

Synthesis of DIBAC analogues with excellent SPAAC rate constants

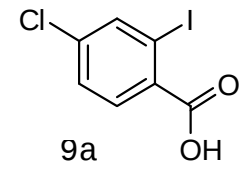
Marjoke F. Debets, Jasper S. Prins, Donny Merkx, Sander S. van Berkel, Floris L.
van Delft, Jan C. M. van Hest, and Floris P. J. T. Rutjes*

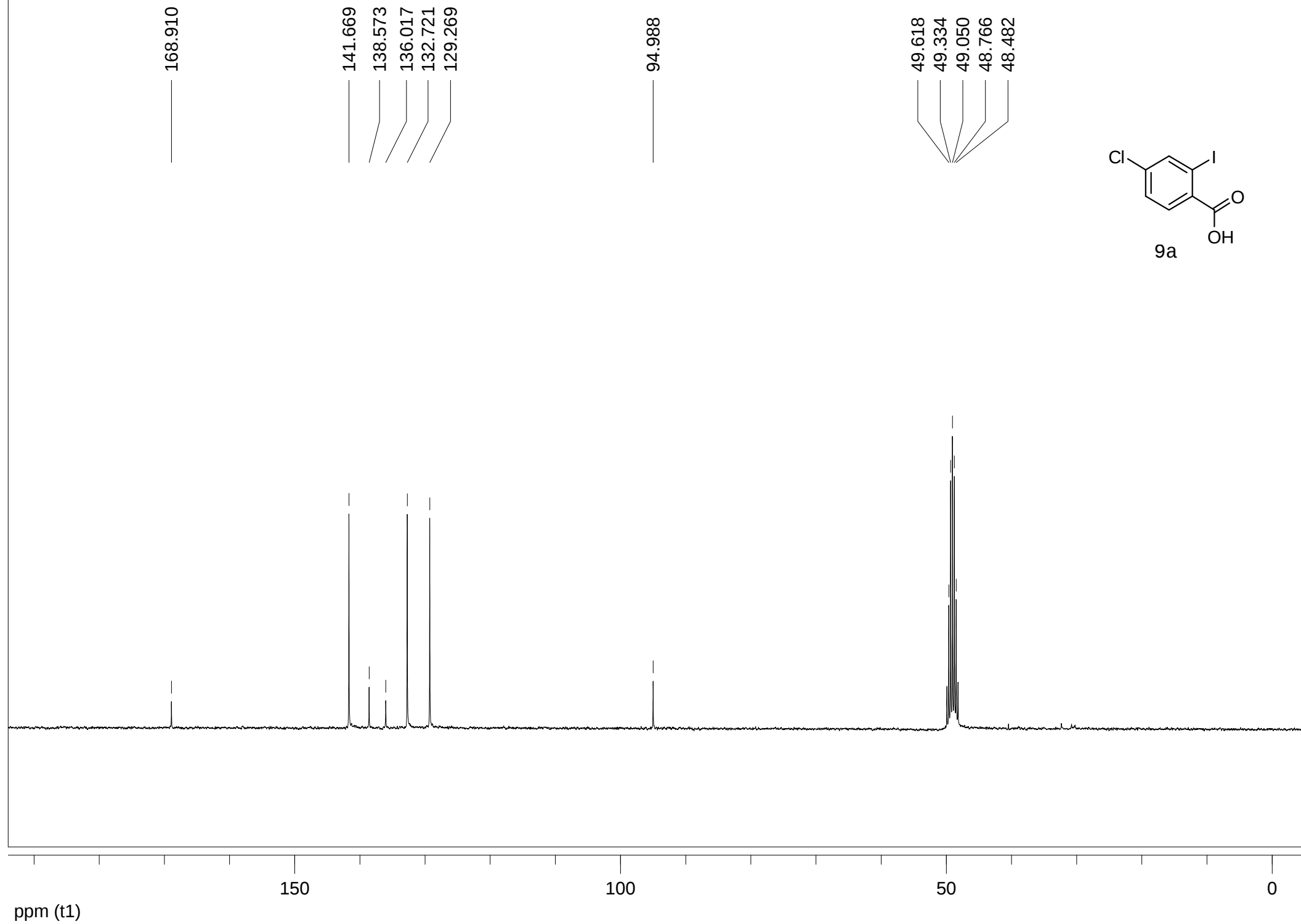
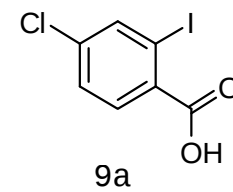
Supporting Information

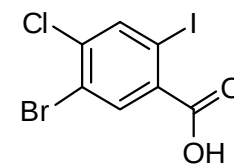
Spectra

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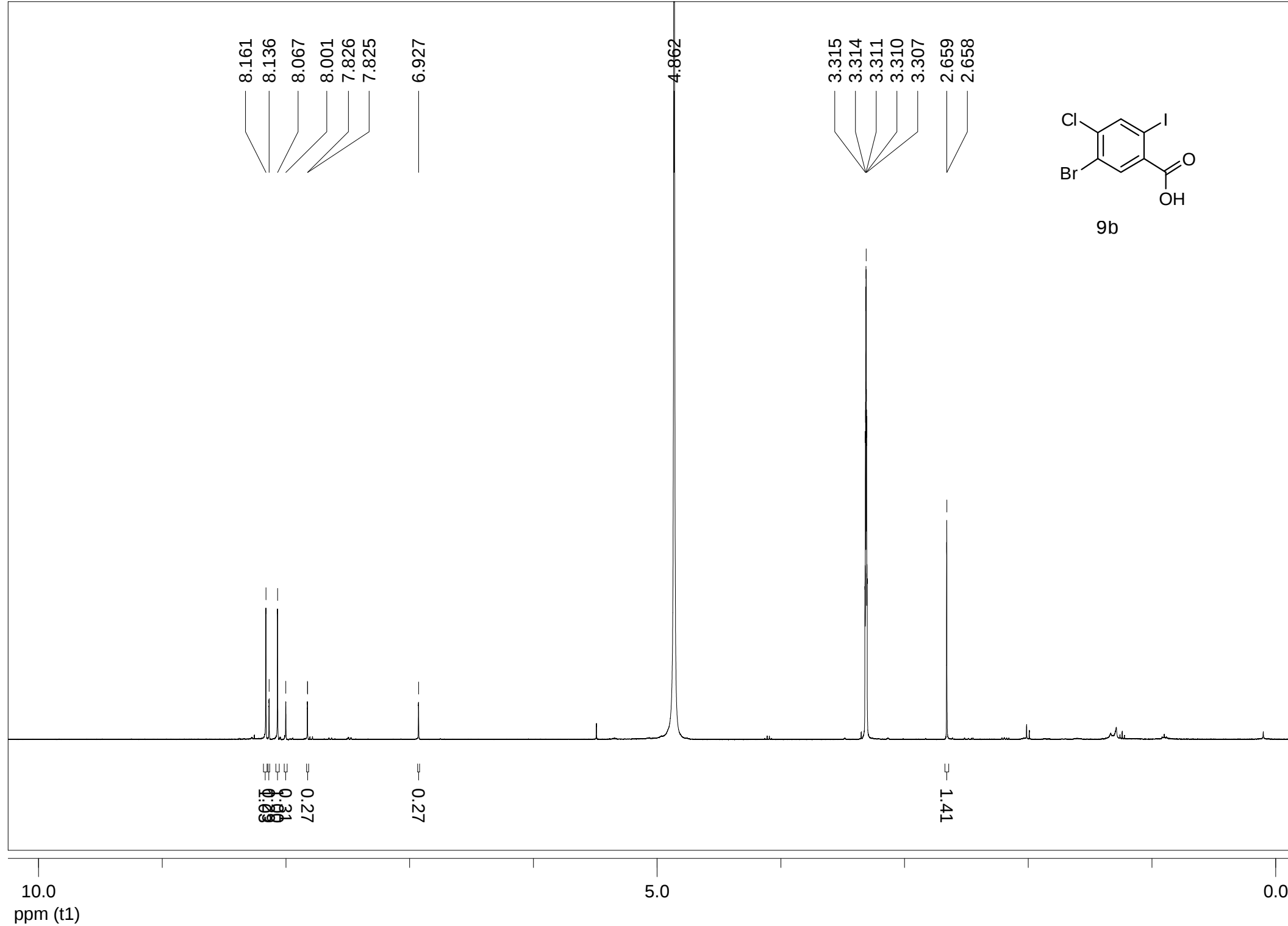
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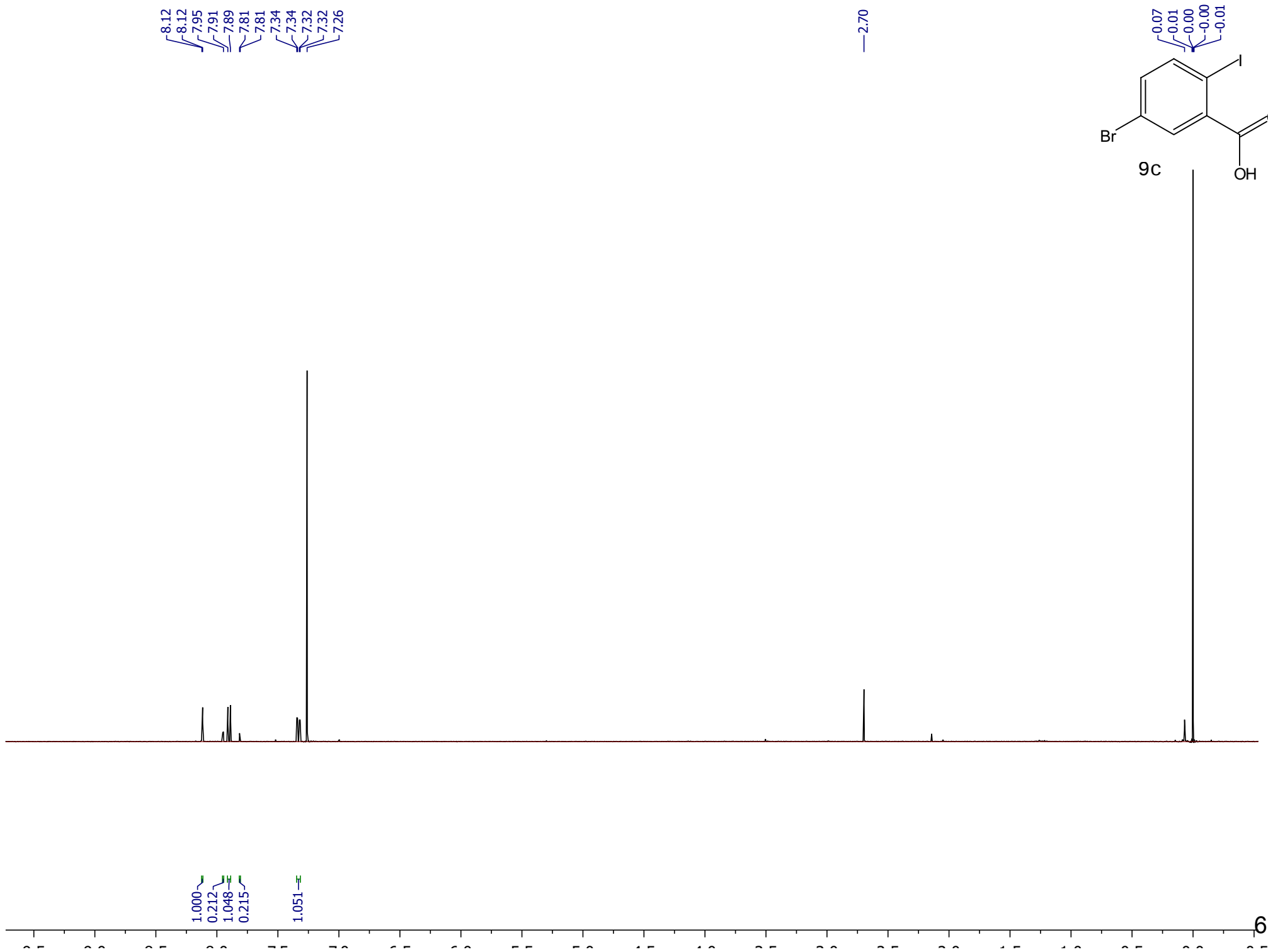


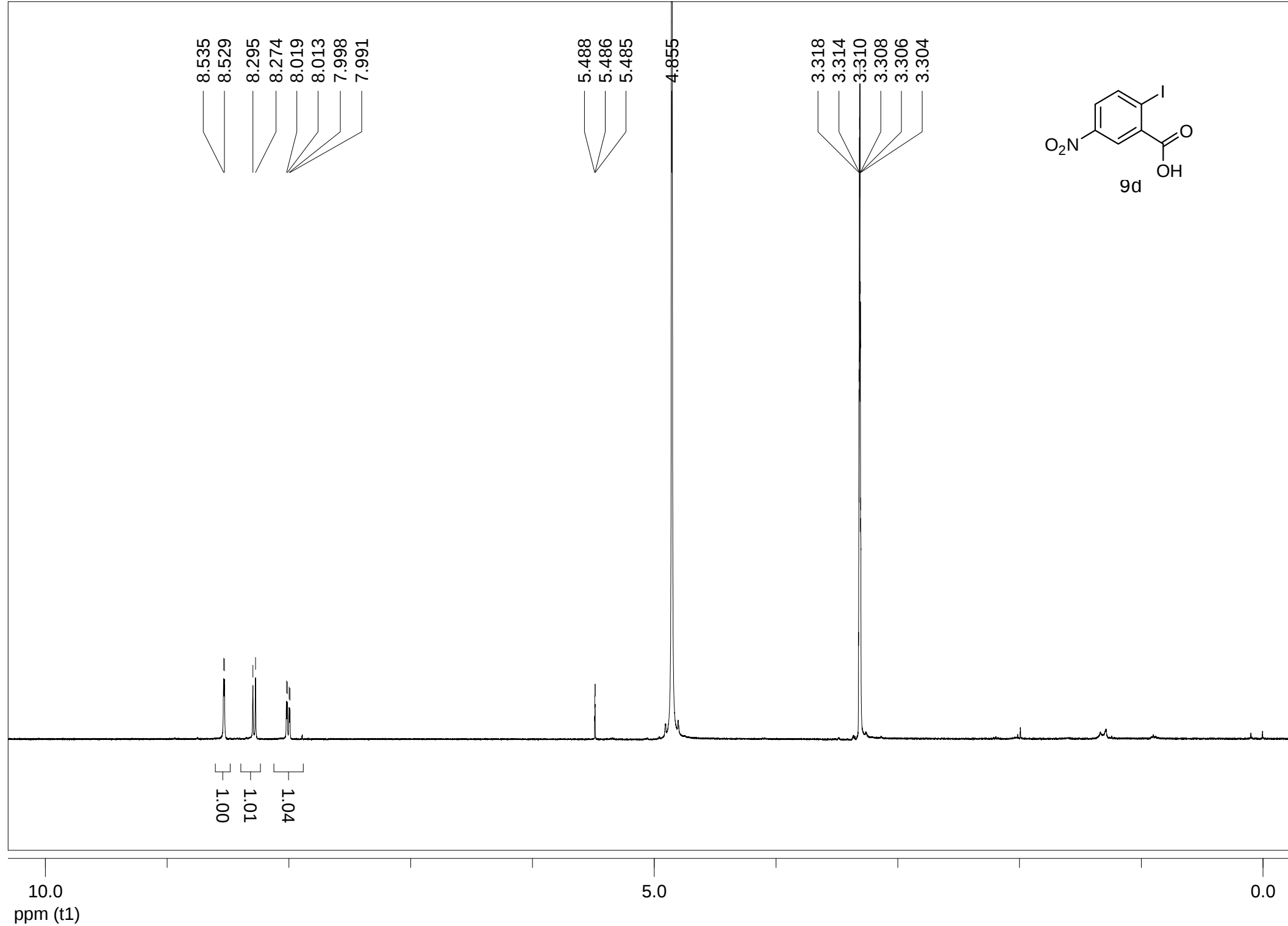
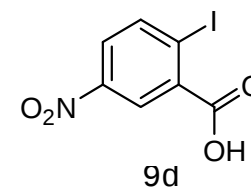


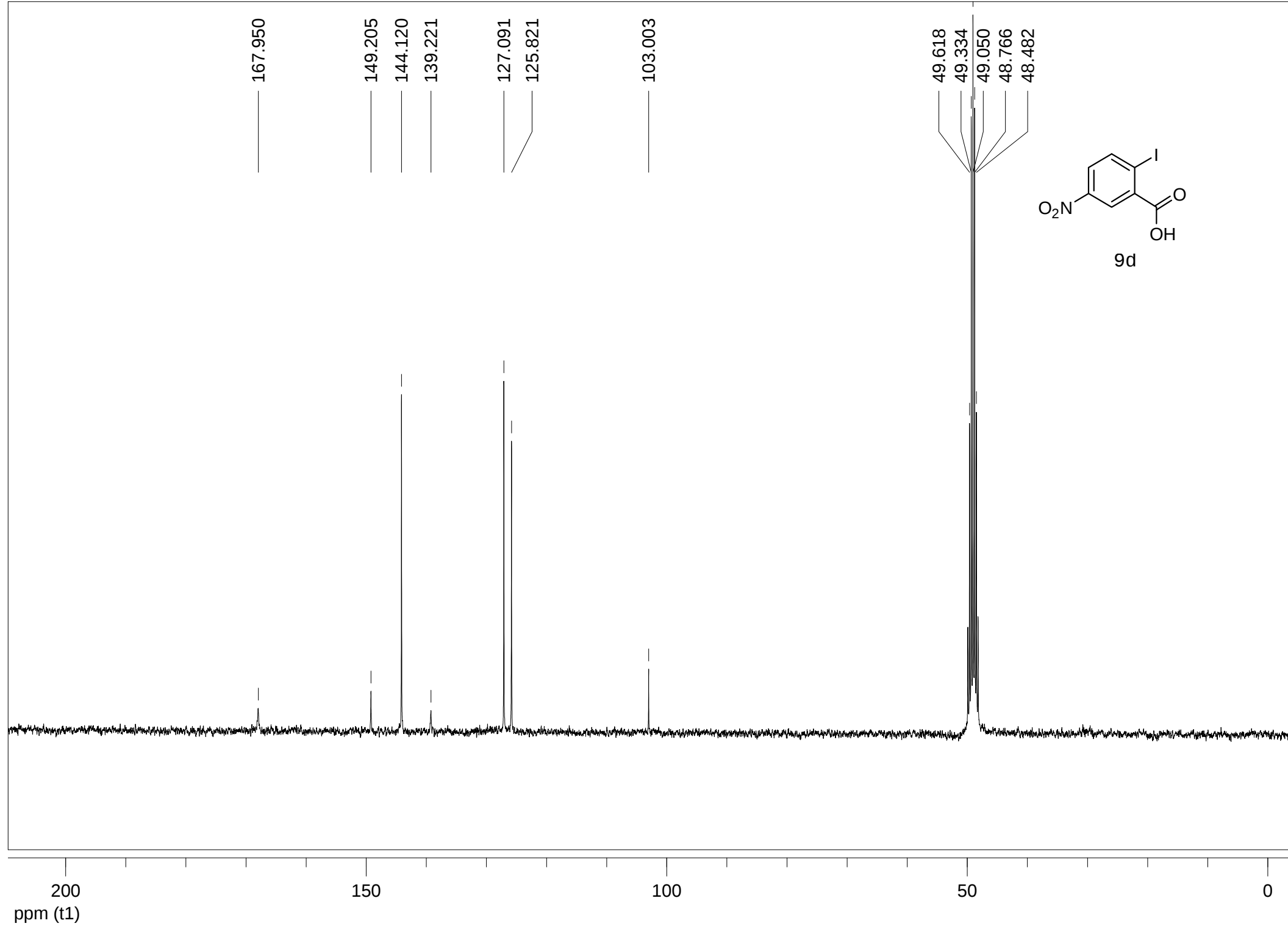


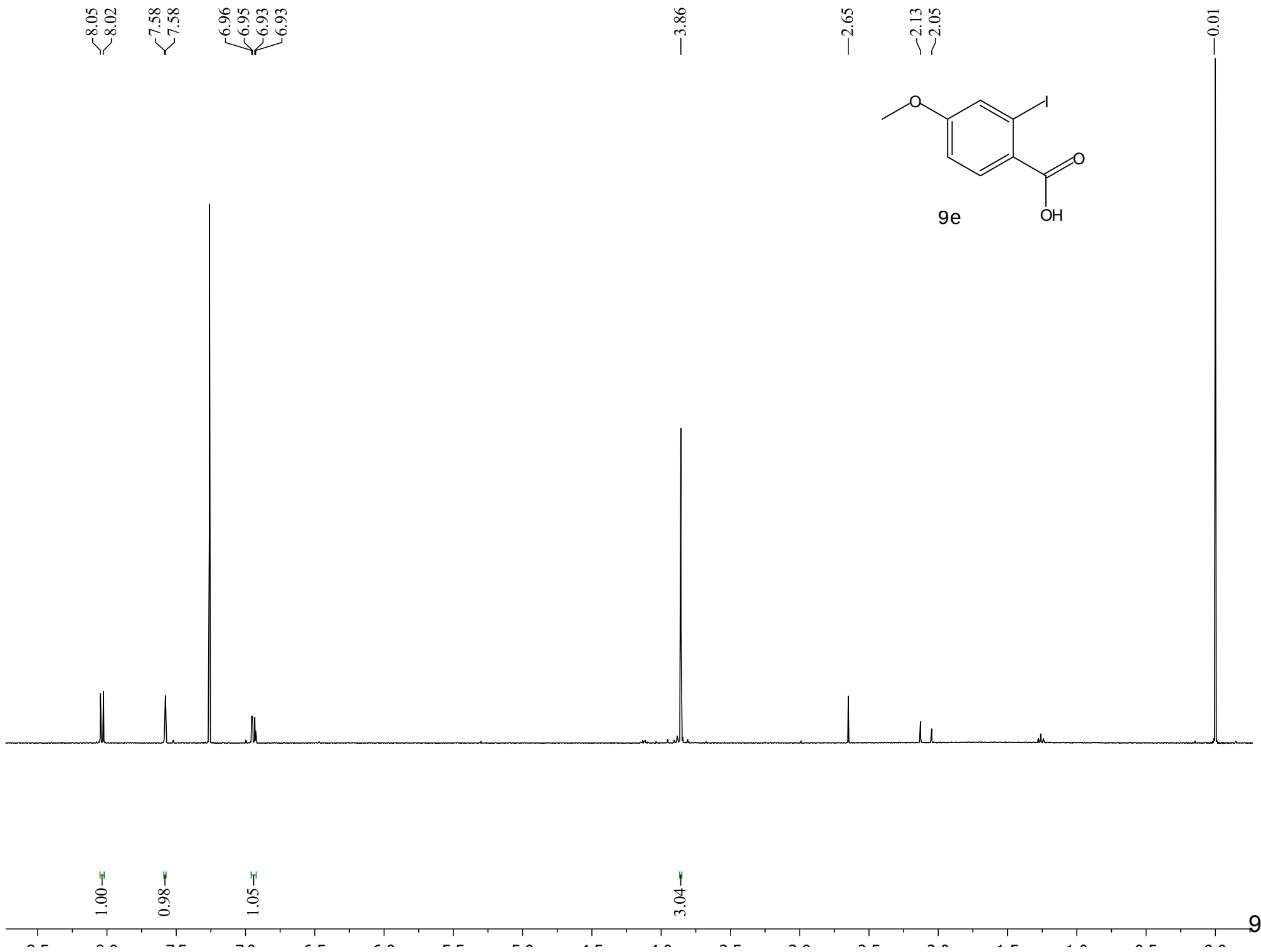
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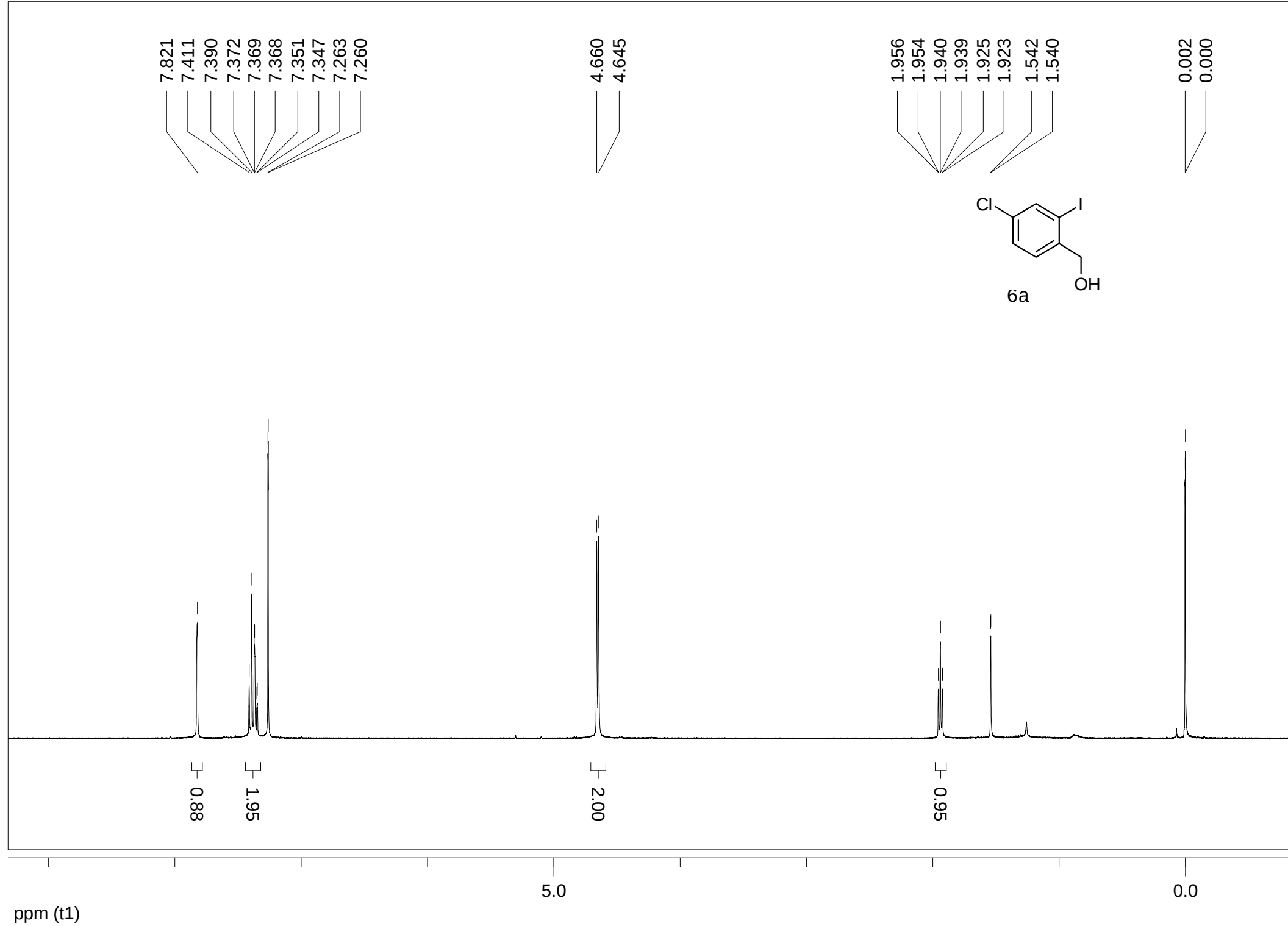


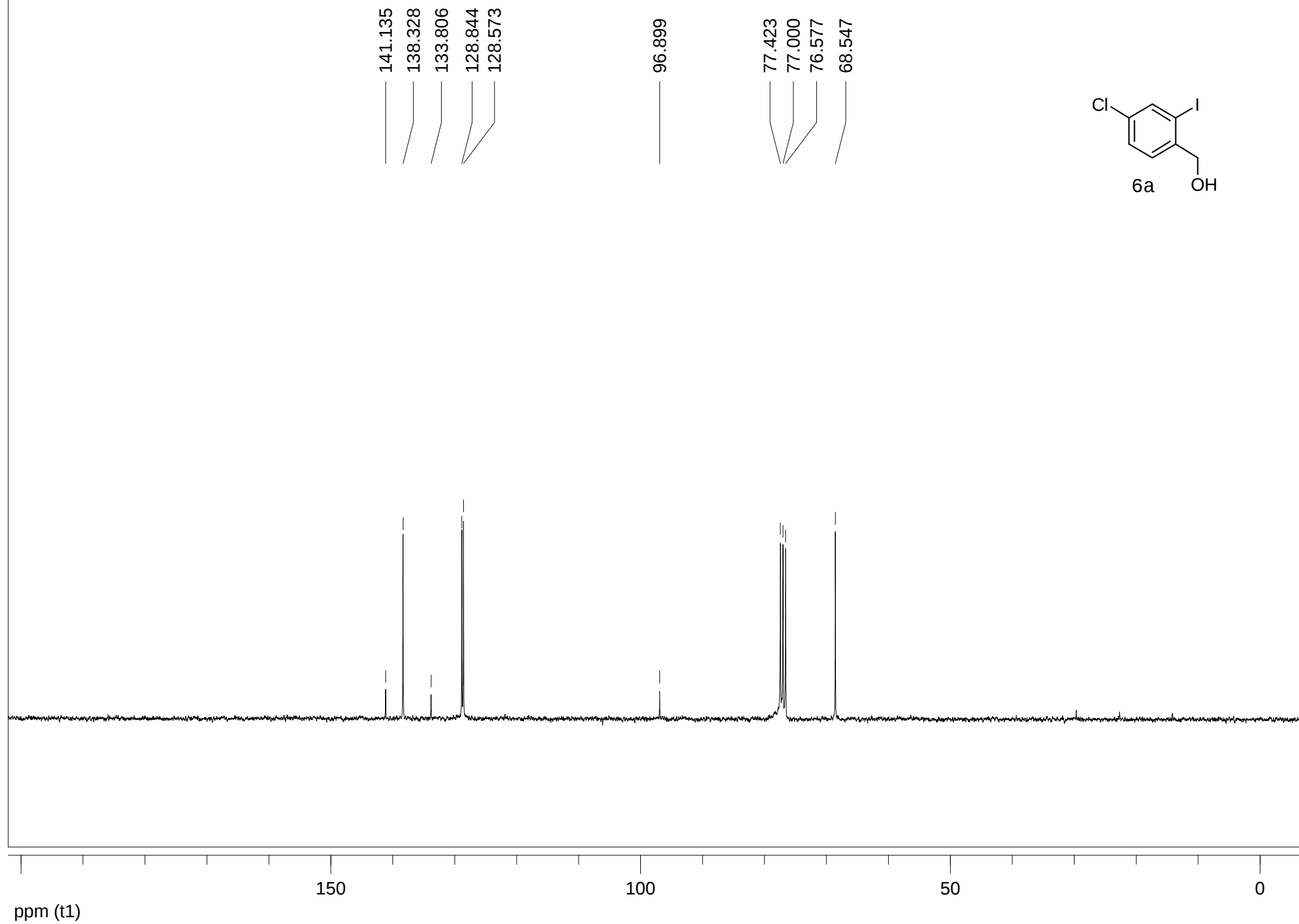
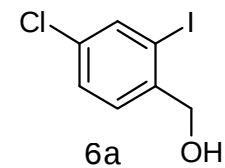


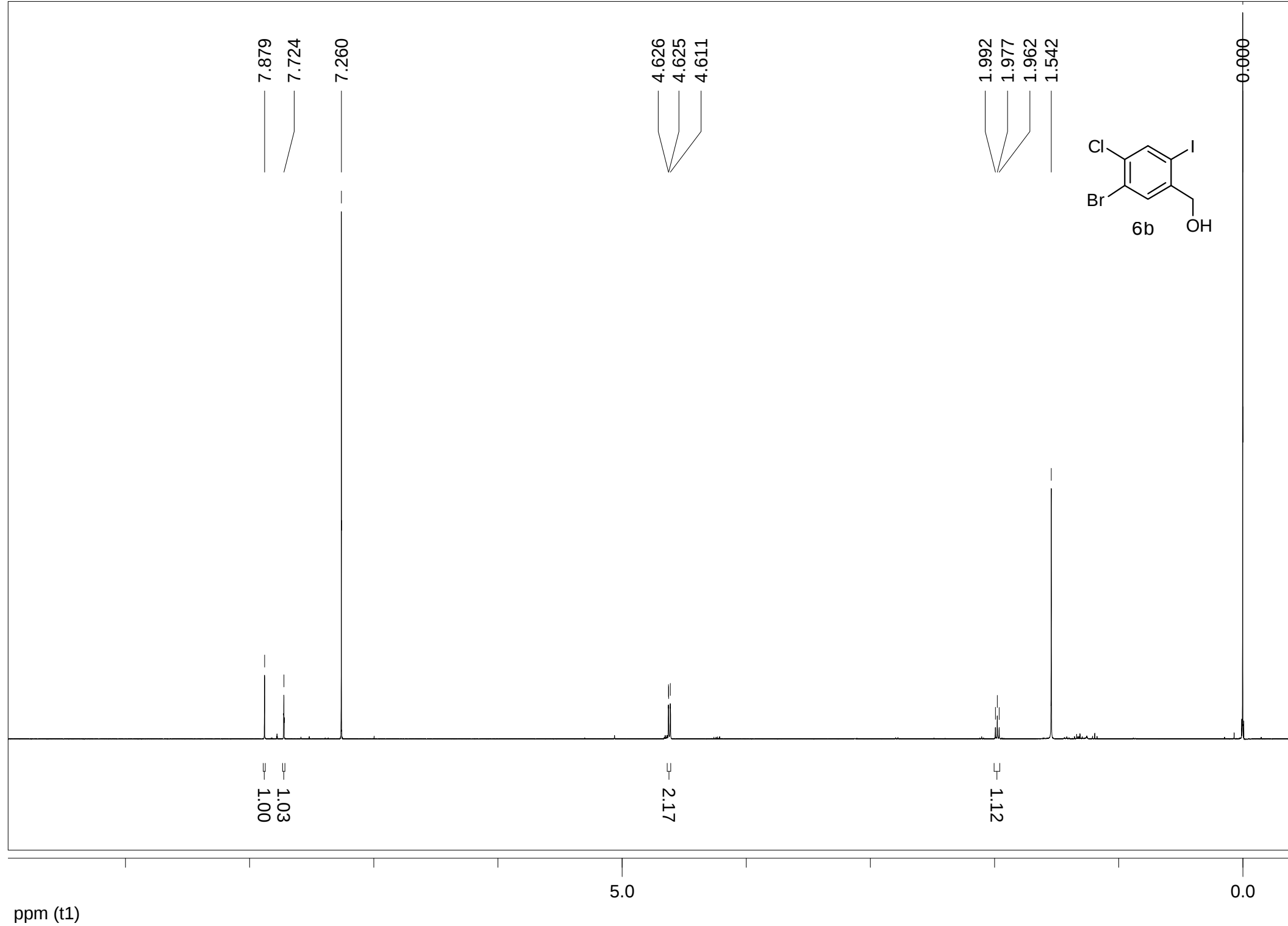
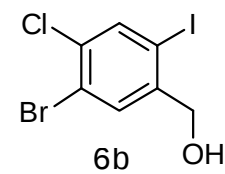


