

Supporting Information File 2

for

Synthesis and chemosensing properties of cinnoline-containing poly(arylene ethynylene)s

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Email: Irina A. Balova* - balova.irina@chem.spbu.ru

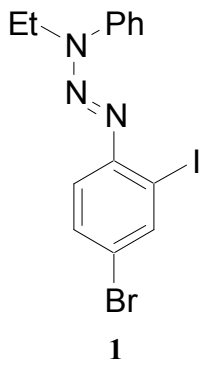
*Corresponding author

Copies of ^1H and ^{13}C NMR spectra for all compounds, copies of DEPT and 2D NMR spectra for compounds 5a,b and 7, copies of IR spectra for compounds 4a,b; 5,b; 7 and 10a,b, copies of GPC chromatograms for PAEs 10a,b.

Table of contents

Copies of NMR and IR spectra – S2

Copies of GPC chromatograms – S45



¹H NMR, 400 MHz

8.06
8.05
7.49
7.38
7.20
7.19
7.17

4.41
4.39
4.38
4.36

1.43
1.41
1.40

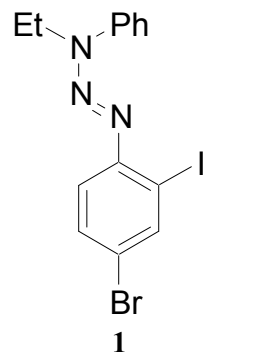
0.94
6.03
1.00

2.05

3.08

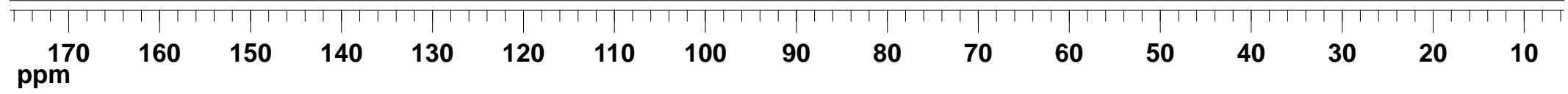
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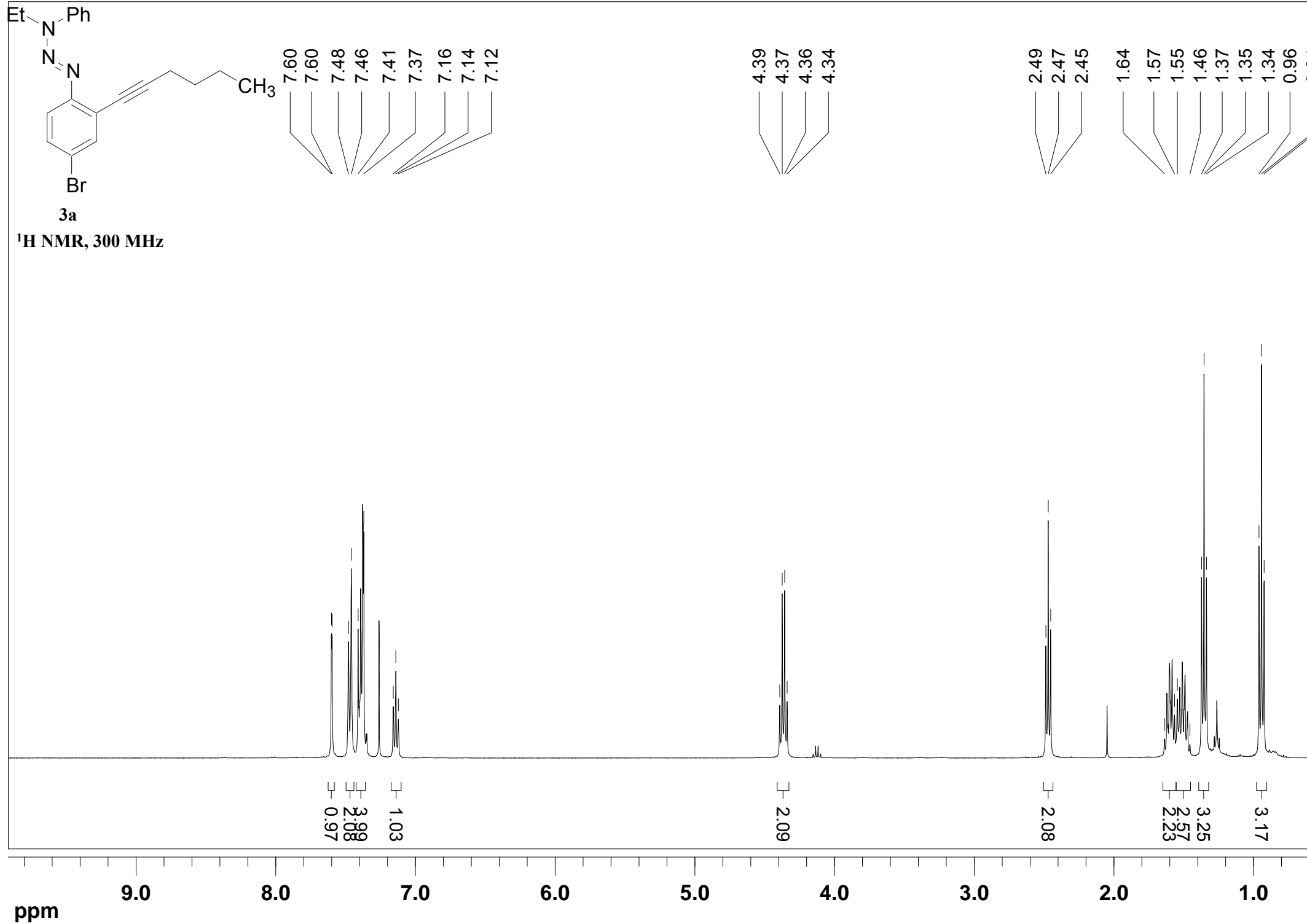
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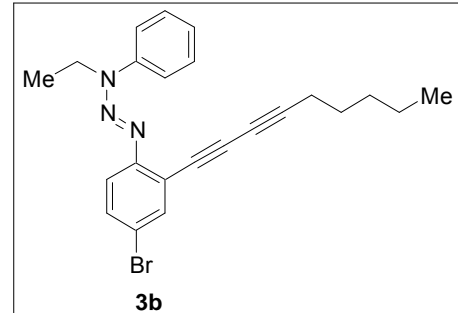


¹³C NMR, 100 MHz

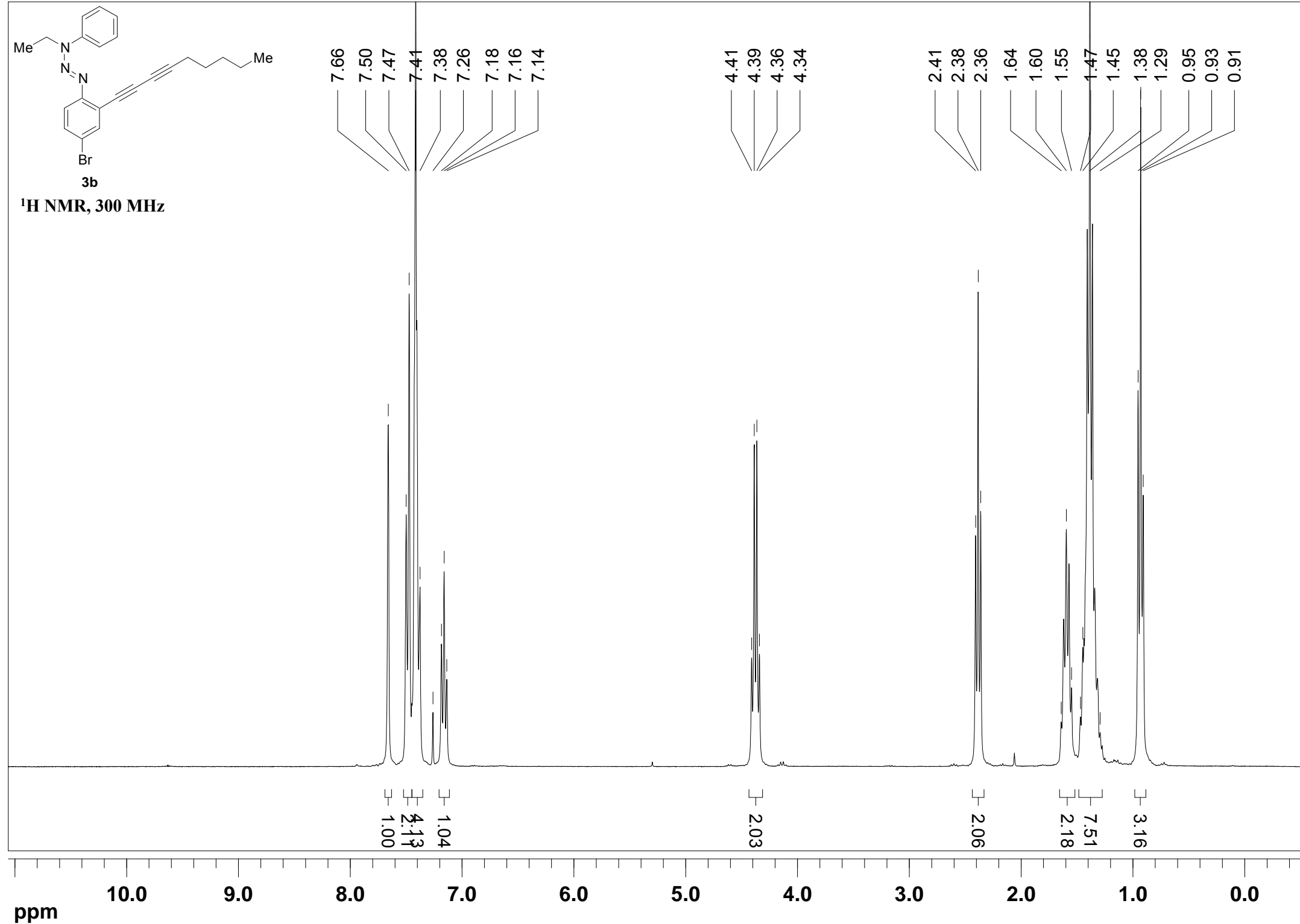
- 148.85
- 143.73
- 140.99
- 131.74
- 129.26
- 124.10
- 119.94
- 118.74
- 117.04
- 98.02
- 41.18
- 10.92

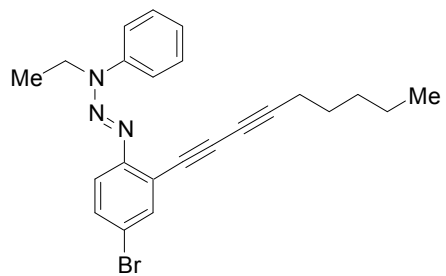






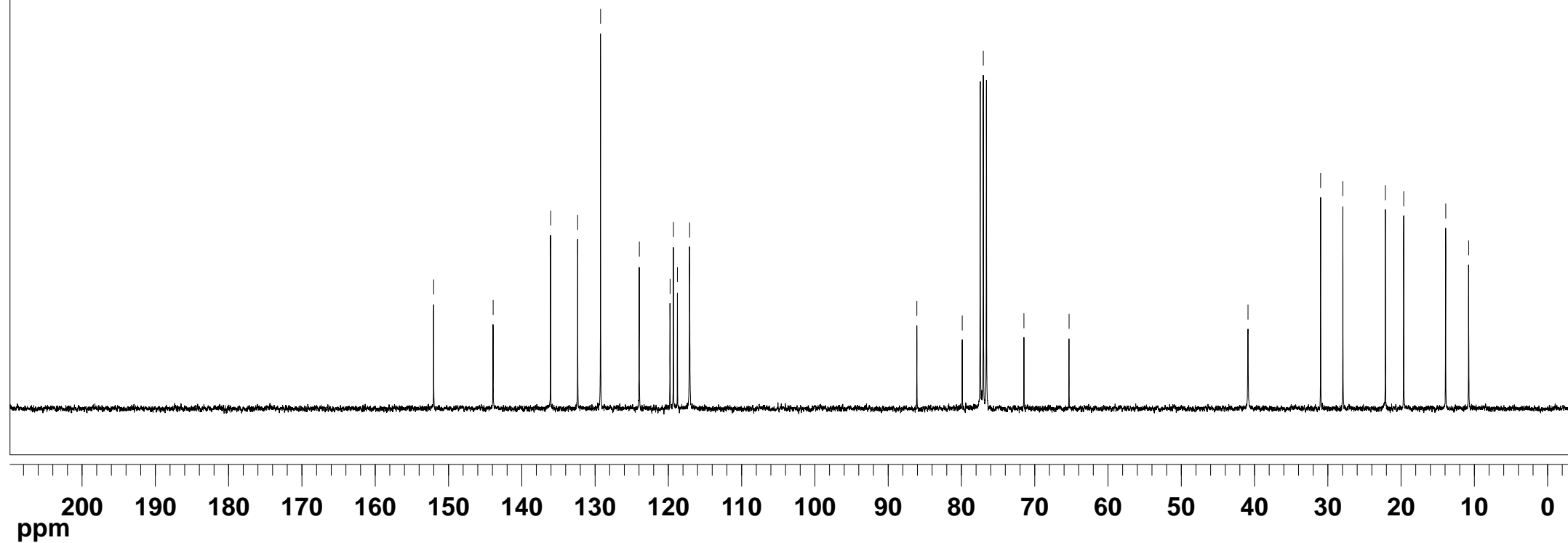
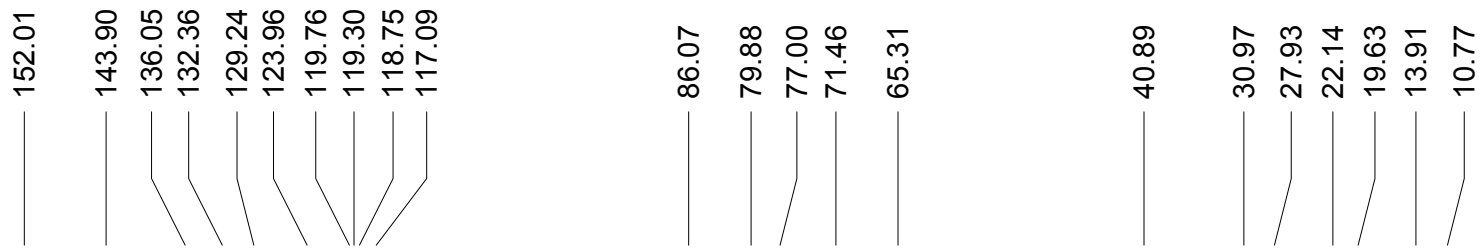
¹H NMR, 300 MHz

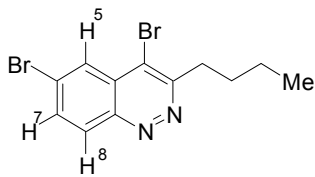




3b

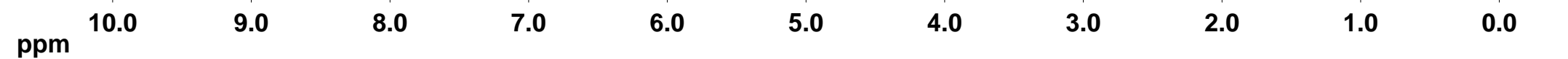
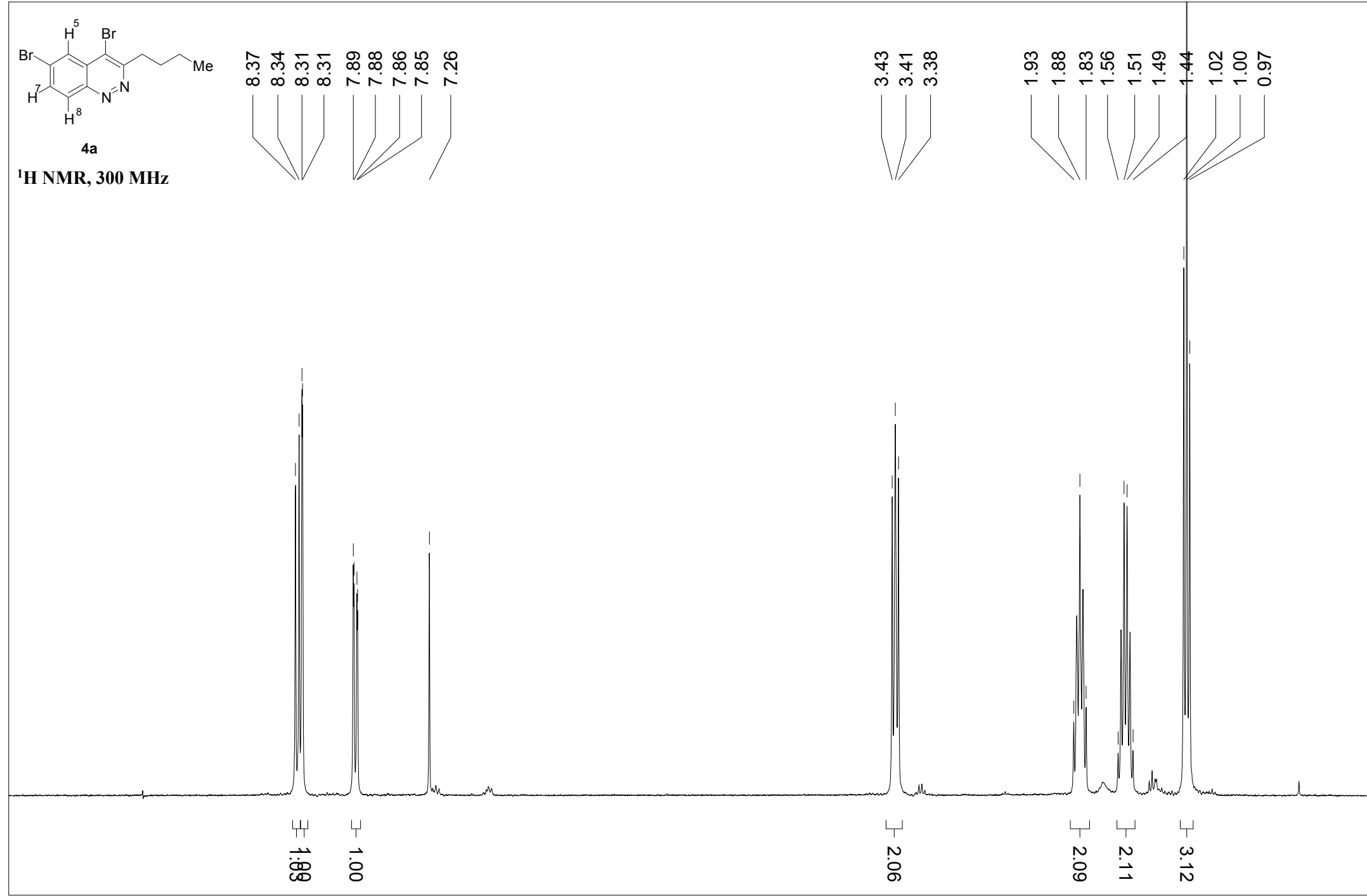
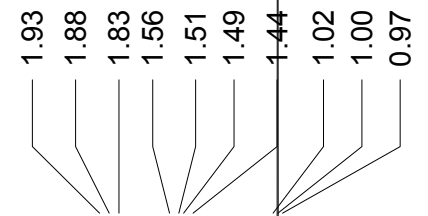
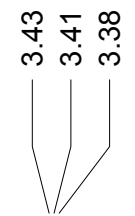
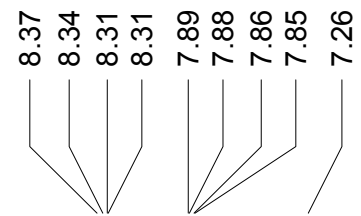
¹³C NMR, 75 MHz

