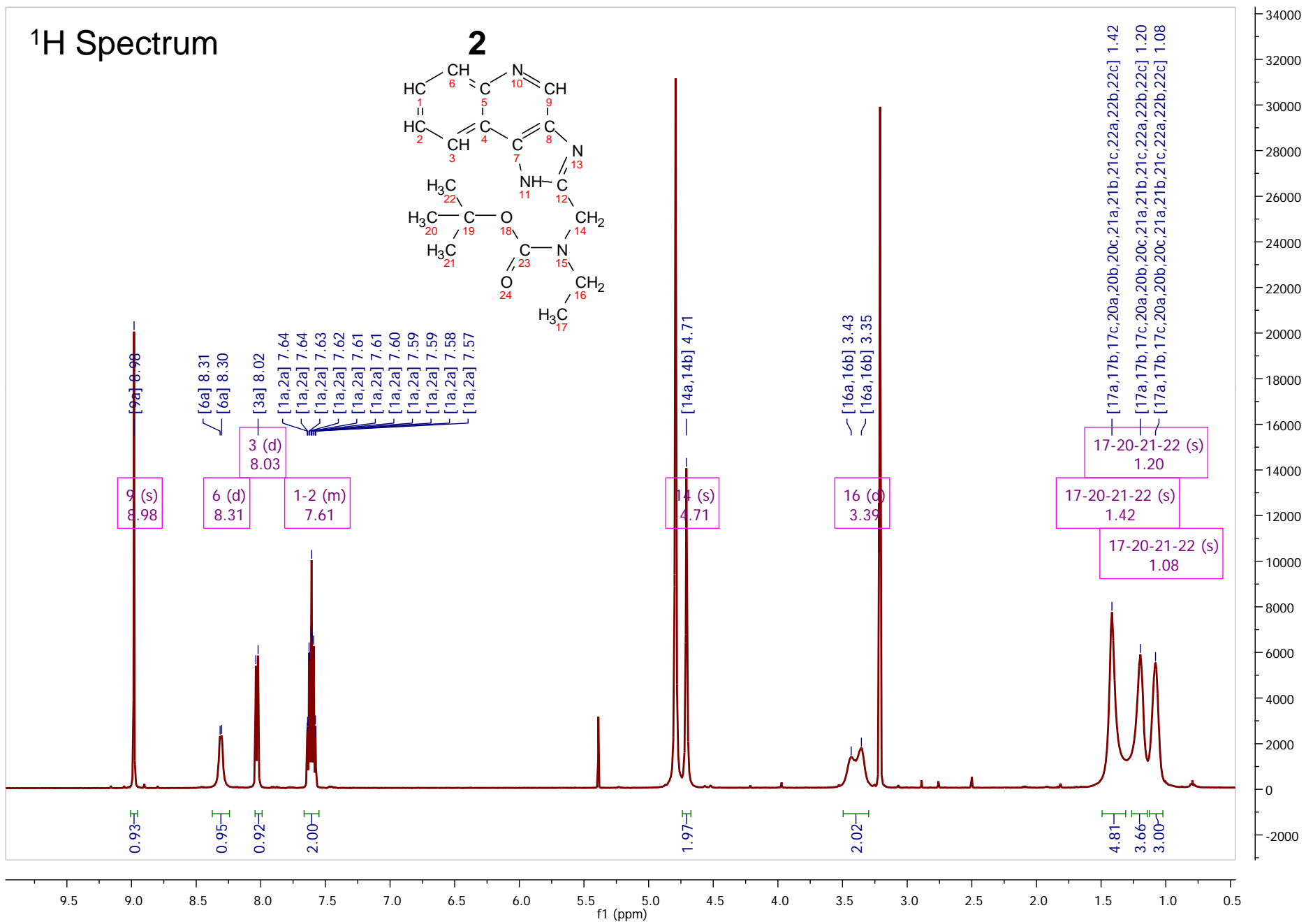
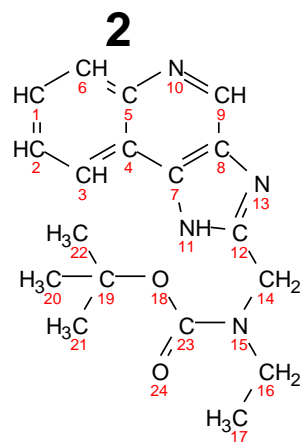


## Supplementary Data

# Preliminary Evaluation of a 3*H* Imidazoquinoline Library as Dual TLR7/TLR8 Antagonists

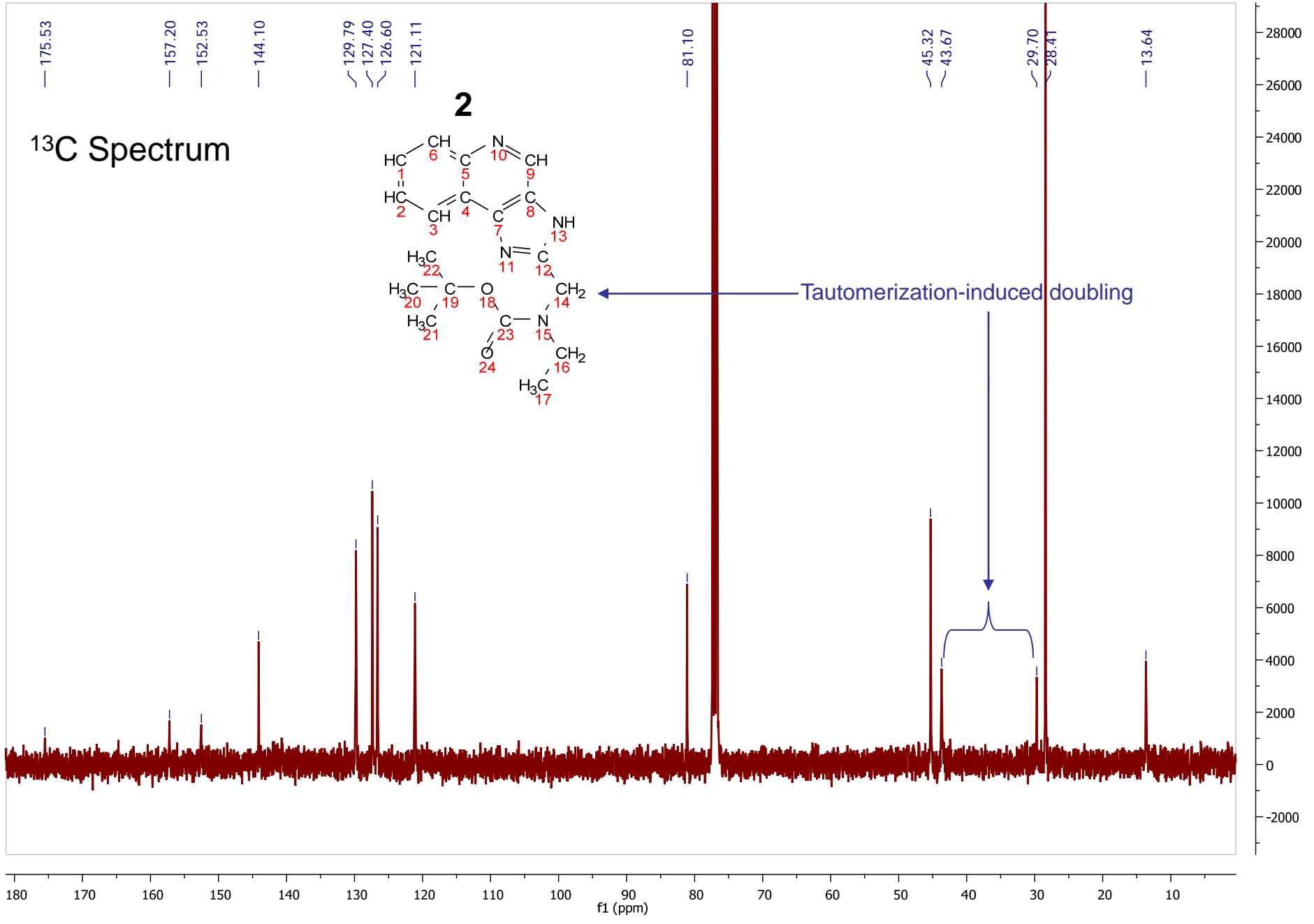
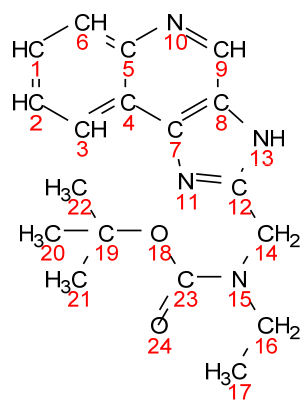
Nikunj M. Shukla, Subbalakshmi S. Malladi, Victor Day, and  
Sunil A. David\*

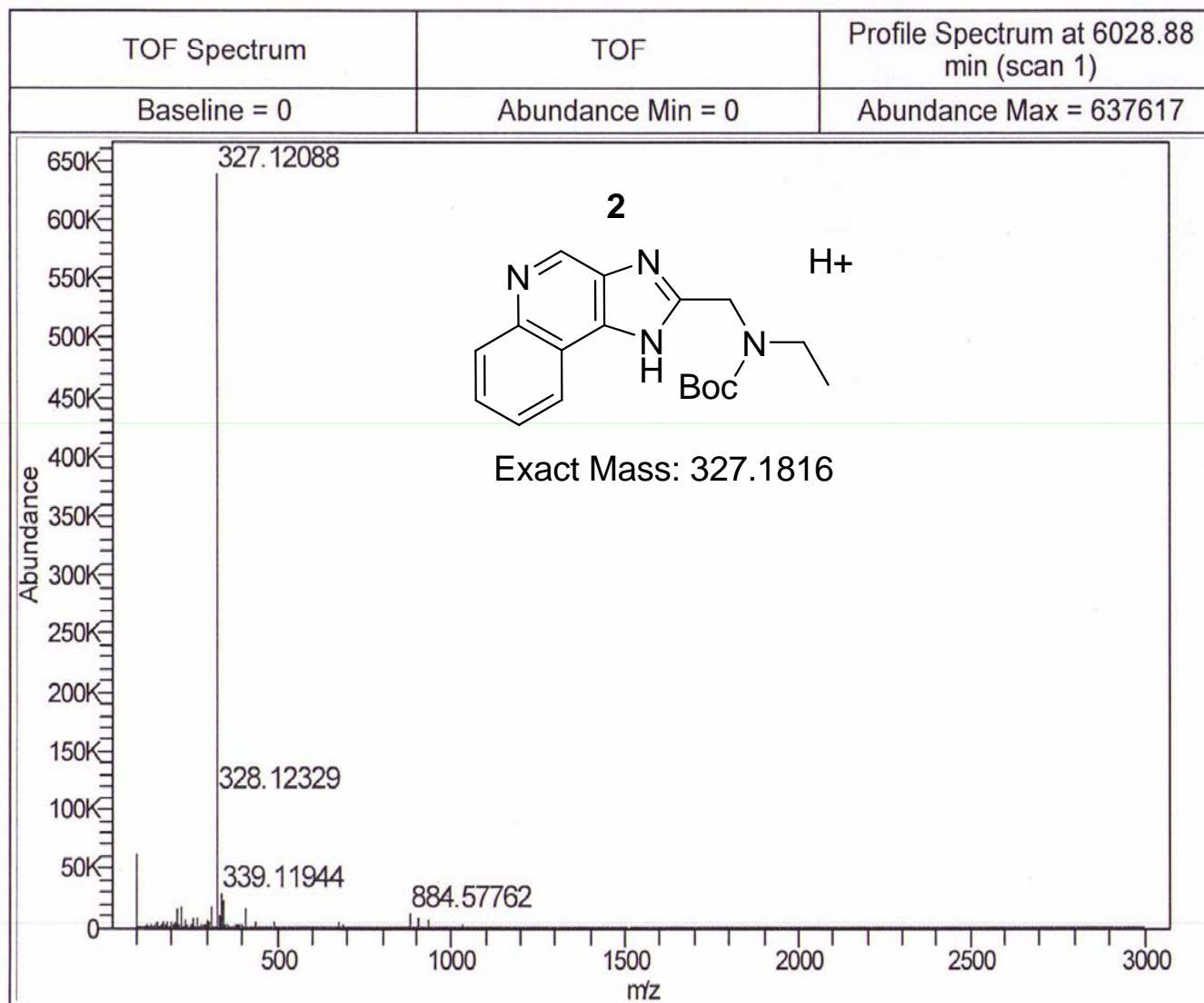
# <sup>1</sup>H Spectrum



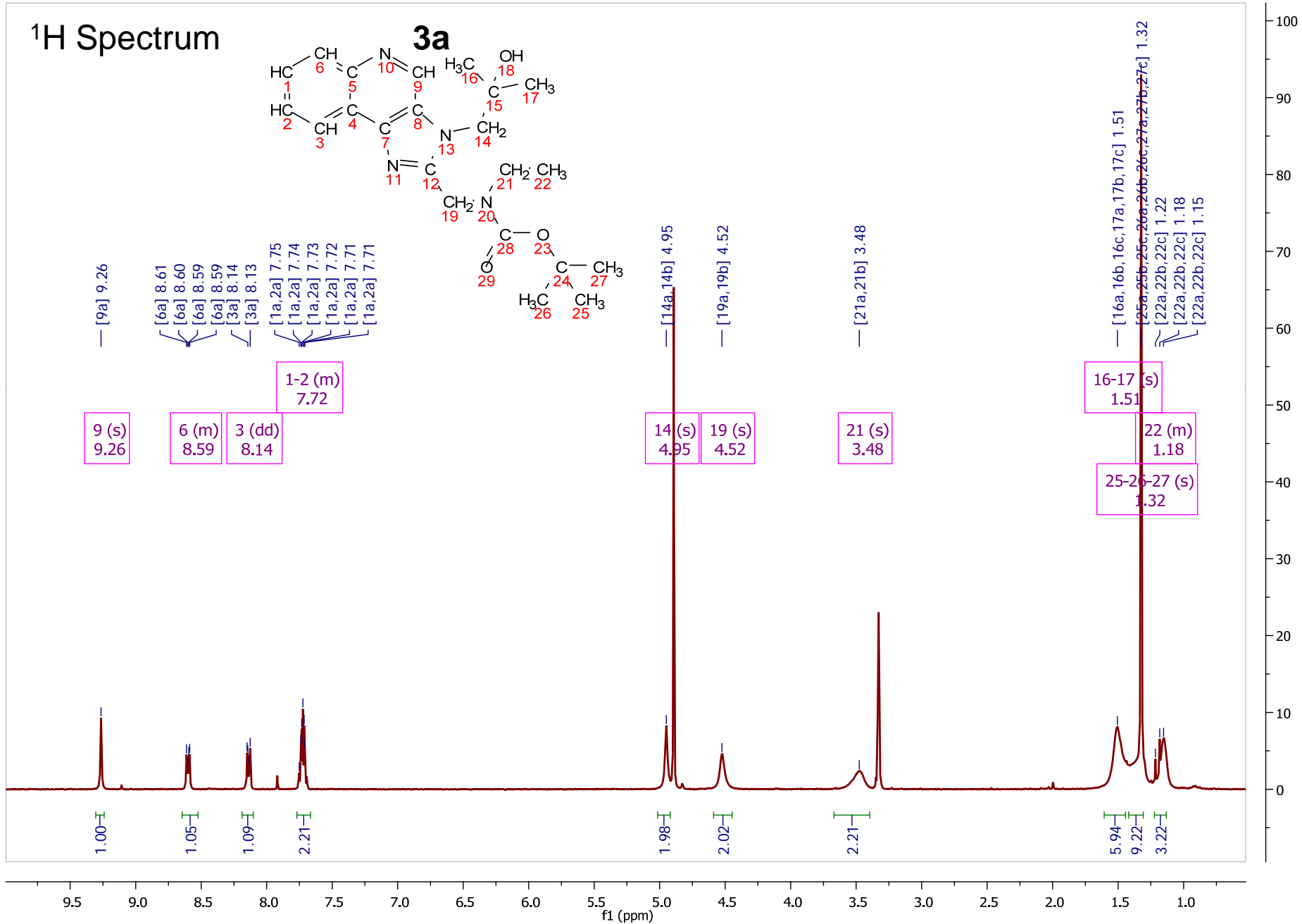
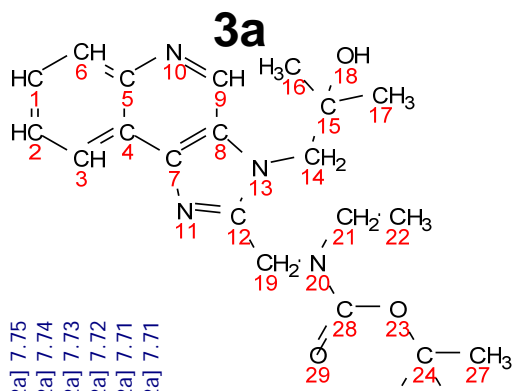
# <sup>13</sup>C Spectrum

**2**

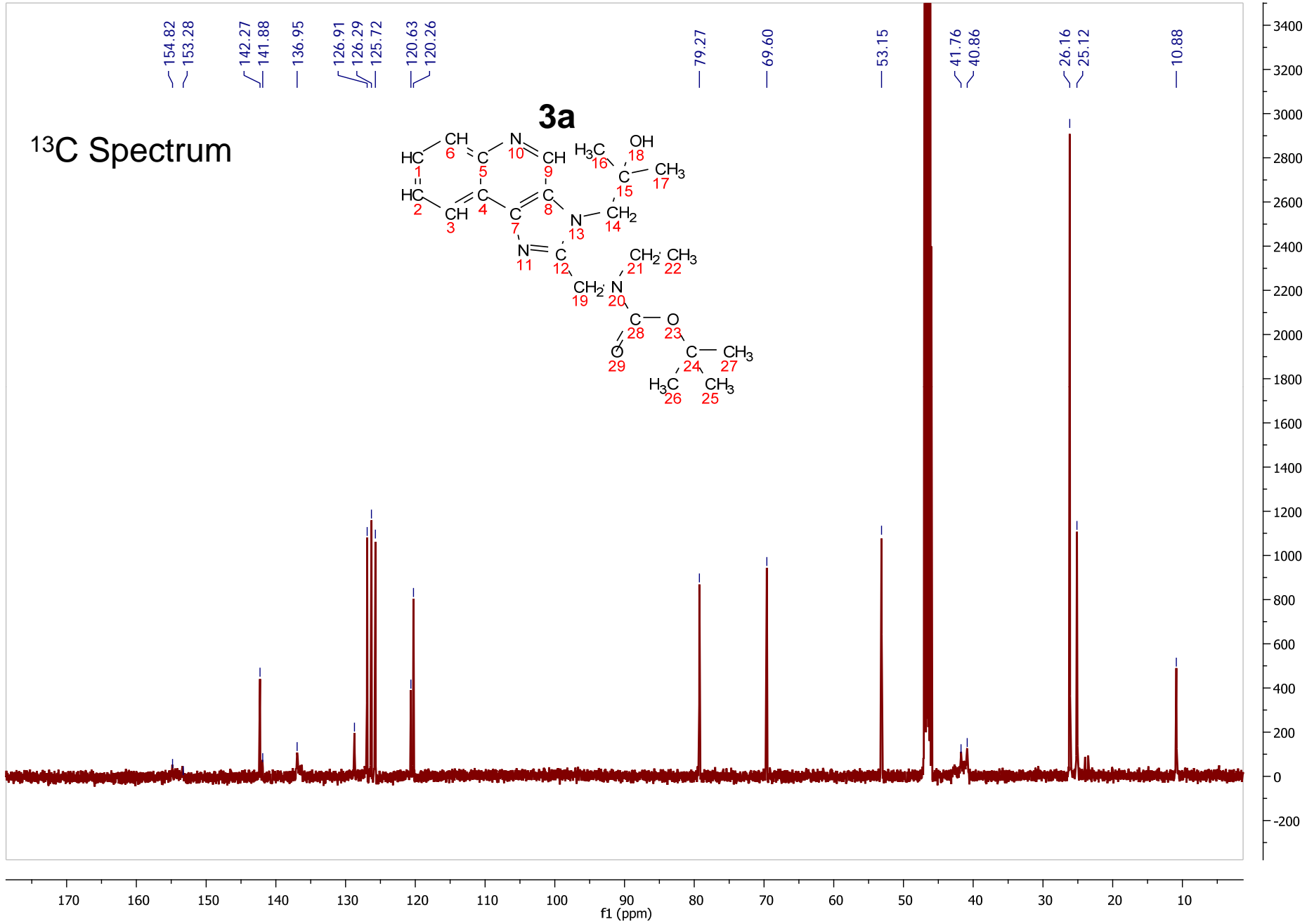
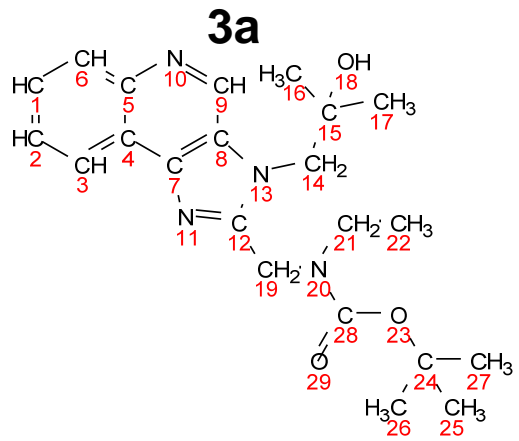


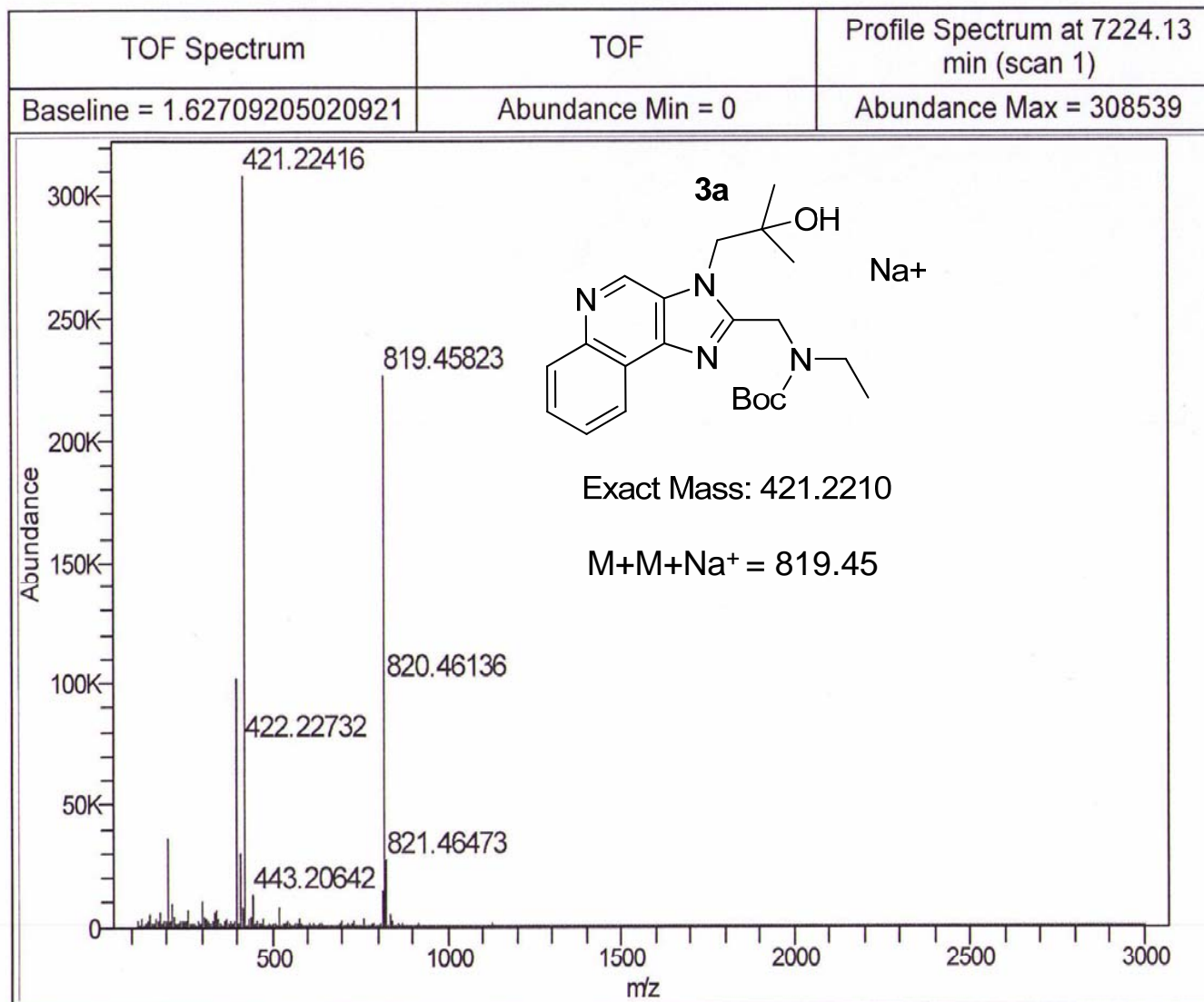


# <sup>1</sup>H Spectrum

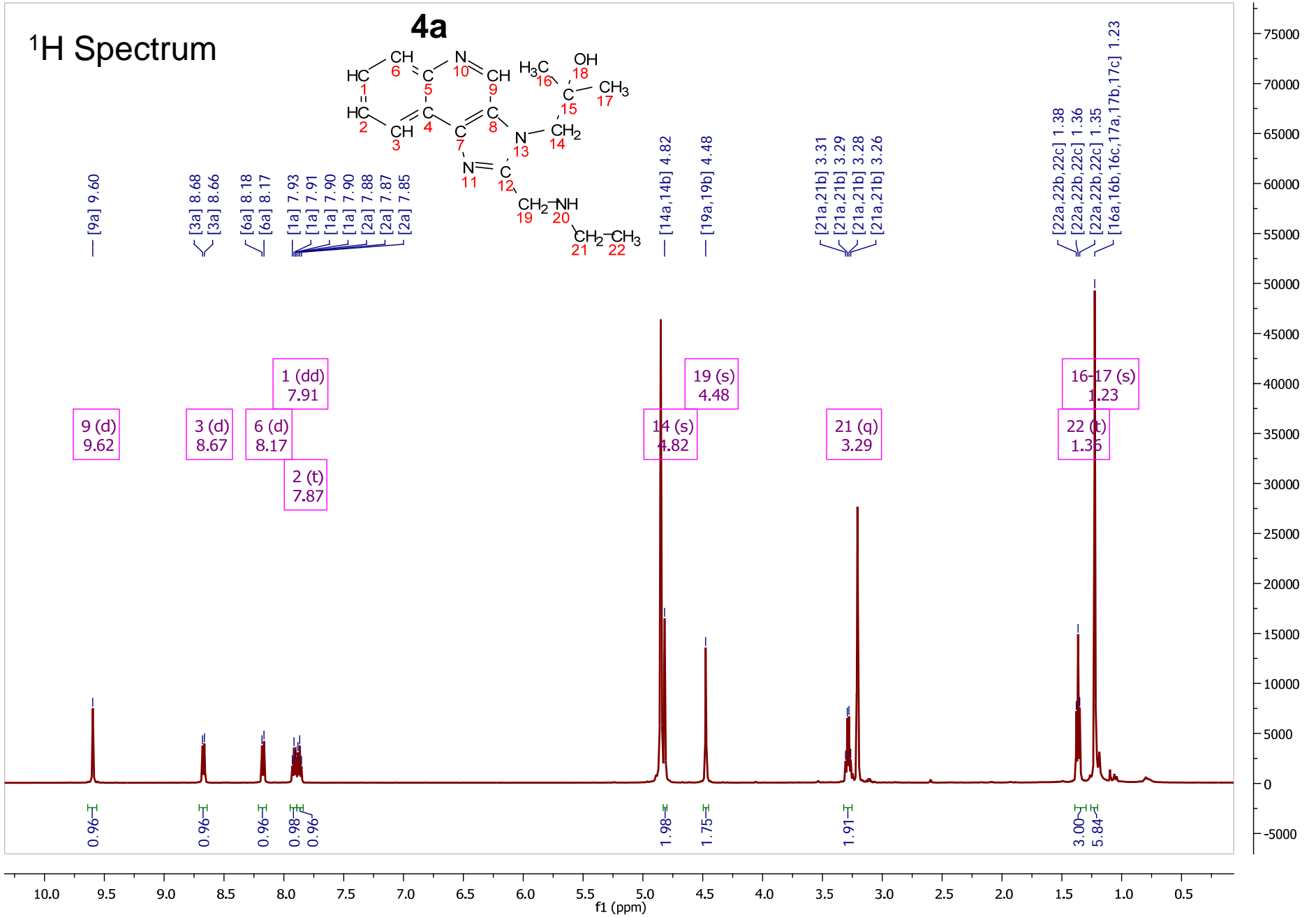
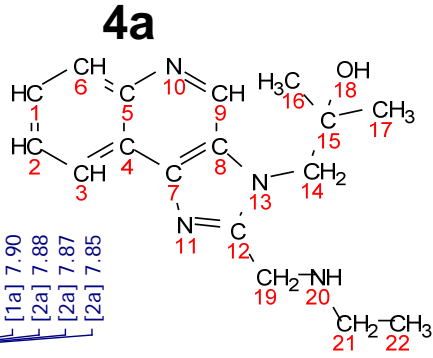


# <sup>13</sup>C Spectrum





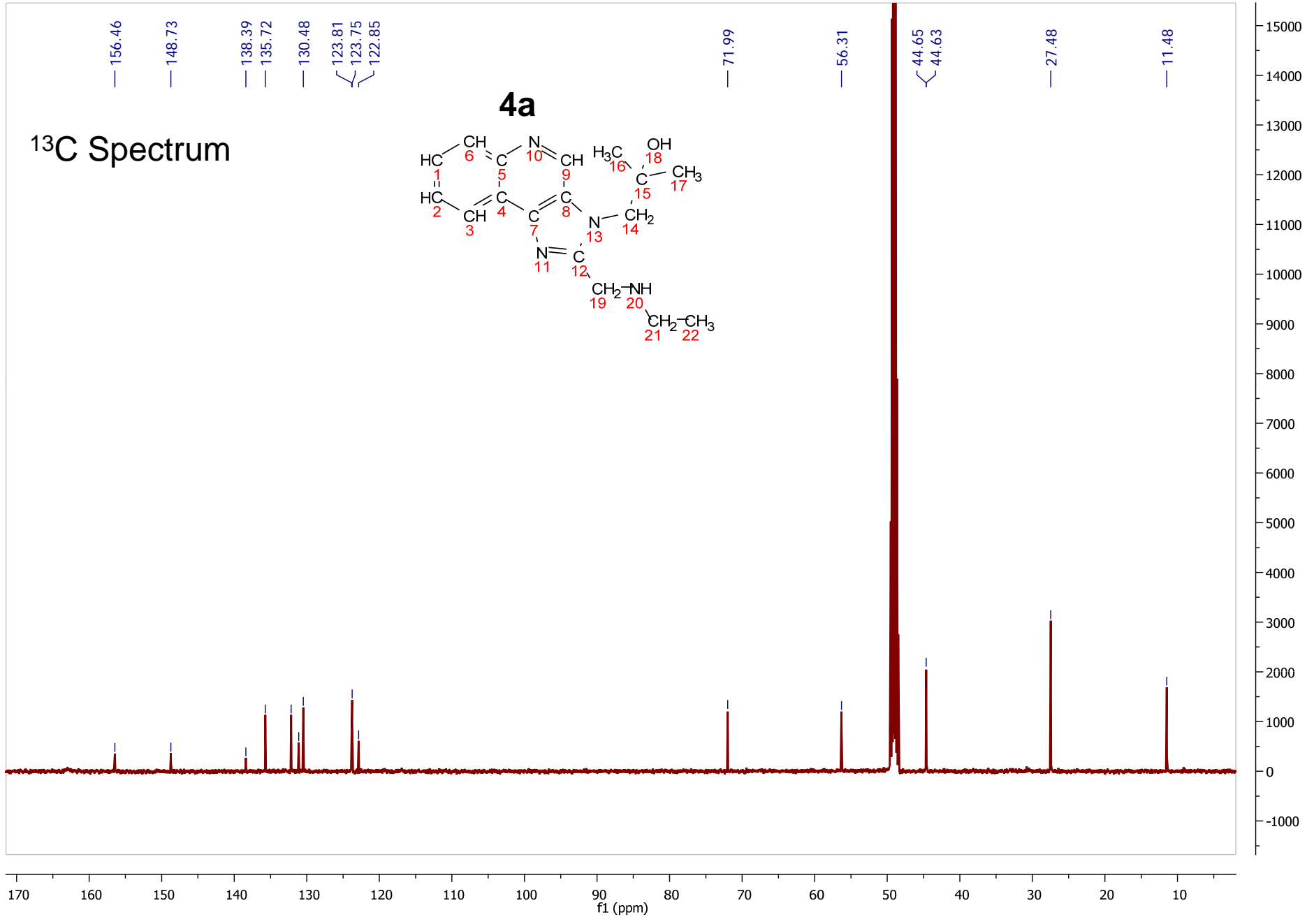
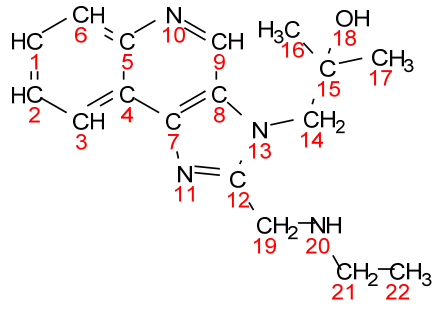
# <sup>1</sup>H Spectrum