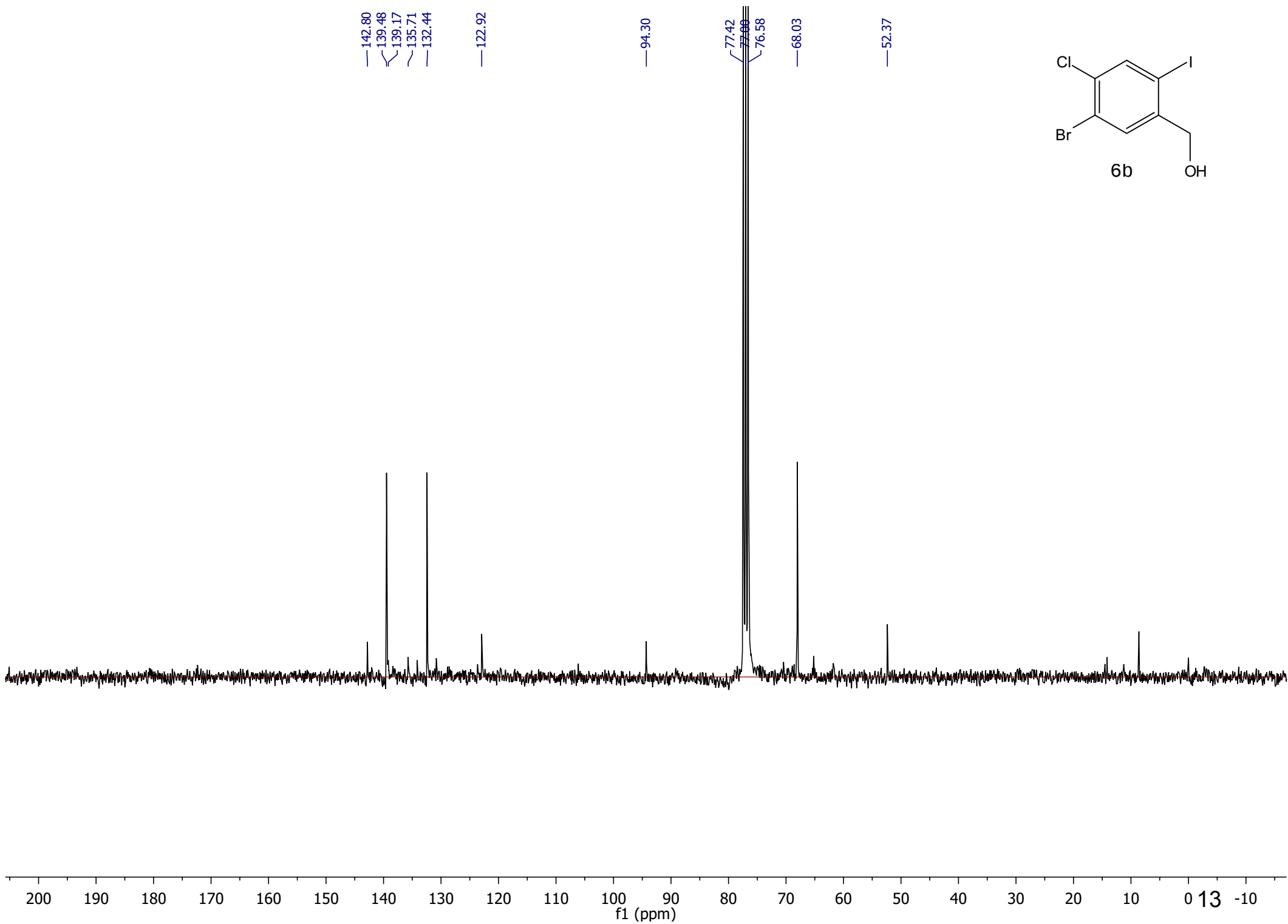




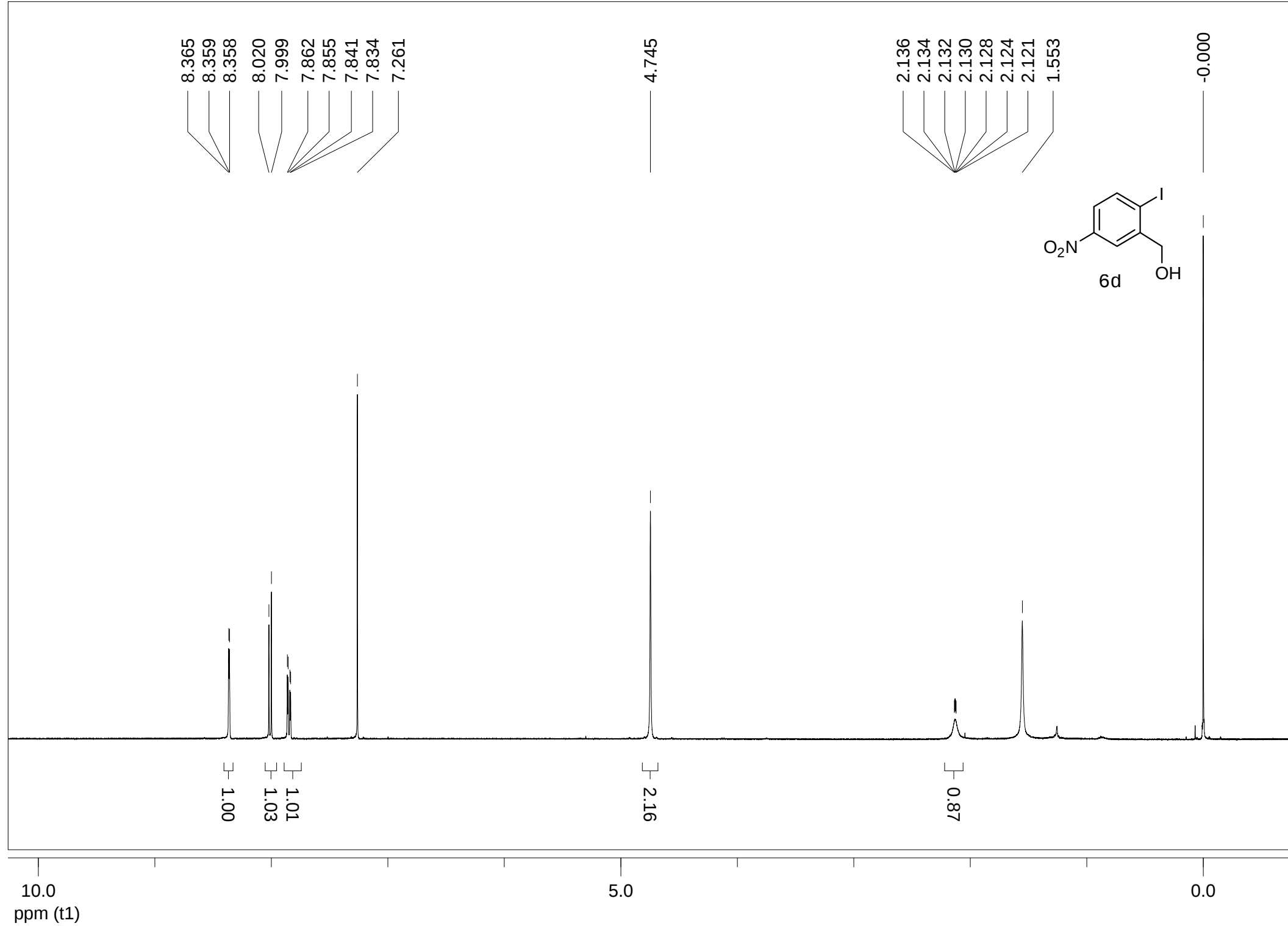


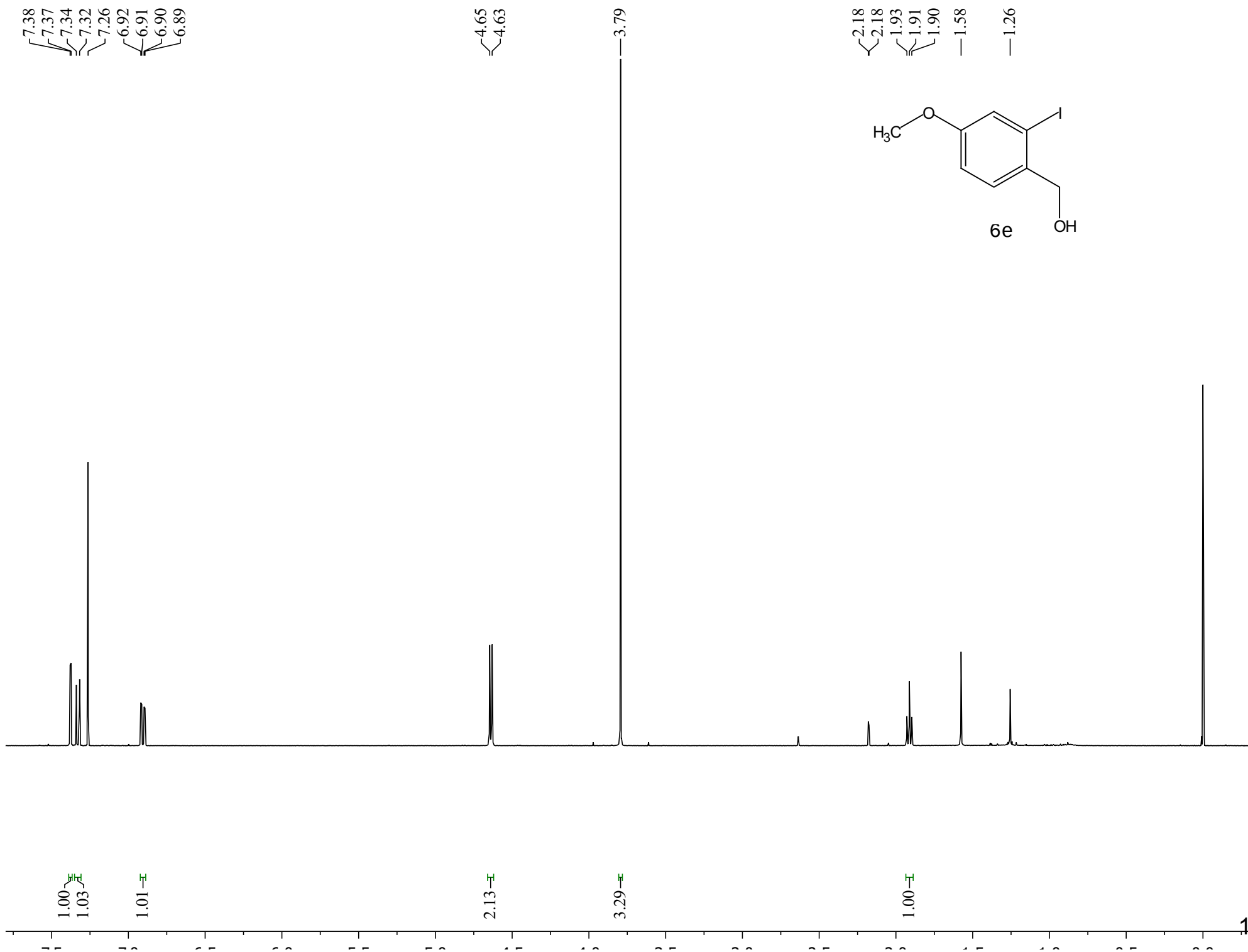


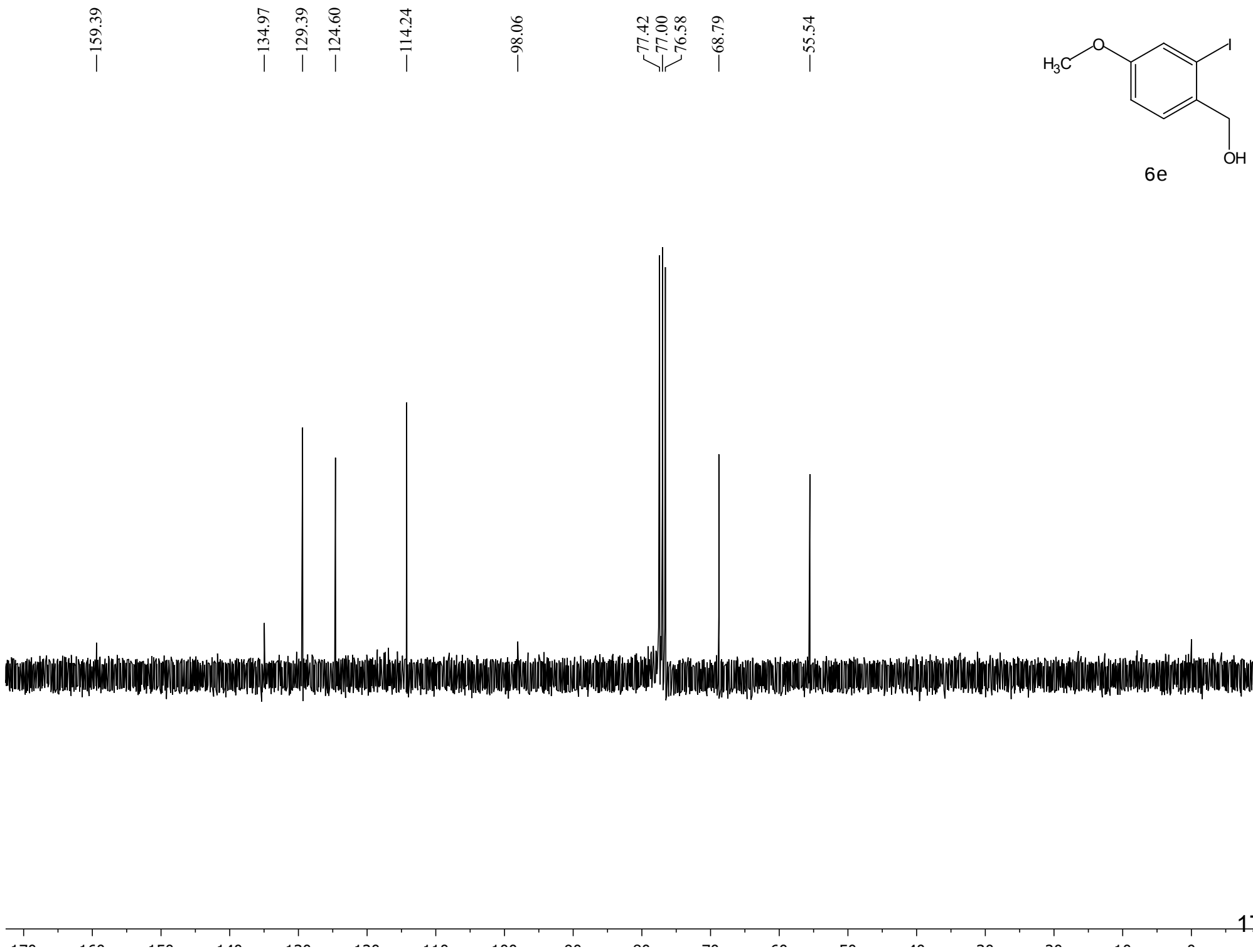


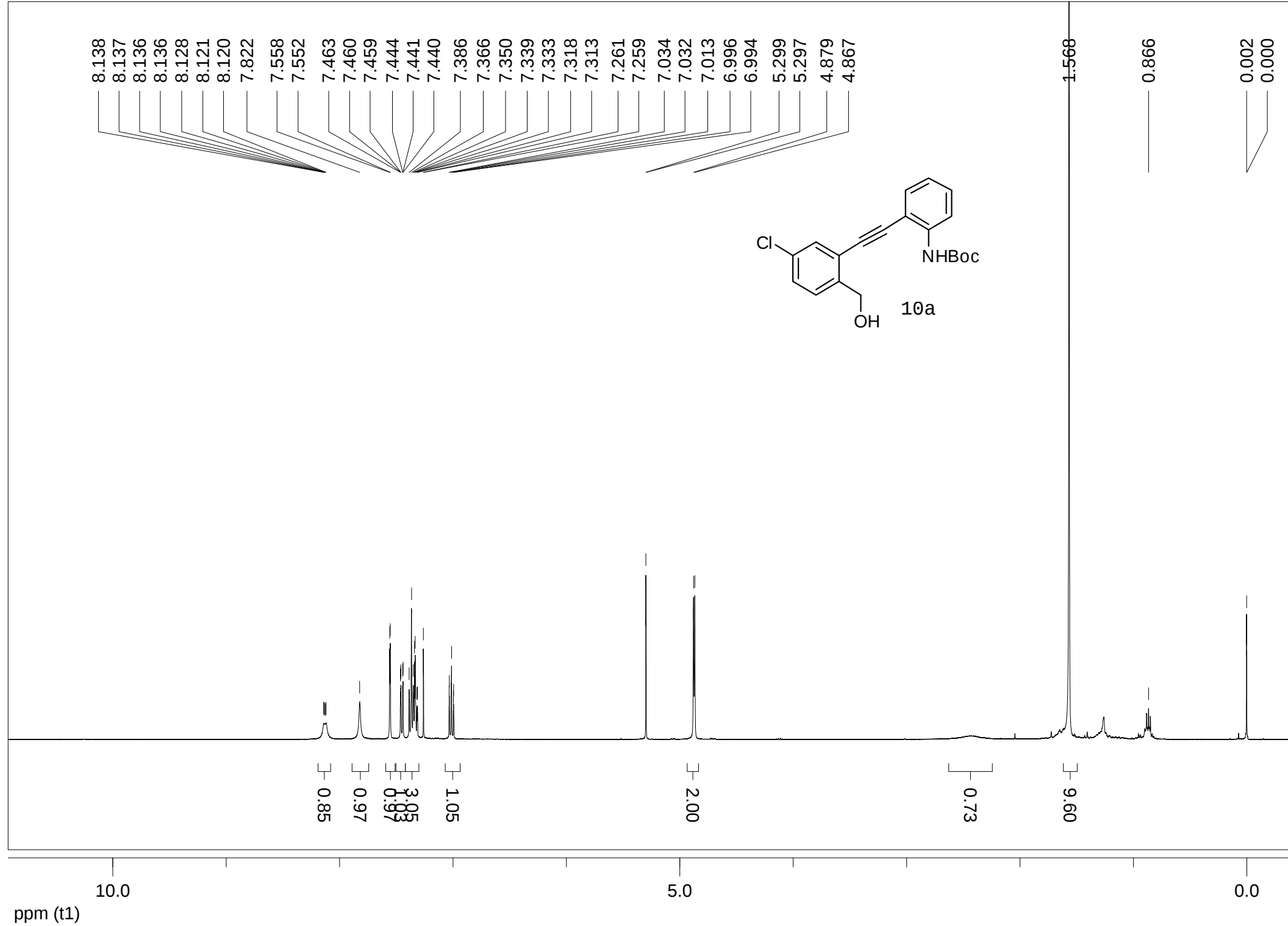


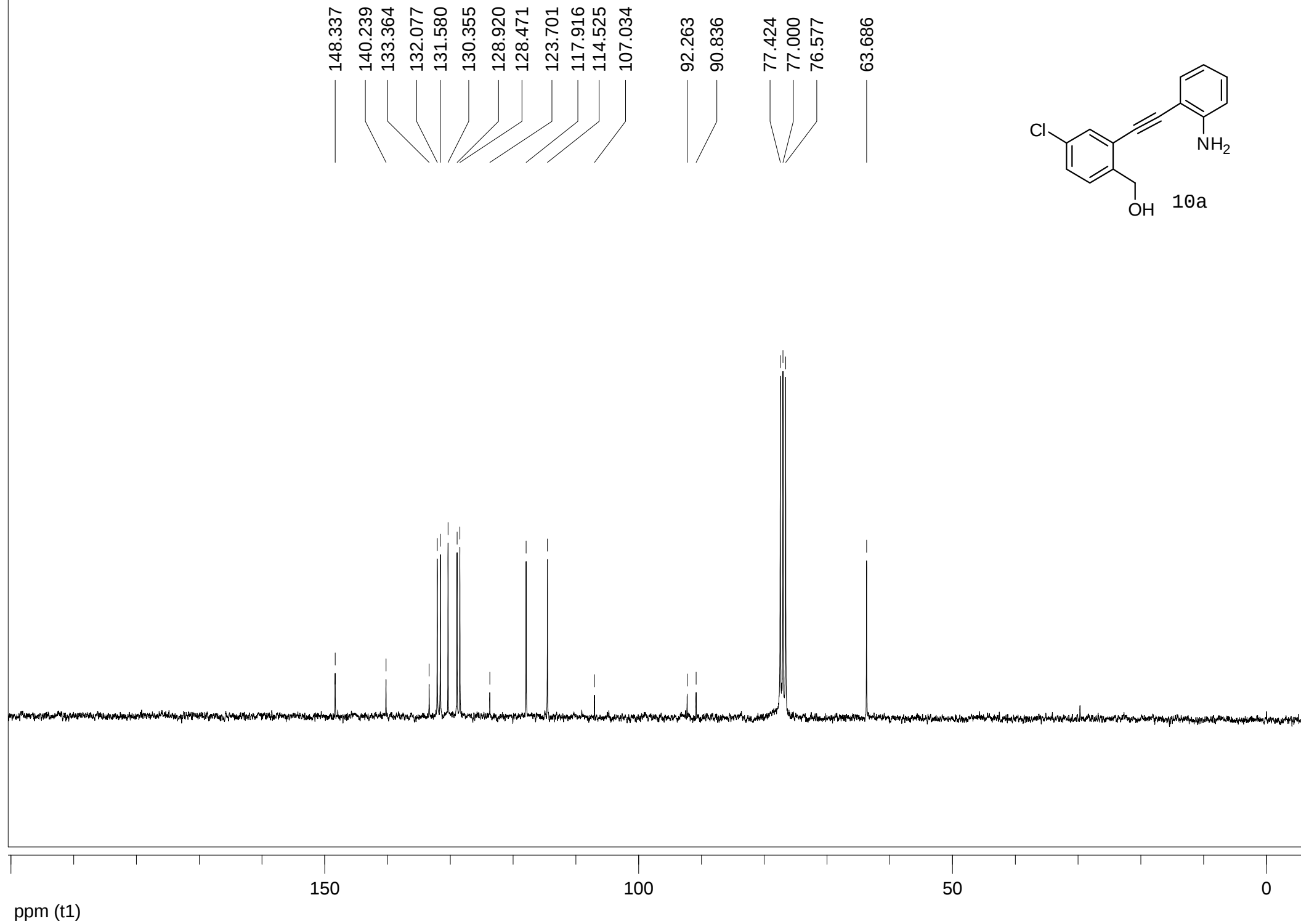
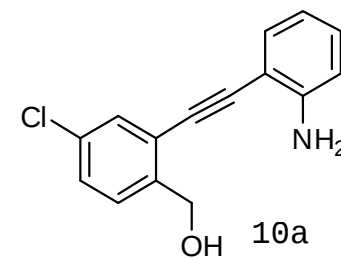


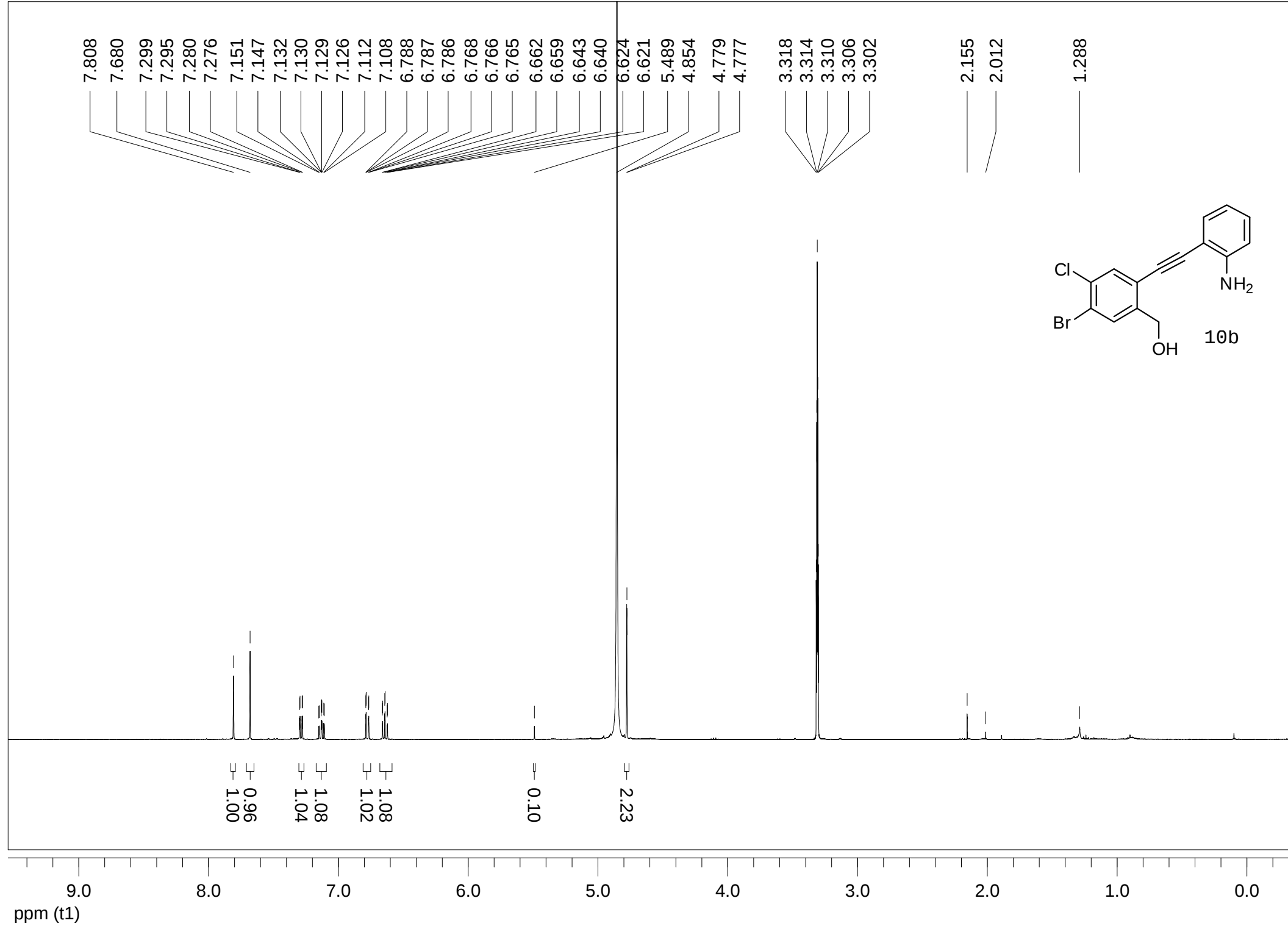


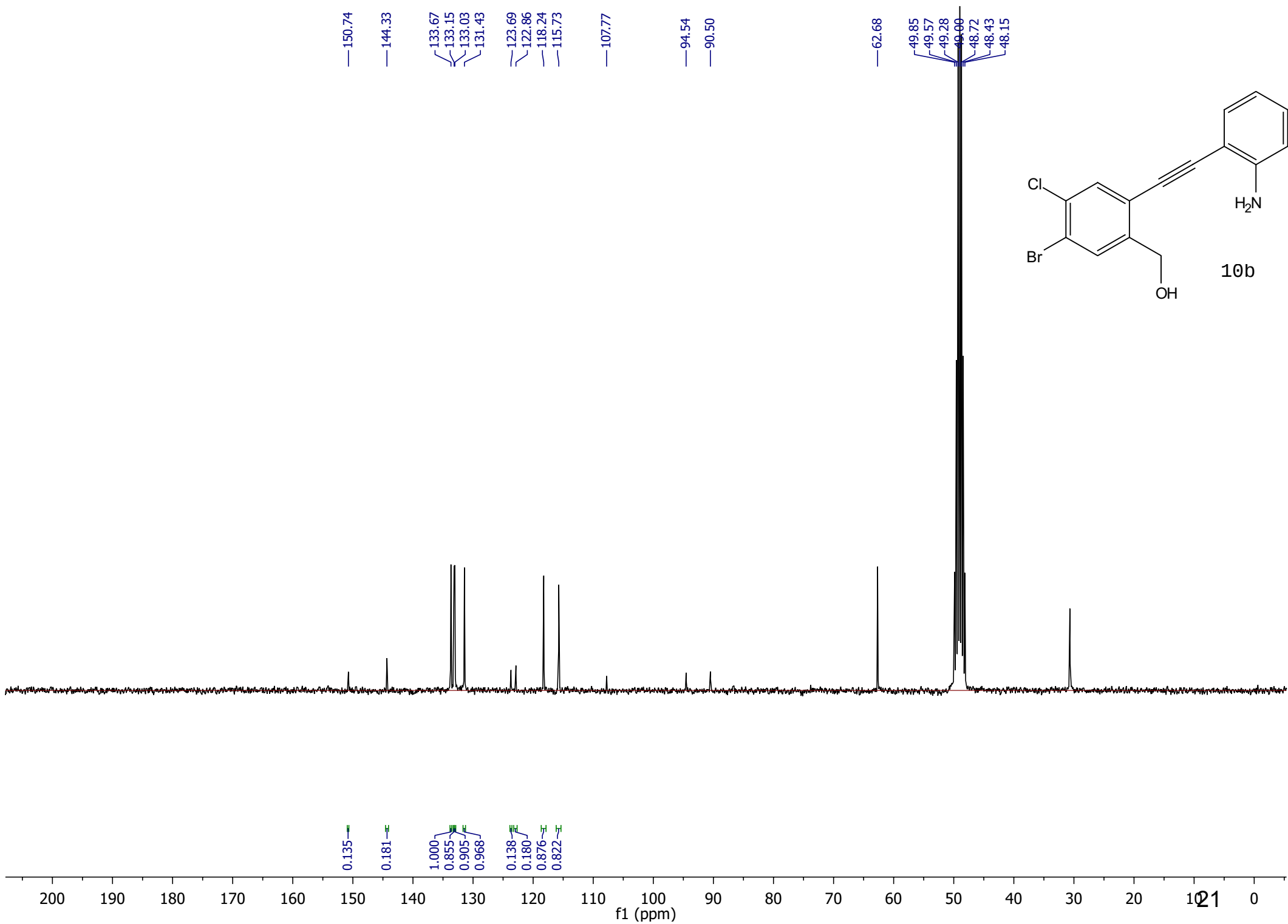


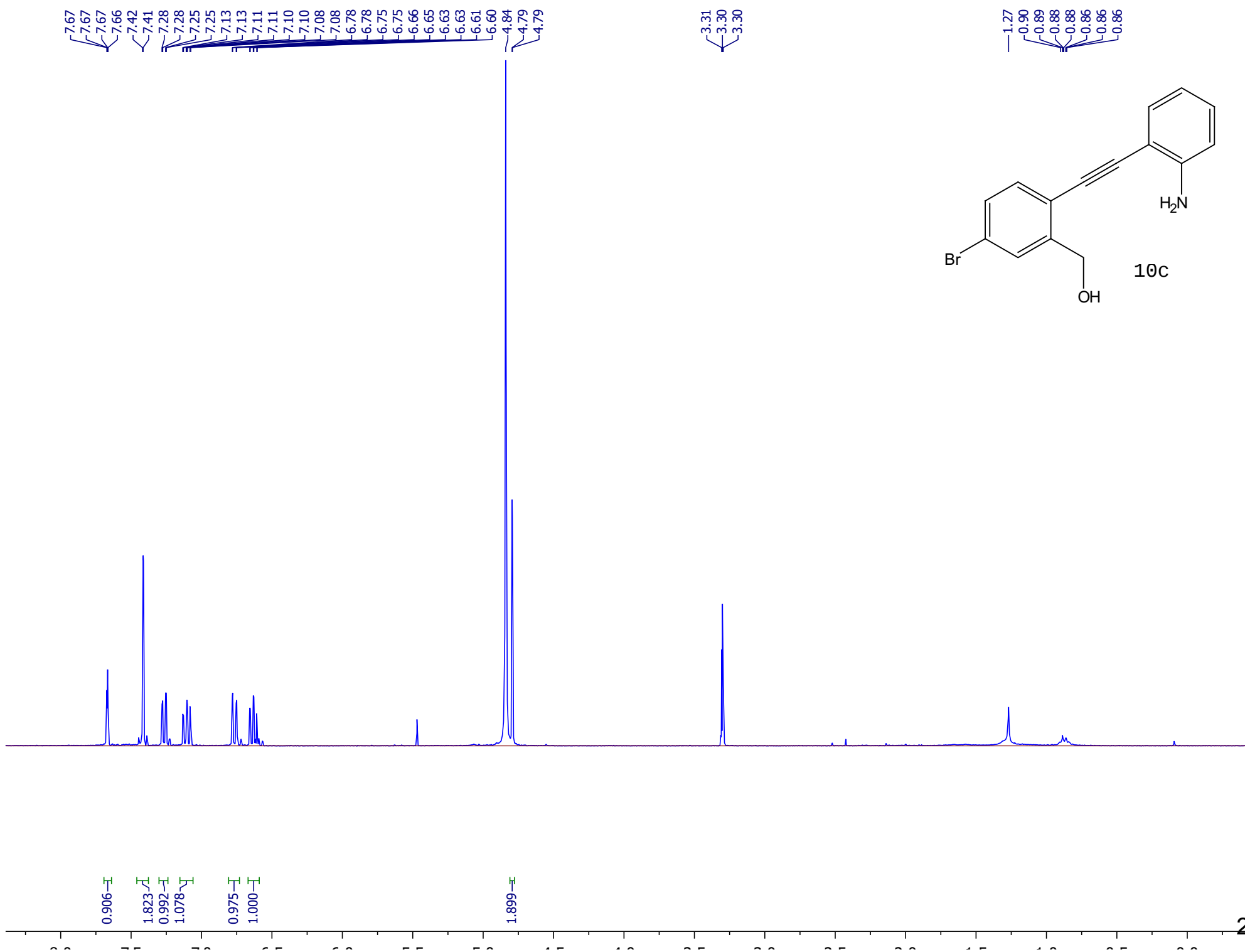


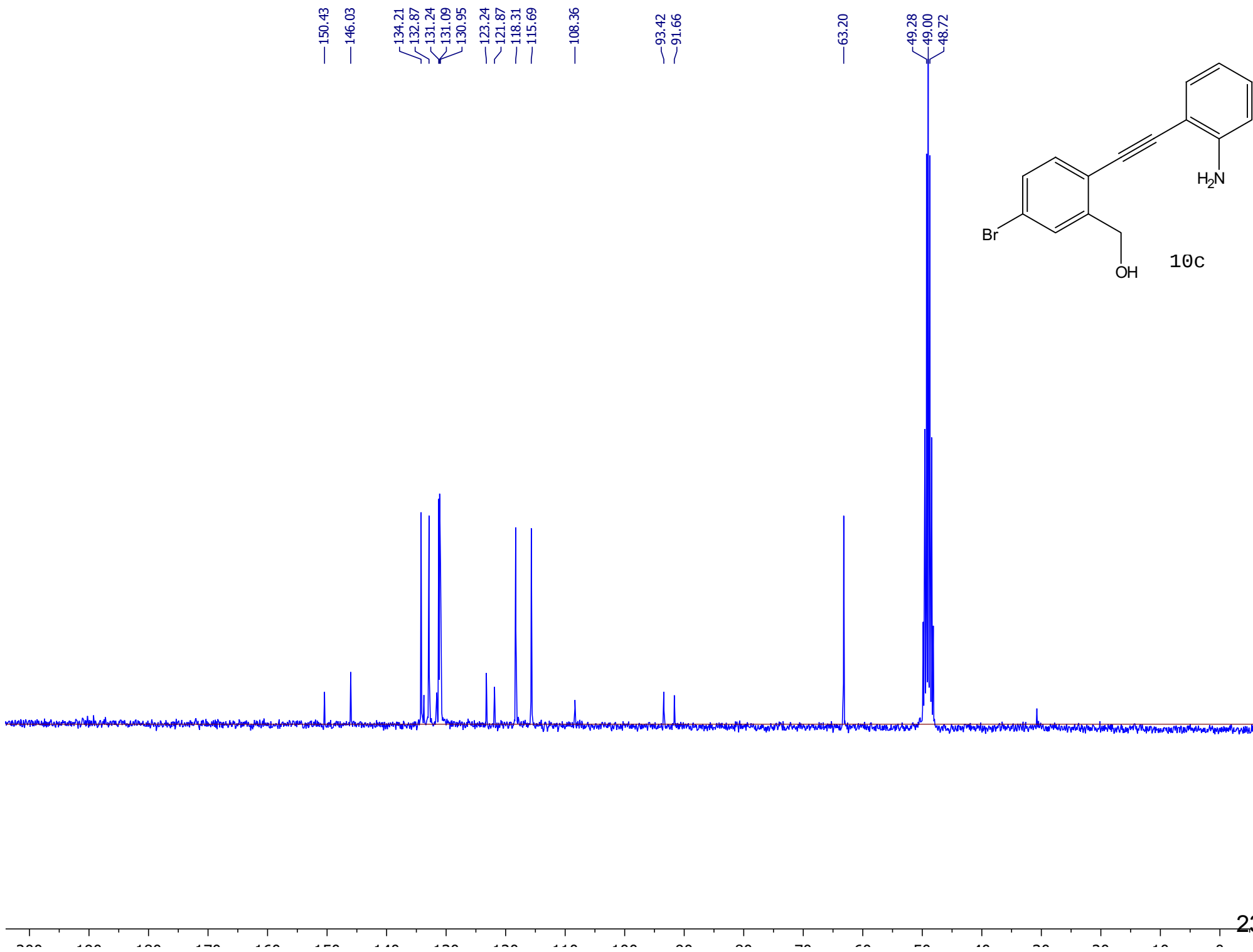


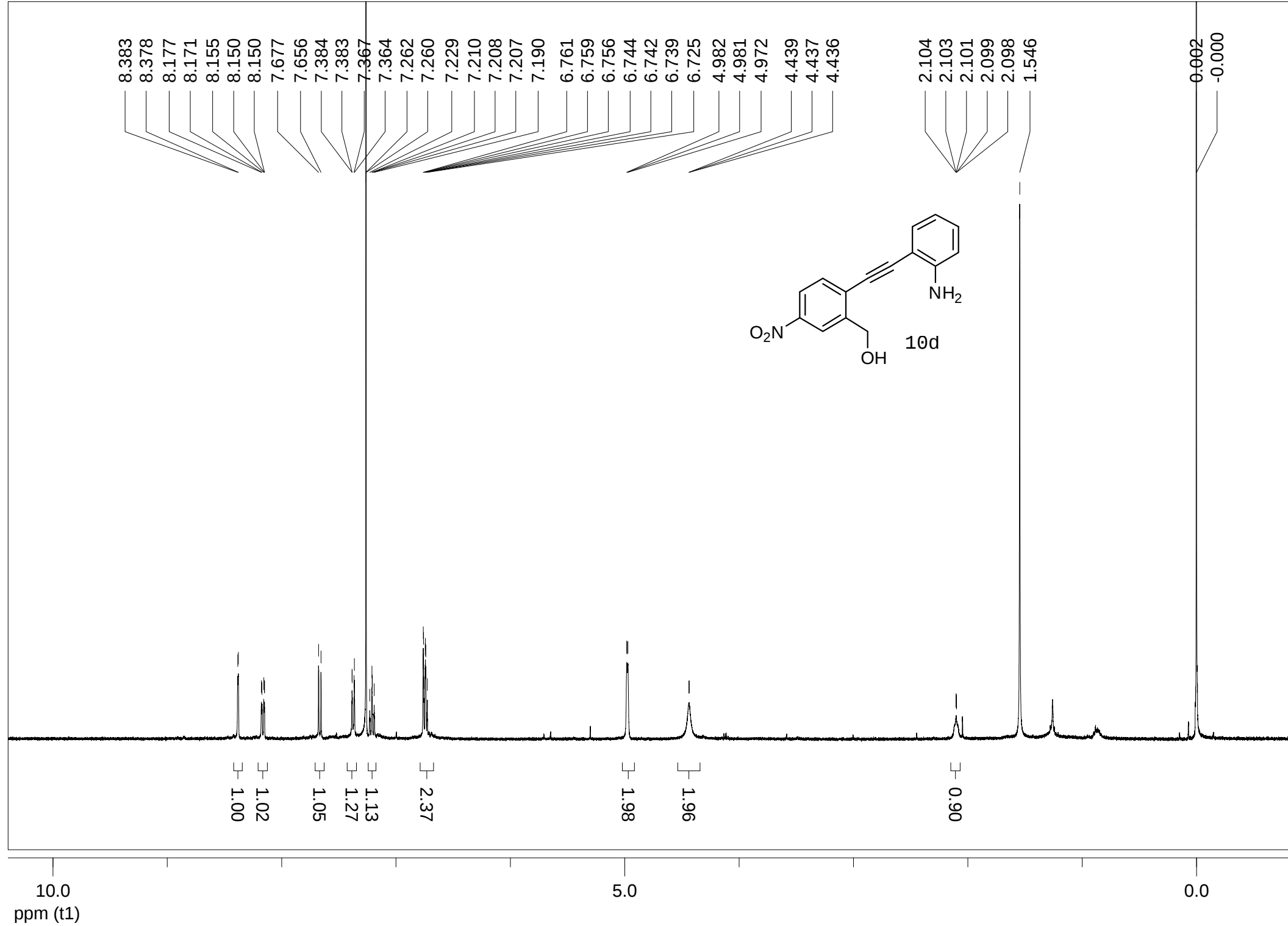


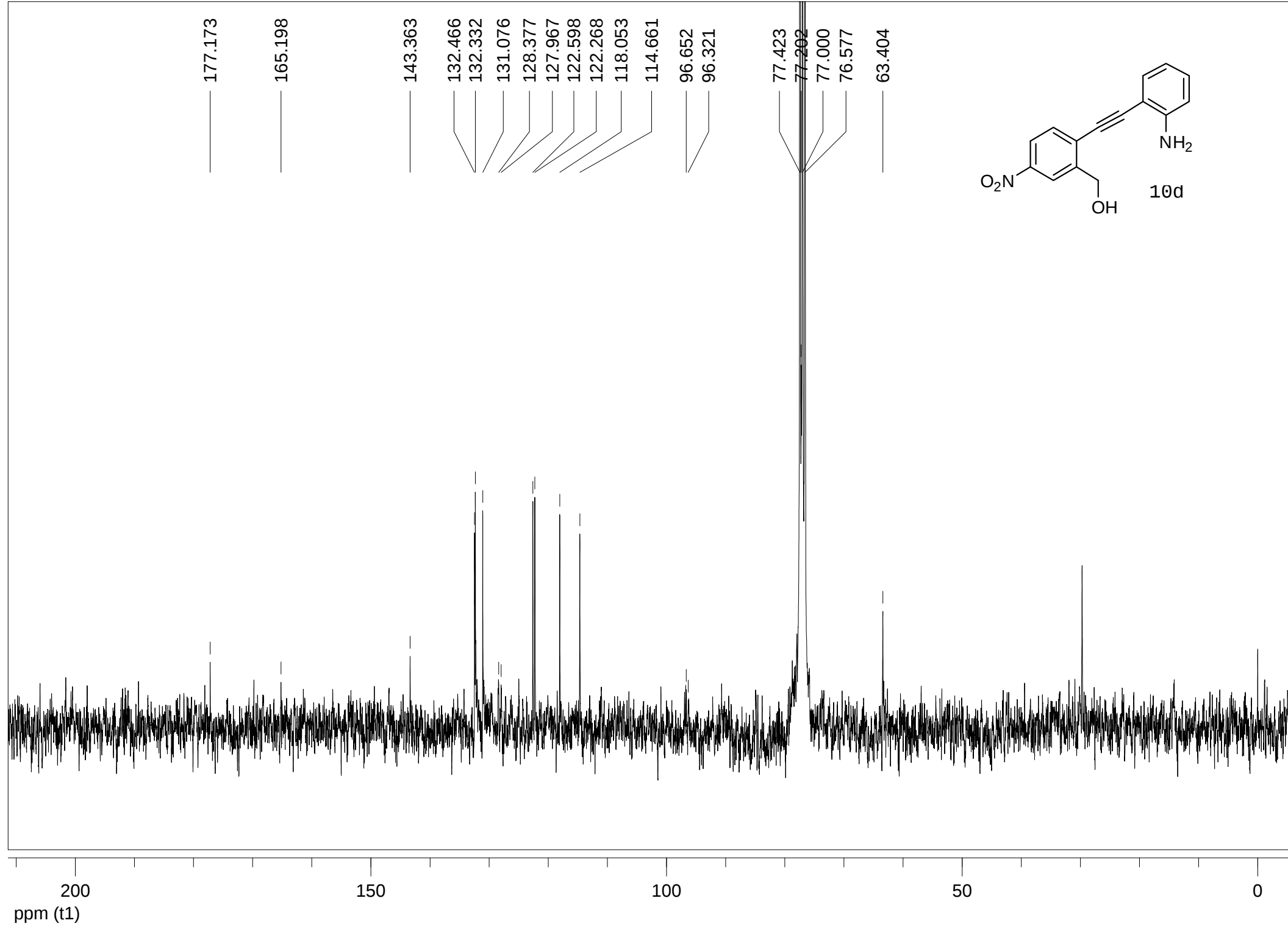










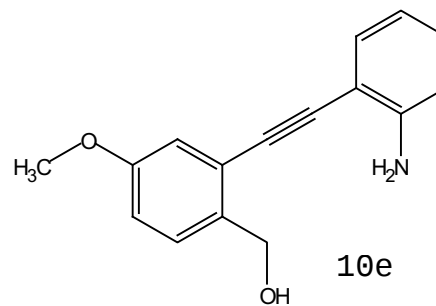


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7.09
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1.85