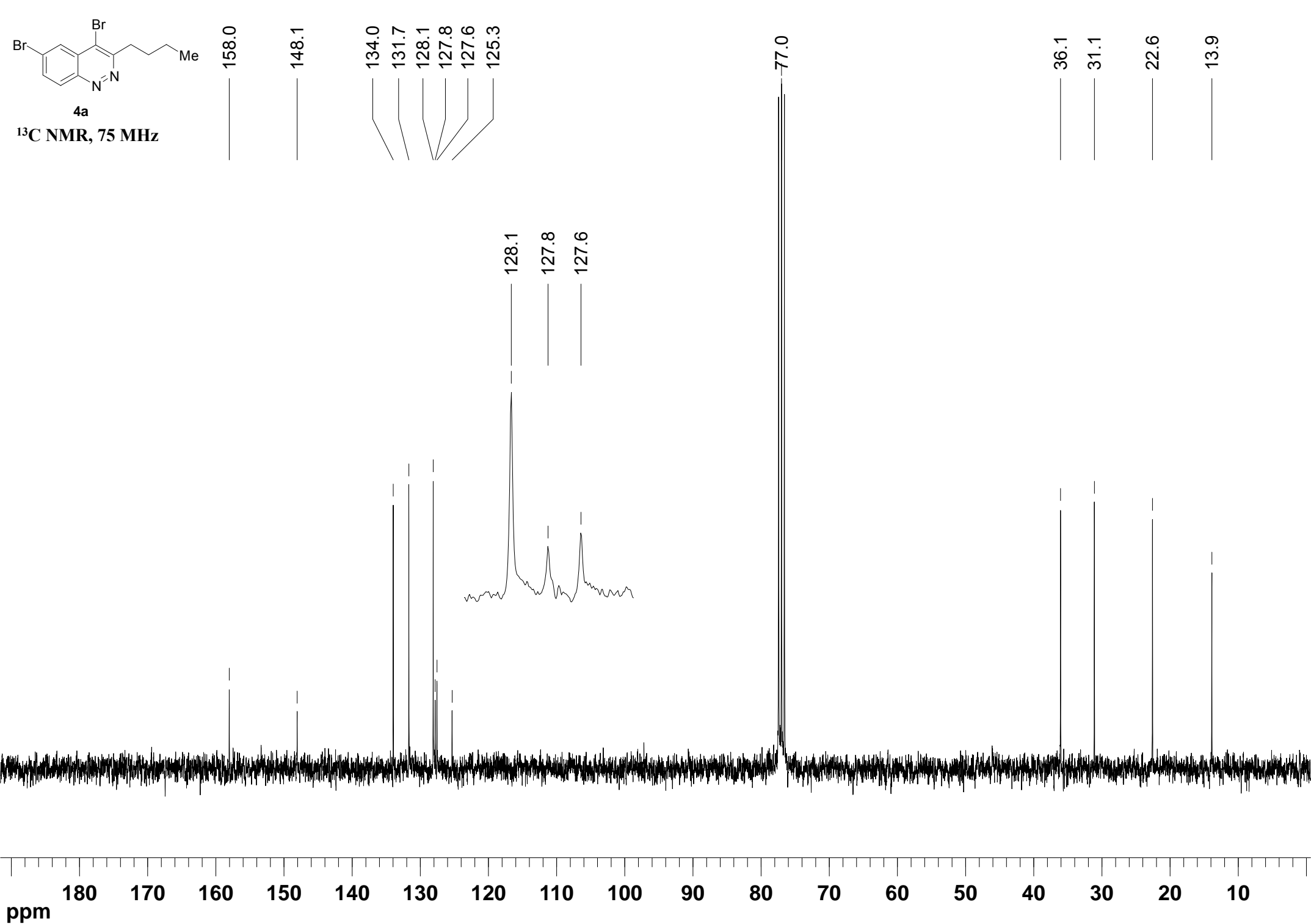


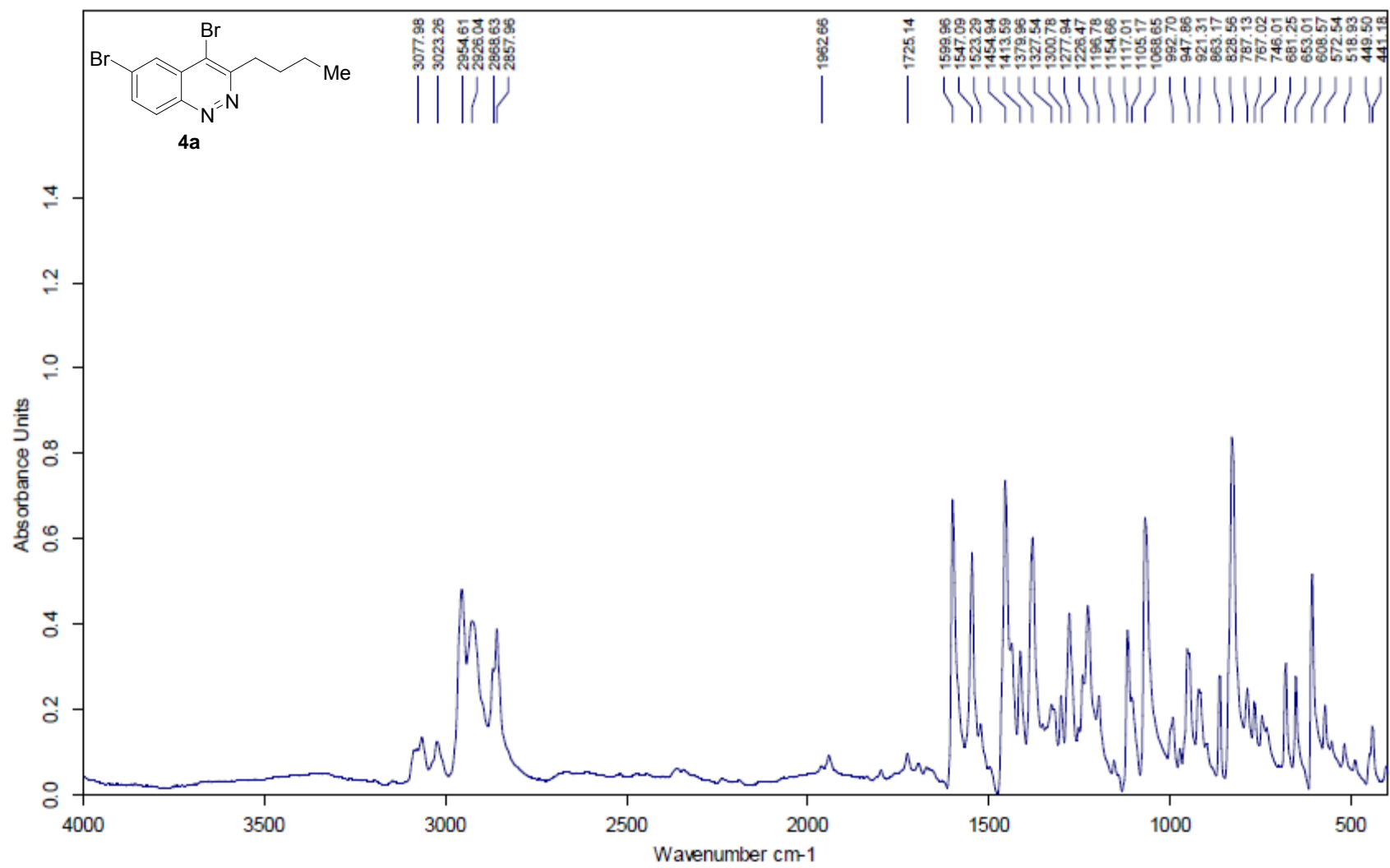


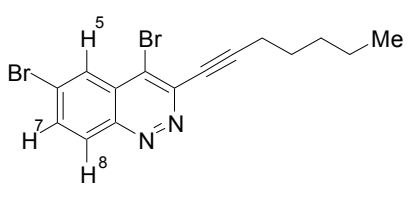
4a

¹H NMR, 300 MHz







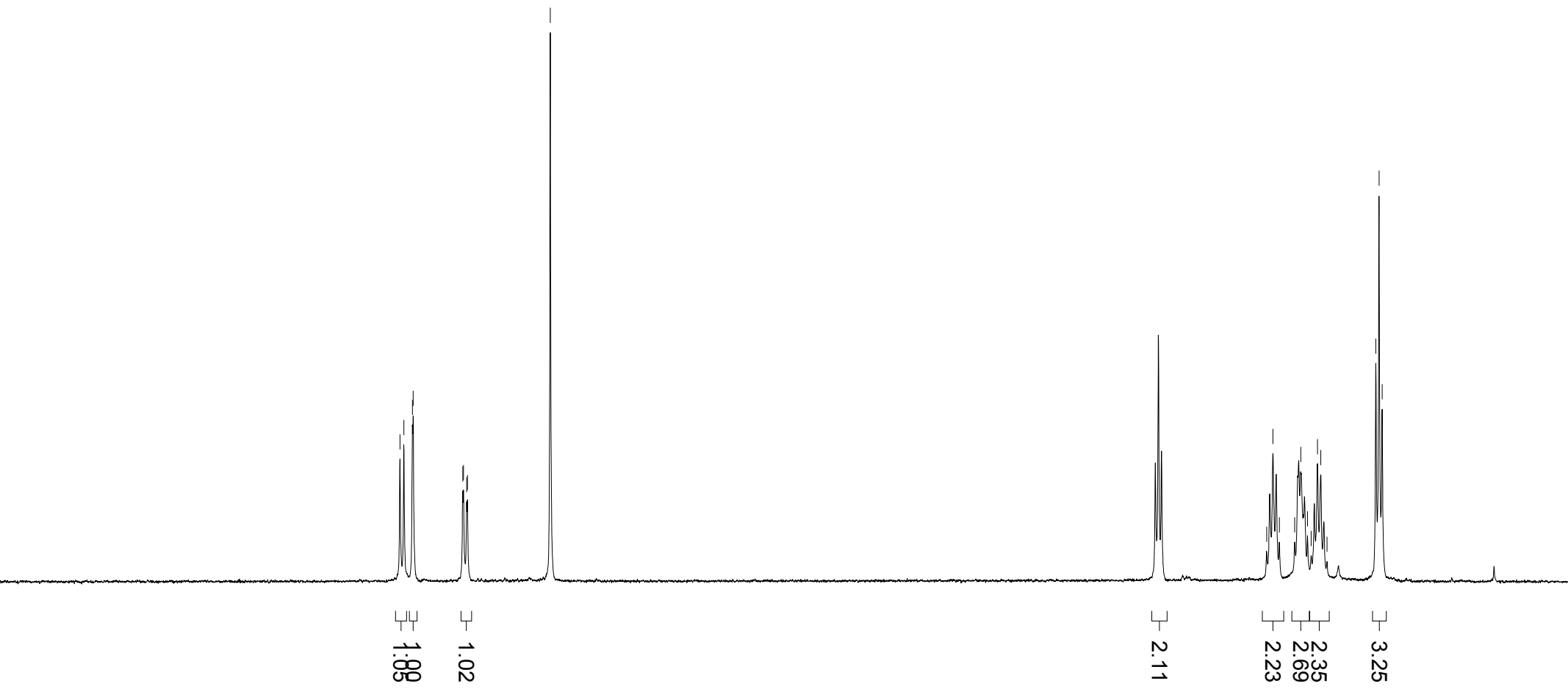


4b

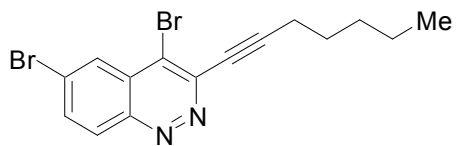
¹H NMR, 300 MHz

8.41
8.38
8.31
8.30
7.93
7.92
7.90
7.89
7.26

1.80
1.75
1.70
1.59
1.54
1.49
1.46
1.41
1.39
1.34
0.97
0.94
0.92



11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm



4b

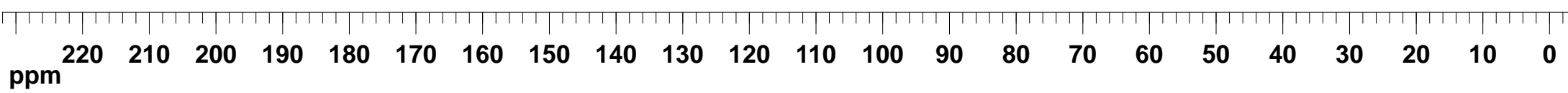
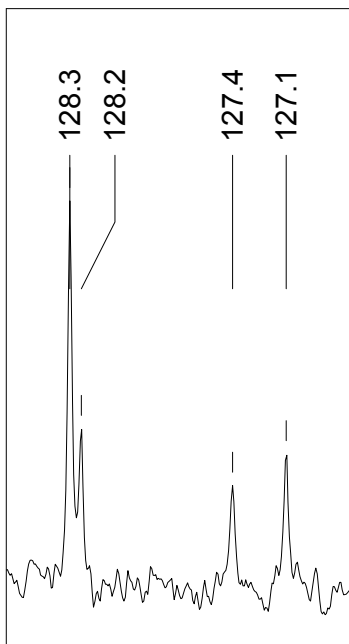
¹³C NMR, 75 MHz

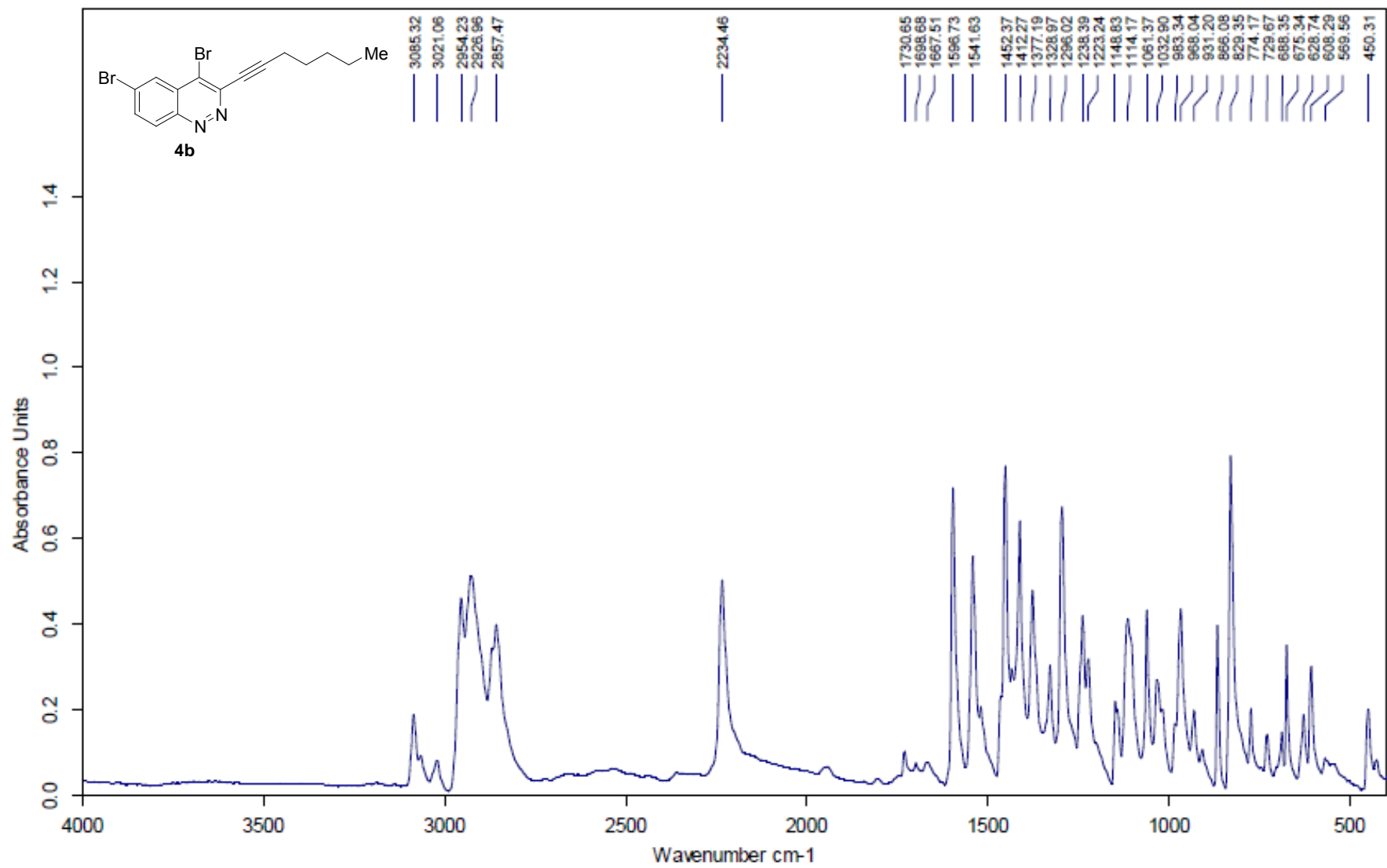
146.9
143.6
134.8
131.9
128.3
128.2
127.4
127.1

