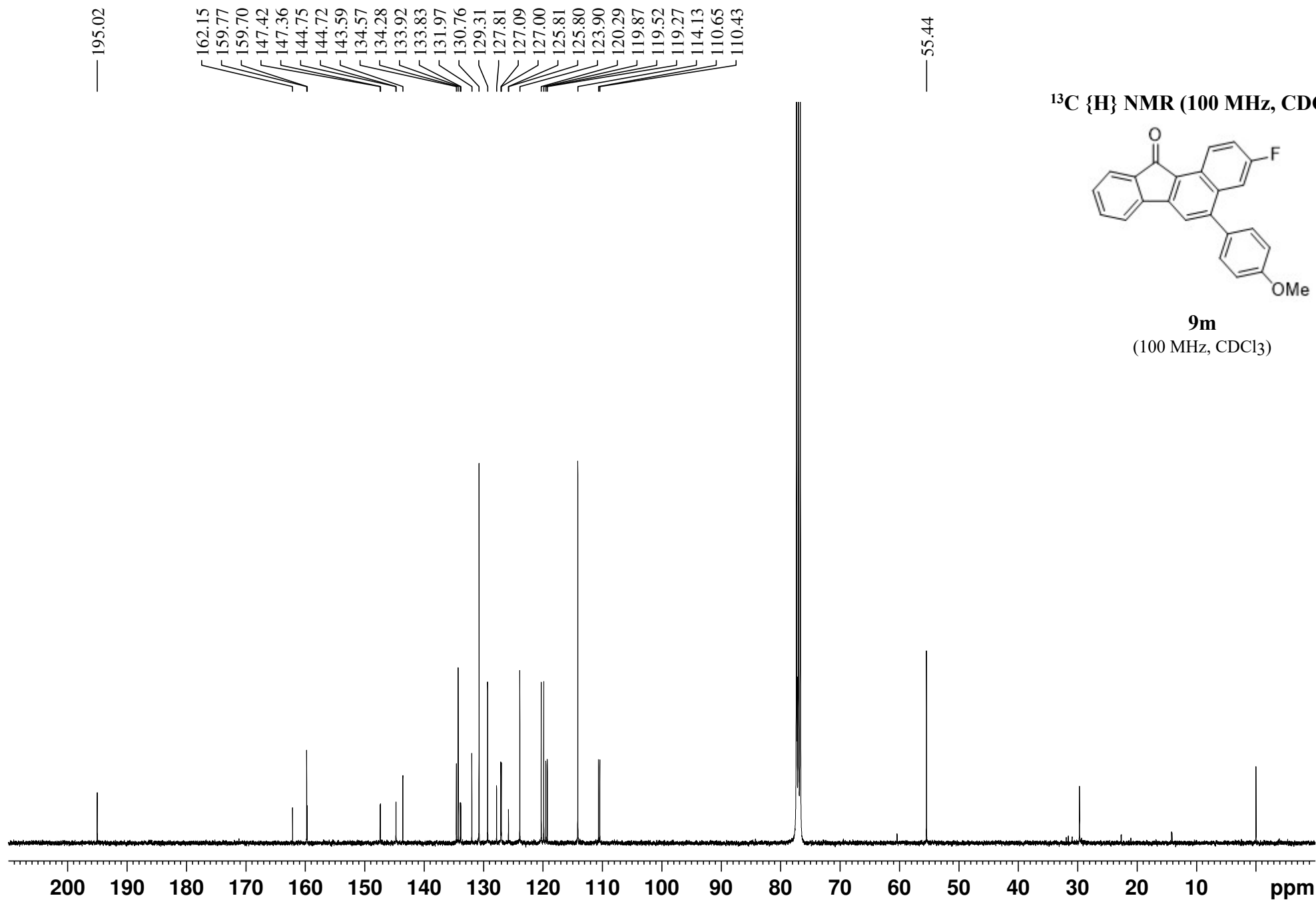


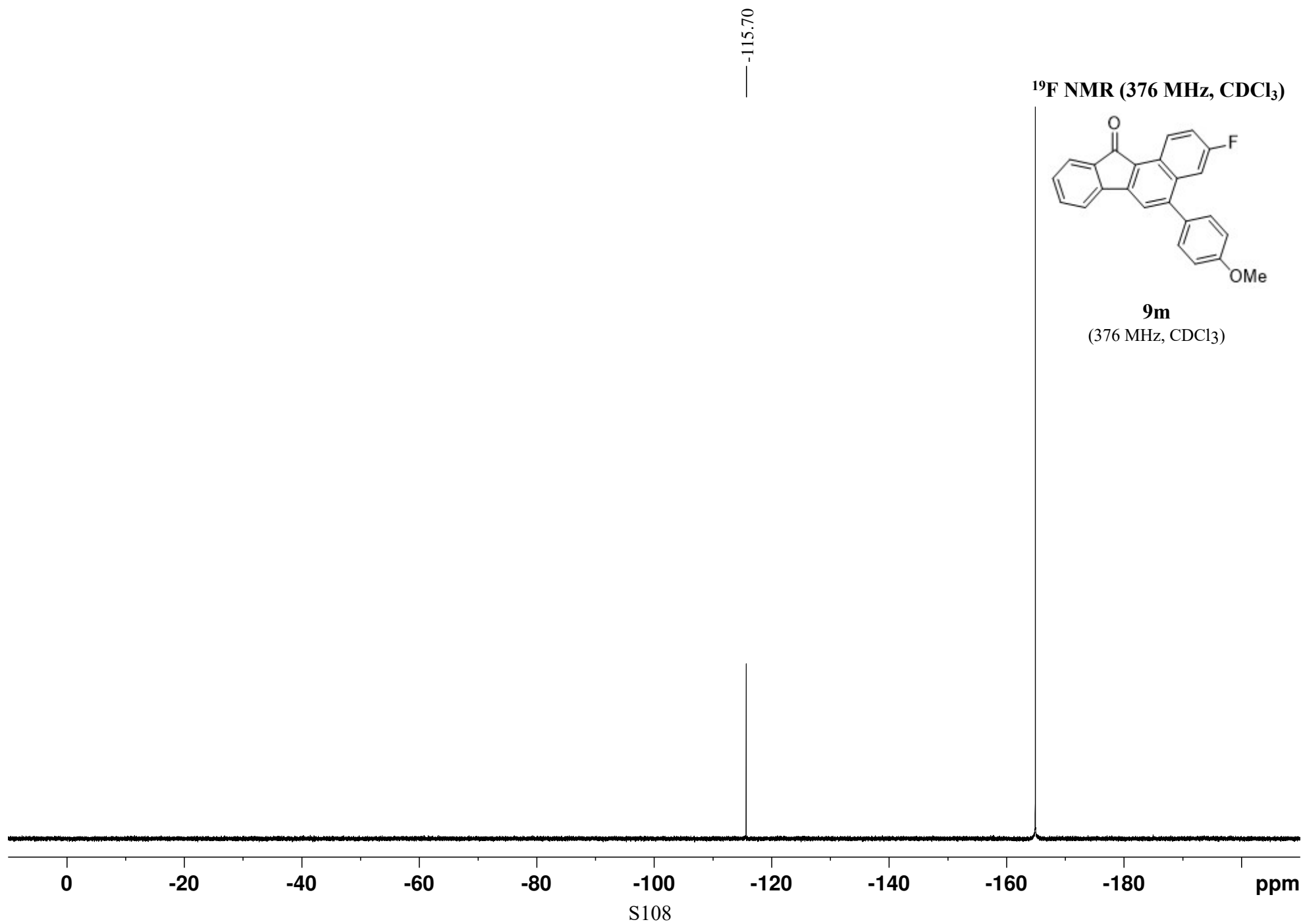


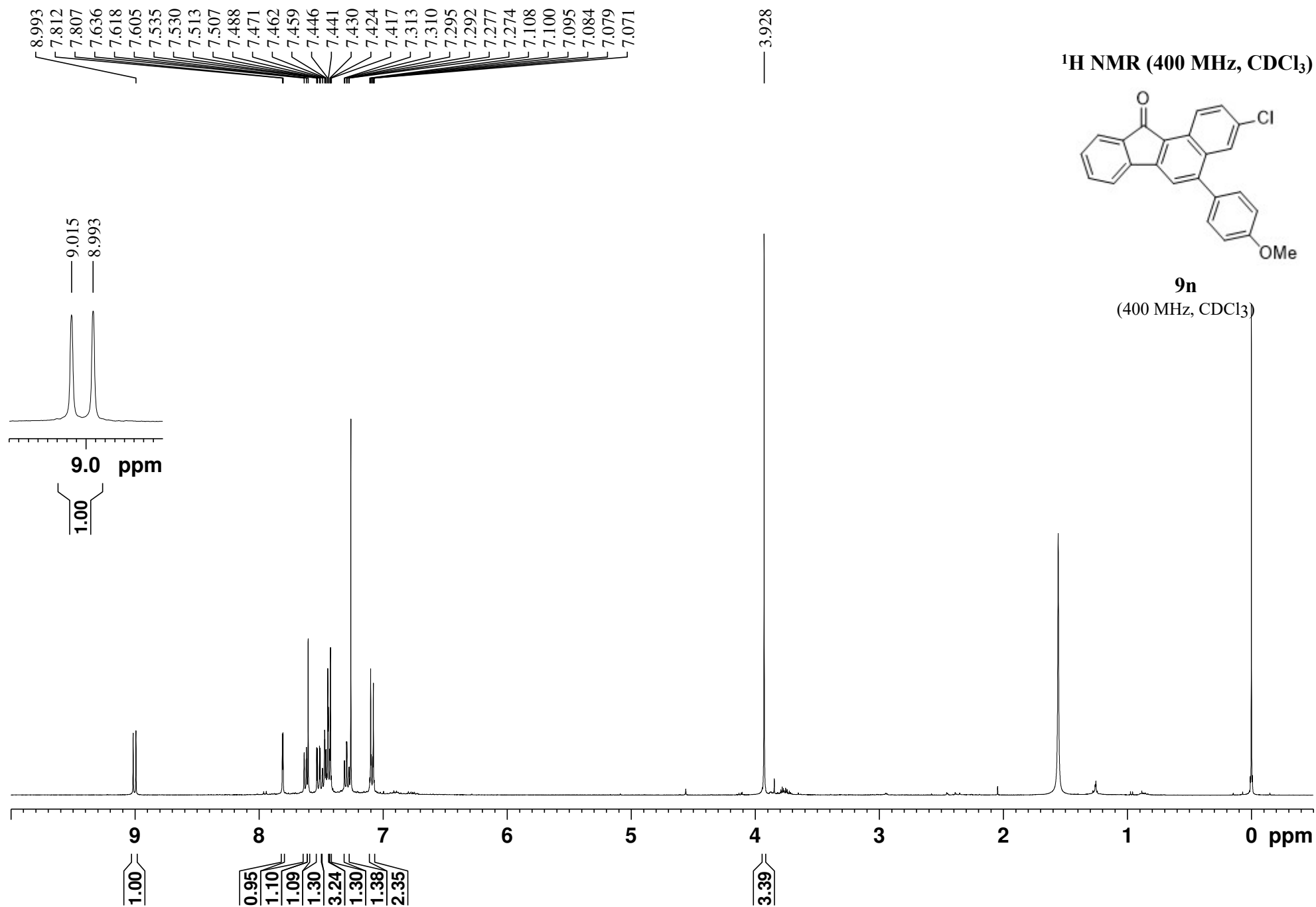


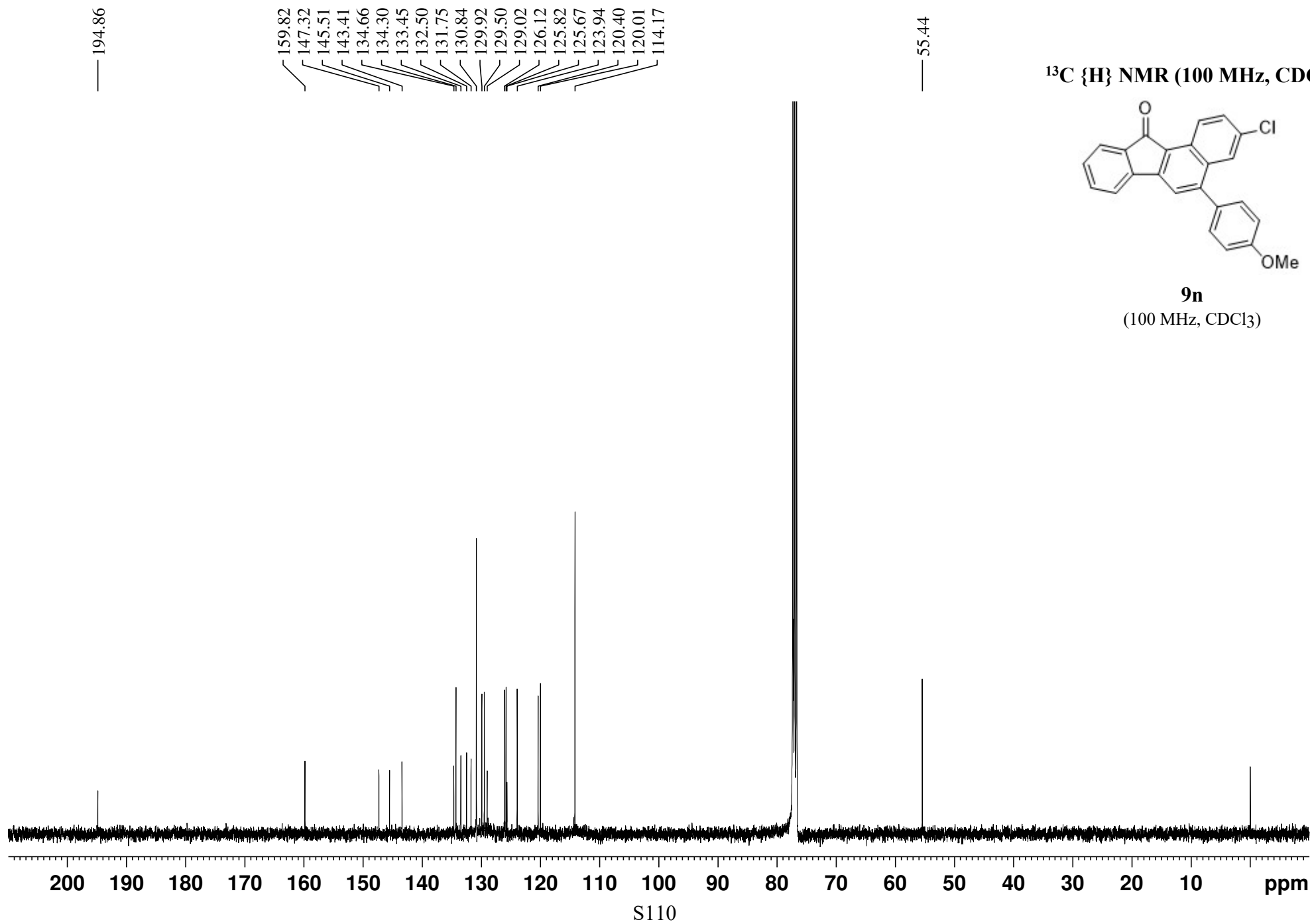








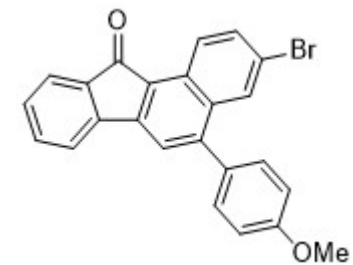