0.00



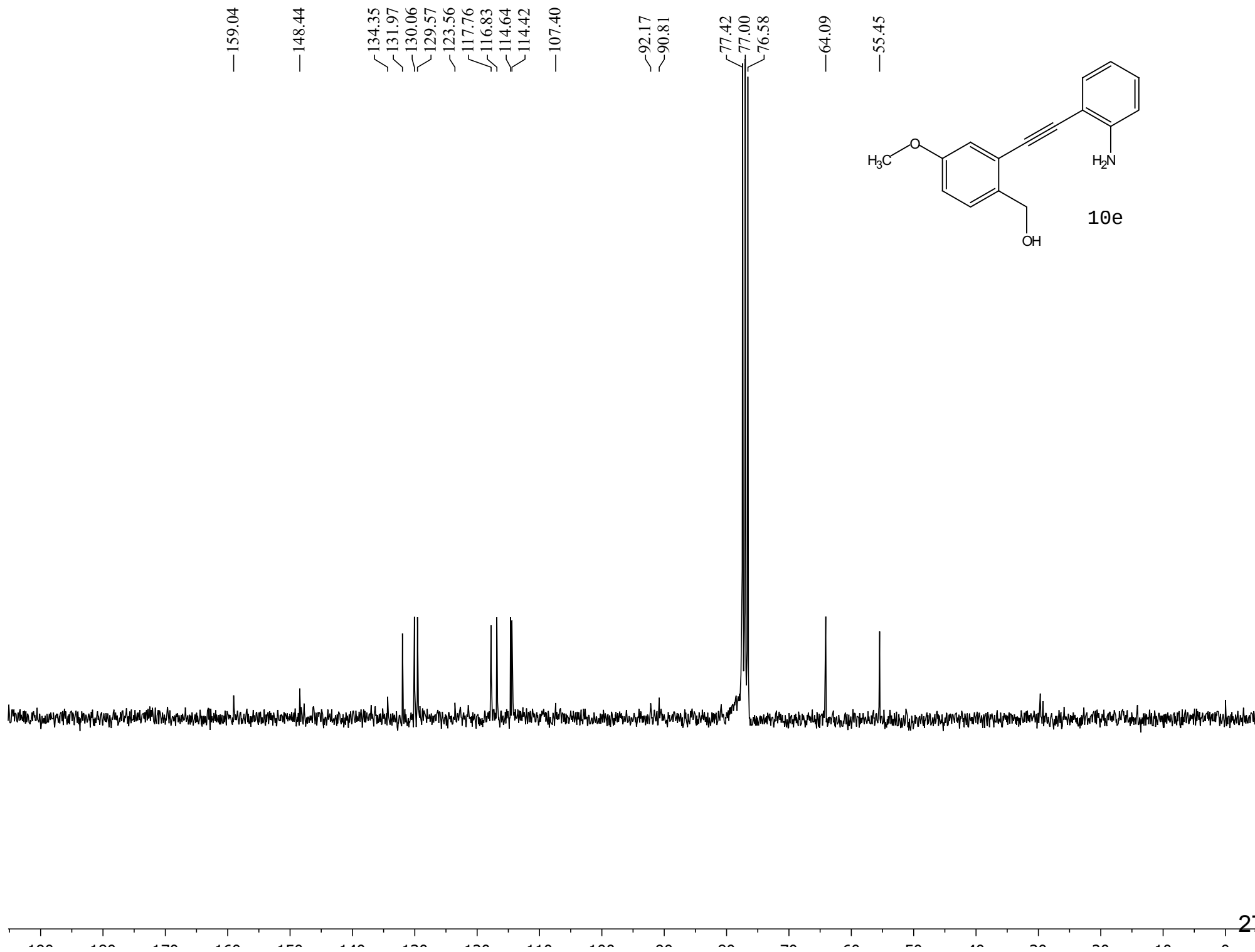
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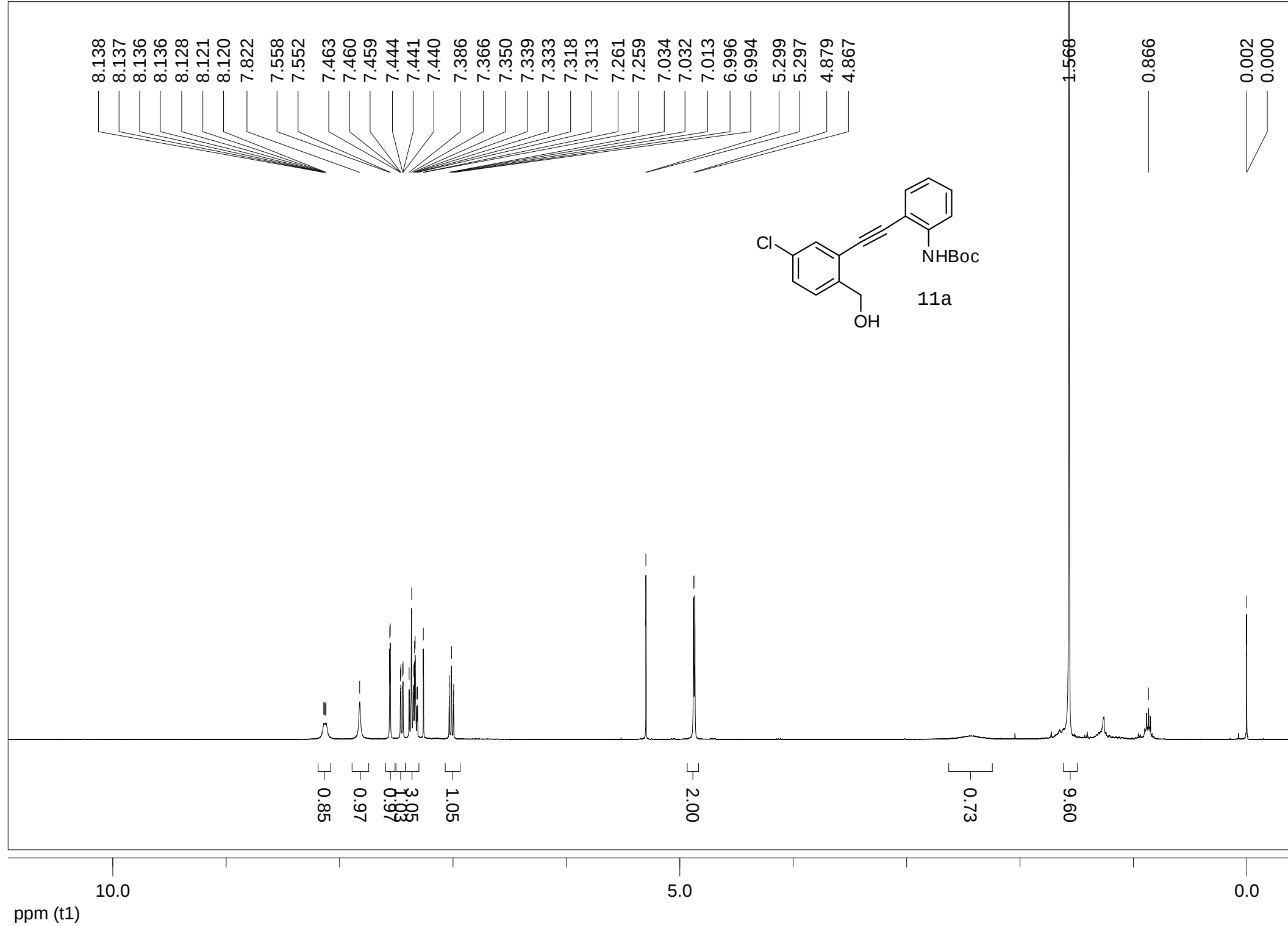
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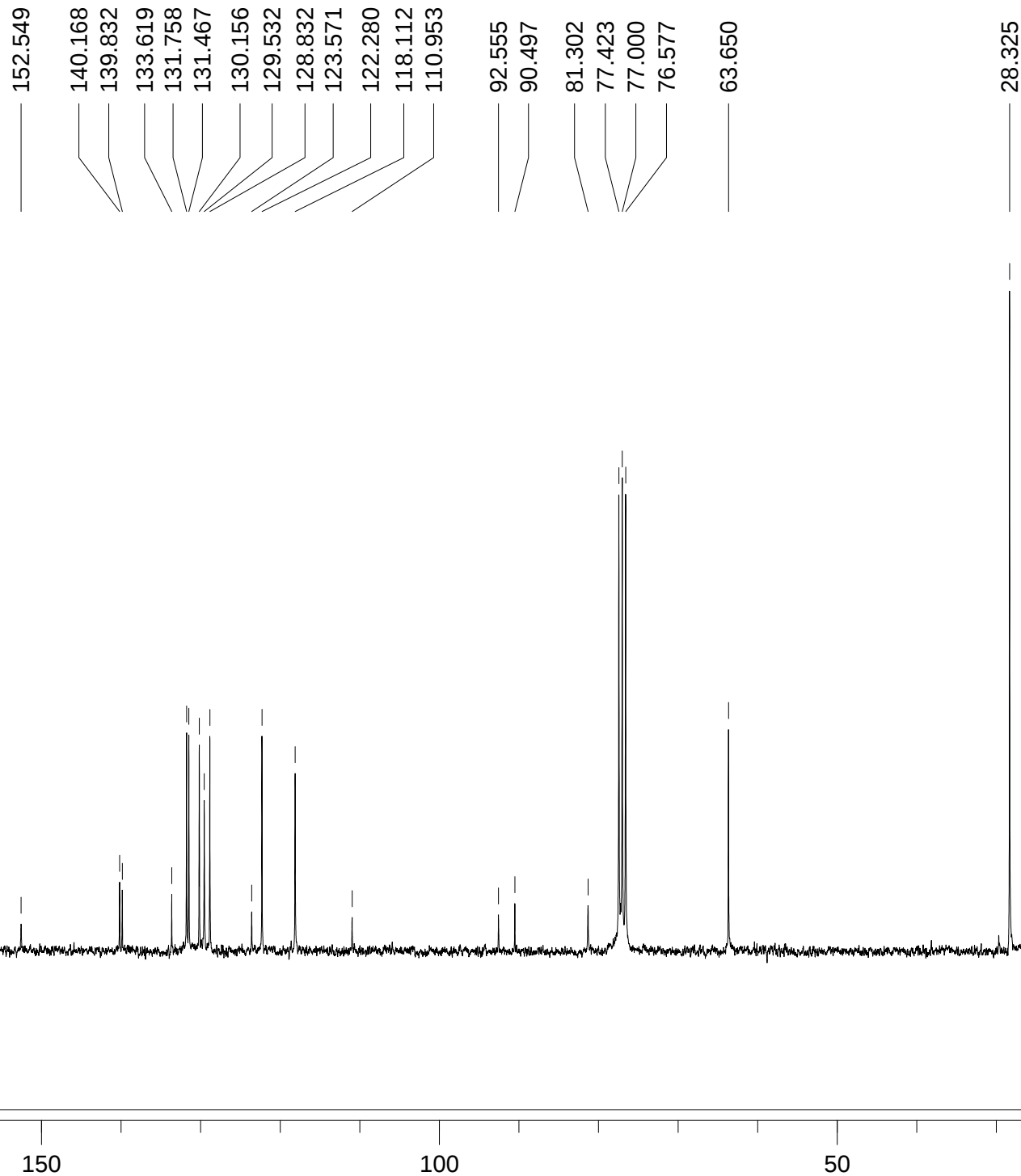
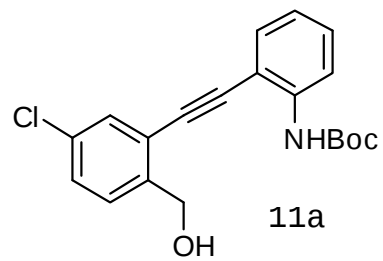
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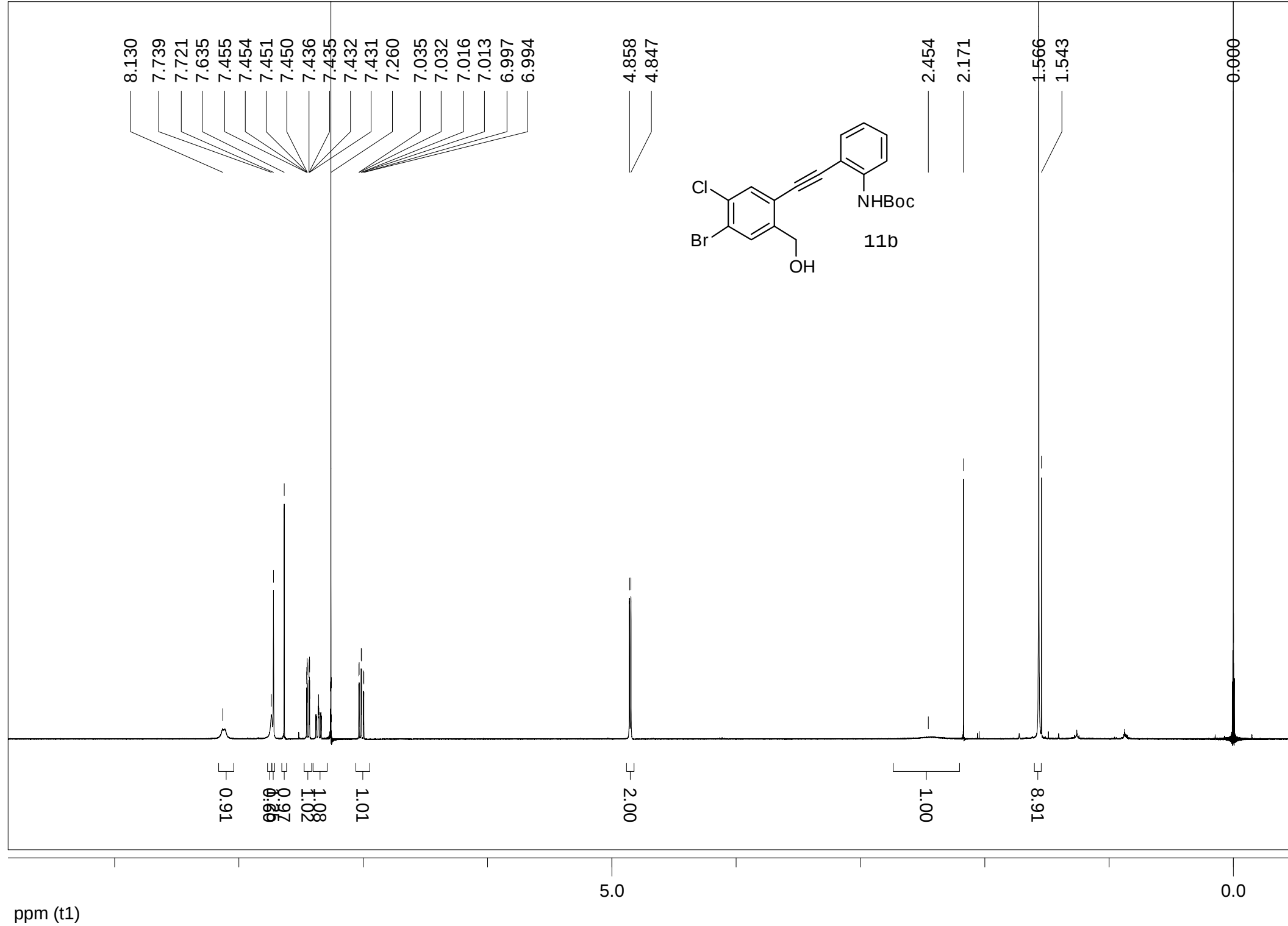
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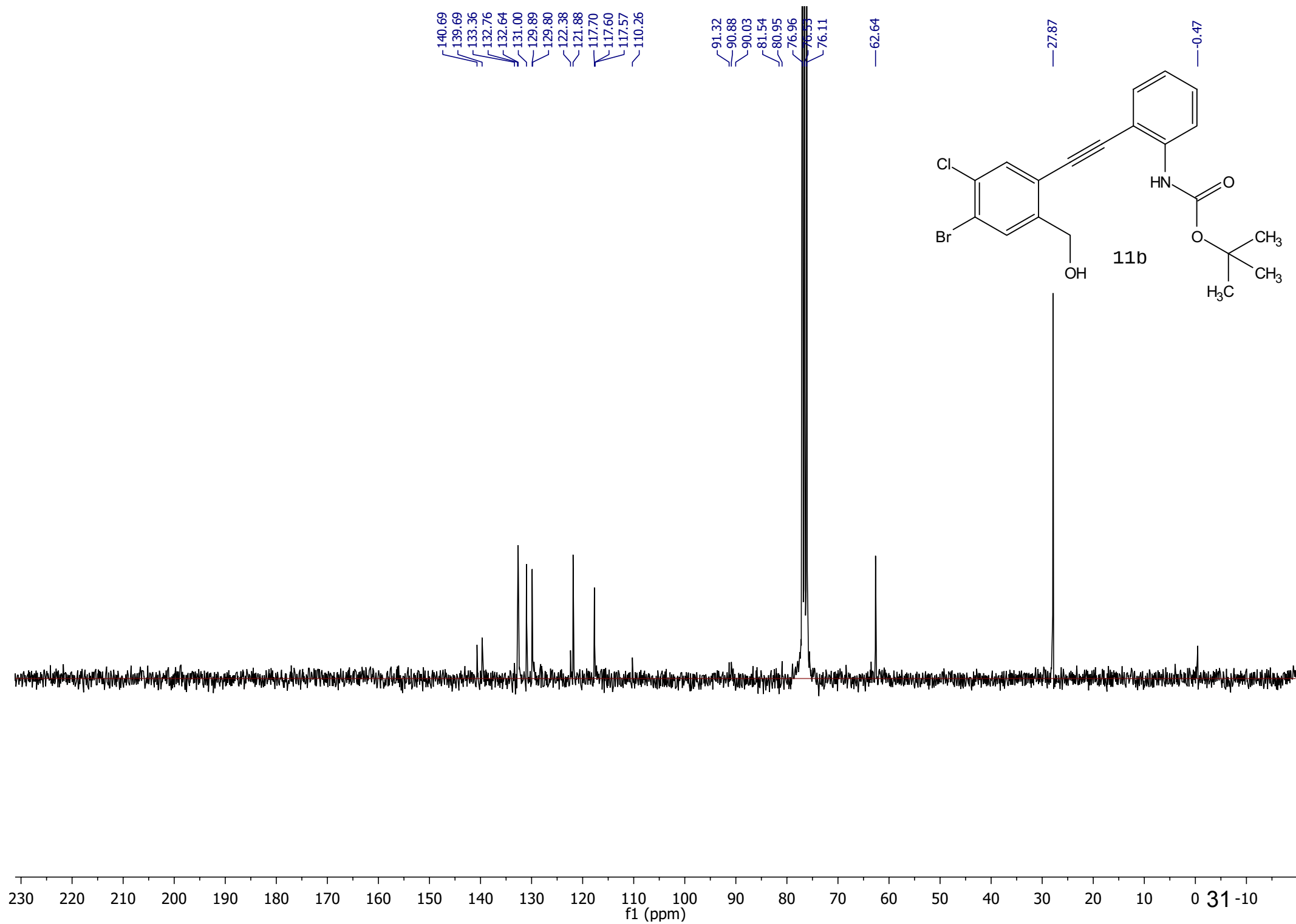
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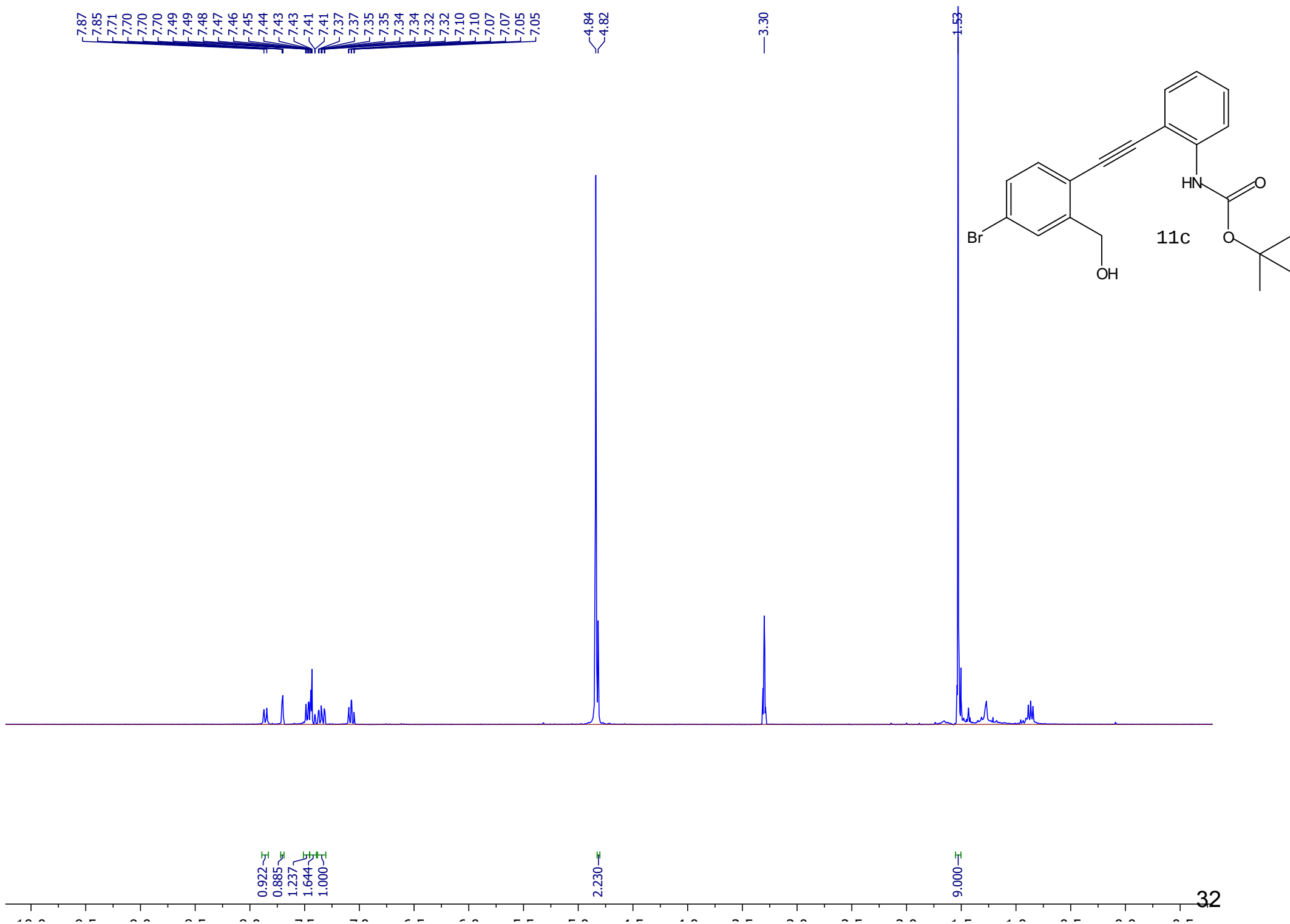


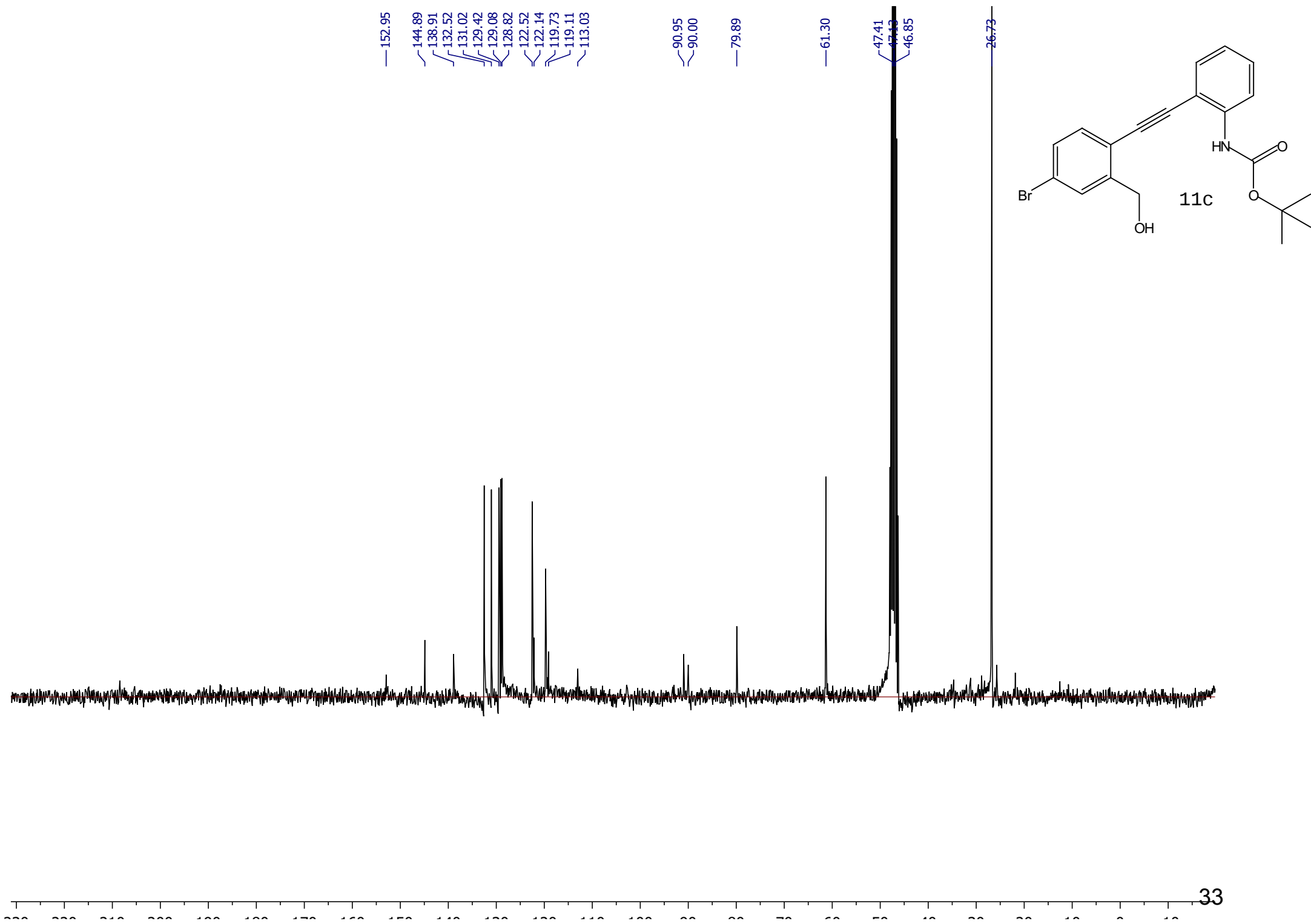


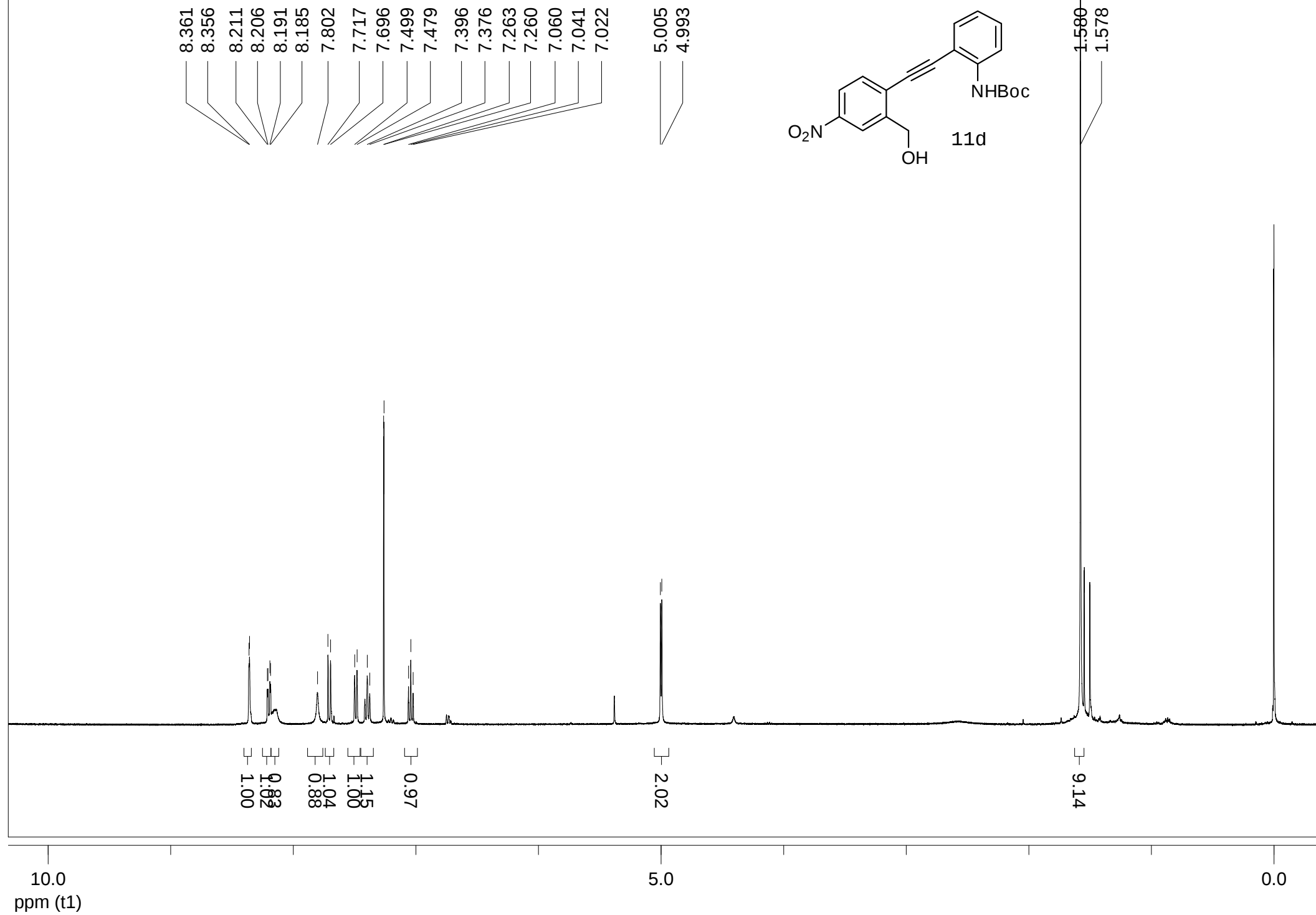
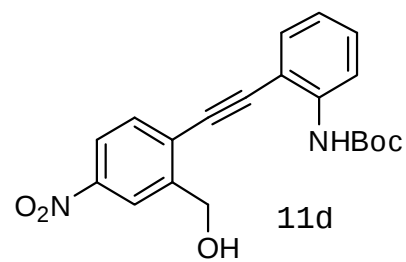


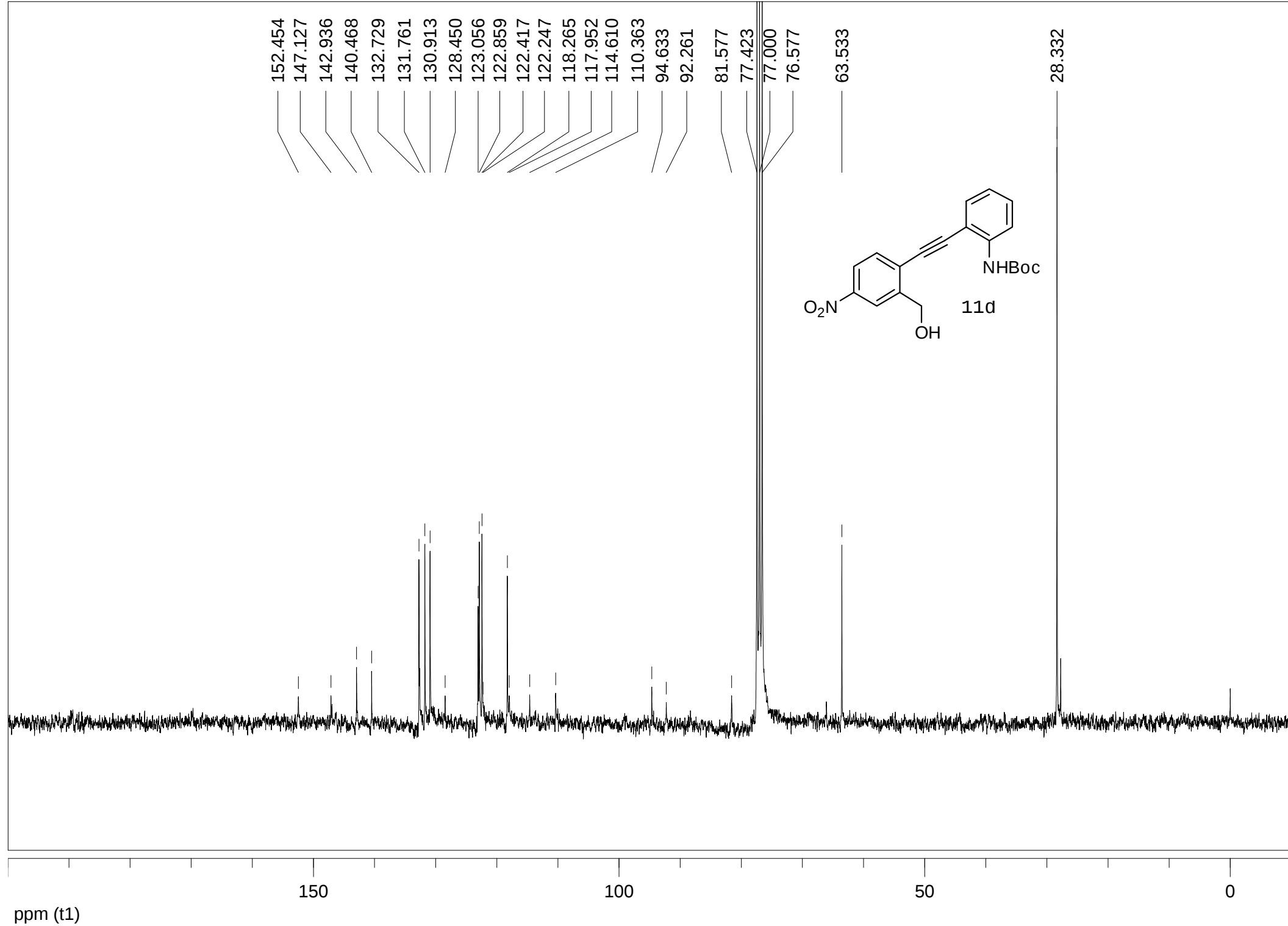


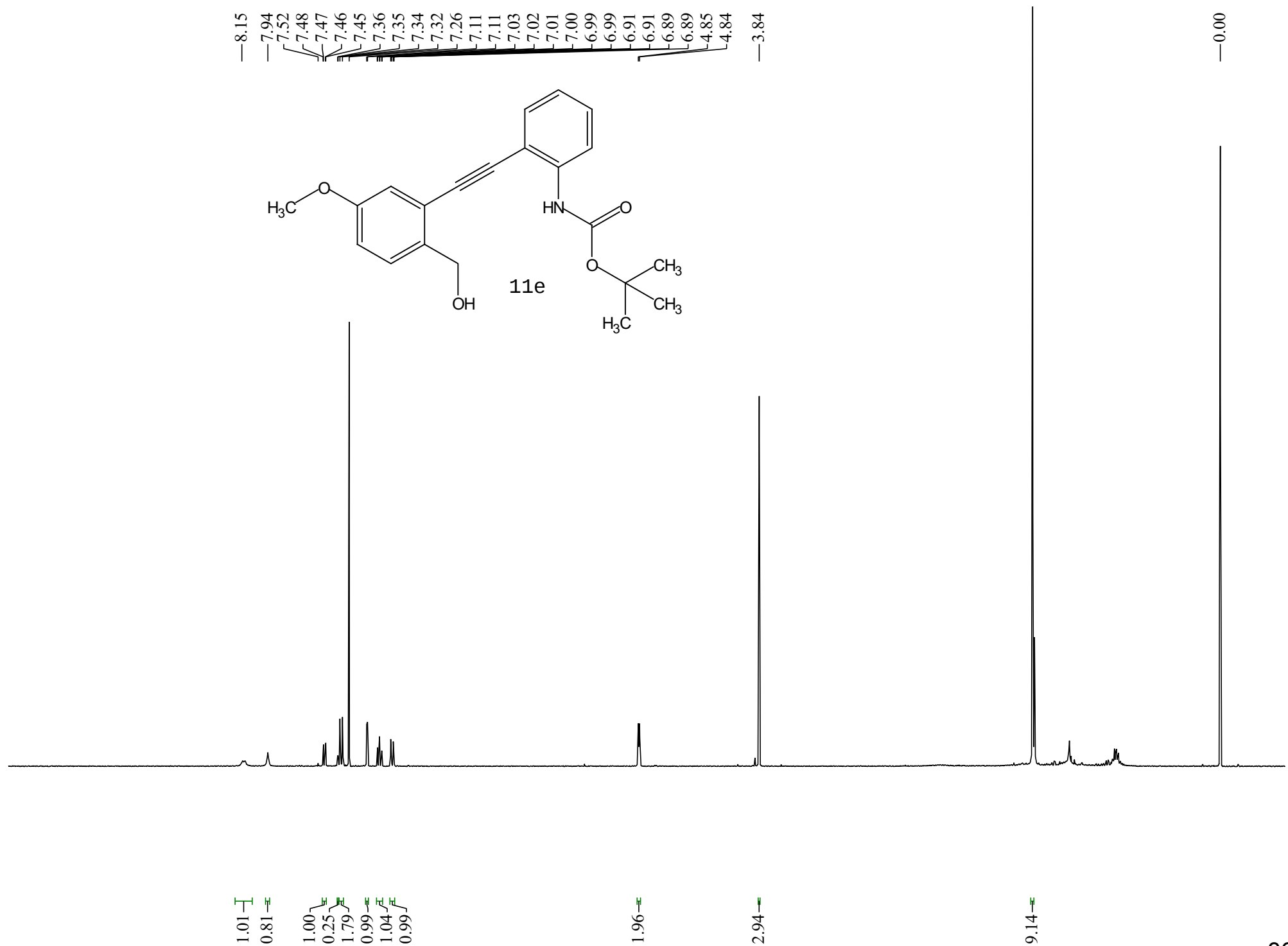


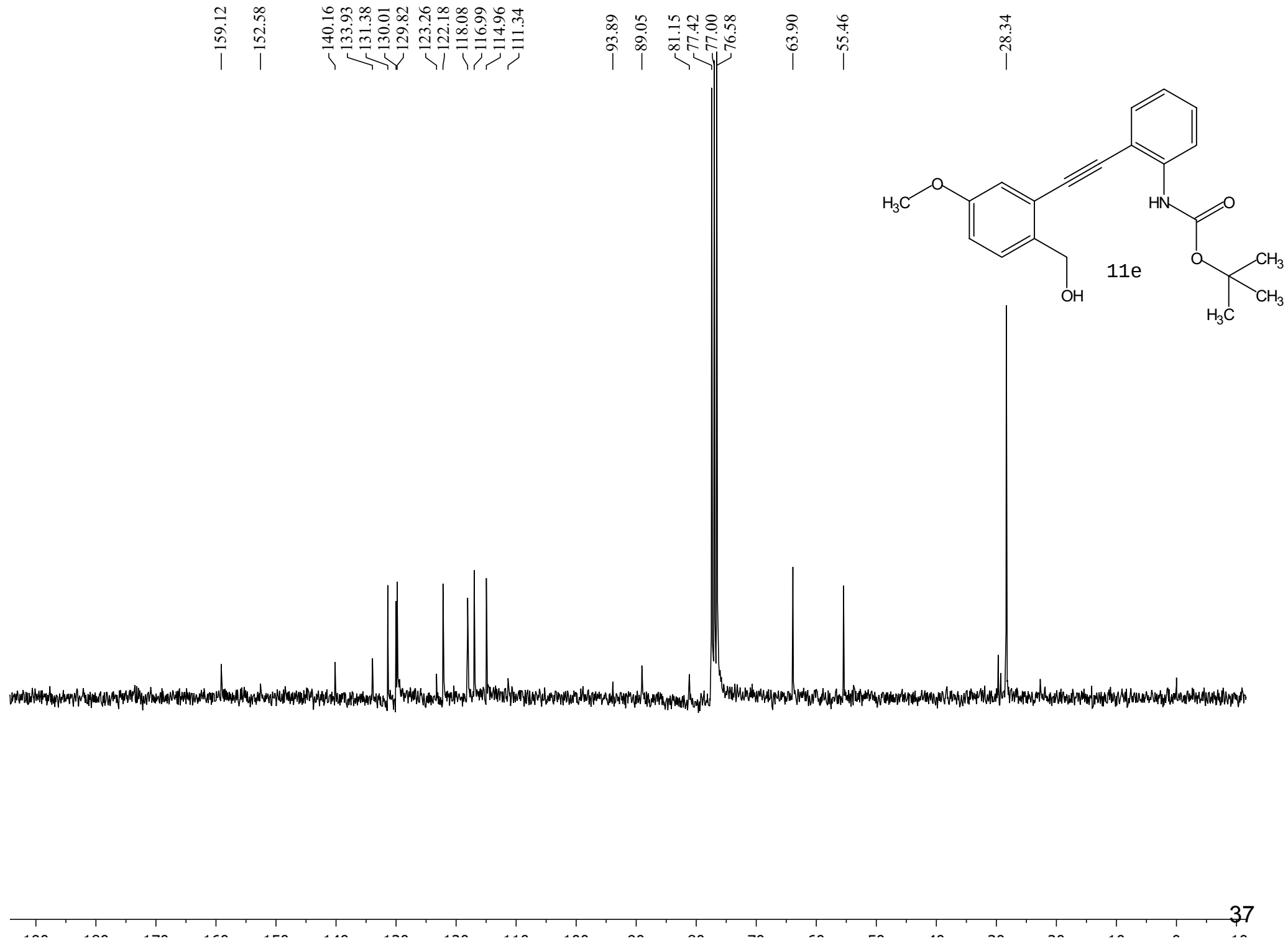


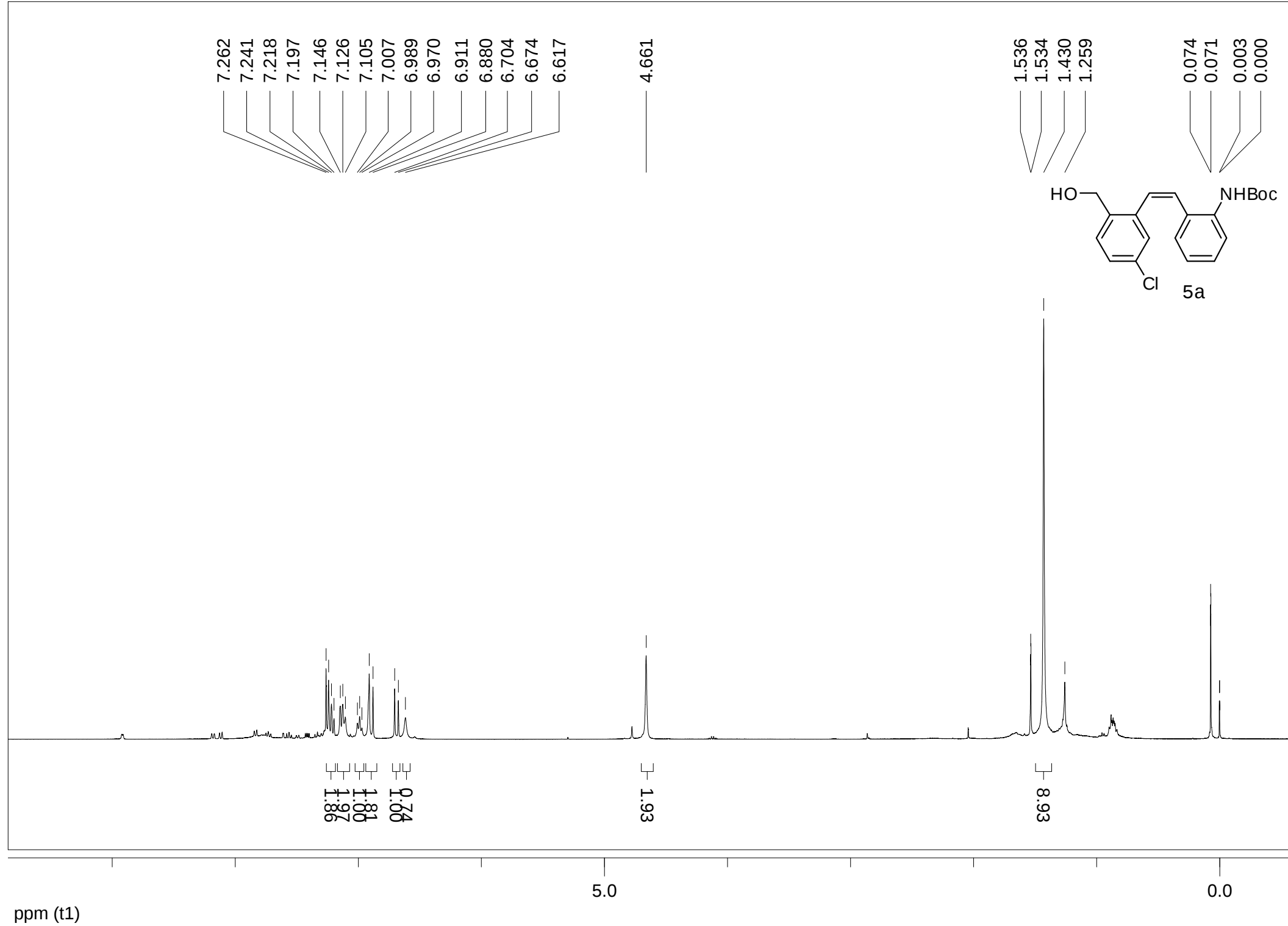


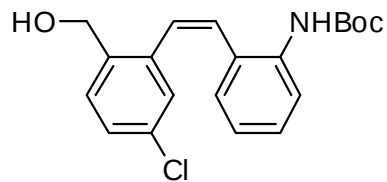




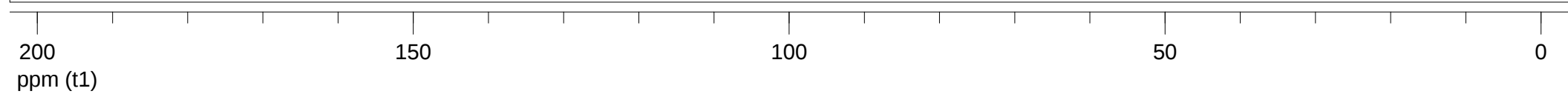
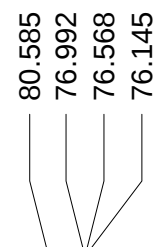
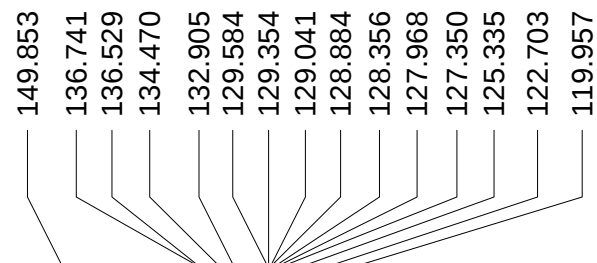