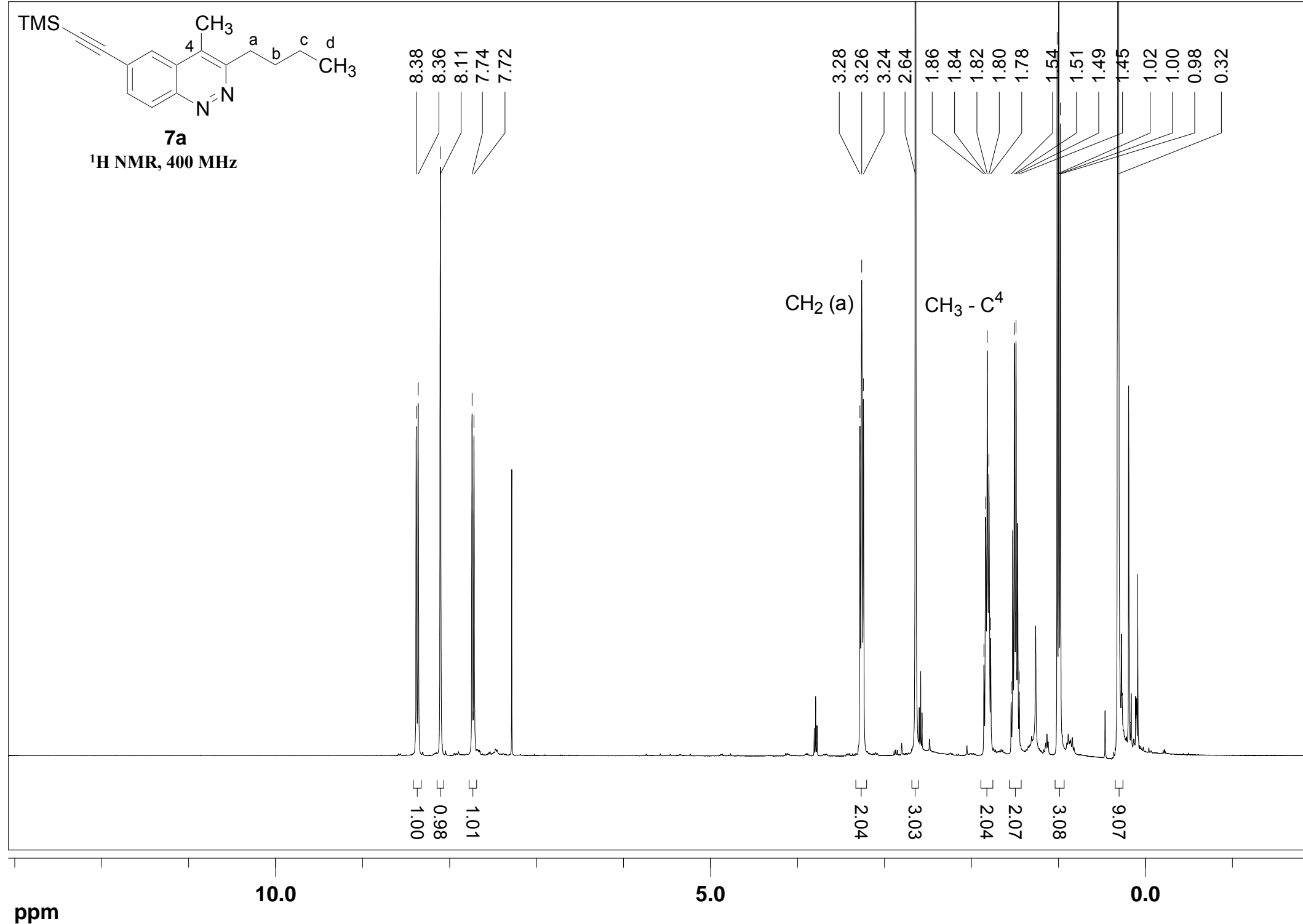
101.0

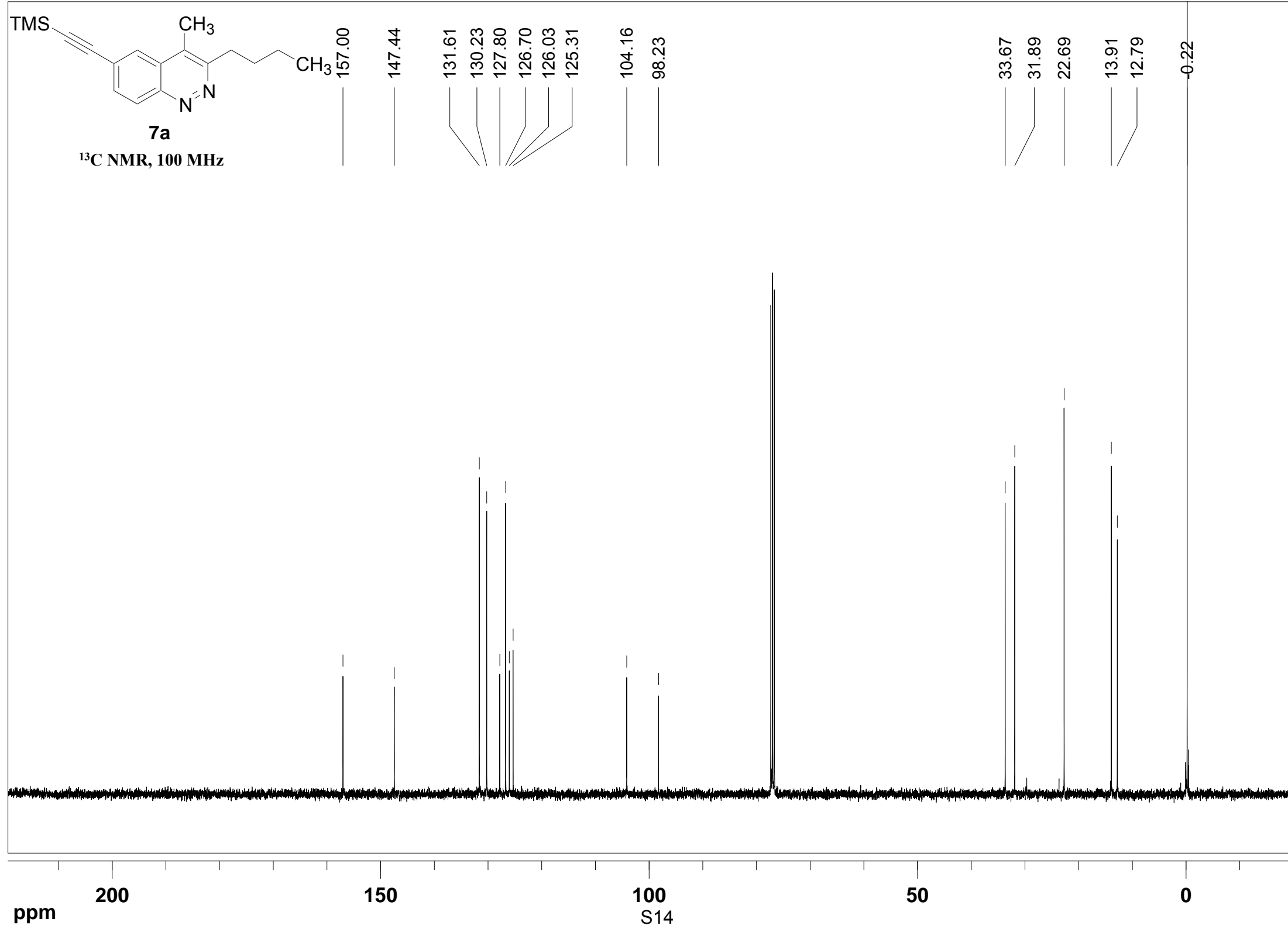
77.8
77.0

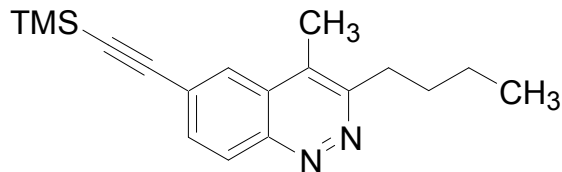
31.1
27.8
22.2
19.8
14.0











7a

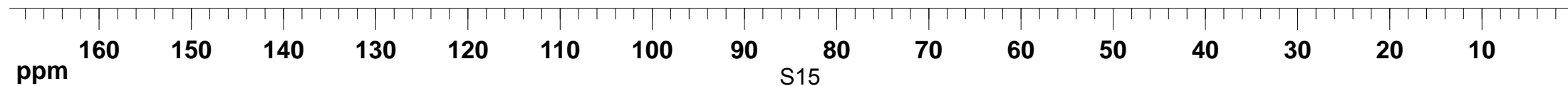
DEPT 135 NMR

131.66
130.28
126.75

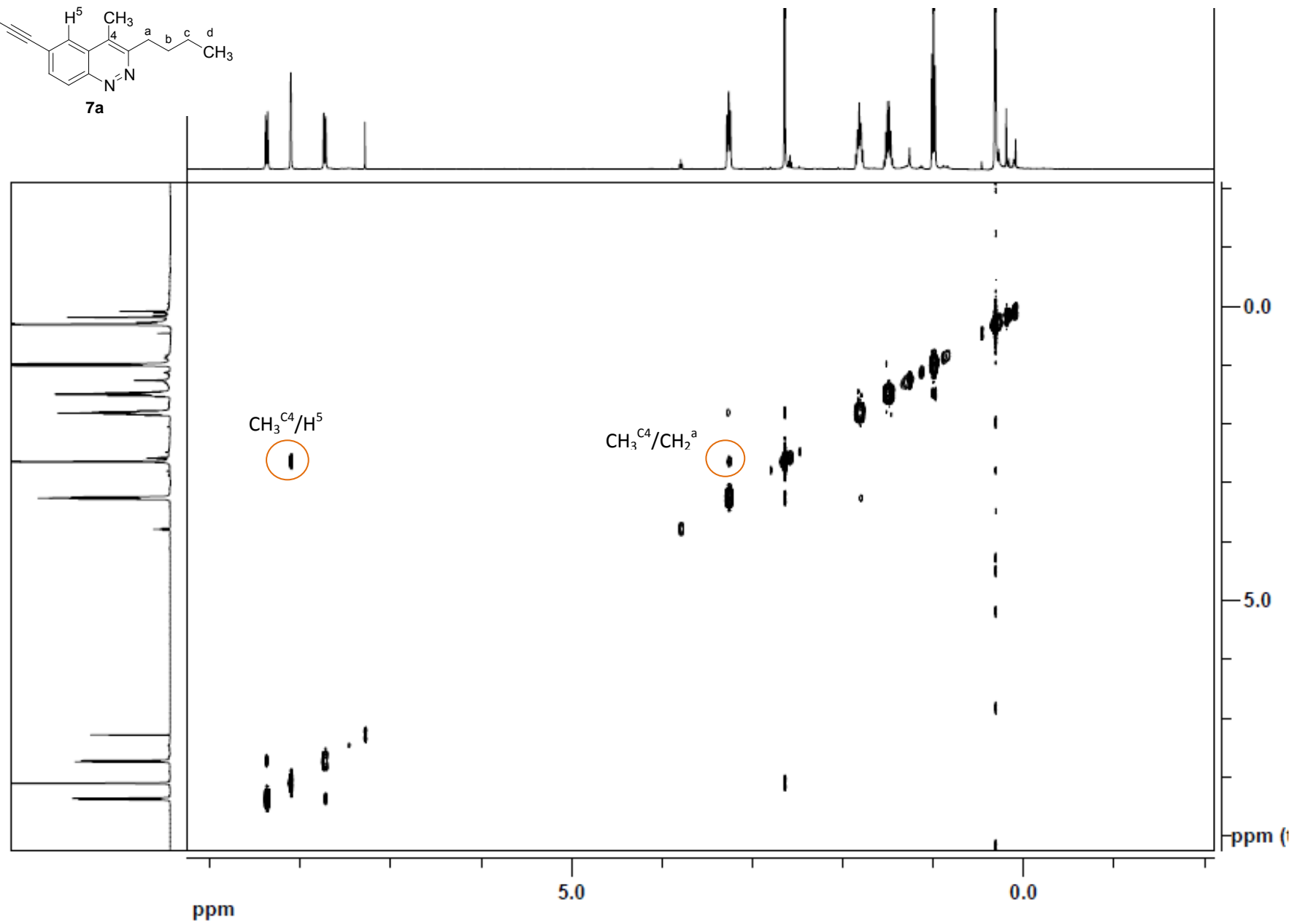
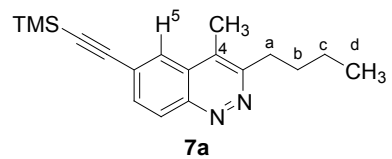
33.72
31.94

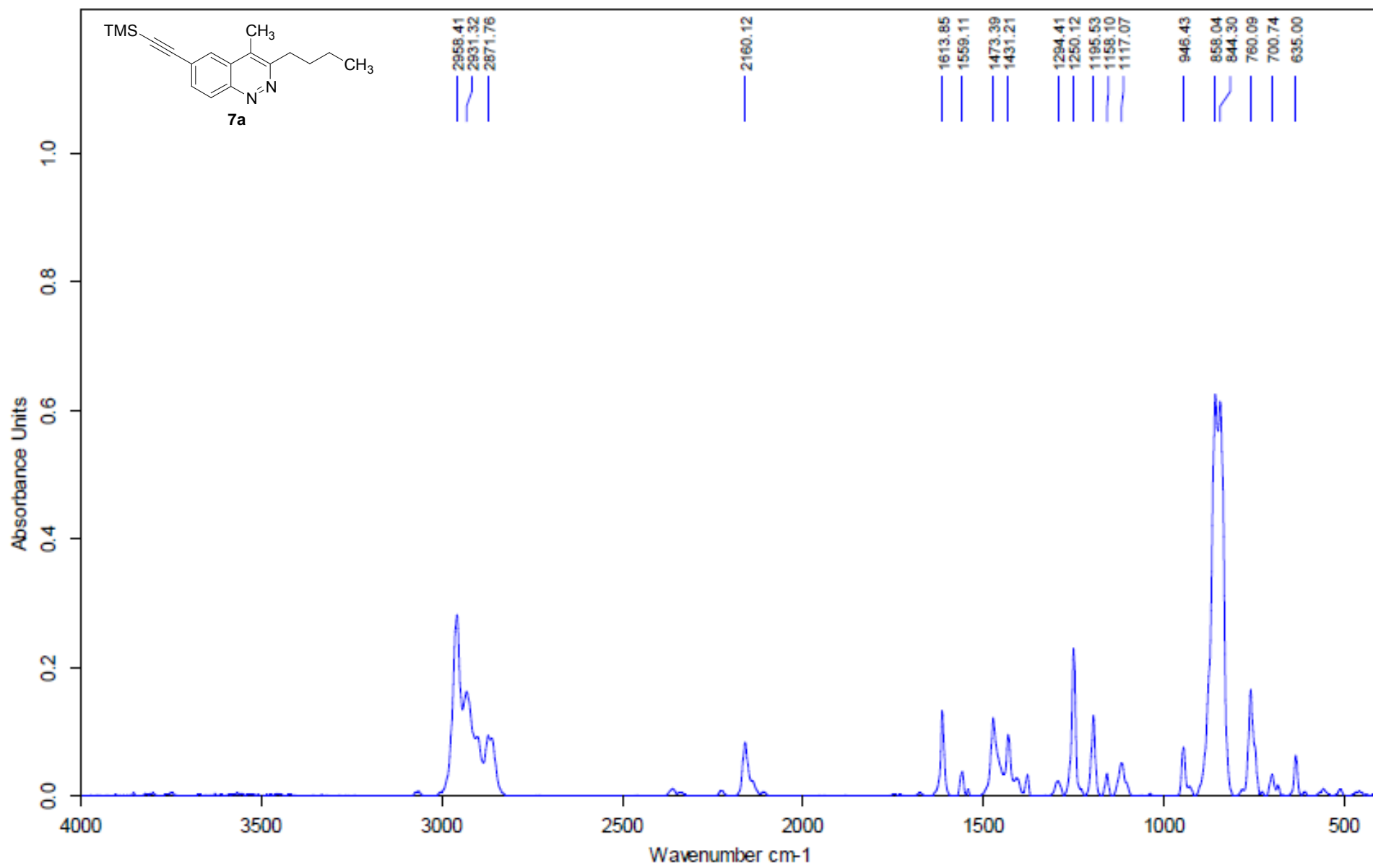
22.74

13.95
12.84



NOESY NMR



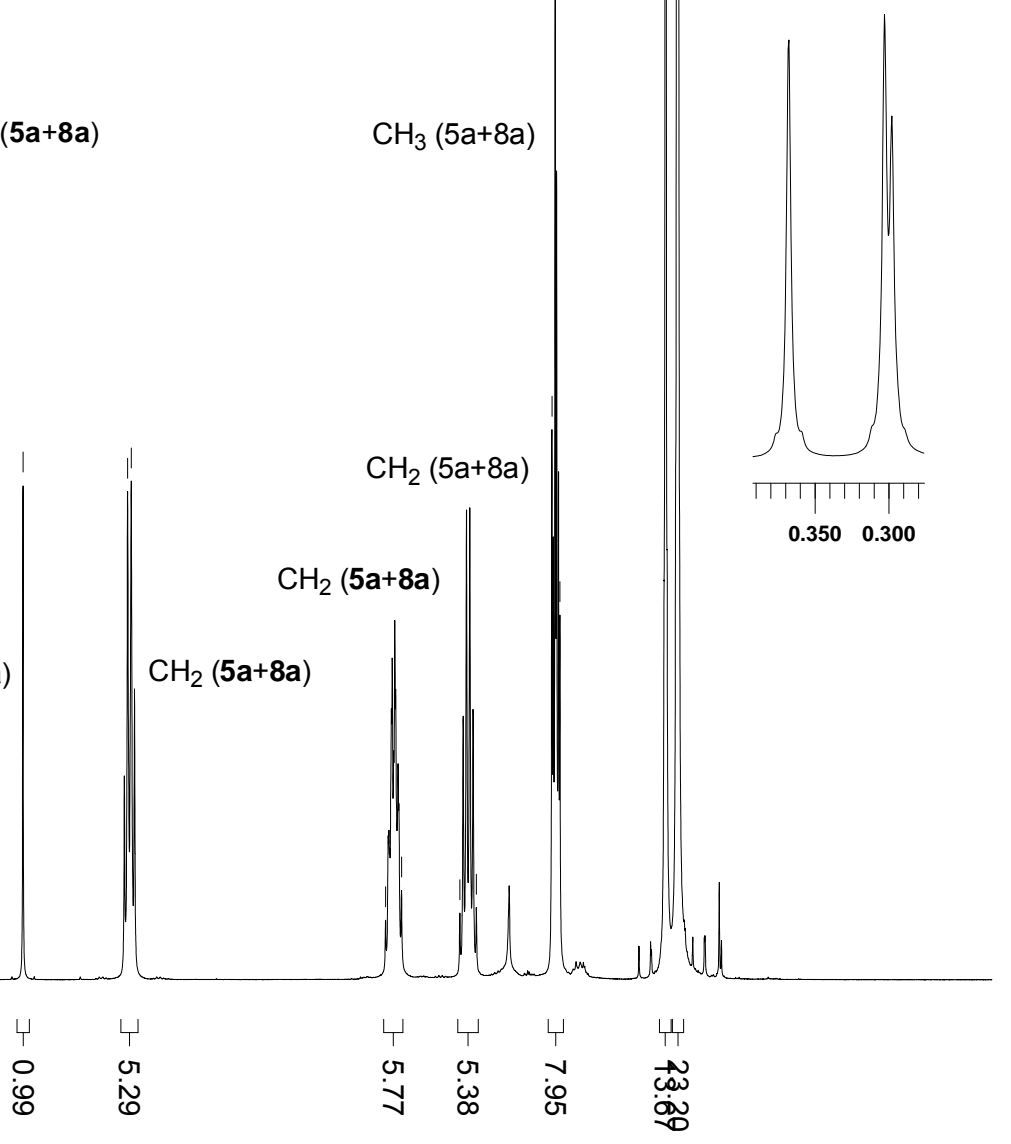
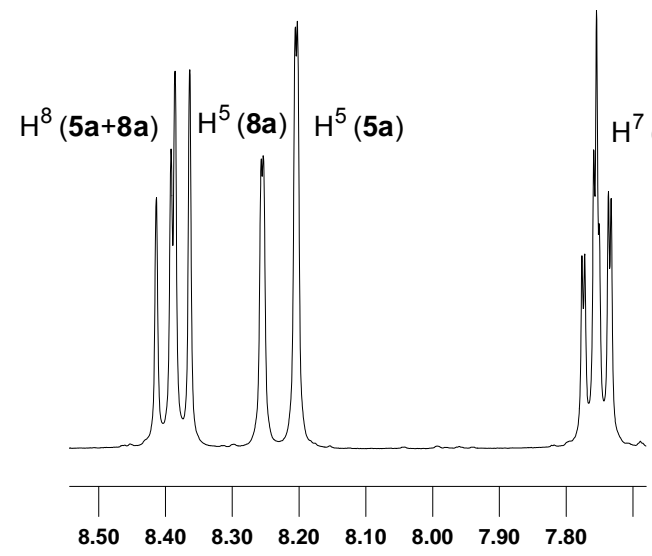
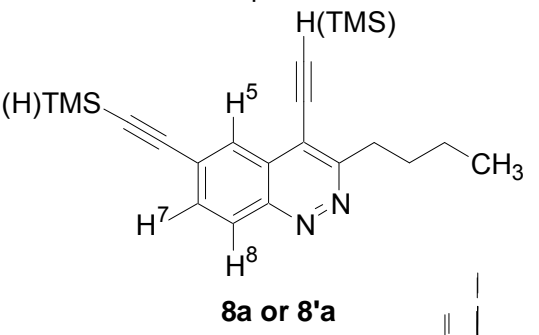
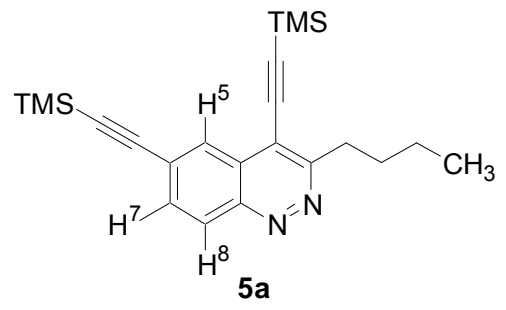