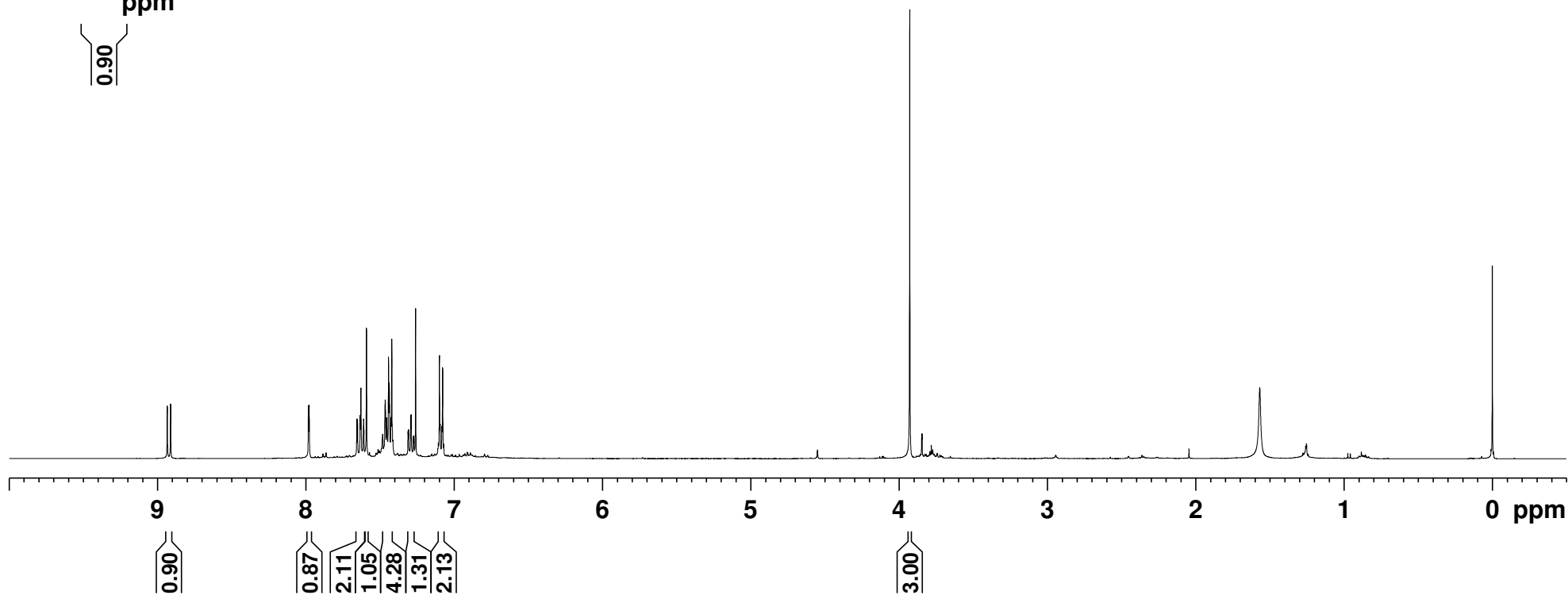
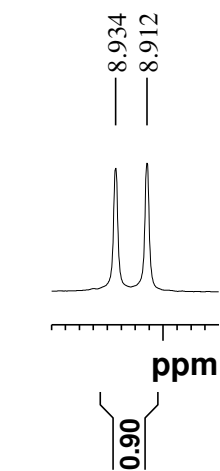
3.928

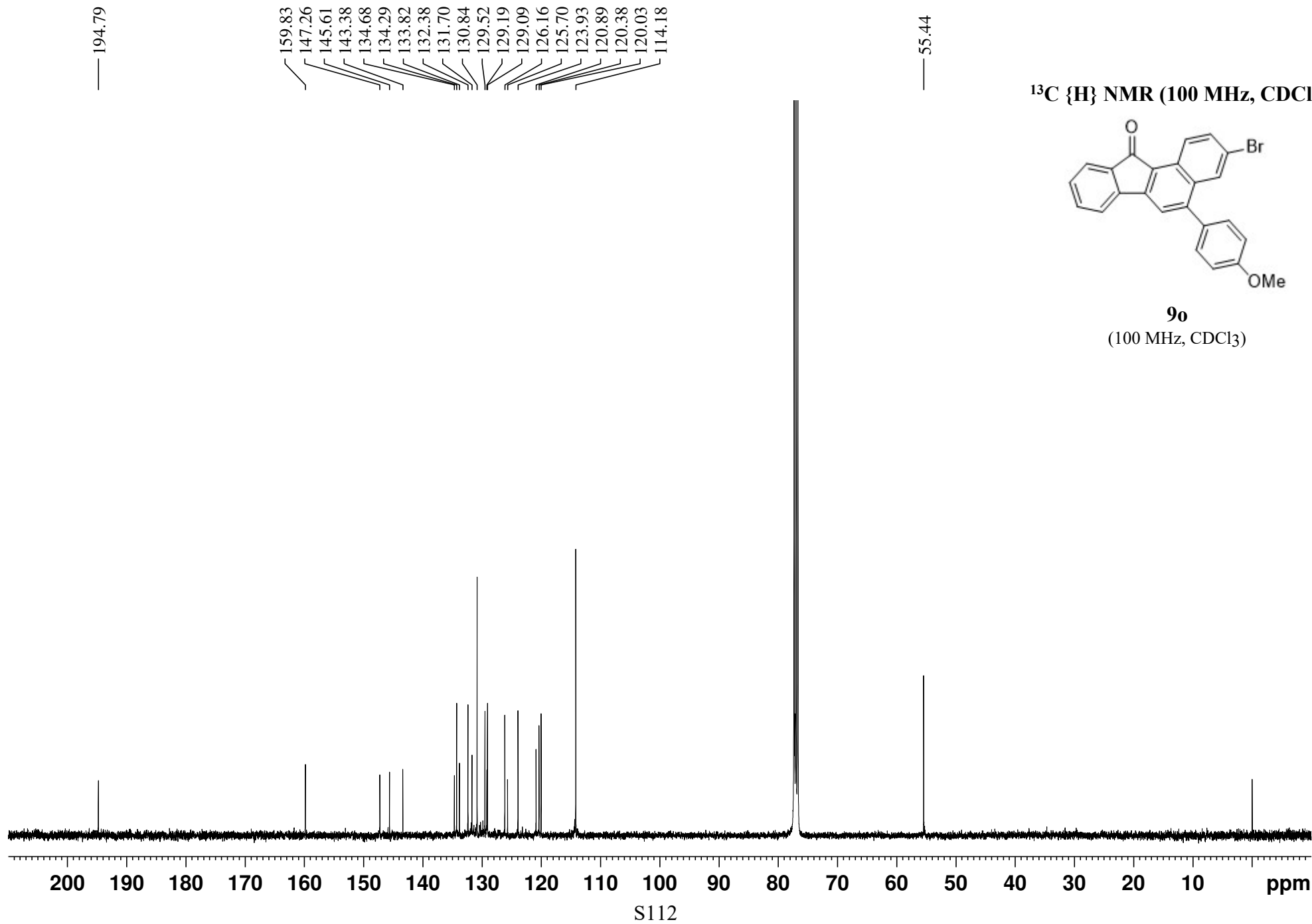
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