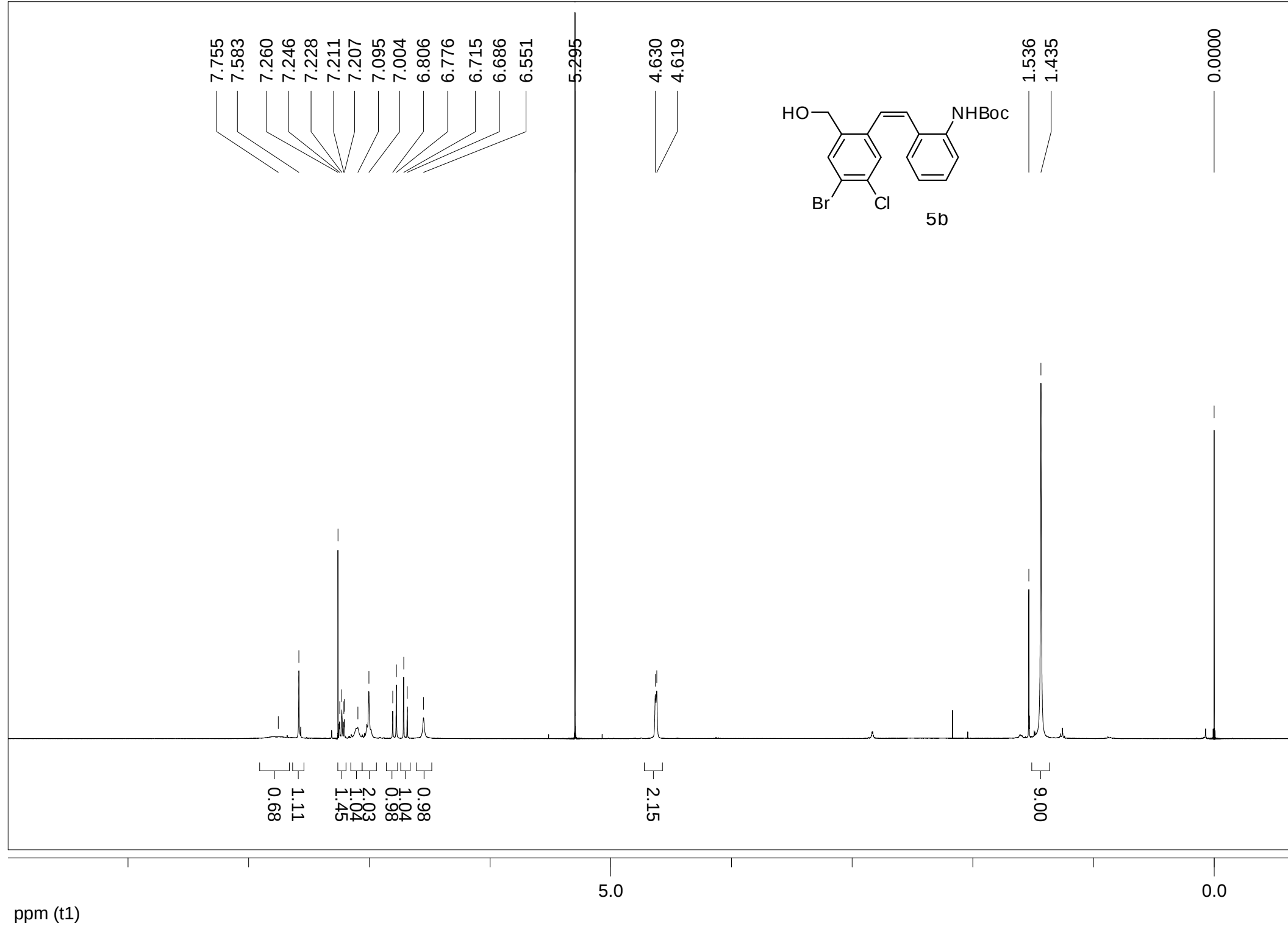




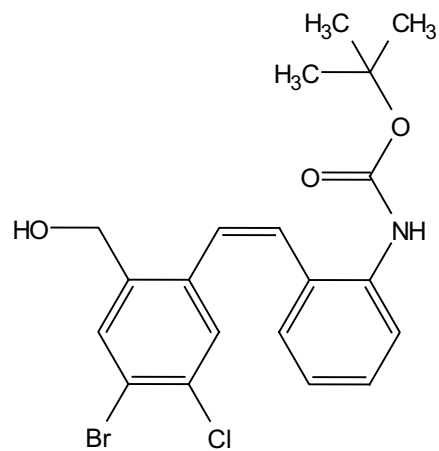


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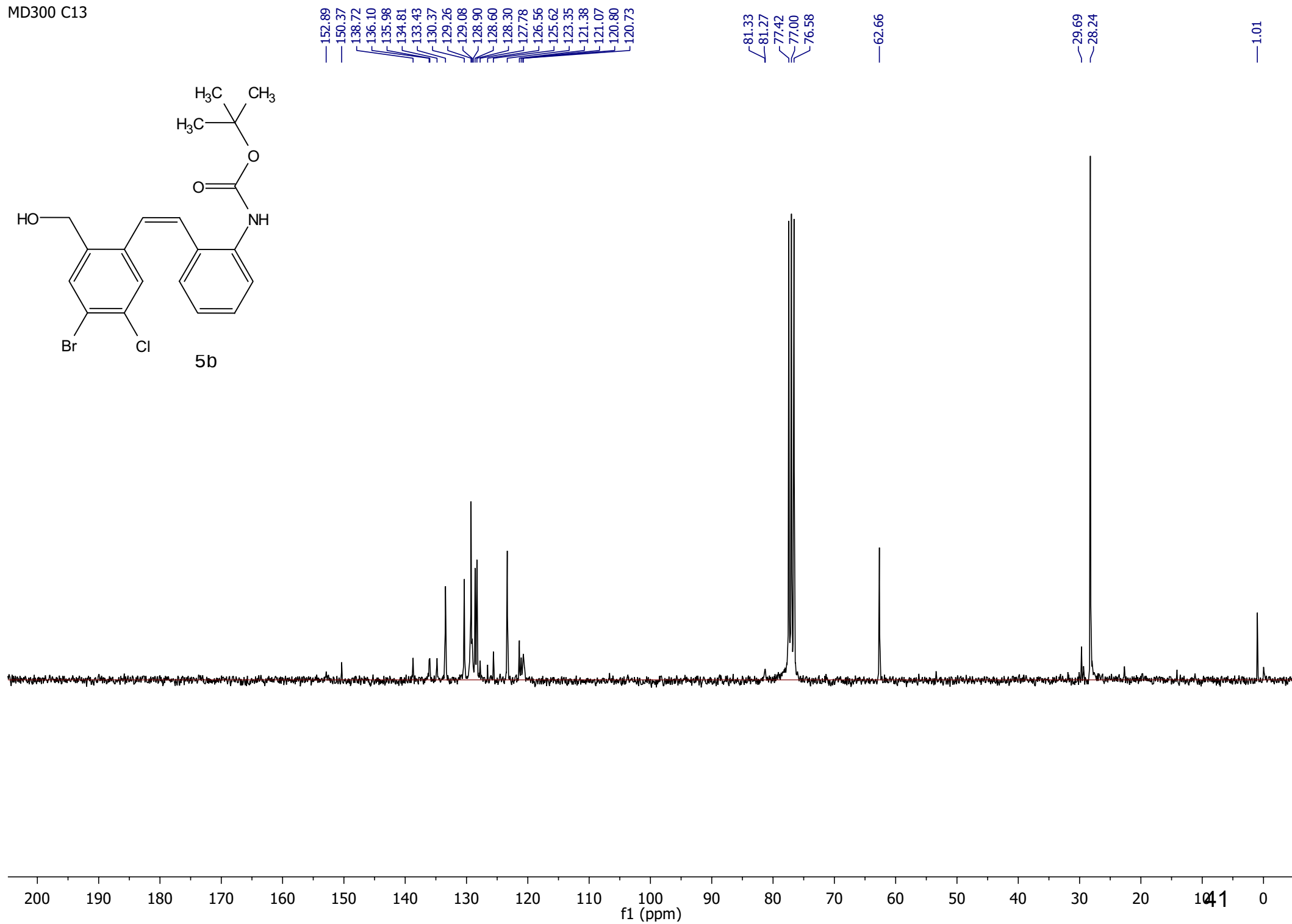


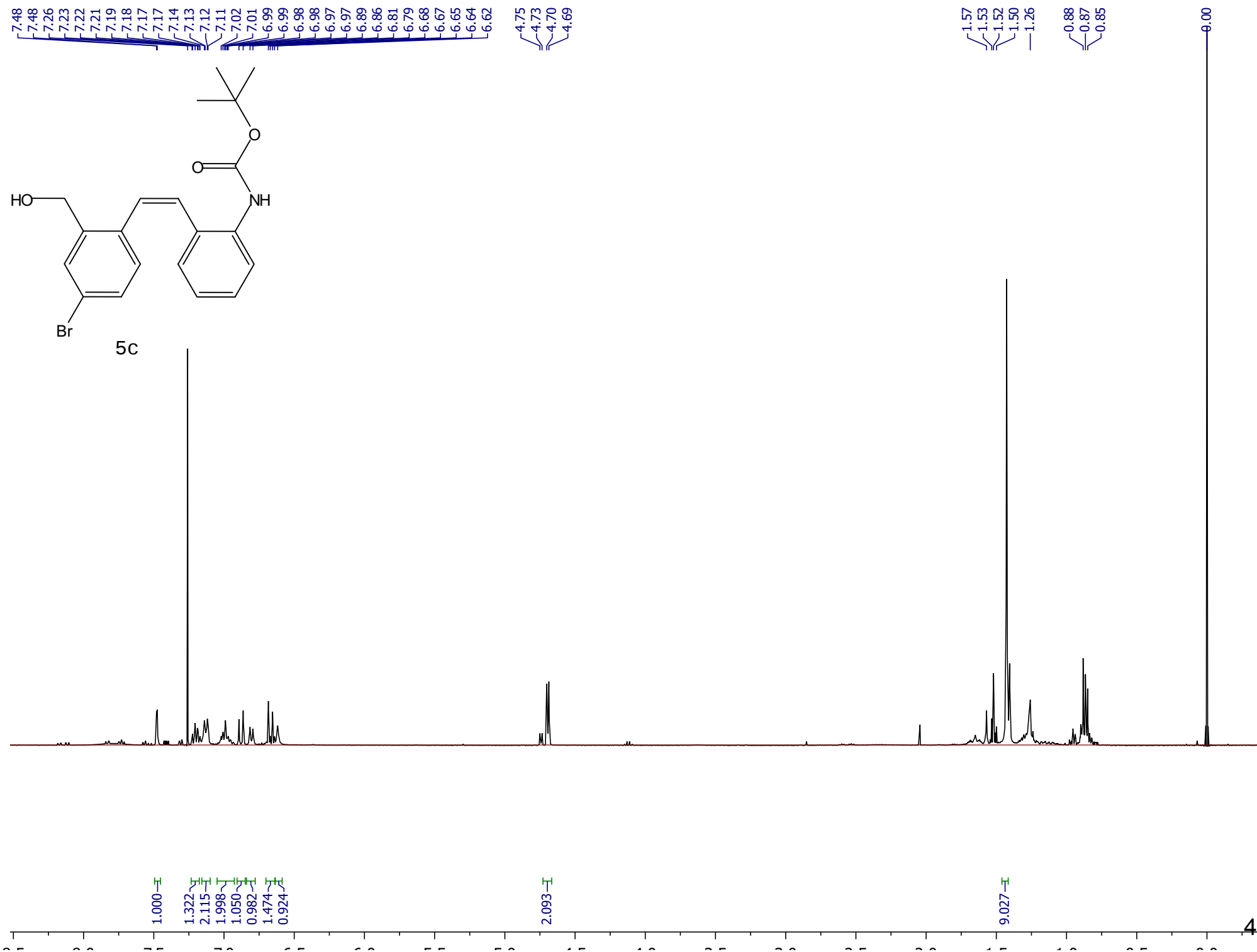


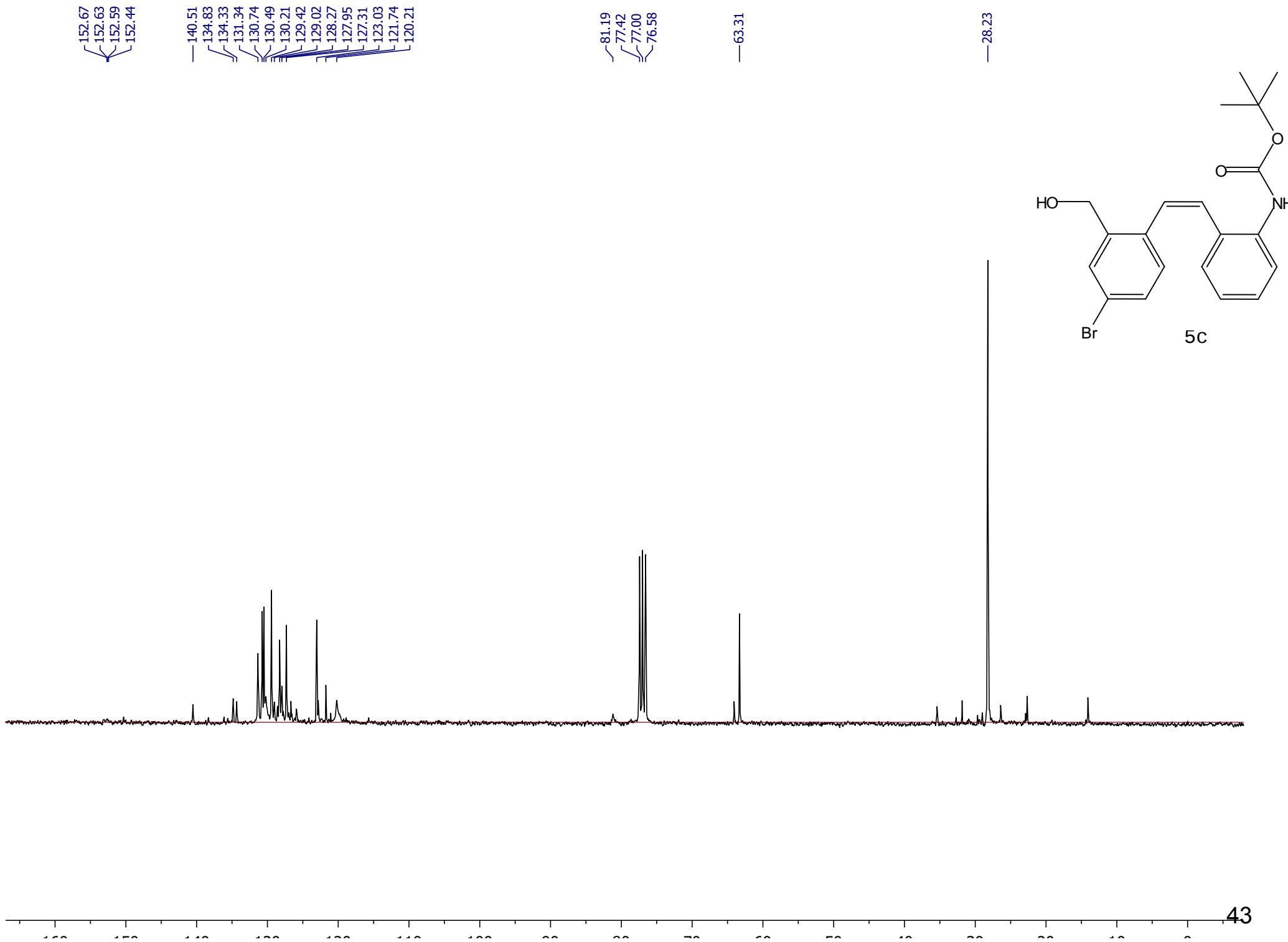
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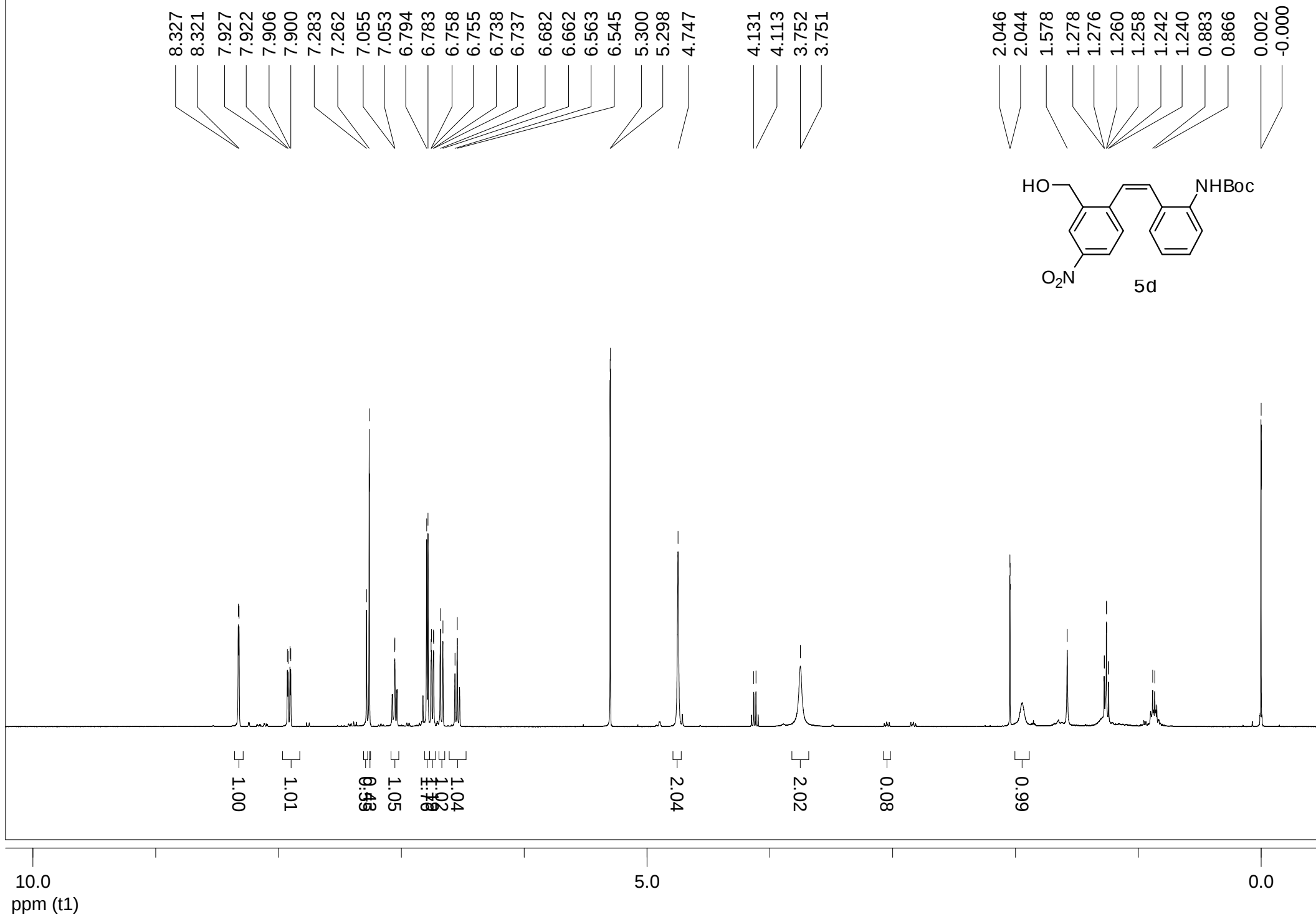


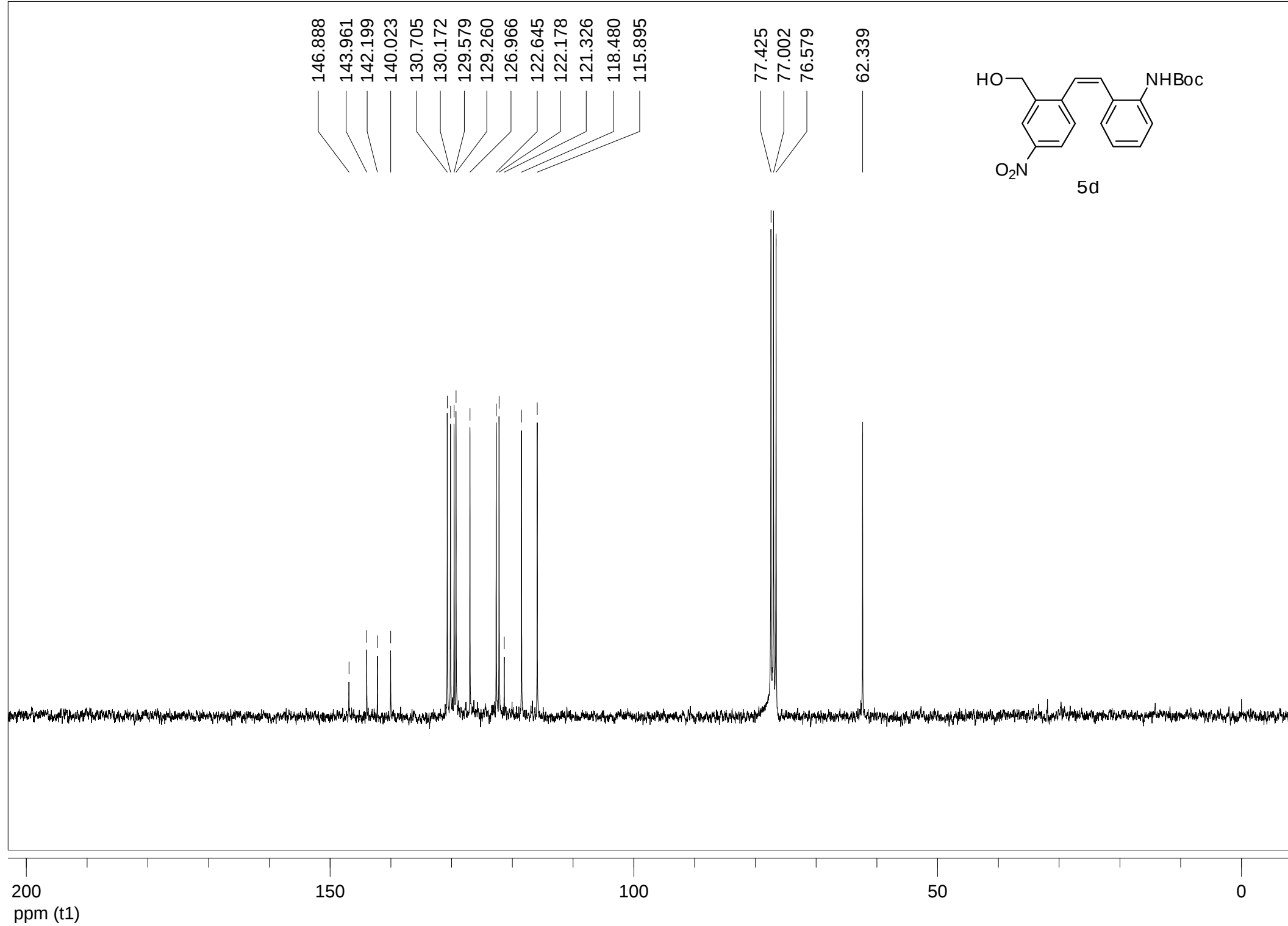
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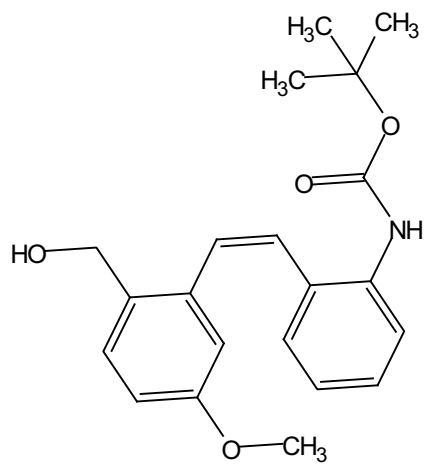




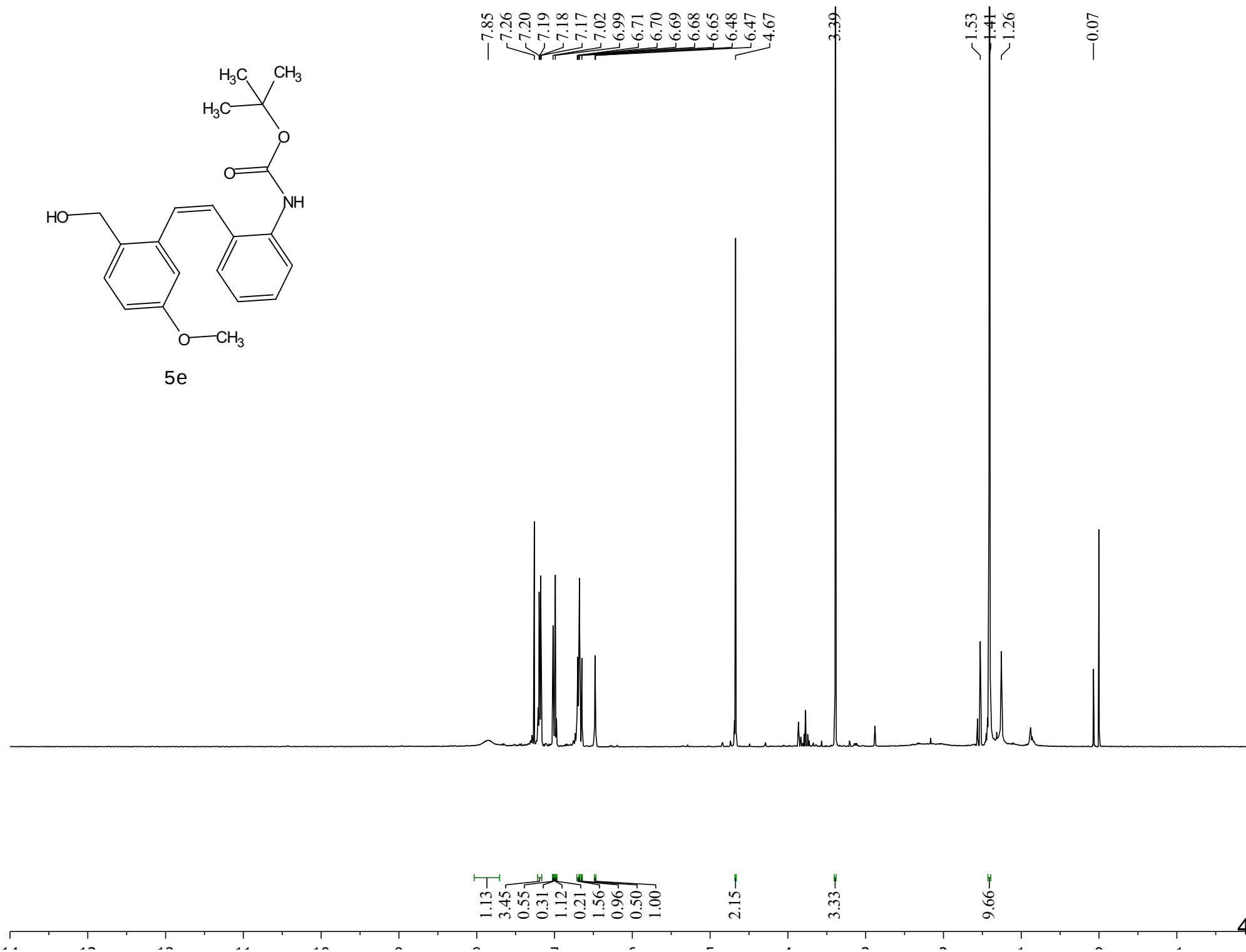


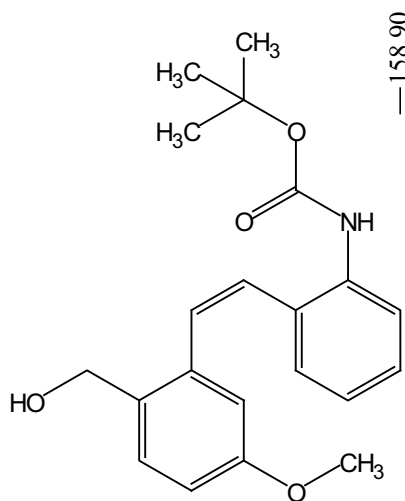






5e





5e

— 158.90

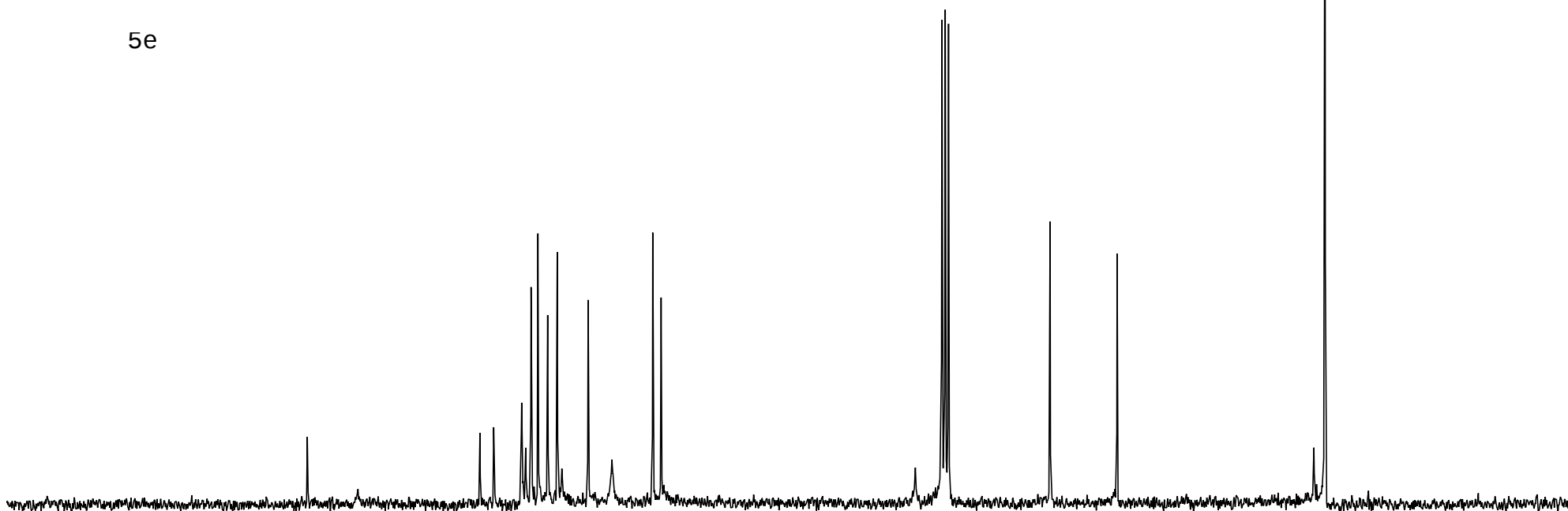
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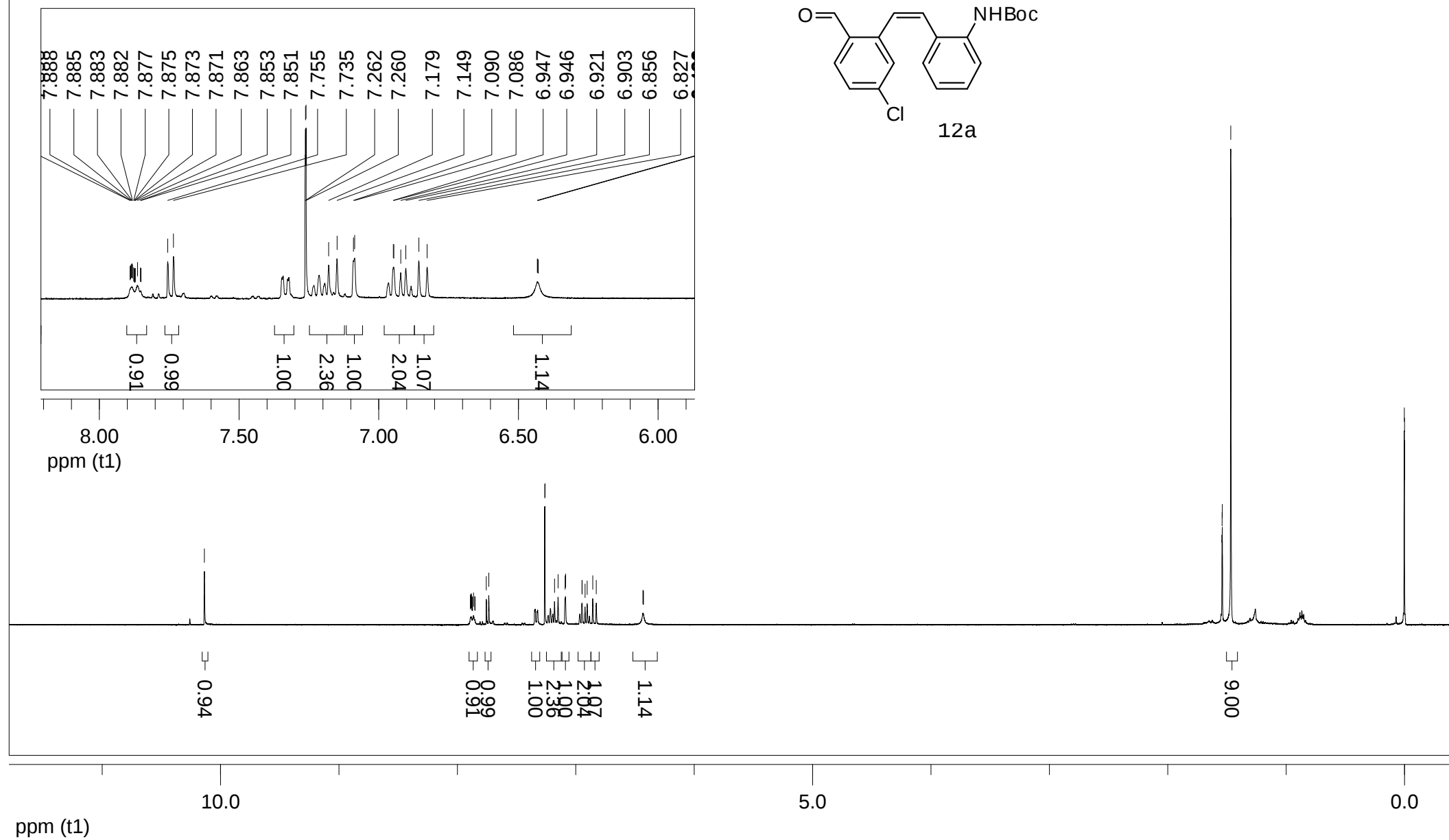
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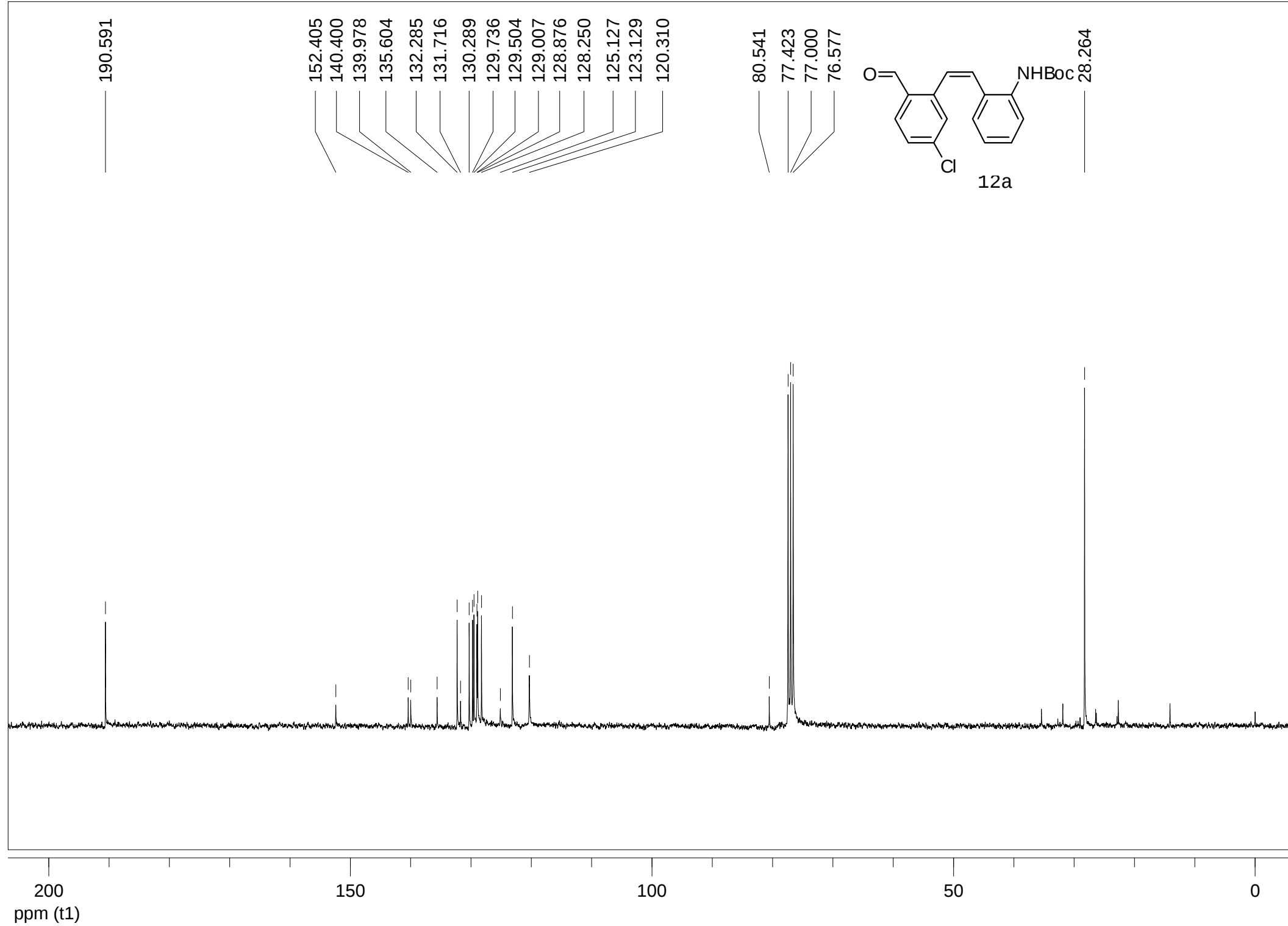
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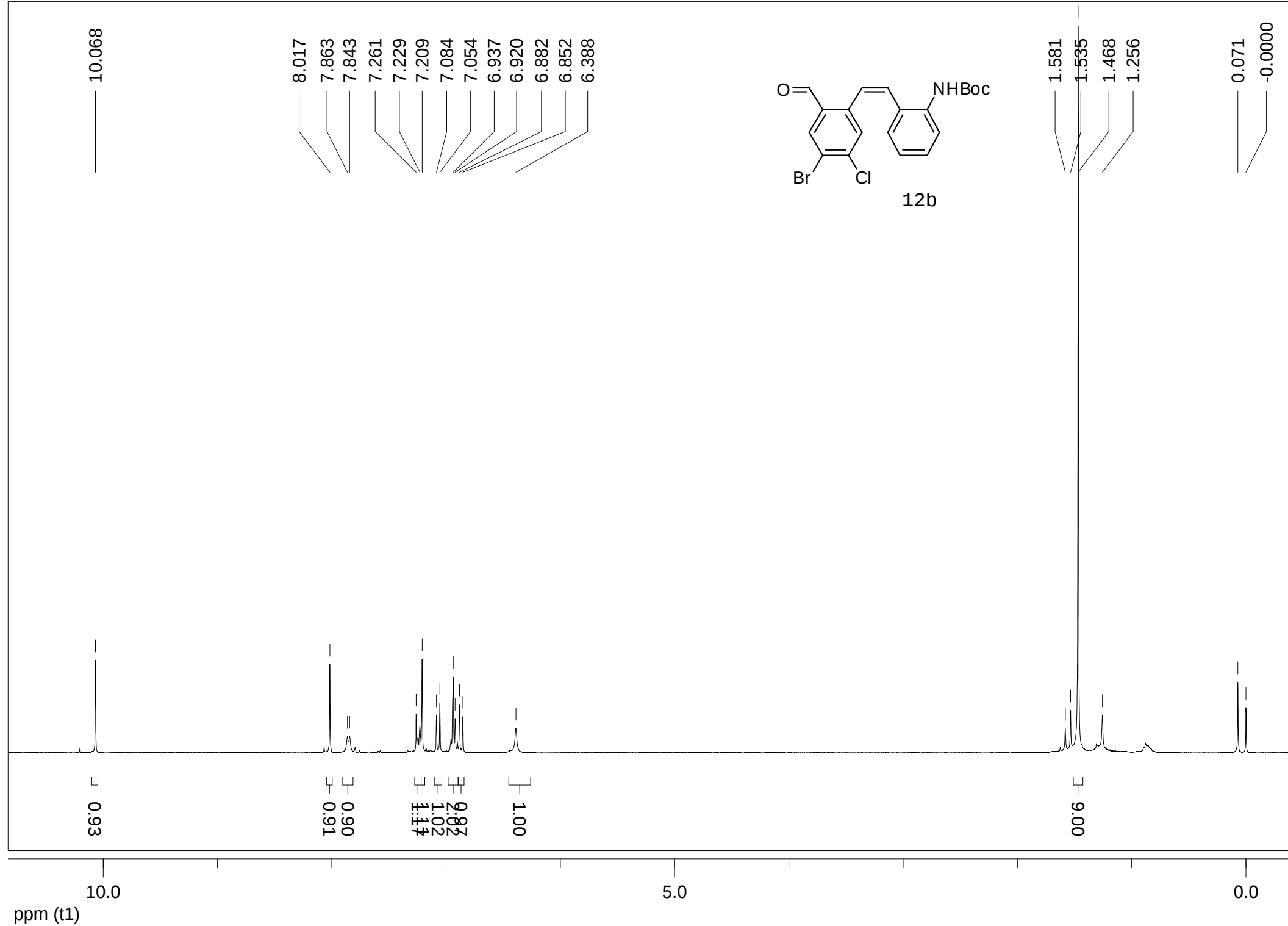
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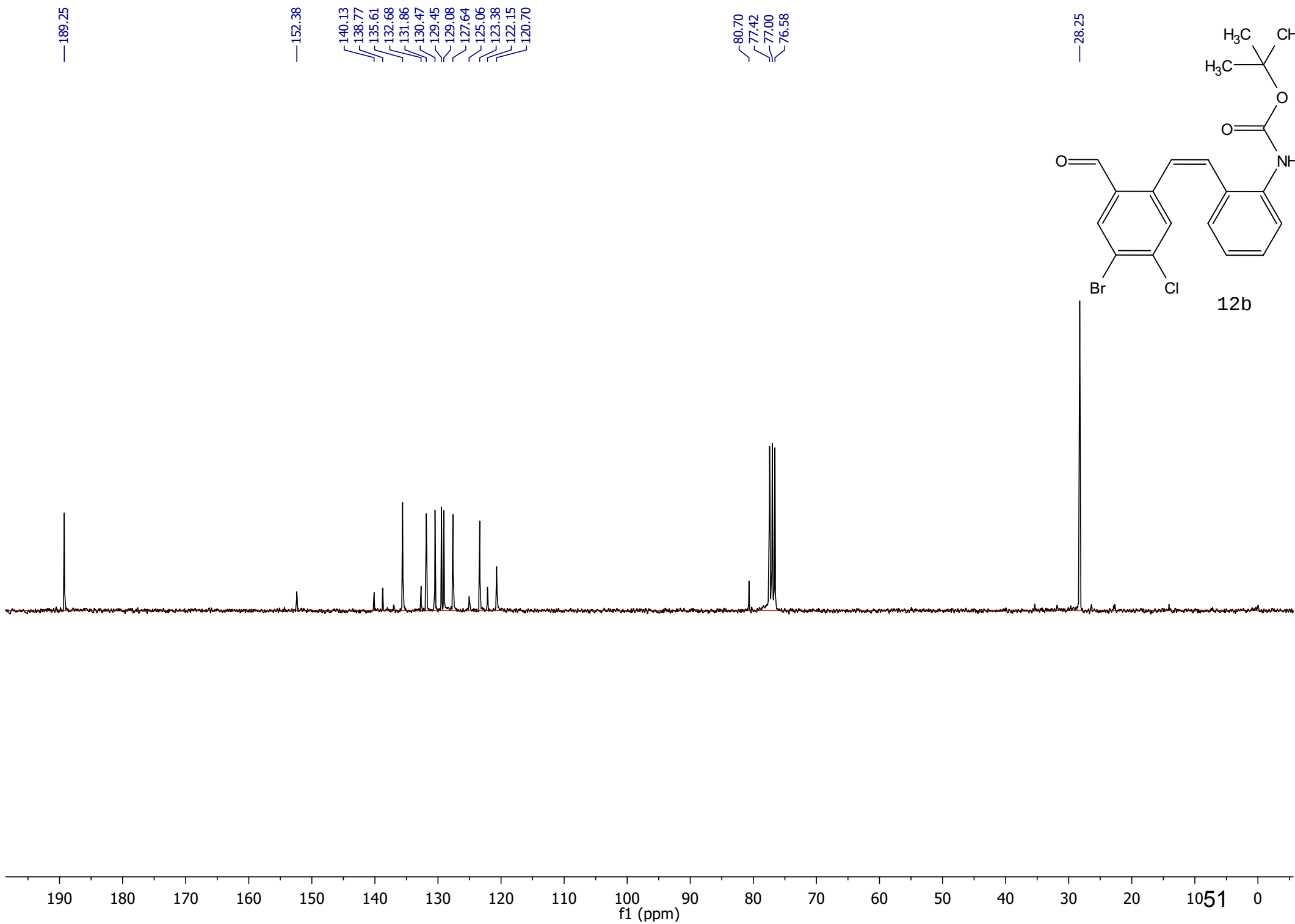
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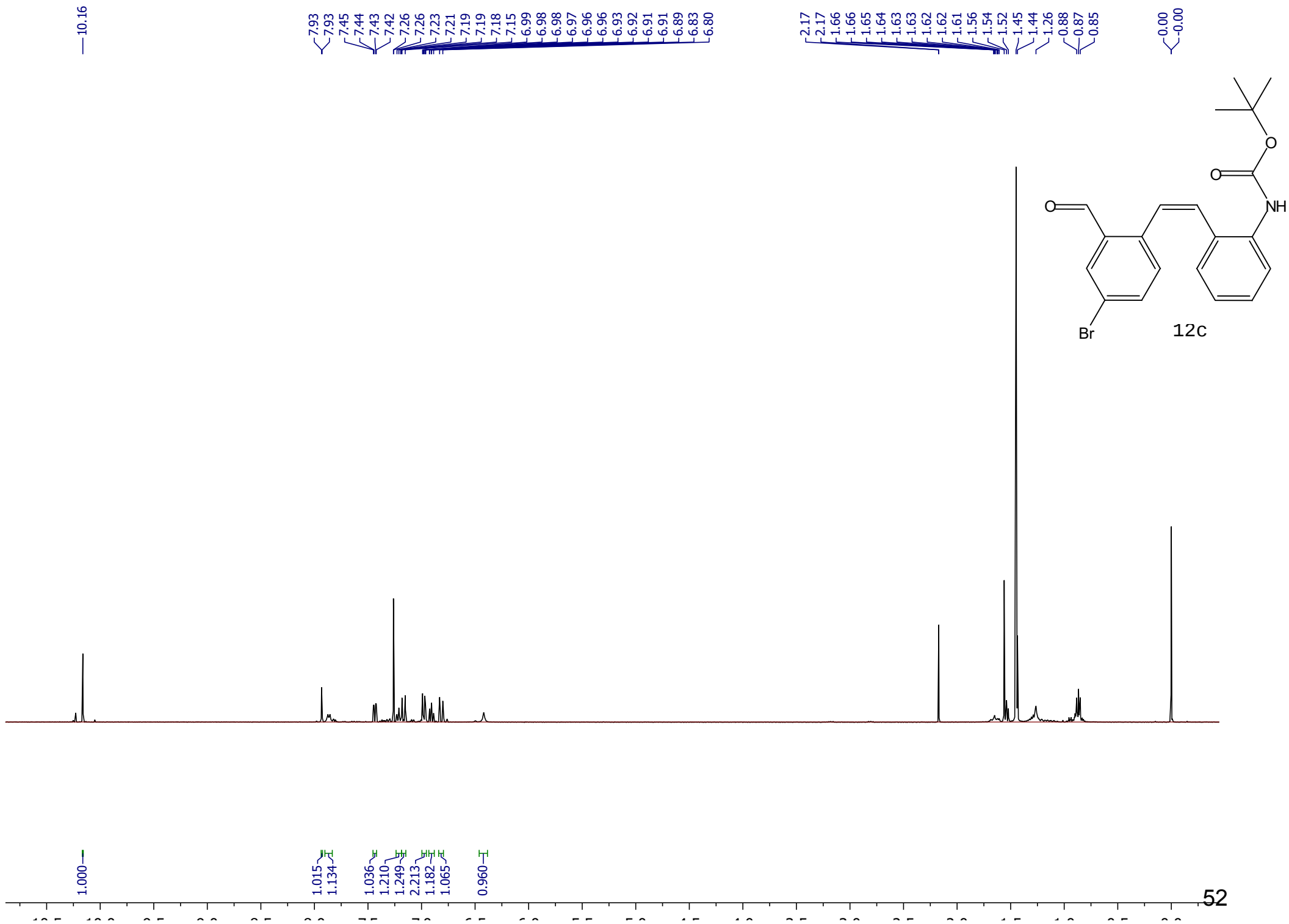