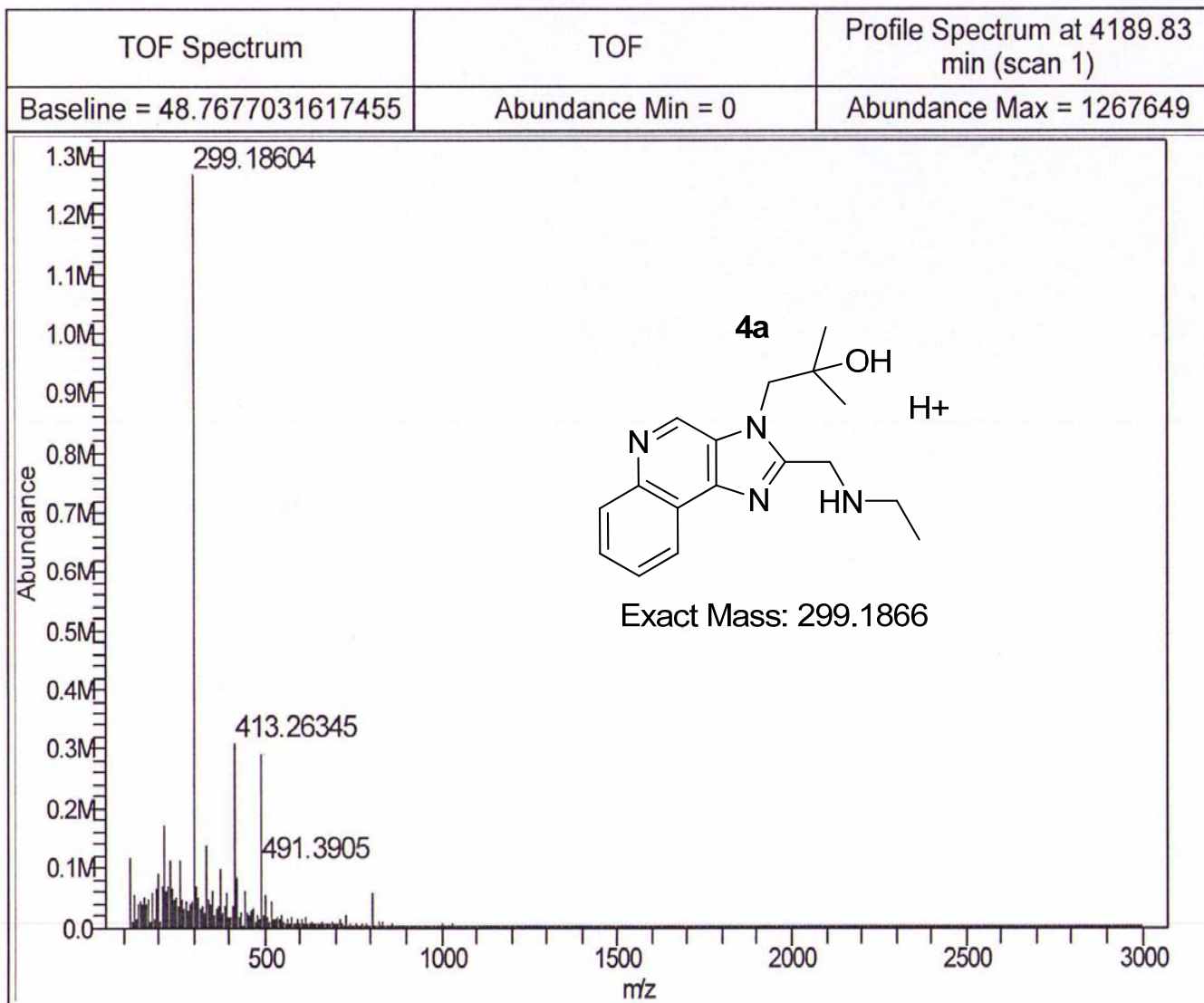




# <sup>13</sup>C Spectrum

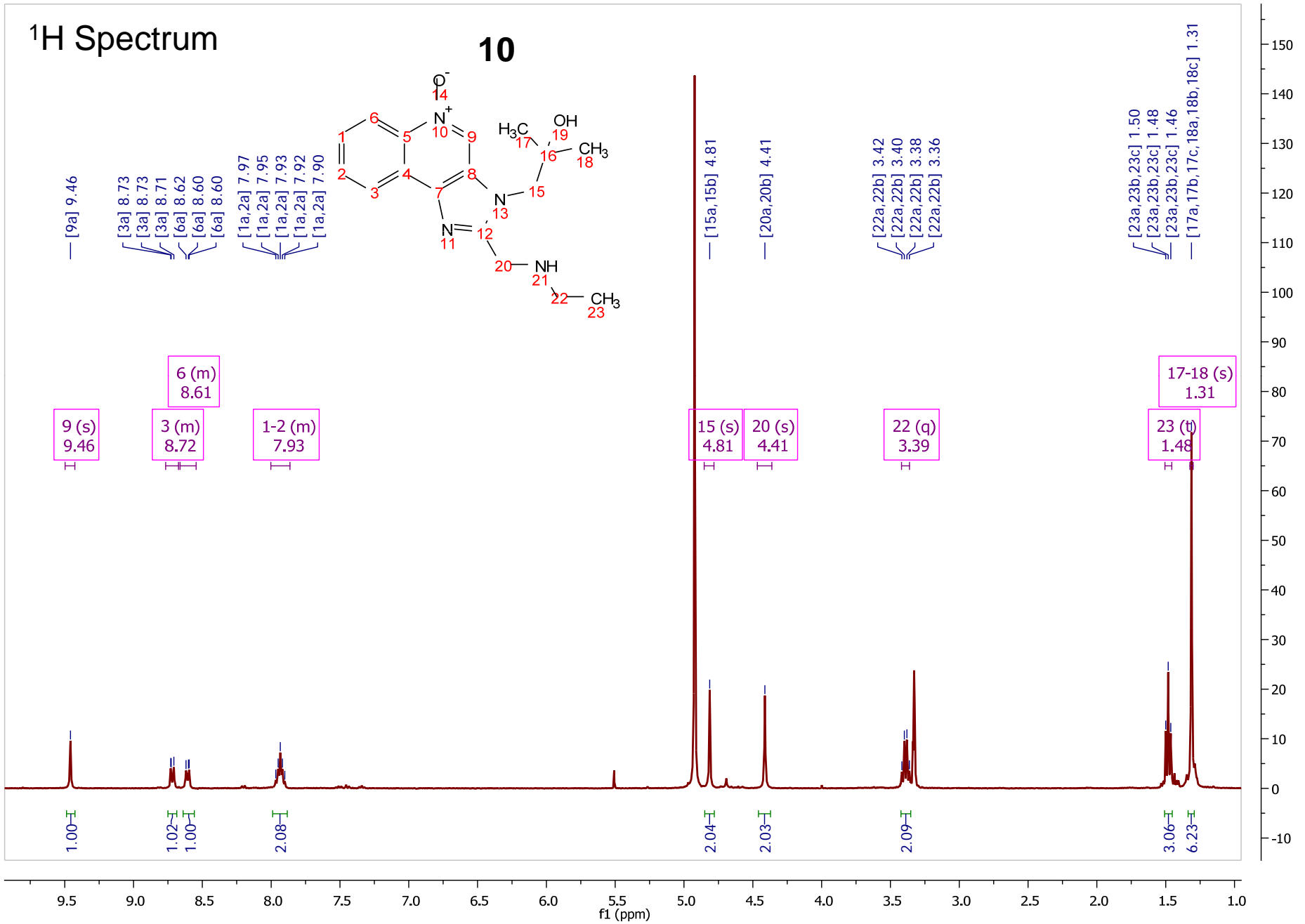
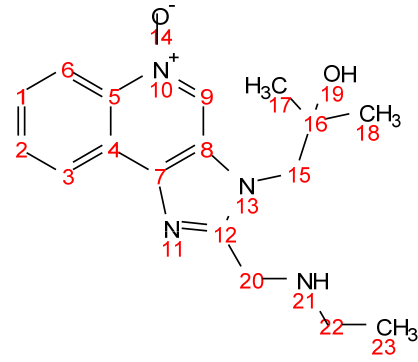
**4a**



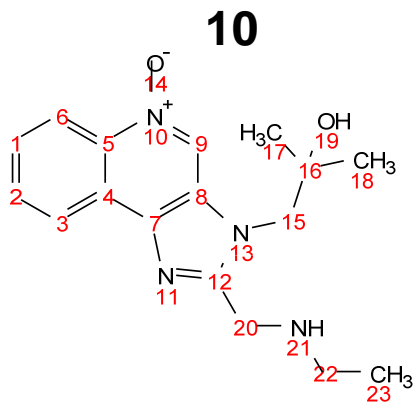


# <sup>1</sup>H Spectrum

## 10

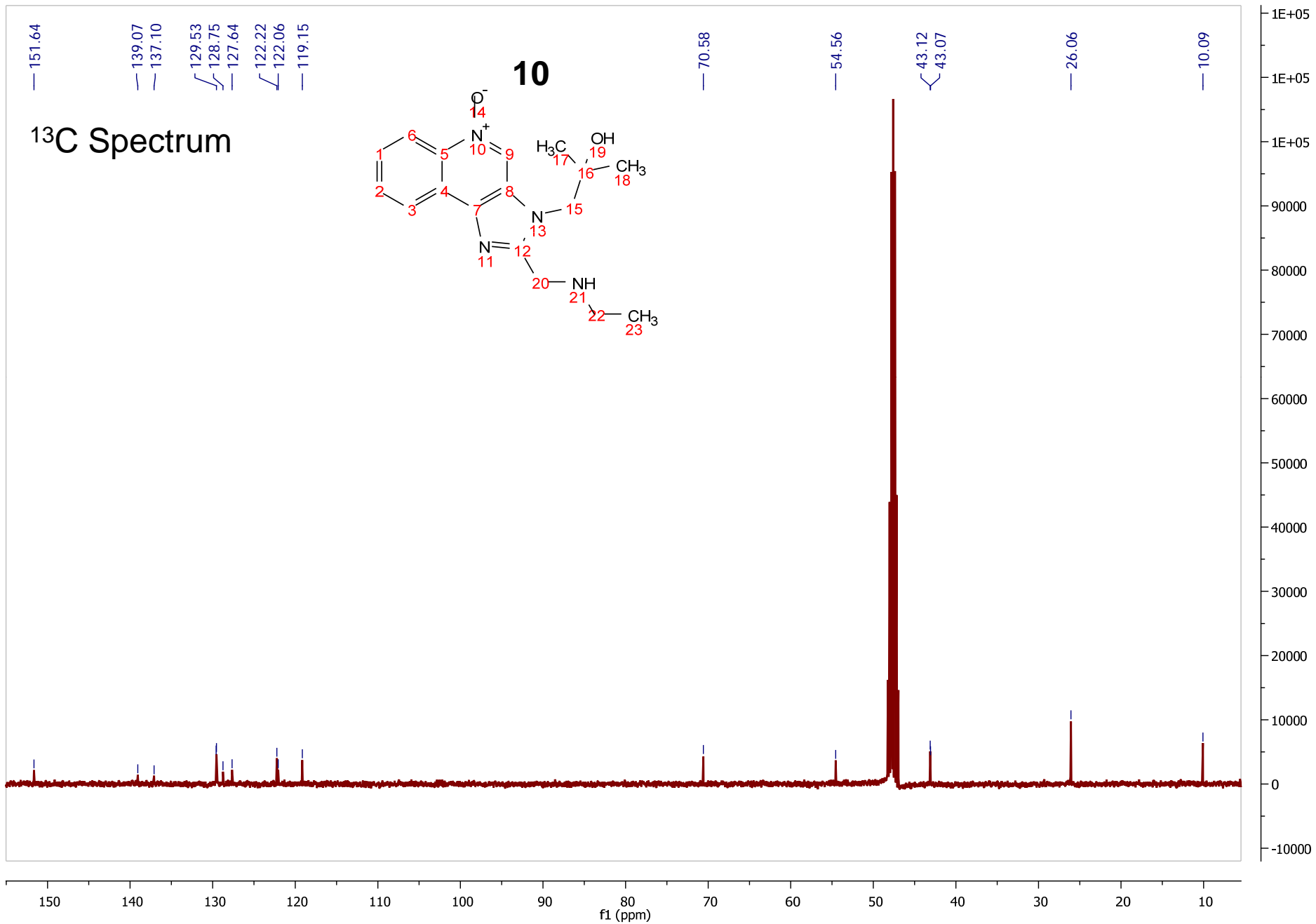


# <sup>13</sup>C Spectrum

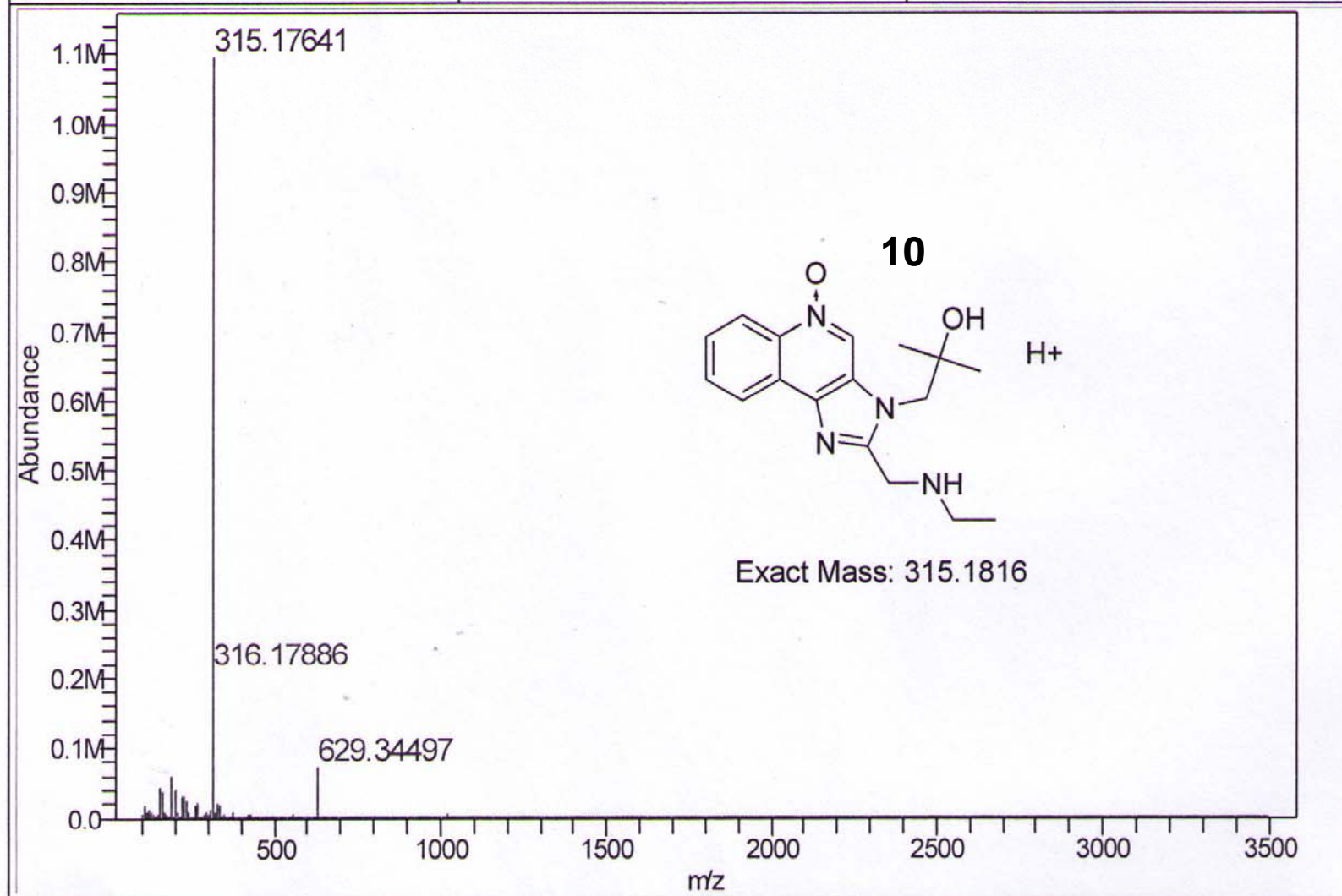


151.64  
139.07  
137.10  
129.53  
128.75  
127.64  
122.22  
122.06  
119.15

70.58  
54.56  
43.12  
43.07  
26.06  
10.09

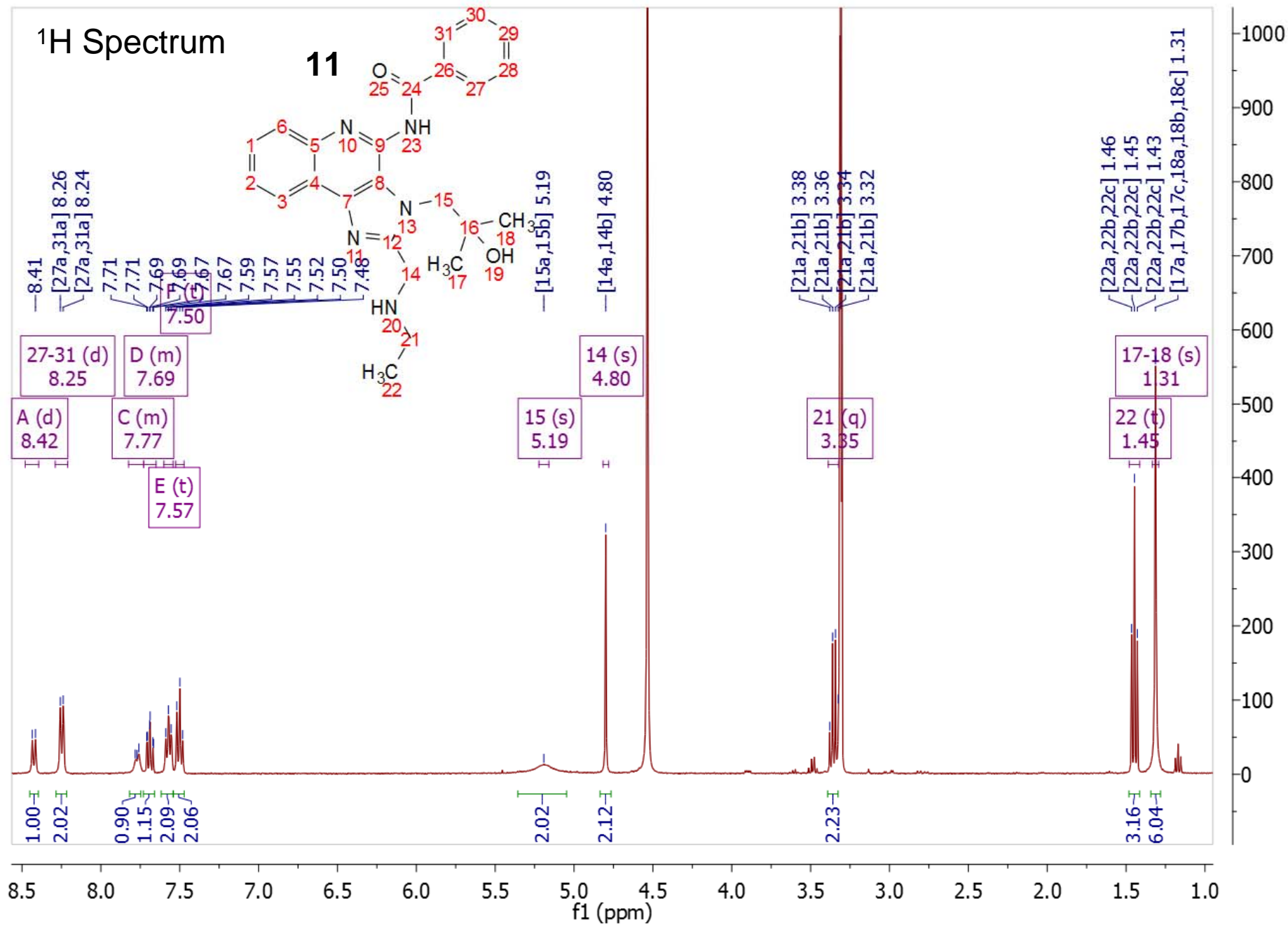
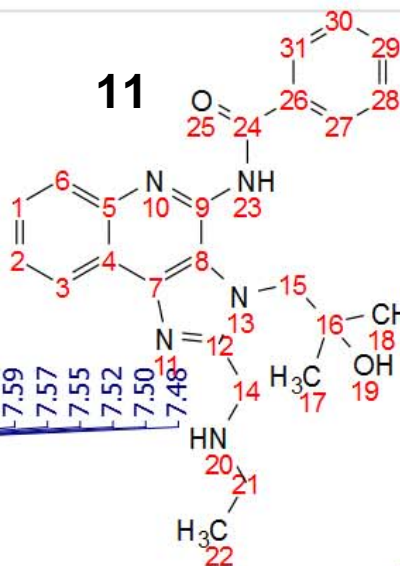


TOF Spectrum	TOF	Profile Spectrum at 4728.97 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 1095820

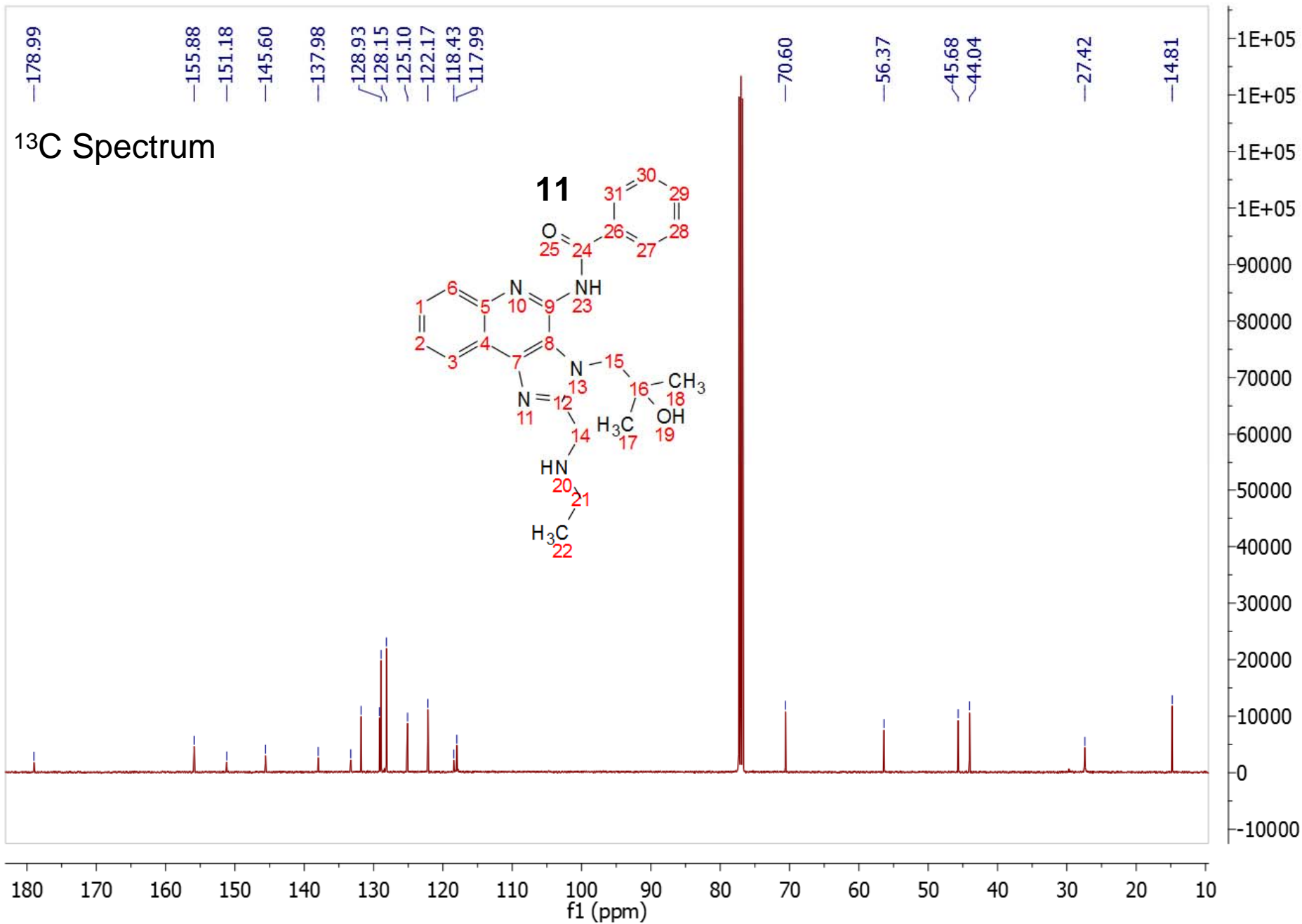


# <sup>1</sup>H Spectrum

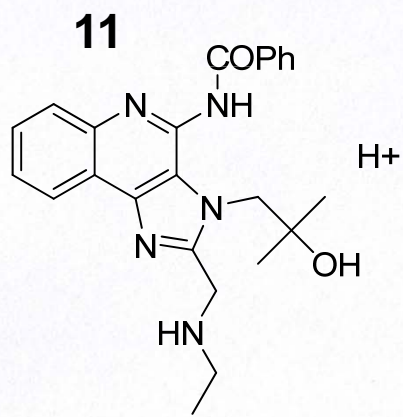
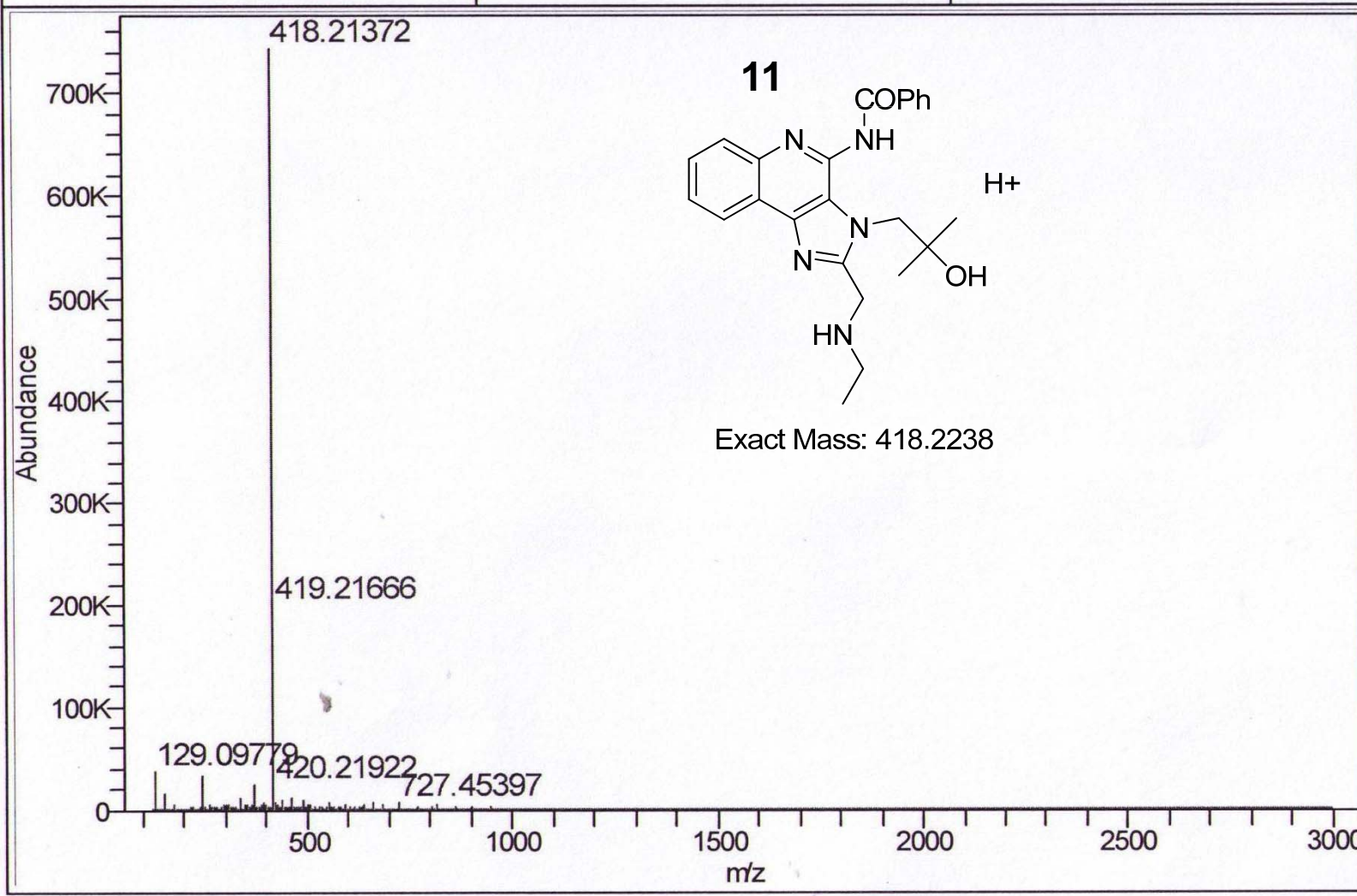
**11**



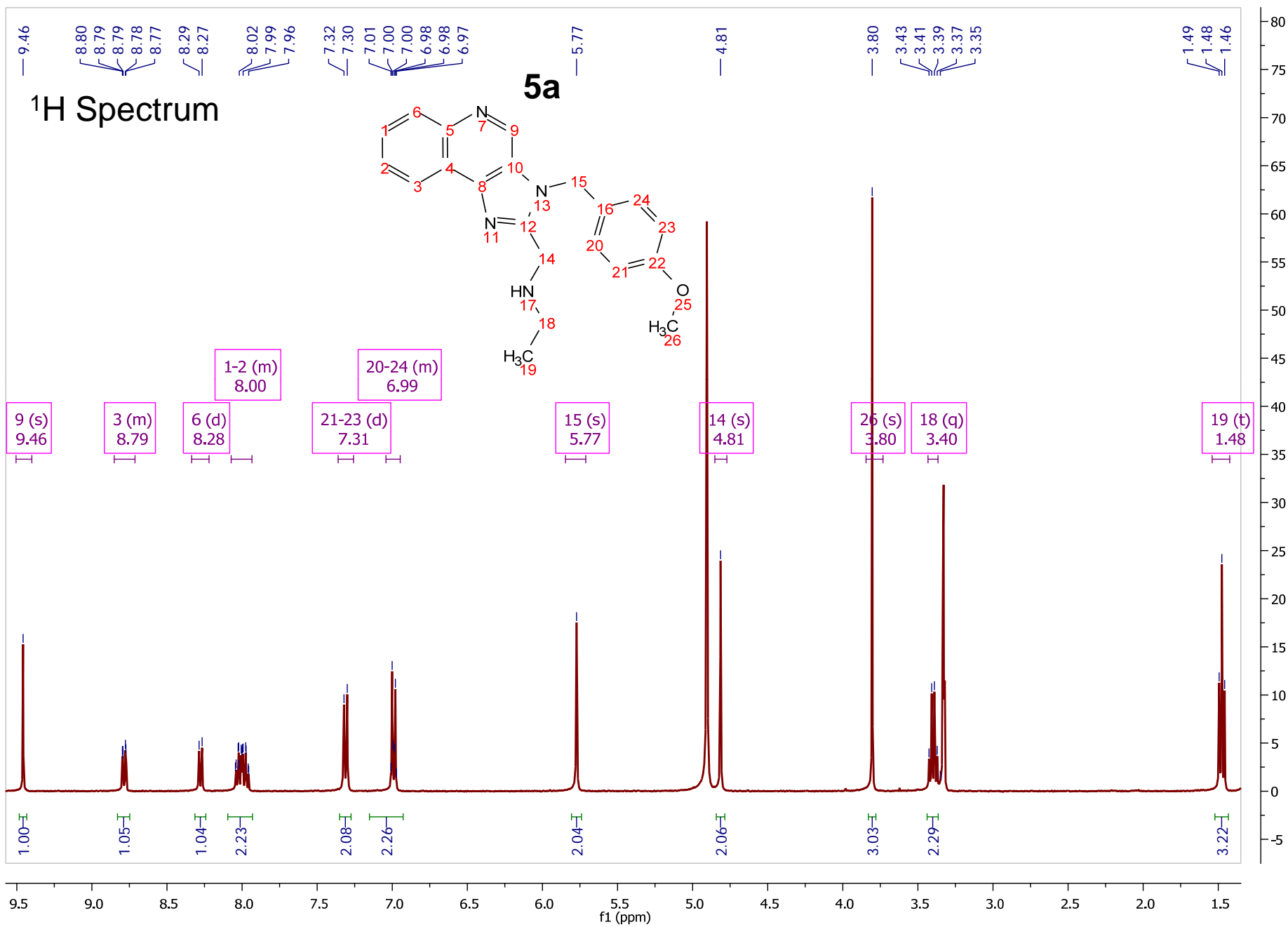
# <sup>13</sup>C Spectrum



TOF Spectrum	TOF	Profile Spectrum at 1280.19 min (scan 1)
Baseline = 0.747896950578339	Abundance Min = 0	Abundance Max = 743096

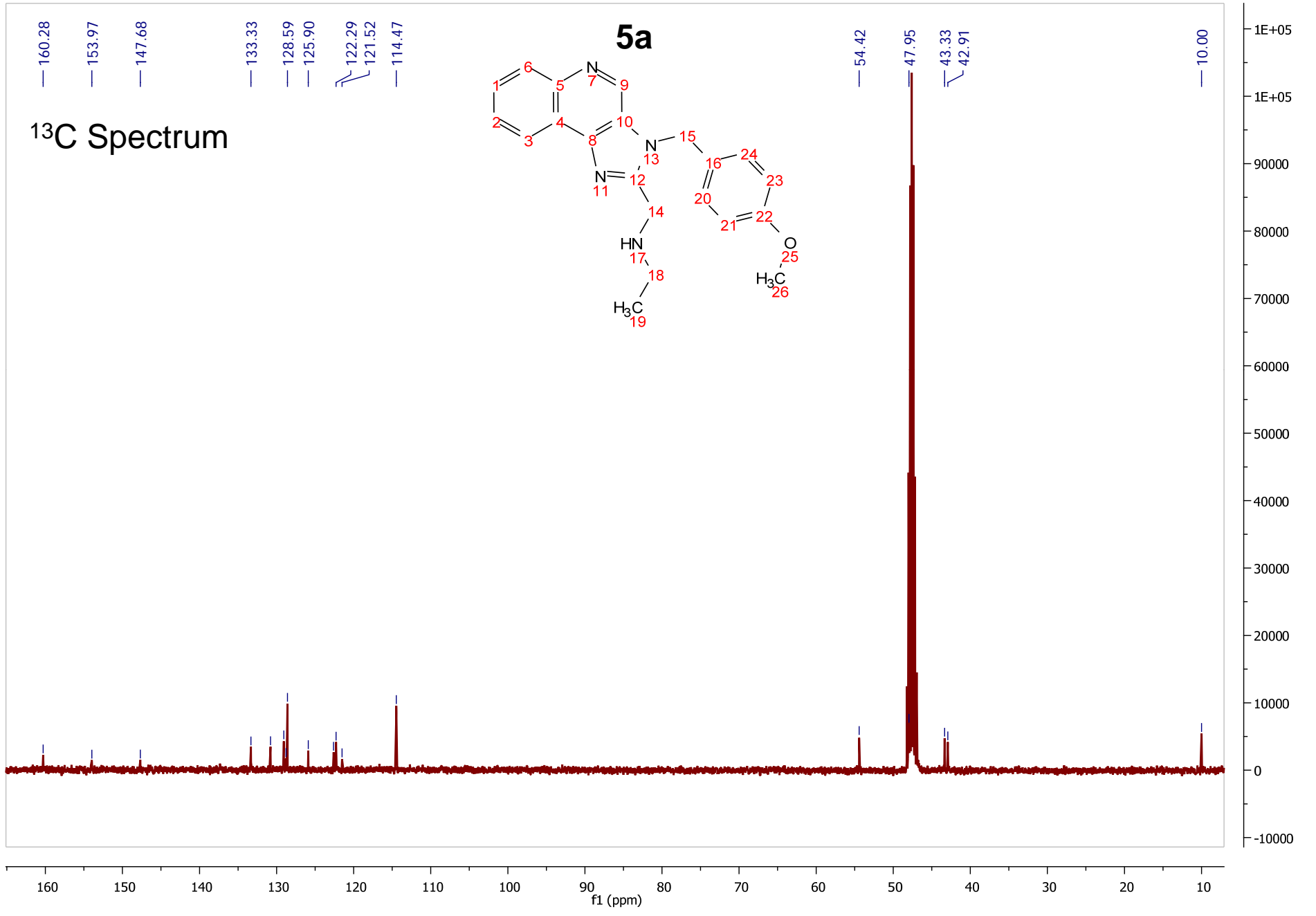
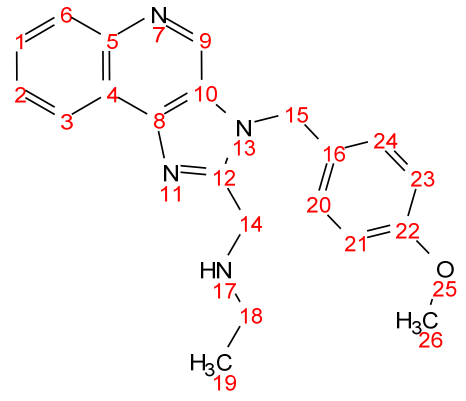