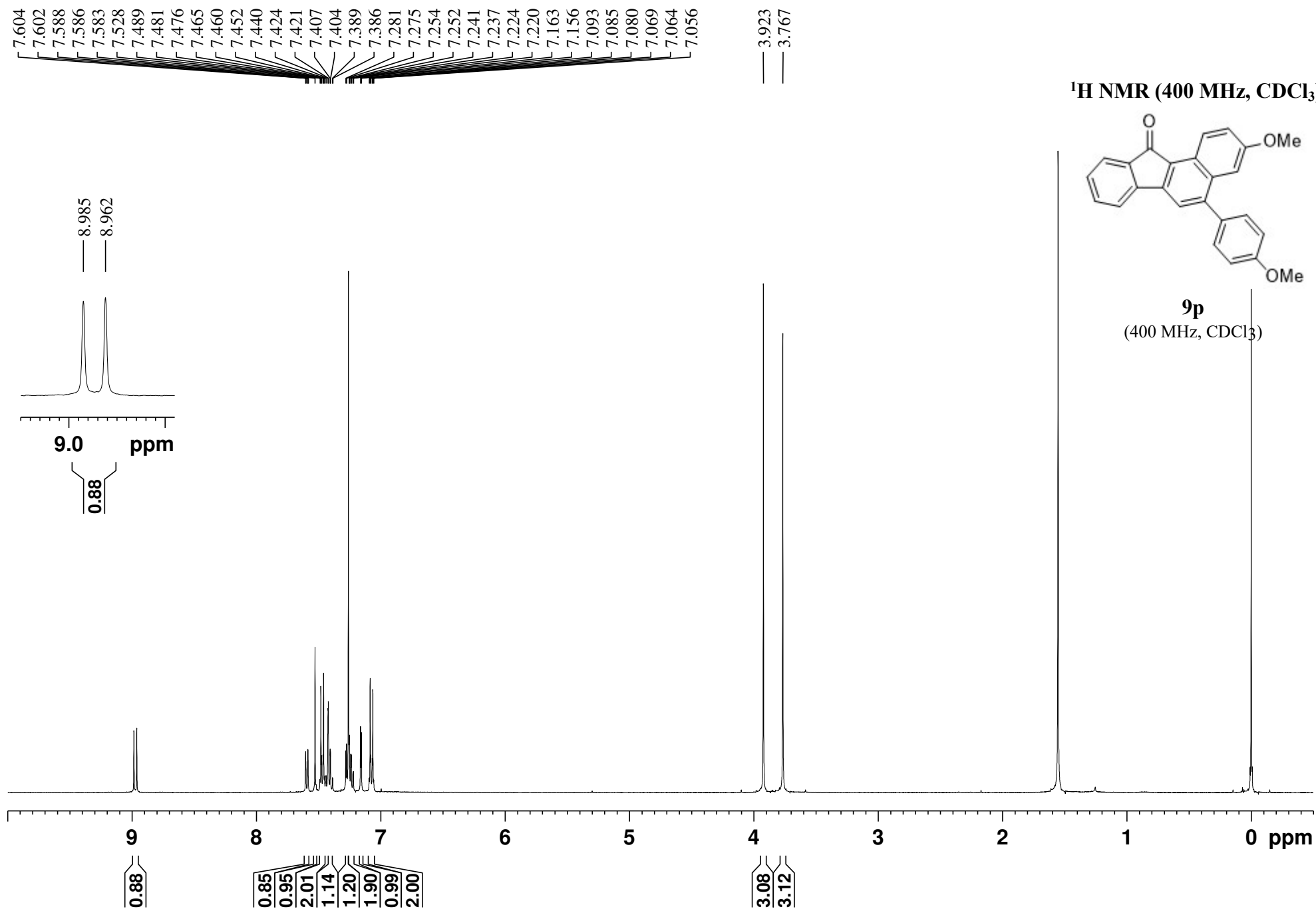


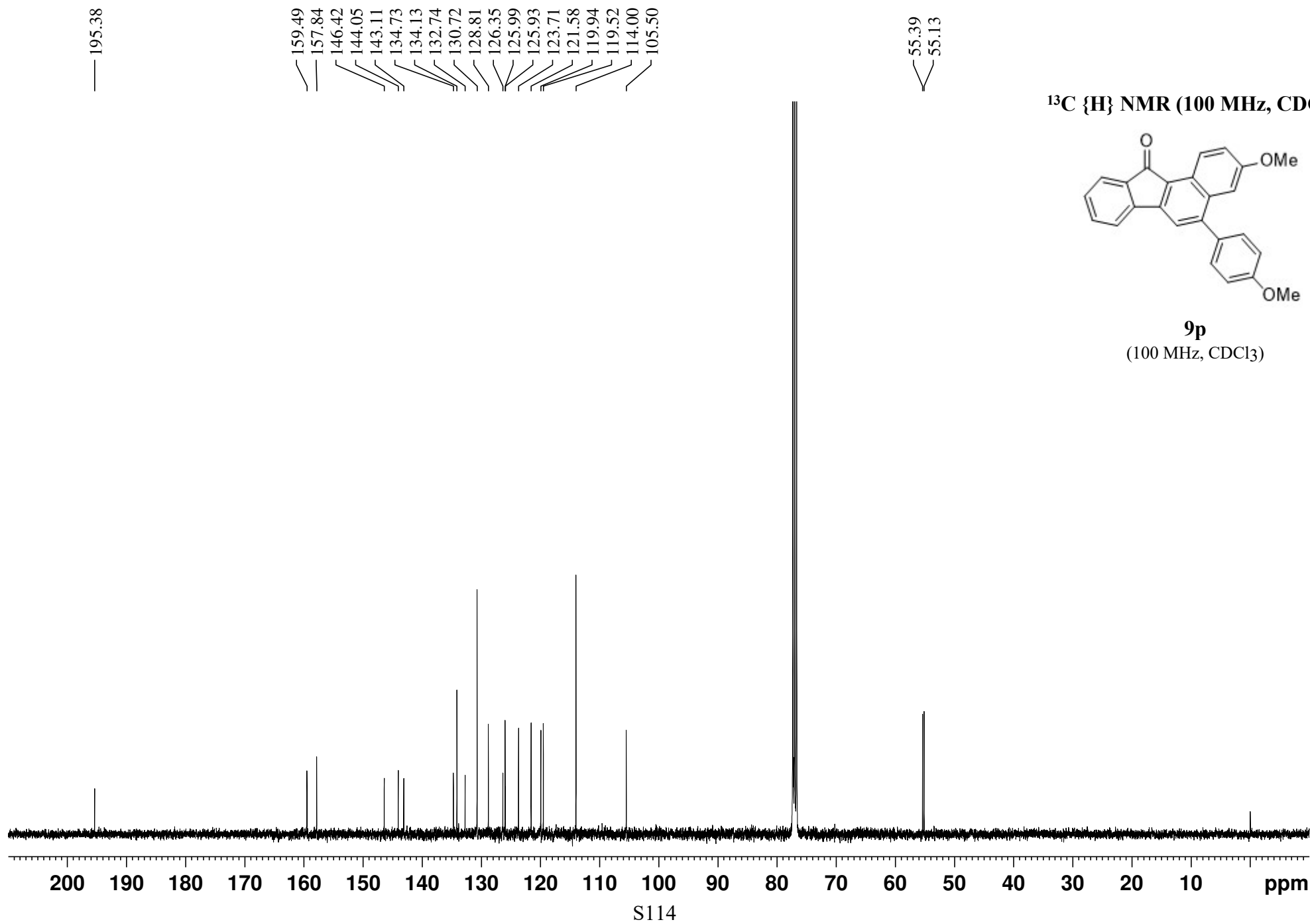
**9o**

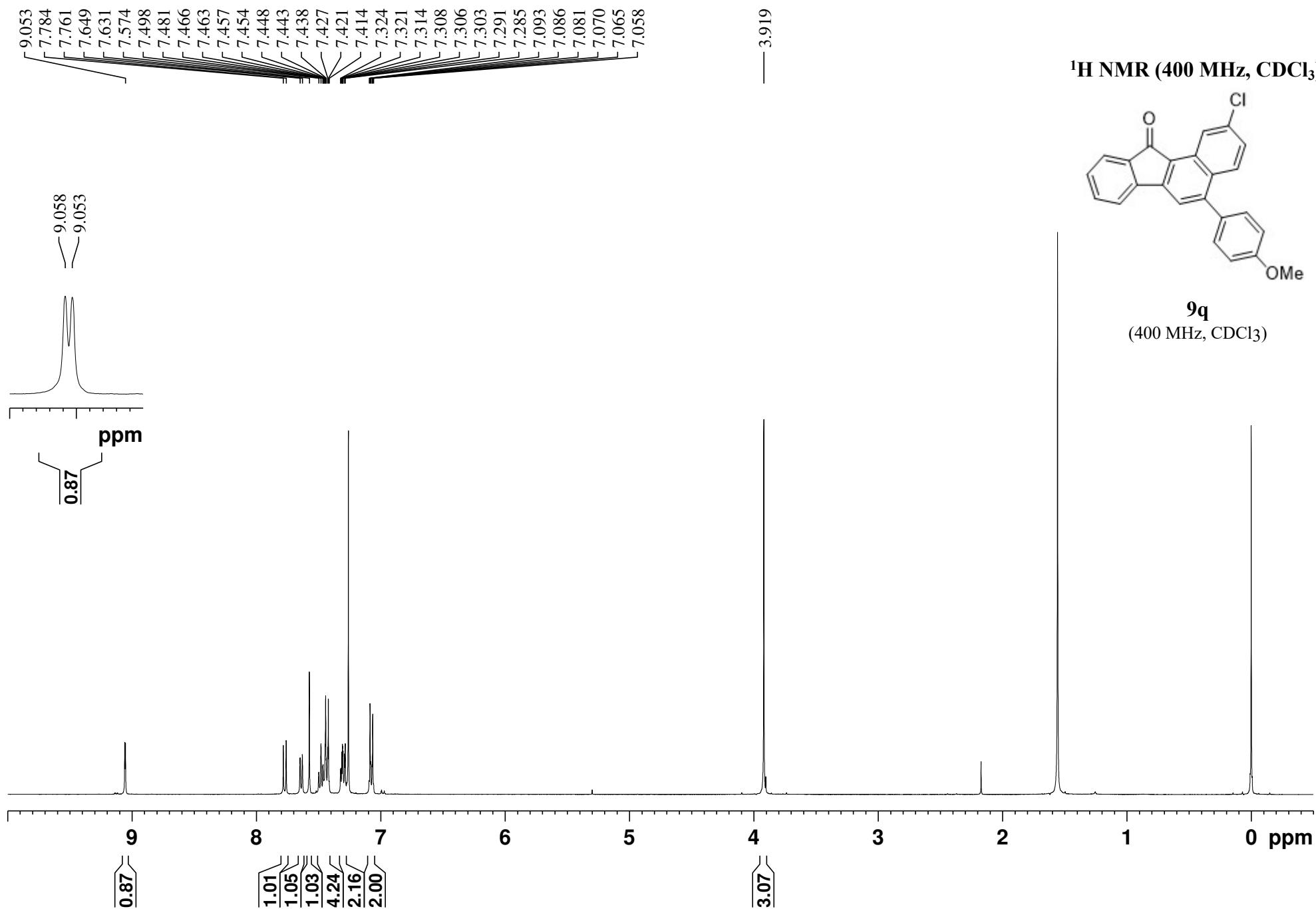
(400 MHz, CDCl<sub>3</sub>)