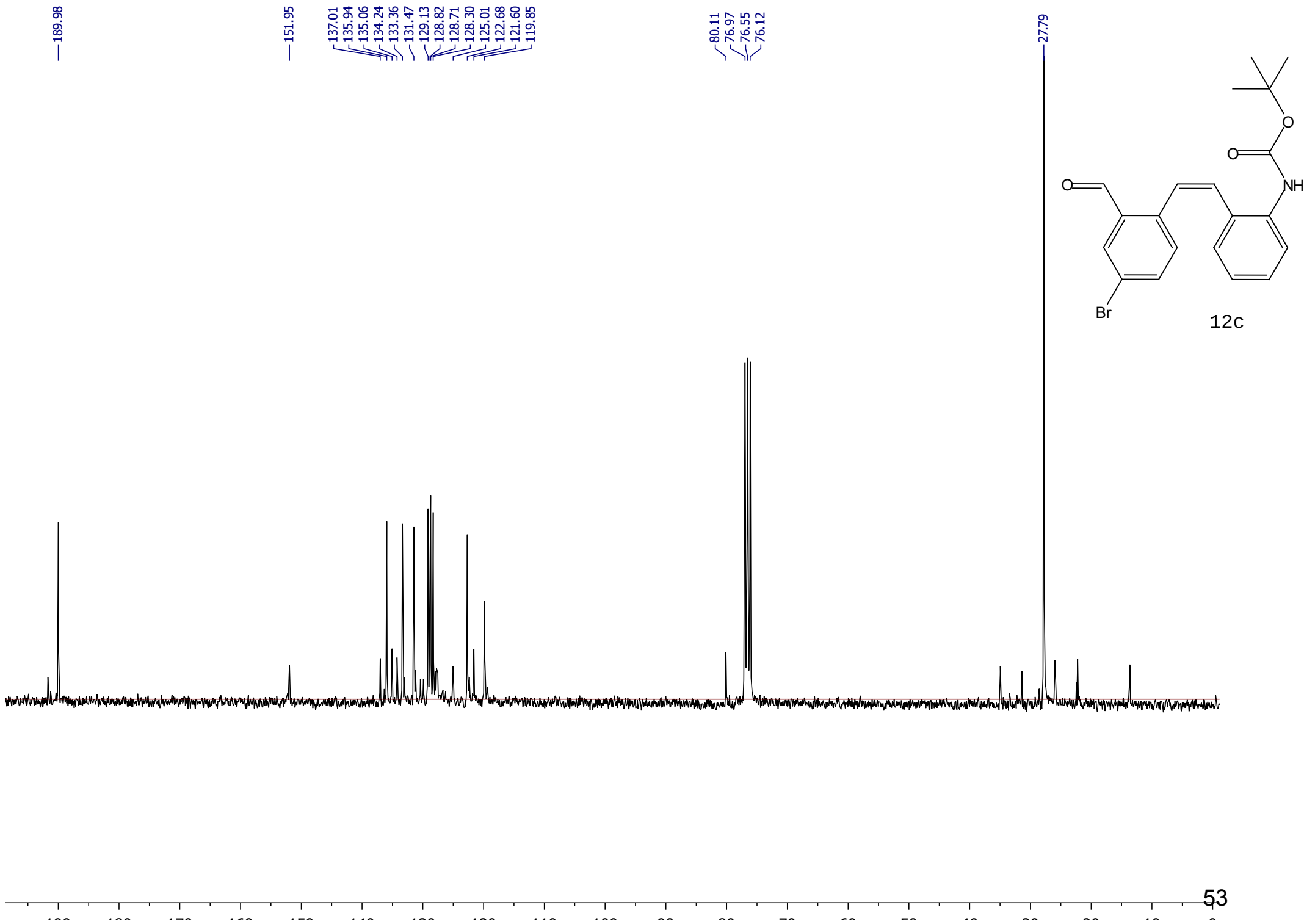


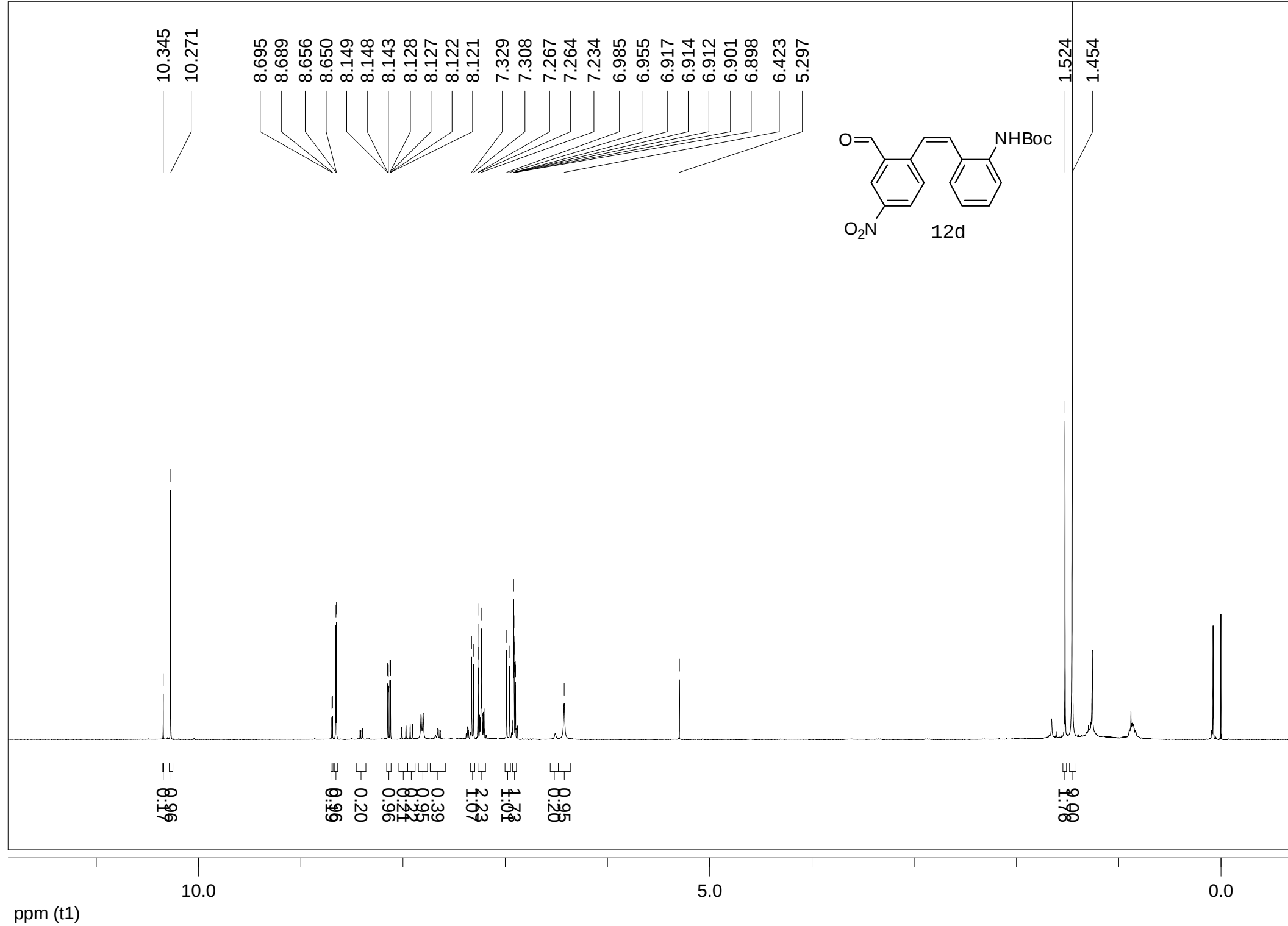


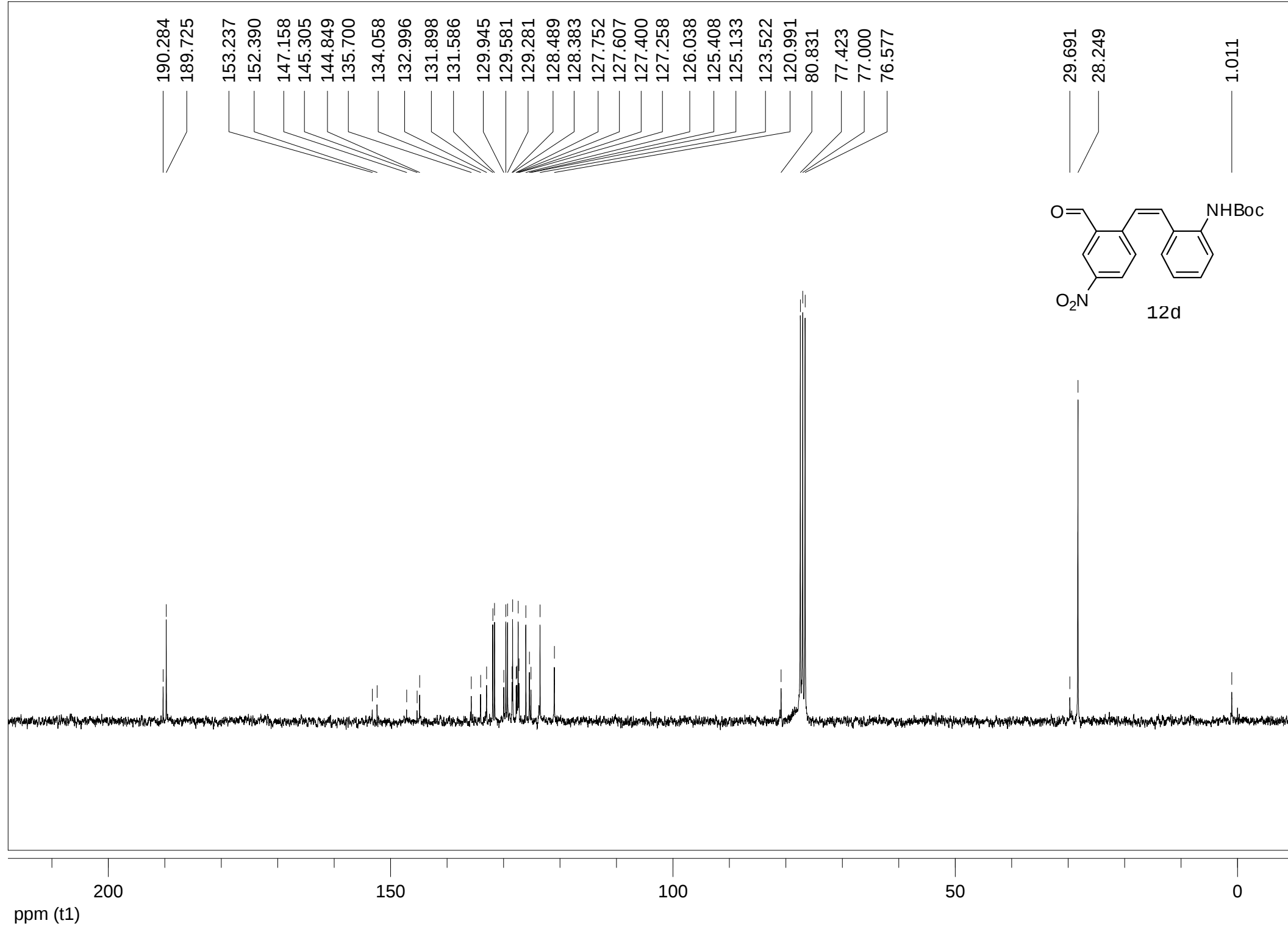


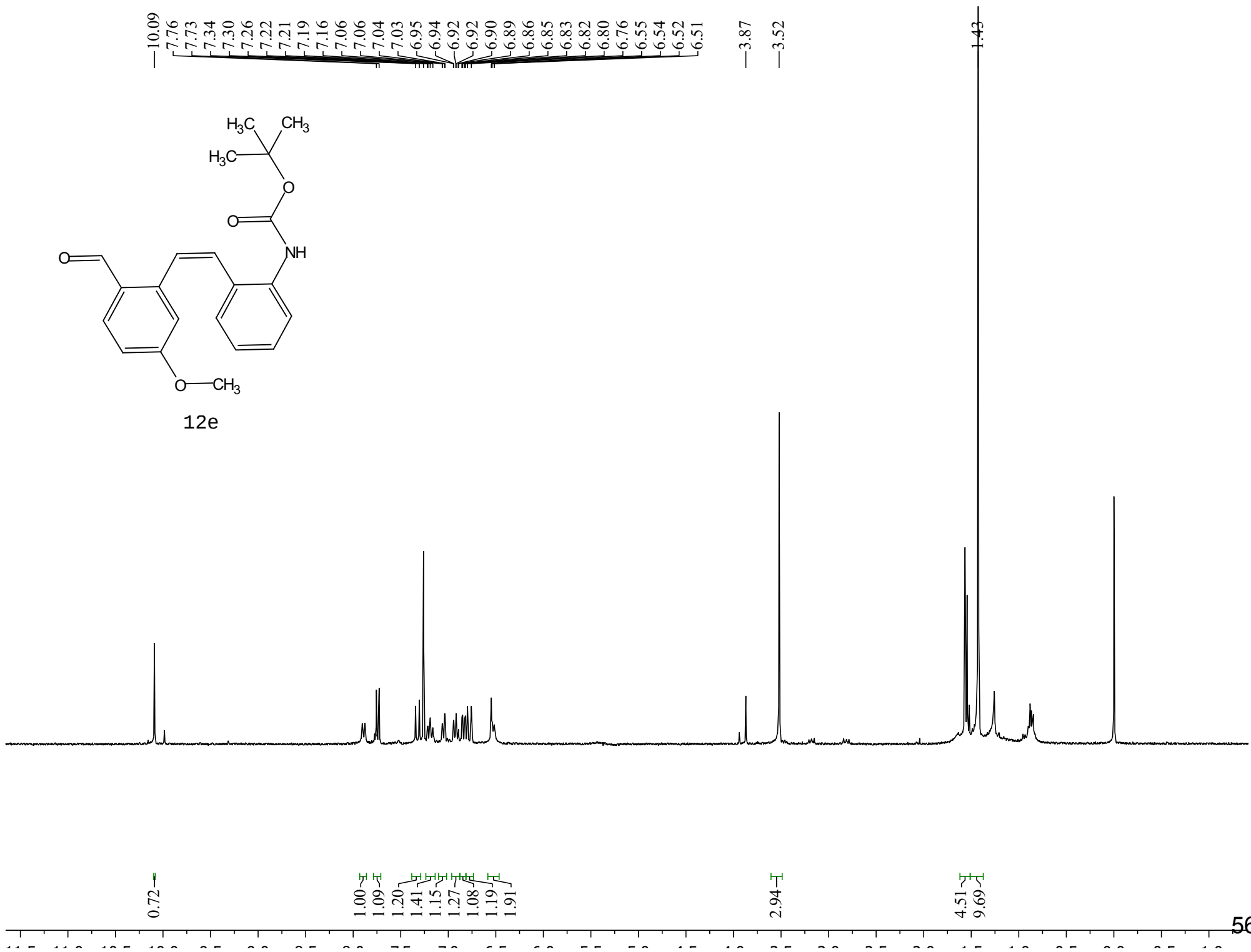


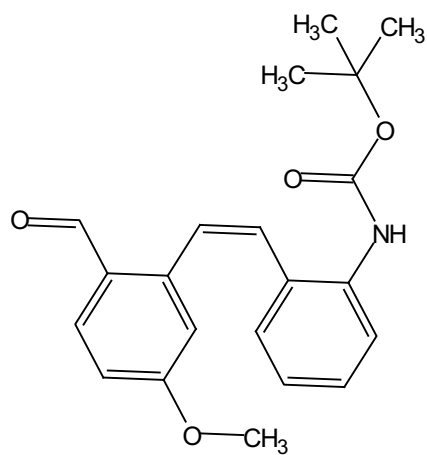












12e

—190.51

—163.19

—152.38

140.60

135.38

134.03

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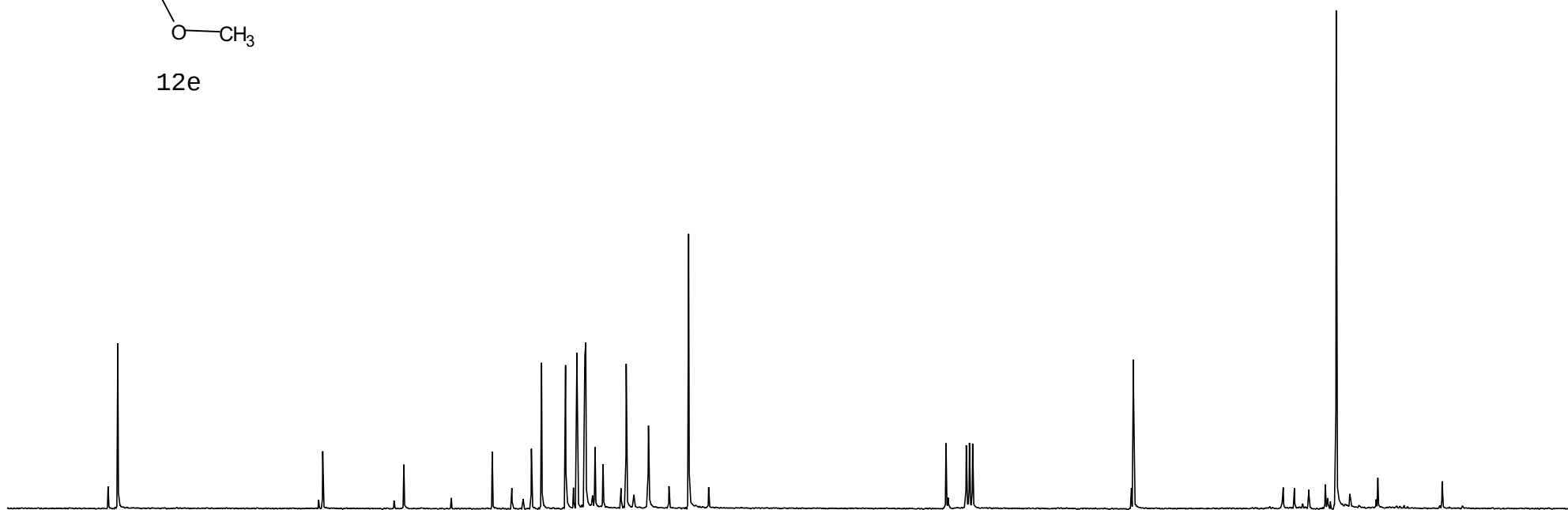
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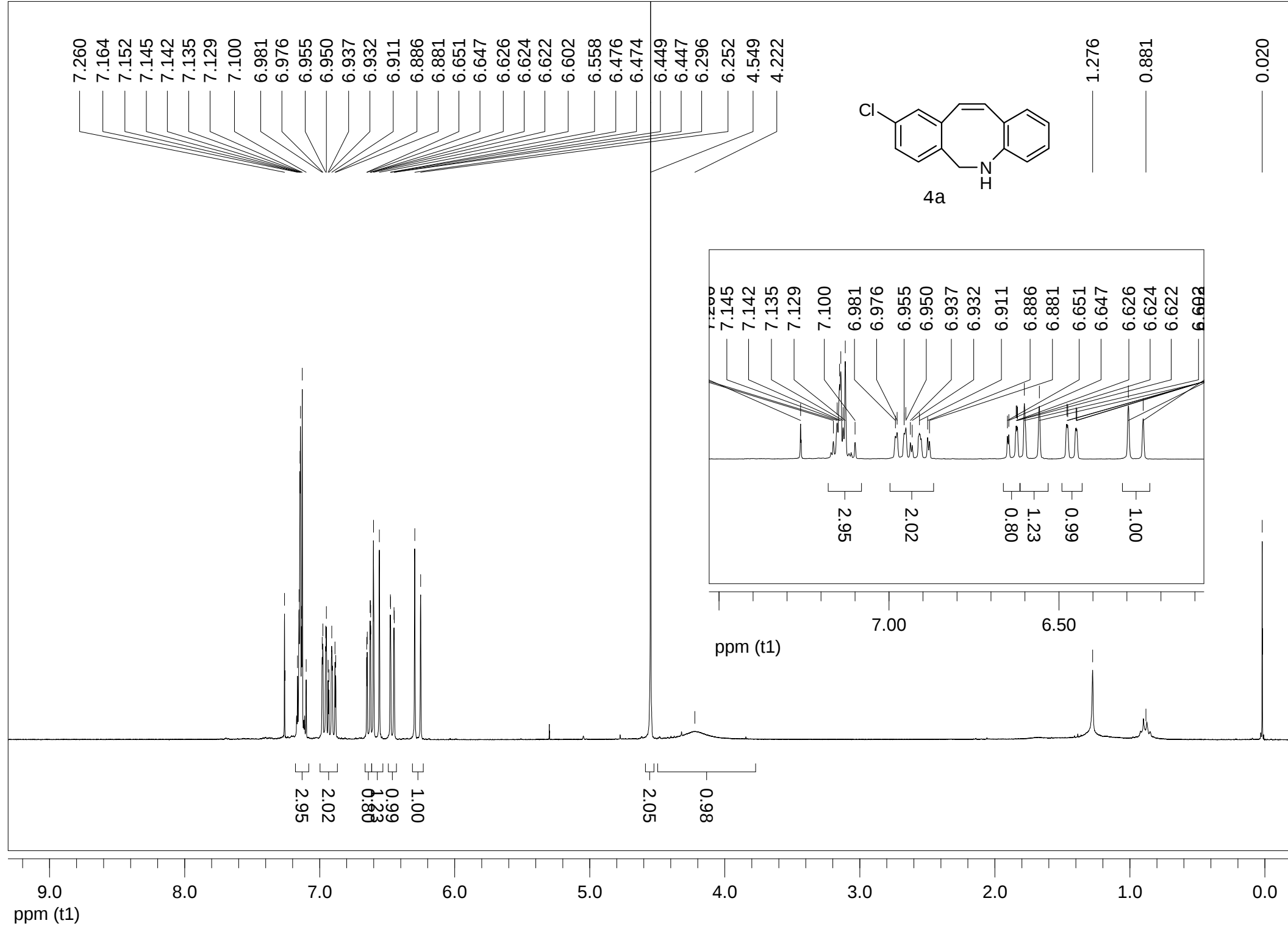
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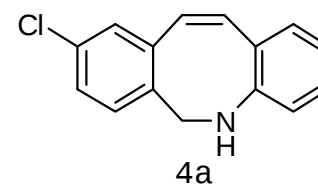
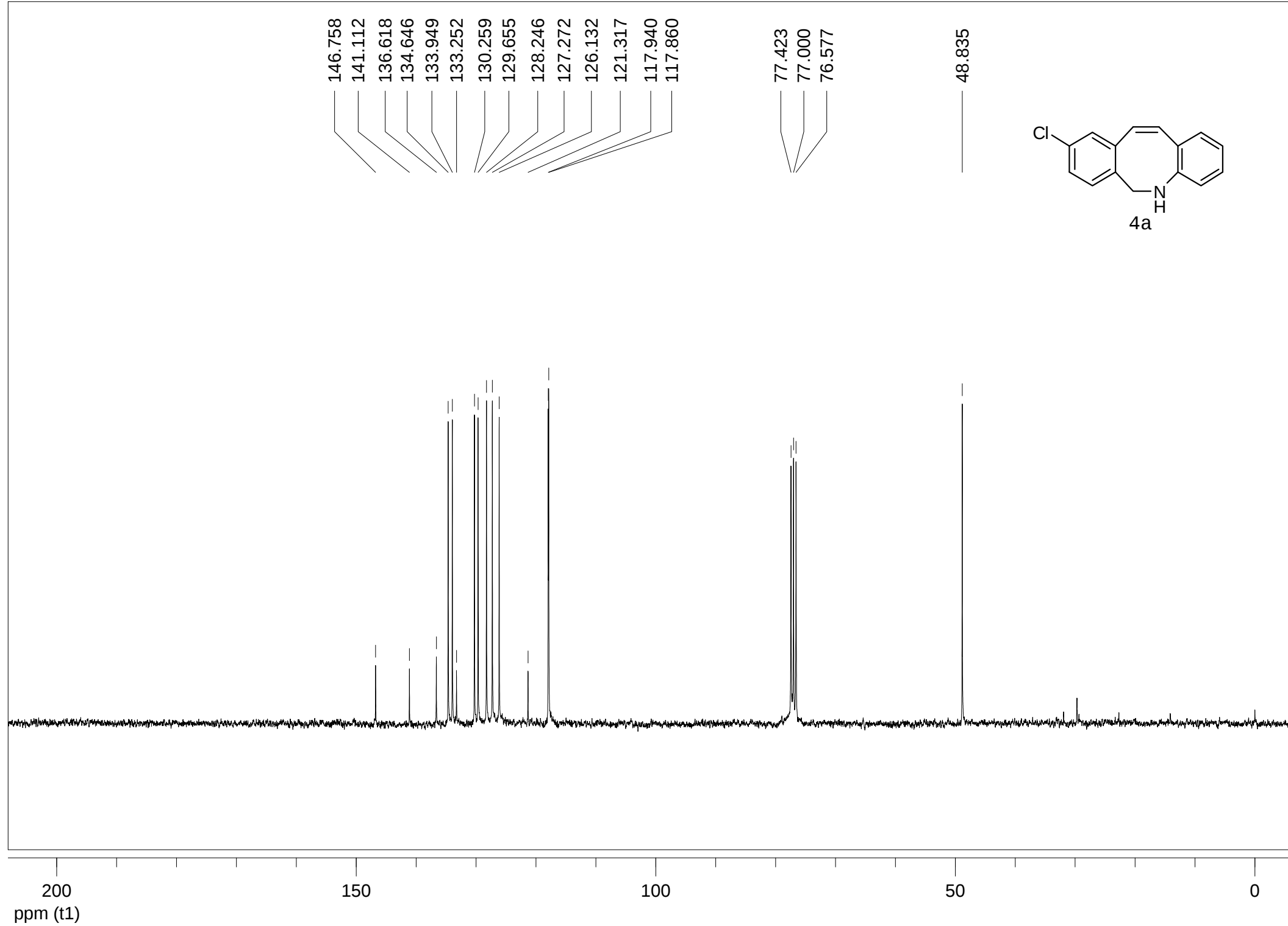
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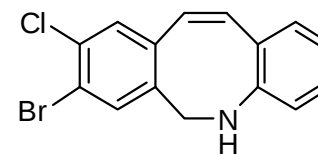
—55.14

—28.12









4b

0.000

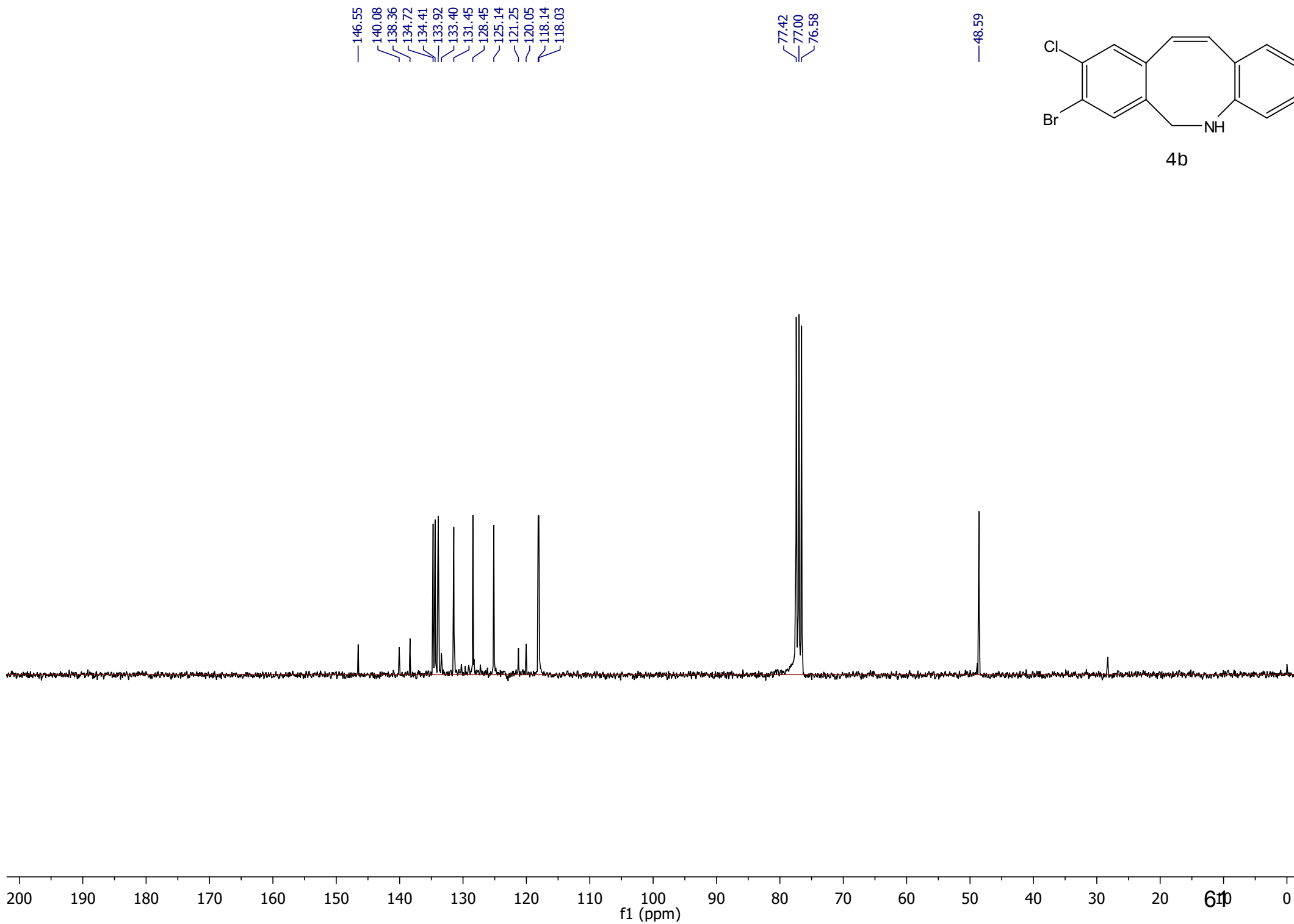
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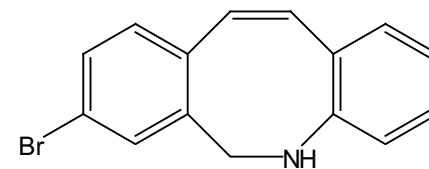
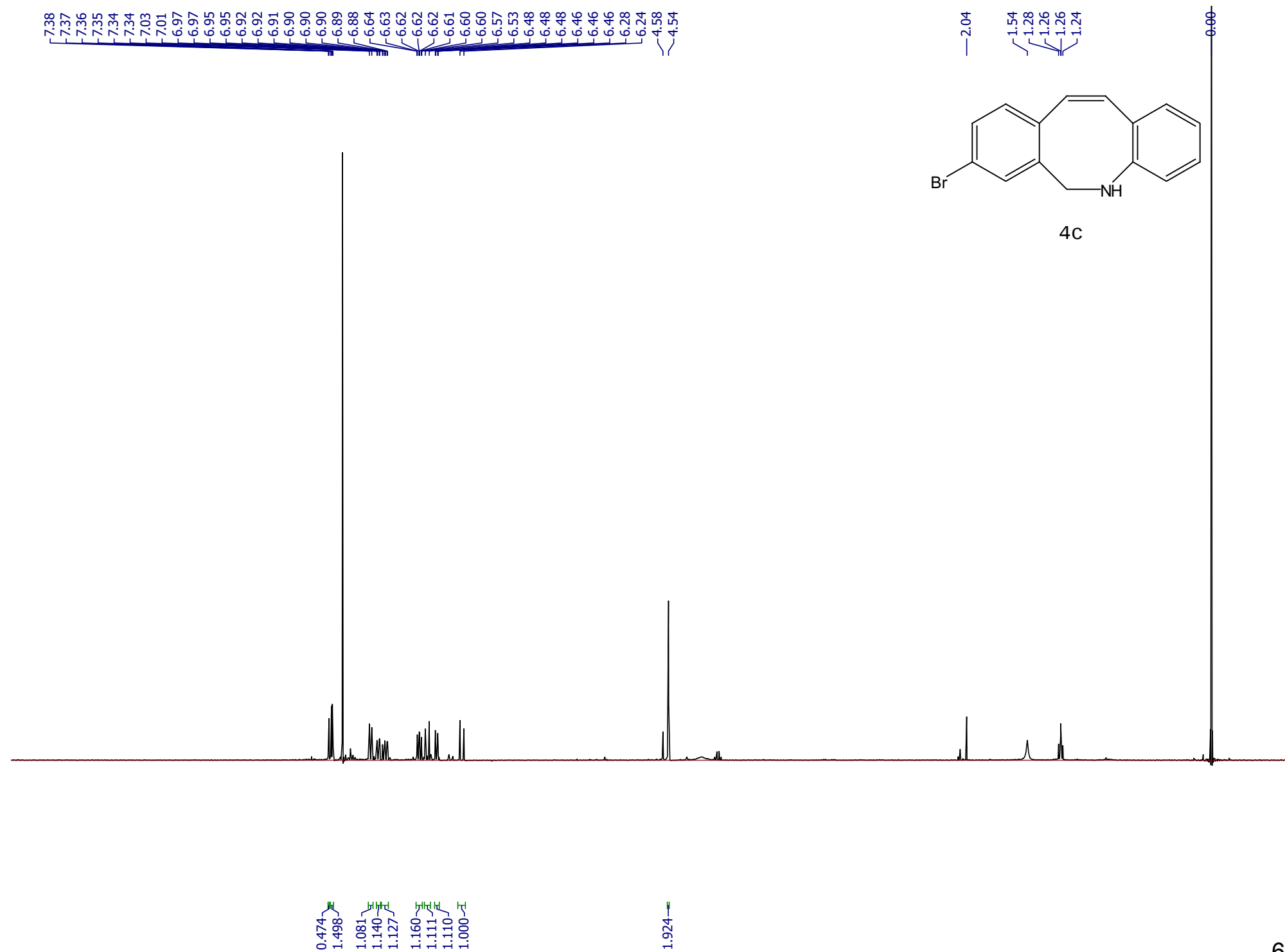
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ppm (t1)