¹H NMR, 400 MHz

8.41
8.39
8.39
8.36
8.26
8.25
8.21
8.20
7.78
7.77
7.76
7.75
7.75
7.74
7.73

3.96
3.38
3.36

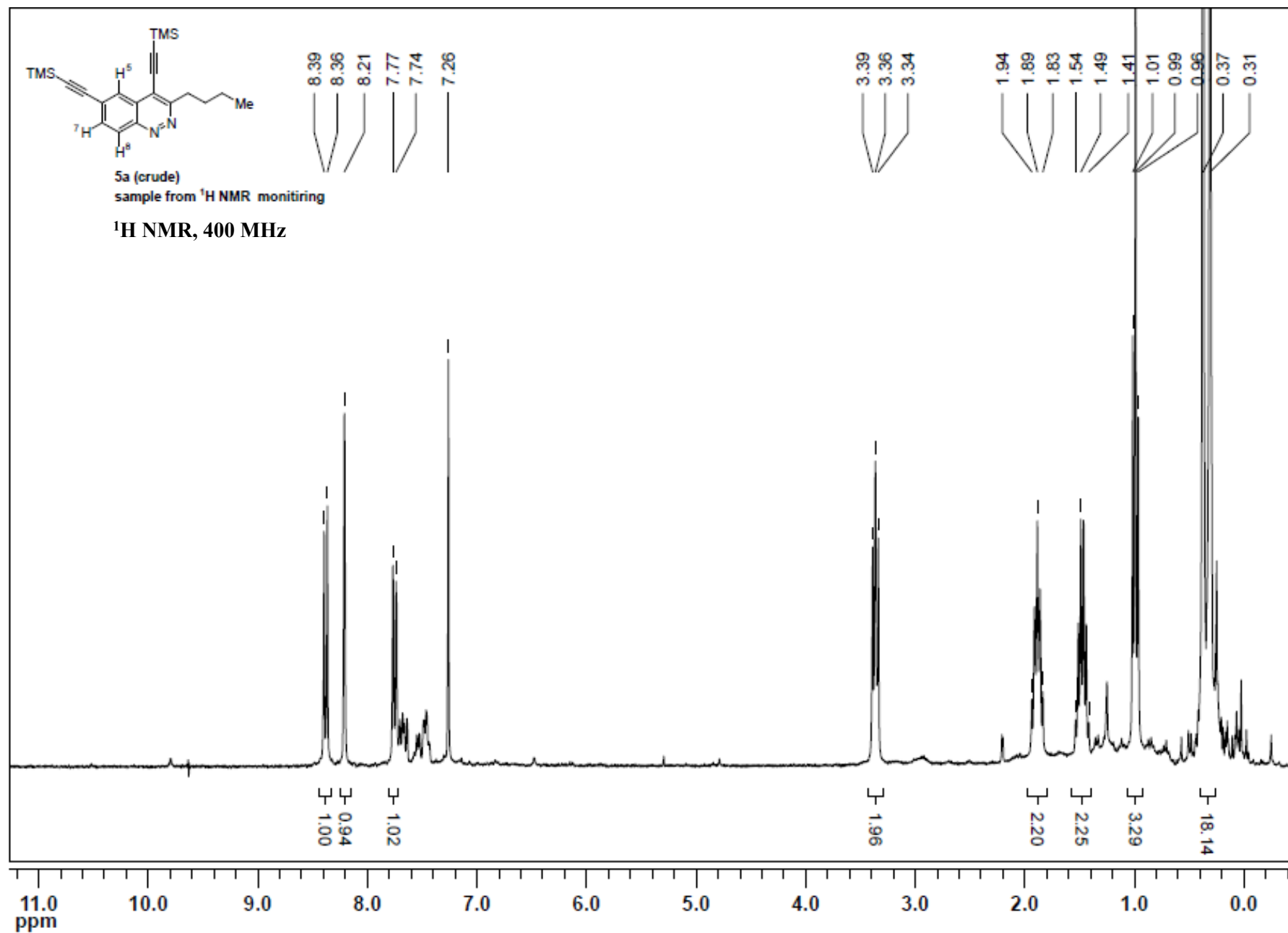
1.93
1.85
1.52
1.43
1.00
0.99
0.96
0.37
0.30
0.30

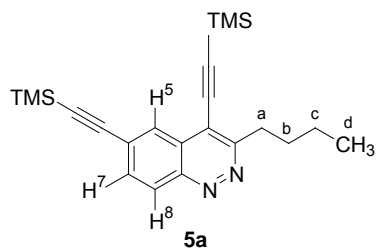


10.0
ppm

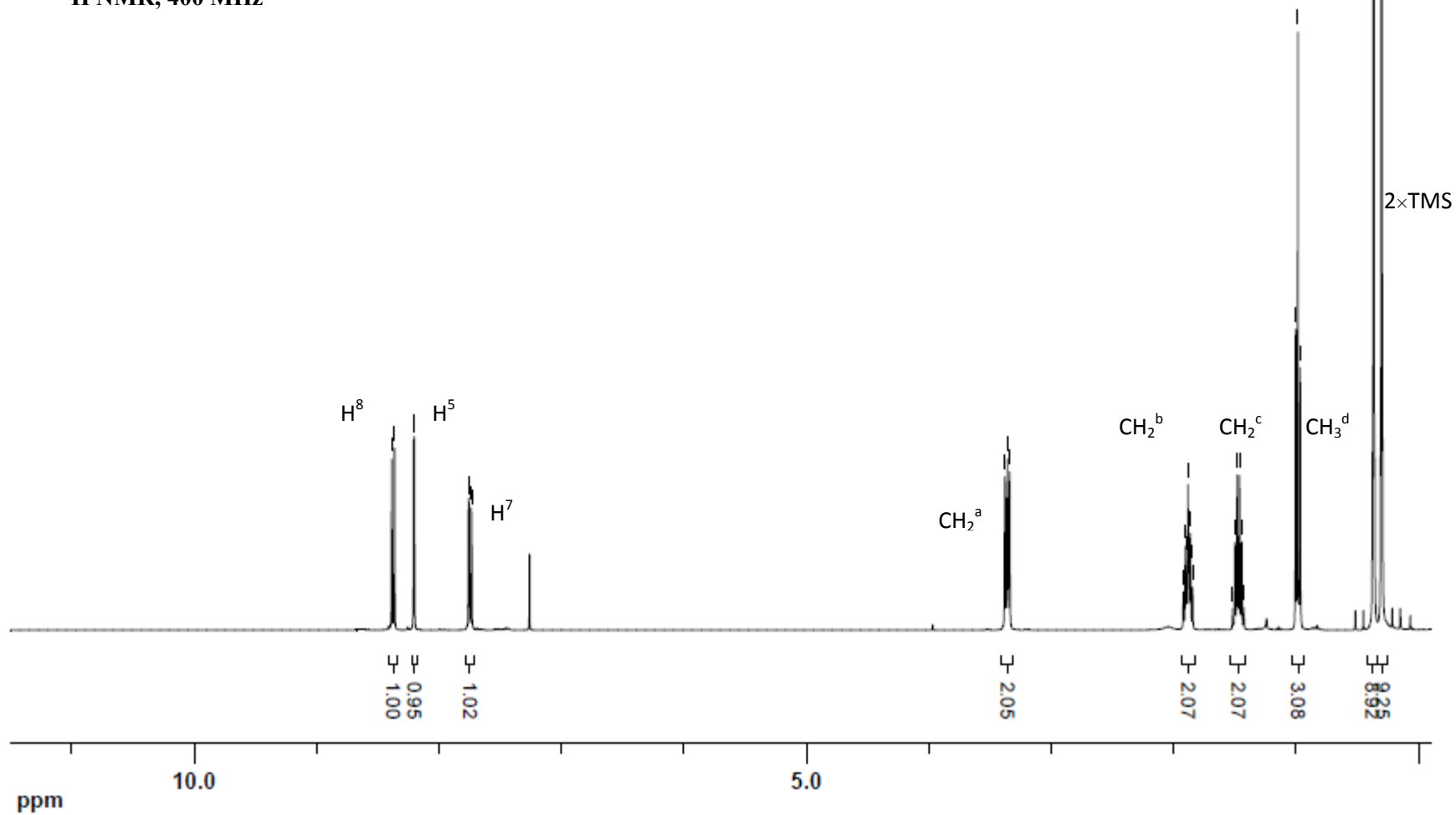
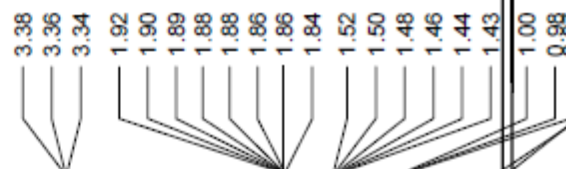
5.0
S18