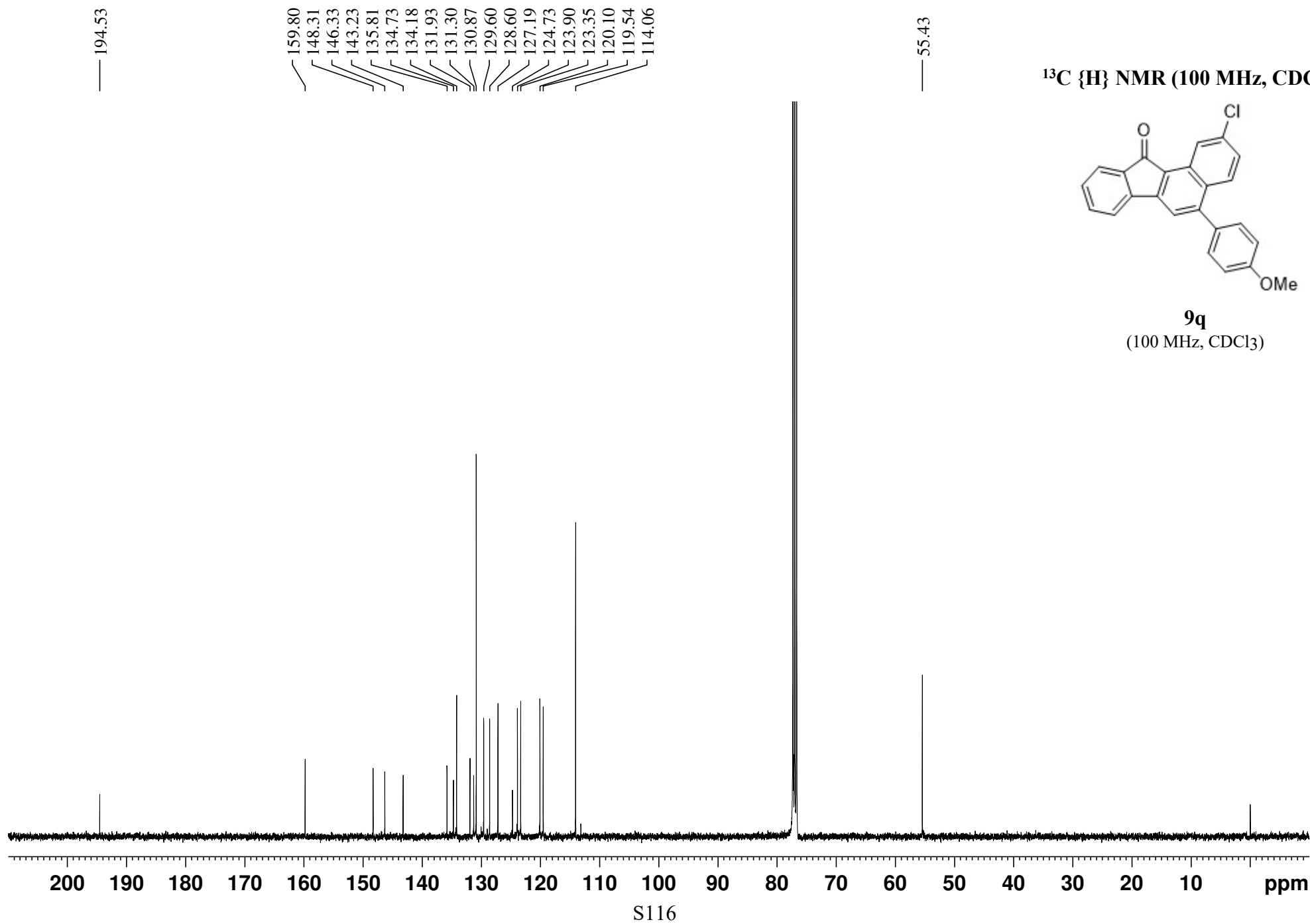


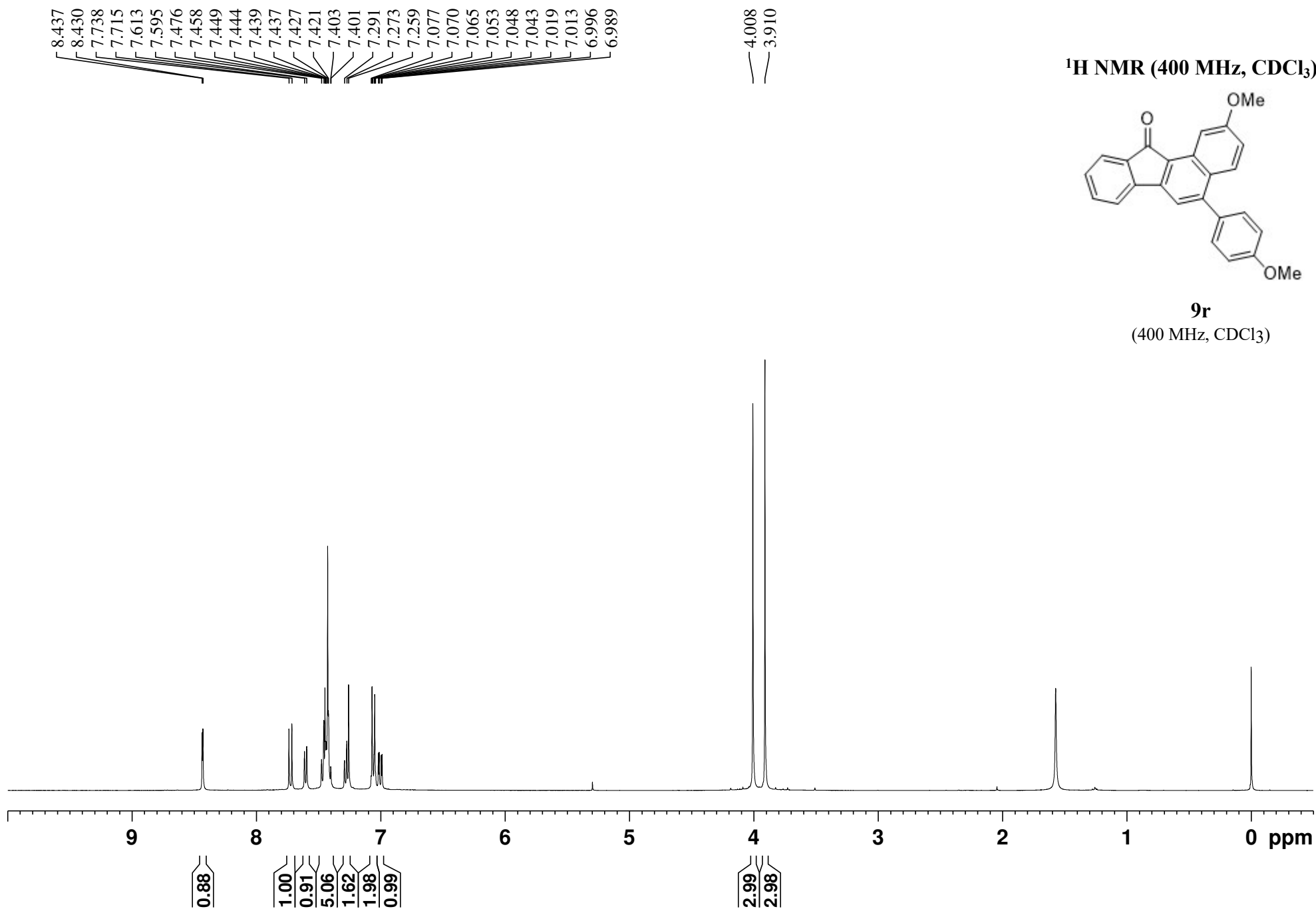


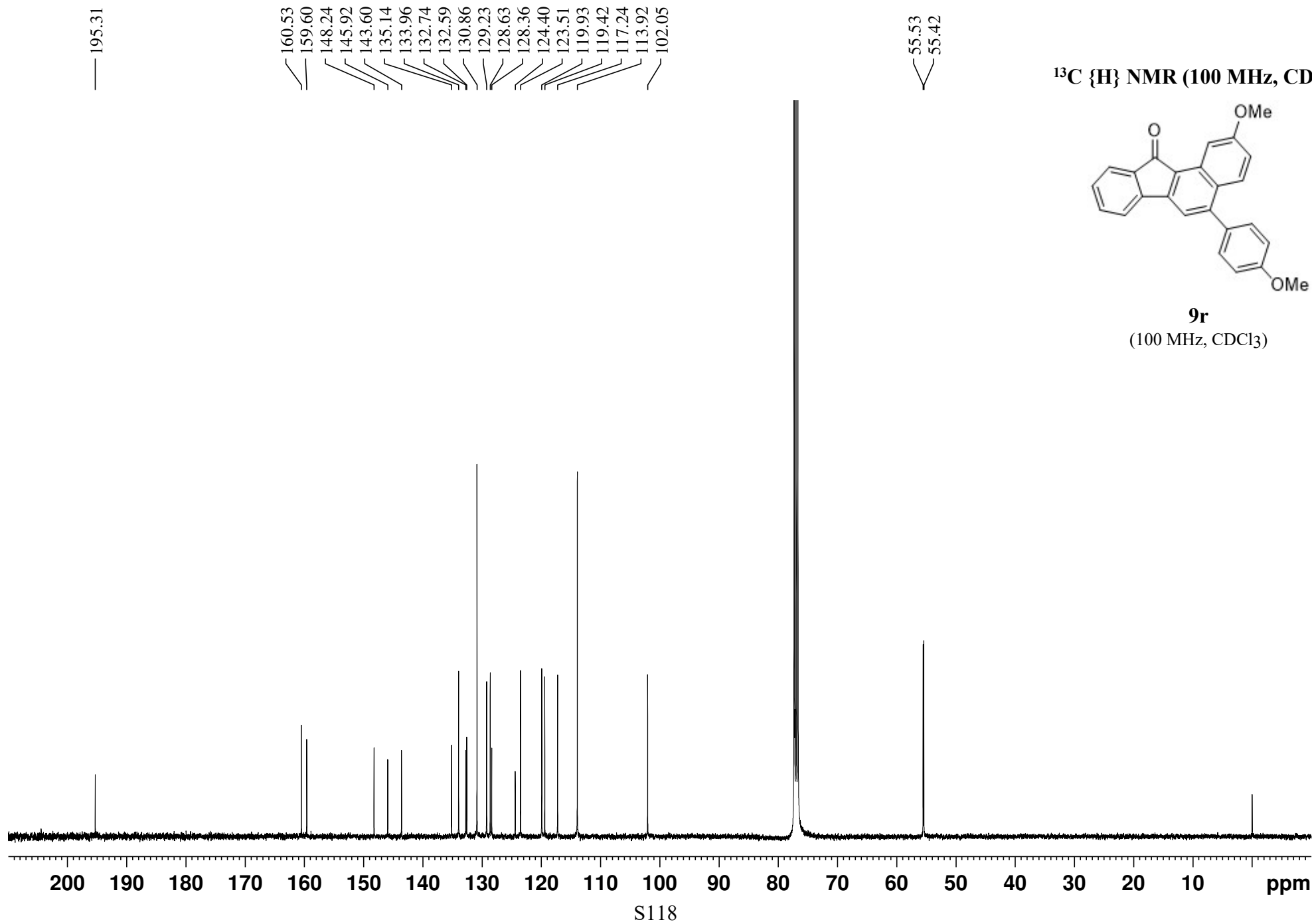


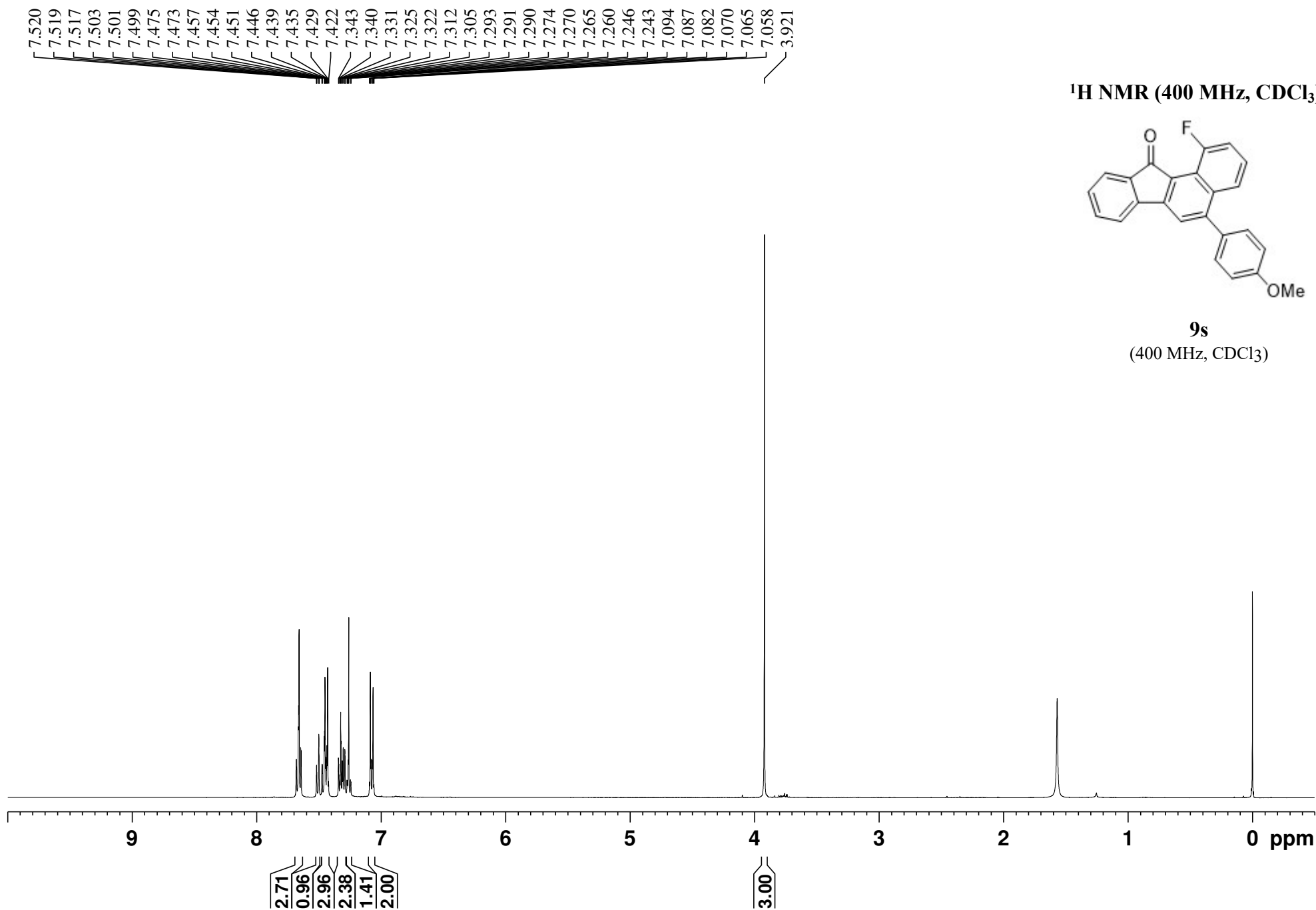


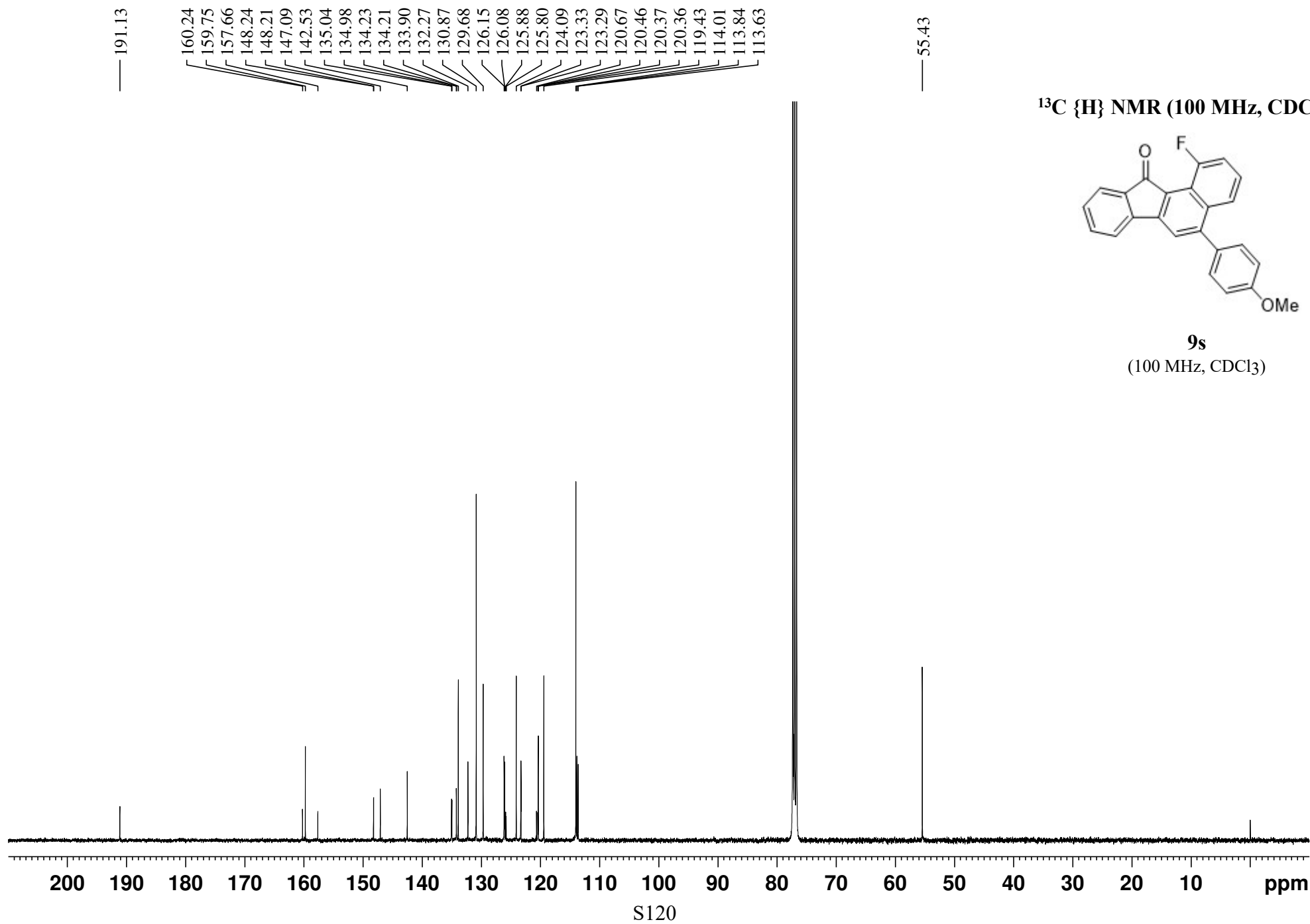