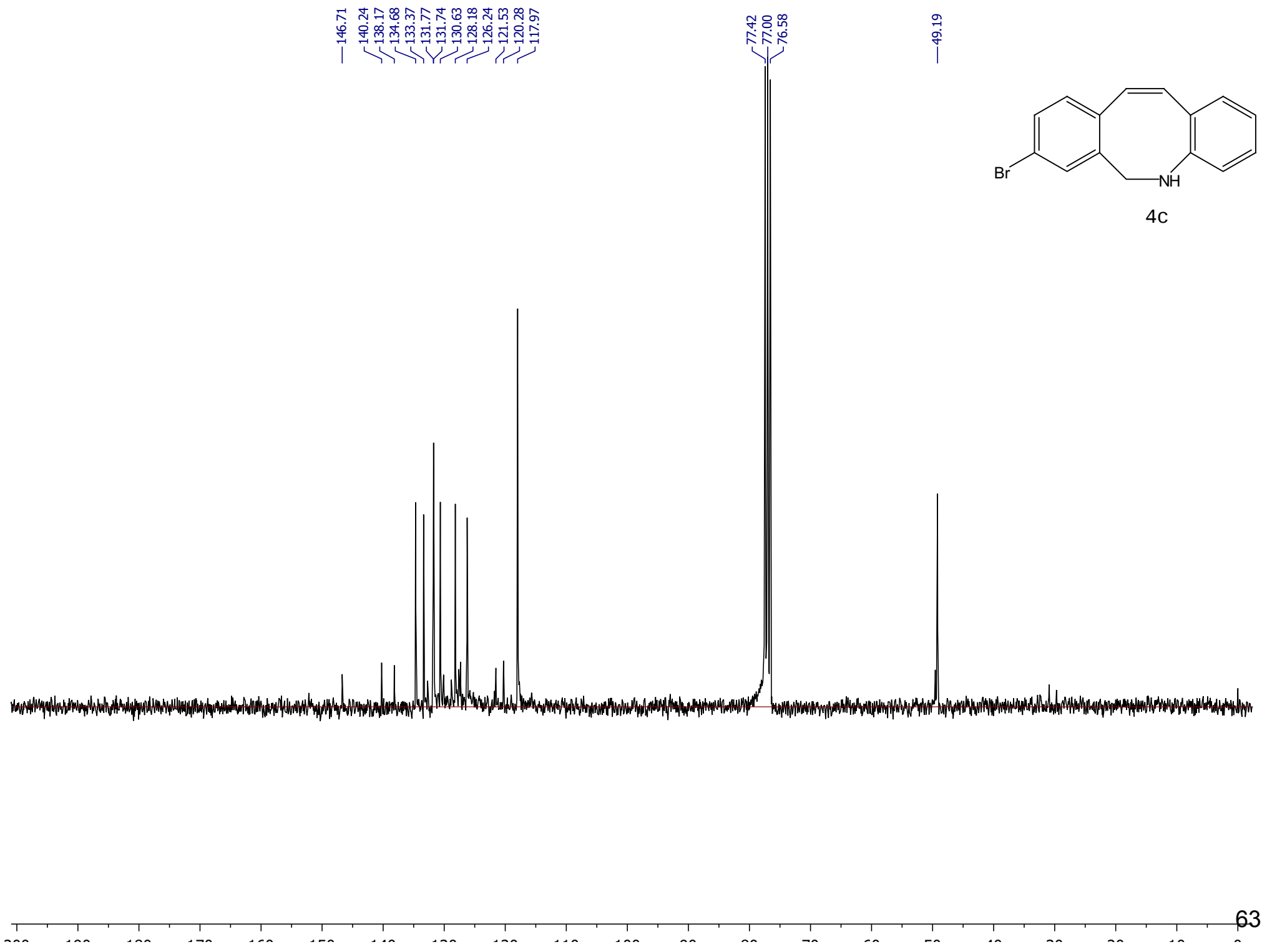
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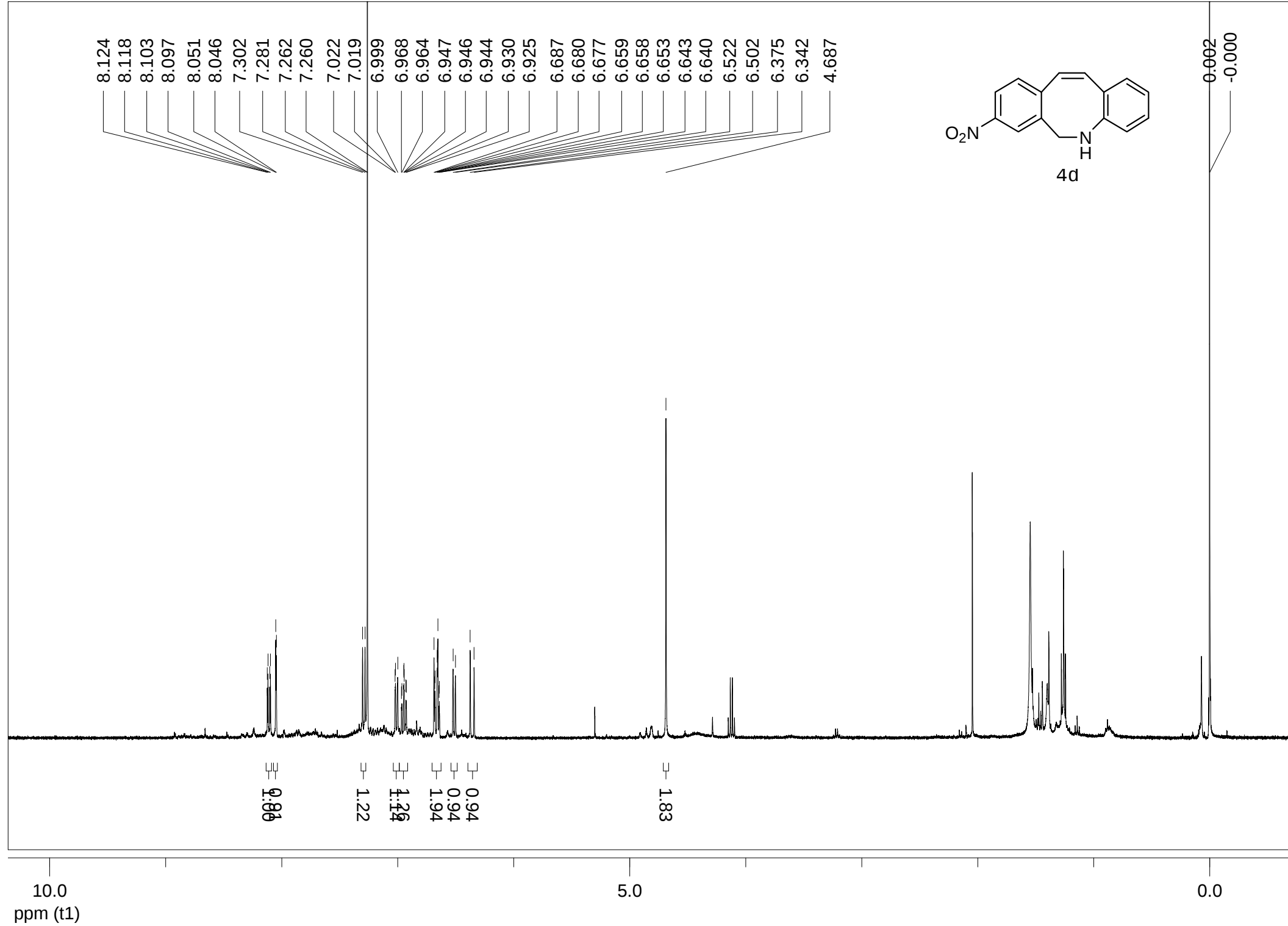
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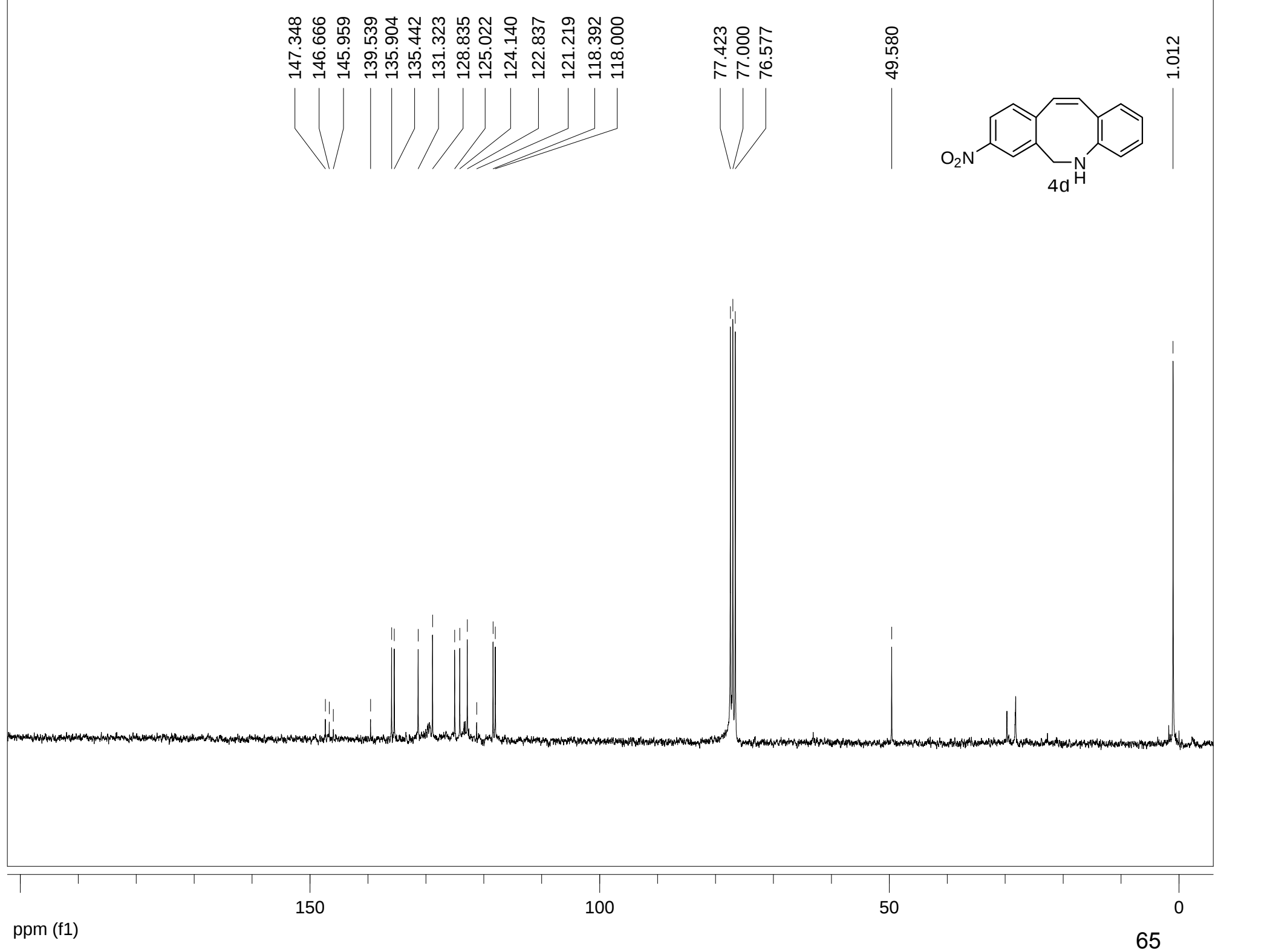


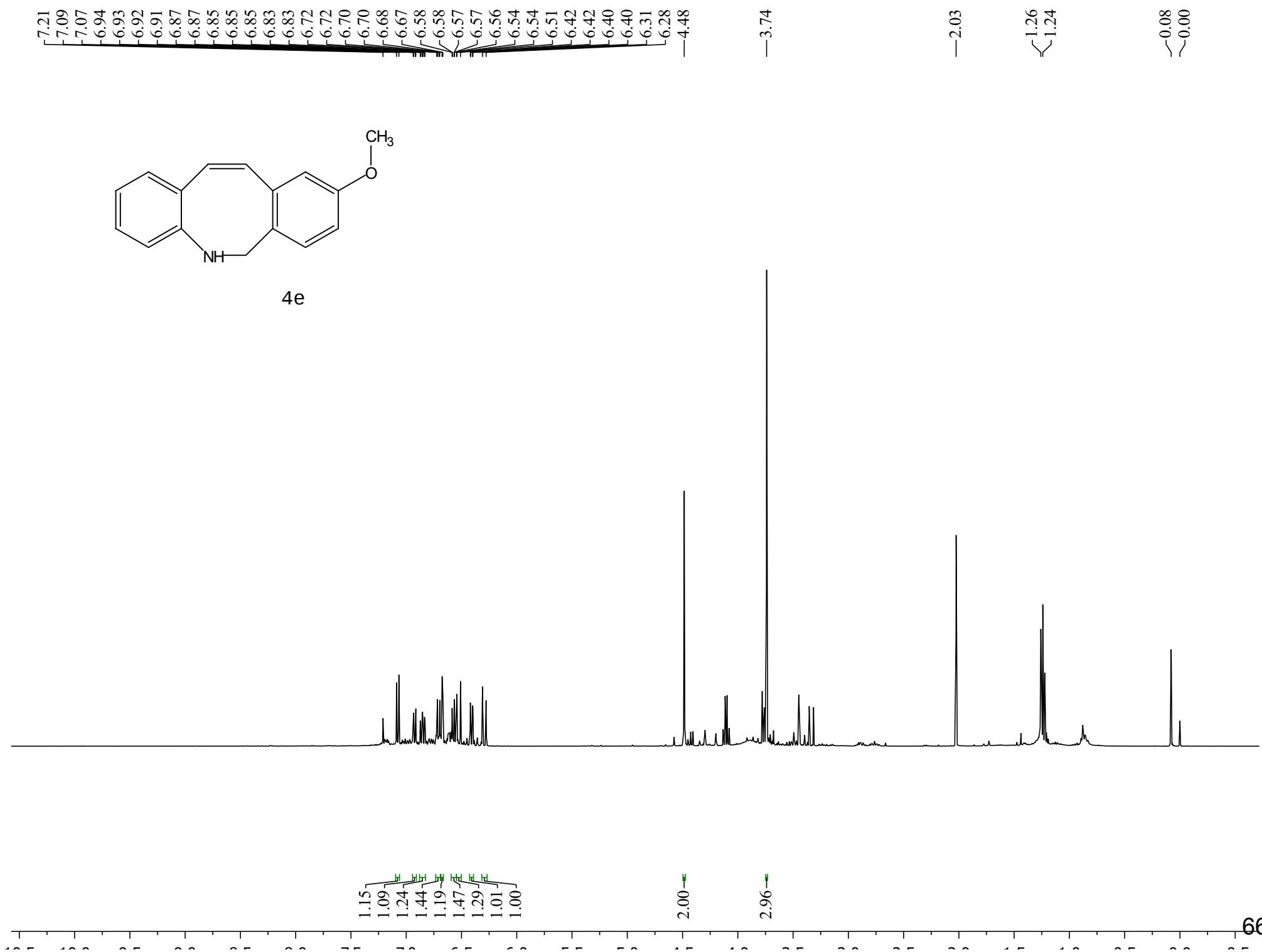


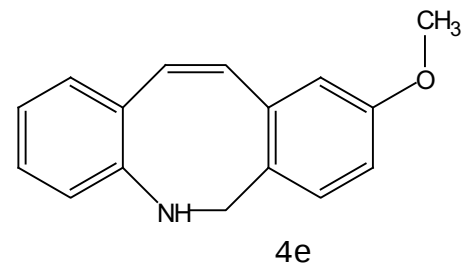
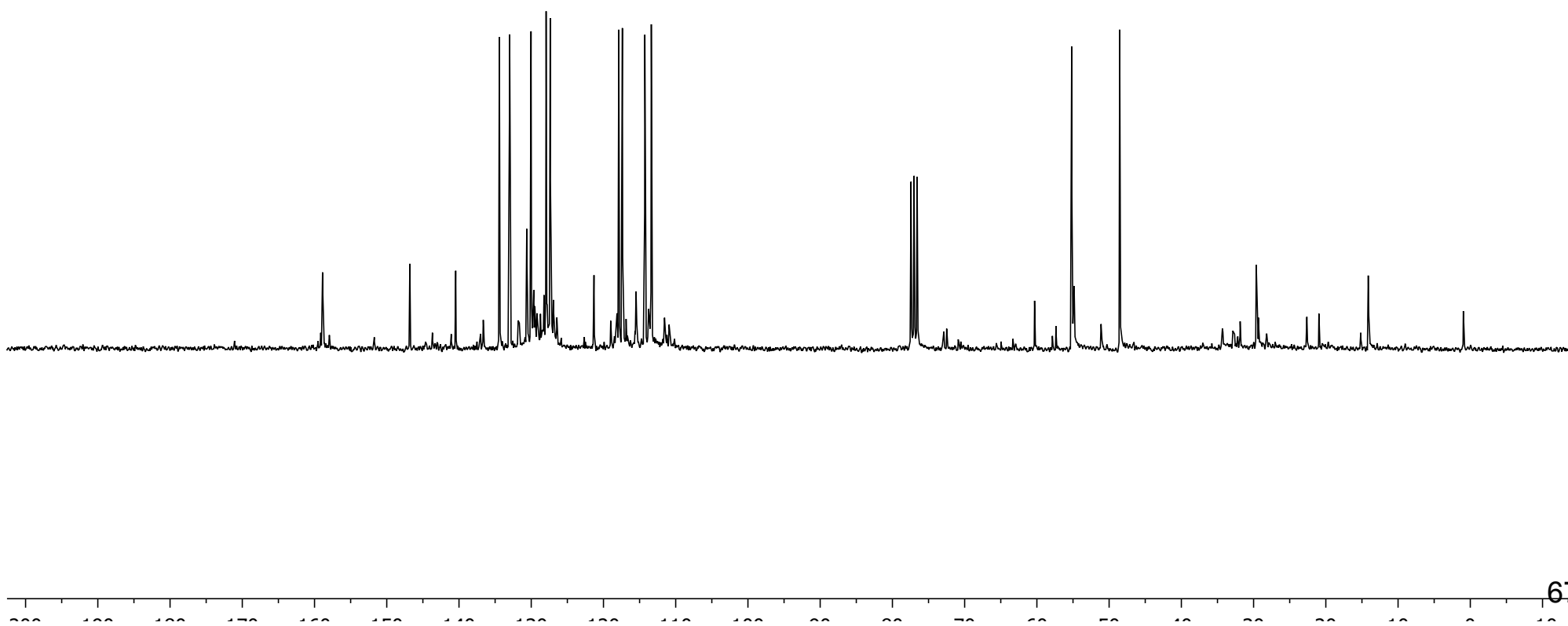
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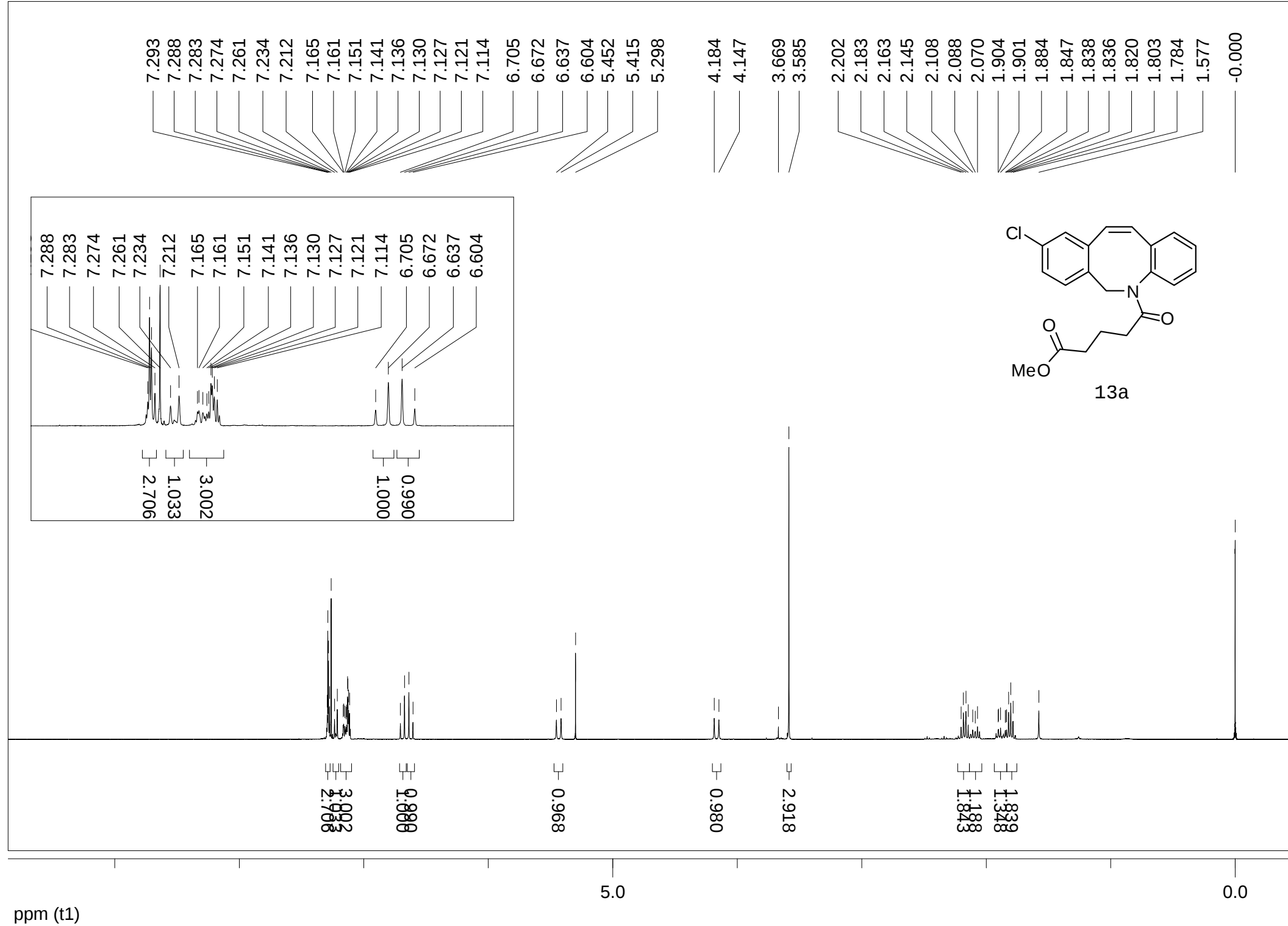


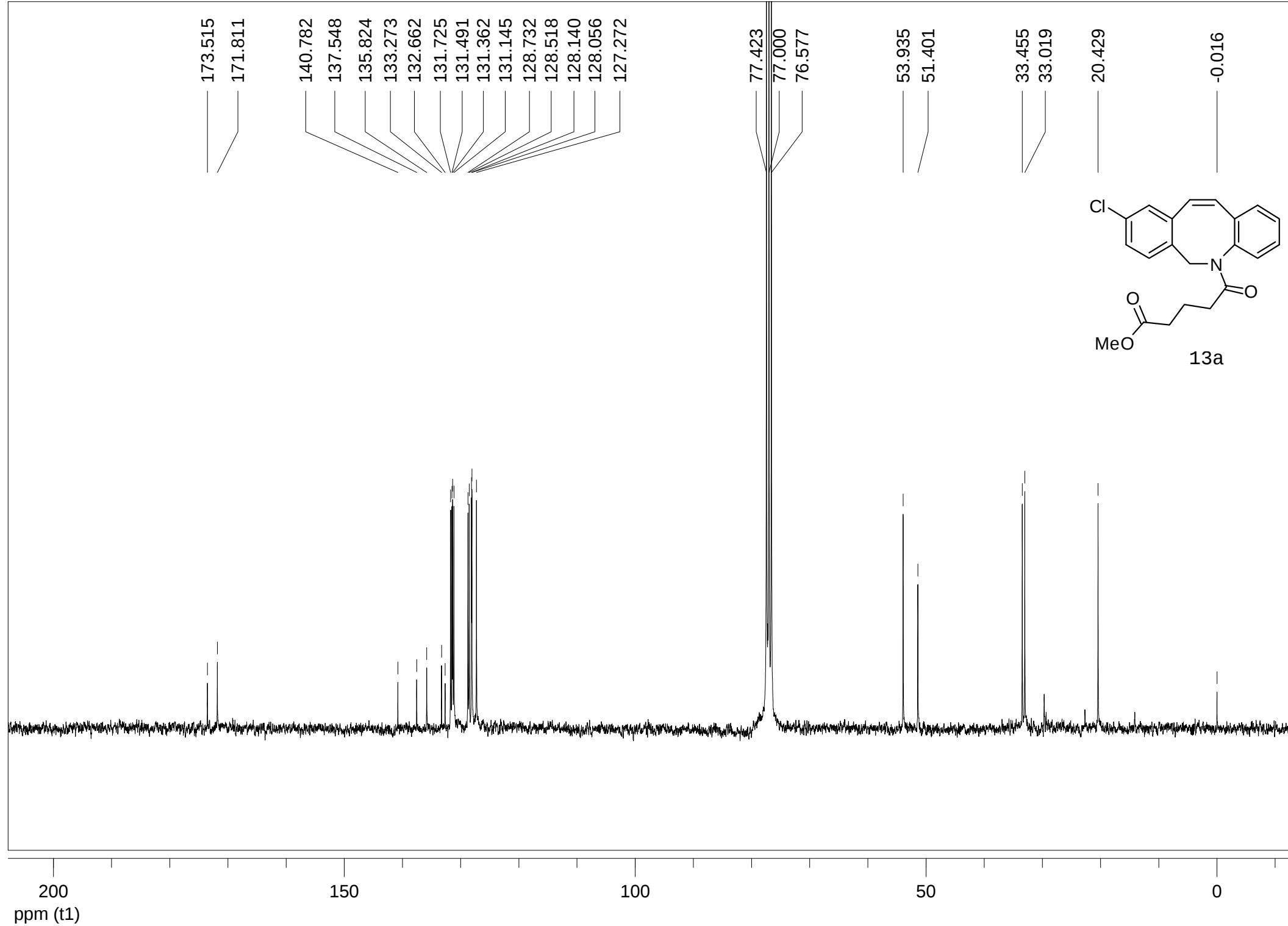


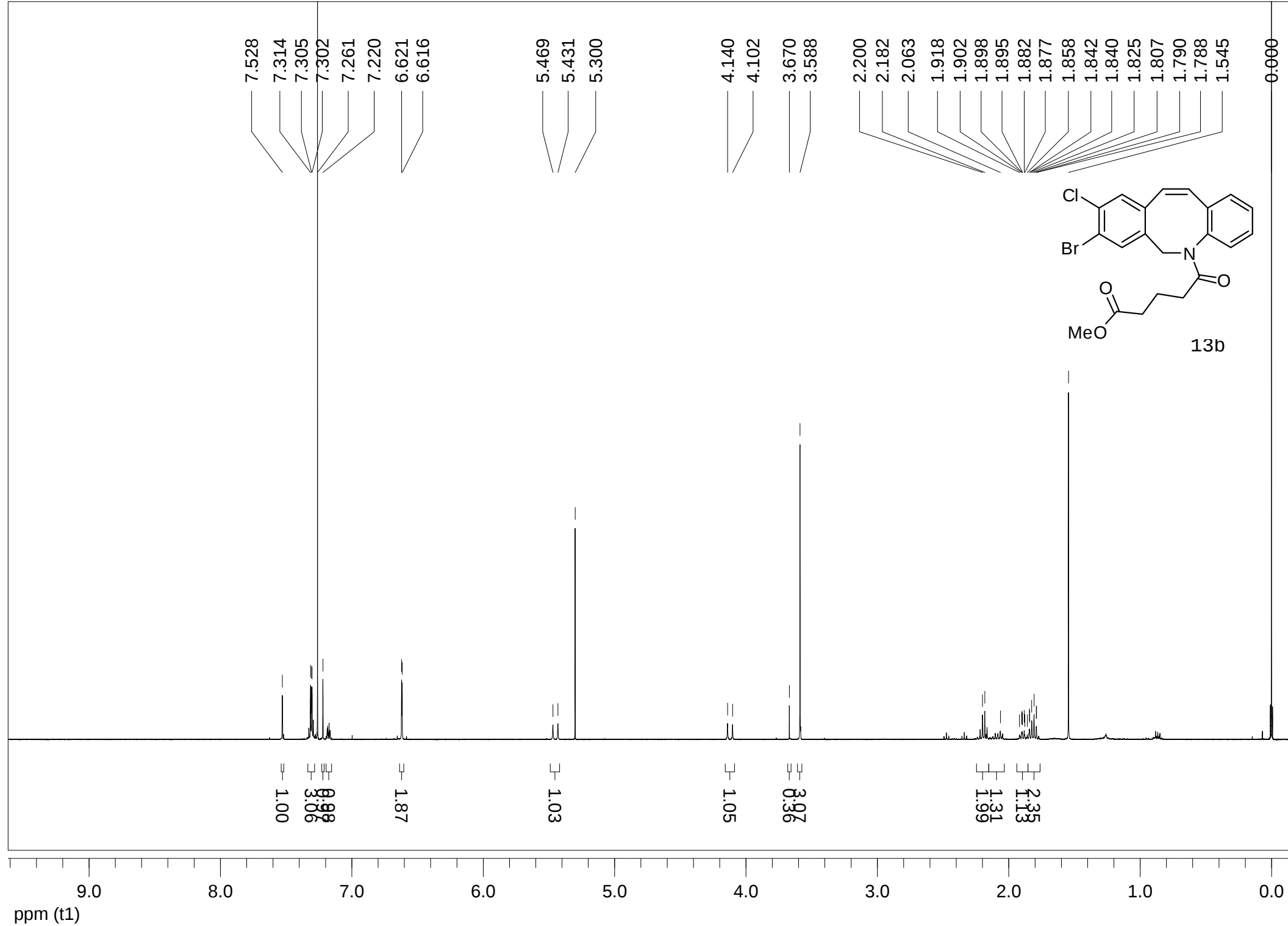


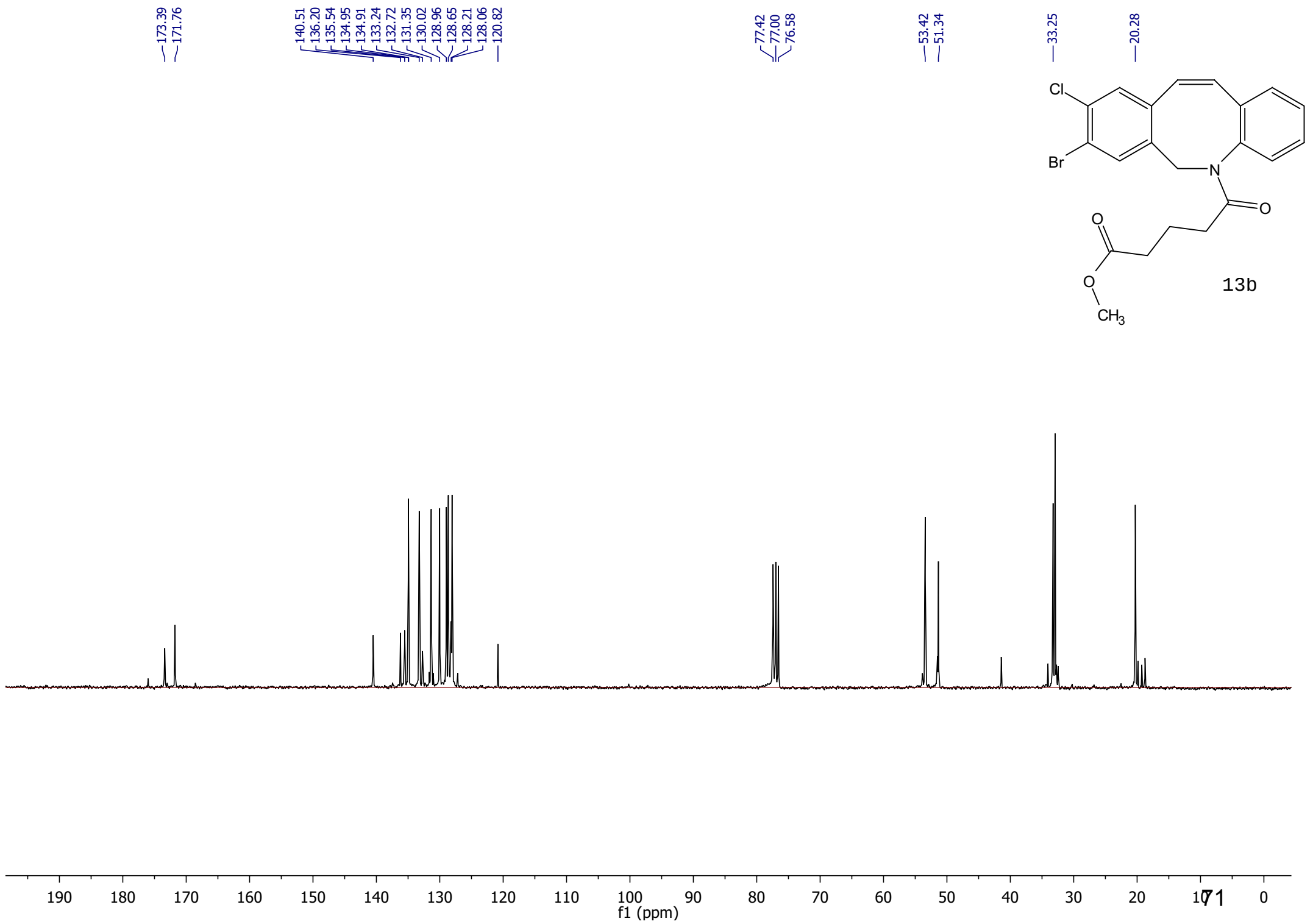












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7.42
7.30
7.29
7.29
7.28
7.27
7.26
7.18
7.17
7.01
6.99
6.70
6.67
6.60
6.57

5.51
5.47

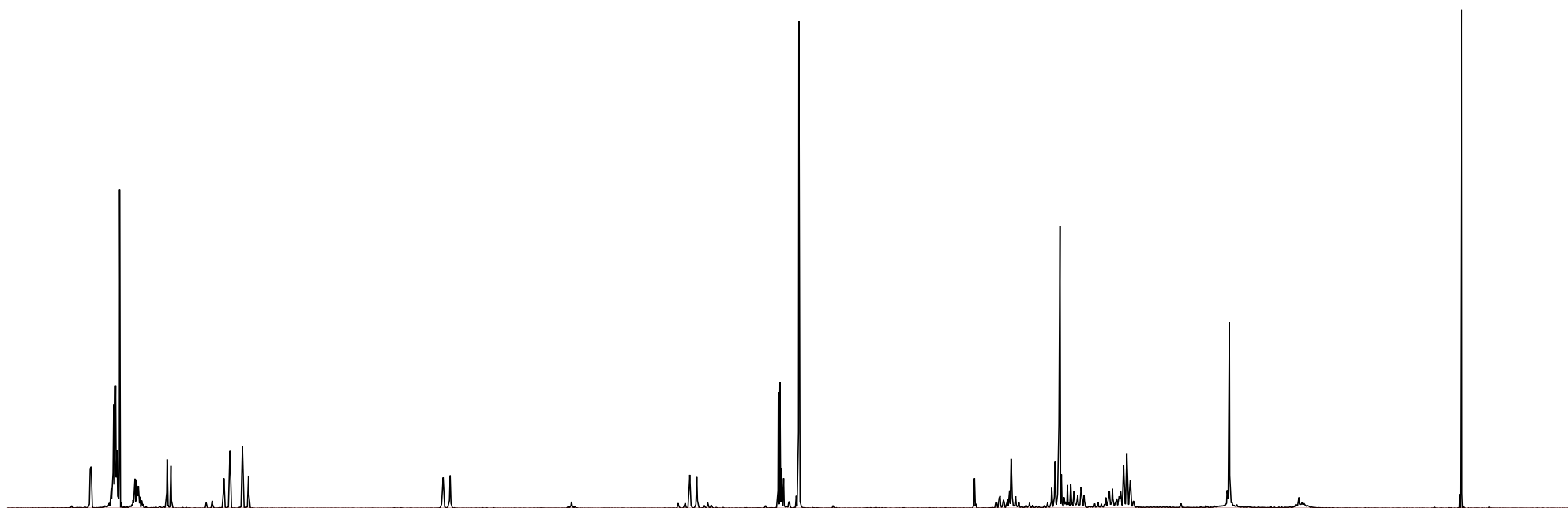
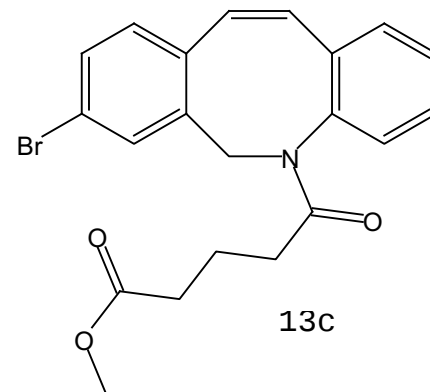
4.18
4.14

3.70
3.69
3.59

2.64
2.20
2.18
2.18
2.18
2.17
2.15
2.13
2.12
2.10
2.08
2.08
2.06

1.85
1.85
1.83
1.81
1.80
1.79
1.26

0.00



0.959
4.264
0.896
1.506
0.991
0.179
1.000
1.126

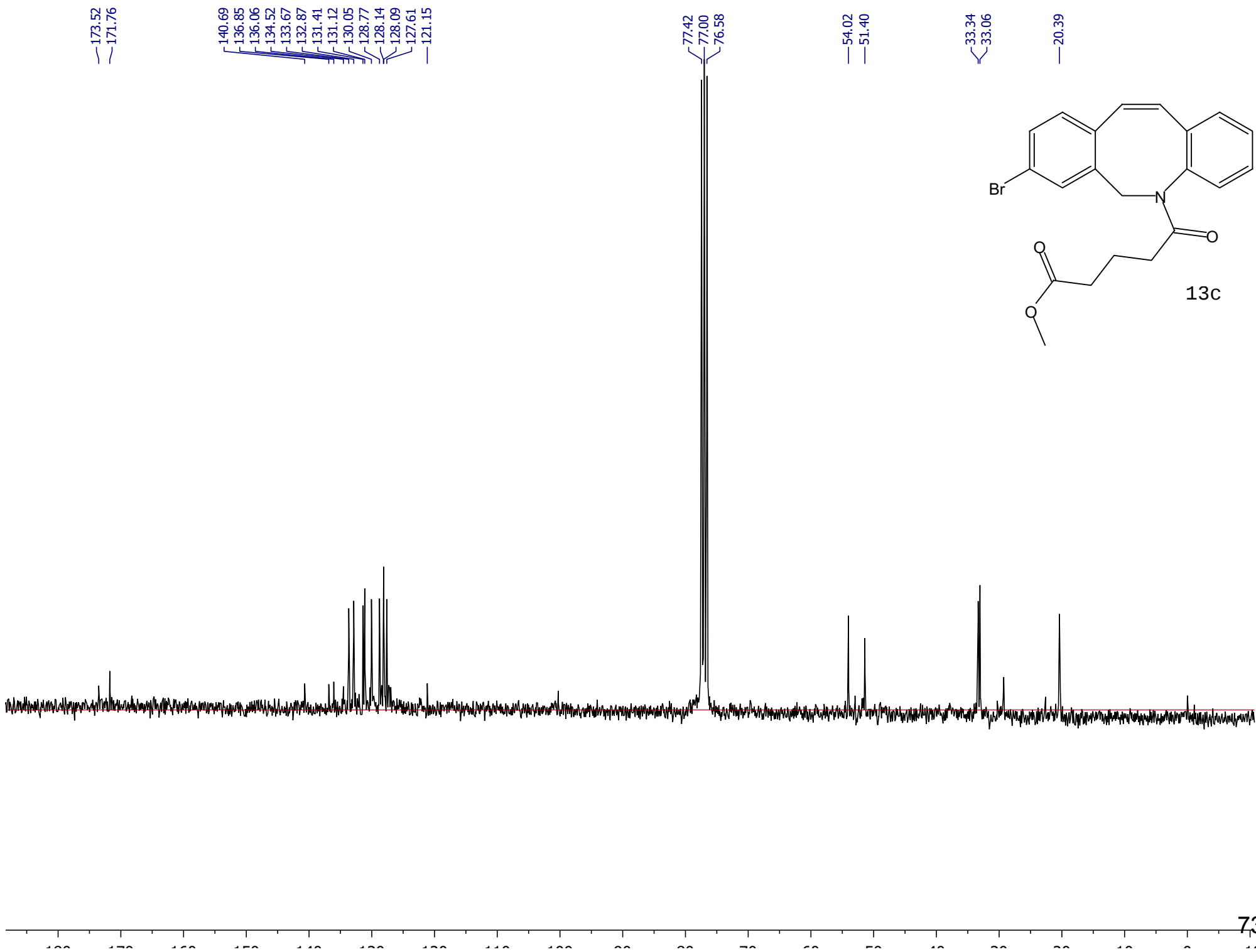
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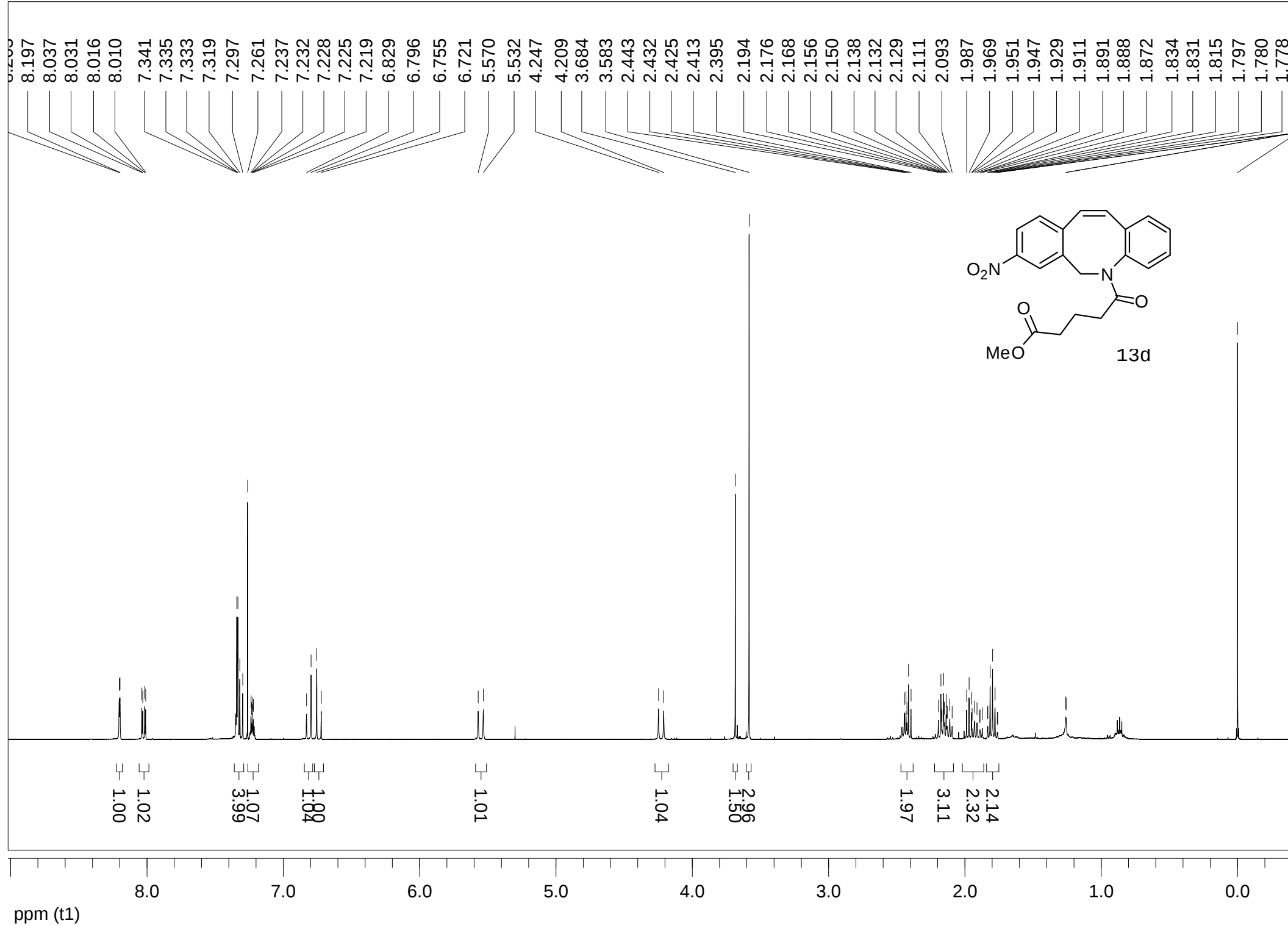
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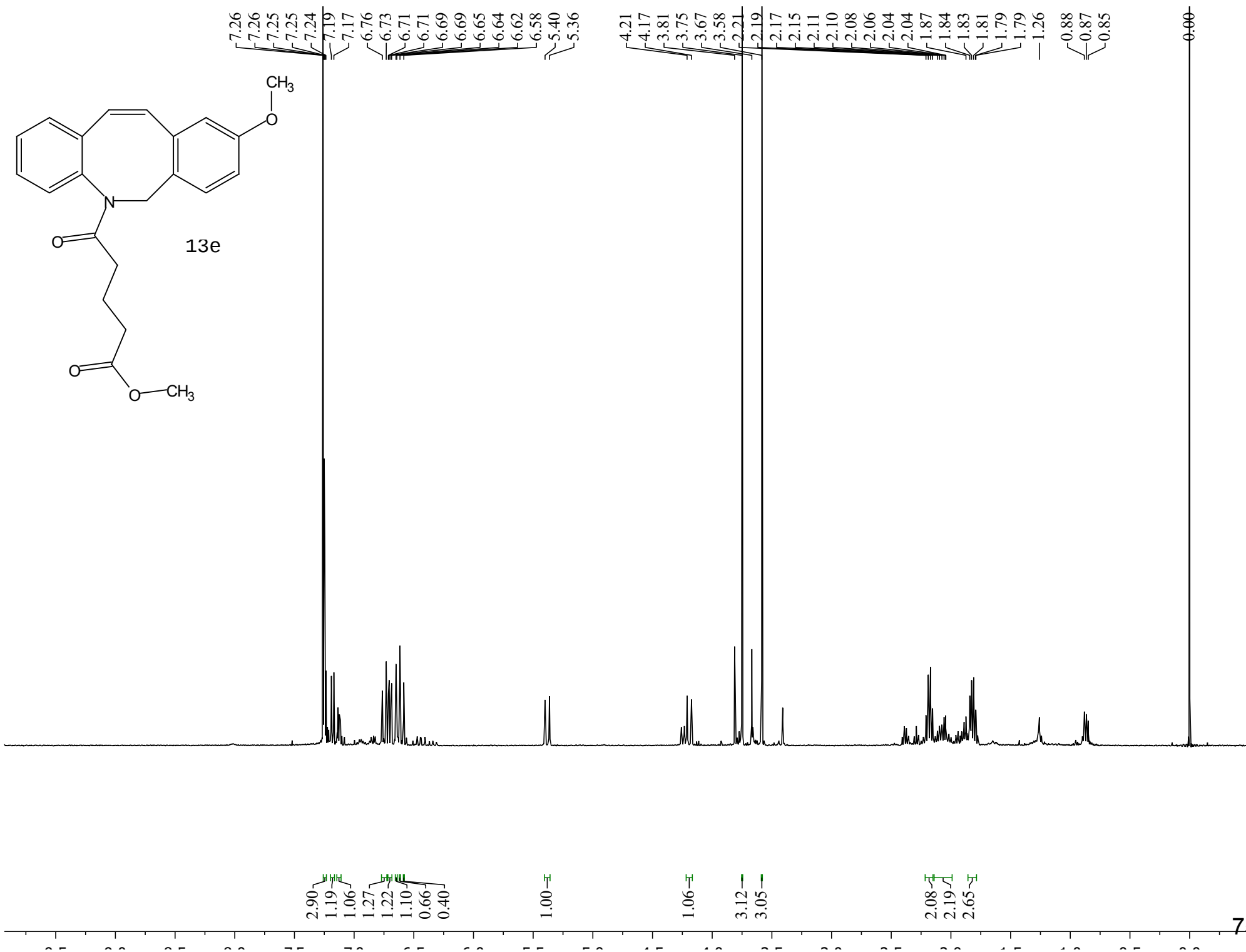
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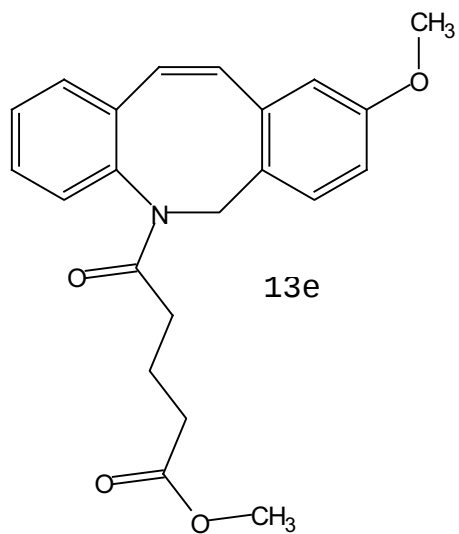
2.148
2.215