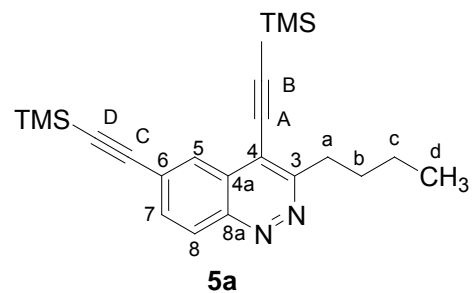
0.0



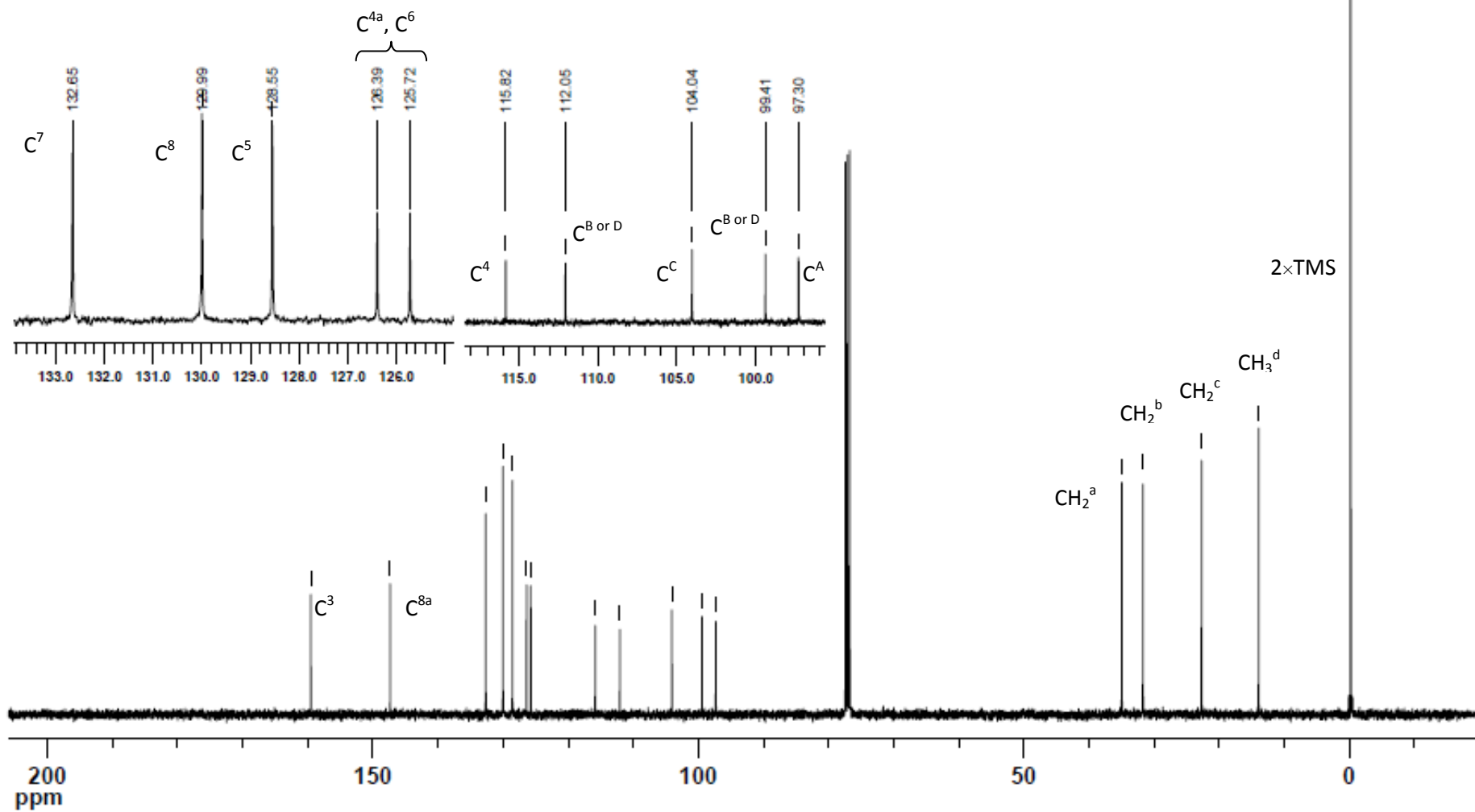


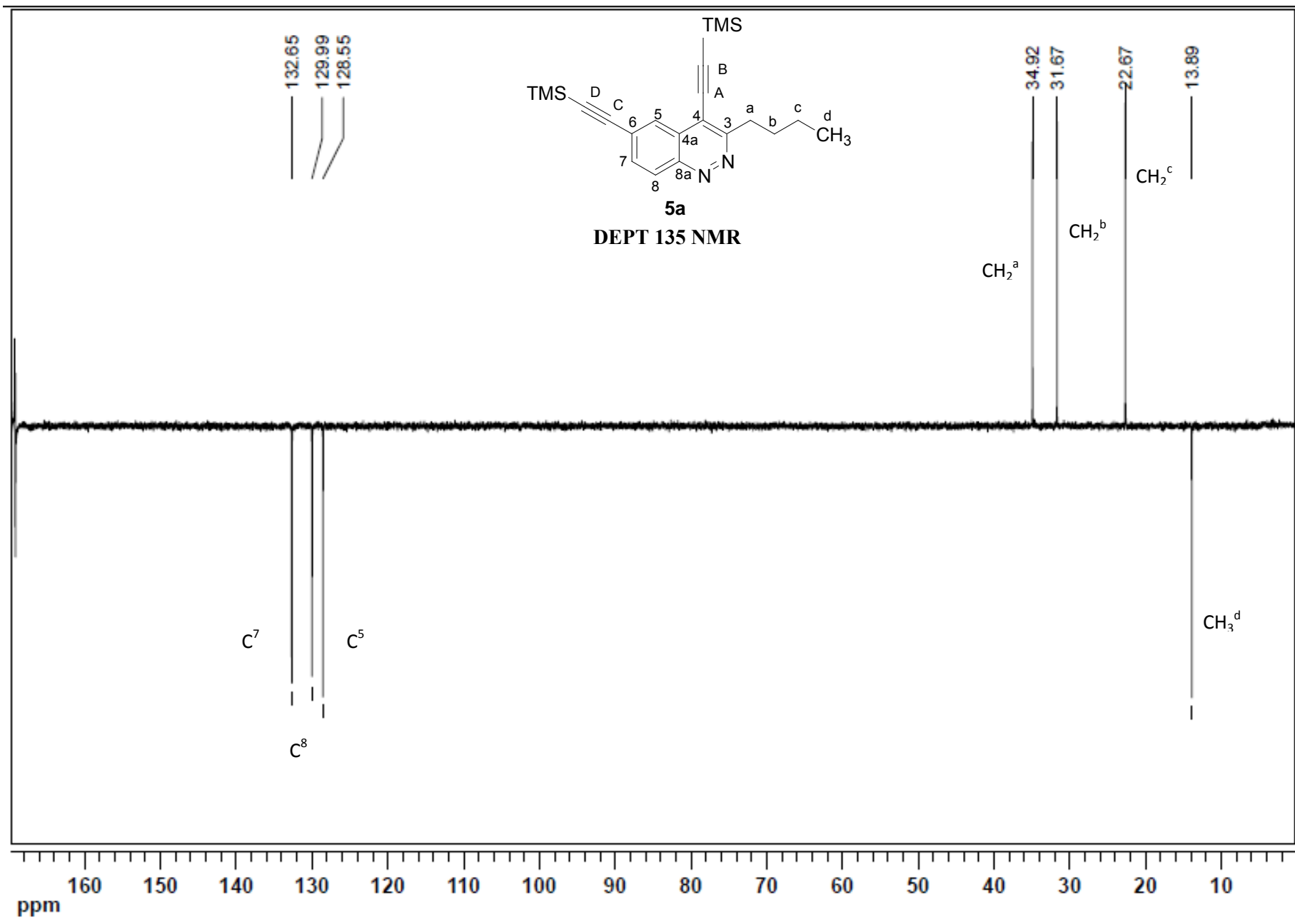
$^1\text{H NMR}$, 400 MHz



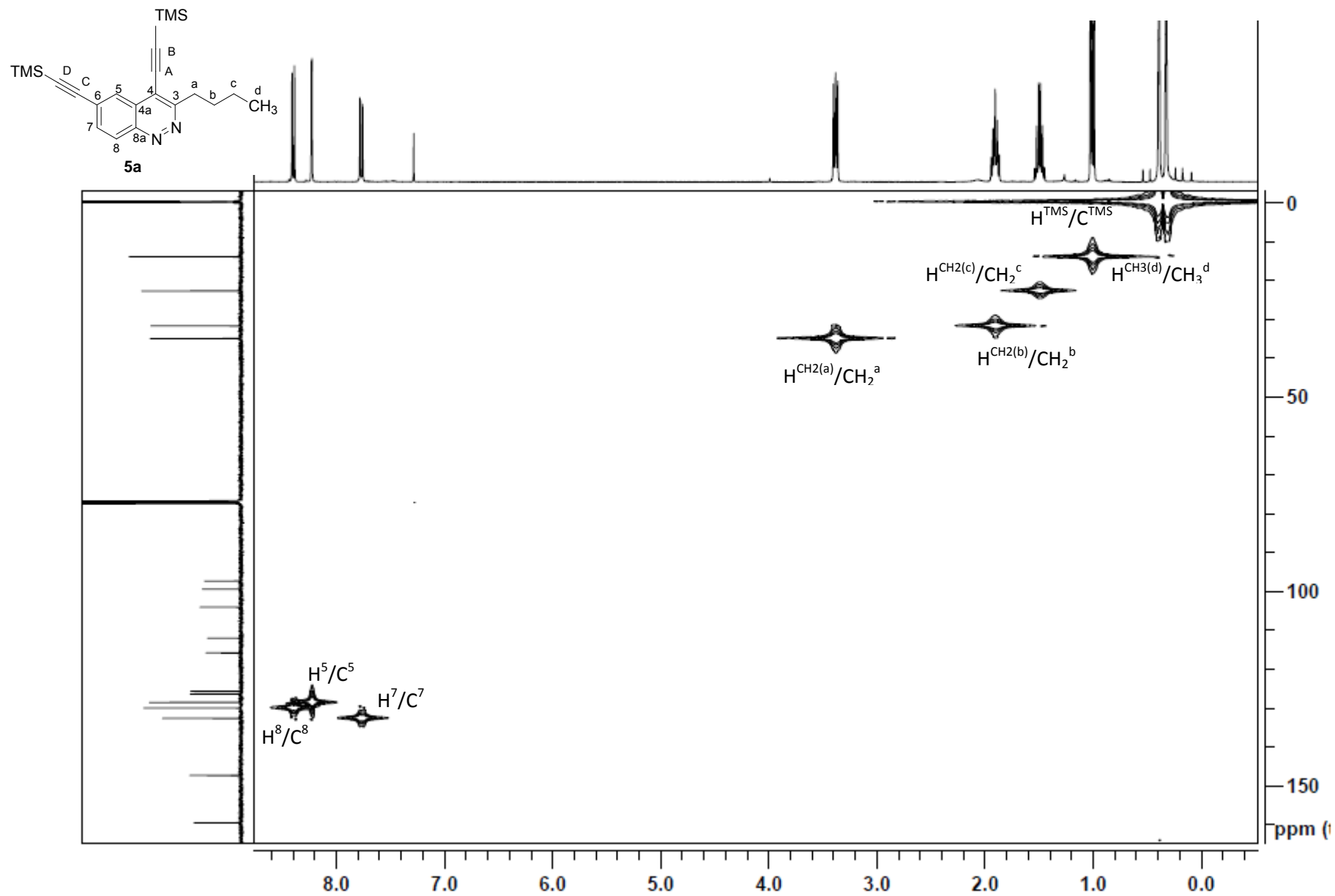


^{13}C NMR, 100 MHz

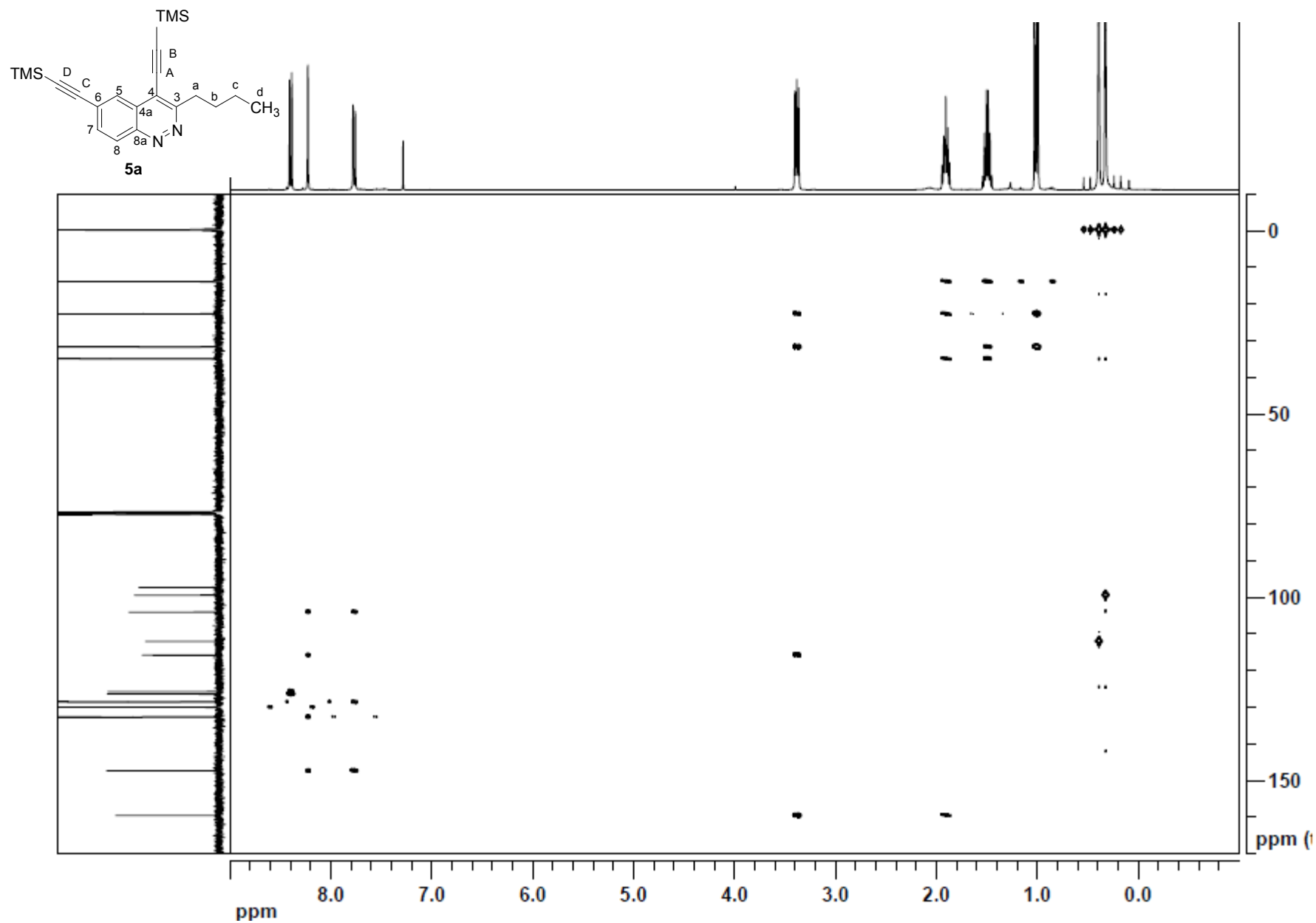




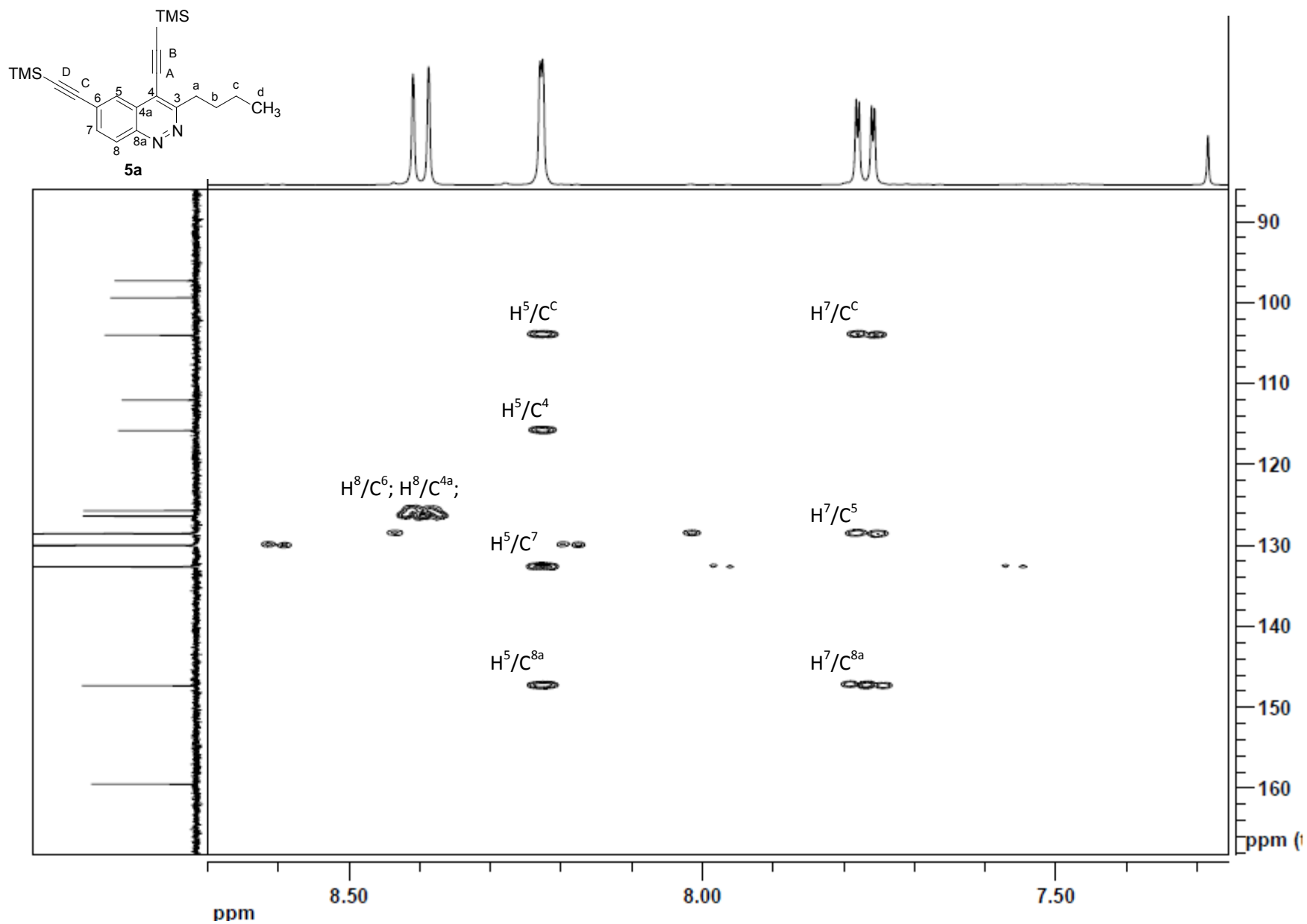
HSQC NMR



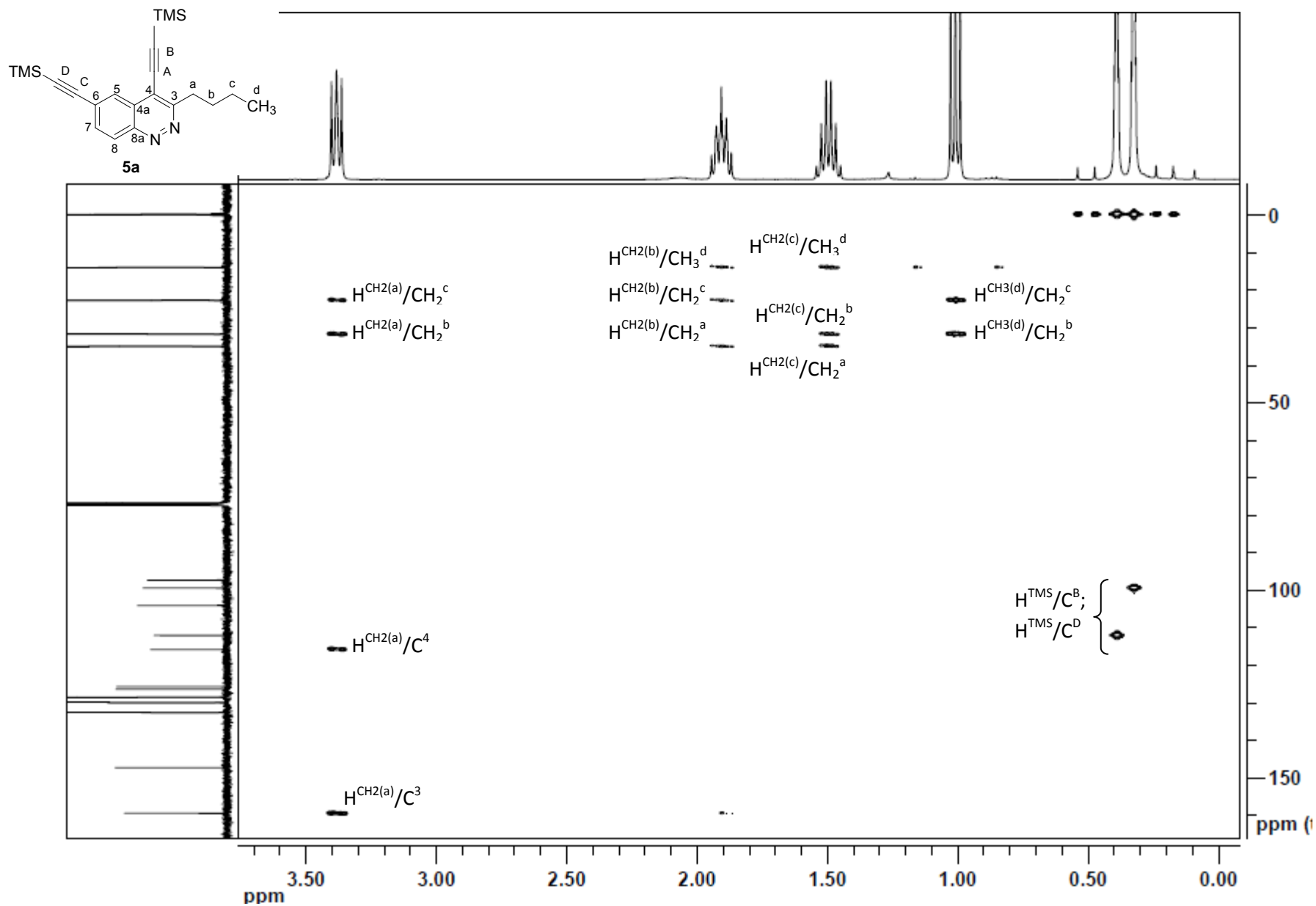
HMBC NMR

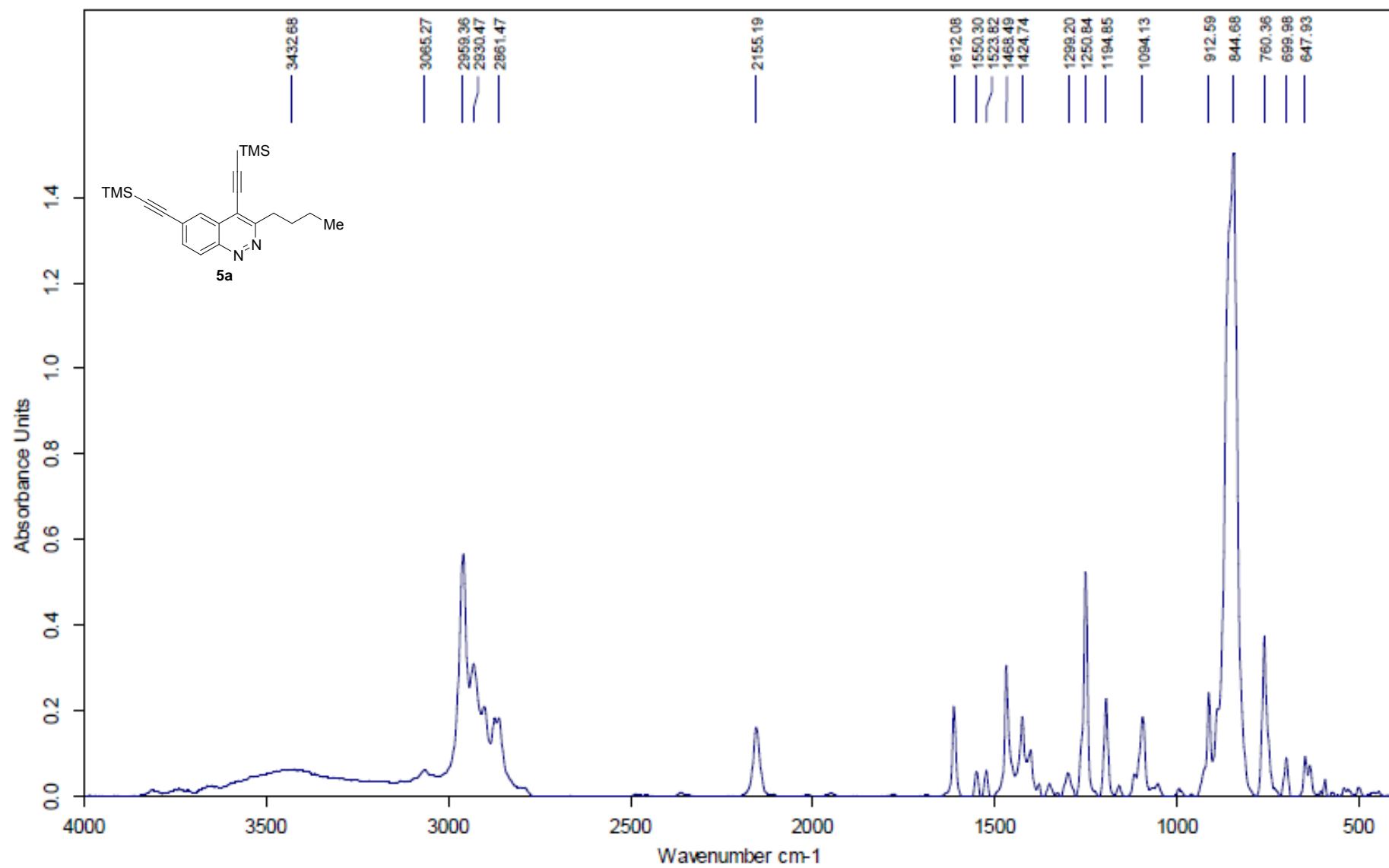


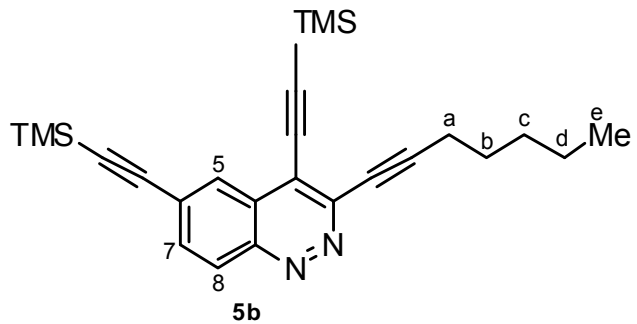
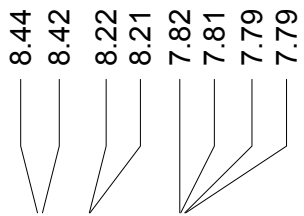
HMBC NMR (Zoom 1)



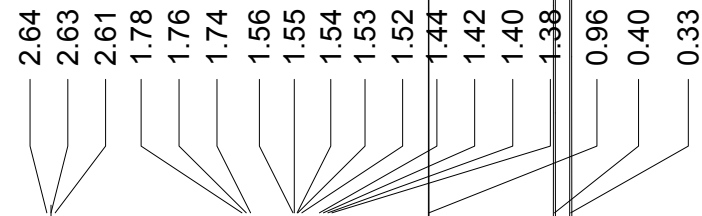
HMBC NMR (Zoom_1)