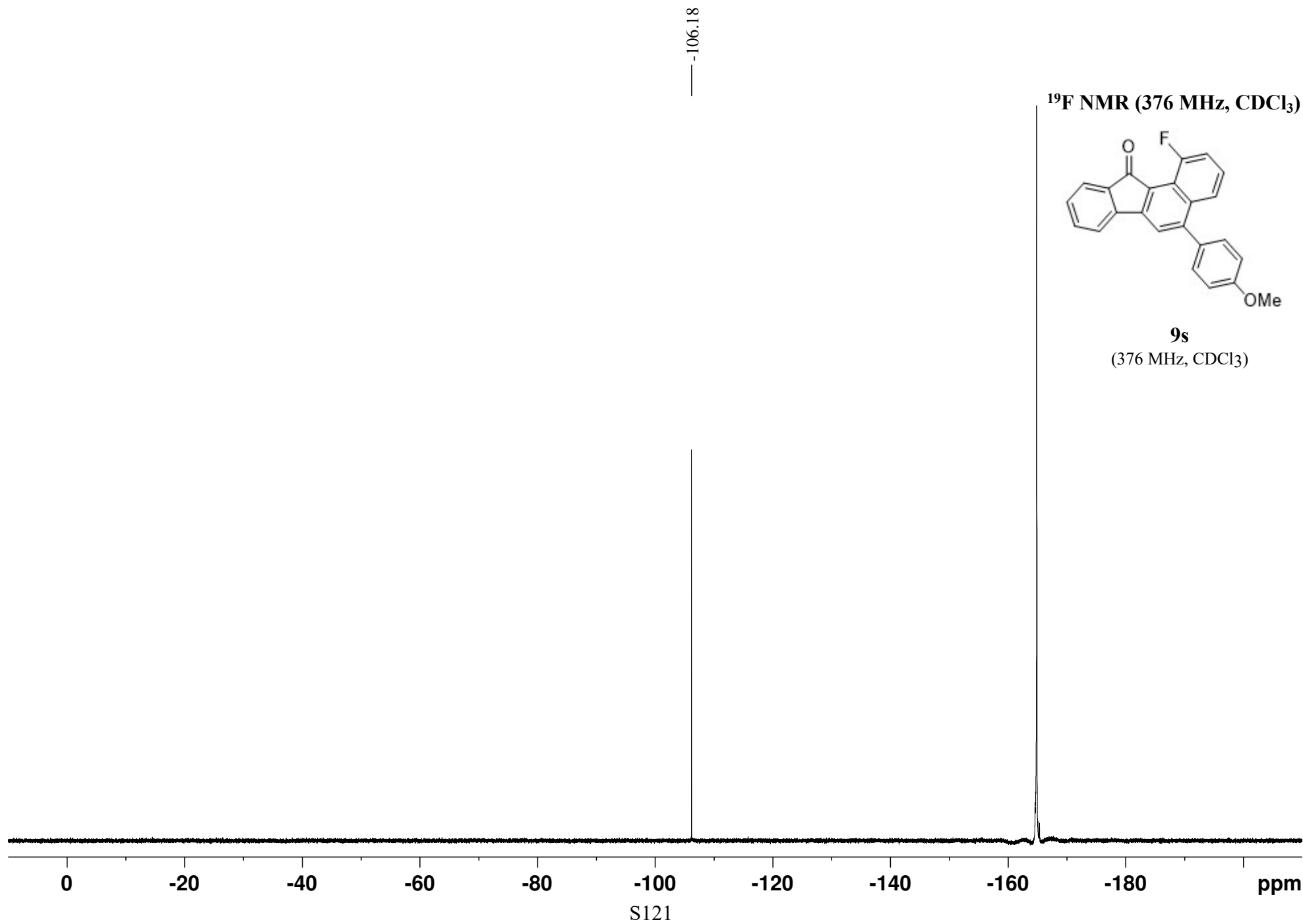


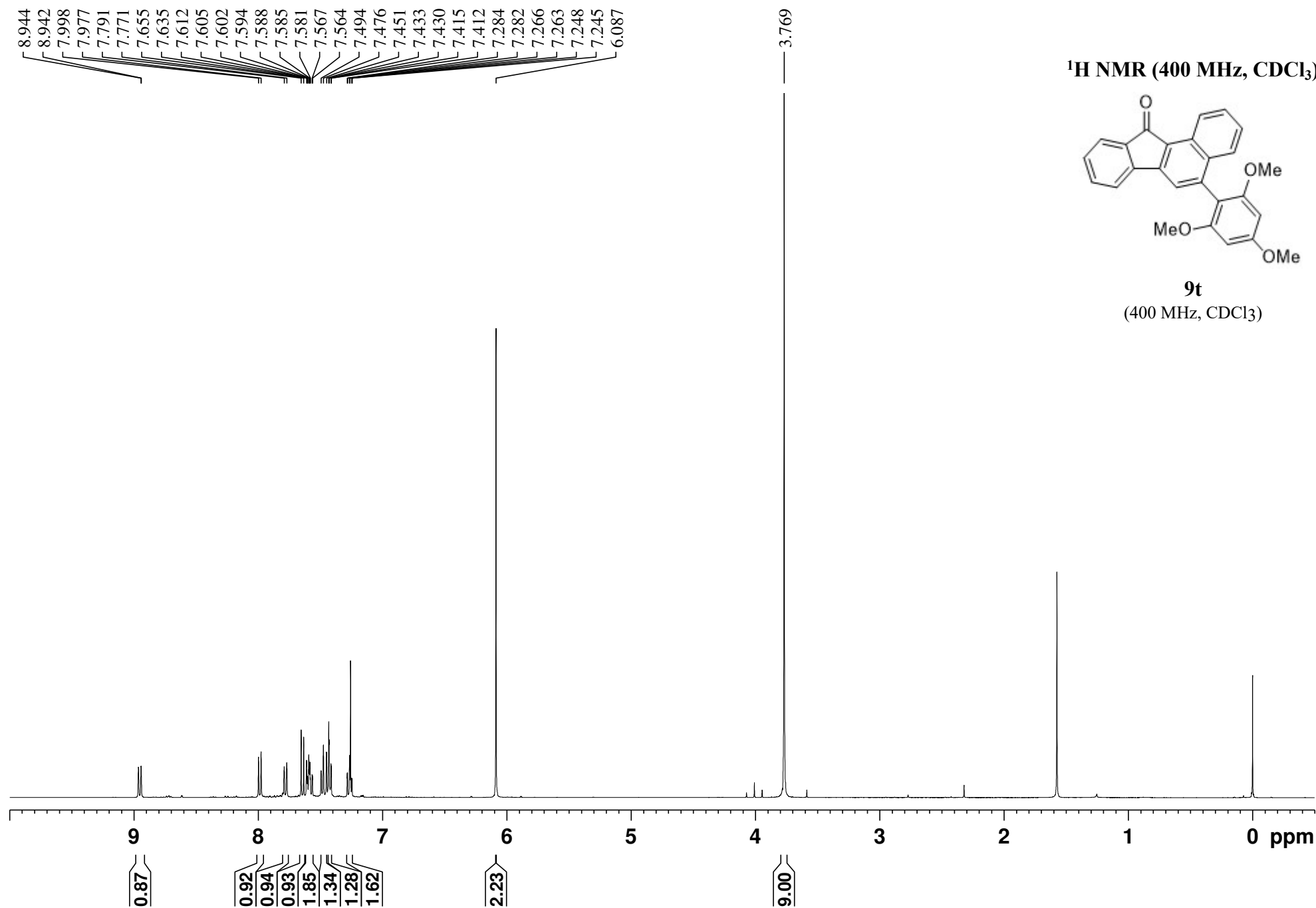


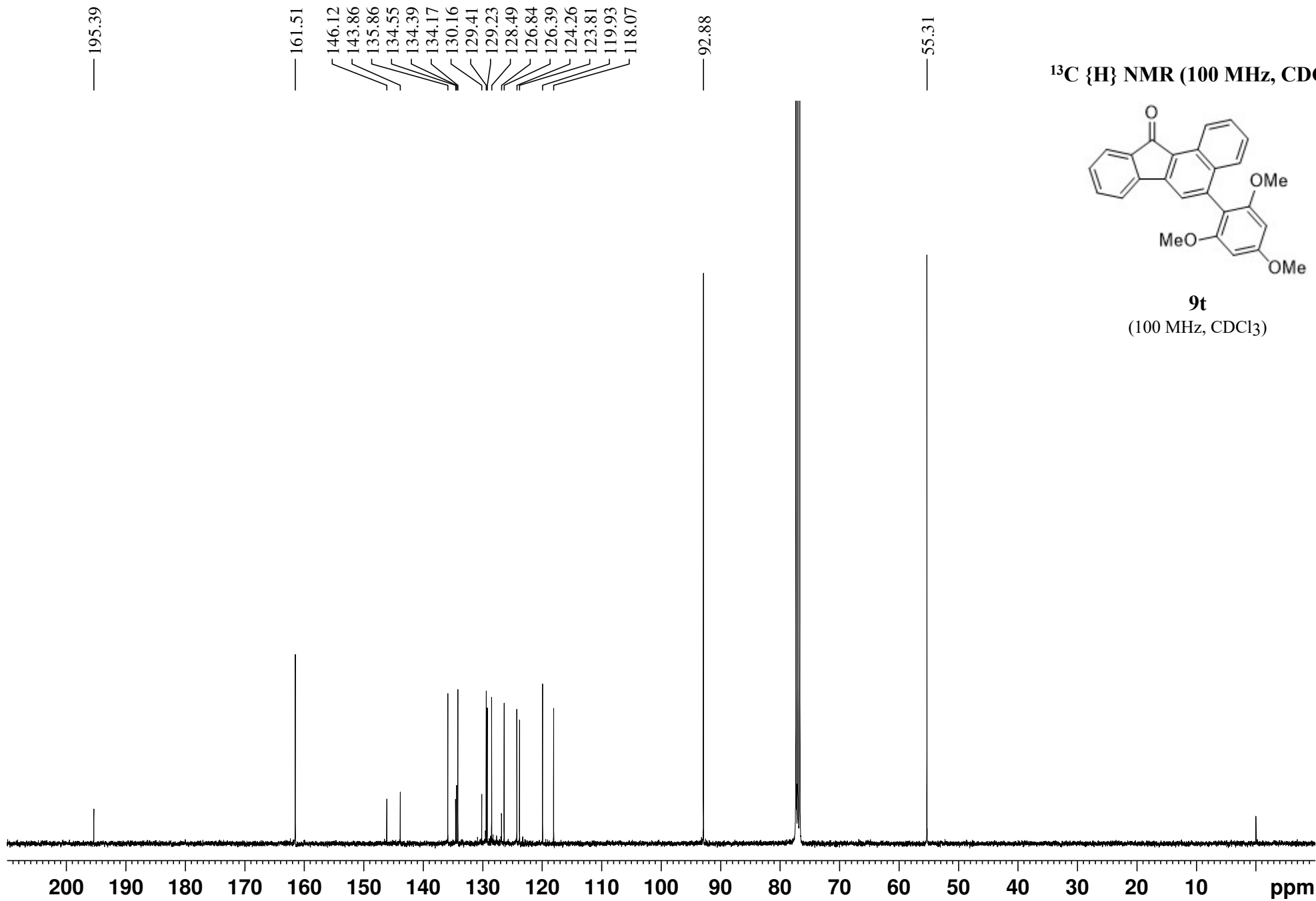


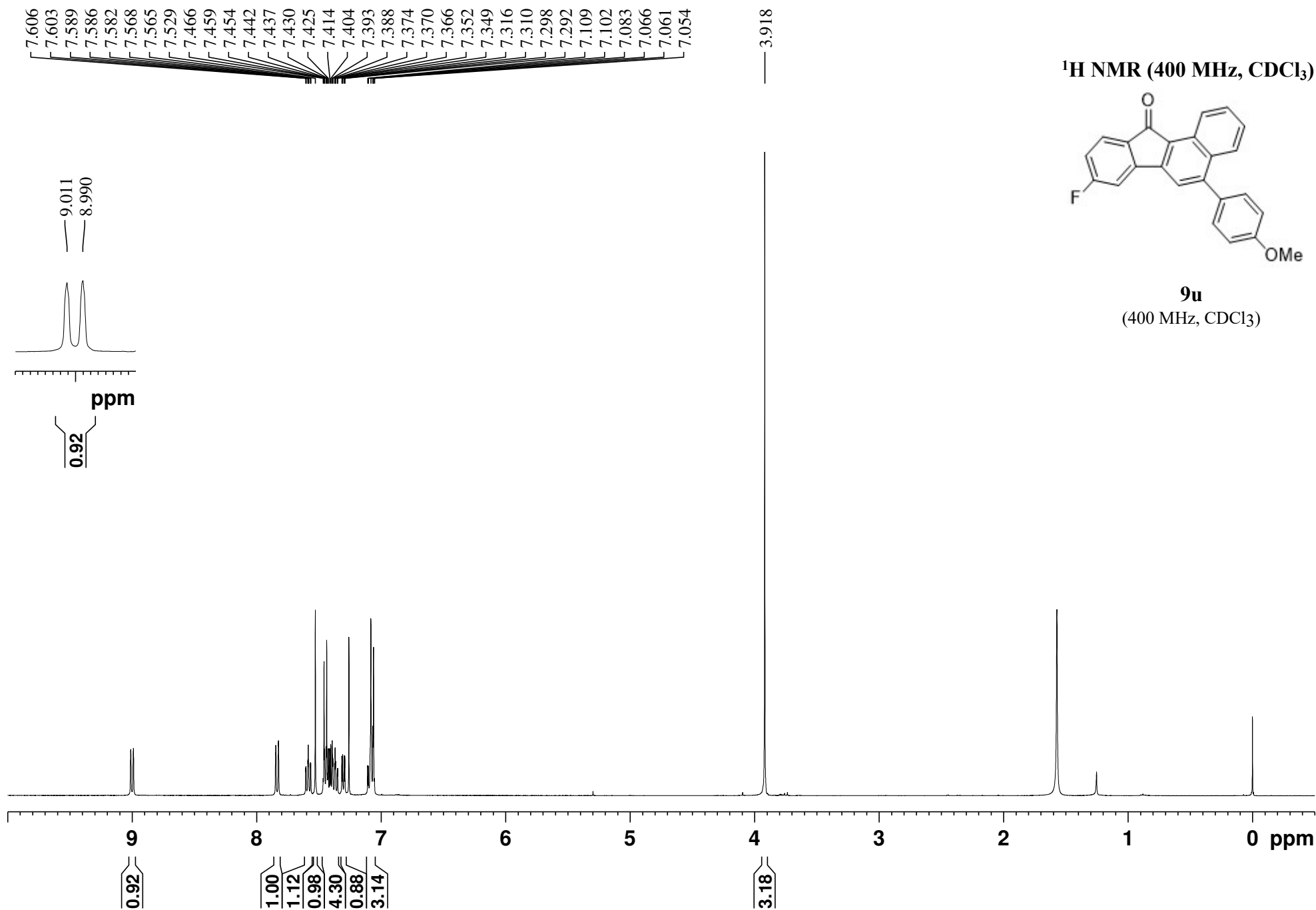


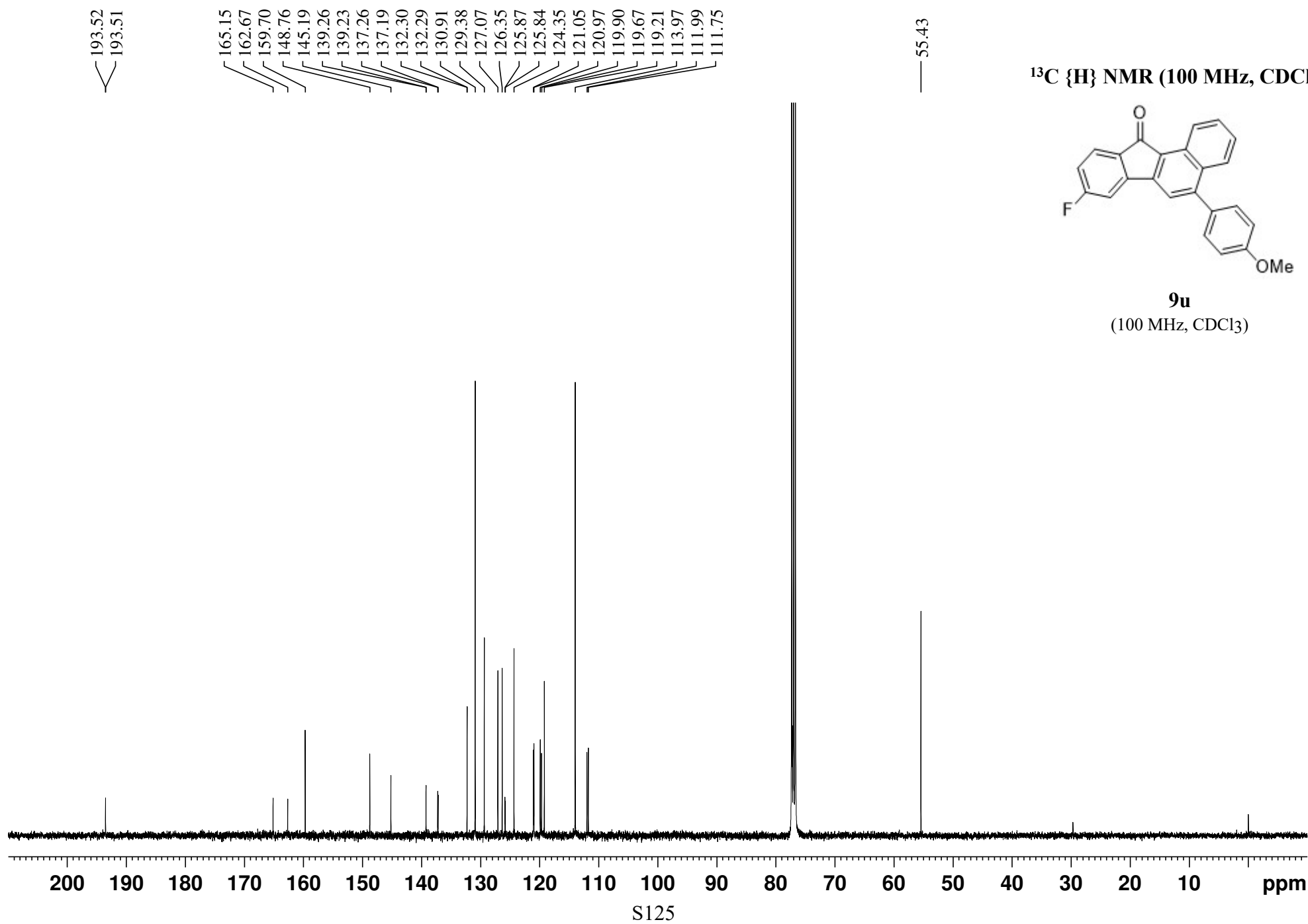


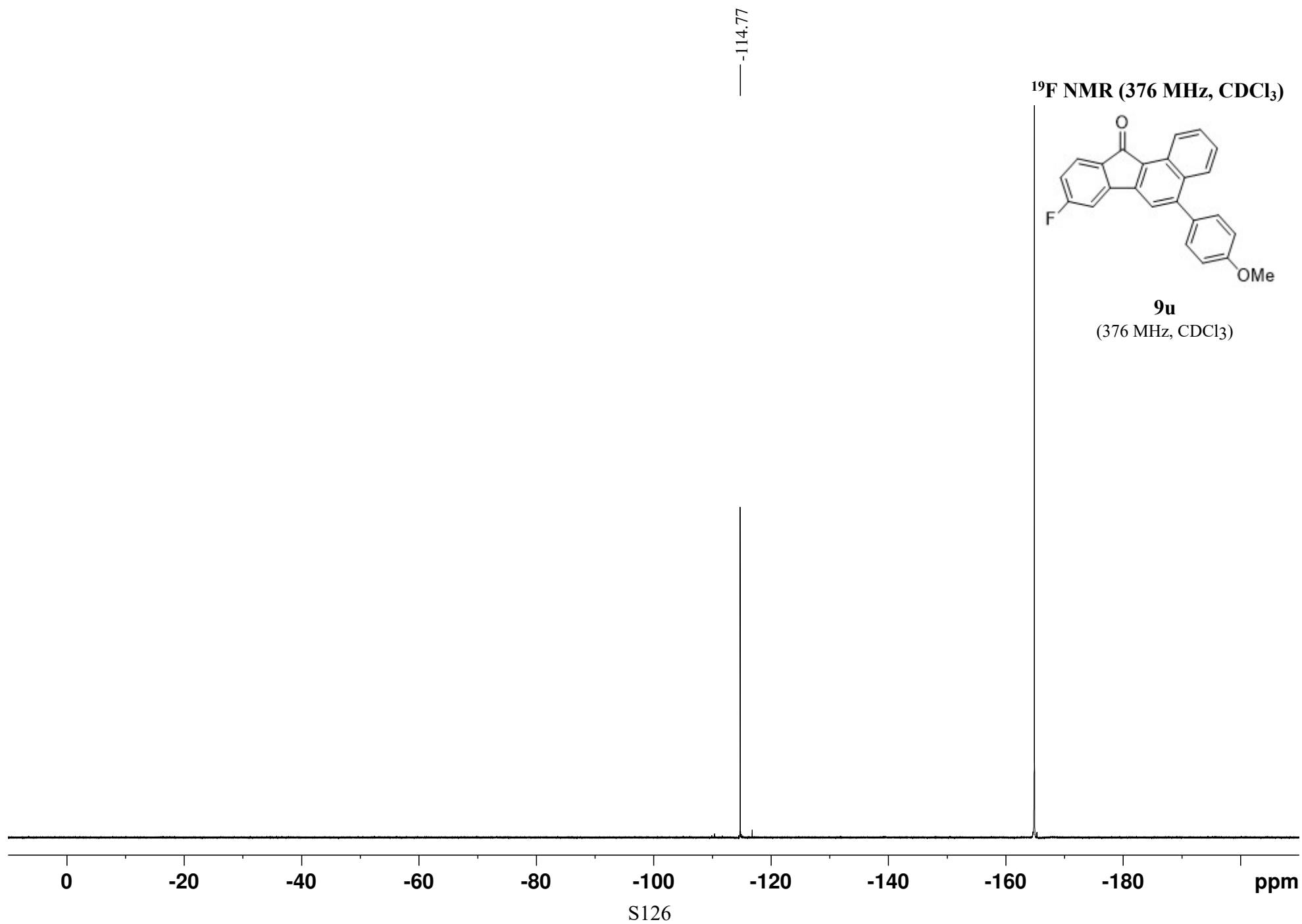