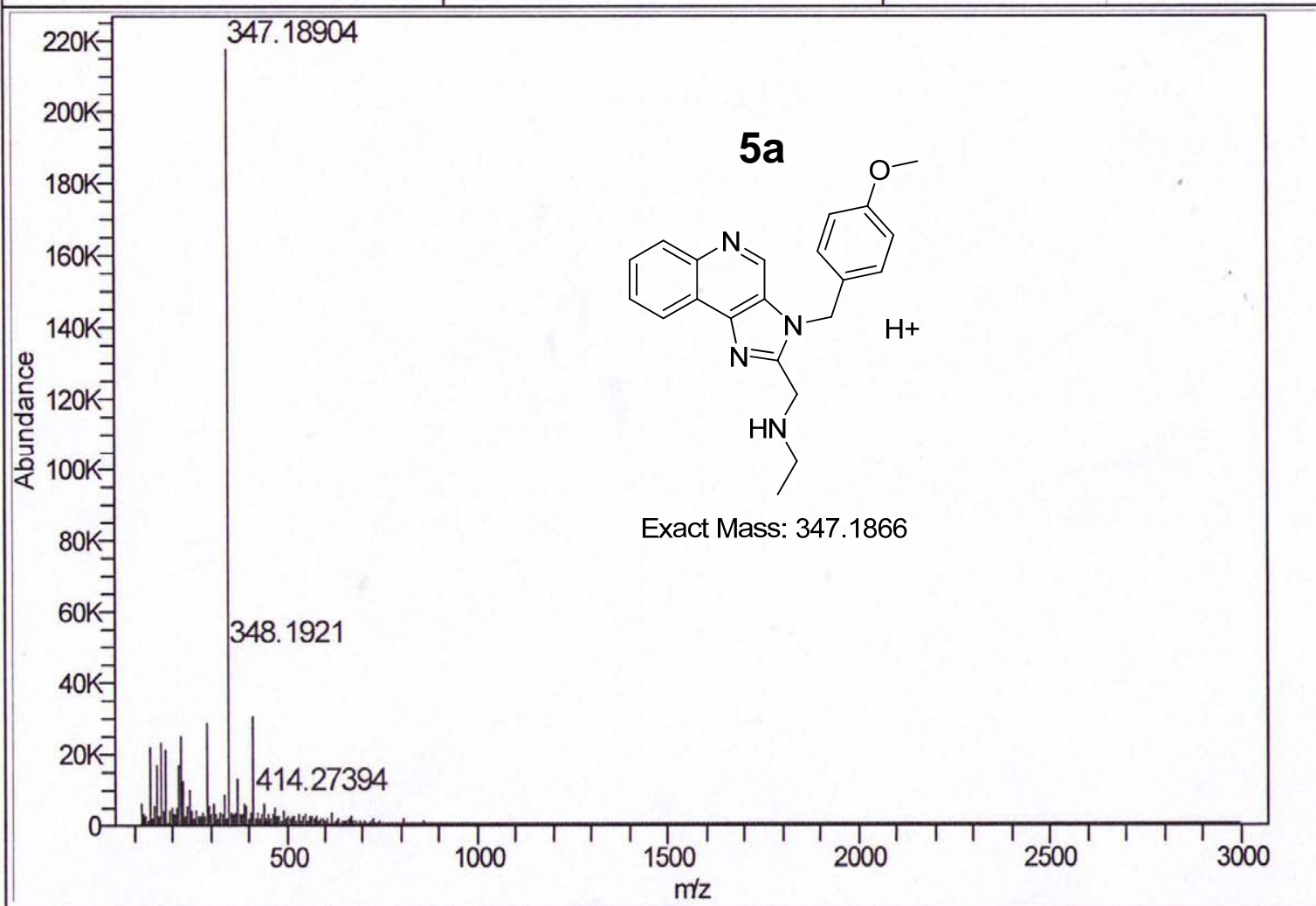


# <sup>13</sup>C Spectrum

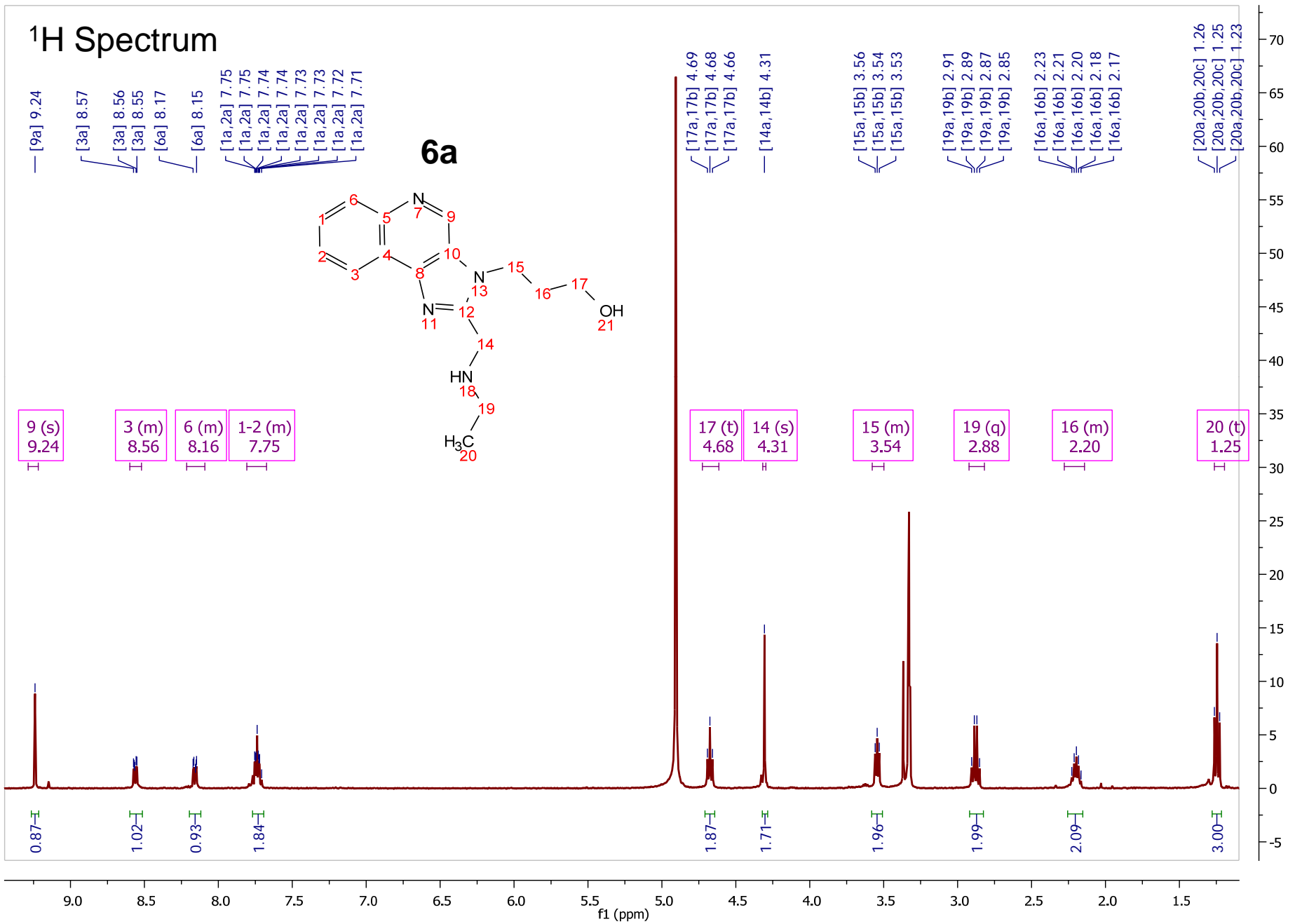
**5a**



TOF Spectrum	TOF	Profile Spectrum at 143.20 min (scan 1)
Baseline = 0.426778242677824	Abundance Min = 0	Abundance Max = 217180

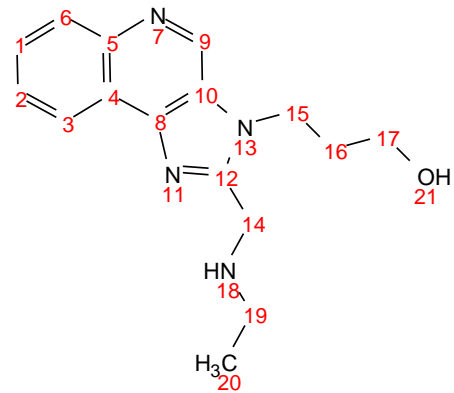


# <sup>1</sup>H Spectrum



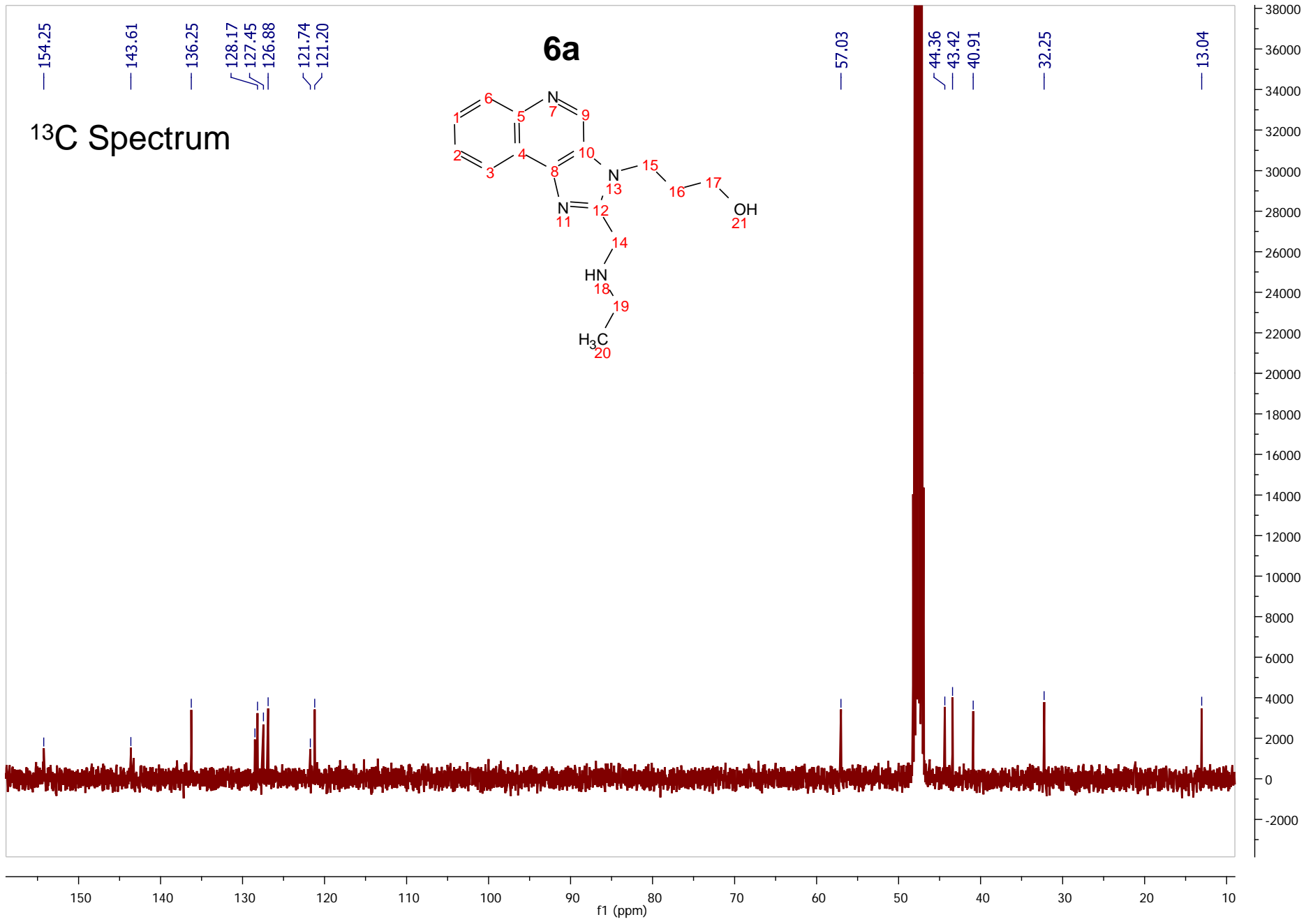
# <sup>13</sup>C Spectrum

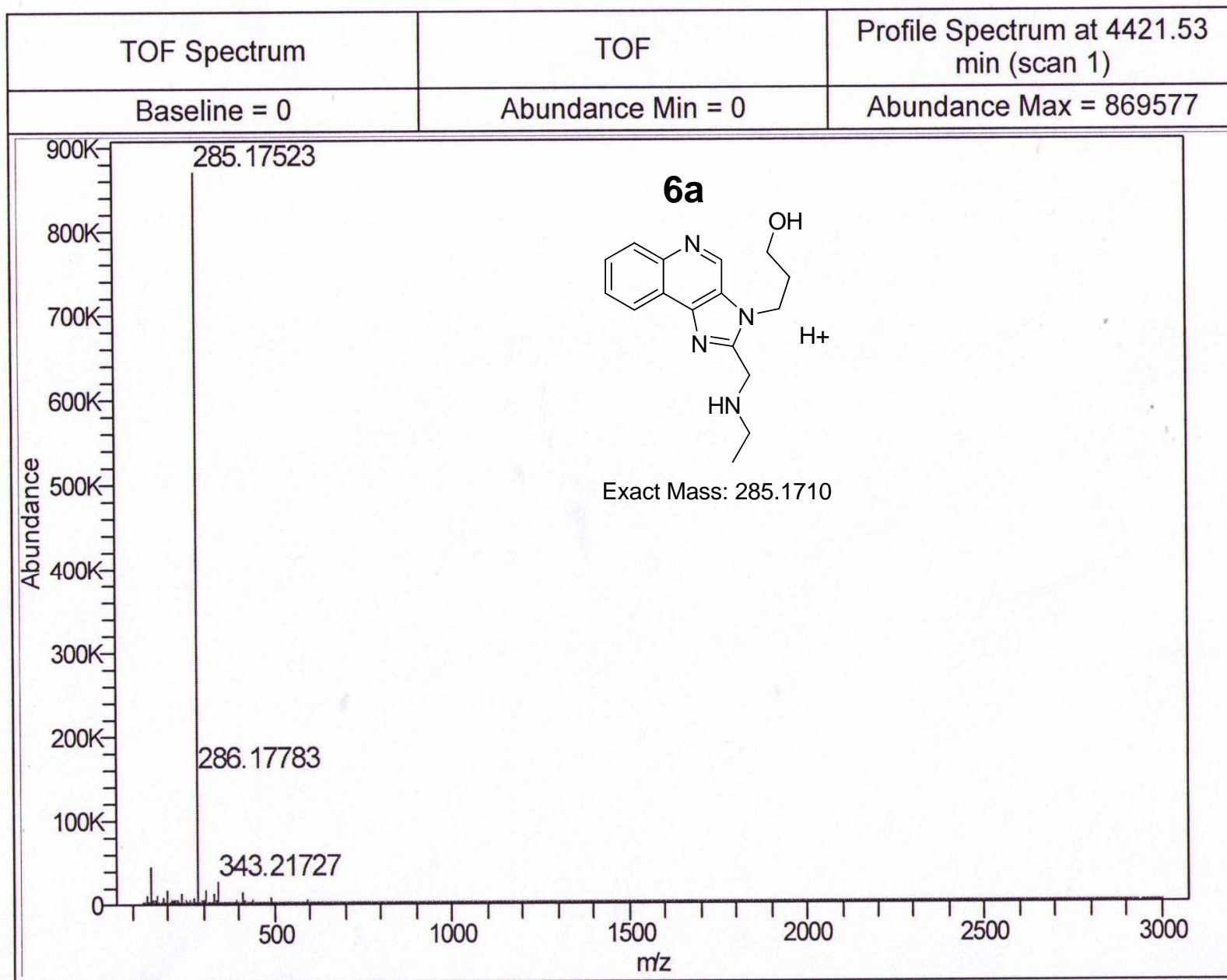
**6a**



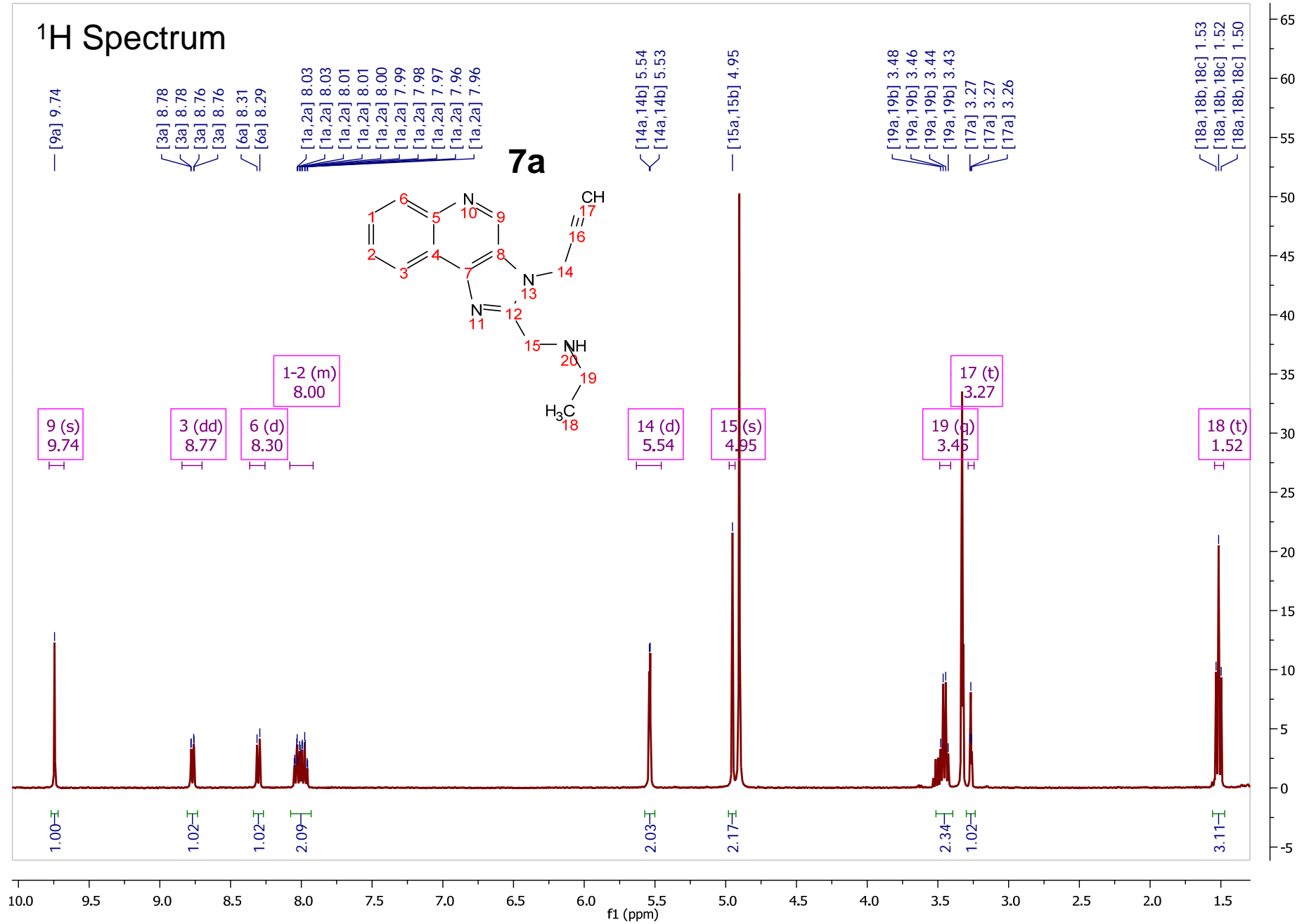
- 154.25
- 143.61
- 136.25
- 128.17
- 127.45
- 126.88
- 121.74
- 121.20

- 57.03
- 44.36
- 43.42
- 40.91
- 32.25
- 13.04



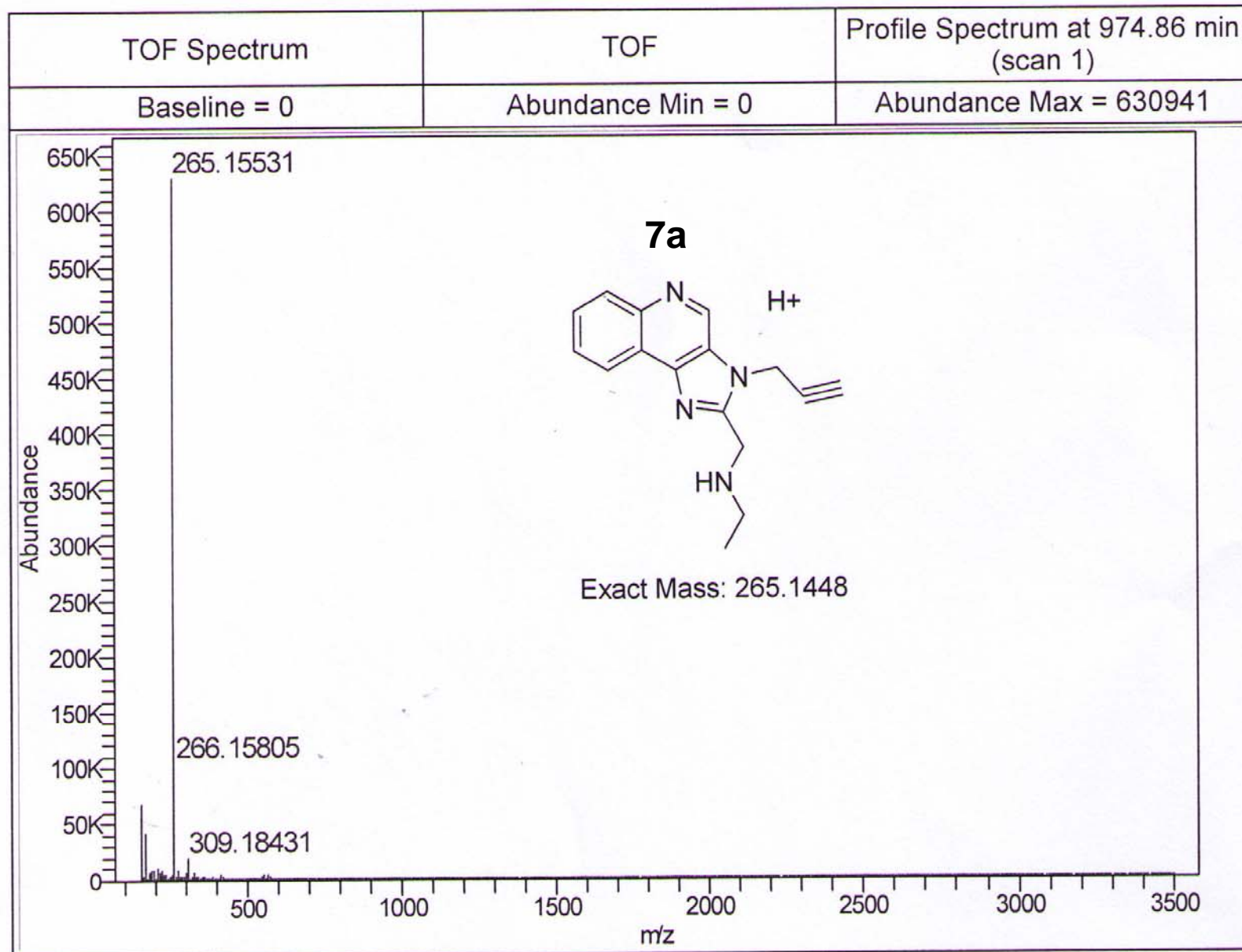


# <sup>1</sup>H Spectrum

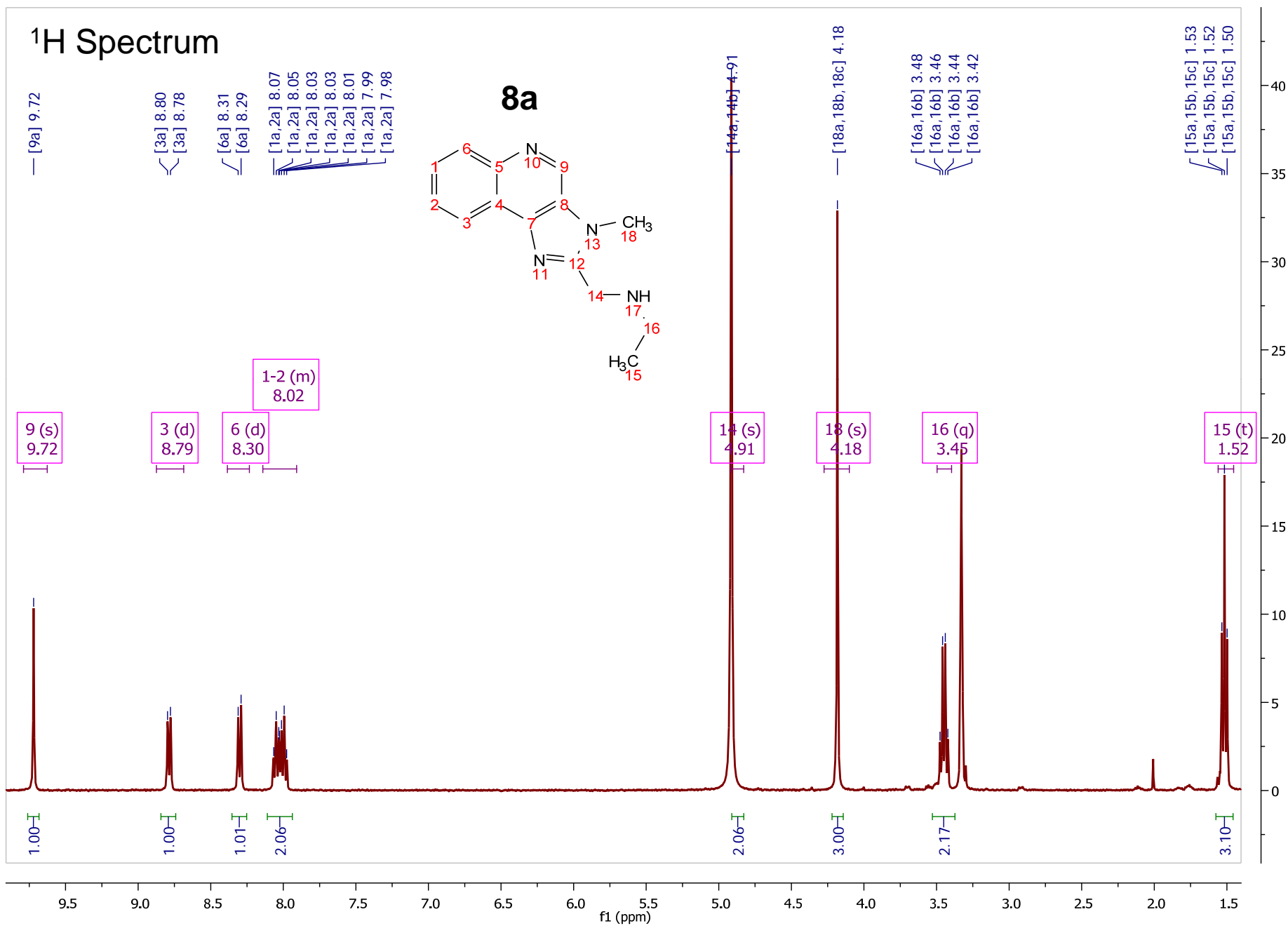




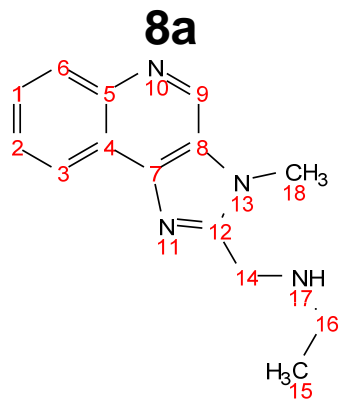




# <sup>1</sup>H Spectrum

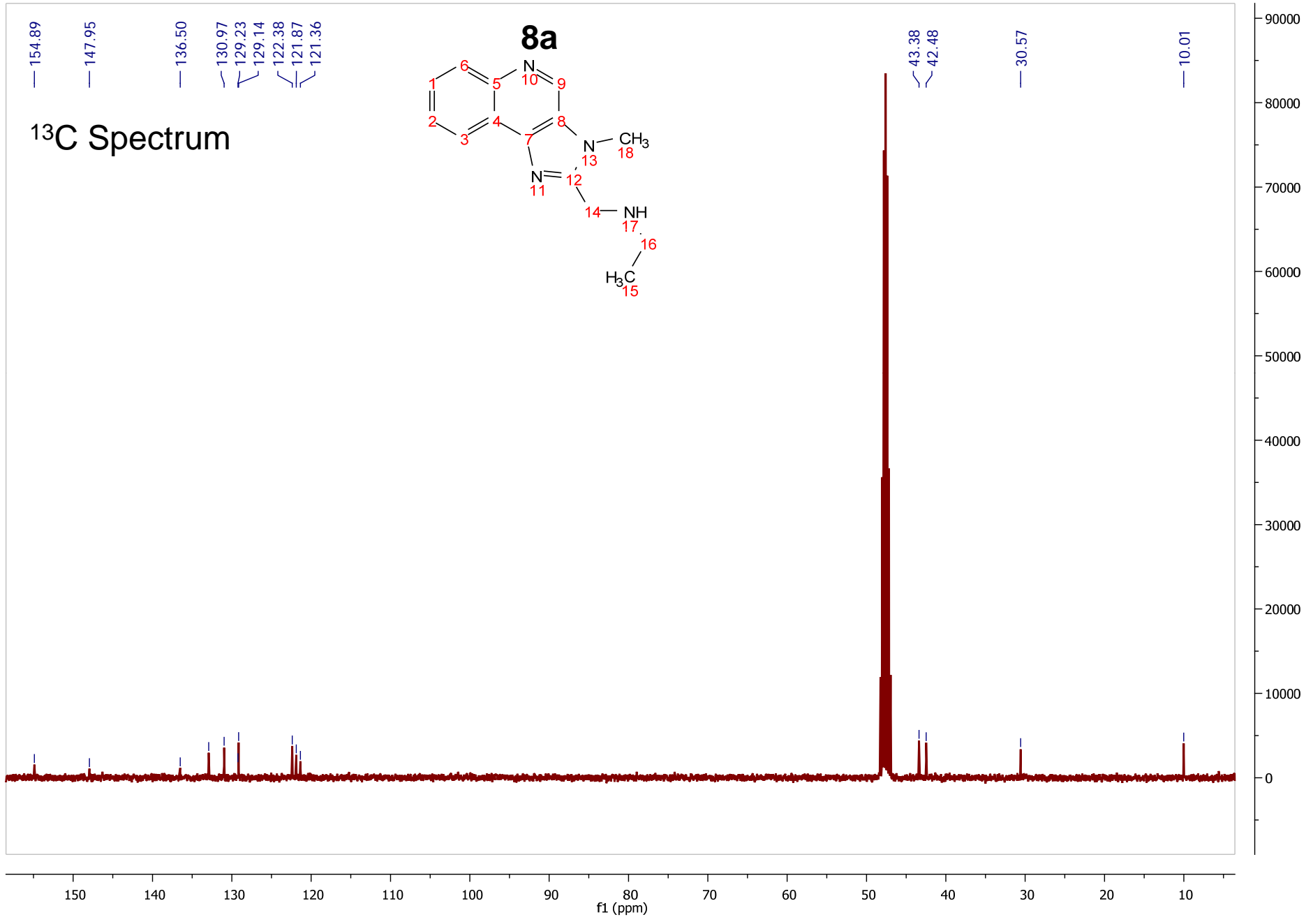


# <sup>13</sup>C Spectrum

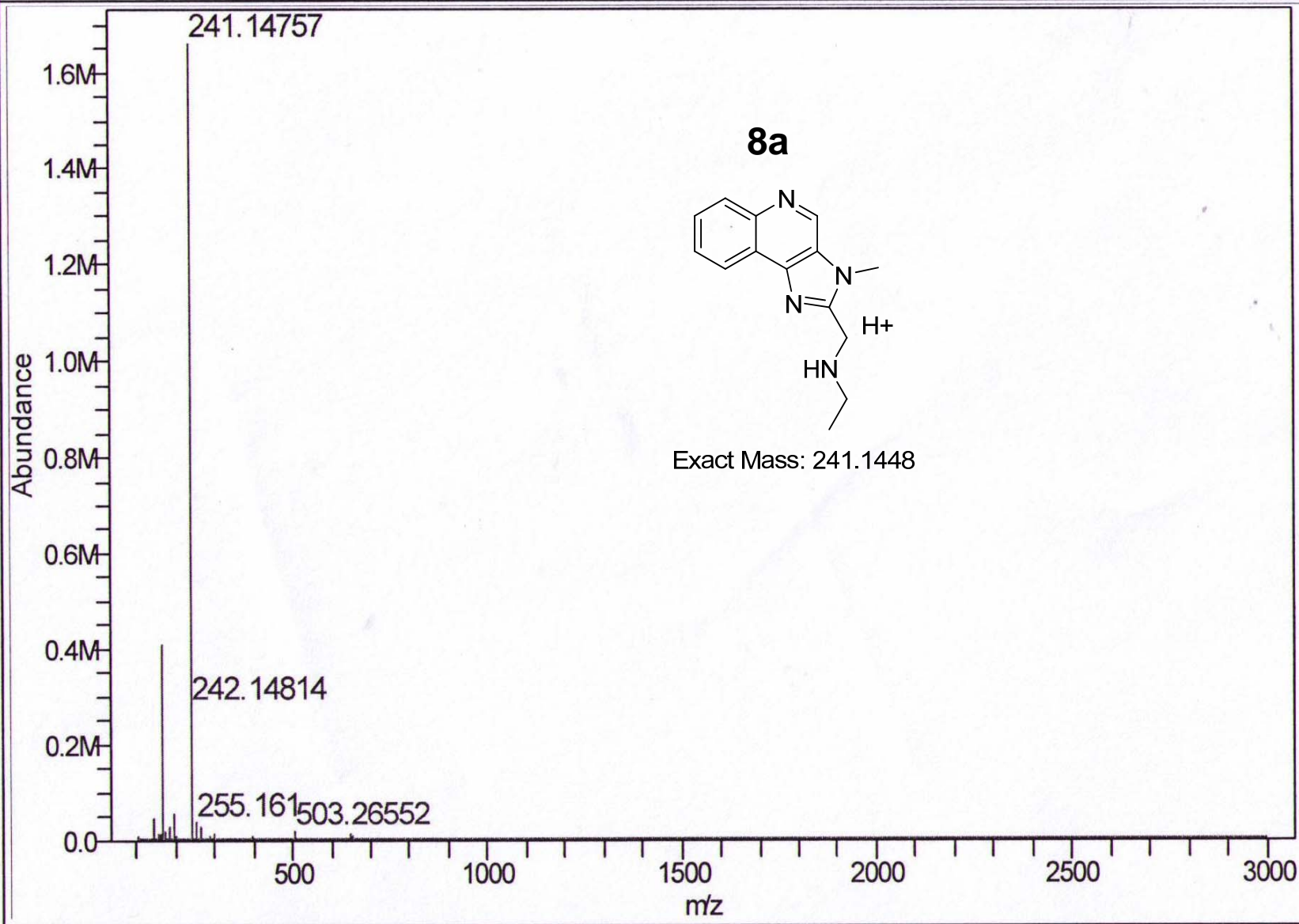


154.89  
147.95  
136.50  
130.97  
129.23  
129.14  
122.38  
121.87  
121.36

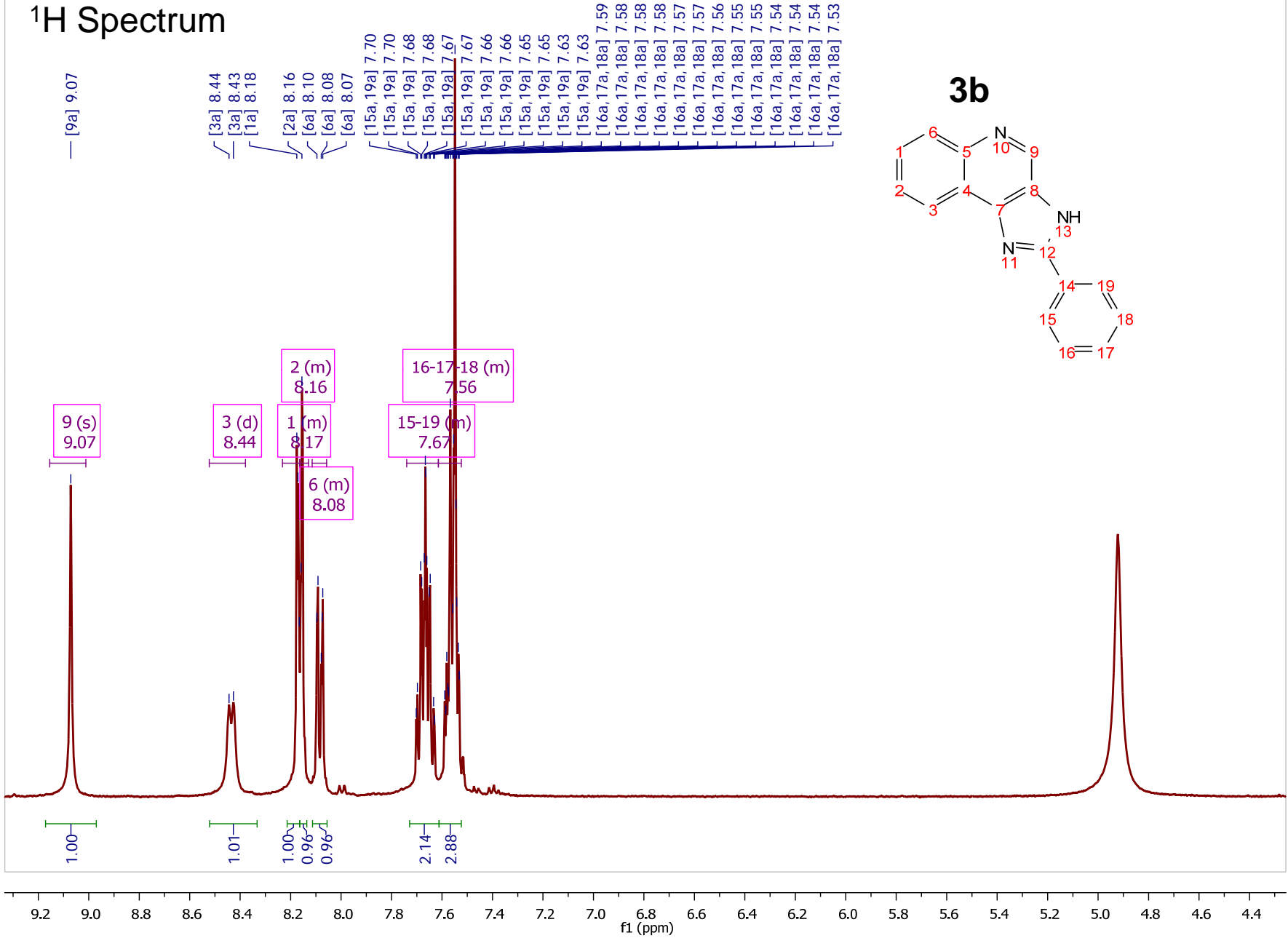
43.38  
42.48  
30.57  
10.01



TOF Spectrum	TOF	Profile Spectrum at 1740.47 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 1661590