2.456









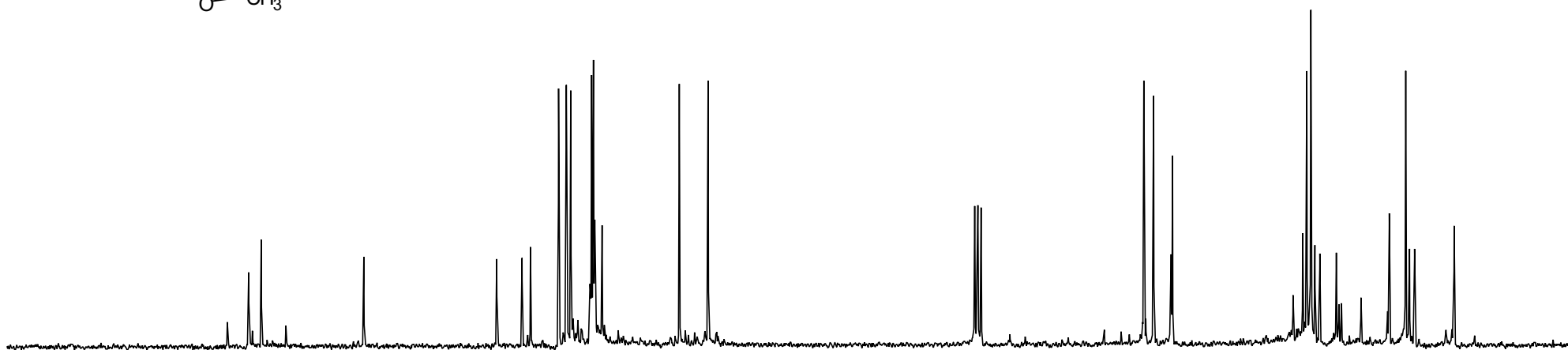
173.46
171.80
158.23
140.66
137.31
136.19
132.47
131.45
130.85
128.27
128.10
127.86
127.71
126.71
116.50
112.69

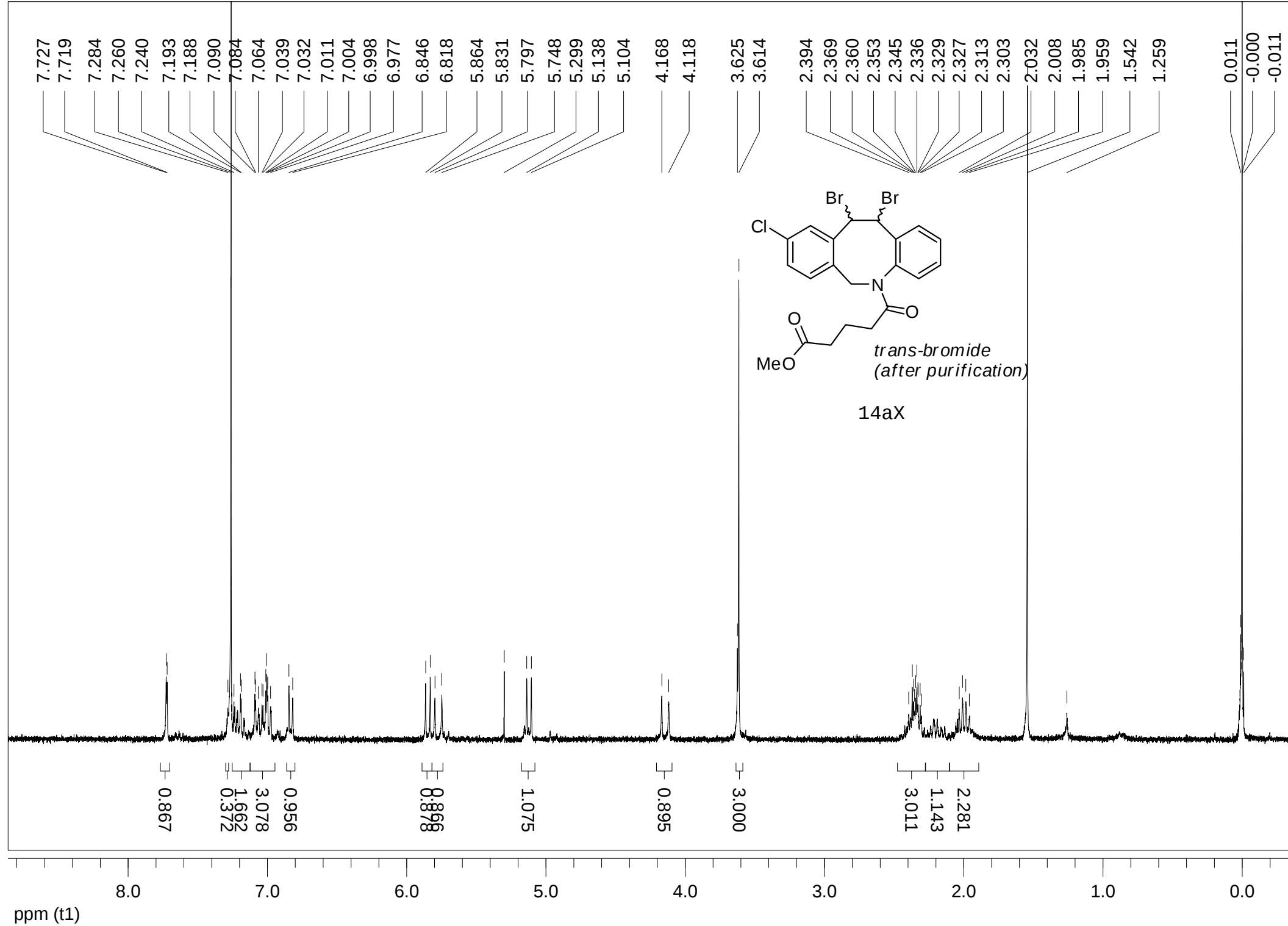
77.42
77.00
76.58

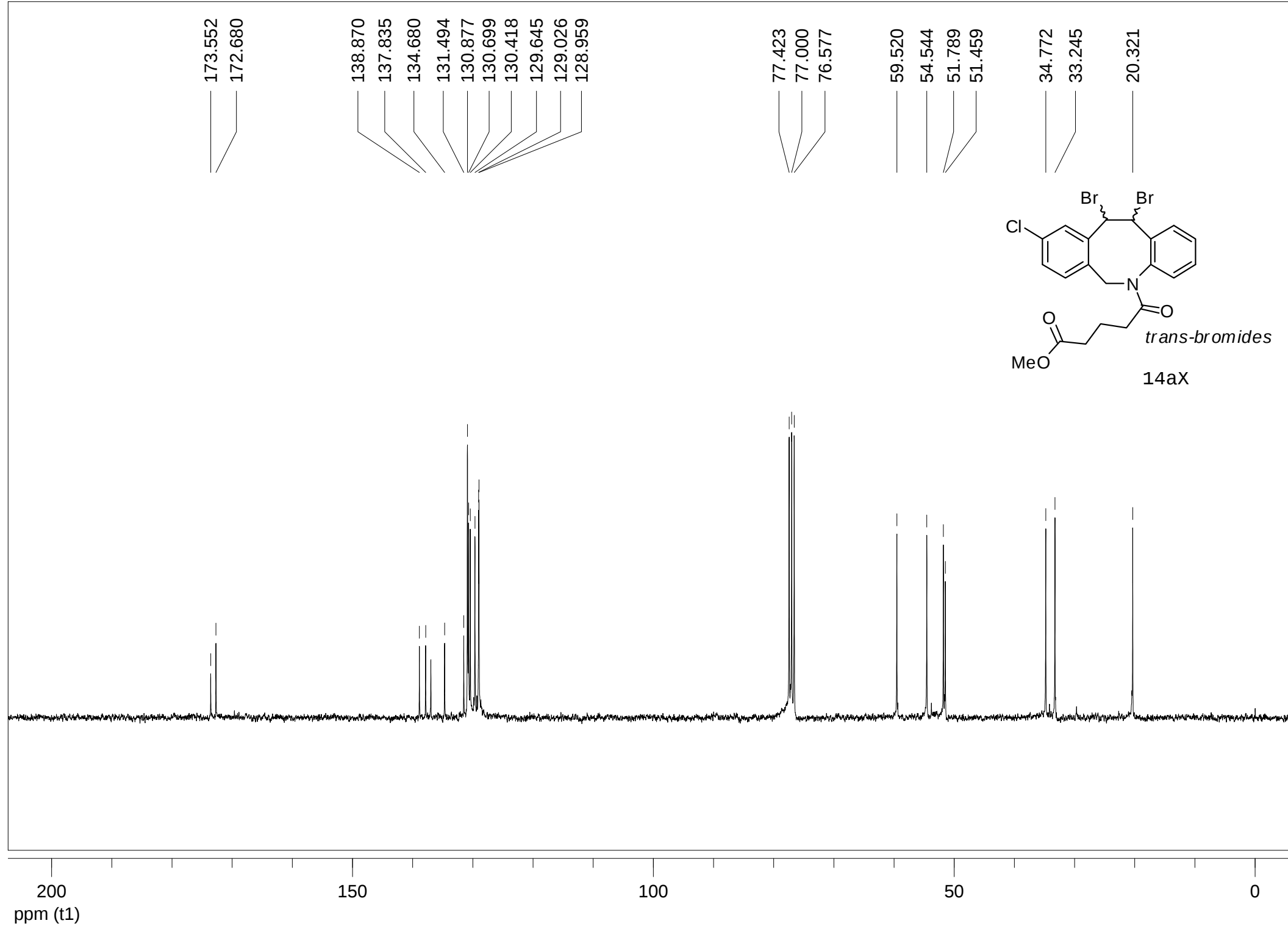
55.05
53.76

33.49
32.96

20.40







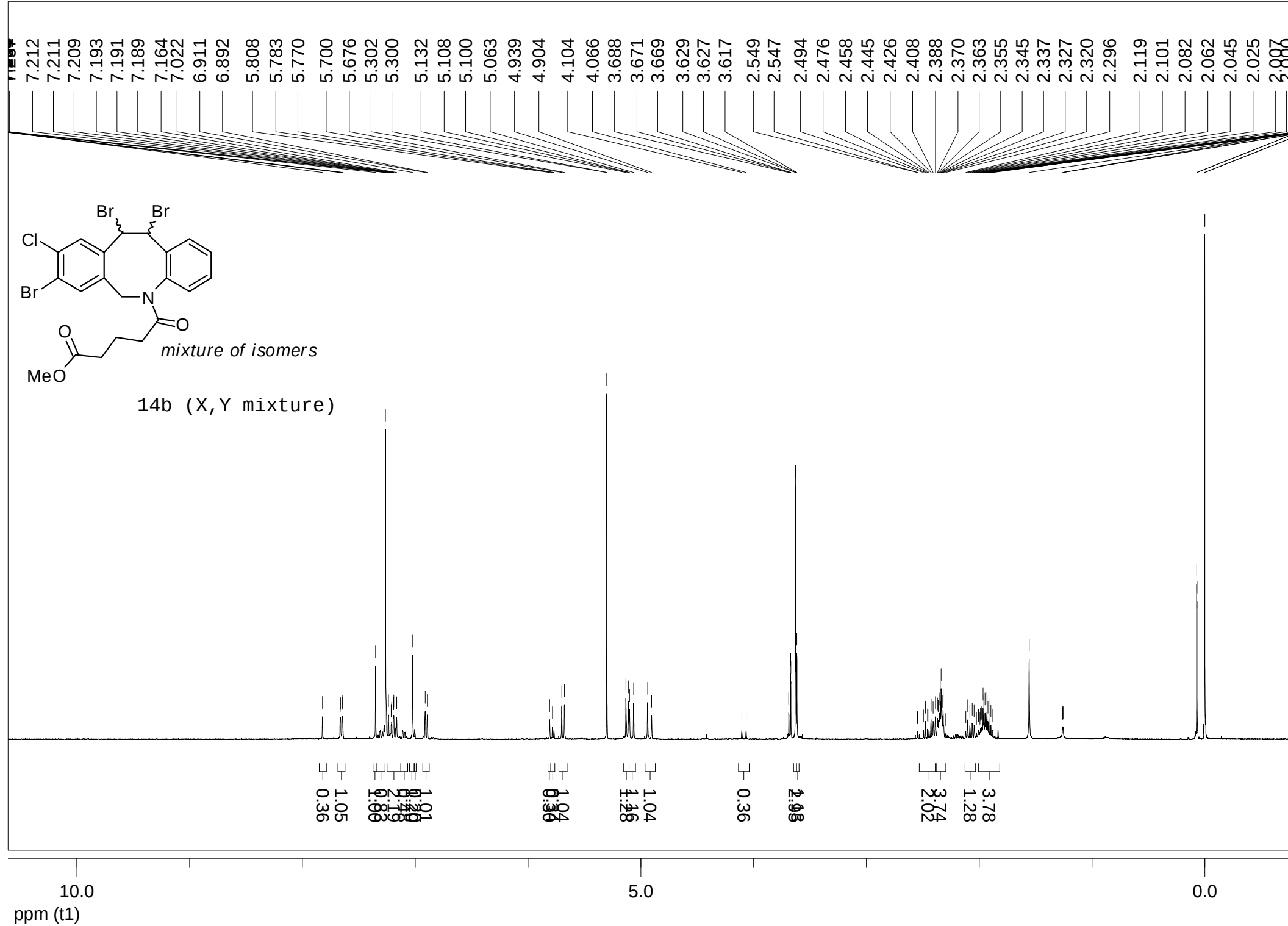
173.552
172.680

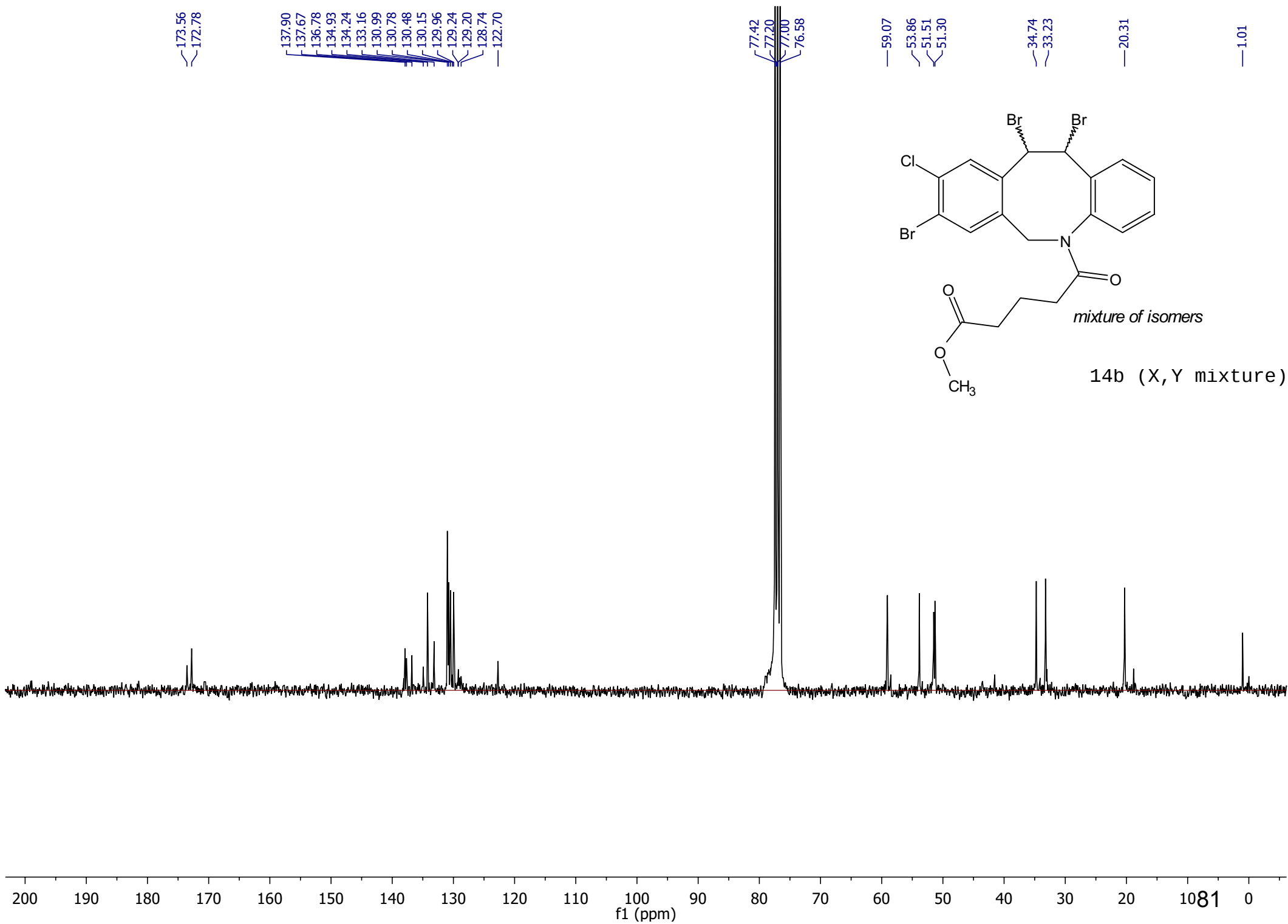
138.870
137.835
134.680
131.494
130.877
130.699
130.418
129.645
129.026
128.959

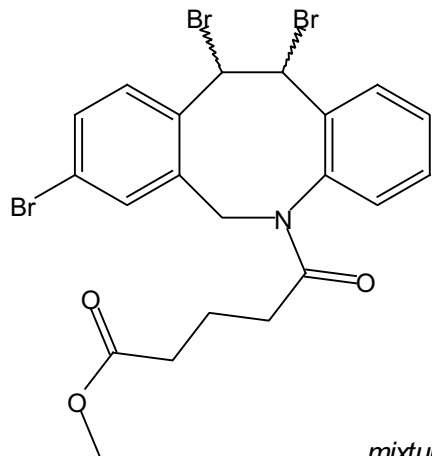
77.423
77.000
76.577

59.520
54.544
51.789
51.459

34.772
33.245
20.321

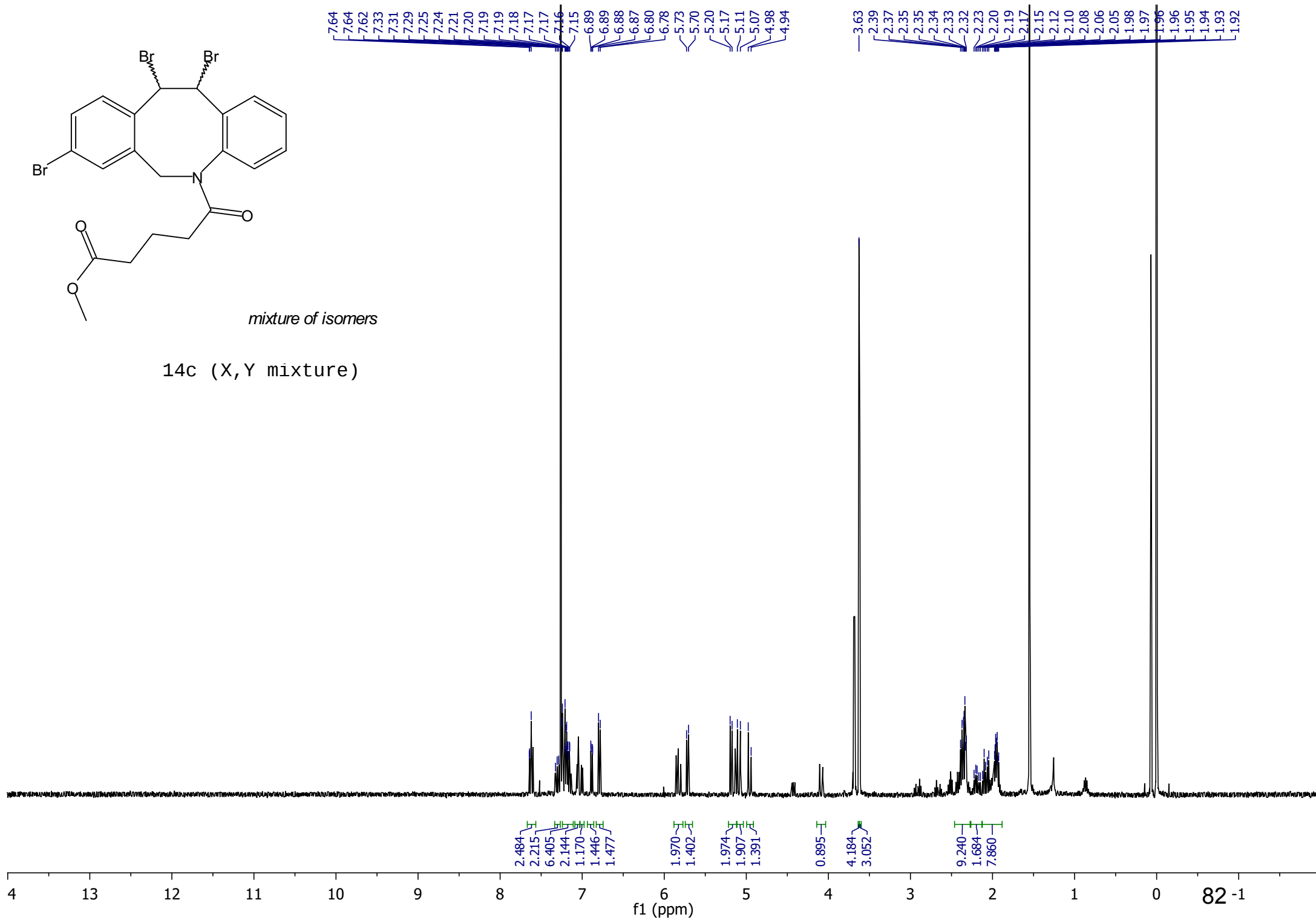


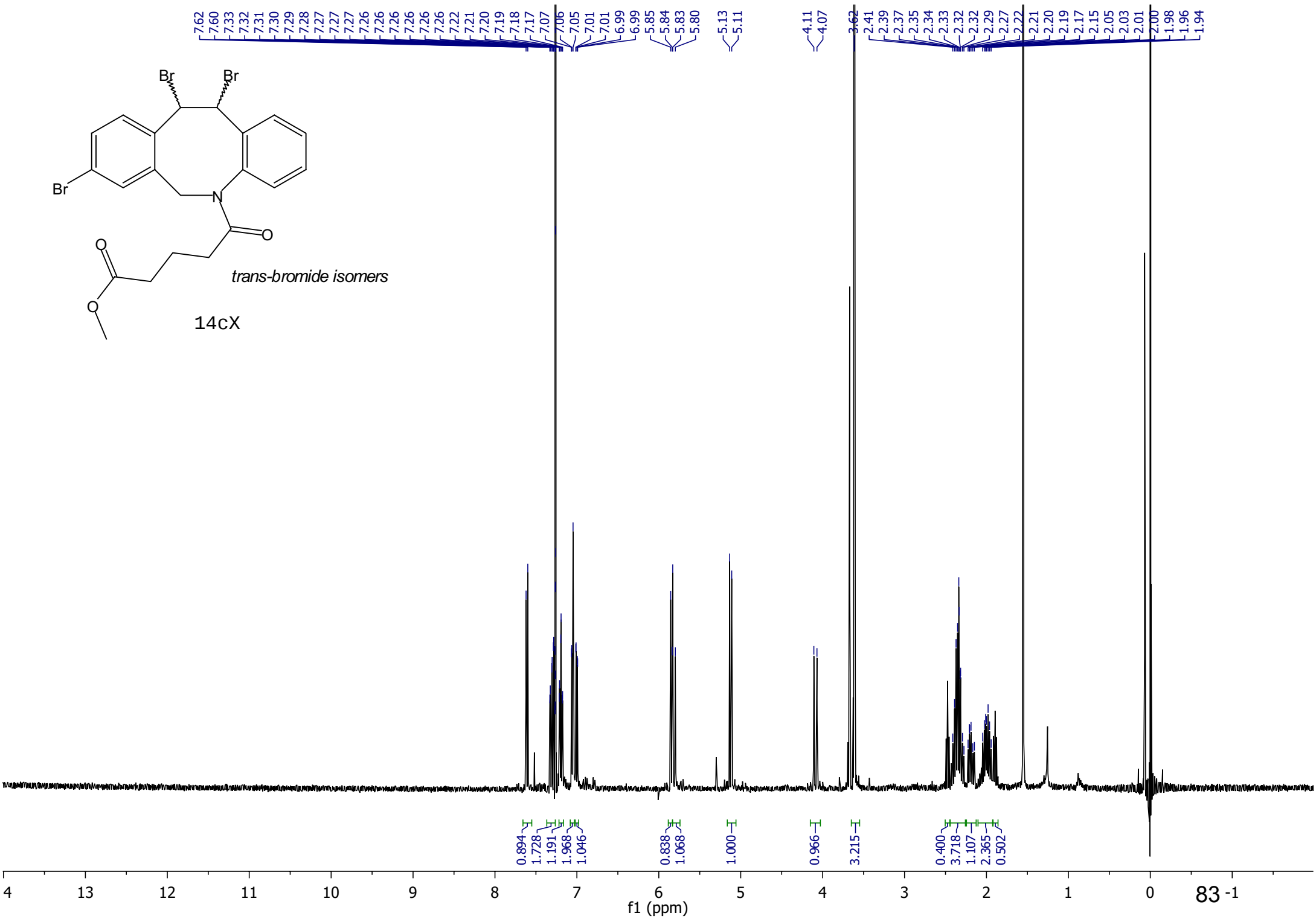


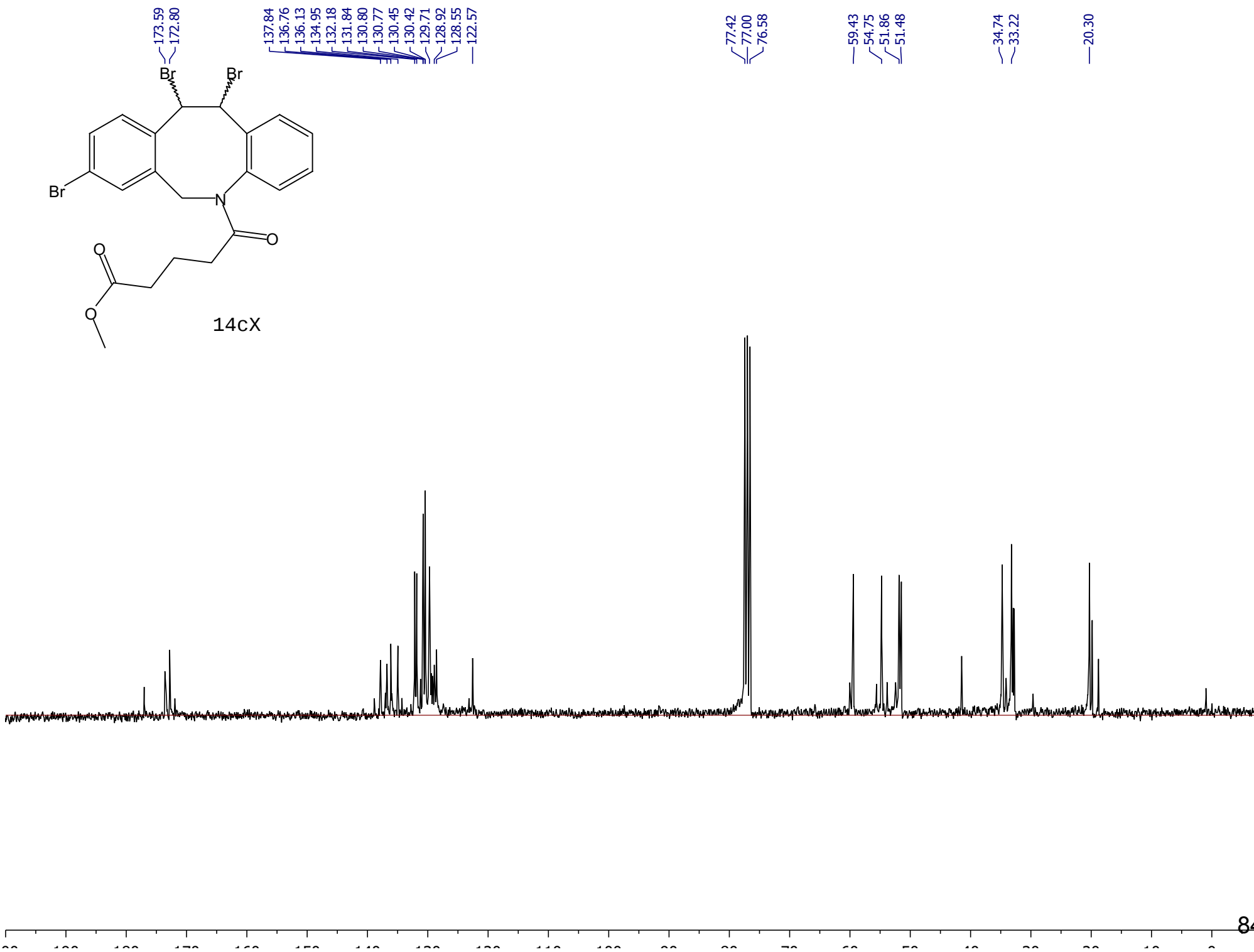
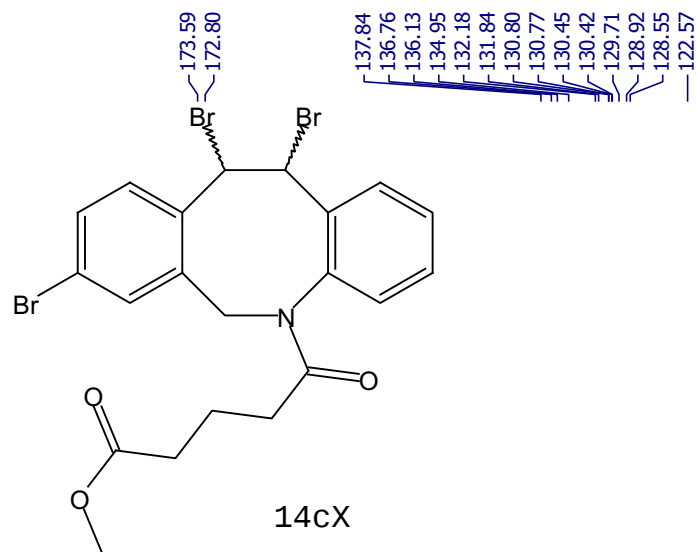


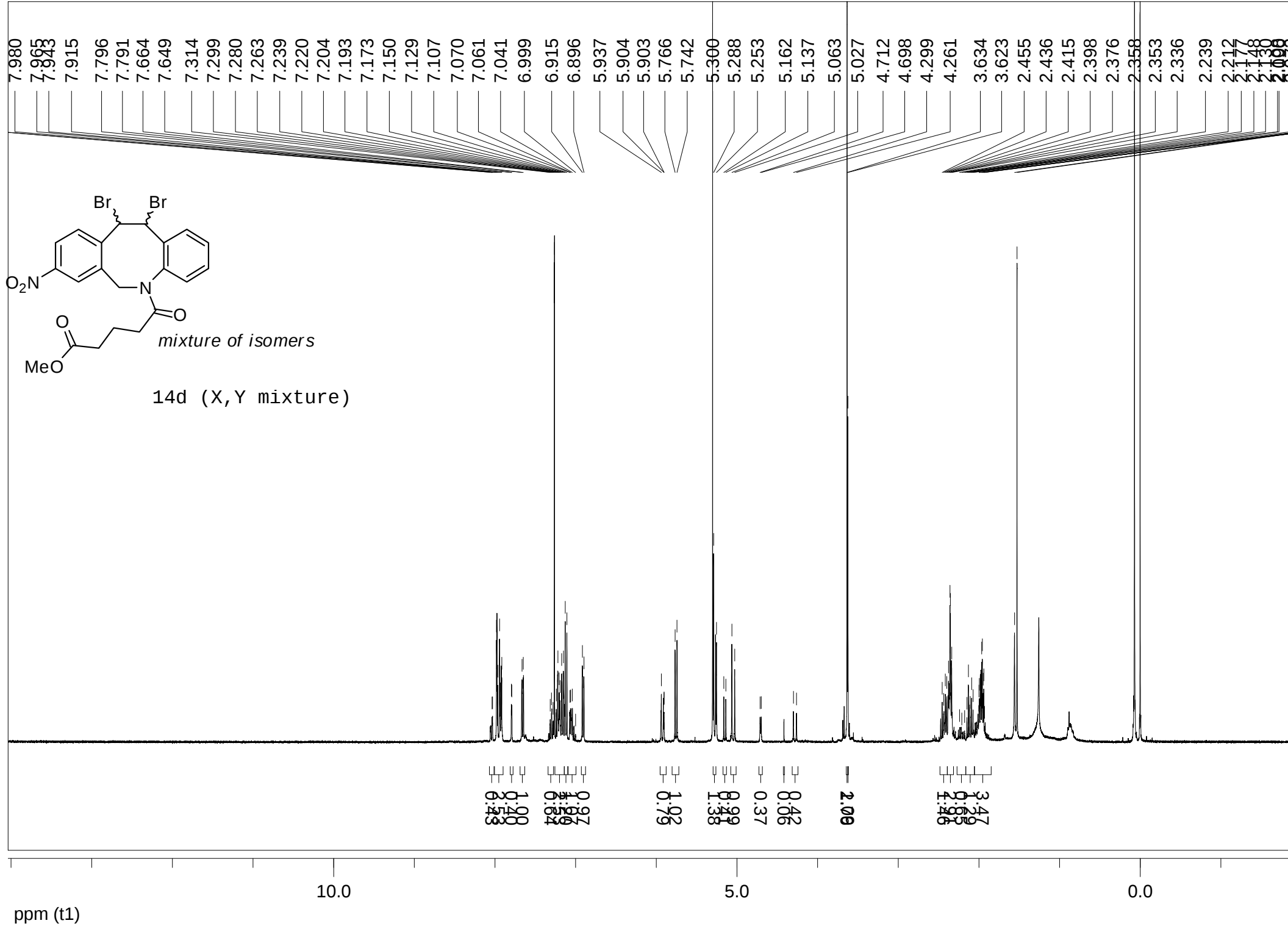
mixture of isomers

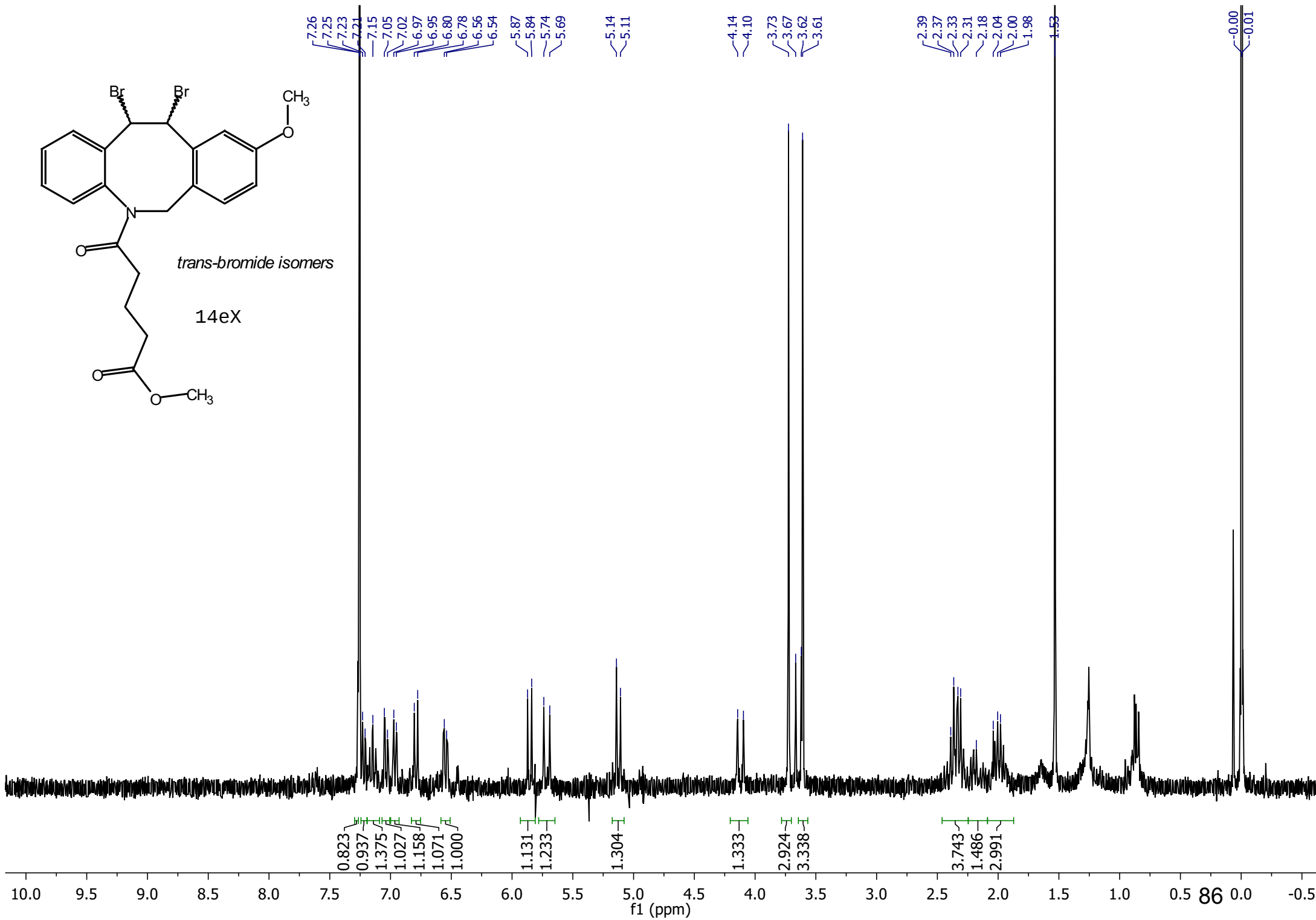
14c (X,Y mixture)

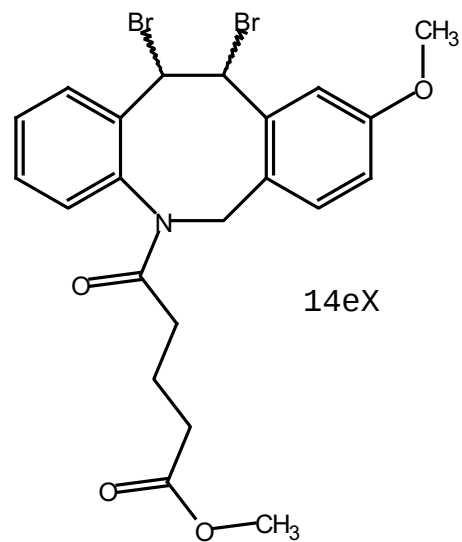












14eX

173.62
172.63

159.80

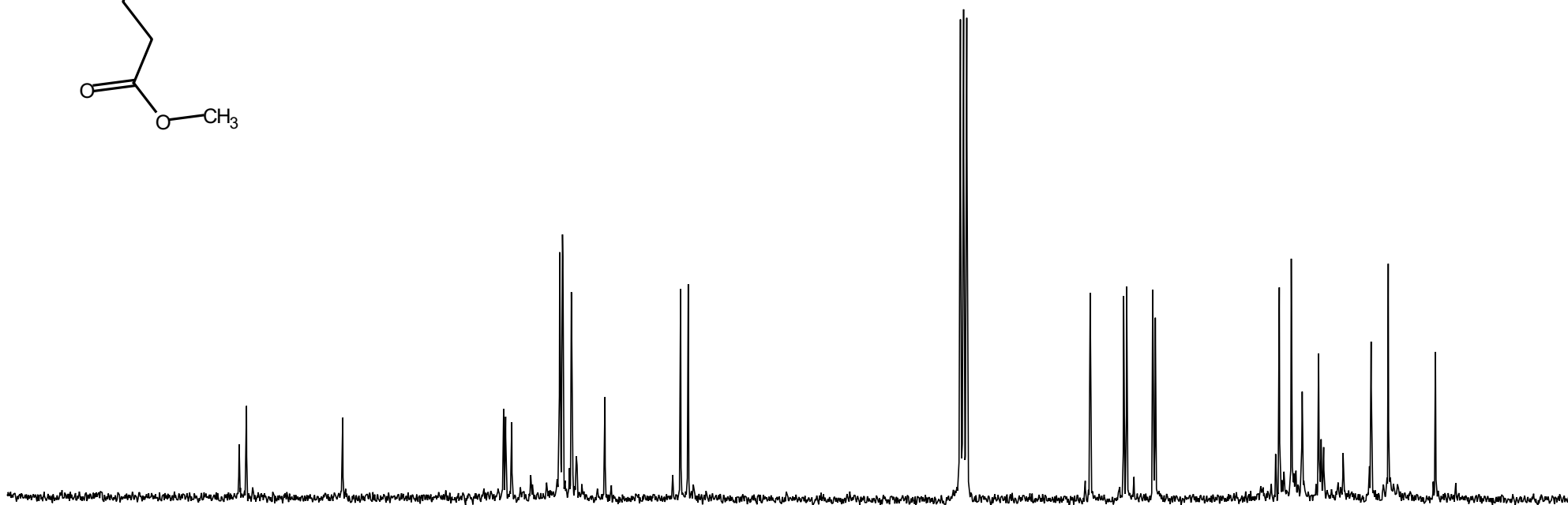
138.34
138.08
137.26
130.87
130.78
130.49
130.44
129.31
124.83
114.74
113.72