¹H NMR, 400 MHz



H⁸

H⁶

H⁷

a

b

c

d

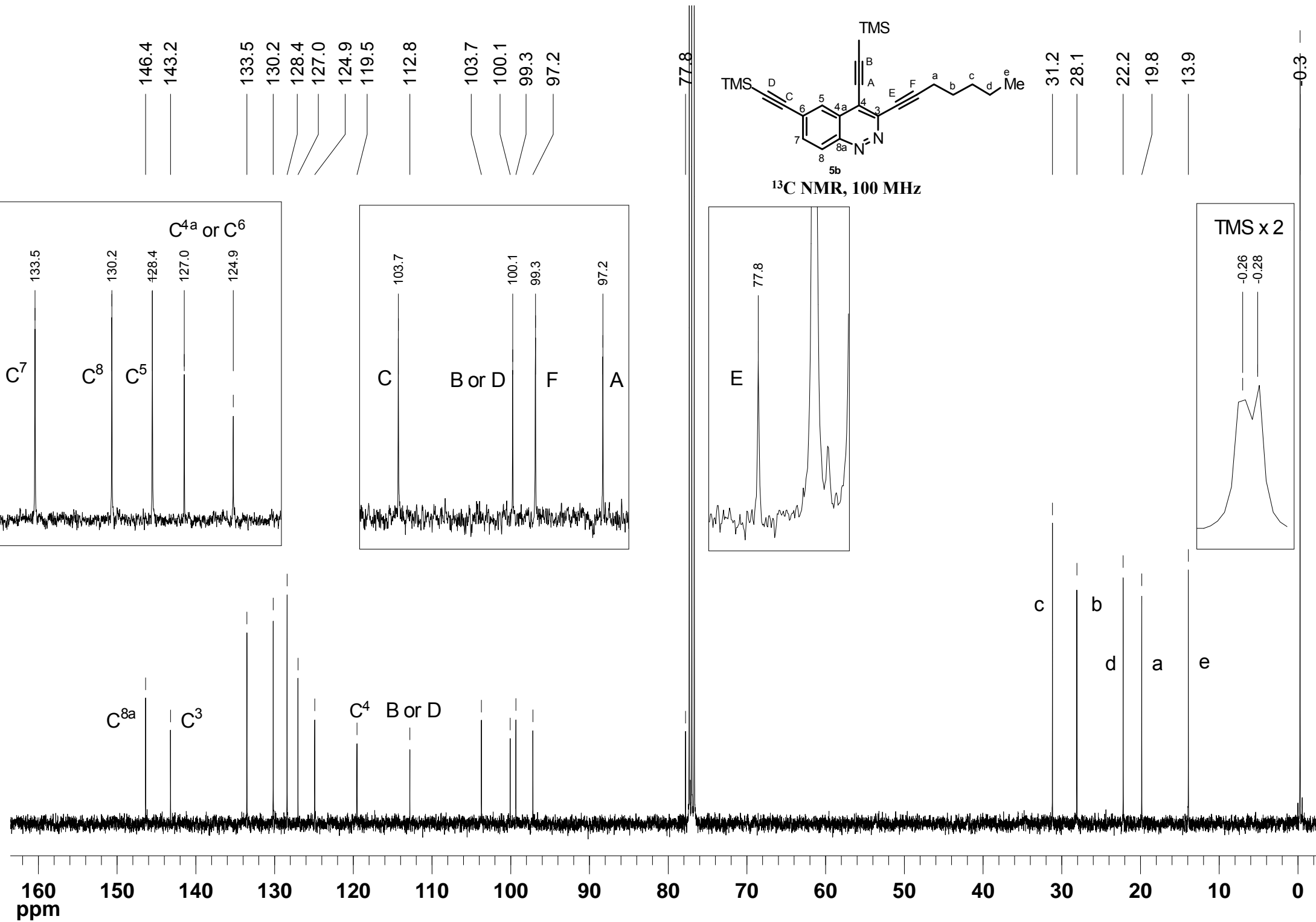
e

1.00
0.96
1.01

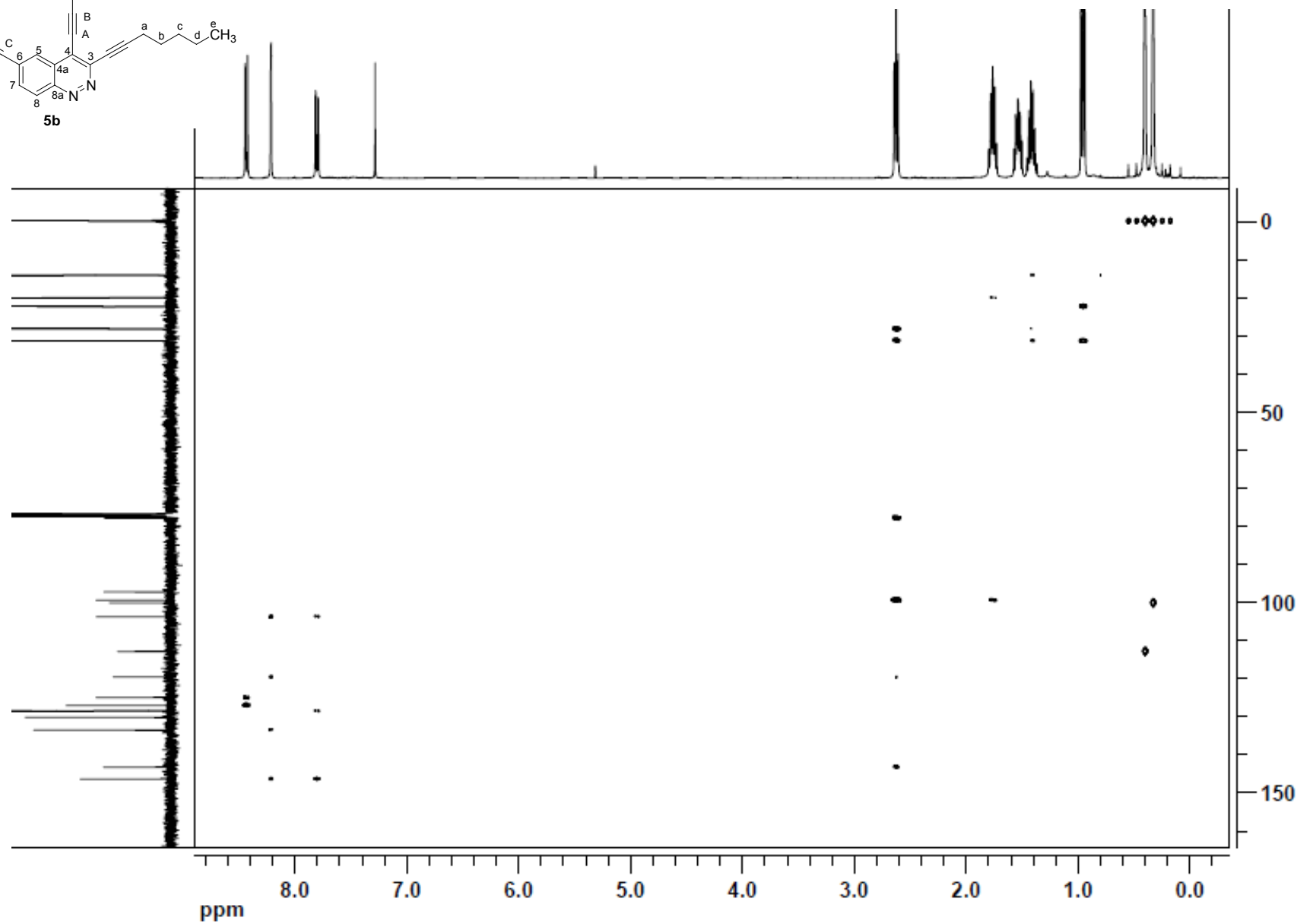
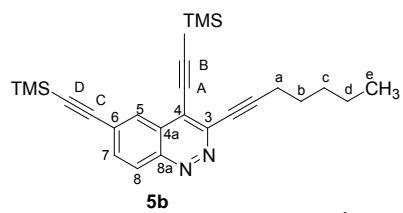
2.04
2.22
2.10
2.10
3.07
9.15

ppm

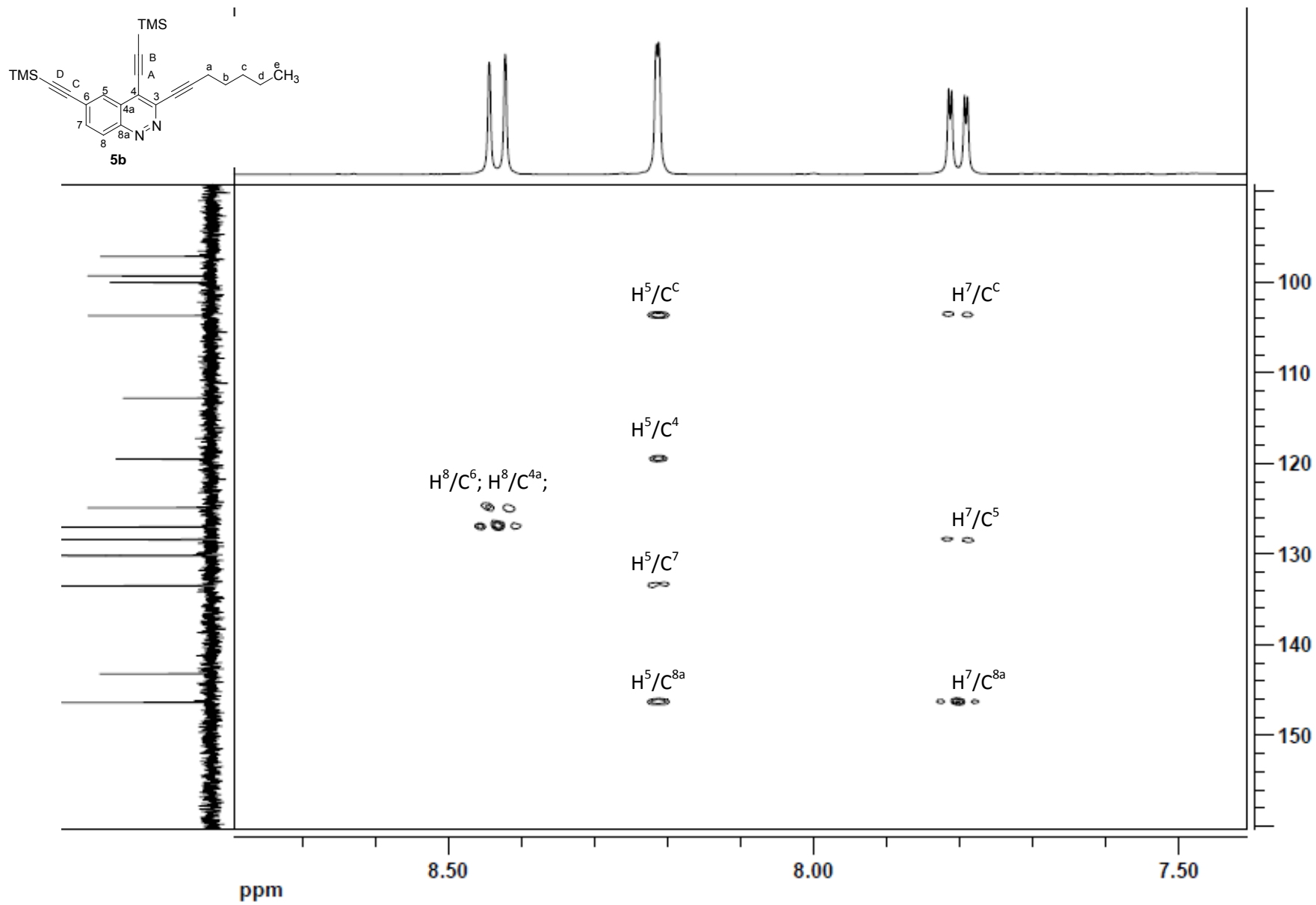
8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0



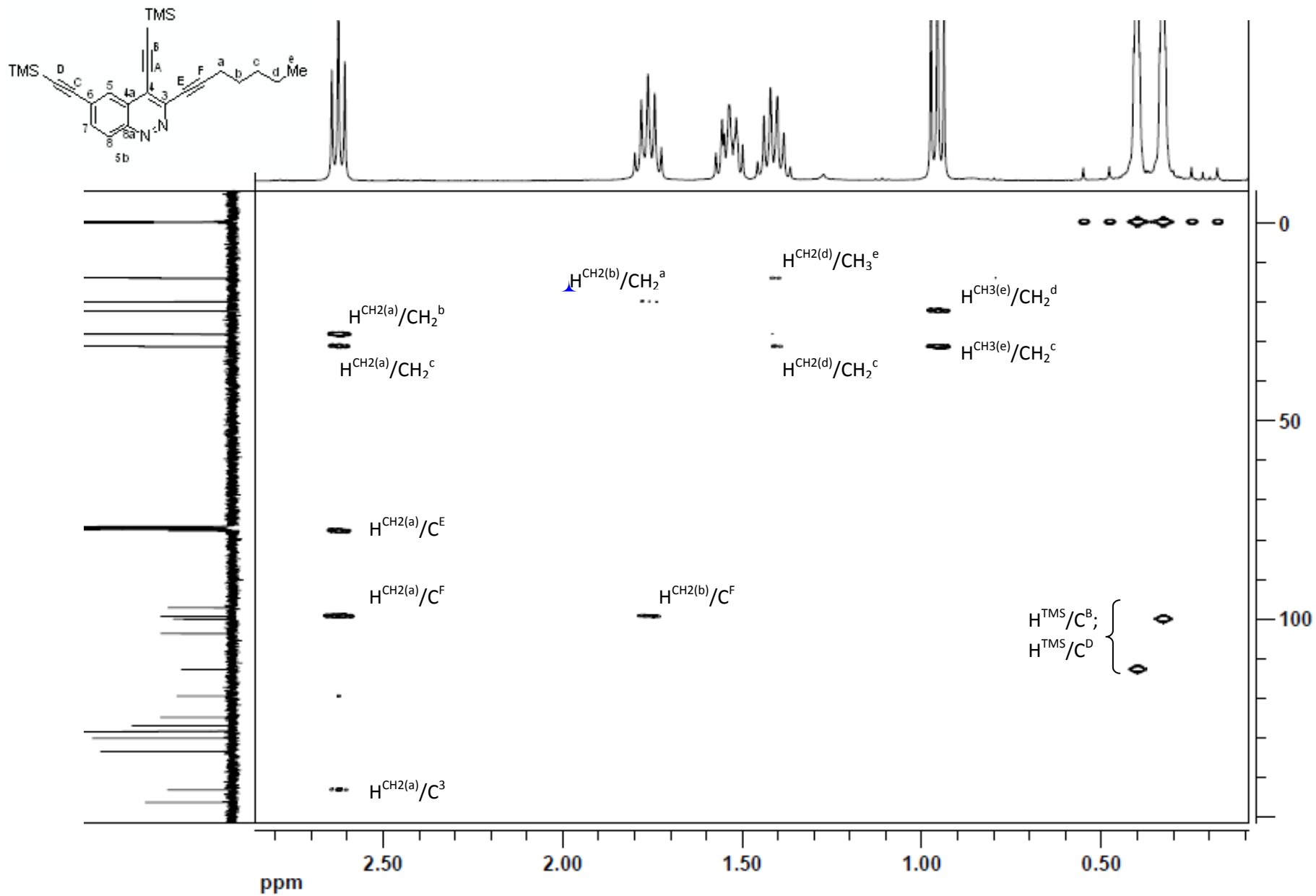
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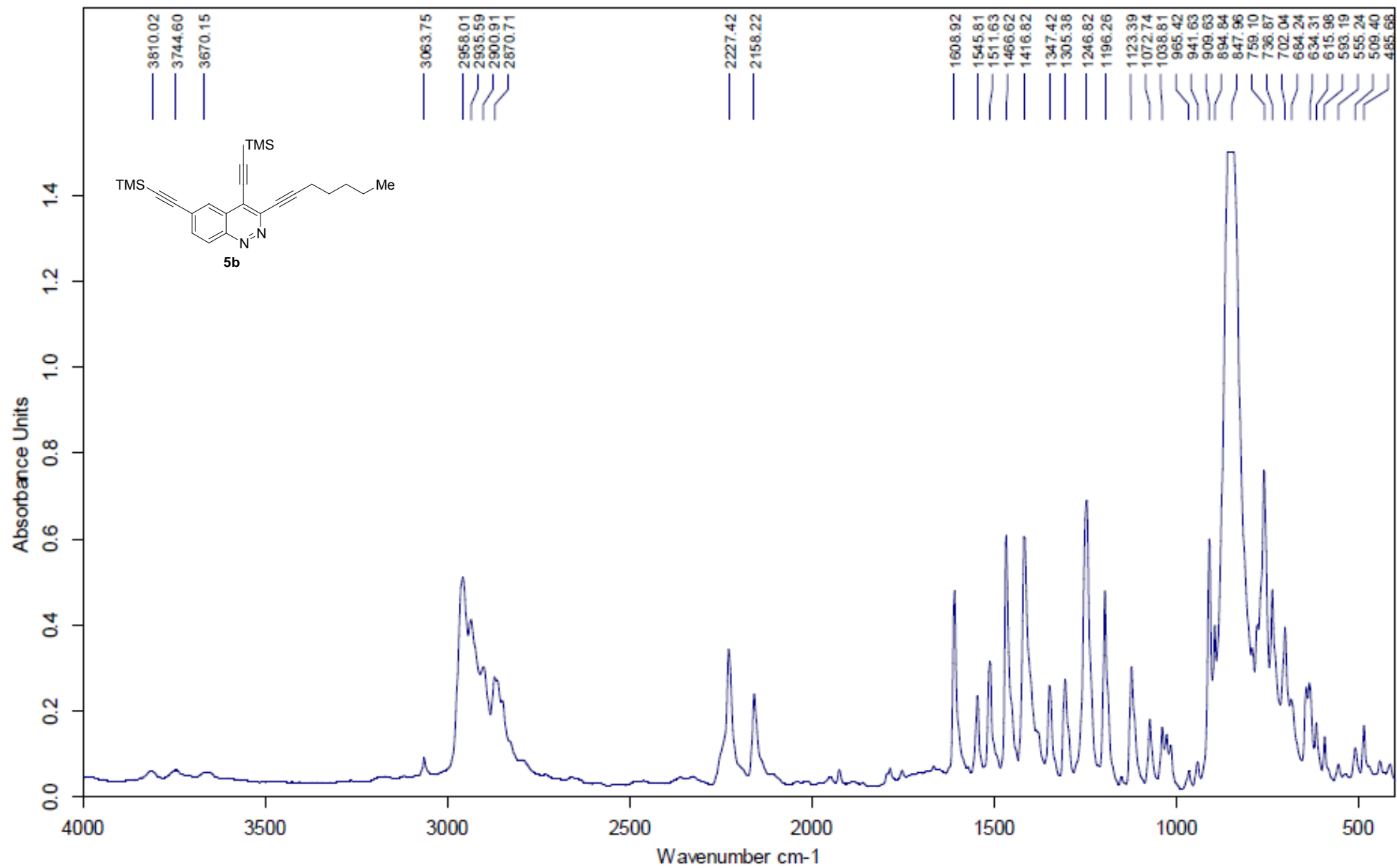