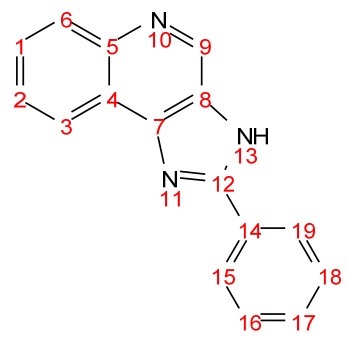


# <sup>1</sup>H Spectrum

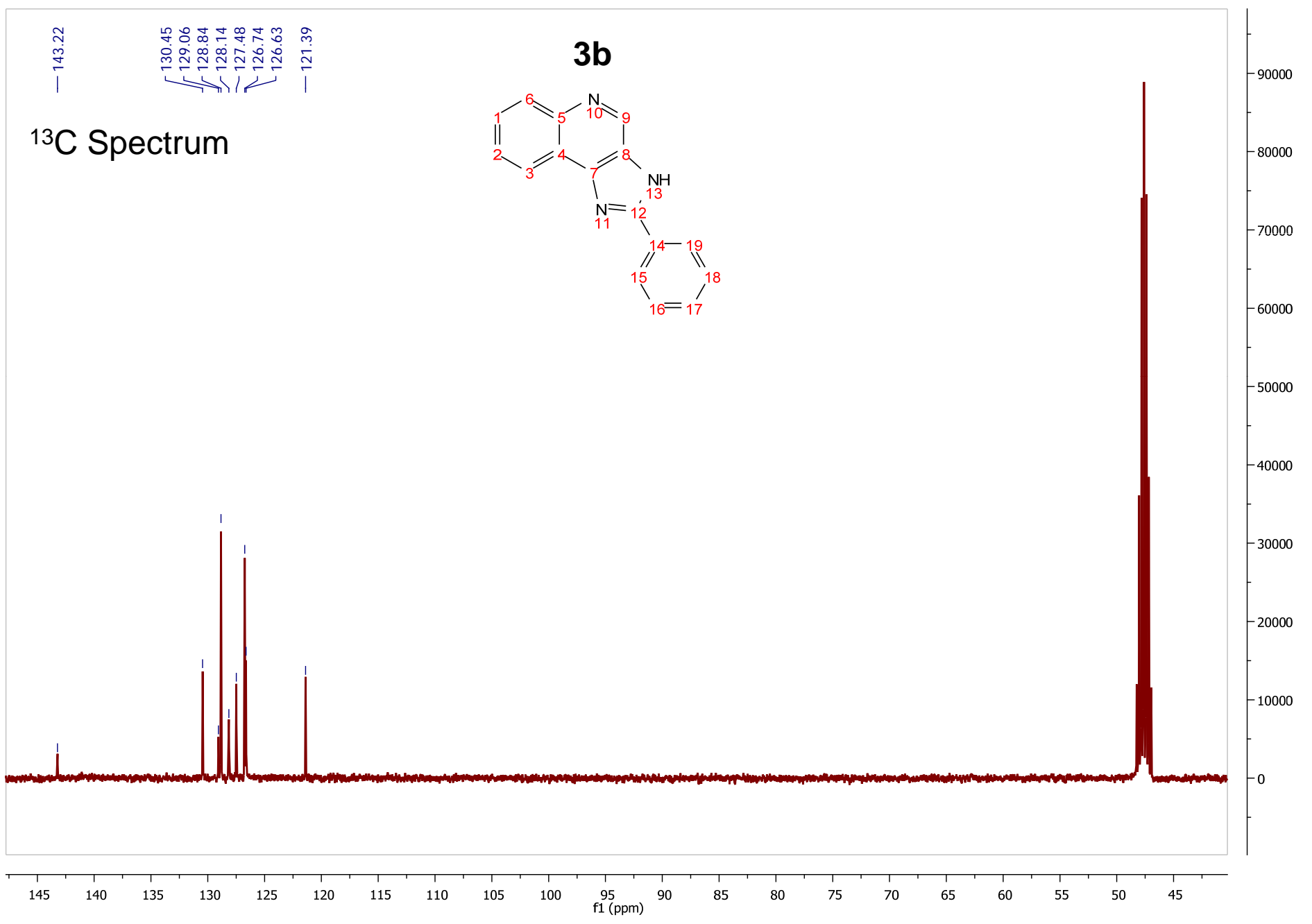


# <sup>13</sup>C Spectrum

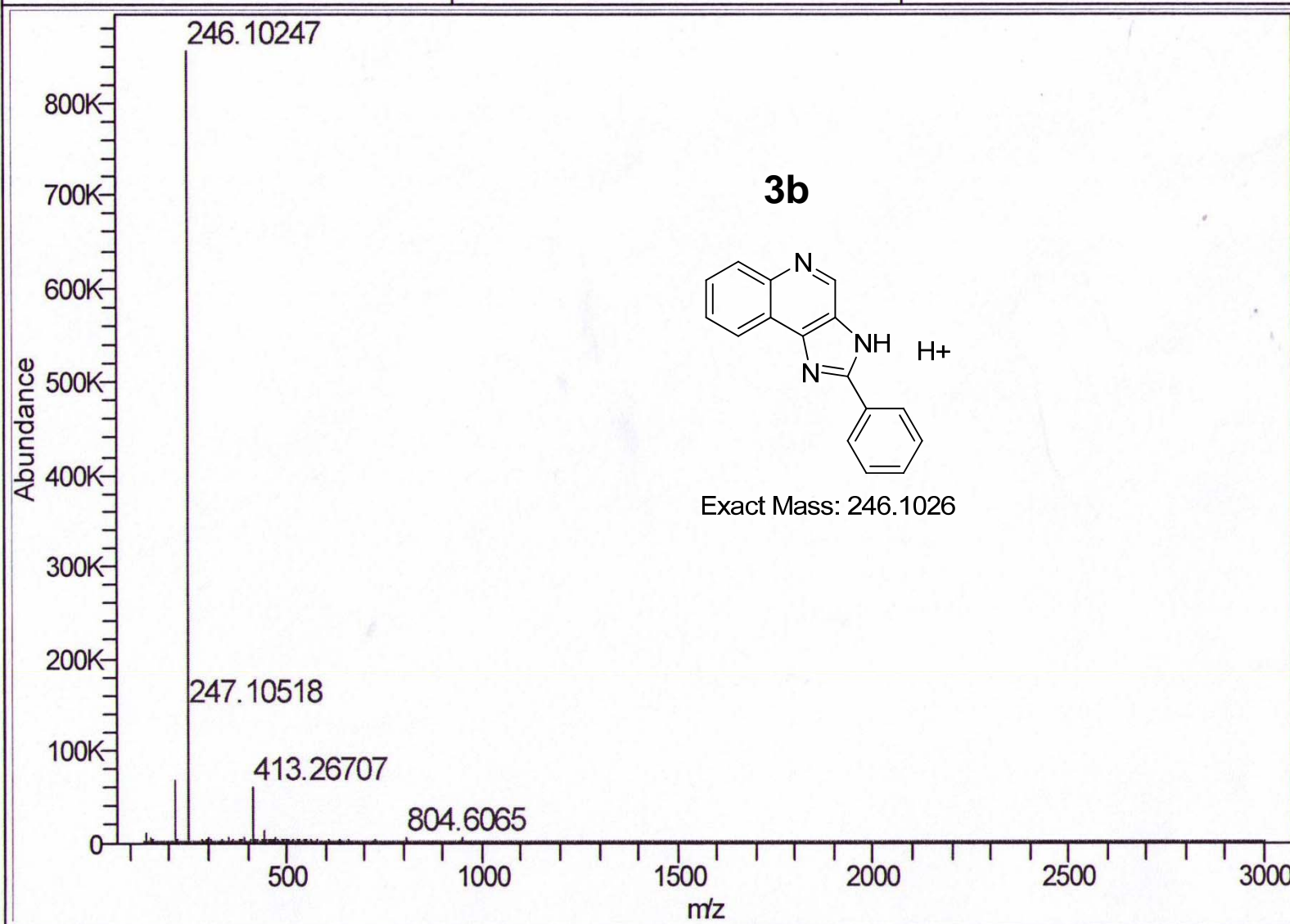
**3b**



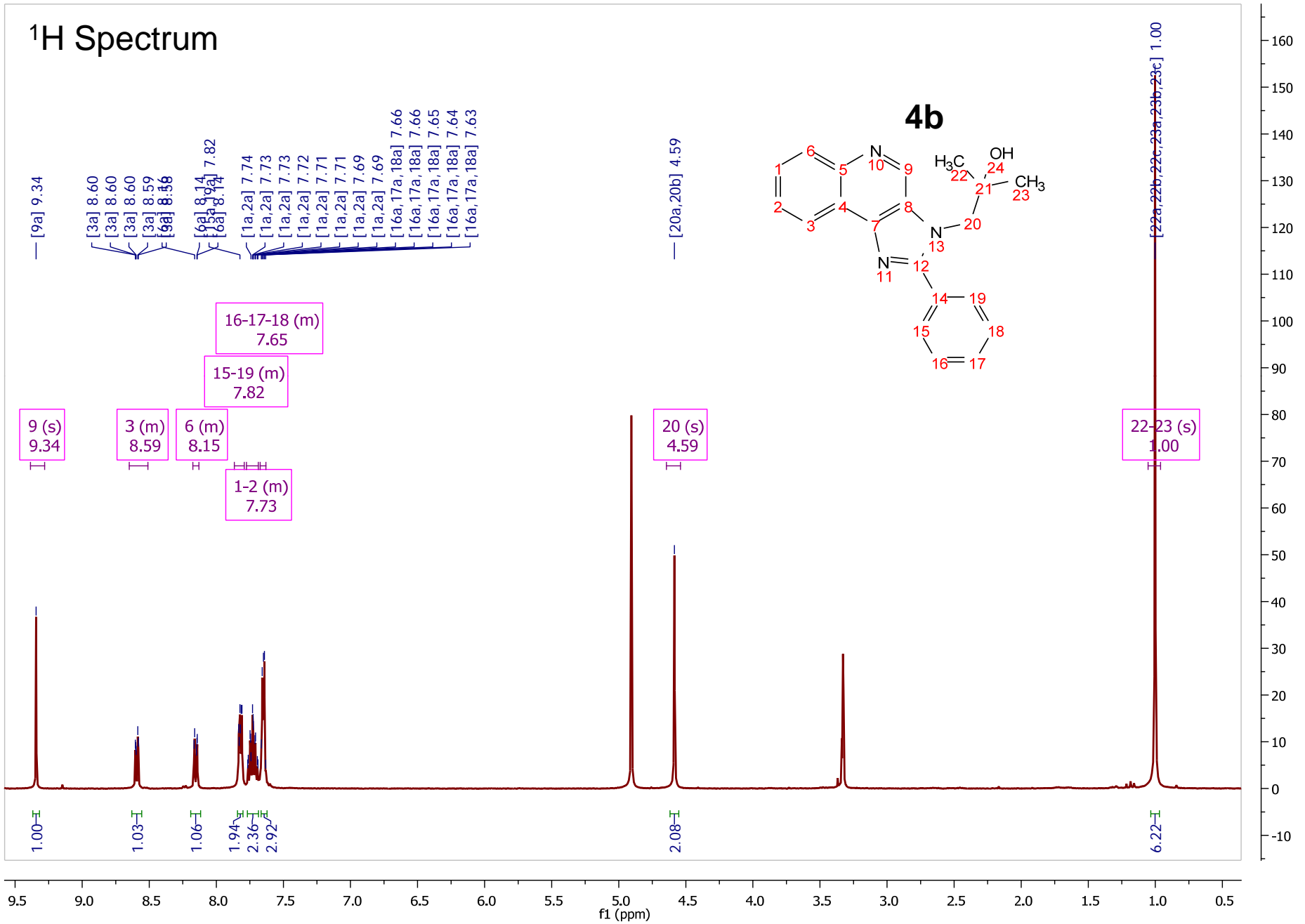
143.22  
130.45  
129.06  
128.84  
128.14  
127.48  
126.74  
126.63  
121.39



TOF Spectrum	TOF	Profile Spectrum at 14285.62 min (scan 1)
Baseline = 8.71720658523632	Abundance Min = 0	Abundance Max = 856918

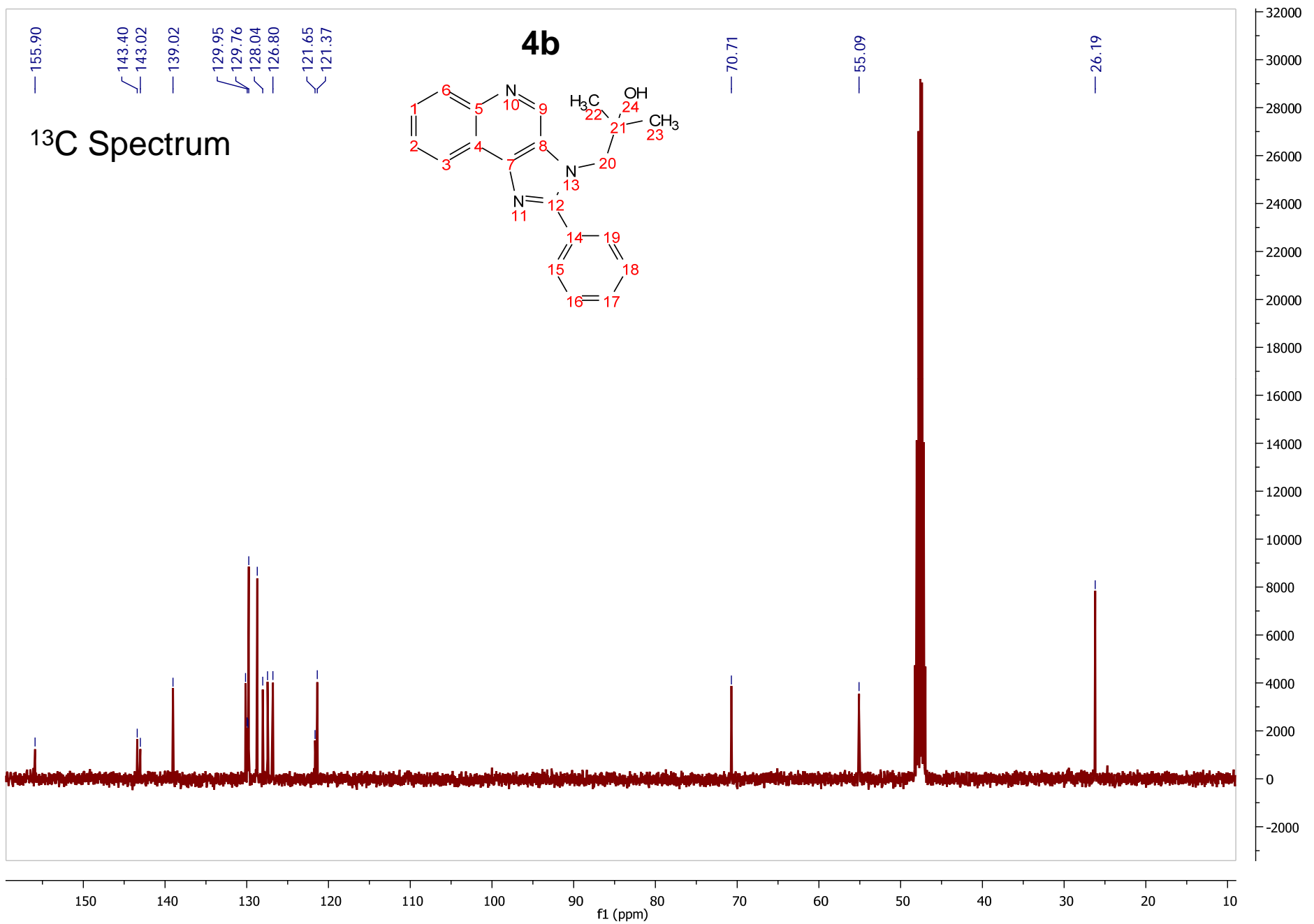
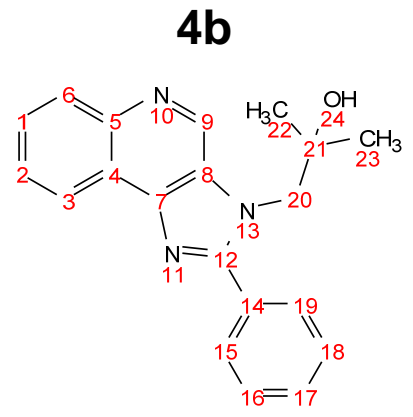


# <sup>1</sup>H Spectrum



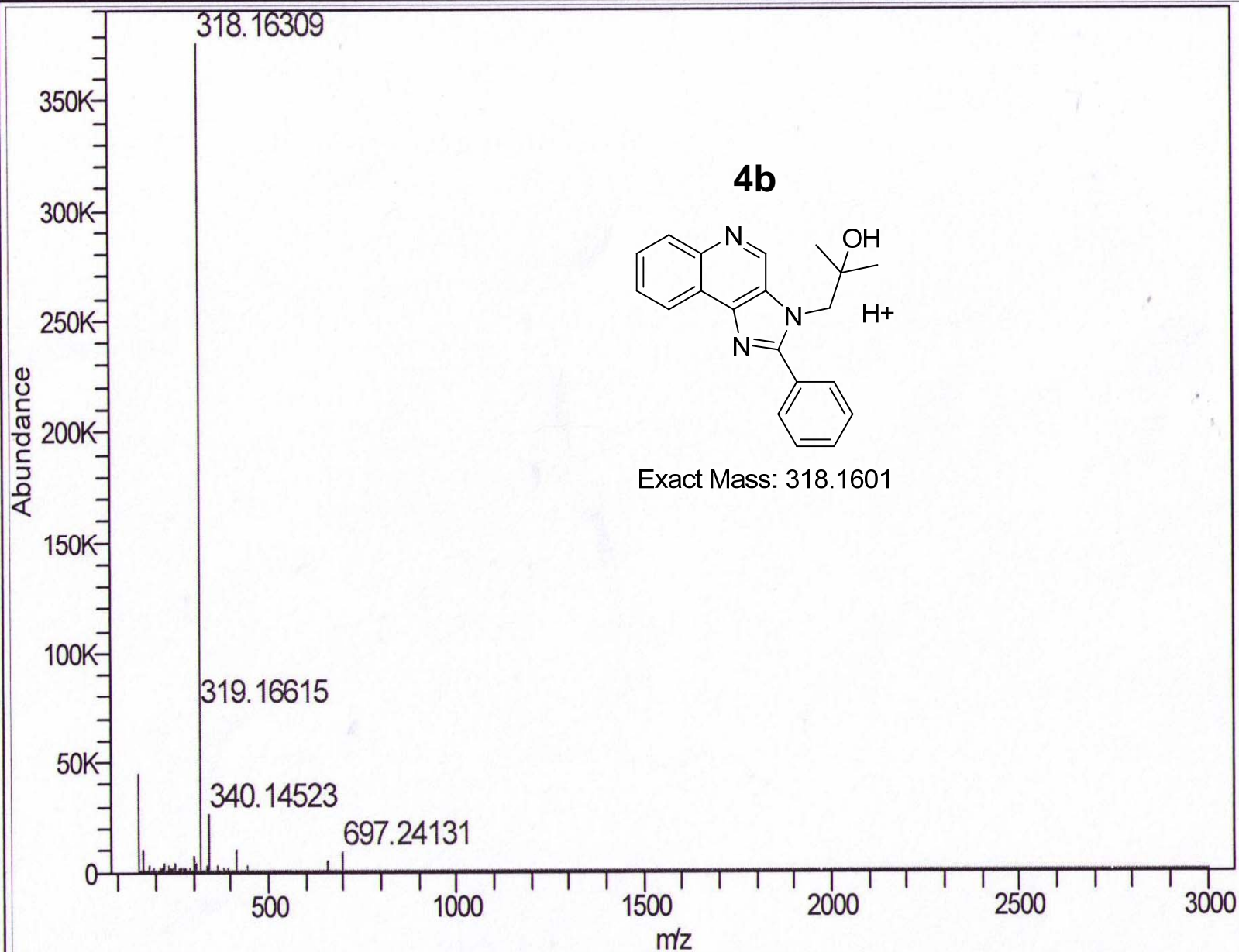


# <sup>13</sup>C Spectrum

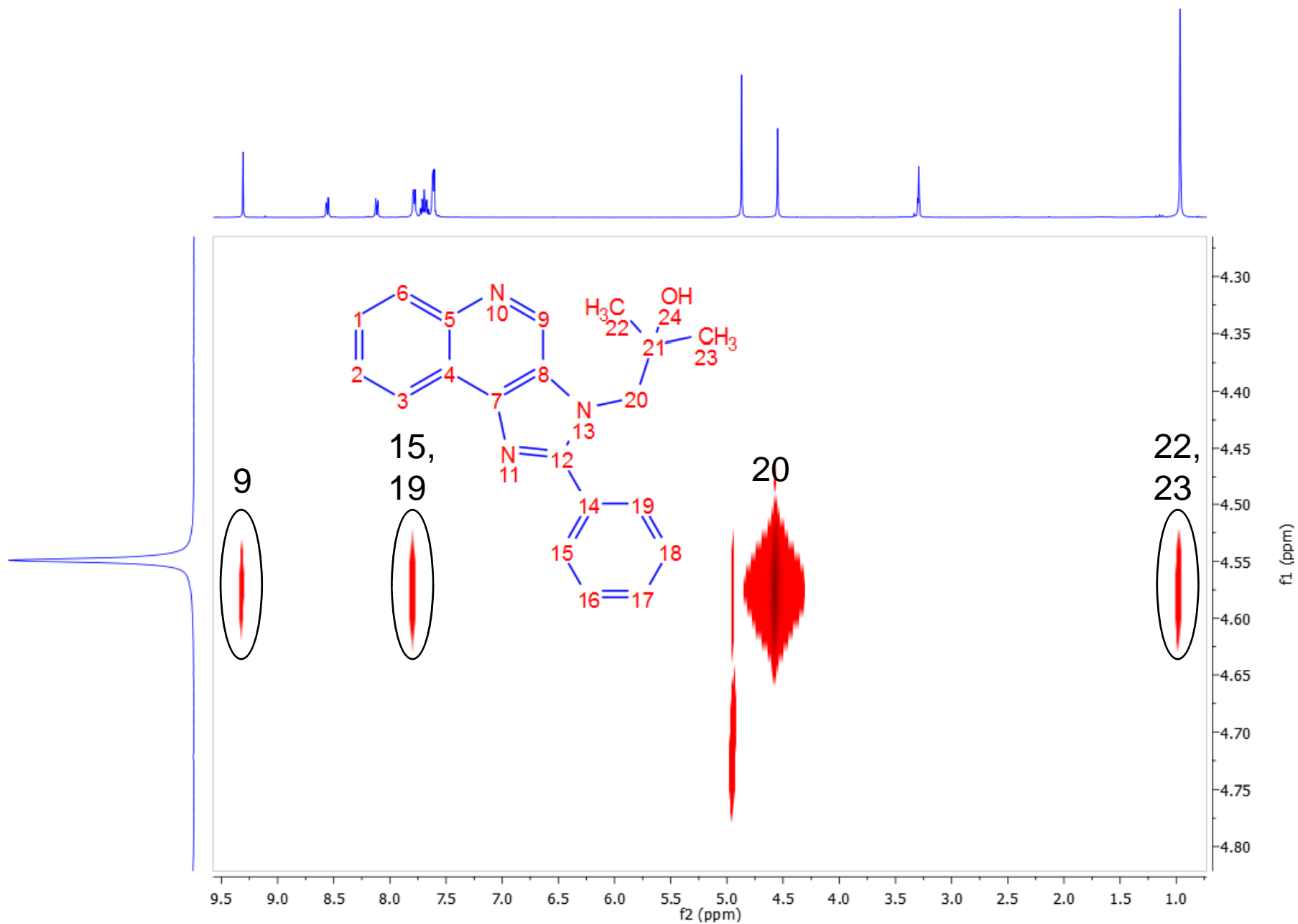


TOF Spectrum

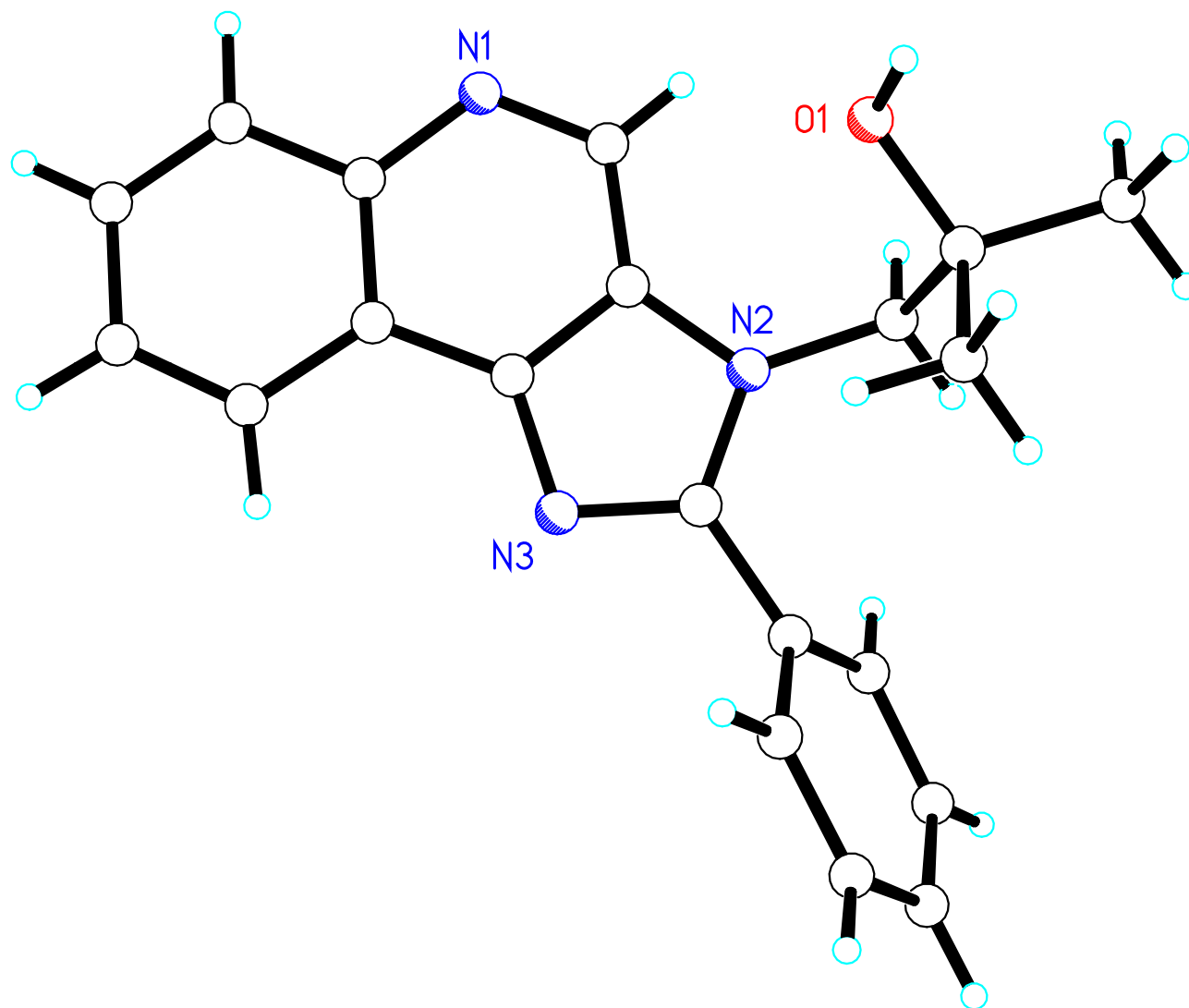
Profile Spectrum at 10393.78 min (scan 1)