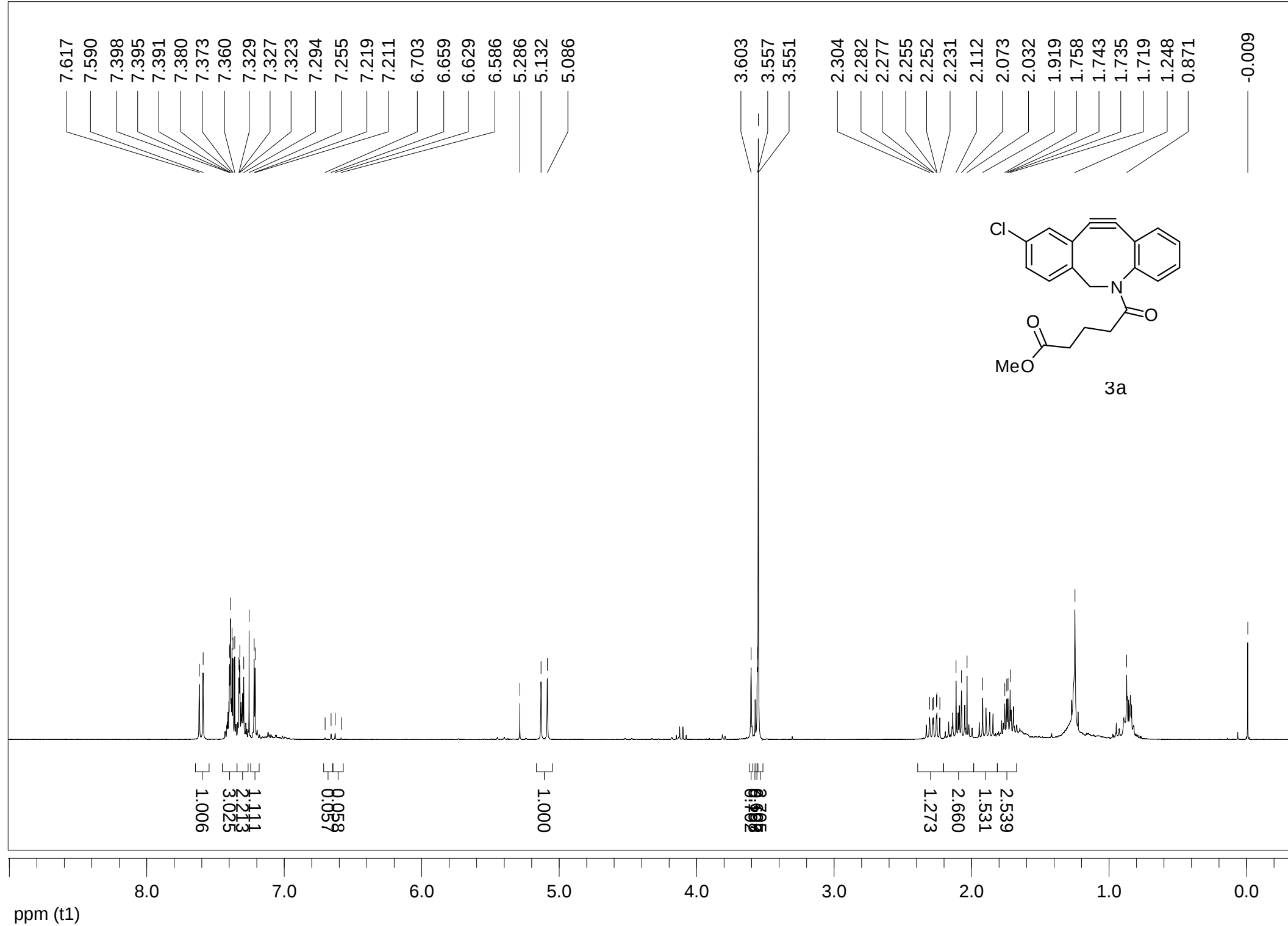
77.42
77.00
76.58

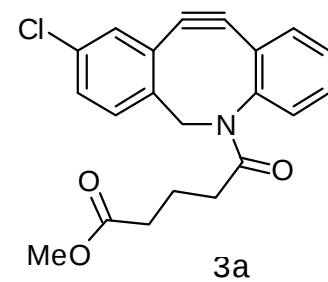
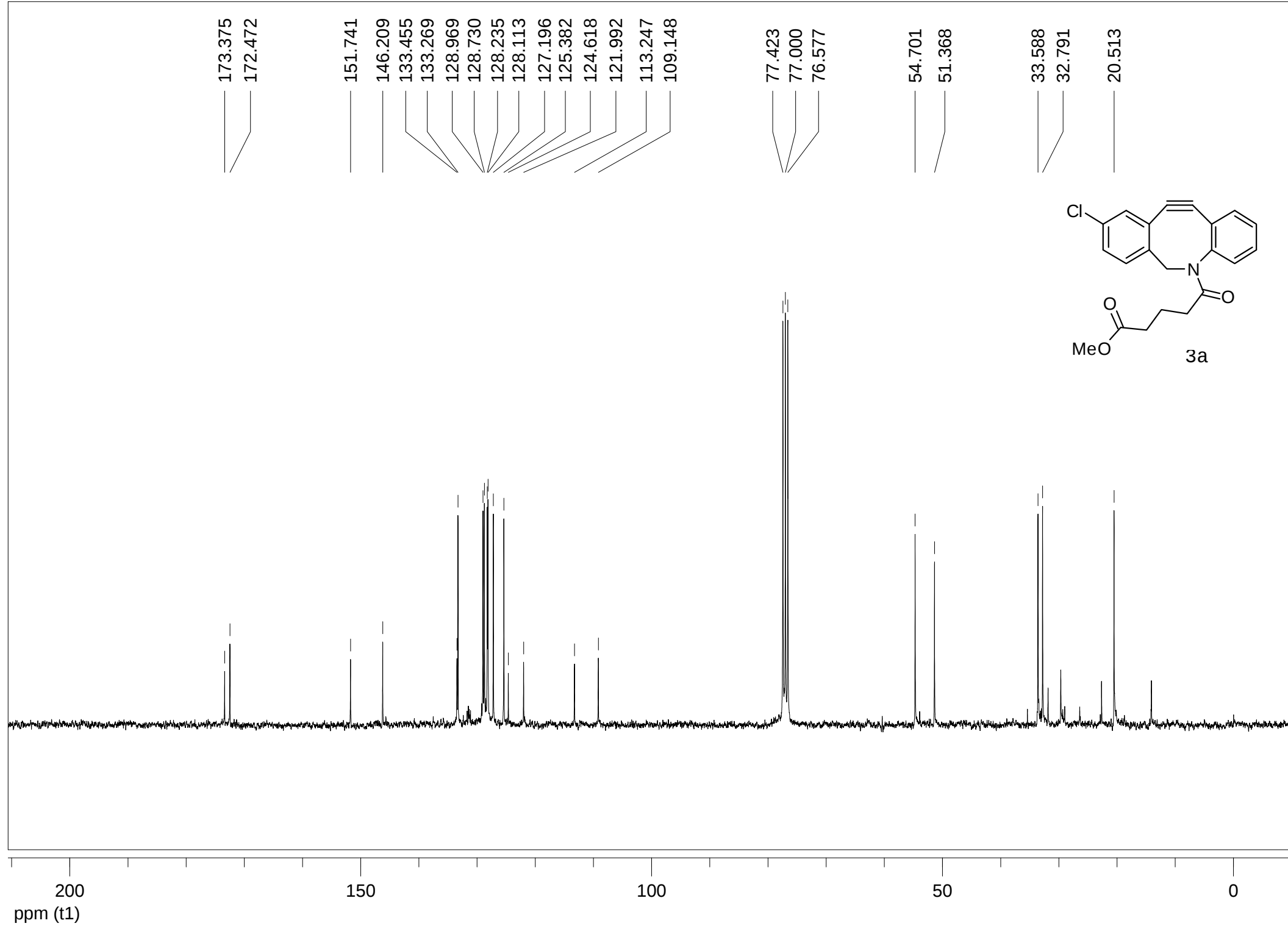
60.12
55.66
55.26
51.78
51.43

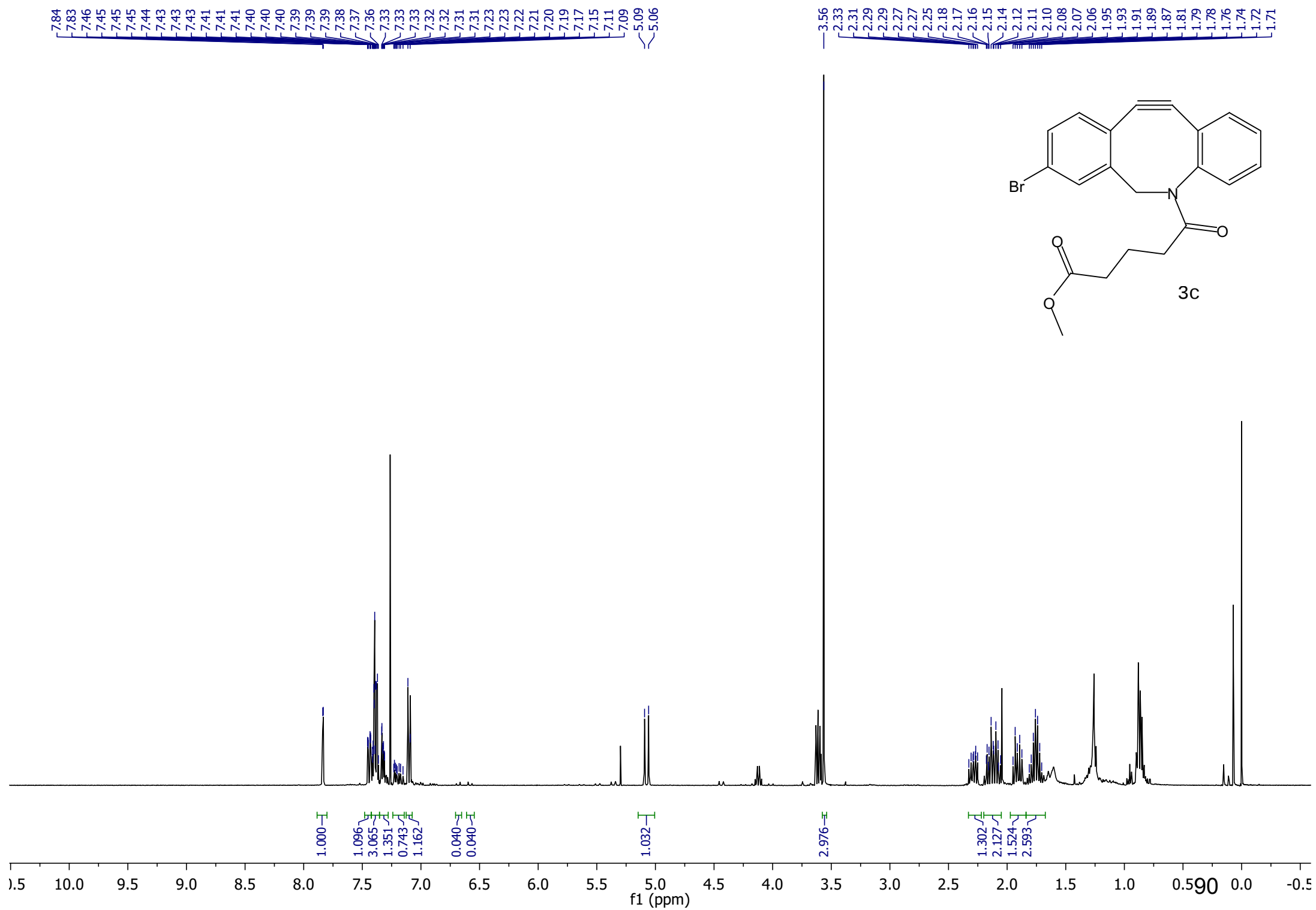
34.90
33.30

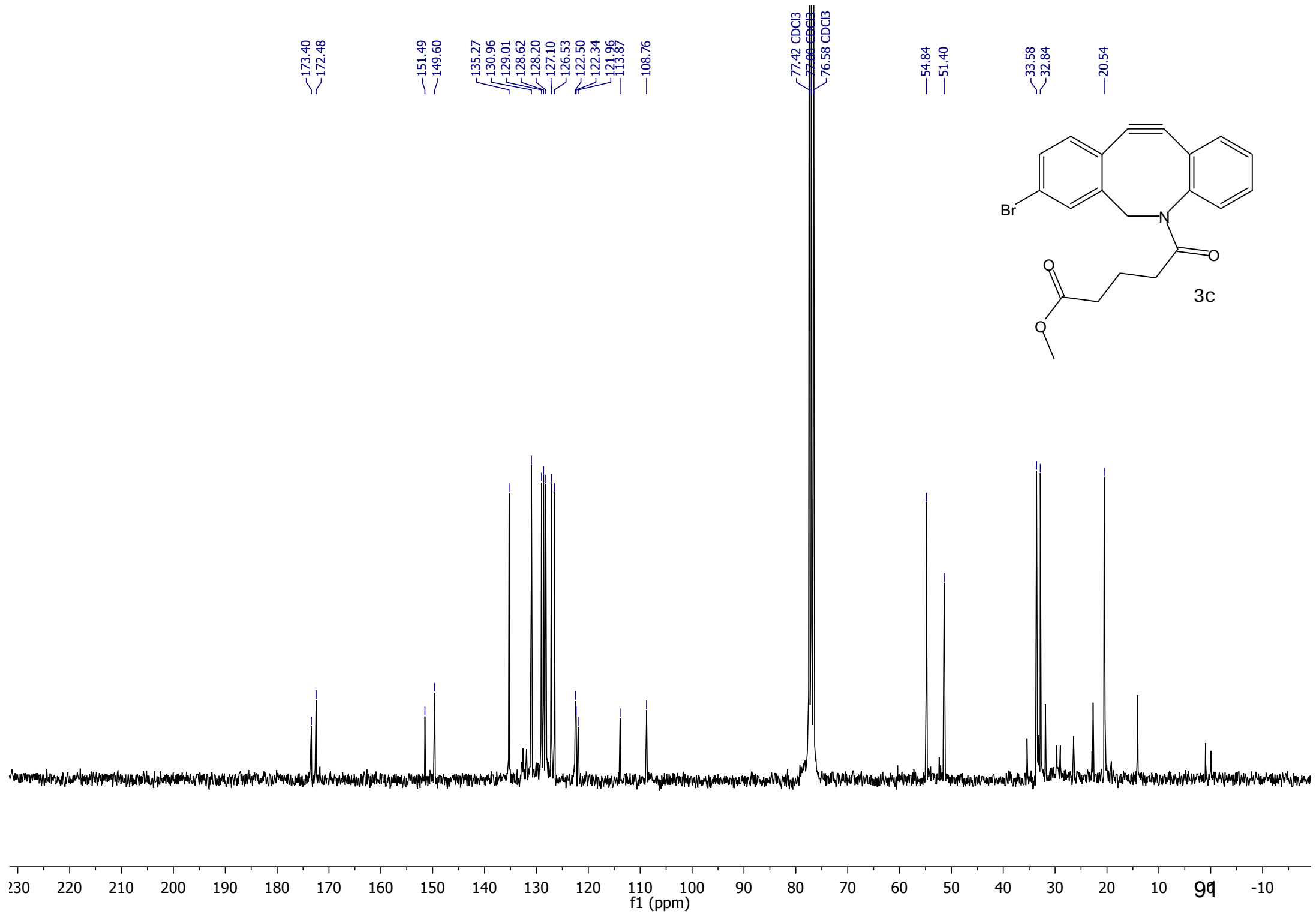
20.37

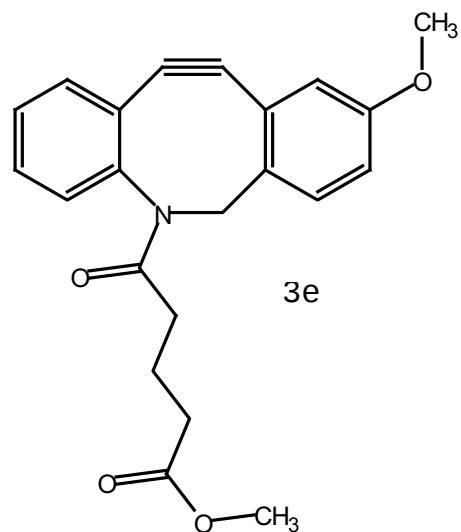




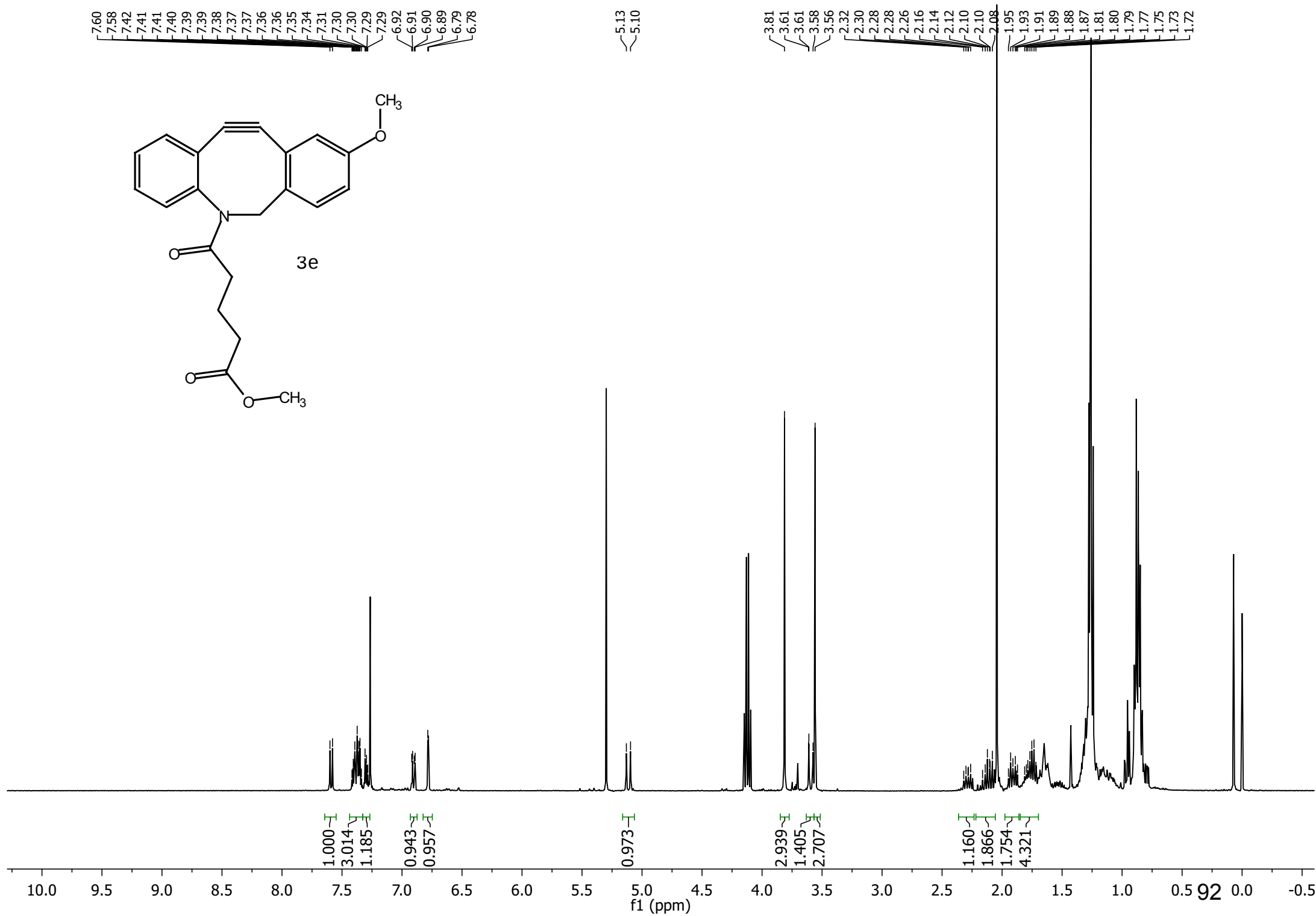


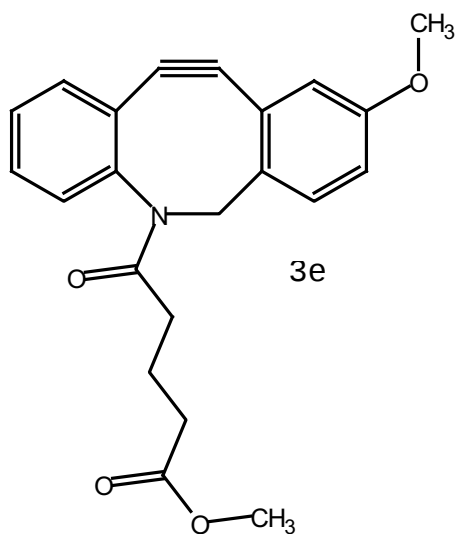






3e





3e

173.05
172.04

158.48

151.44

139.96

132.66

128.51

127.95

127.49

126.68

123.53

121.96

114.24

113.49

110.48

107.53

54.98

54.27

50.93

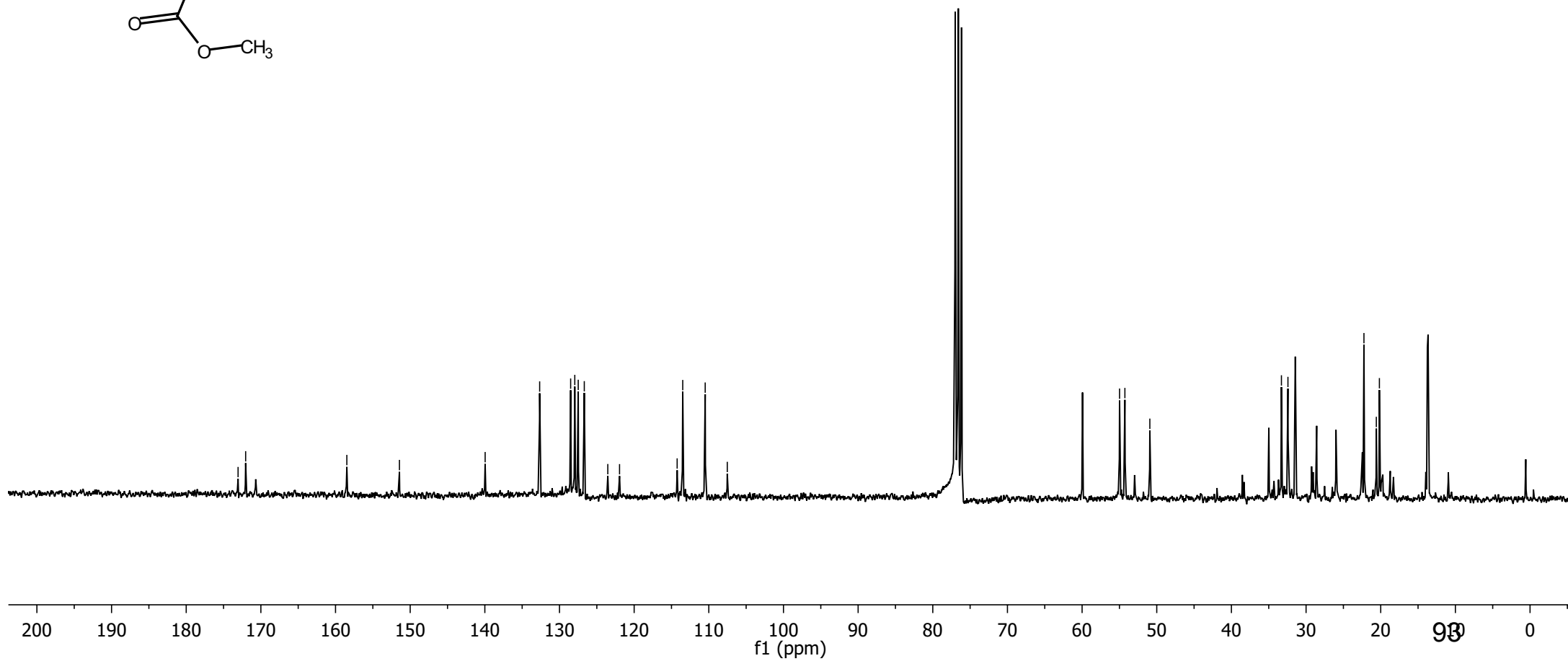
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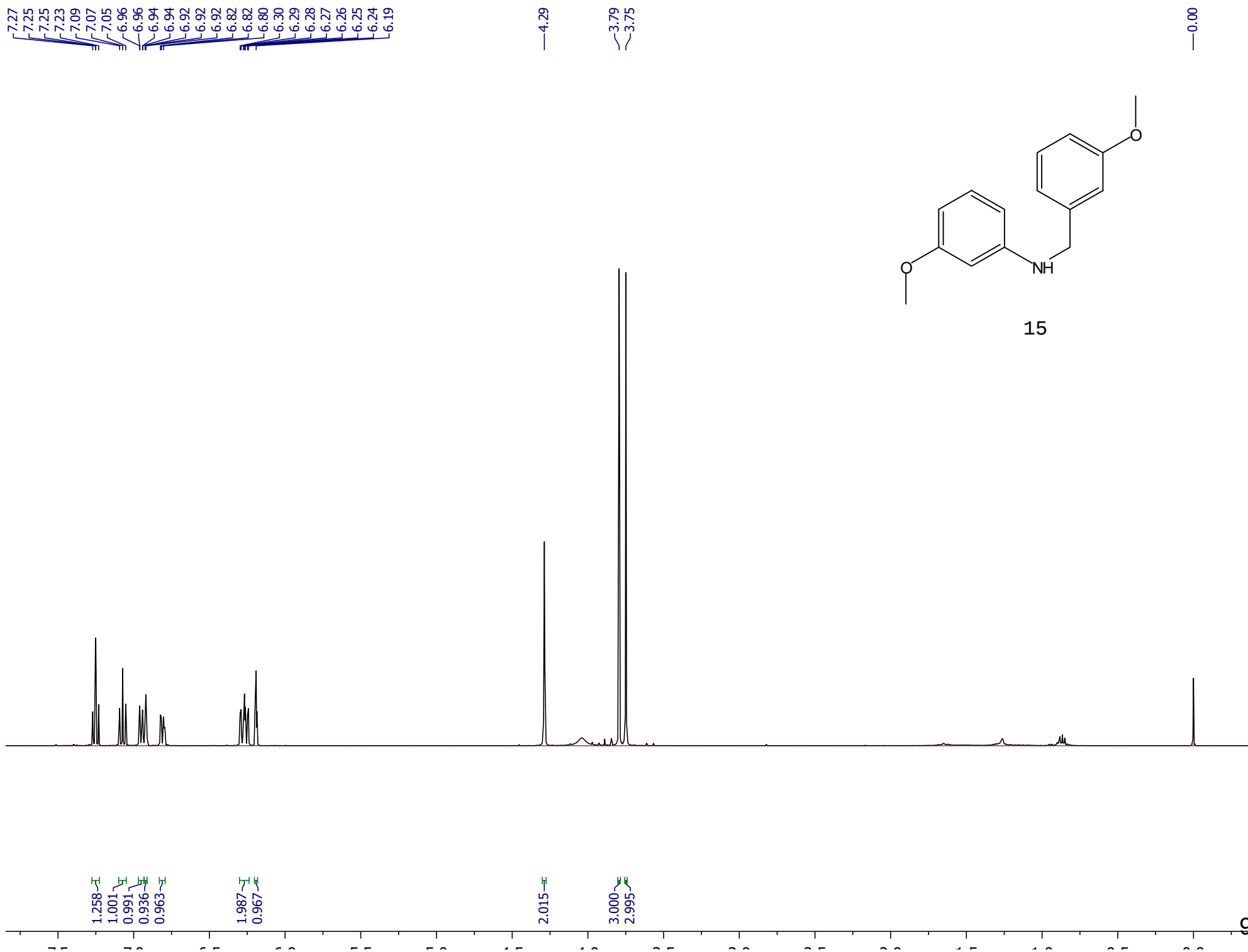
32.43

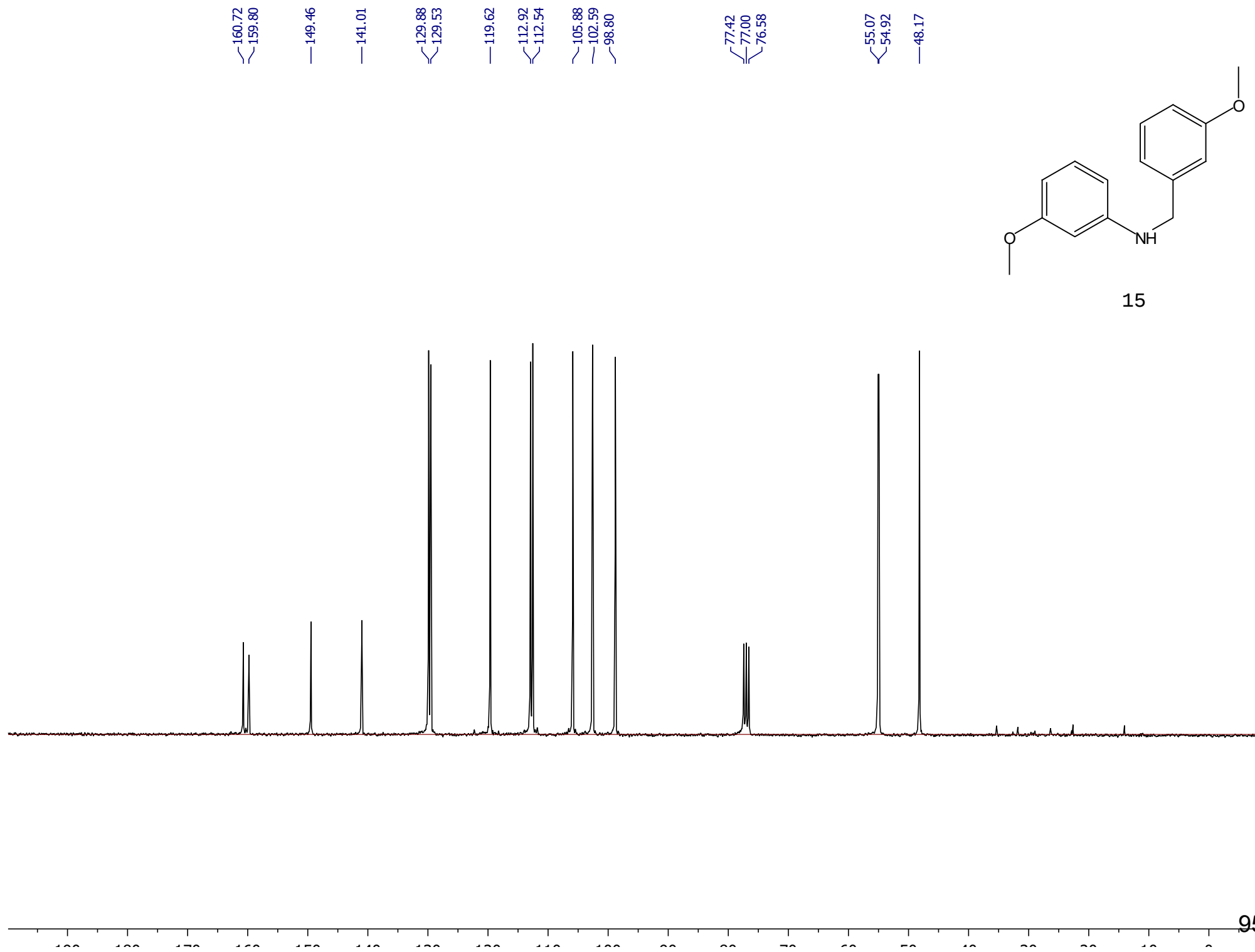
22.25

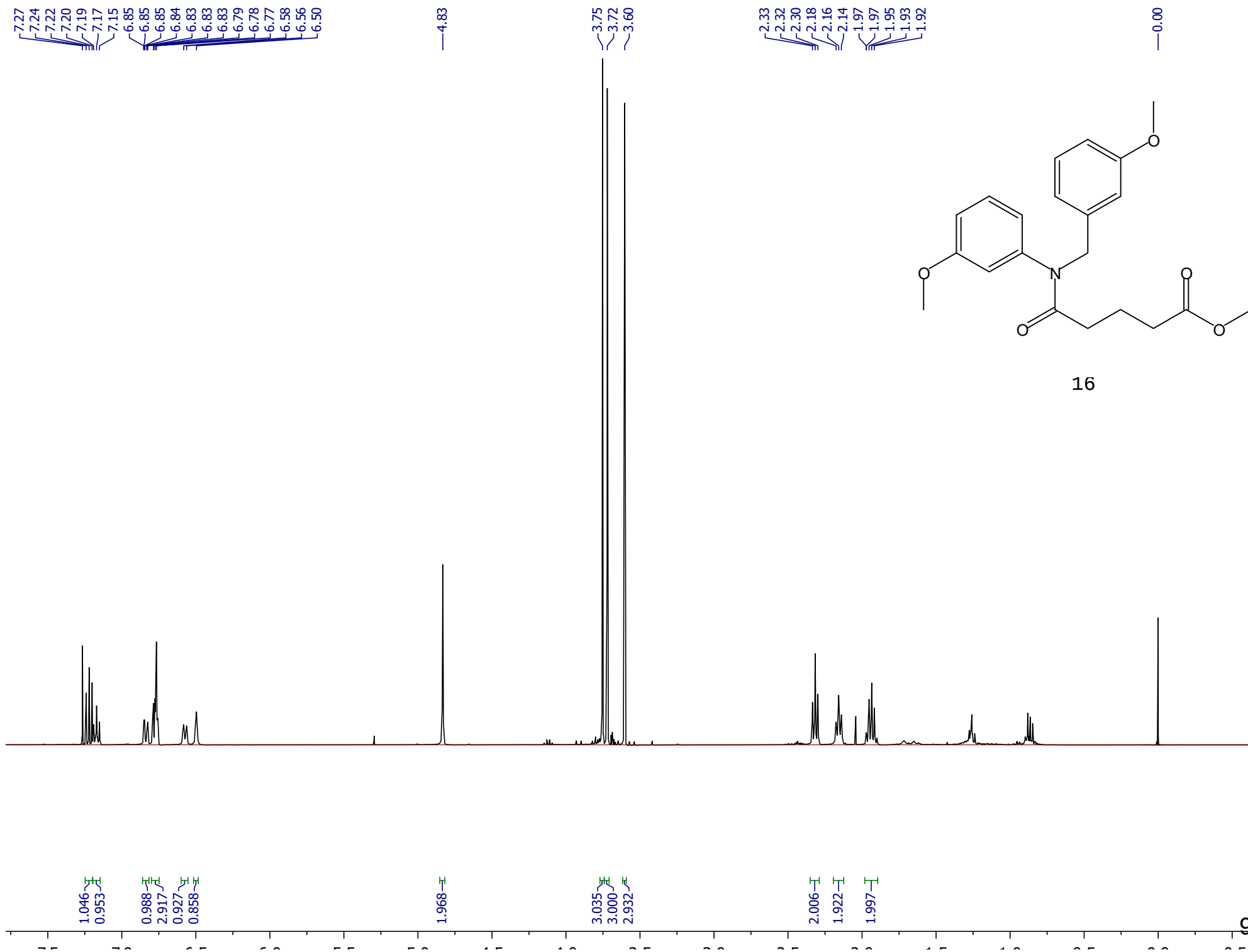
20.59

20.18









173.55
171.89

160.29
159.58

143.35
139.14

130.14
129.27

121.09
120.54

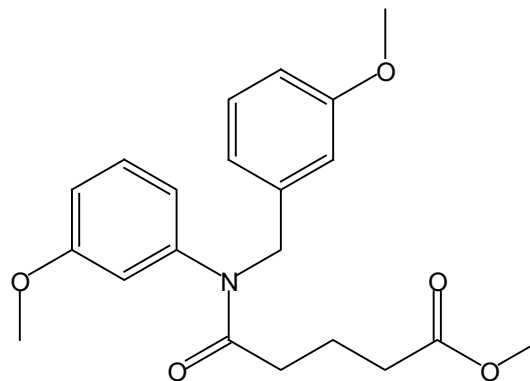
114.07
113.48
113.02

77.42
77.00
76.58

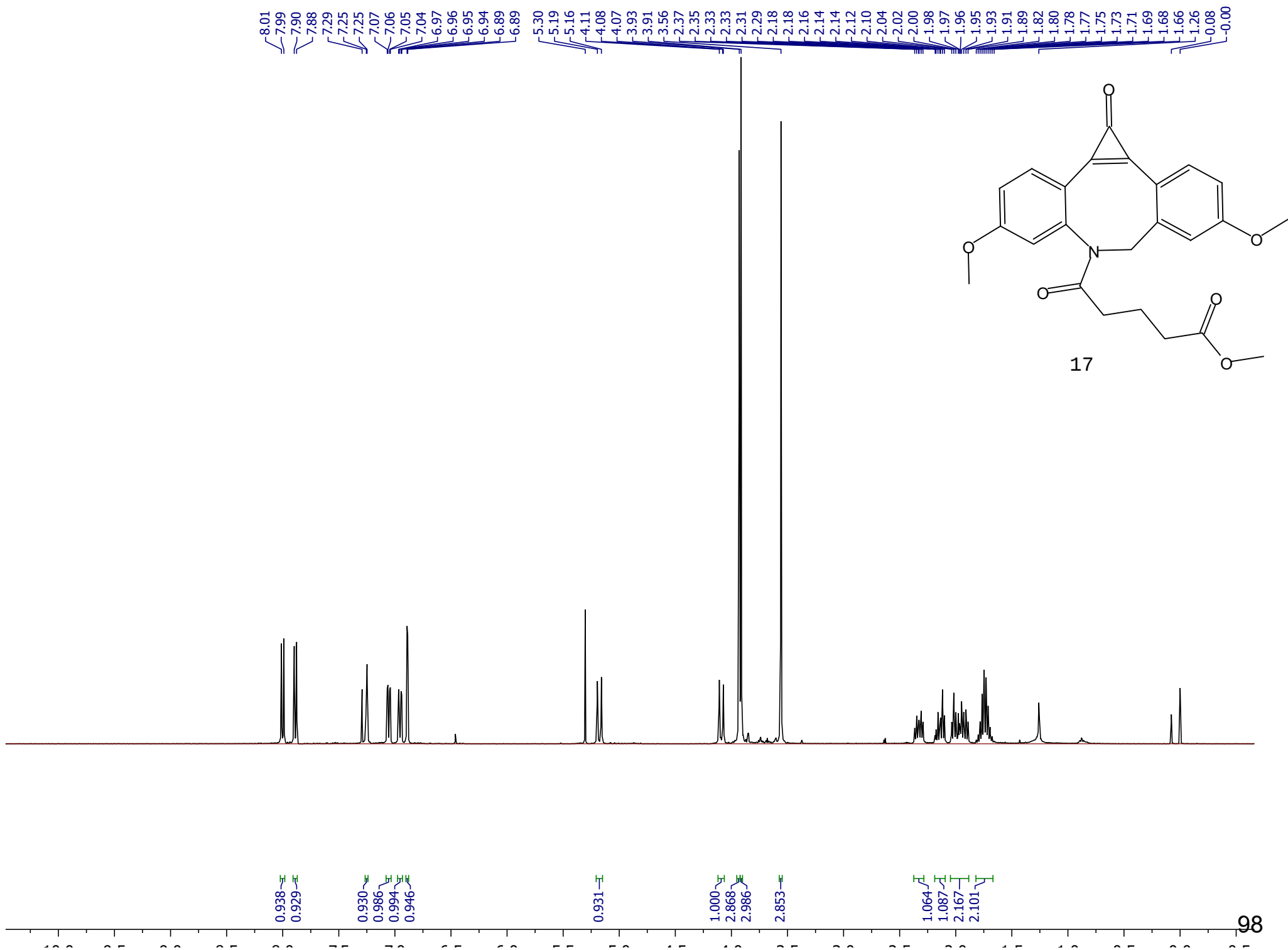
55.29
55.15
52.83
51.40

33.24
33.16

20.72



16



173.14
172.49

162.89
162.55

152.41

145.81

143.14

141.45

138.91

135.65

135.07

118.08

115.43

115.22

114.87

113.74

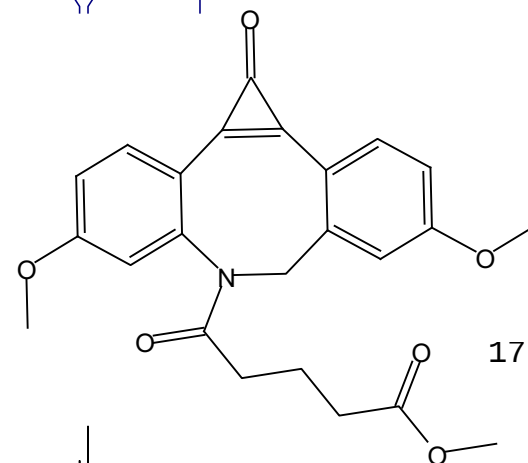
113.57

77.42
77.00
76.58

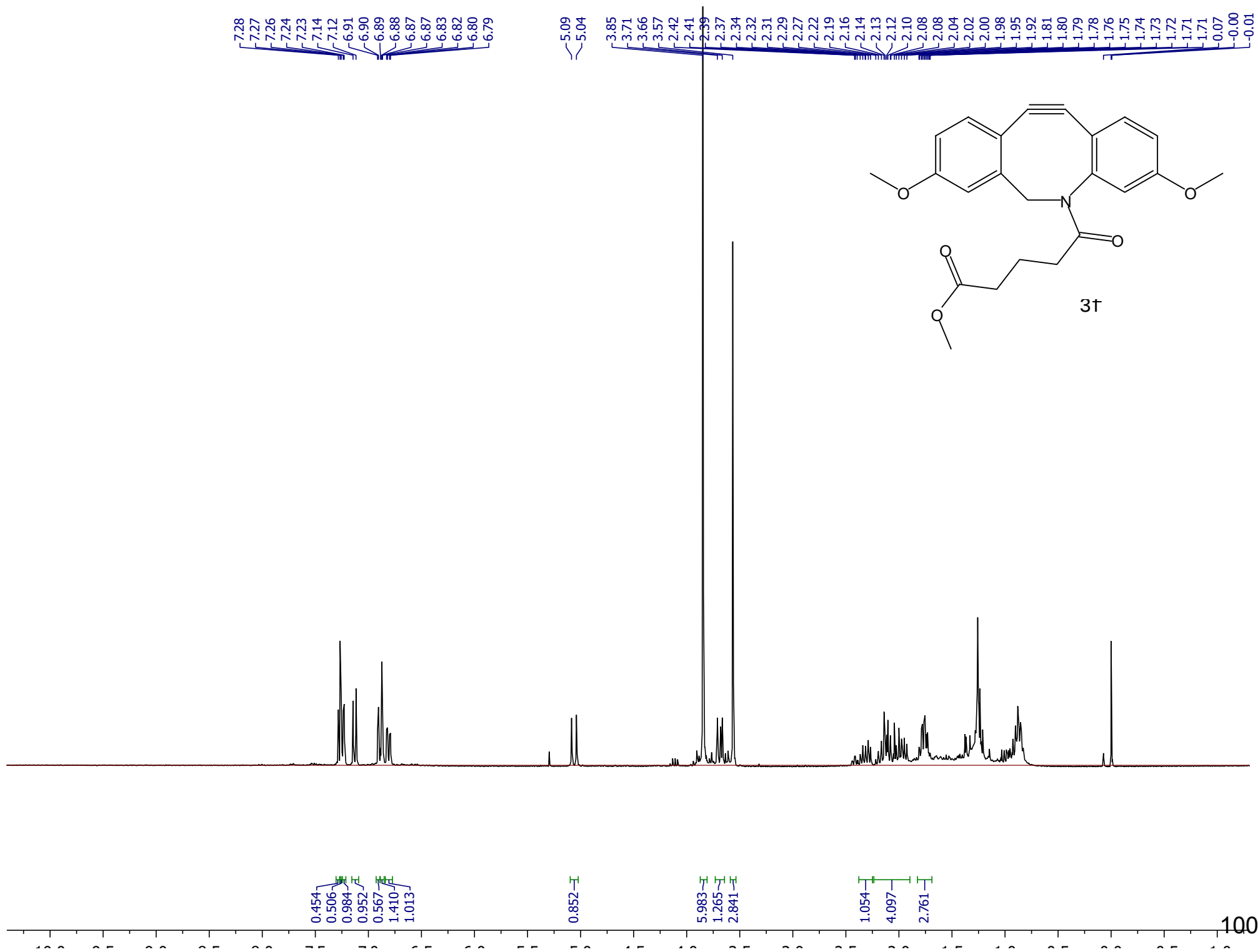
56.00
55.84
55.49
51.40

33.38
32.48

20.47



17



173.46
172.64

159.34
159.28

152.39
149.55

127.23
126.08
118.27
115.83
115.13
114.95
113.91
113.29
113.12
106.46

77.42
77.00
76.58

55.60
55.31
51.34

33.59
32.82

20.60