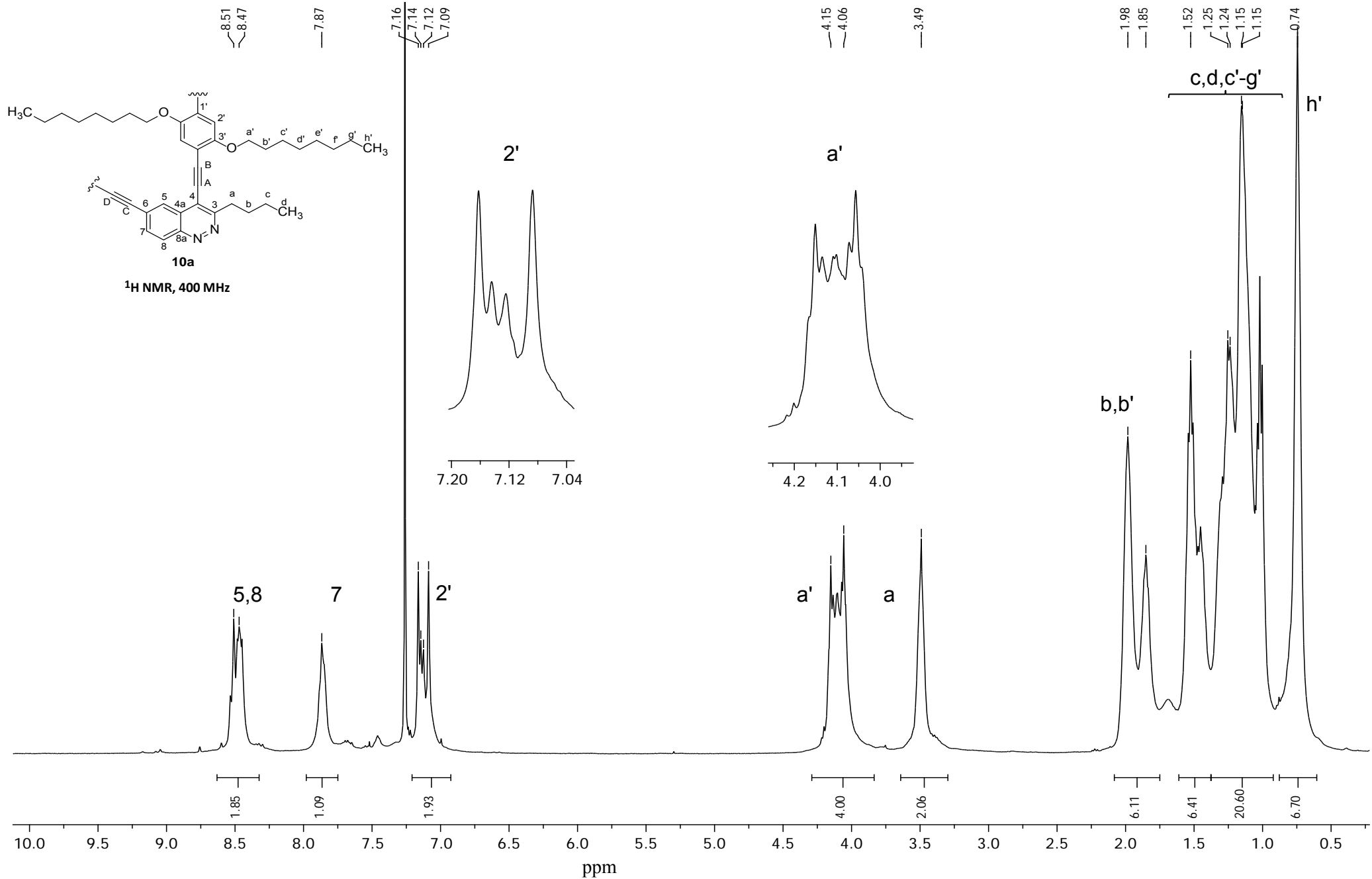
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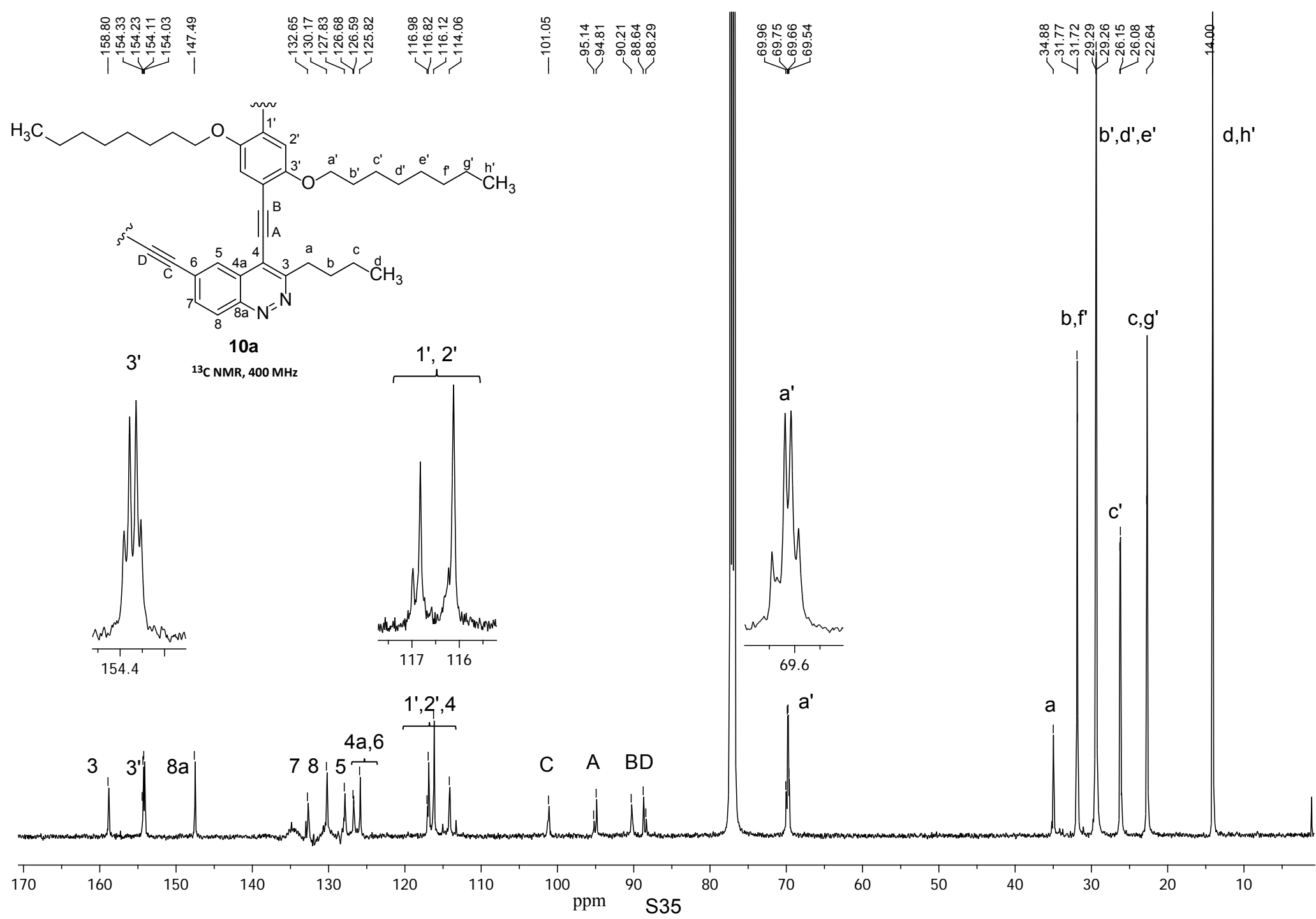


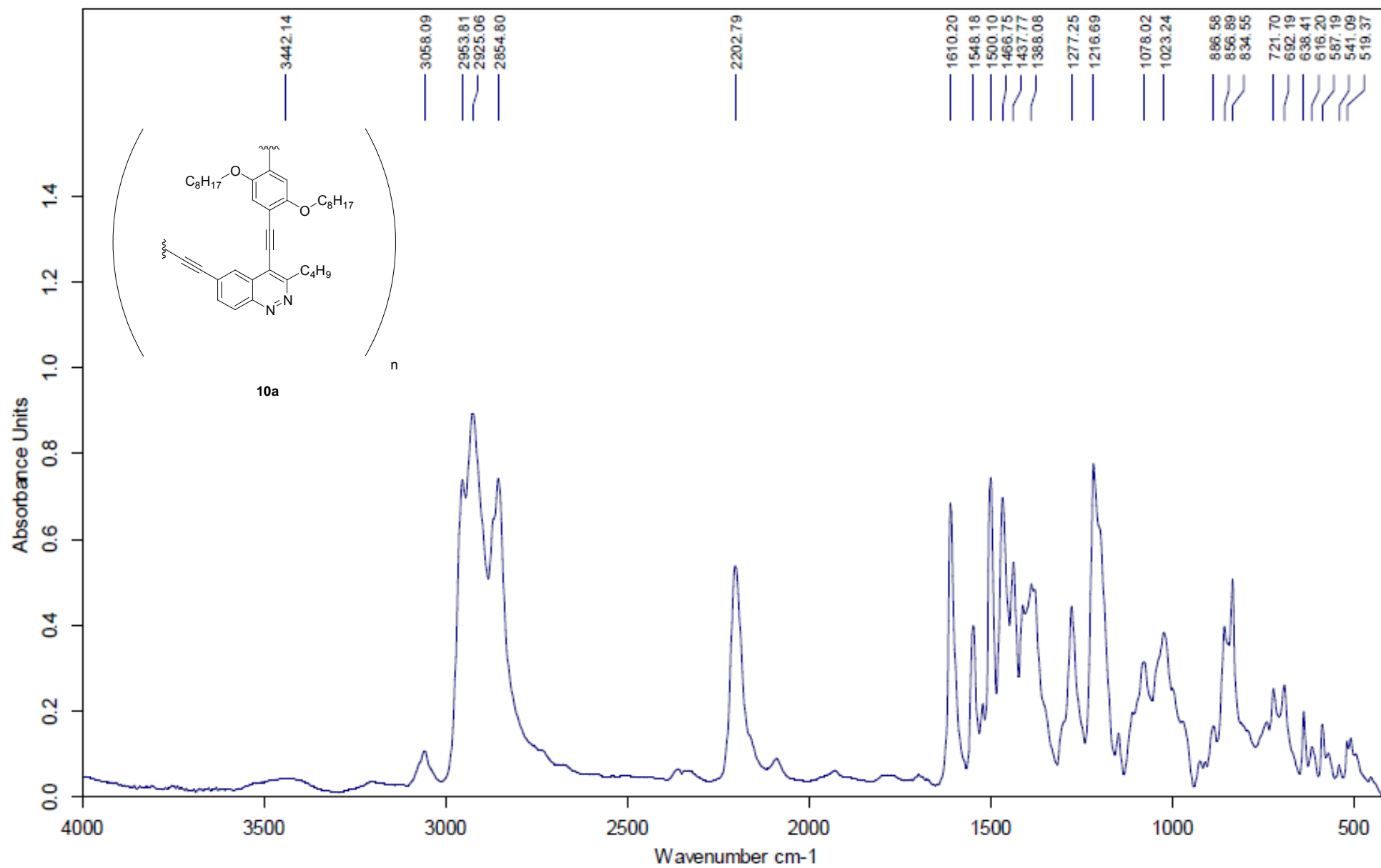
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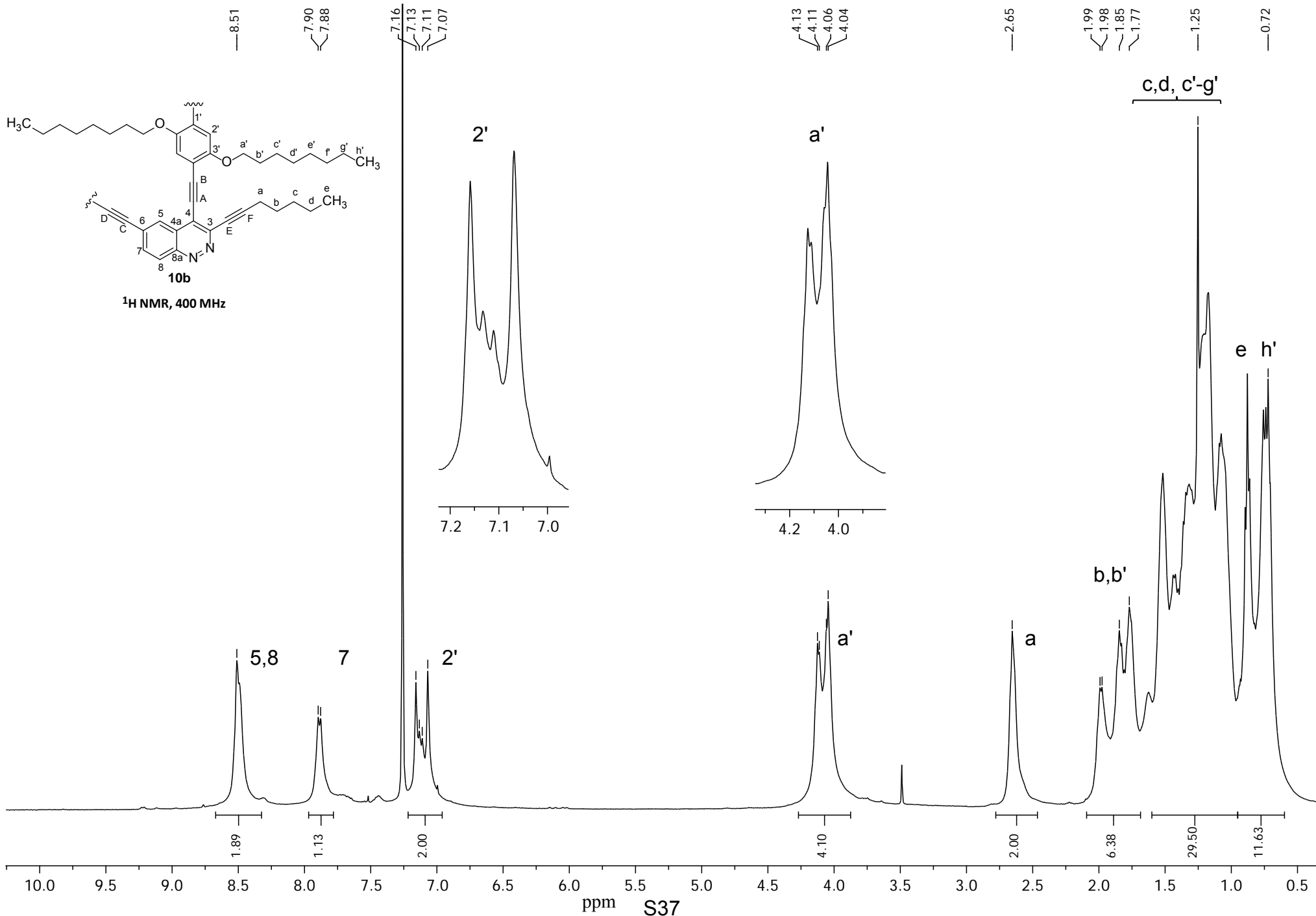