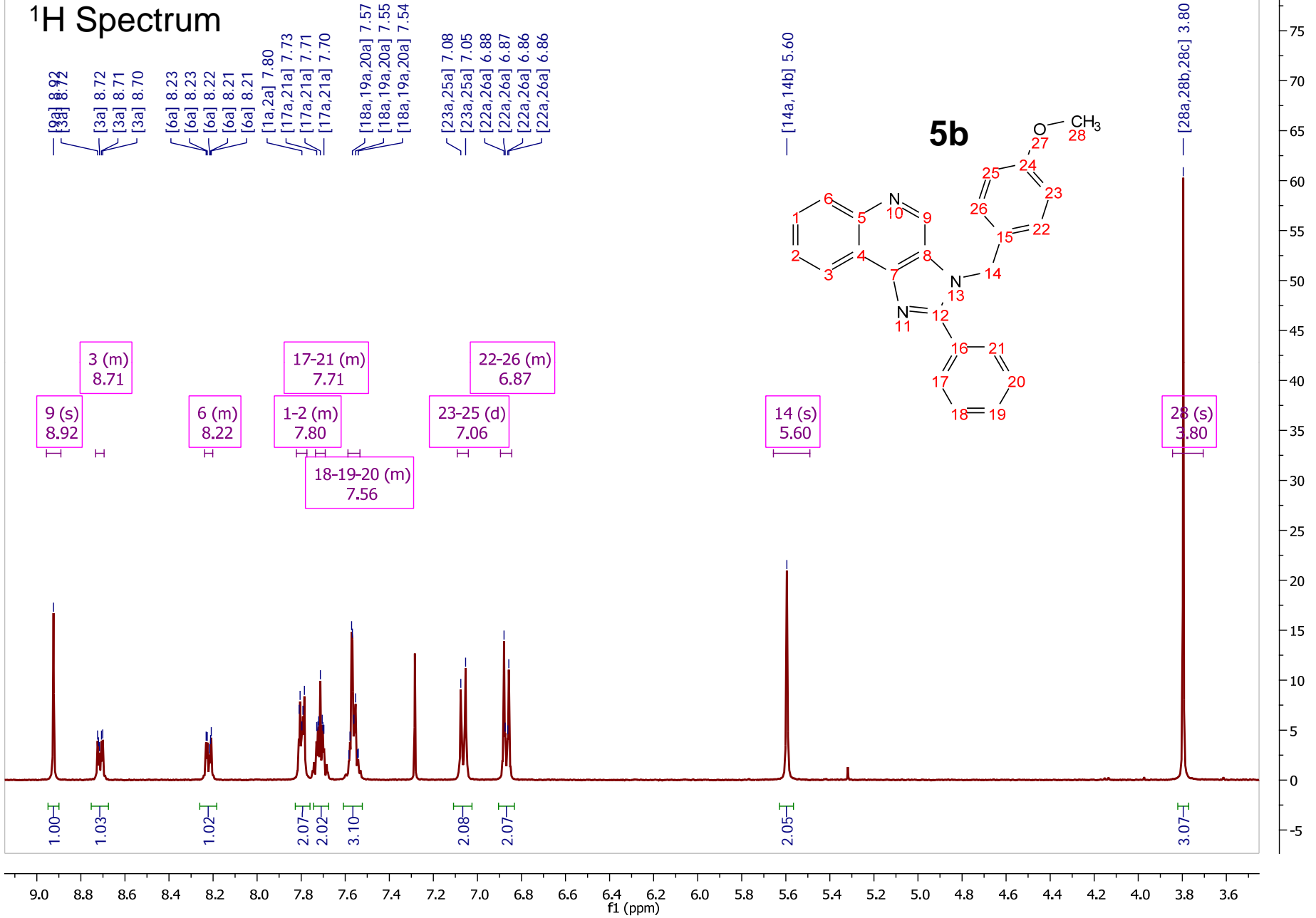
# 2D-NOESY Spectrum of Compound **4b**



# Crystal Structure of Compound 4b

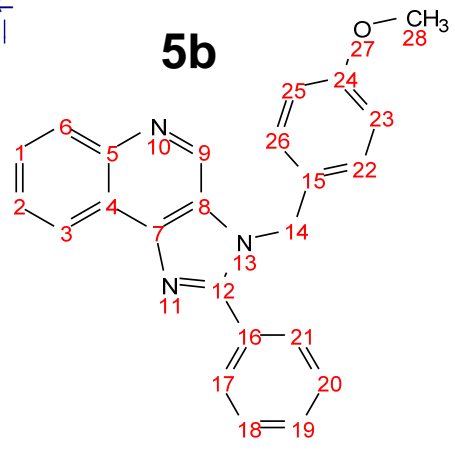


# <sup>1</sup>H Spectrum



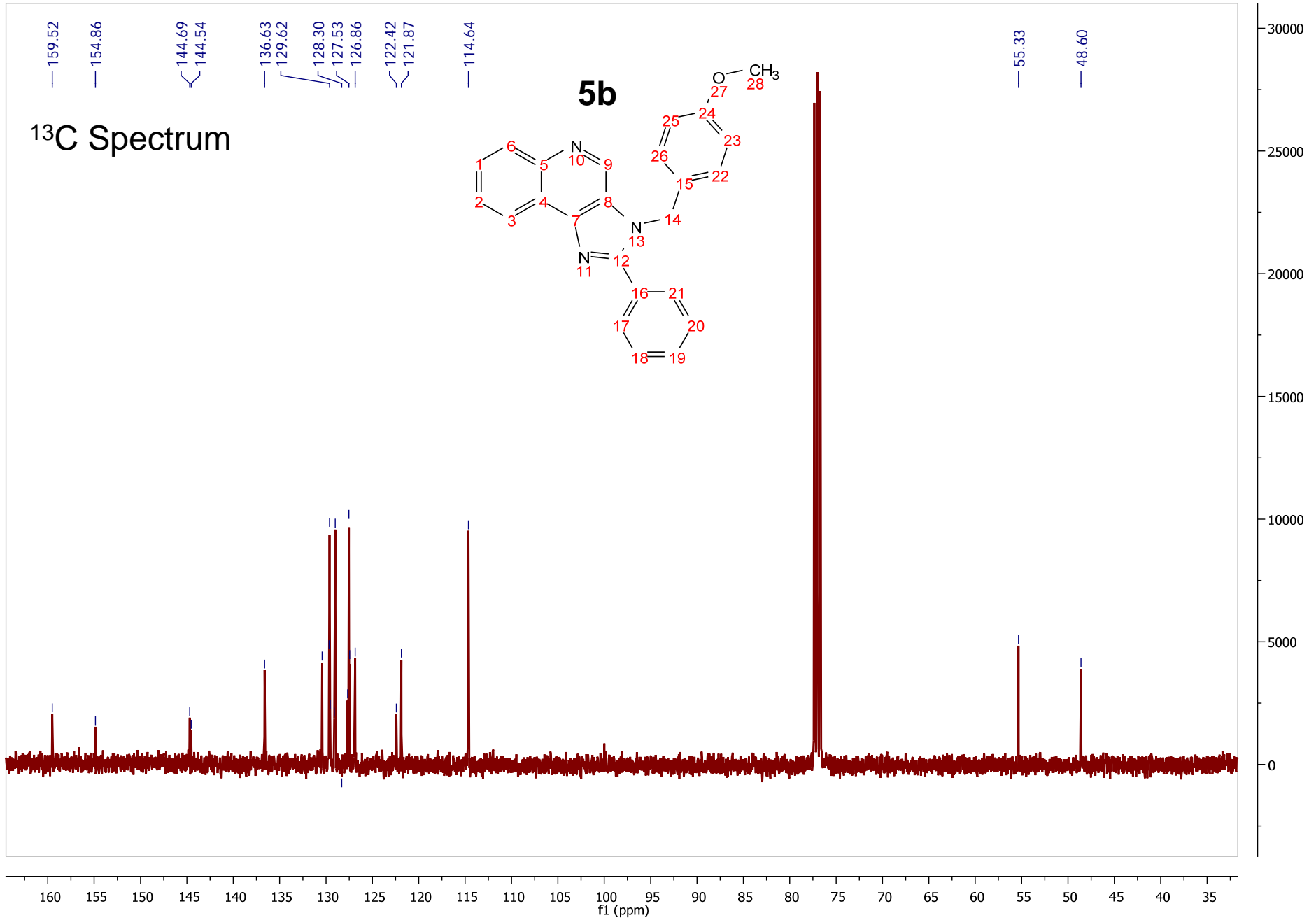
# <sup>13</sup>C Spectrum

**5b**

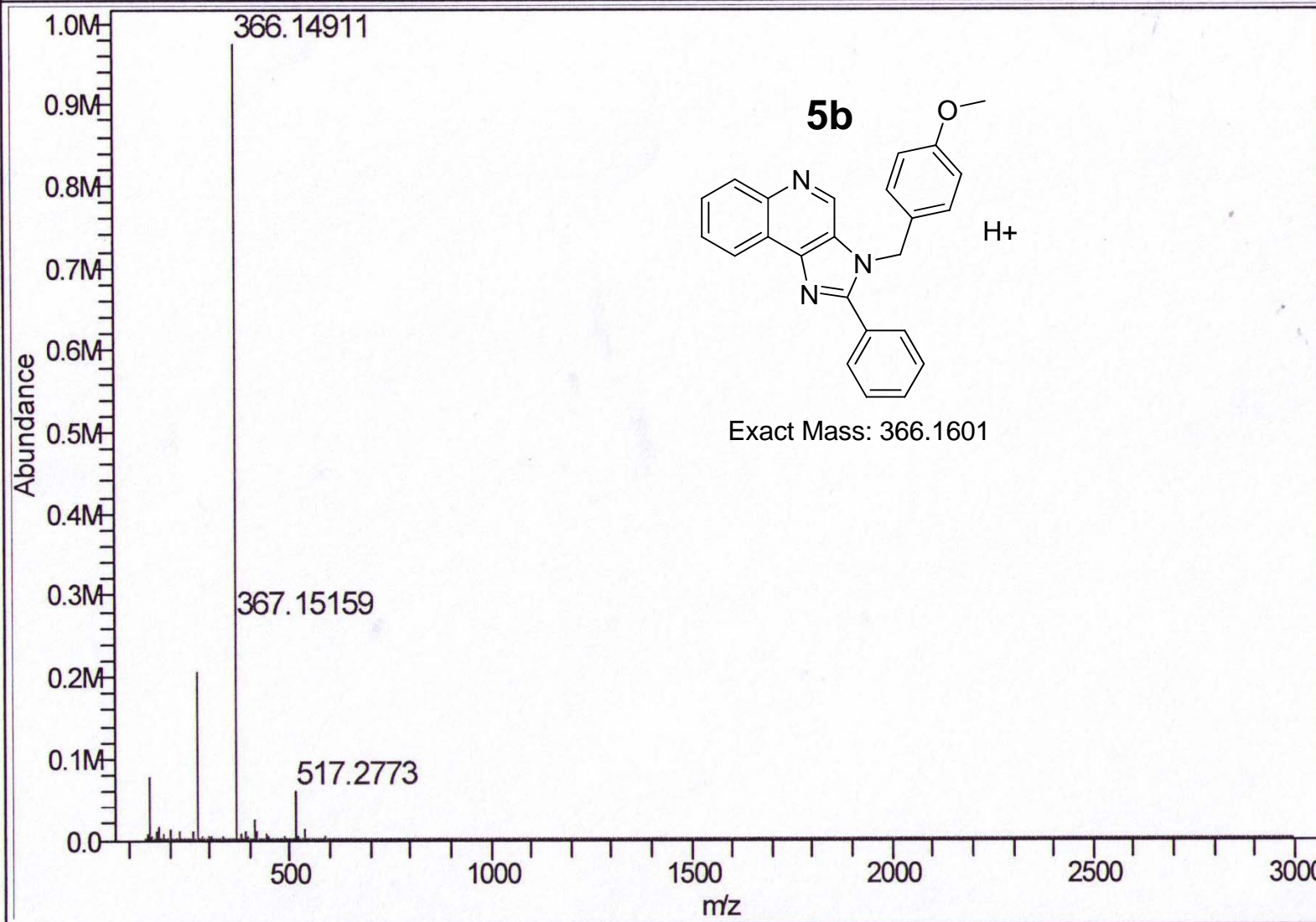


- 159.52
- 154.86
- 144.69
- 144.54
- 136.63
- 129.62
- 128.30
- 127.53
- 126.86
- 122.42
- 121.87
- 114.64

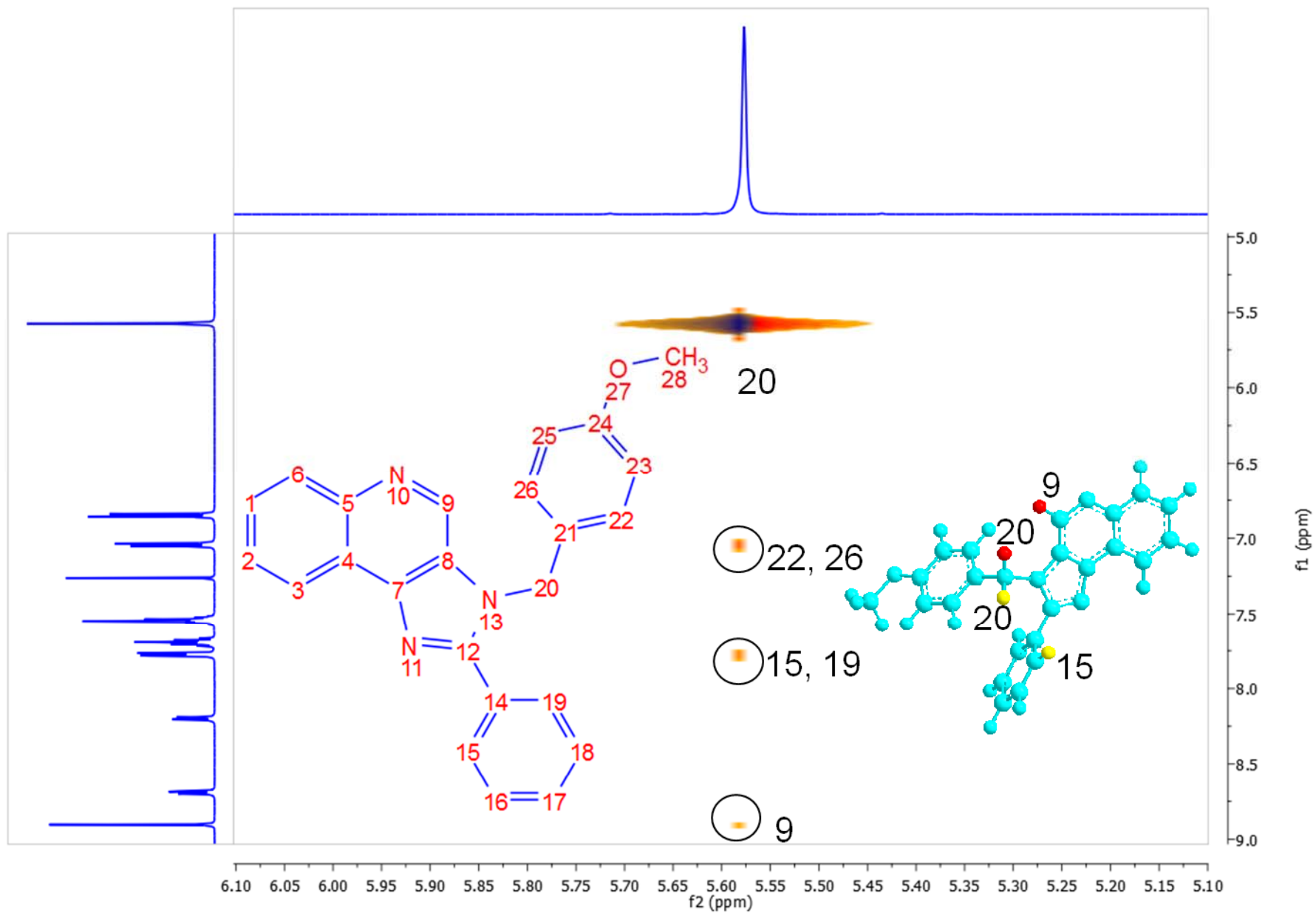
- 55.33
- 48.60



TOF Spectrum	TOF	Profile Spectrum at 1424.65 min (scan 1)
Baseline = 1.006107275624	Abundance Min = 0	Abundance Max = 973383

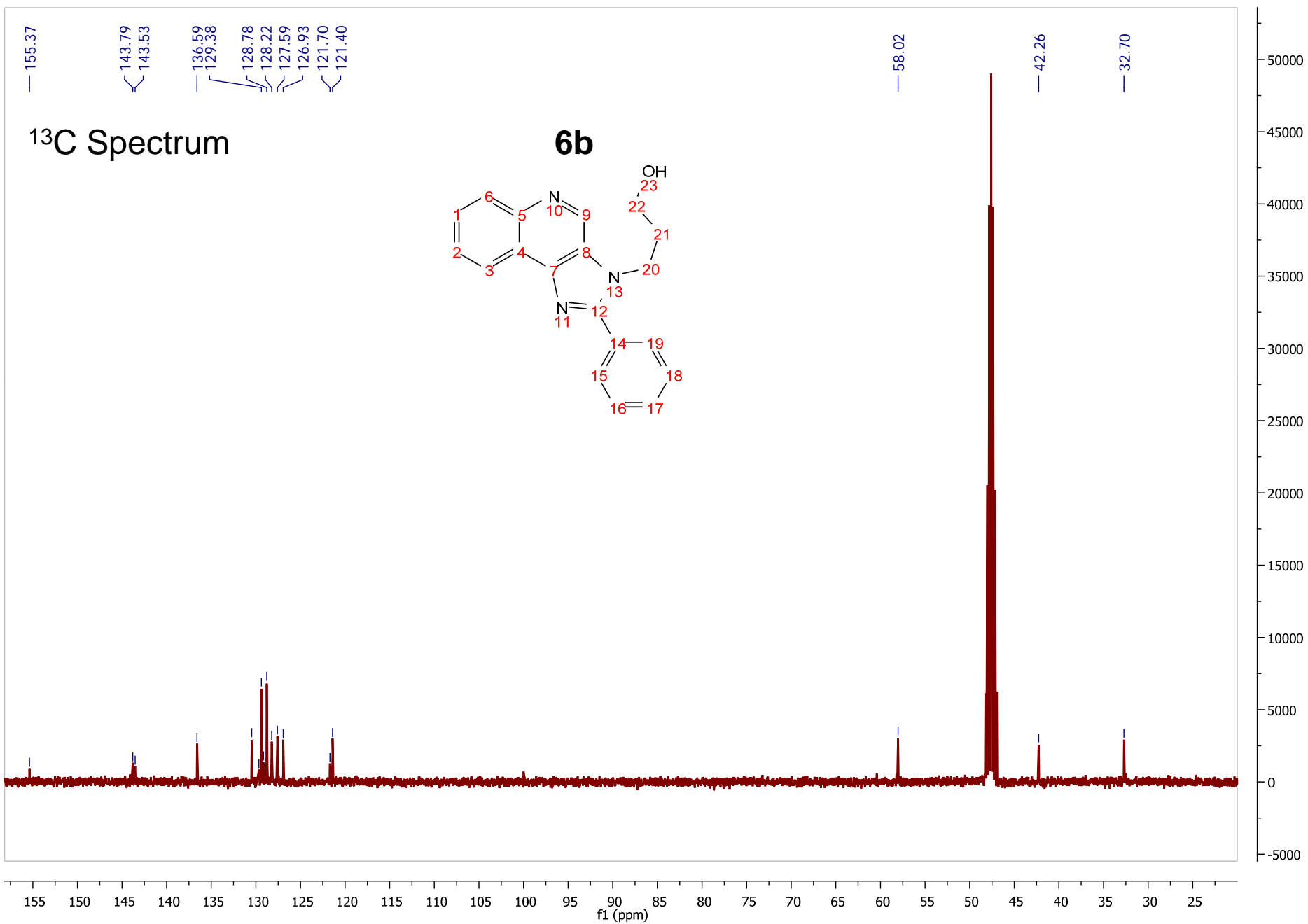


# 2D-NOESY Spectrum of Compound **5b**

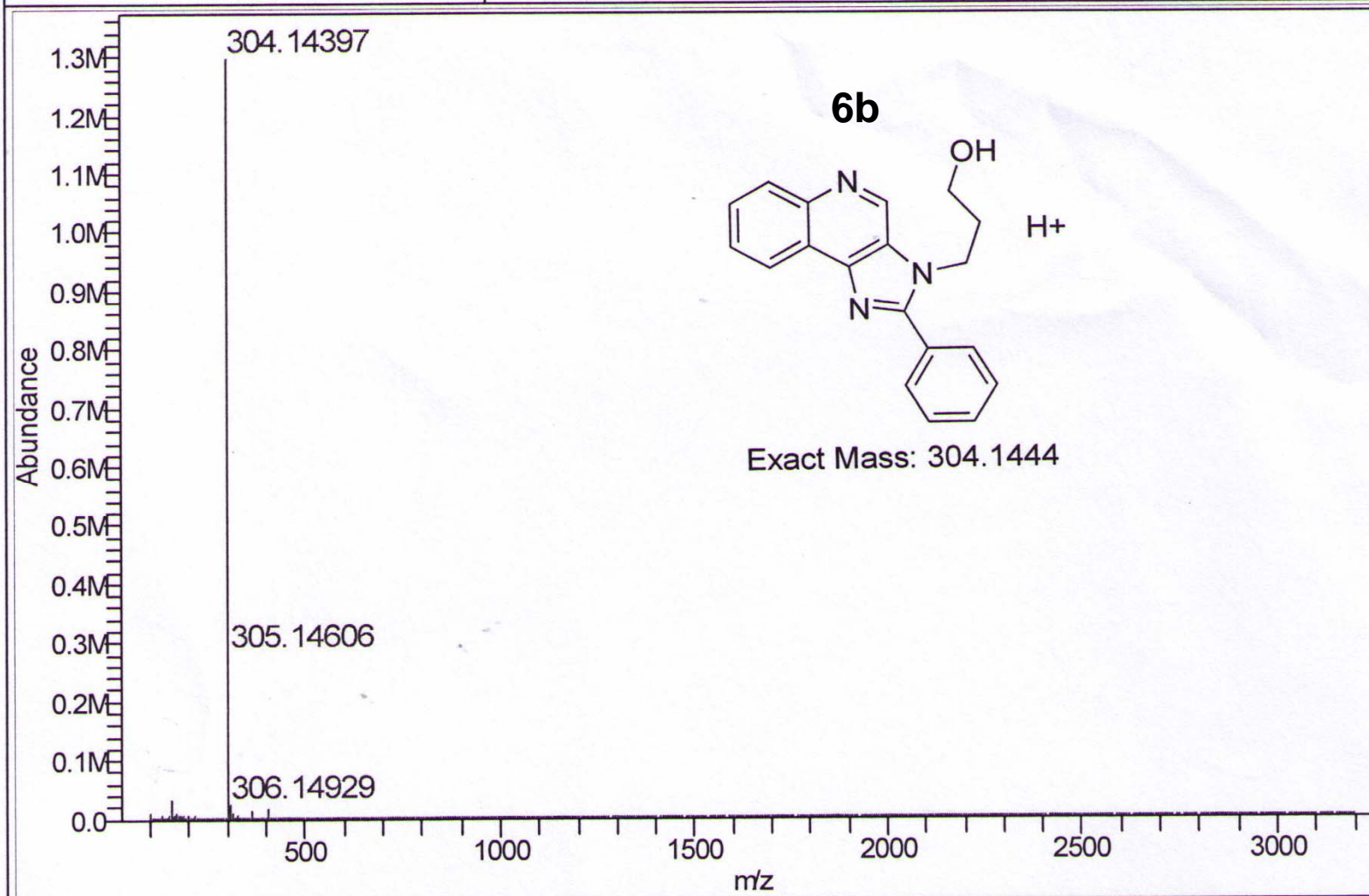




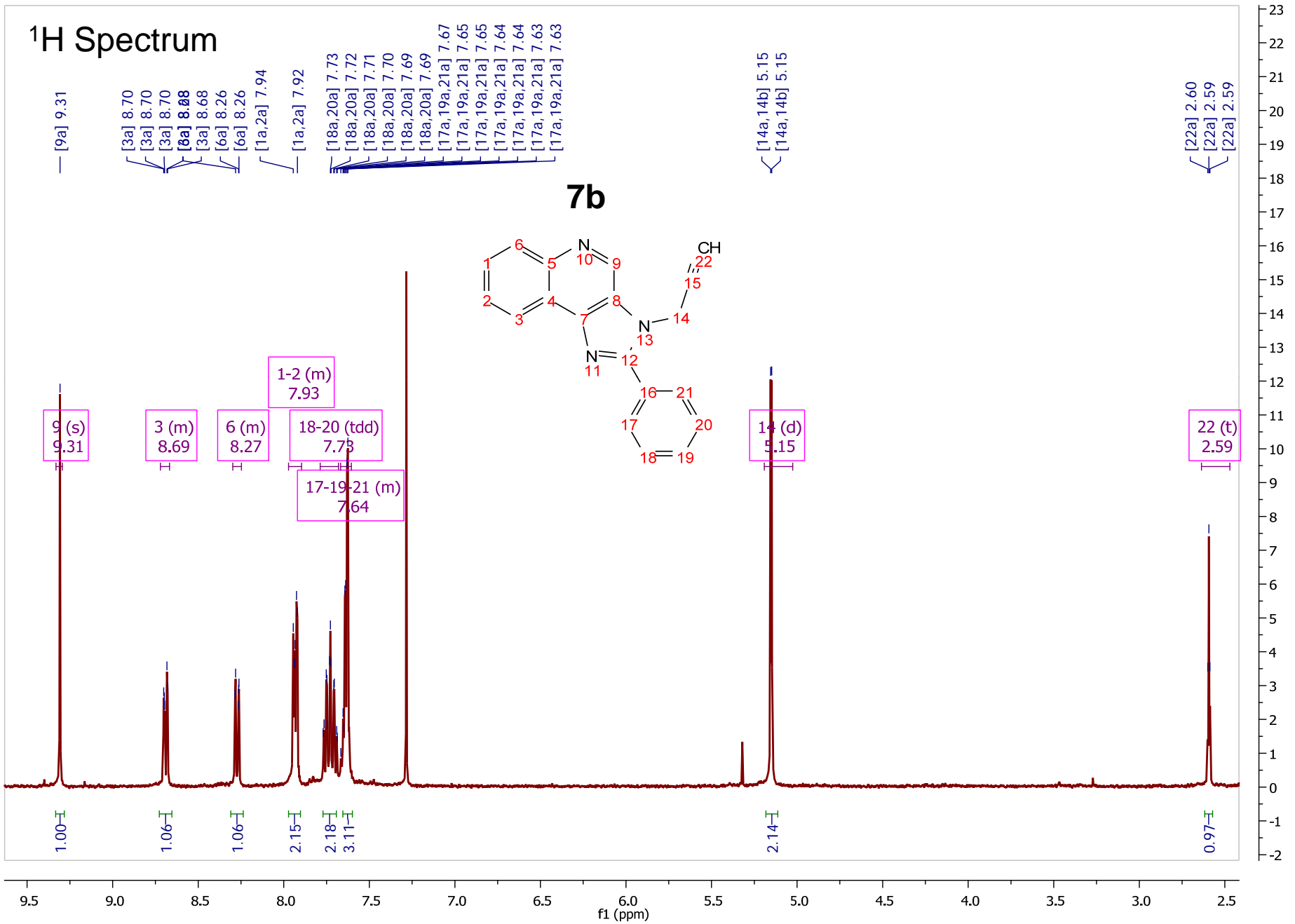


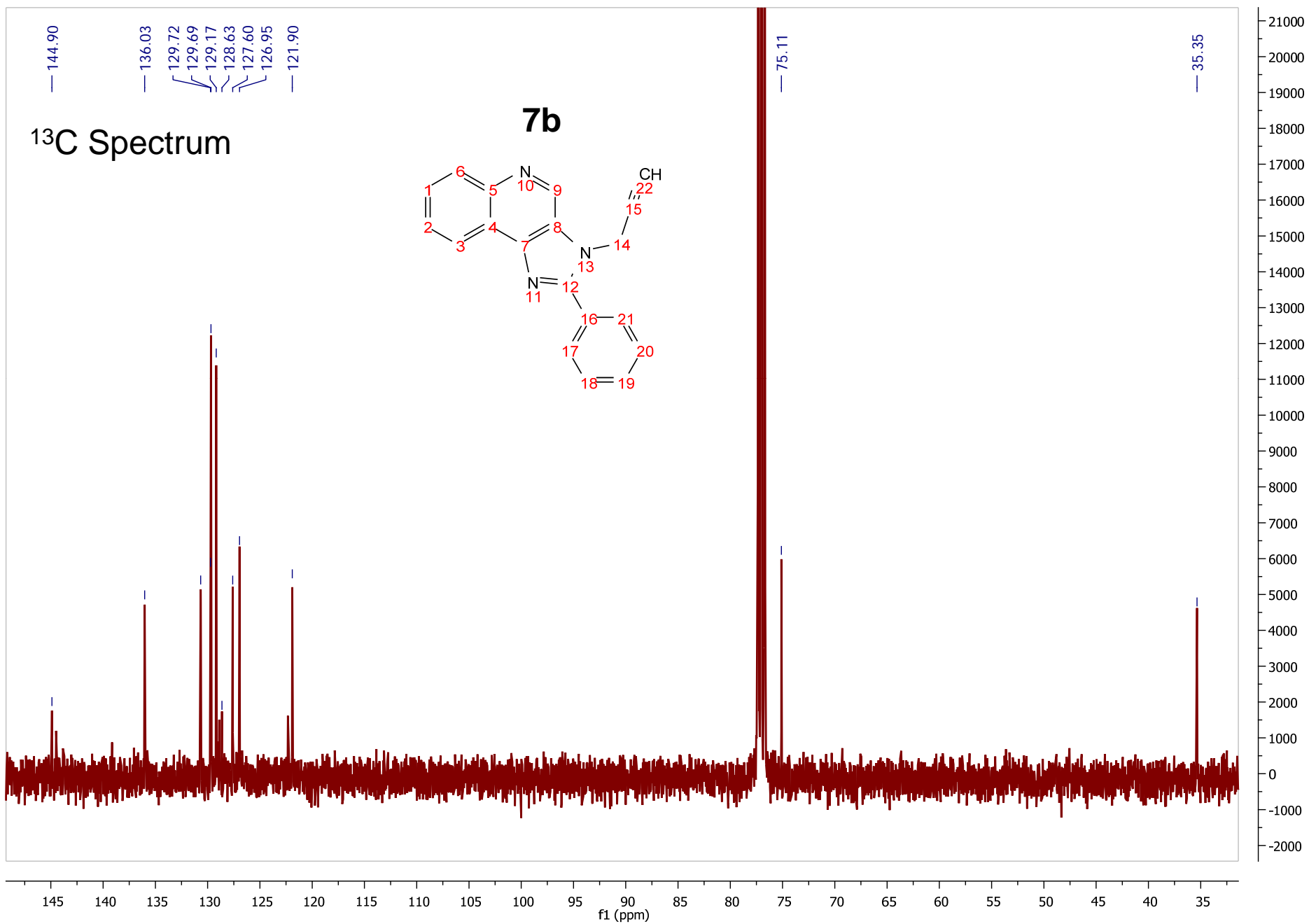


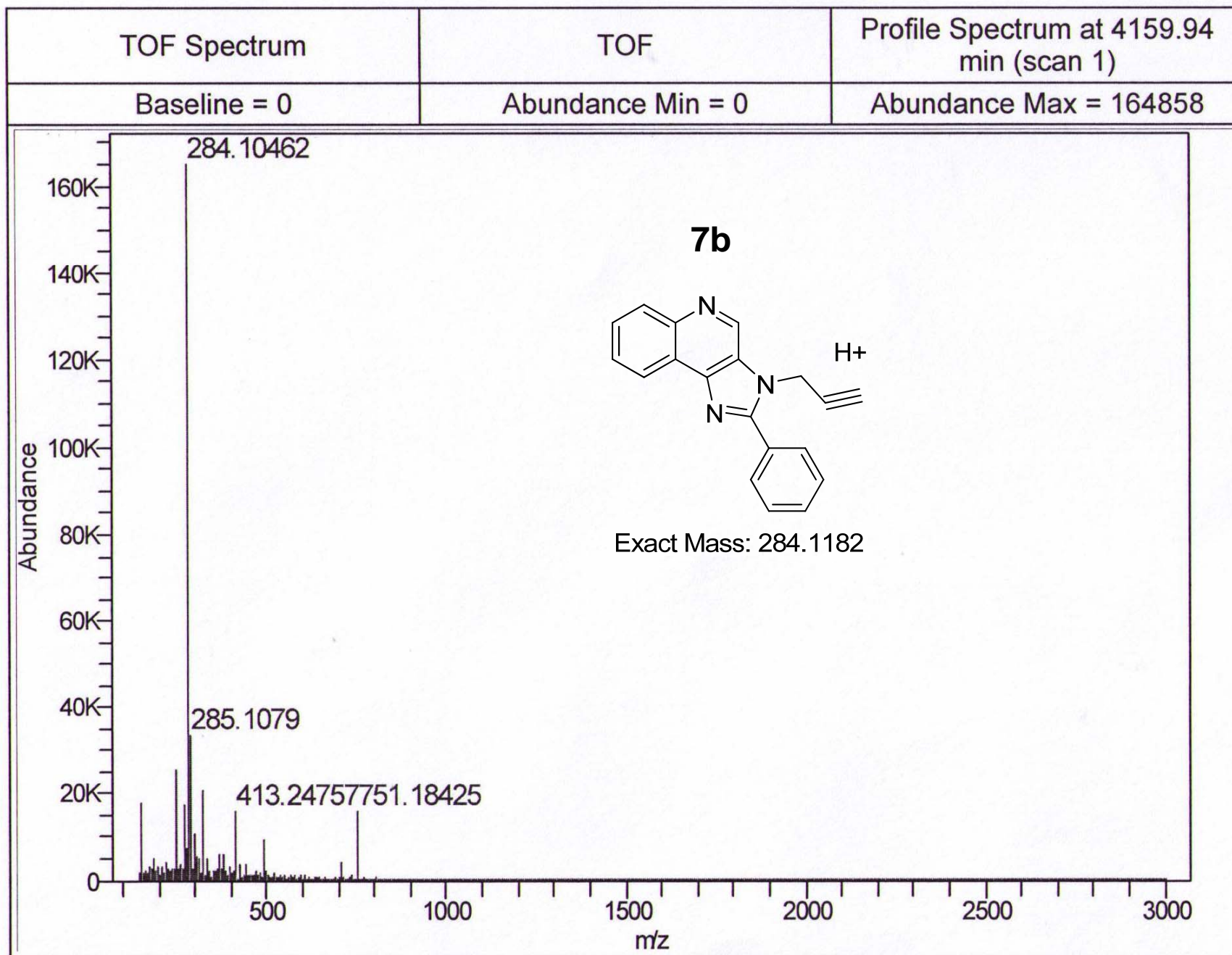
TOF Spectrum	TOF	Profile Spectrum at 1021.48 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 1298370



# <sup>1</sup>H Spectrum

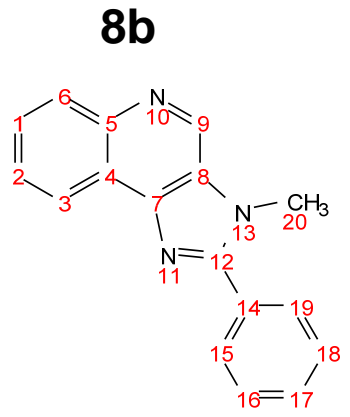






# <sup>1</sup>H Spectrum

[3a] 8.89  
[3a] 8.89  
[3a] 8.87  
[3a] 8.87  
[9a] 8.75  
[2a] 8.54  
[2a] 8.54  
[2a] 8.52  
[2a] 8.52  
[6a] 7.81  
[15a,19a] 7.76  
[15a,19a] 7.74  
[15a,19a] 7.72  
[15a,19a] 7.71  
[15a,19a] 7.70  
[15a,19a] 7.68  
[16a,17a,18a] 7.53  
[16a,17a,18a] 7.53  
[16a,17a,18a] 7.52  
[16a,17a,18a] 7.51  
[16a,17a,18a] 7.51  
[16a,17a,18a] 7.49  
[16a,17a,18a] 7.47  
[16a,17a,18a] 7.47  
[16a,17a,18a] 7.47  
[16a,17a,18a] 7.46  
[16a,17a,18a] 7.45  
[16a,17a,18a] 7.45