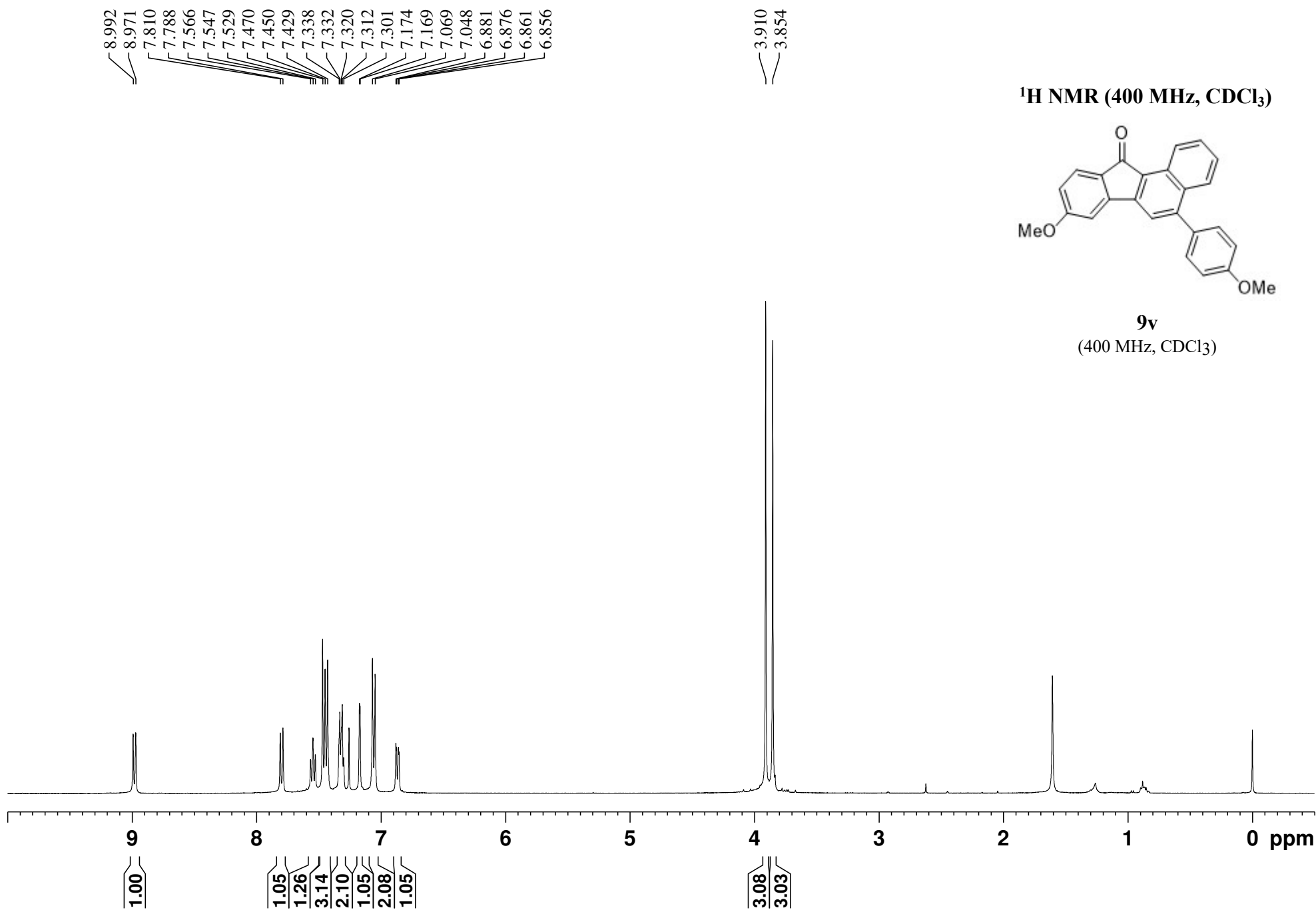


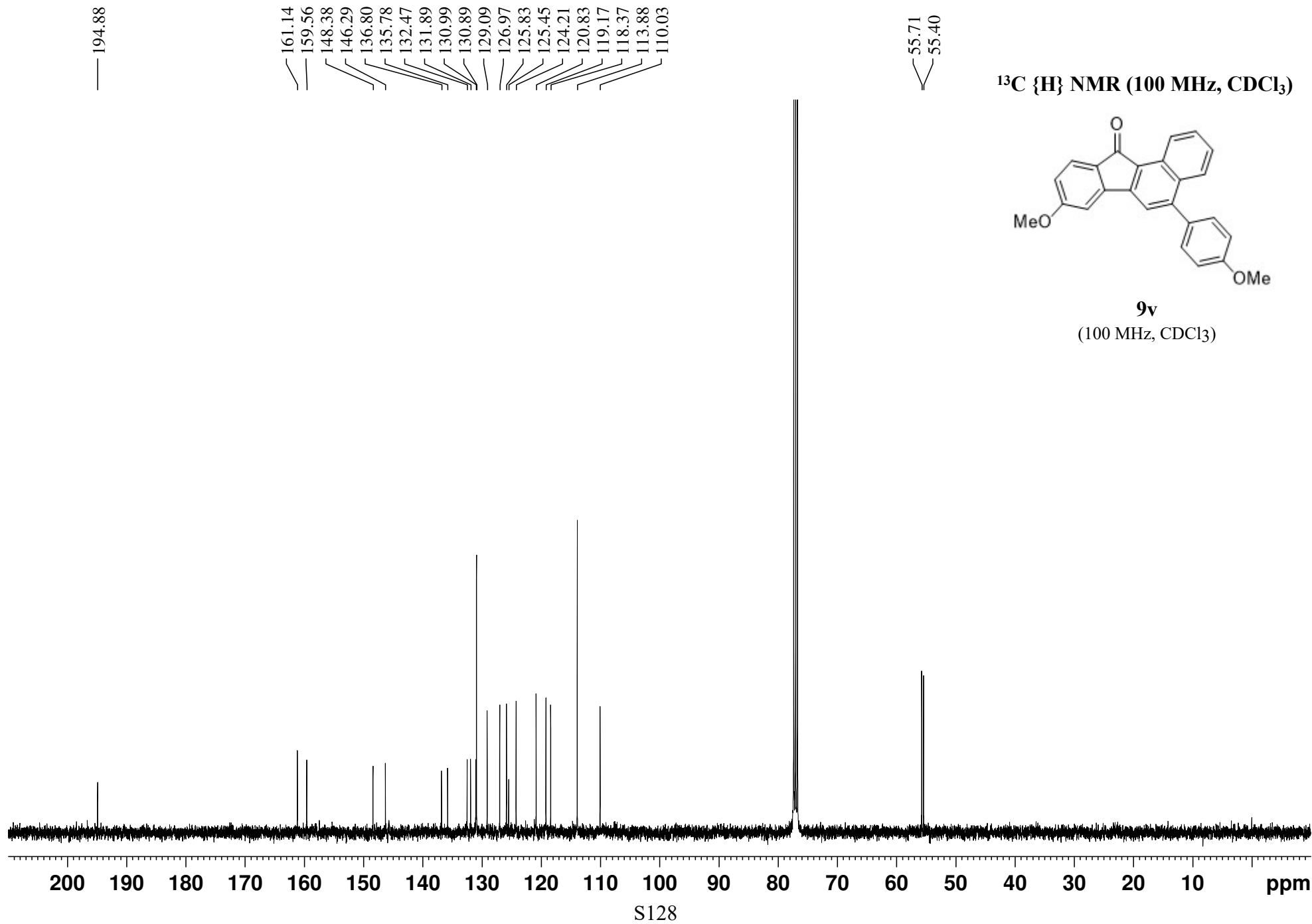






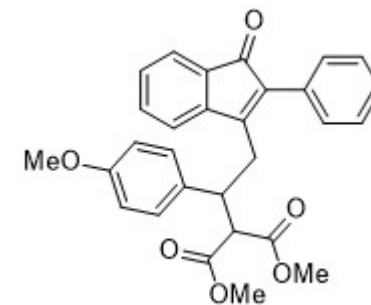






7.584  
7.496  
7.494  
7.477  
7.476  
7.459  
7.457  
7.445  
7.427  
7.272  
7.269  
7.264  
7.260  
7.256  
7.252  
7.233  
6.825  
6.815  
6.807  
6.801  
6.798  
6.791  
6.781  
6.665  
6.658  
6.654  
6.642  
6.636  
6.629  
6.488  
6.481  
6.477  
6.465  
6.459  
6.454  
3.822  
3.798  
3.790  
3.771  
3.763  
3.758  
3.743  
3.730  
3.698  
3.390  
3.179  
3.148  
3.119  
3.027  
3.019  
2.996  
2.987

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



**11e**

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