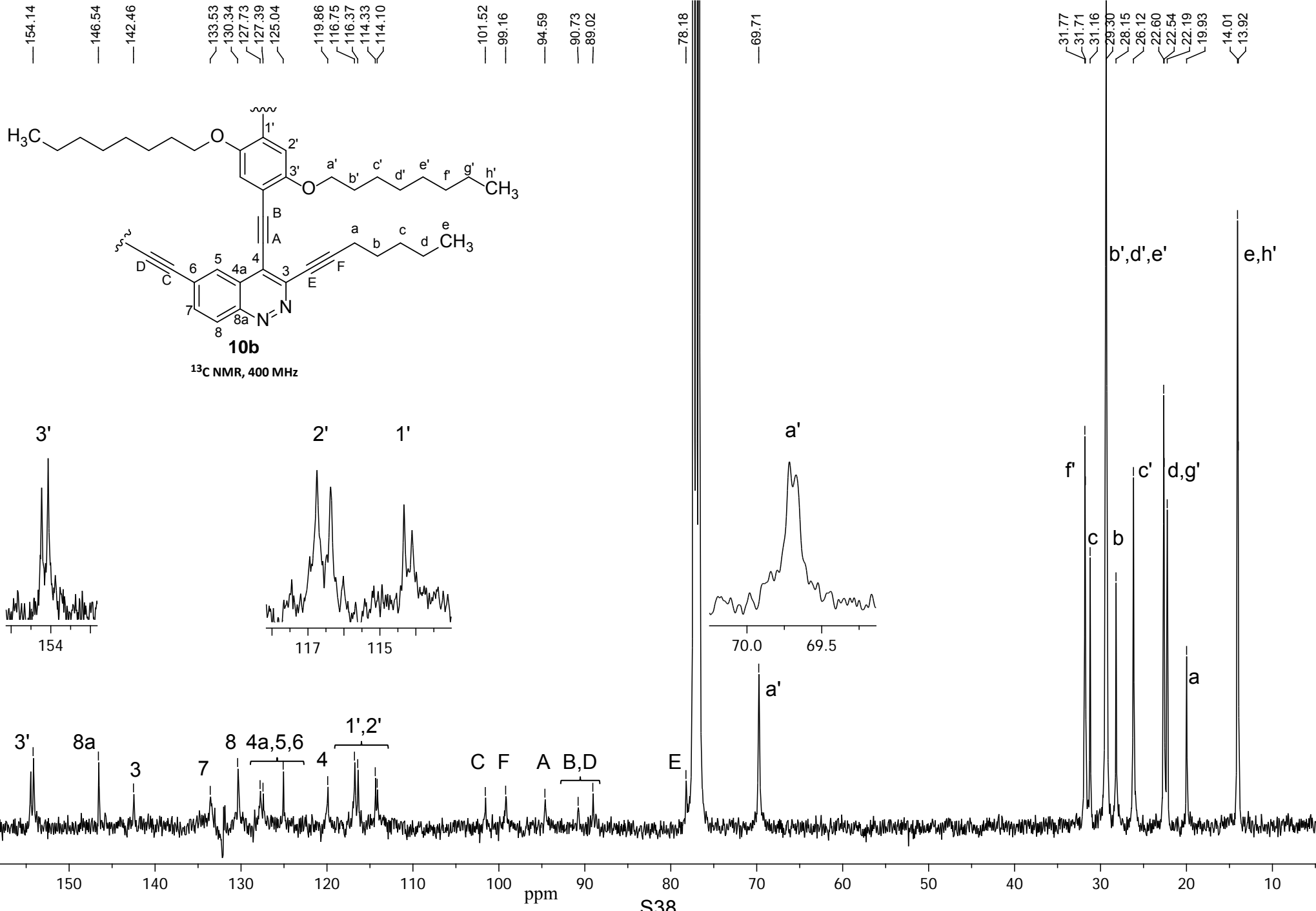


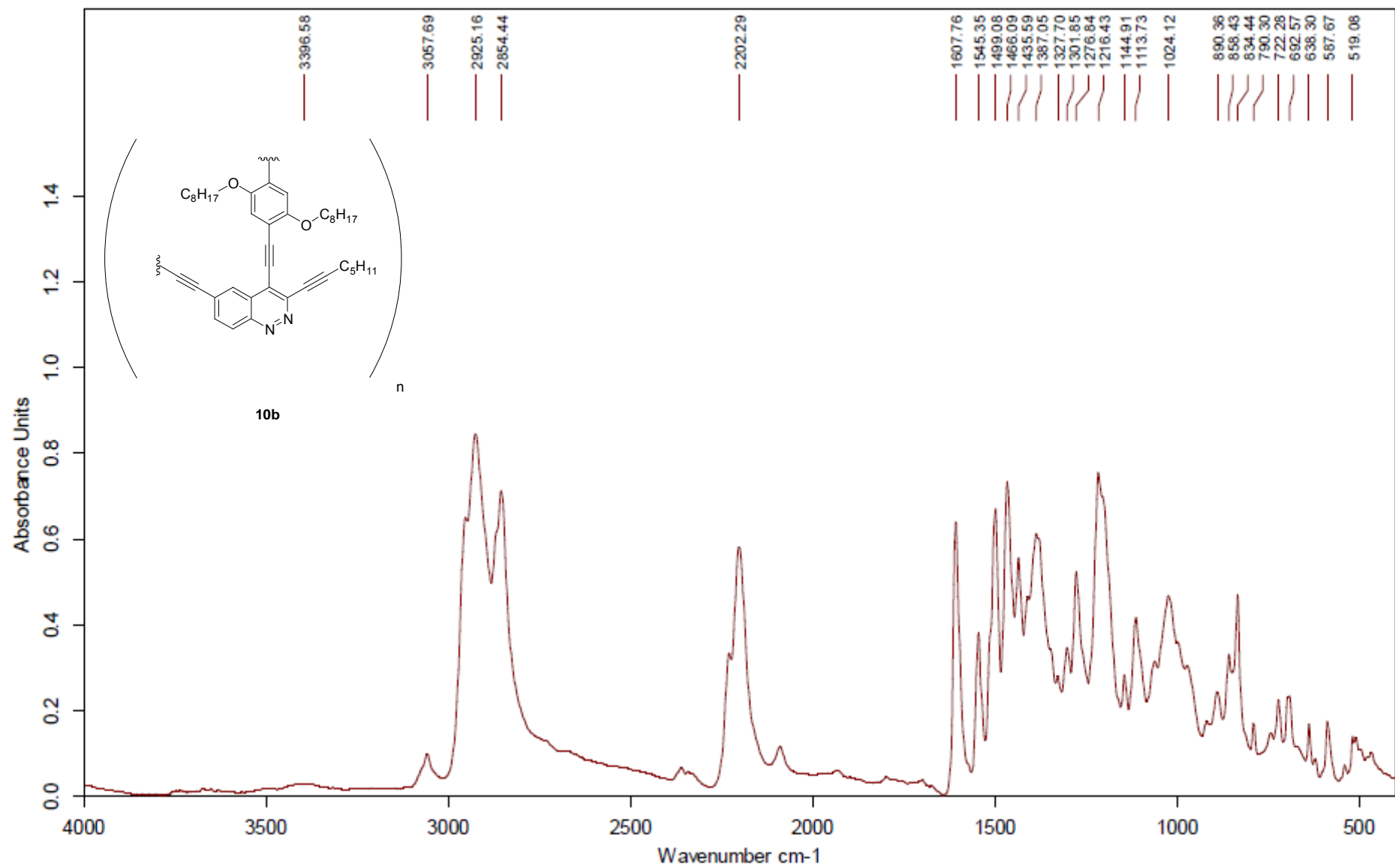


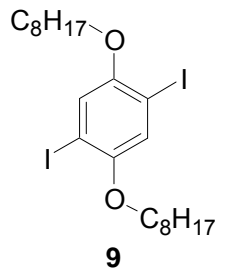






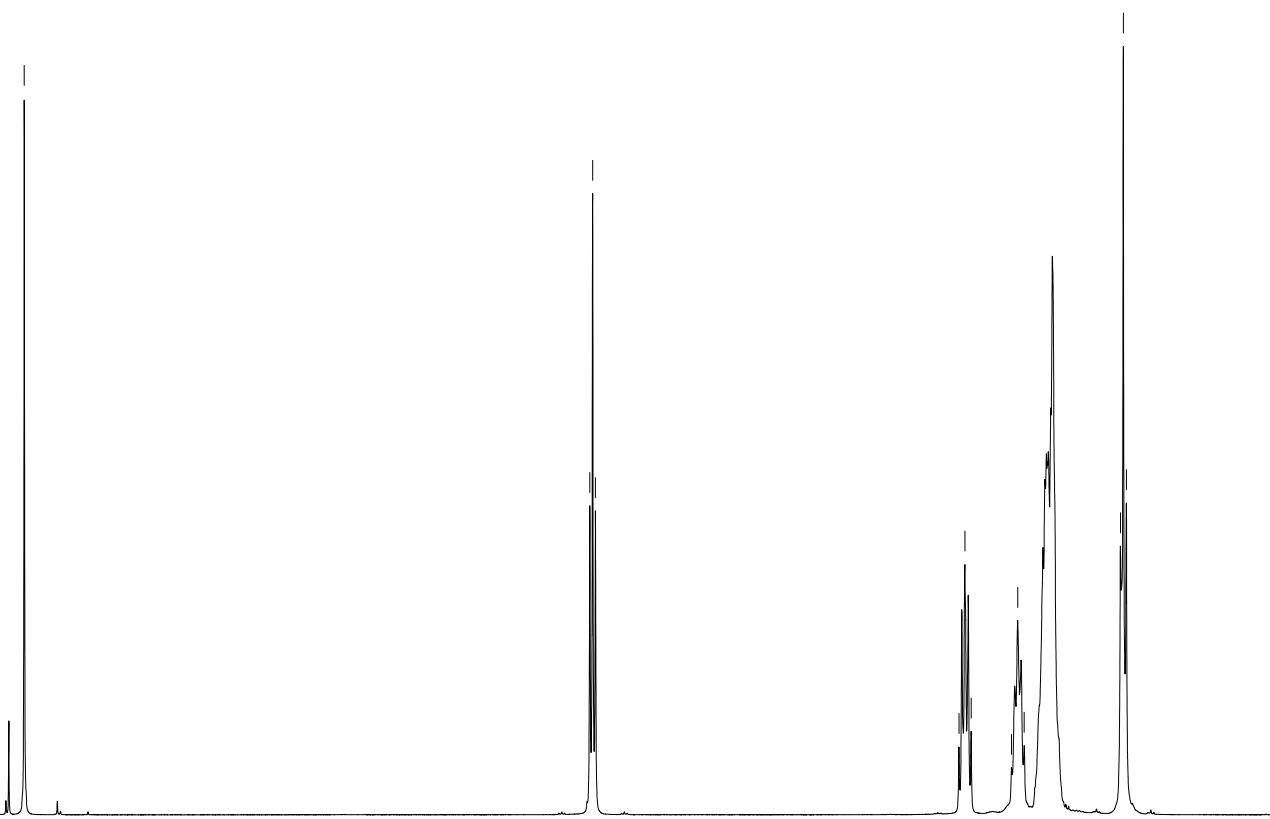






¹H NMR, 400 MHz

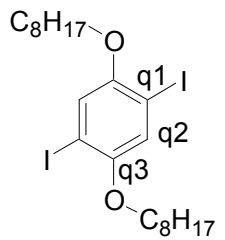
7.17
3.94
3.92
3.91
1.83
1.80
1.76
1.53
1.49
1.46
0.91
0.89
0.87



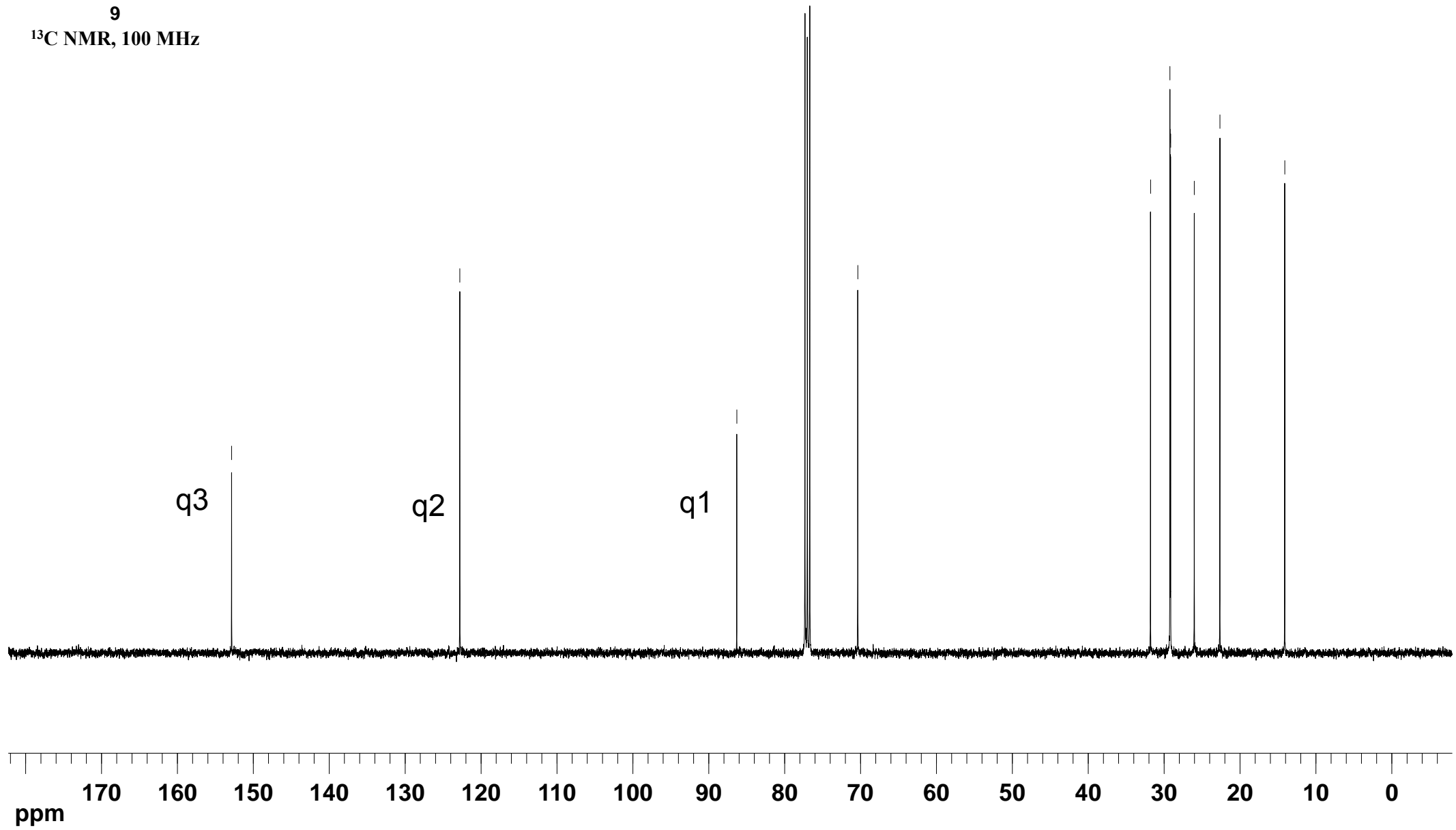
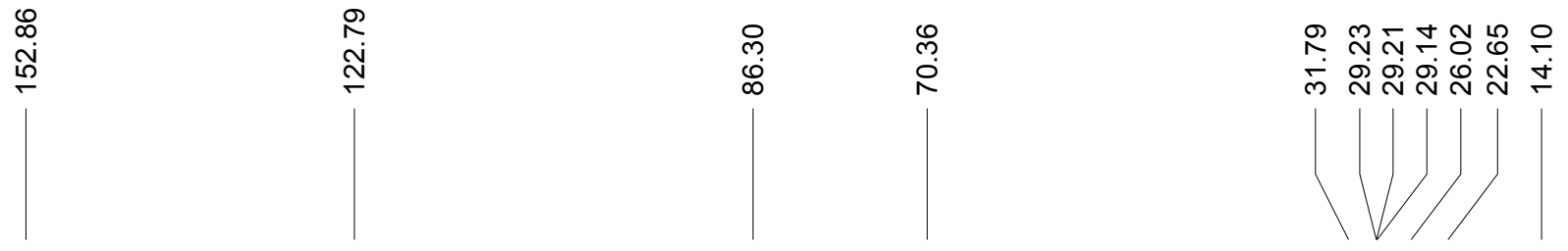
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ppm

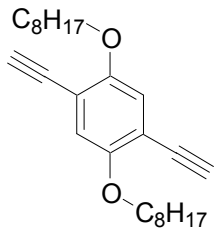
5.0

0.0



9
¹³C NMR, 100 MHz





¹H NMR, 400 MHz

6.95

3.97

3.33

1.80

1.46

1.28

0.88

2.00

4.08

1.85

4.10

4.28

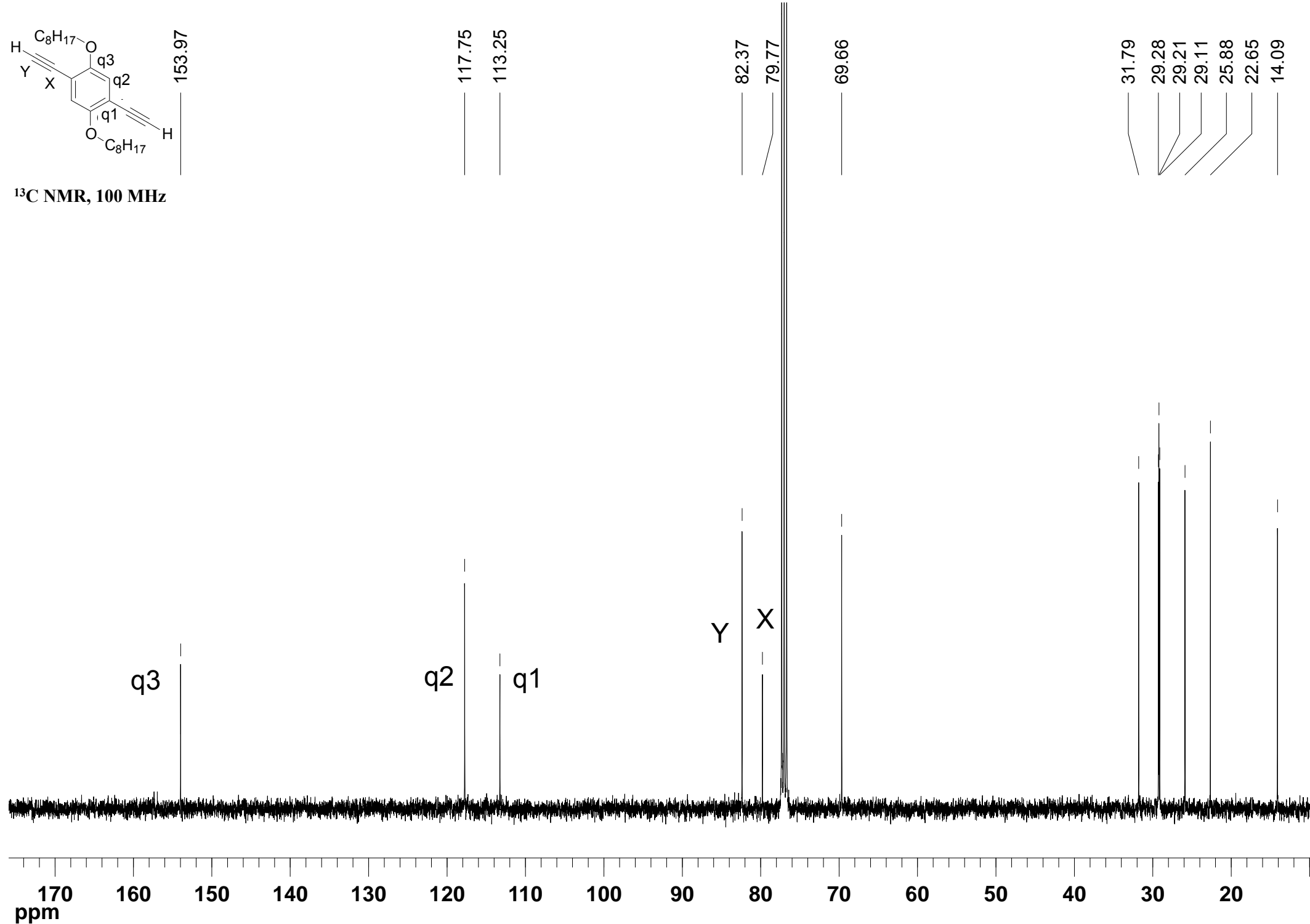
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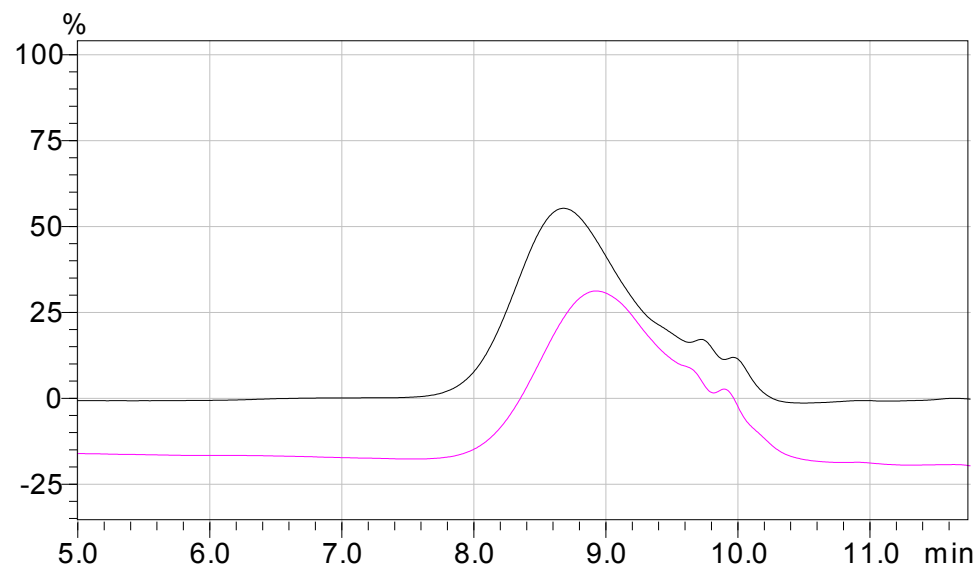
6.25

ppm

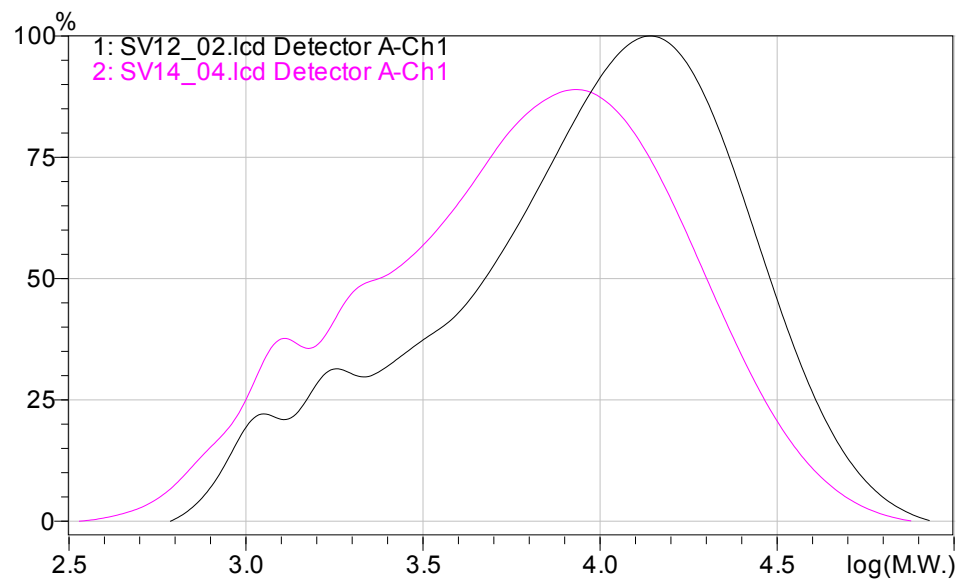
5.0

0.0





GPC analysis of PAEs **10a,b**. Elution curves for **10a** (black) and **10b** (pink) are shown



GPC analysis of PAEs **10a,b**. Mw distribution curves for **10a** (black) and **10b** (pink) are shown.