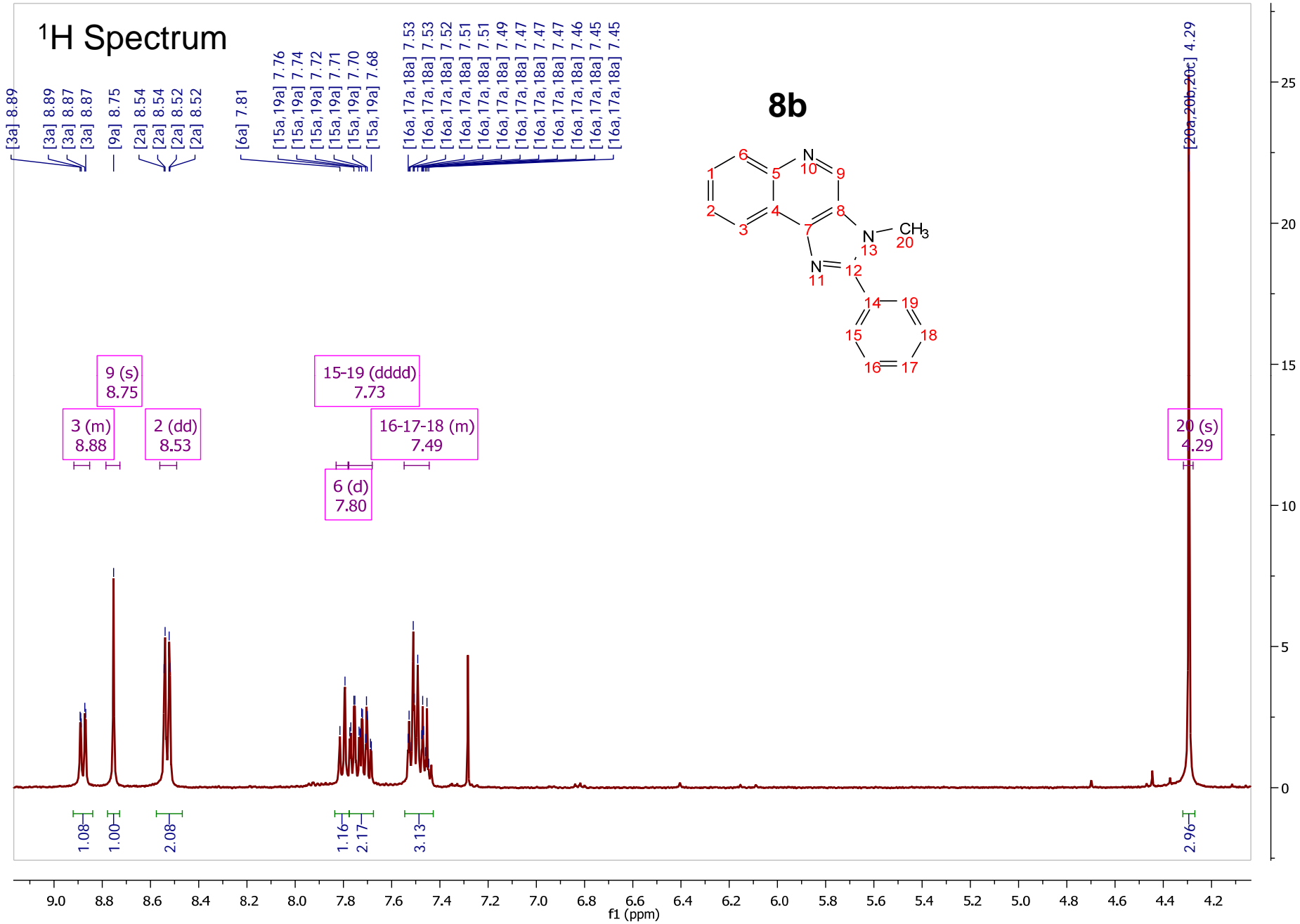


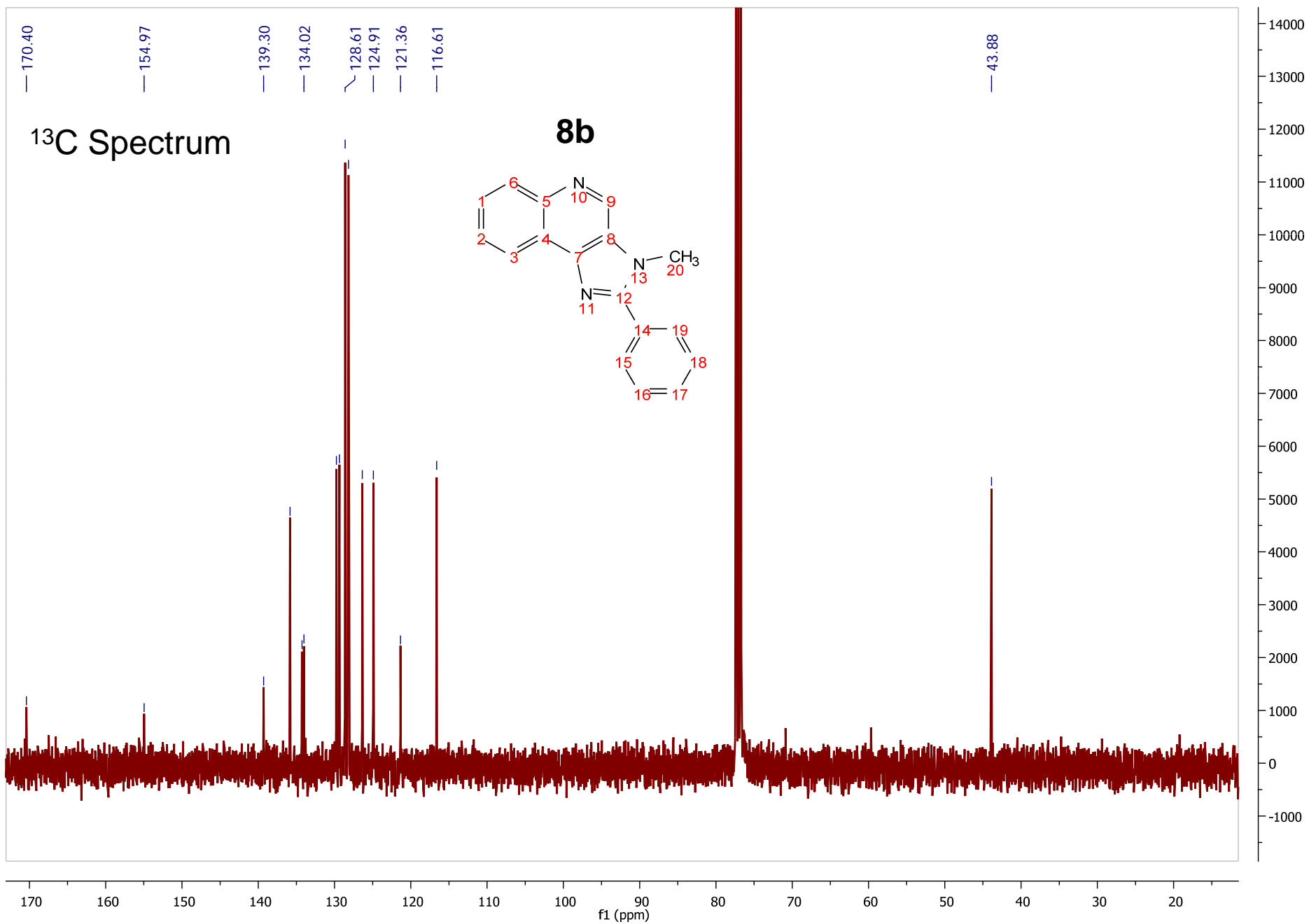
9 (s)  
8.75  
3 (m)  
8.88  
2 (dd)  
8.53  
15-19 (dddd)  
7.73  
16-17-18 (m)  
7.49  
6 (d)  
7.80  
20 (s)  
4.29

1.08  
1.00  
2.08

1.16  
2.17  
3.13

2.96

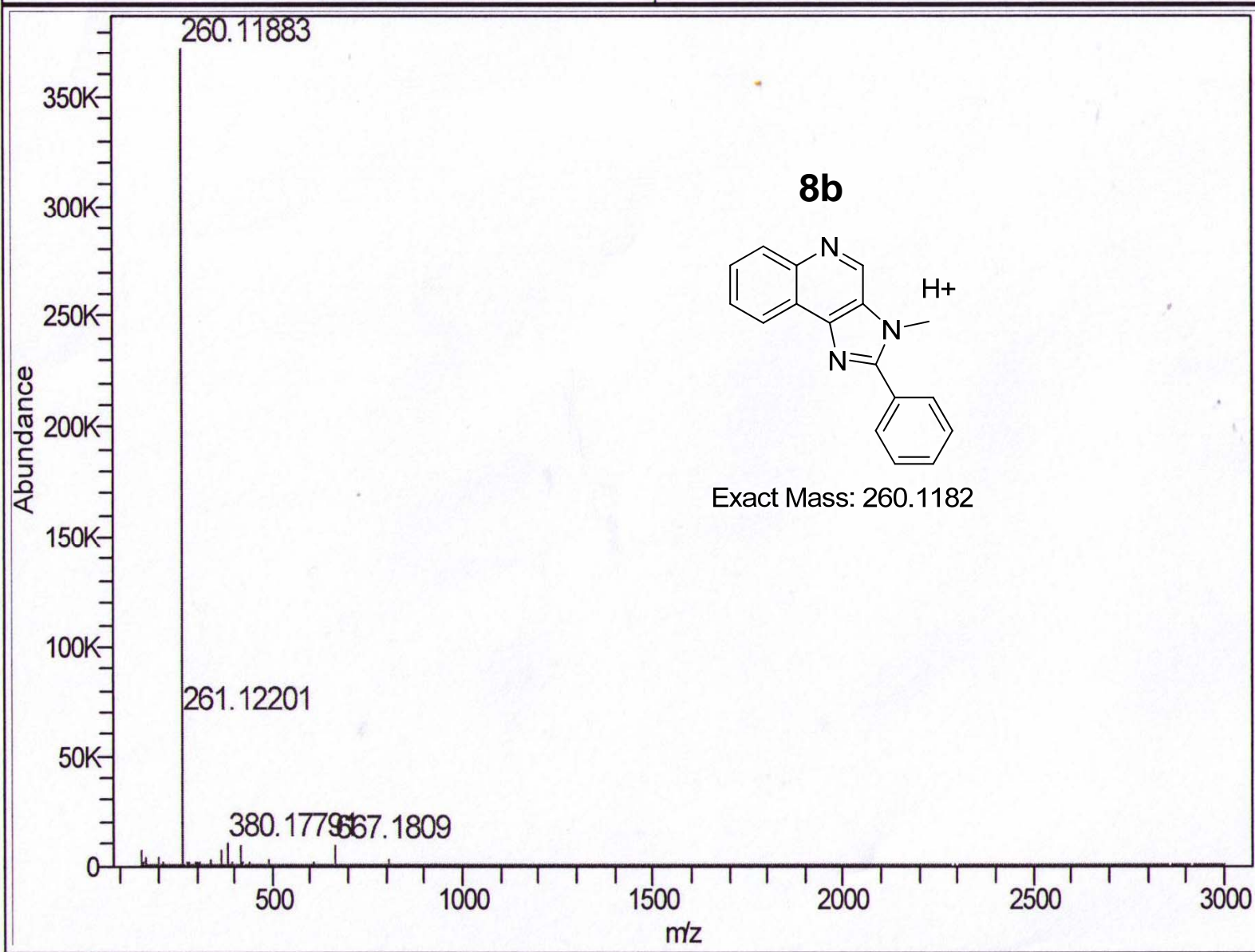






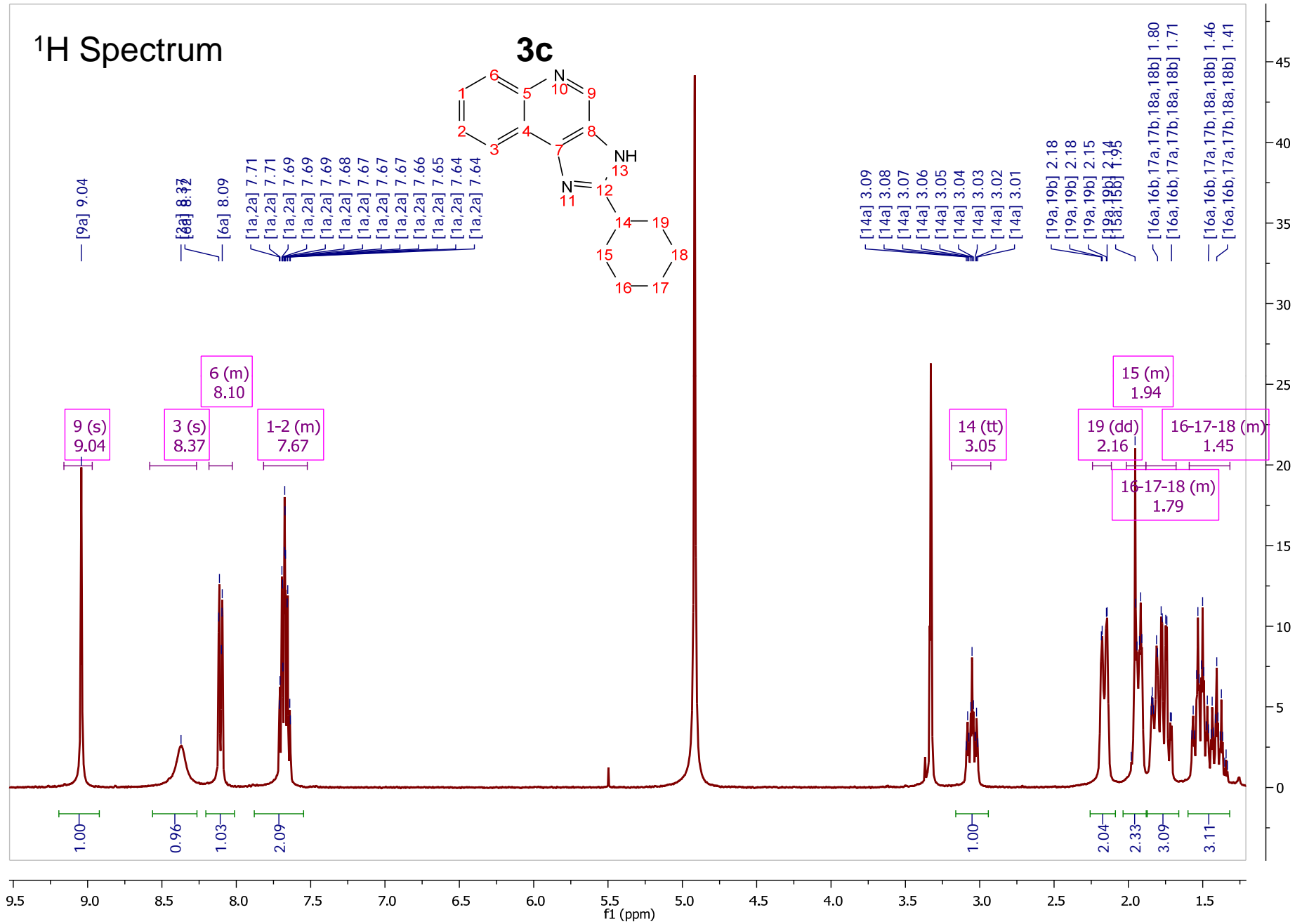
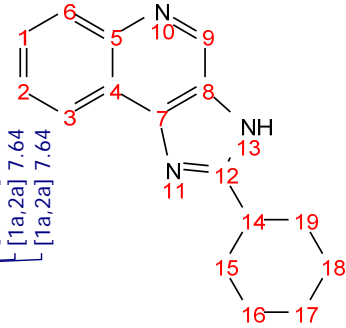
TOF Spectrum

Profile Spectrum at 16295.88 min (scan 1)

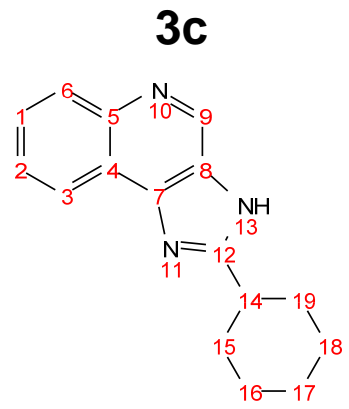


# <sup>1</sup>H Spectrum

**3c**

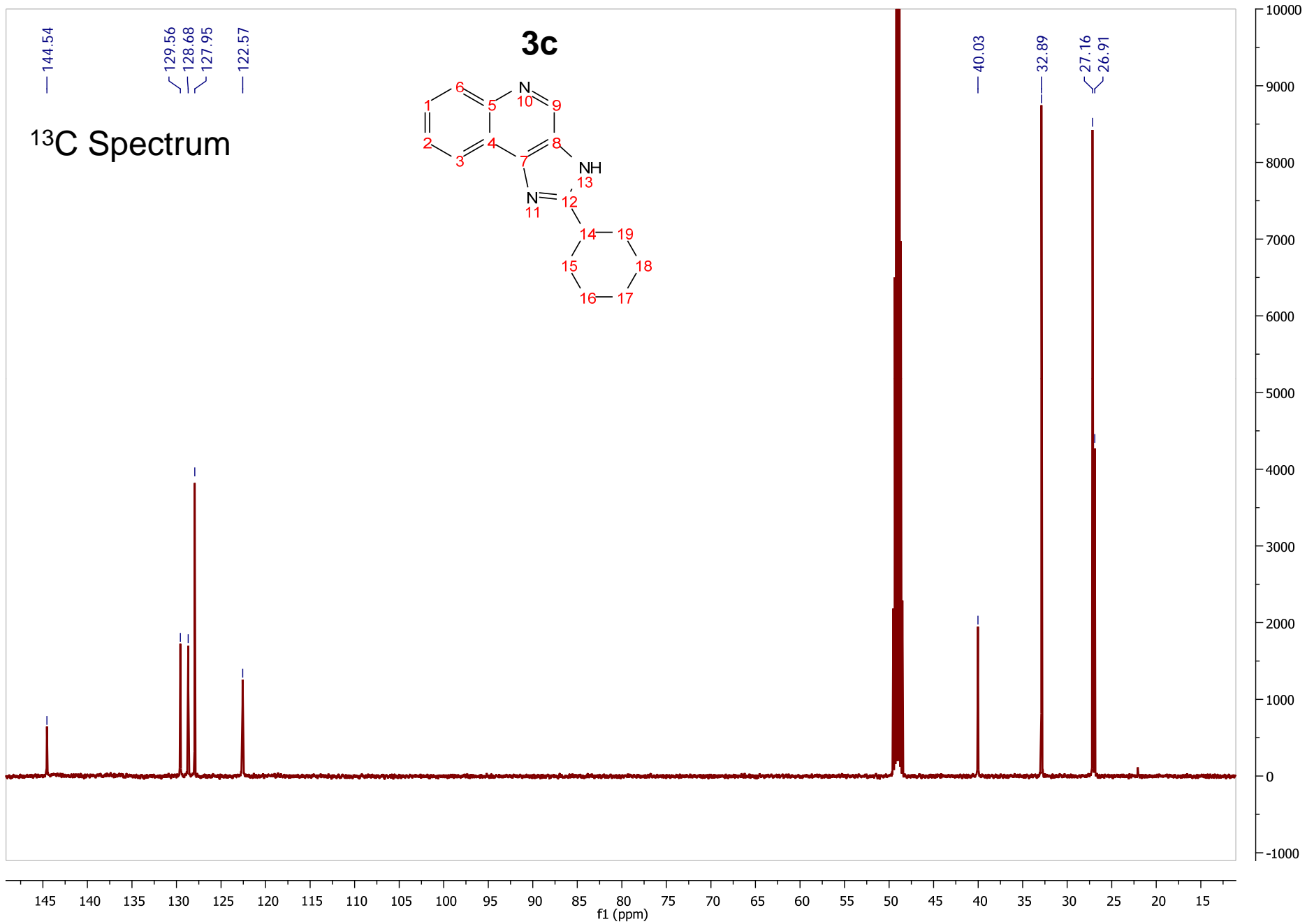


# <sup>13</sup>C Spectrum

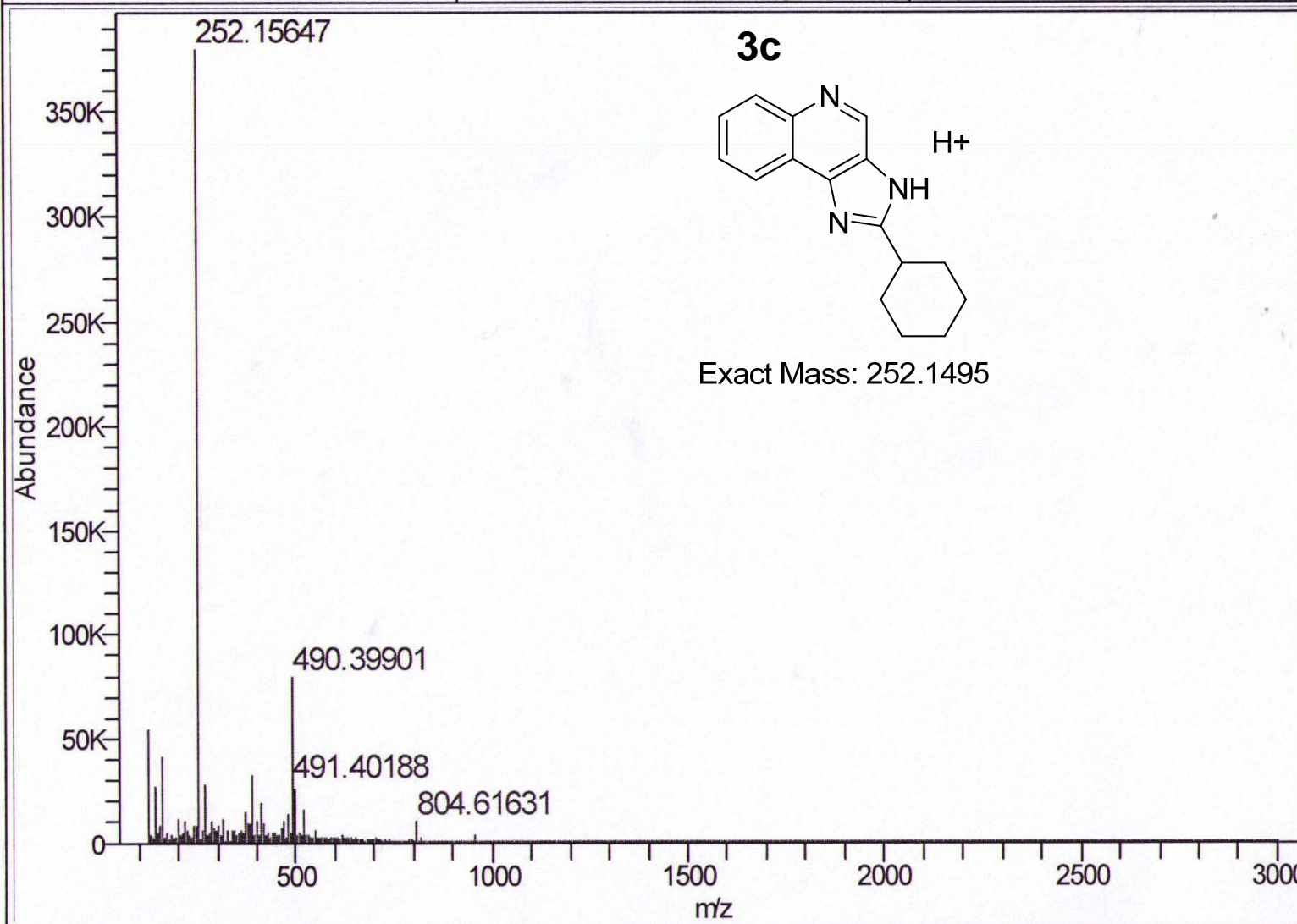


144.54  
129.56  
128.68  
127.95  
122.57

40.03  
32.89  
27.16  
26.91

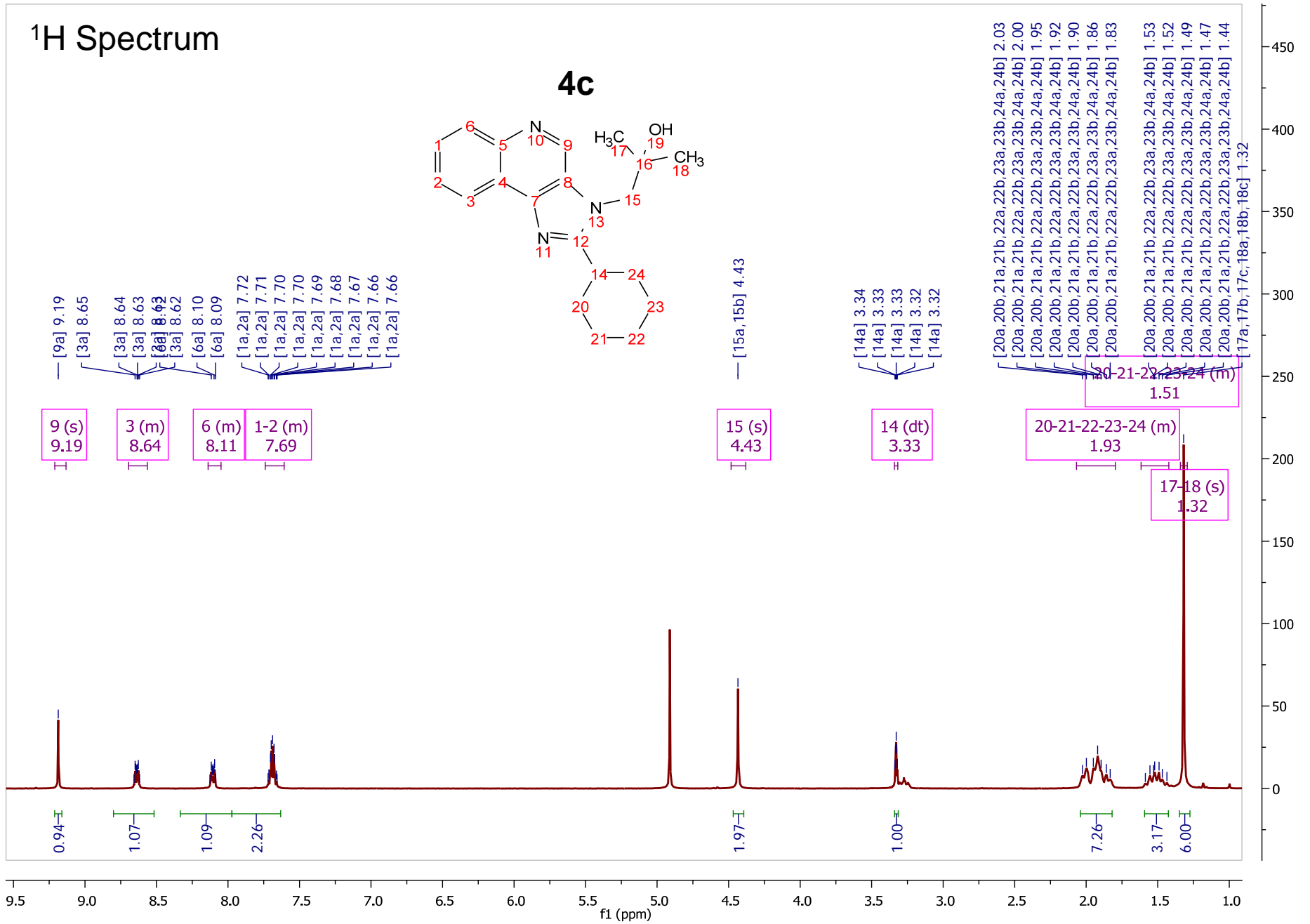
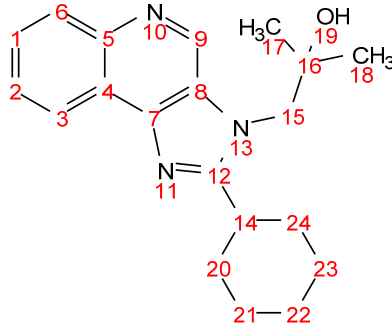


TOF Spectrum	TOF	Profile Spectrum at 12617.38 min (scan 1)
Baseline = 9.02798117154812	Abundance Min = 0	Abundance Max = 380358



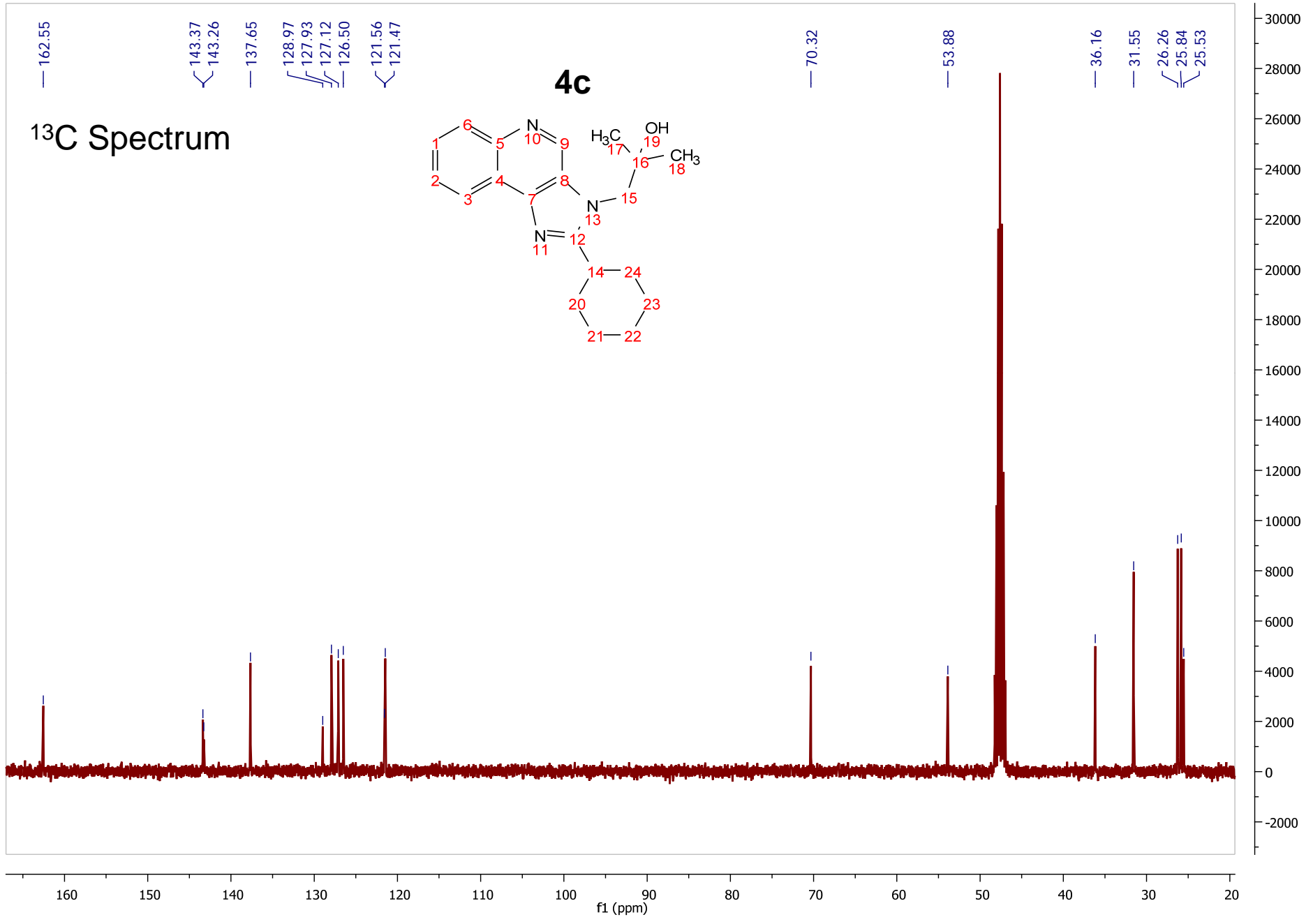
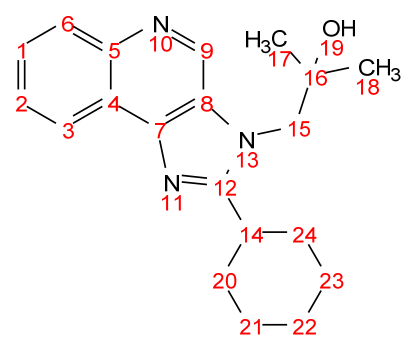
# <sup>1</sup>H Spectrum

**4c**



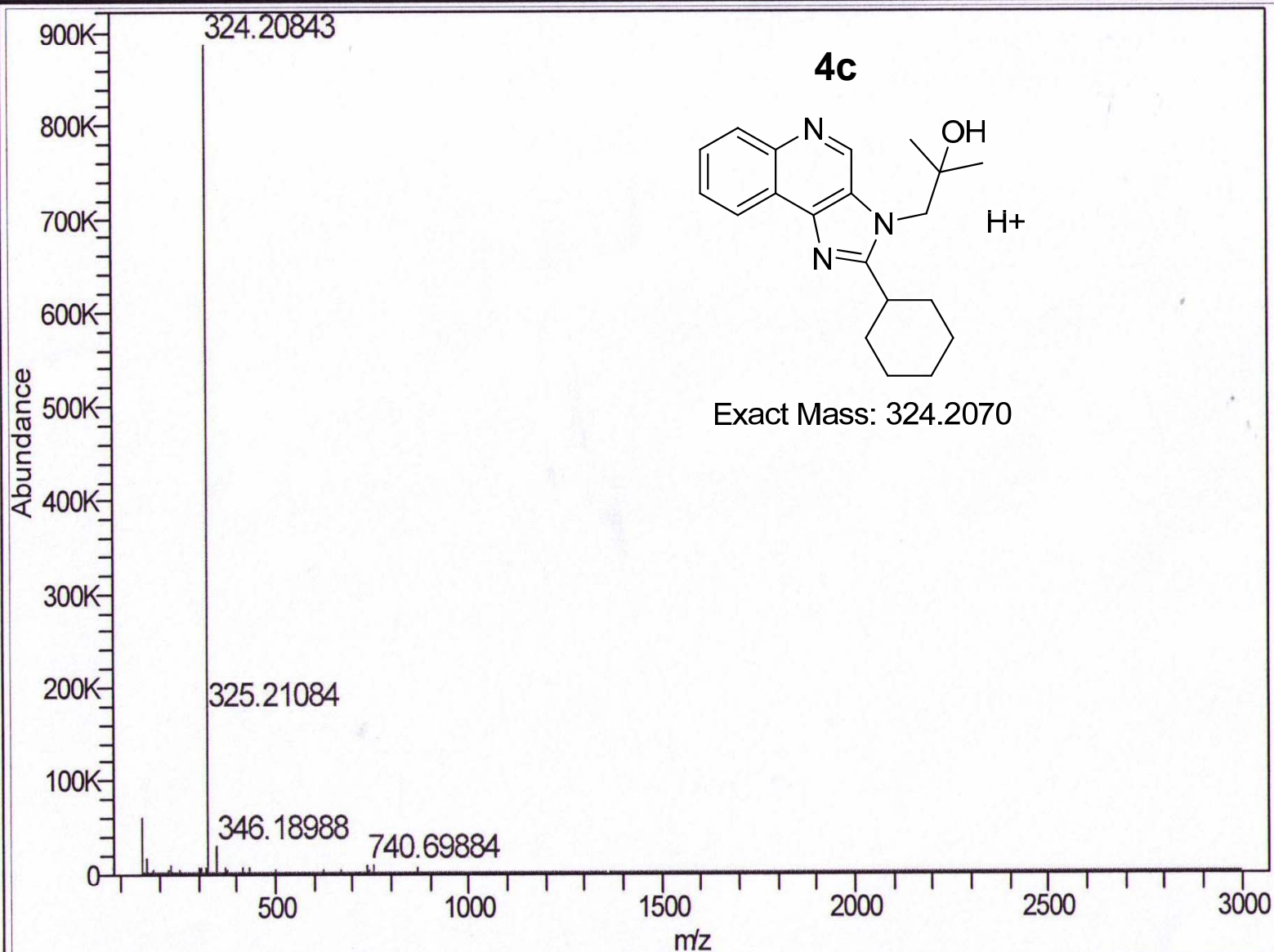
# <sup>13</sup>C Spectrum

**4c**

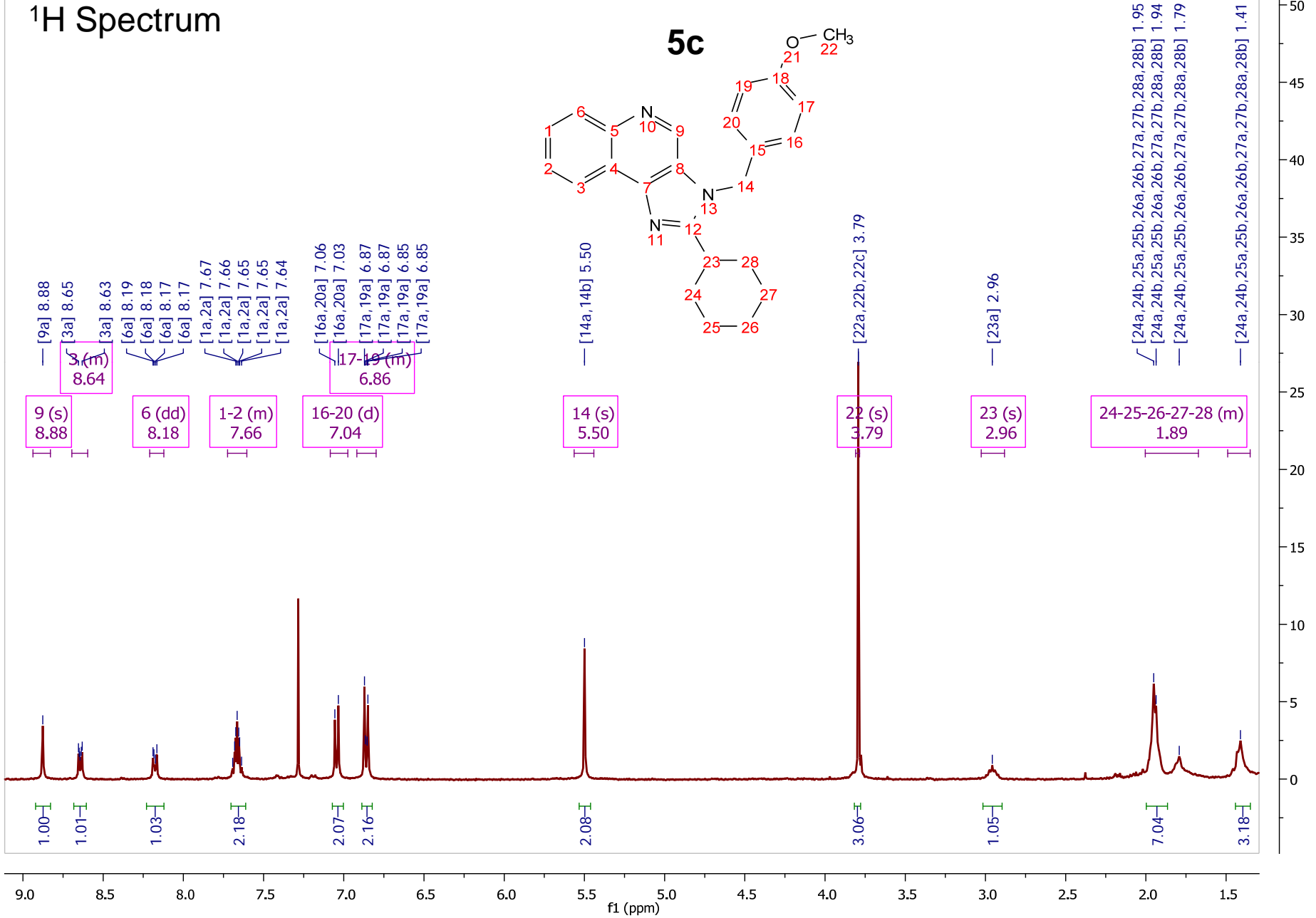
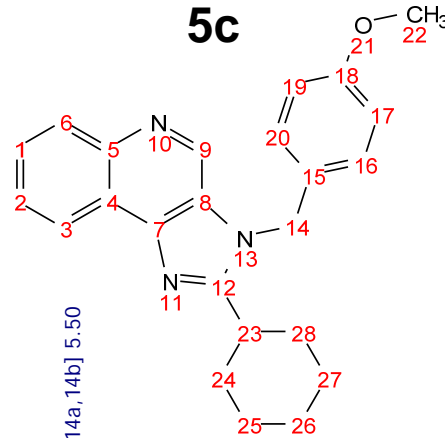


TOF Spectrum

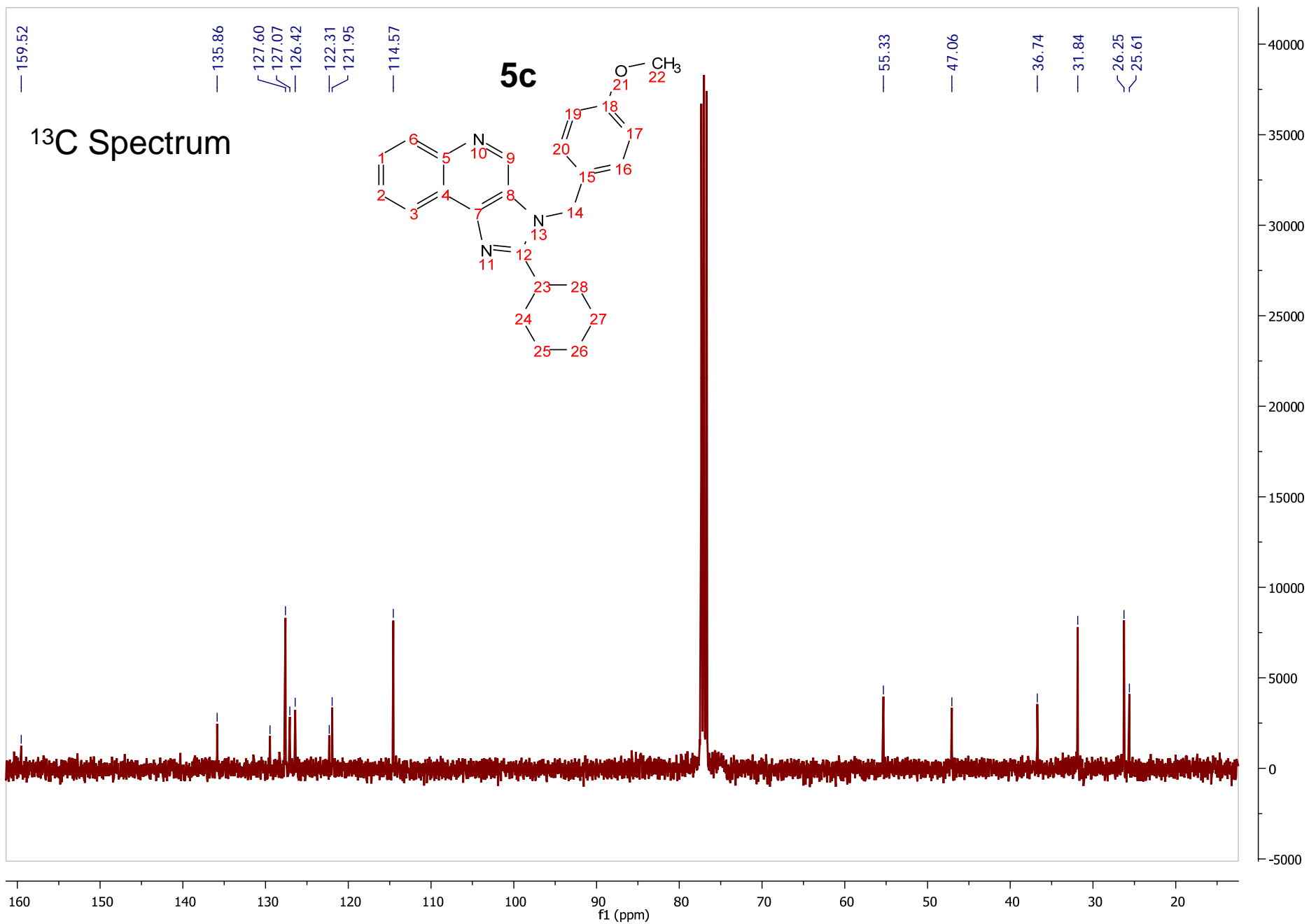
Profile Spectrum at 10481.55 min (scan 1)

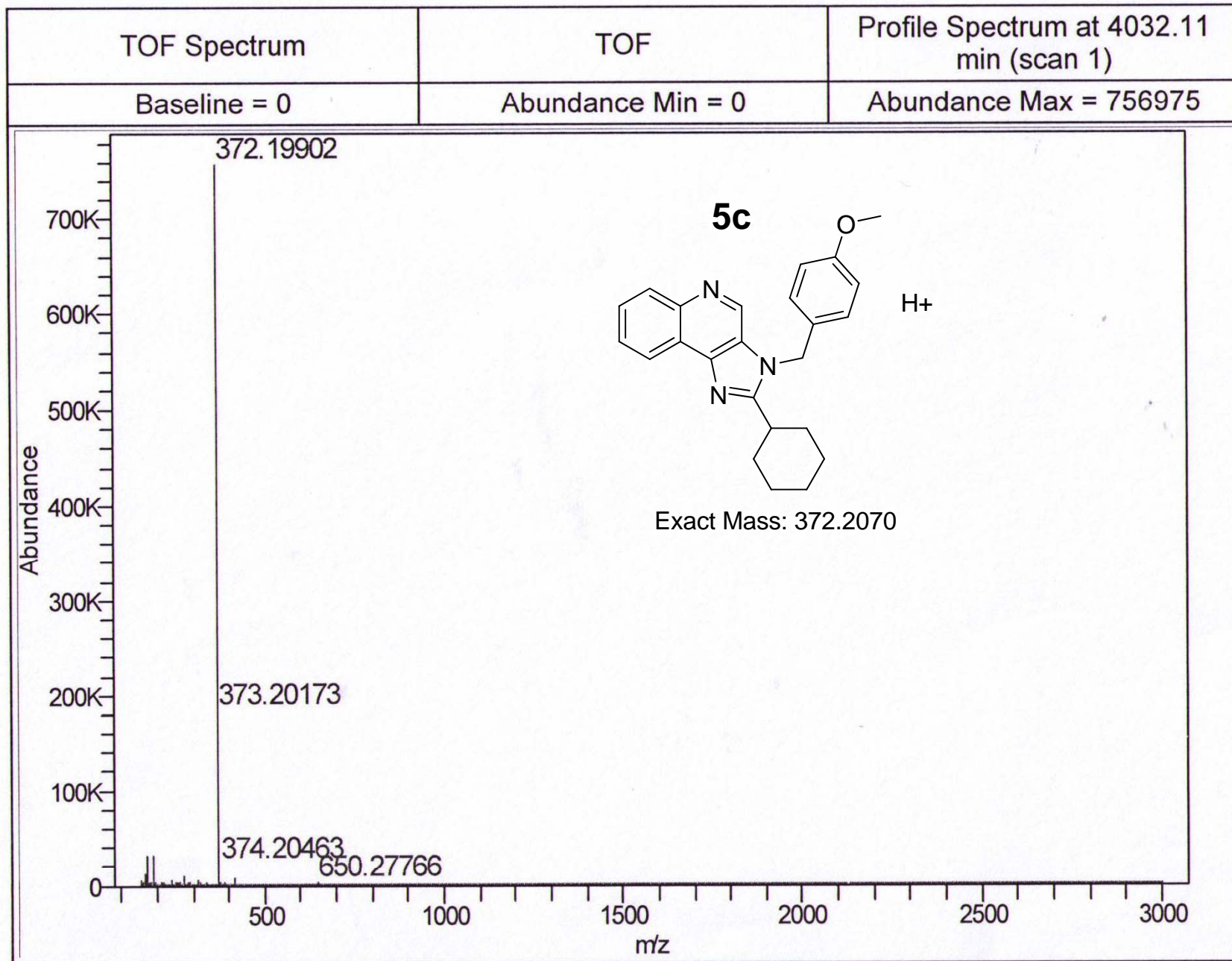


# <sup>1</sup>H Spectrum

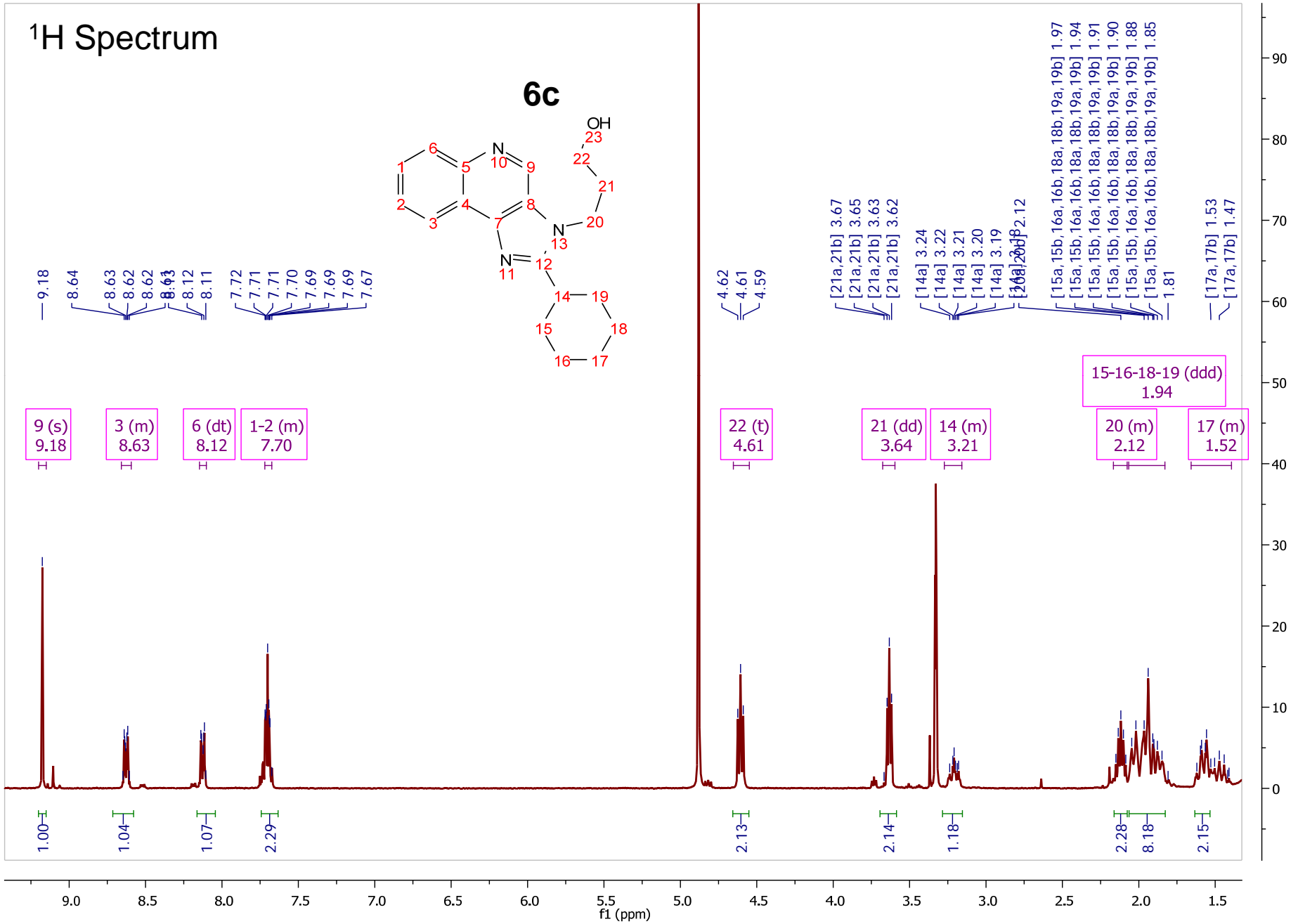
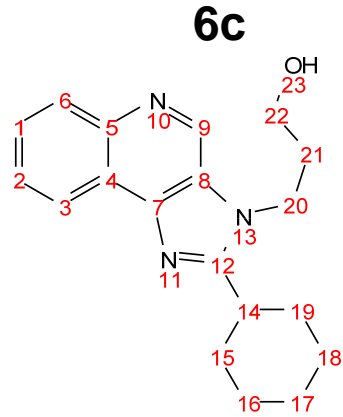




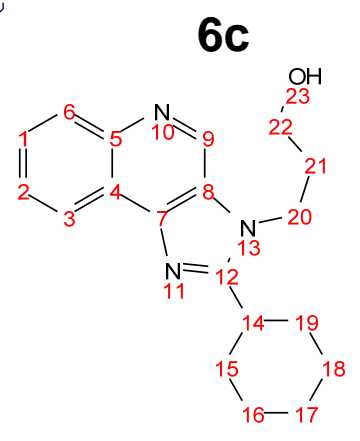




# <sup>1</sup>H Spectrum

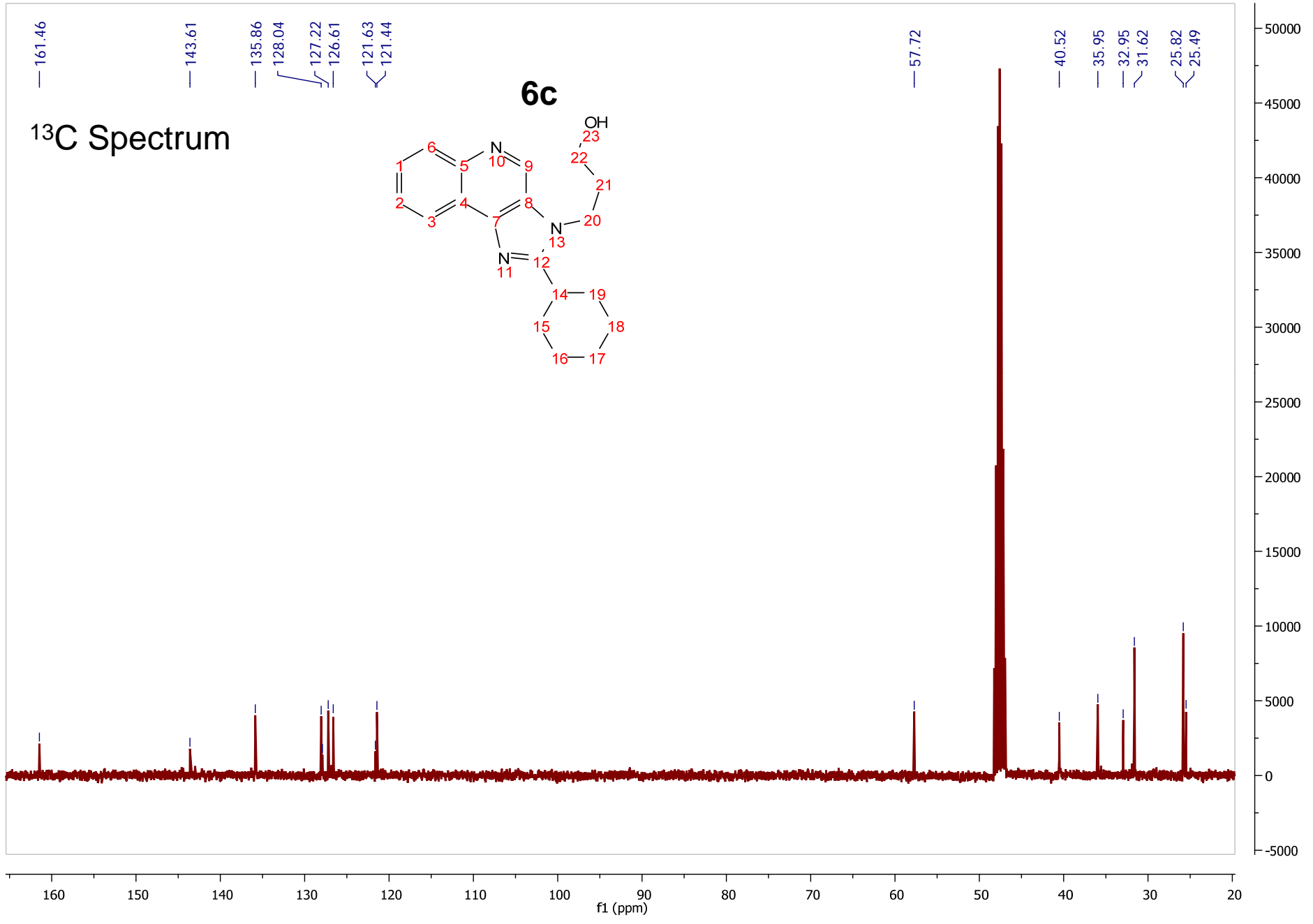


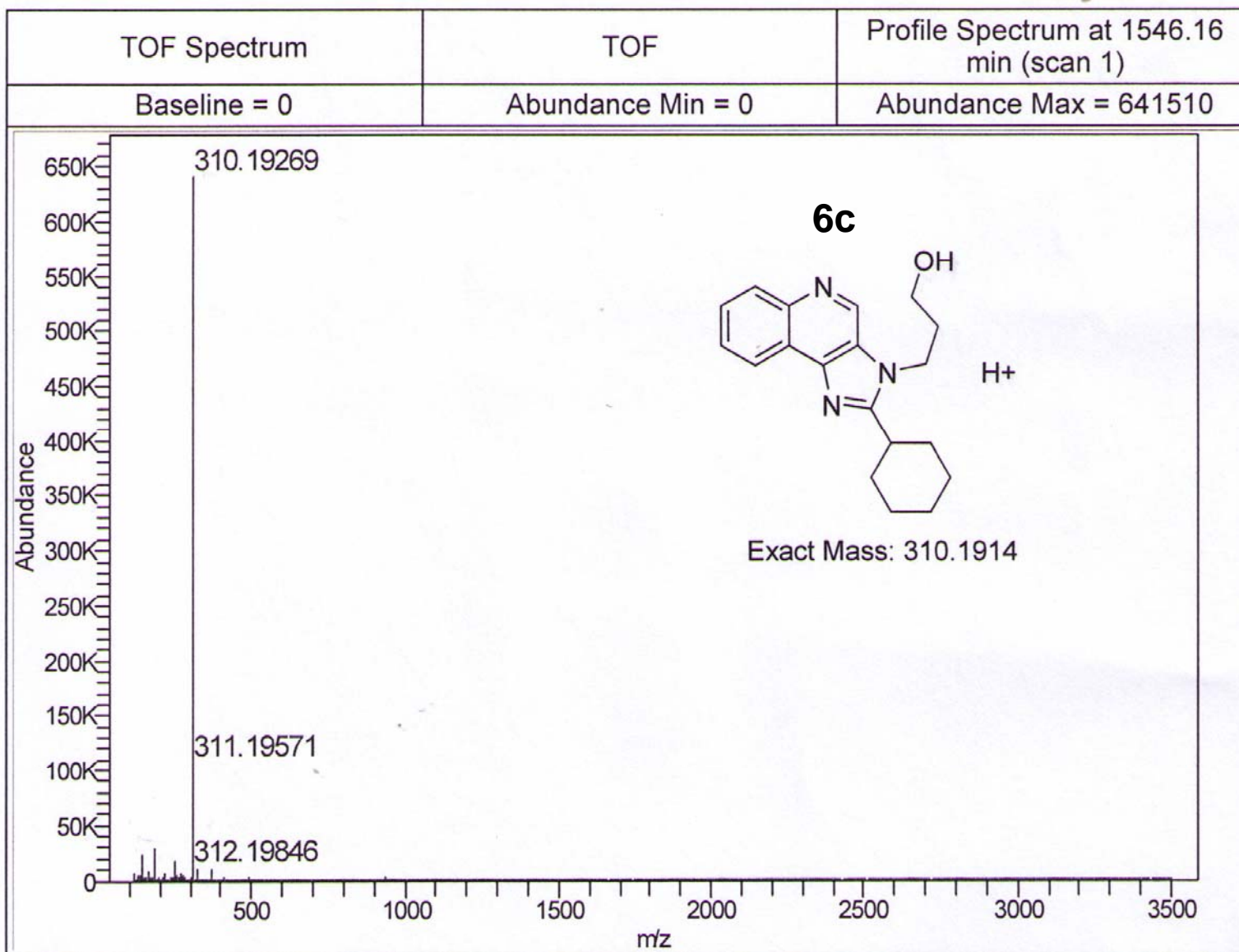
# <sup>13</sup>C Spectrum



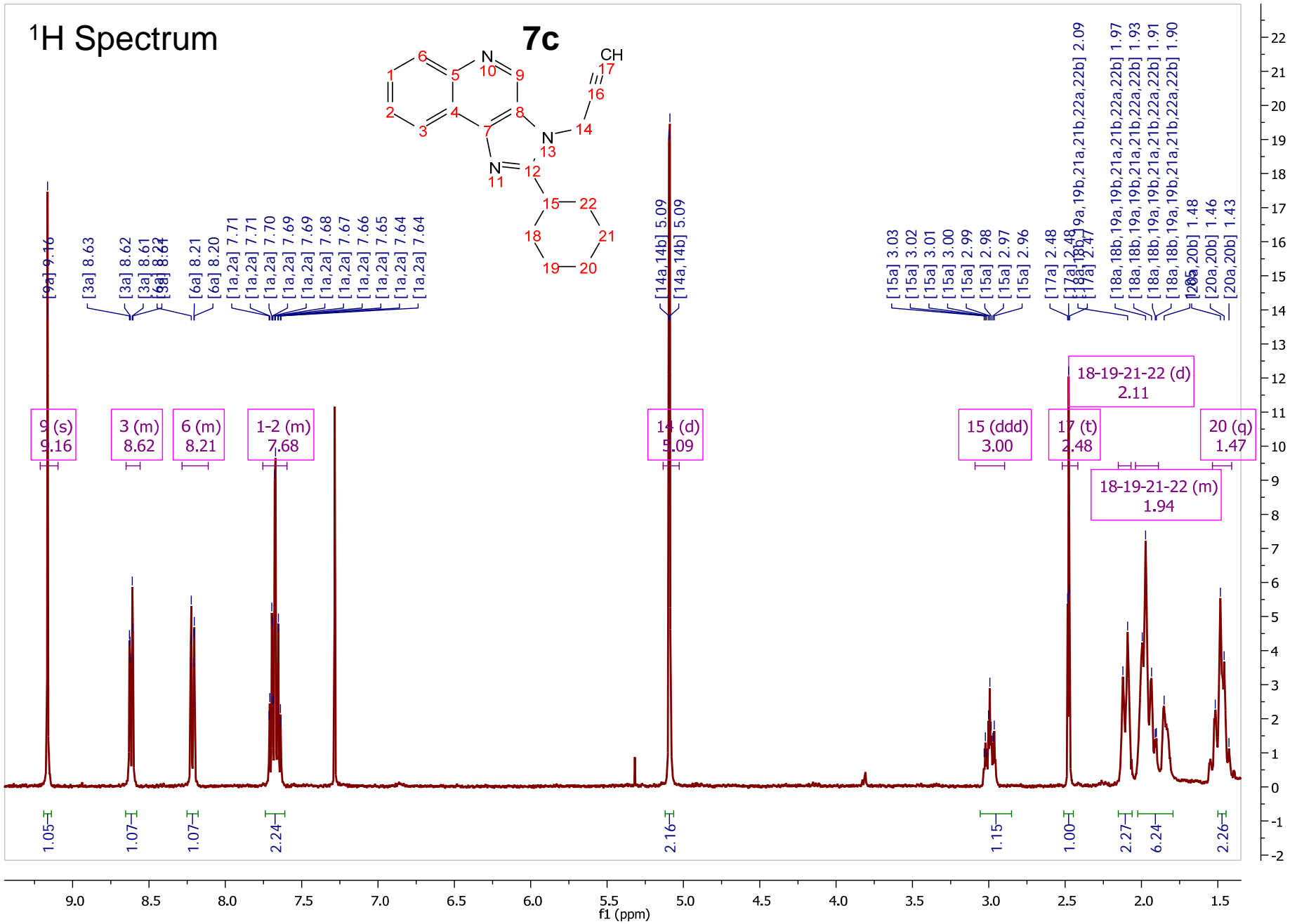
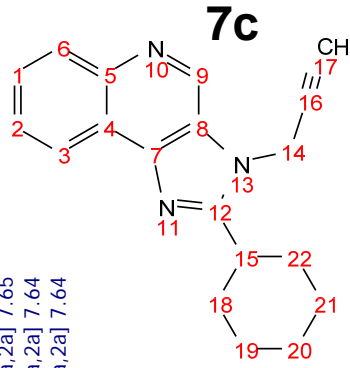
161.46  
143.61  
135.86  
128.04  
127.22  
126.61  
121.63  
121.44

57.72  
40.52  
35.95  
32.95  
31.62  
25.82  
25.49



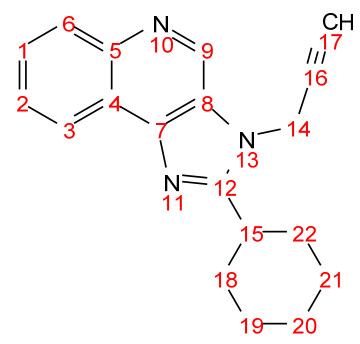


# <sup>1</sup>H Spectrum



# <sup>13</sup>C Spectrum

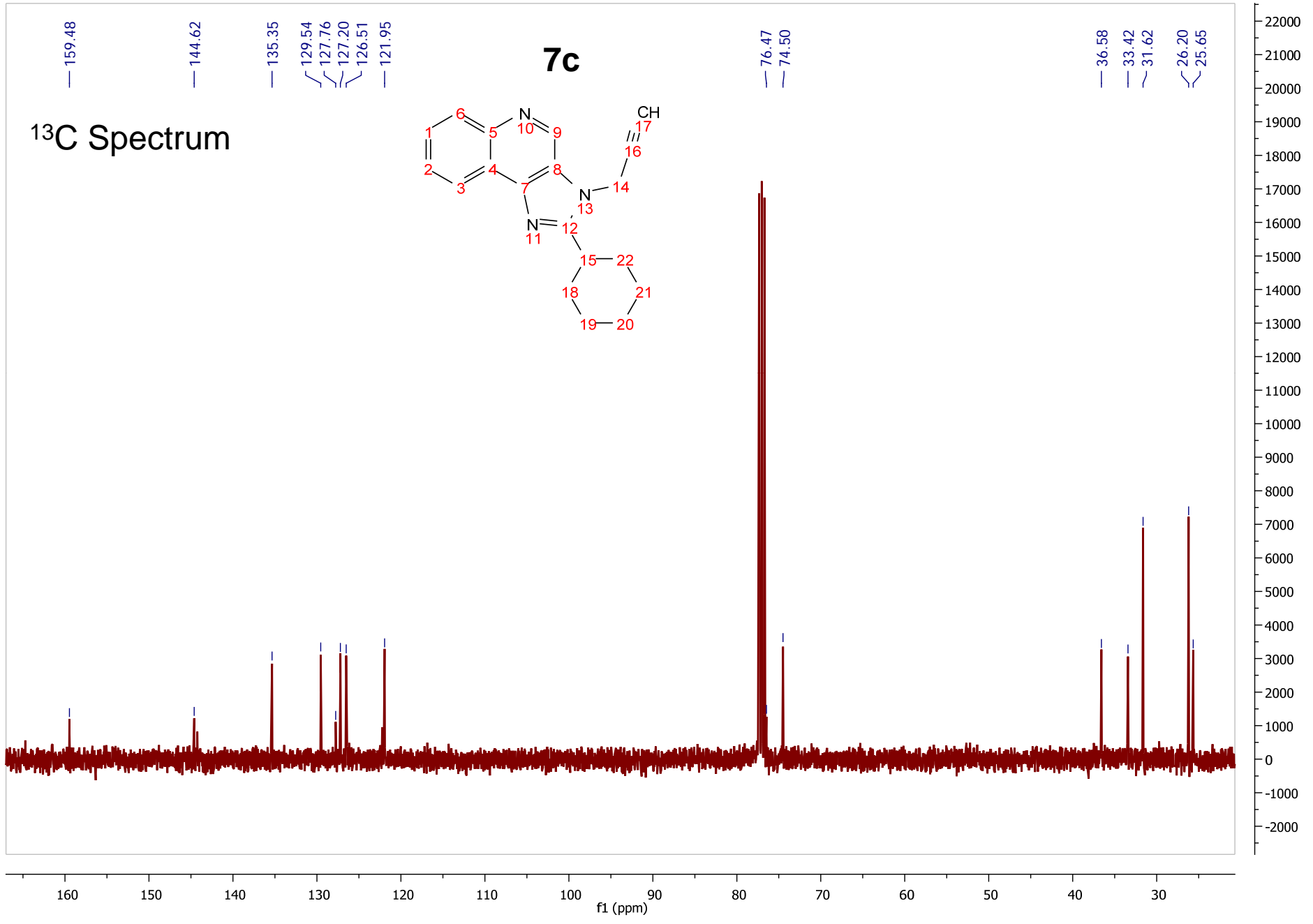
**7c**

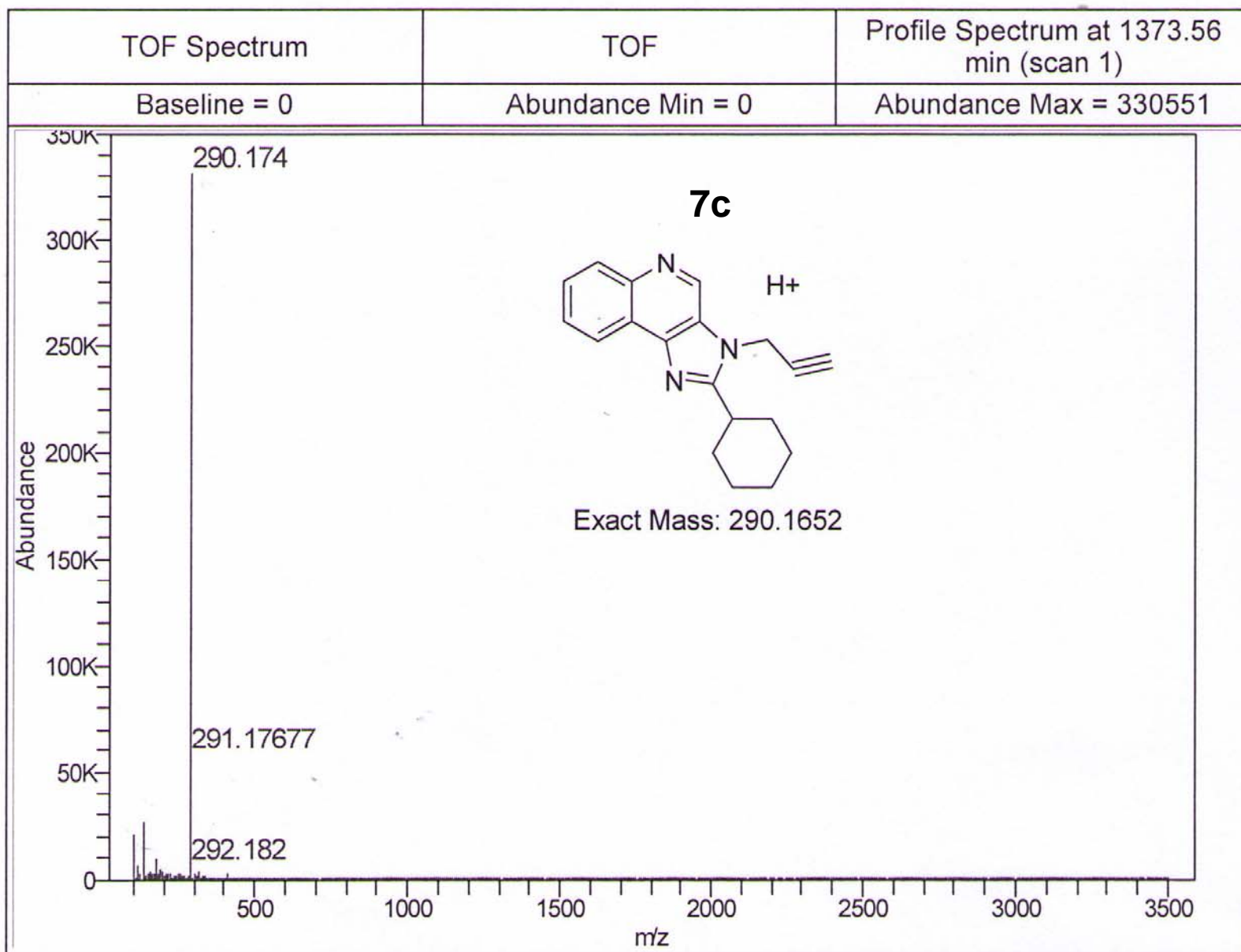


— 159.48  
— 144.62  
— 135.35  
— 129.54  
— 127.76  
— 127.20  
— 126.51  
— 121.95

— 76.47  
— 74.50

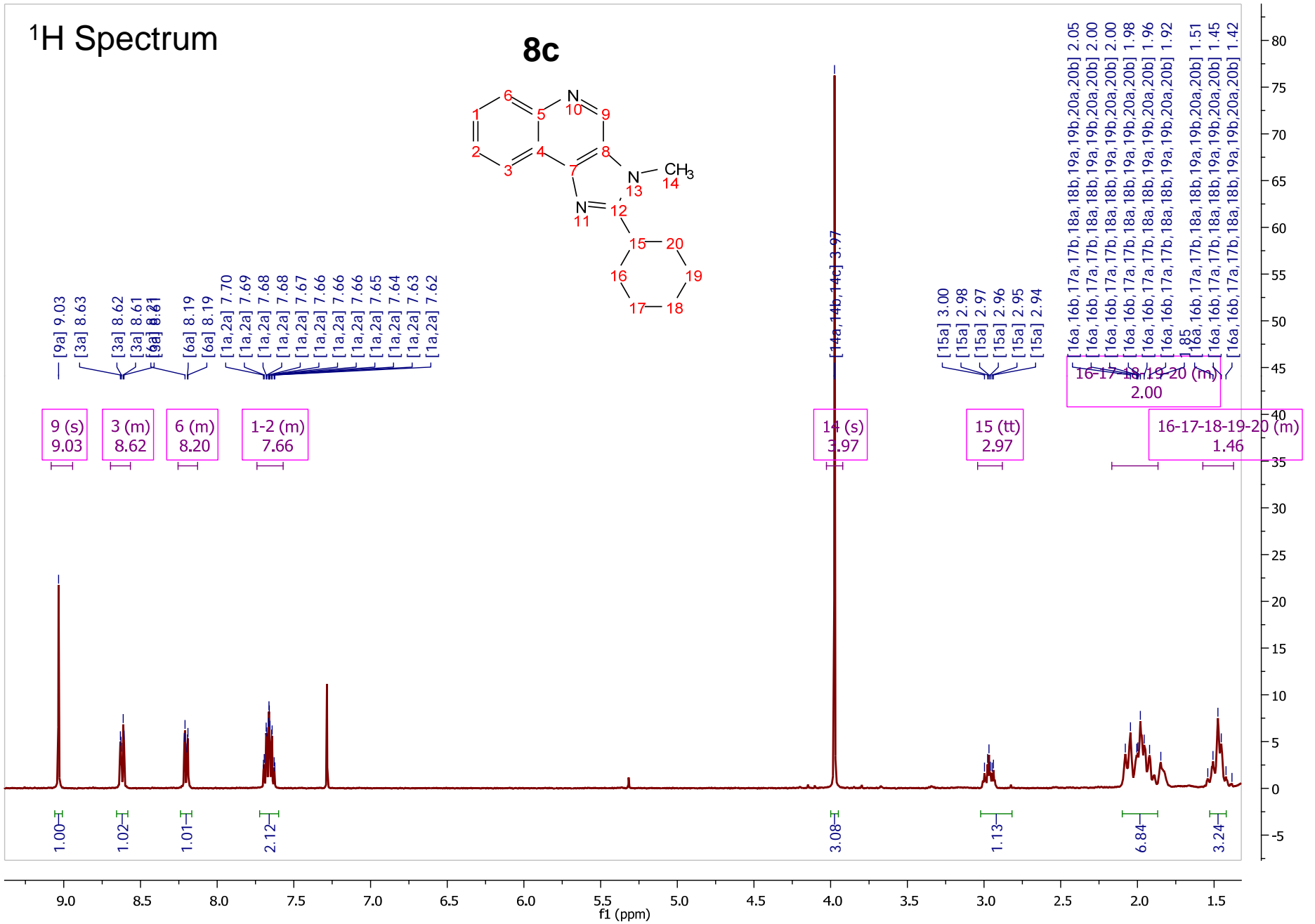
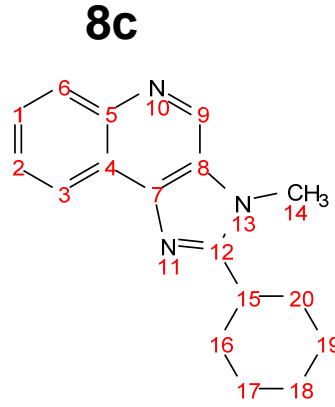
— 36.58  
— 33.42  
— 31.62  
— 26.20  
— 25.65



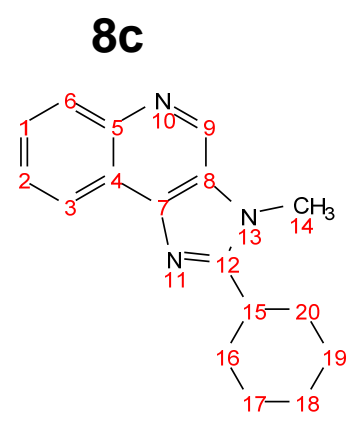




# <sup>1</sup>H Spectrum

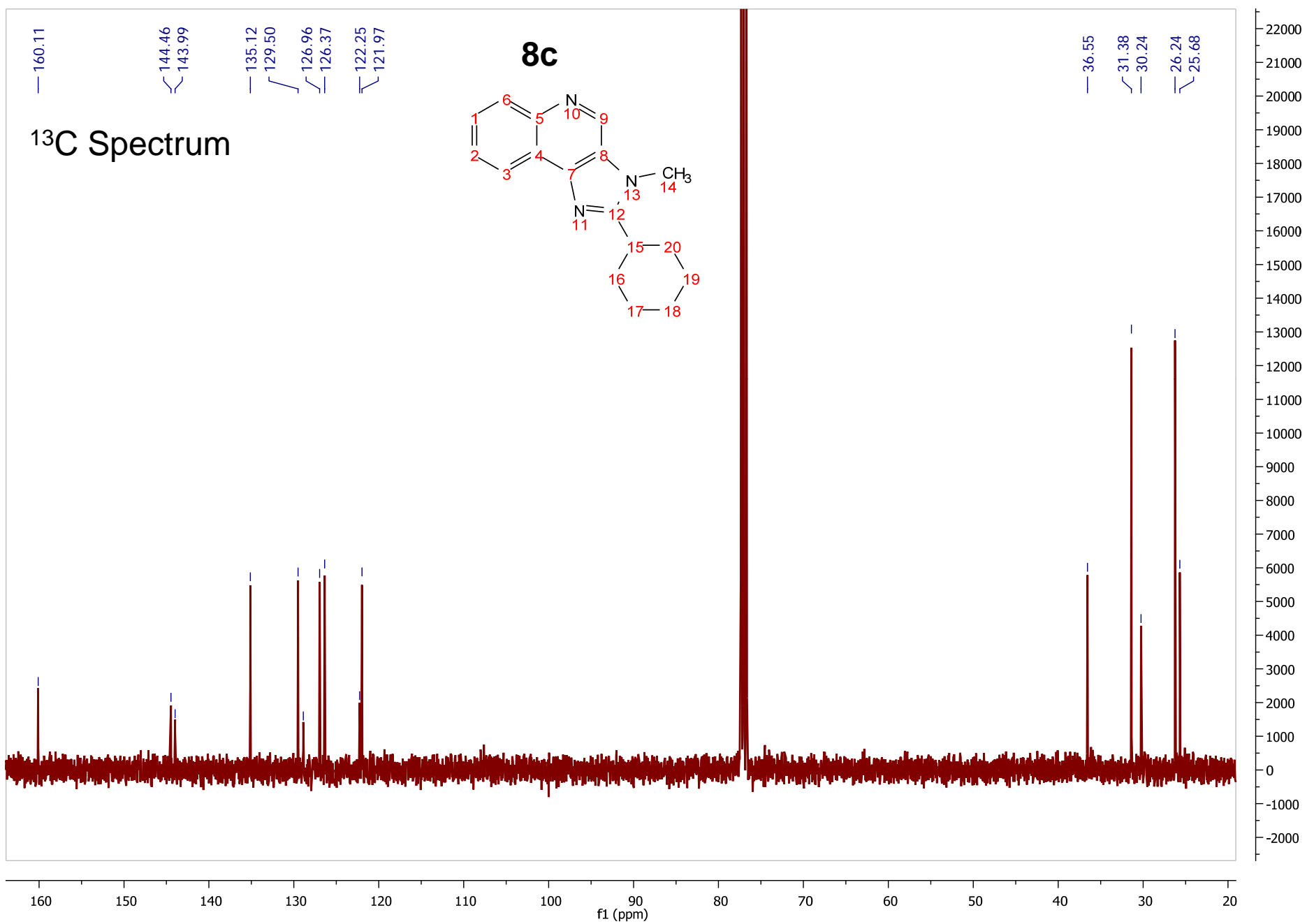


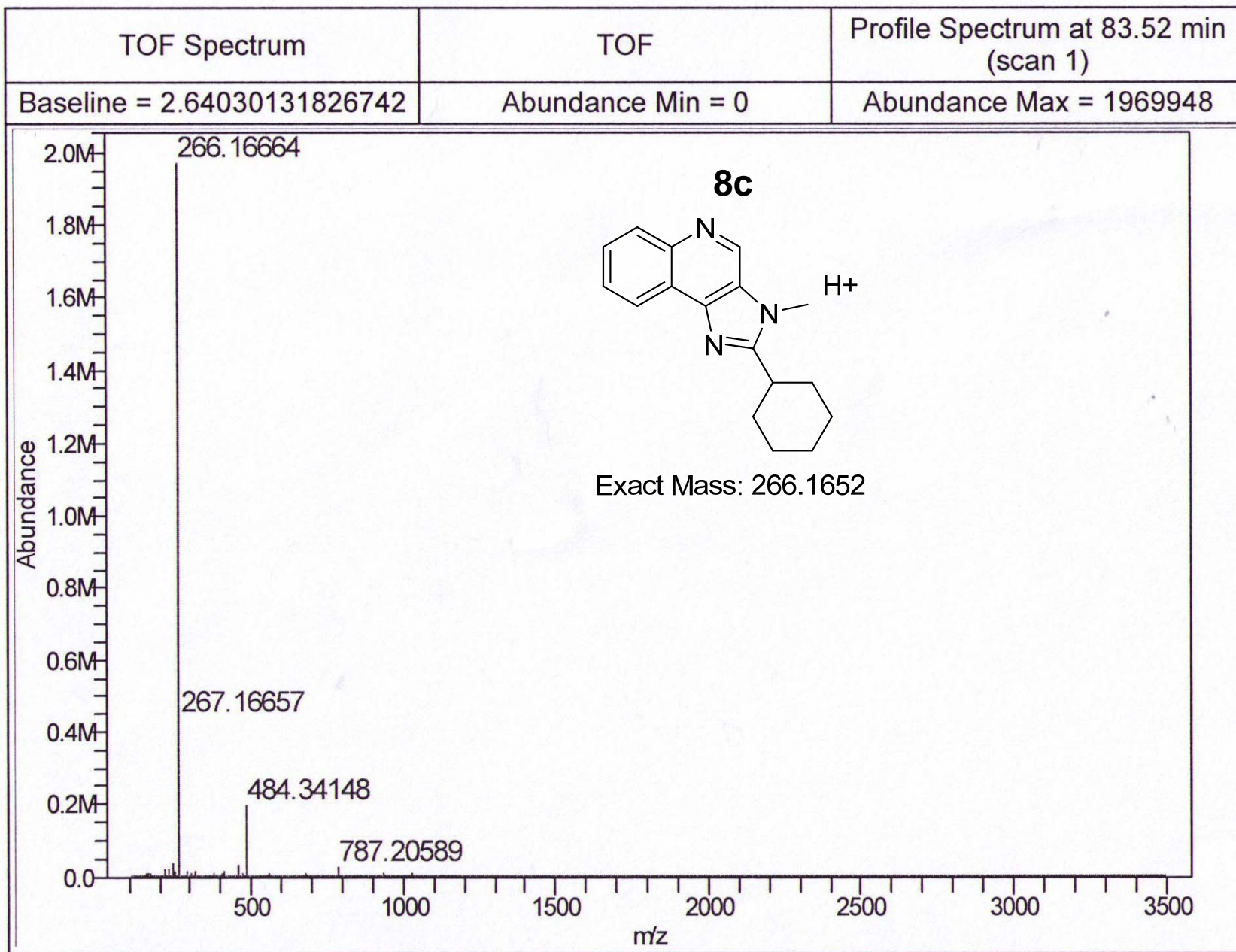
# <sup>13</sup>C Spectrum



160.11  
144.46  
143.99  
135.12  
129.50  
126.96  
126.37  
122.25  
121.97

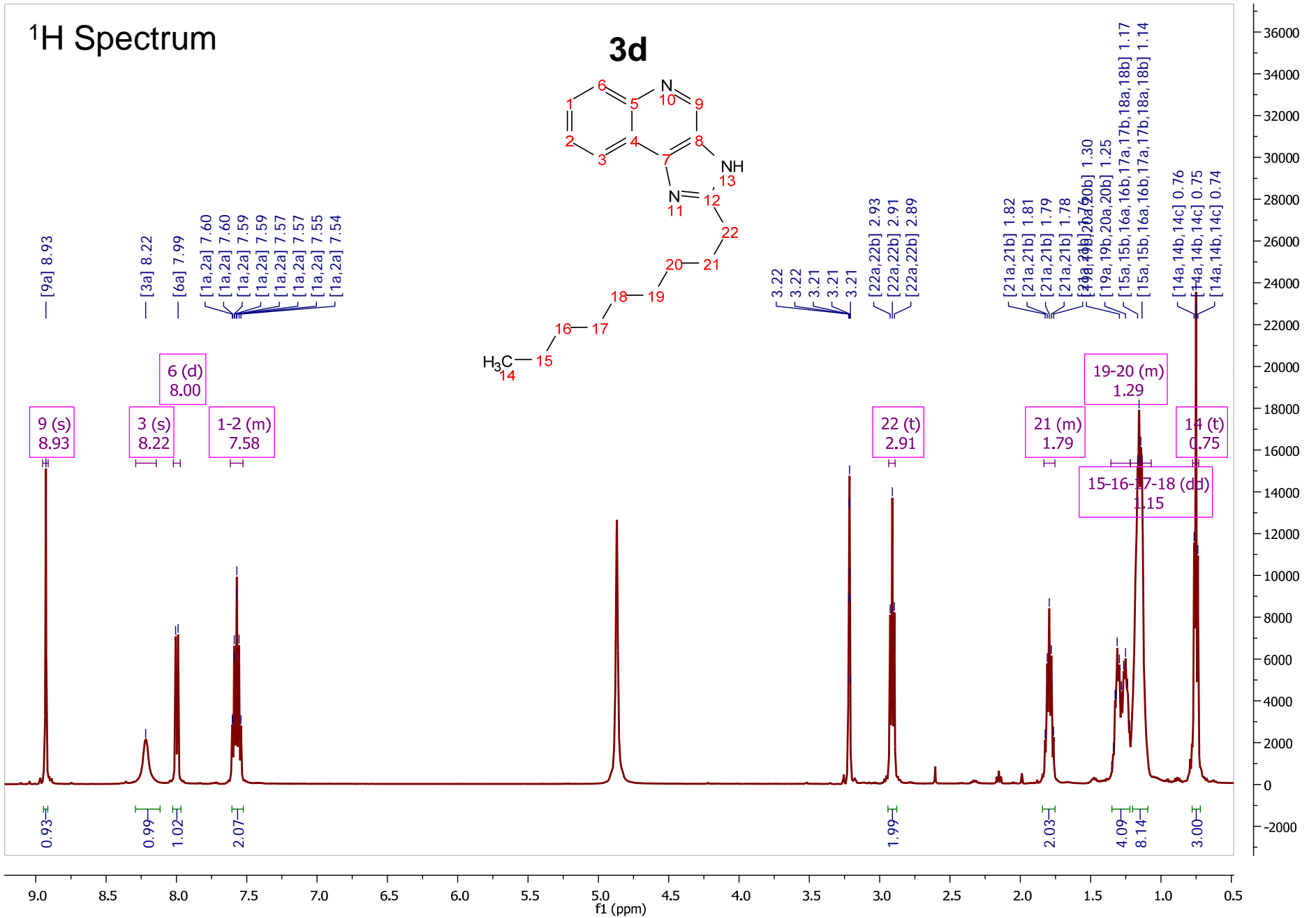
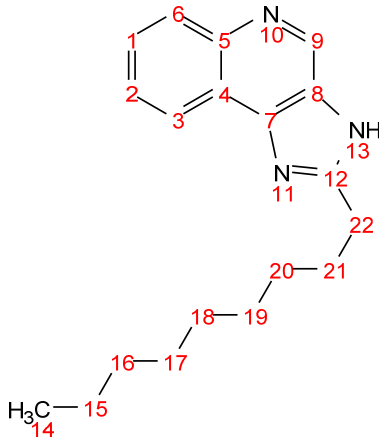
36.55  
31.38  
30.24  
26.24  
25.68

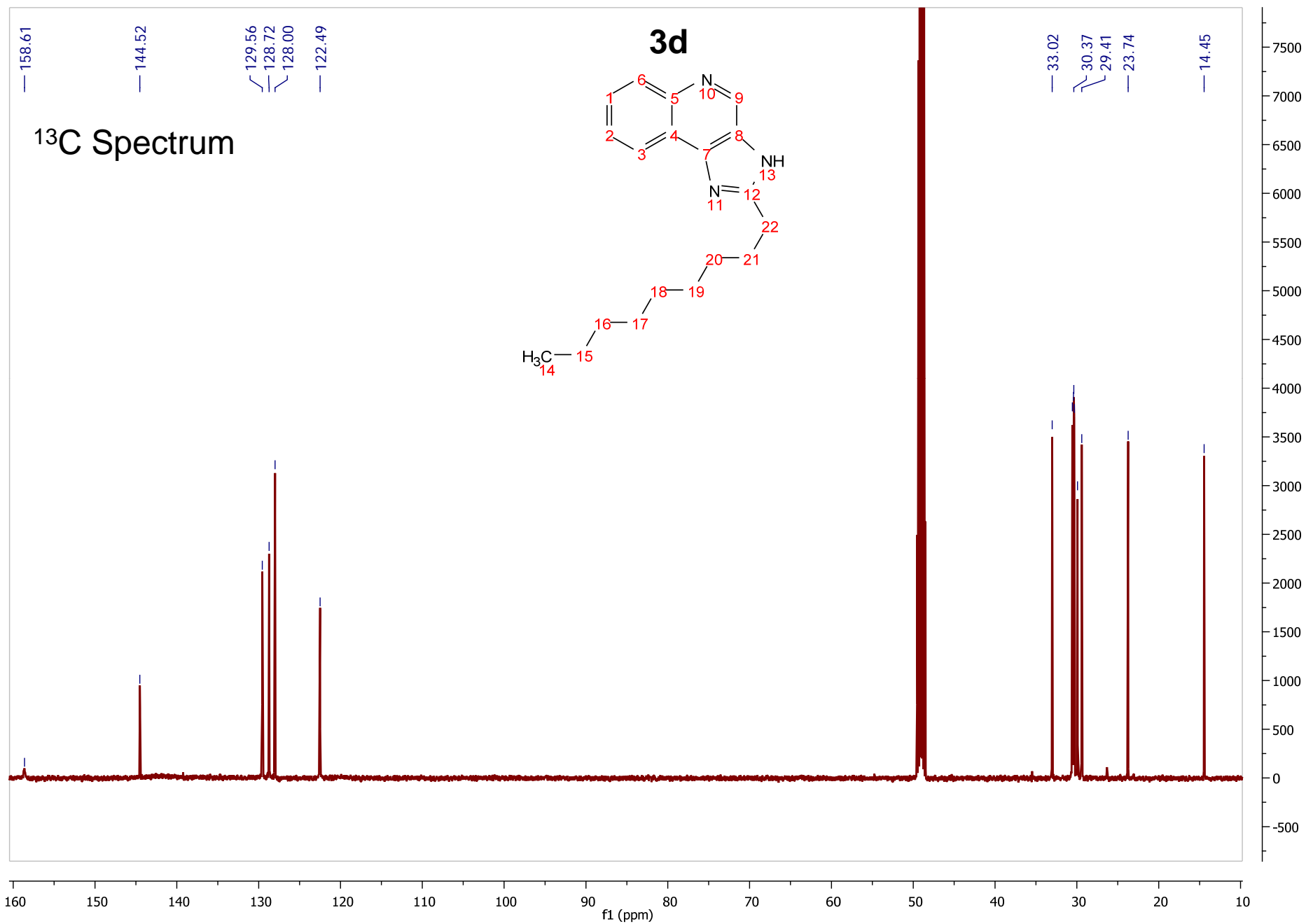


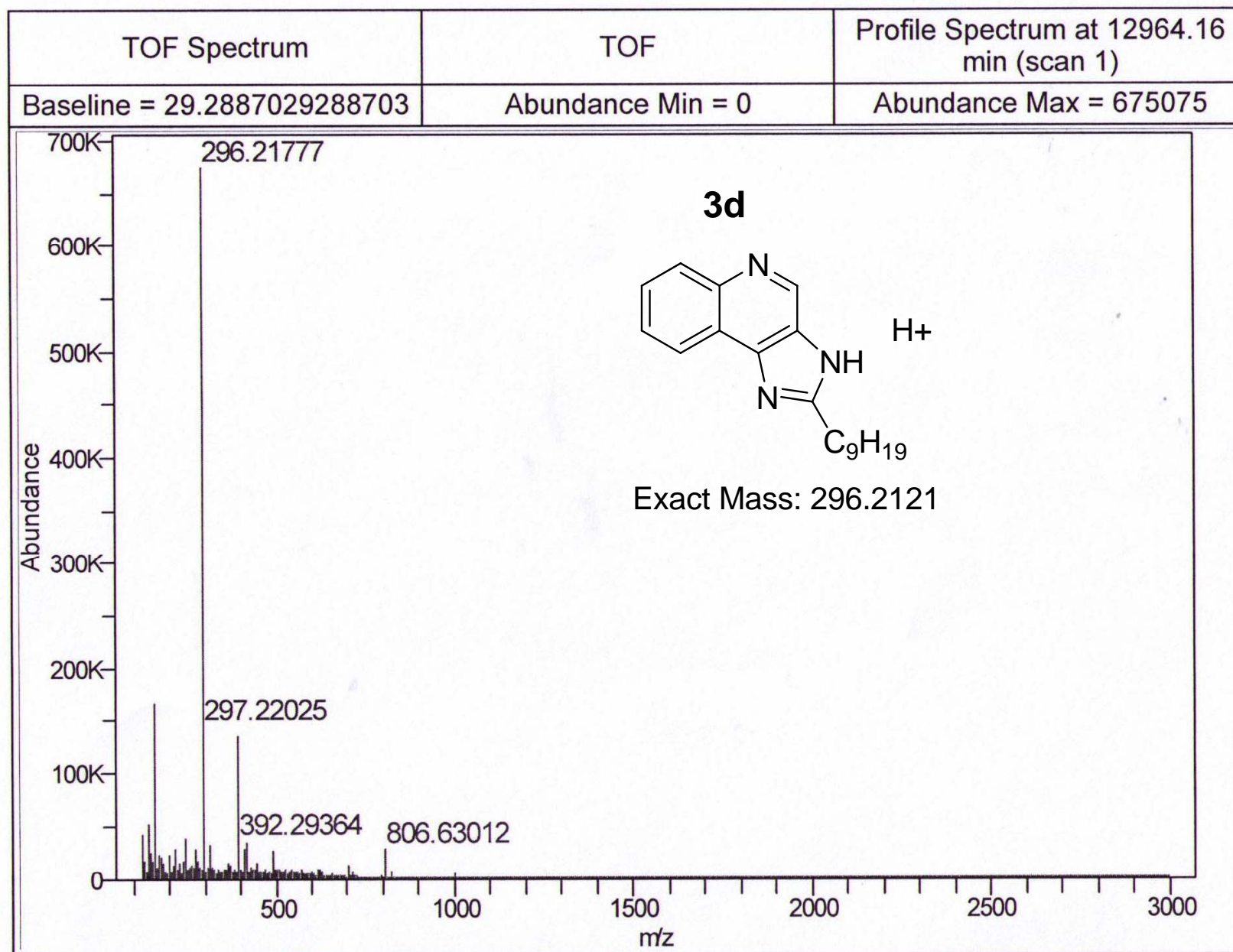


# <sup>1</sup>H Spectrum

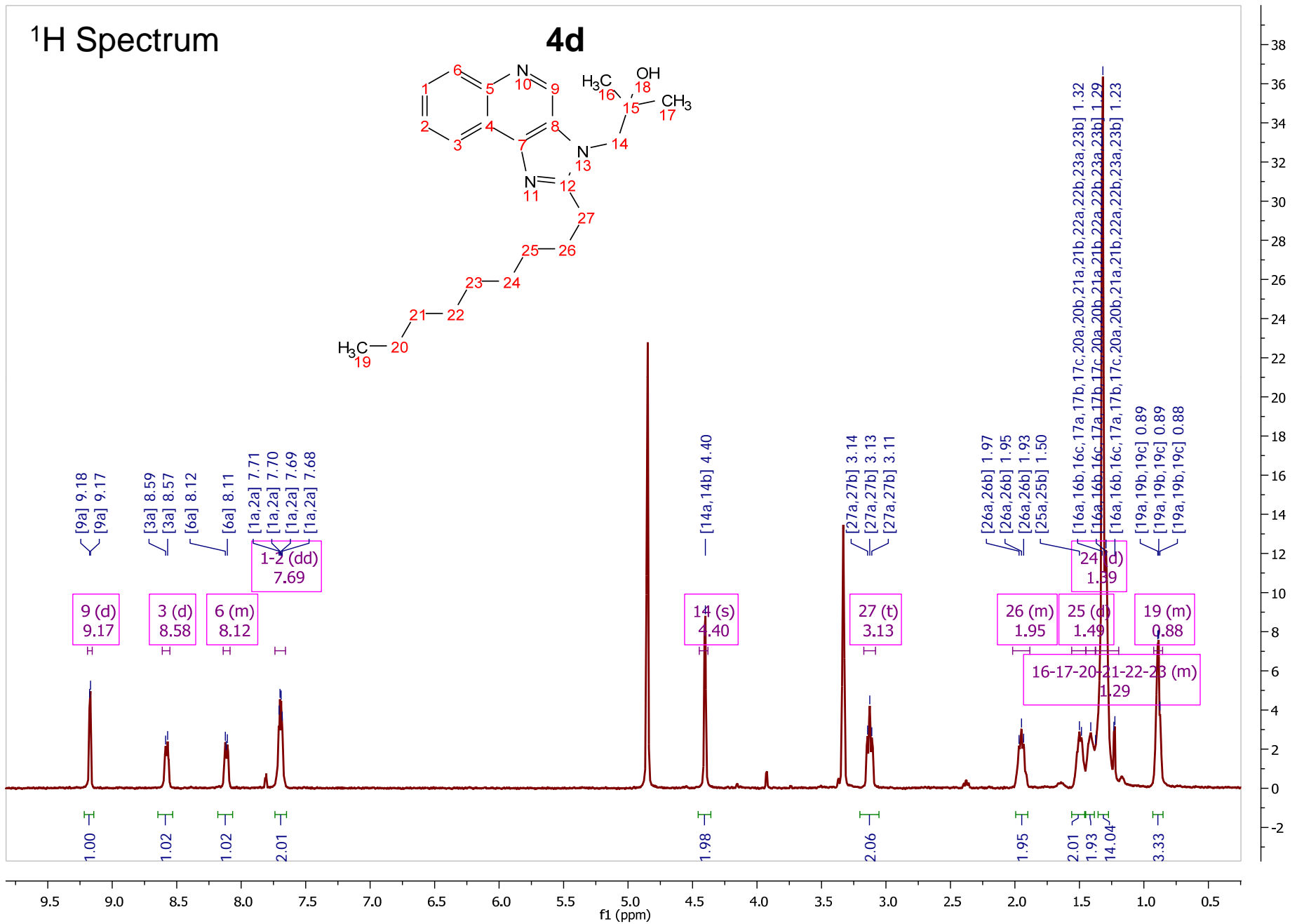
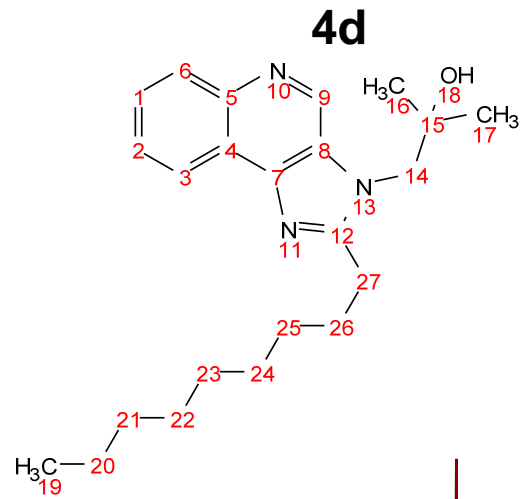
**3d**



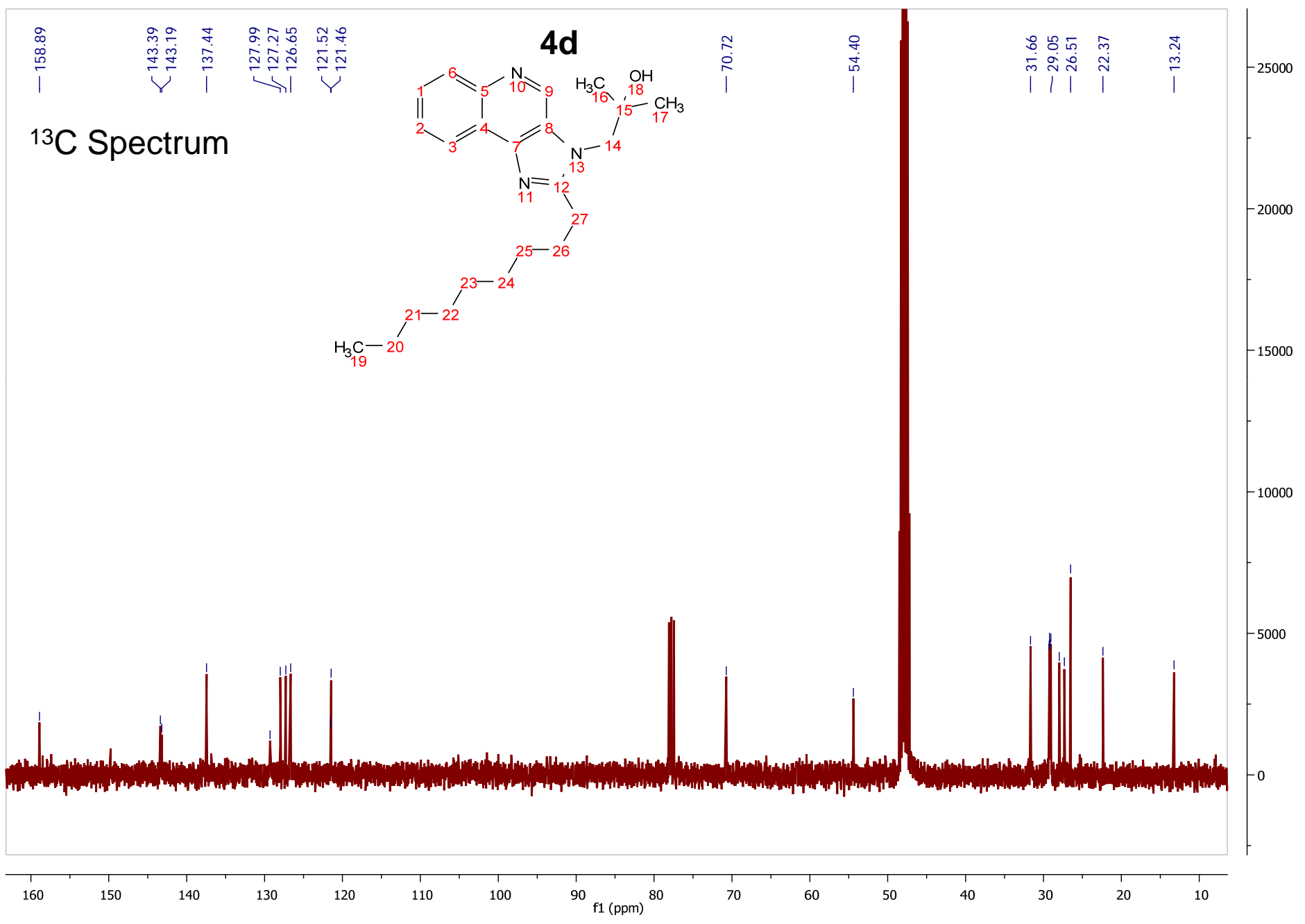
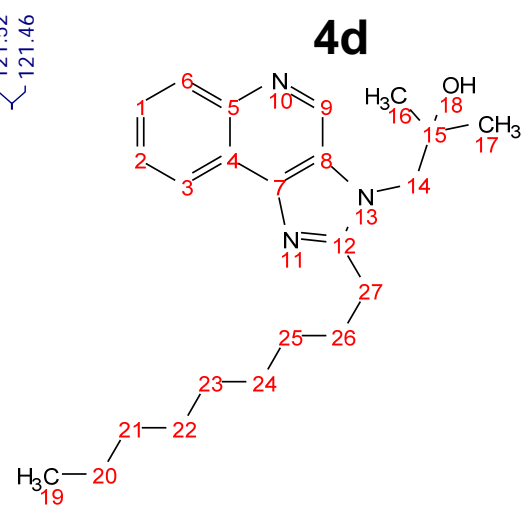




# <sup>1</sup>H Spectrum



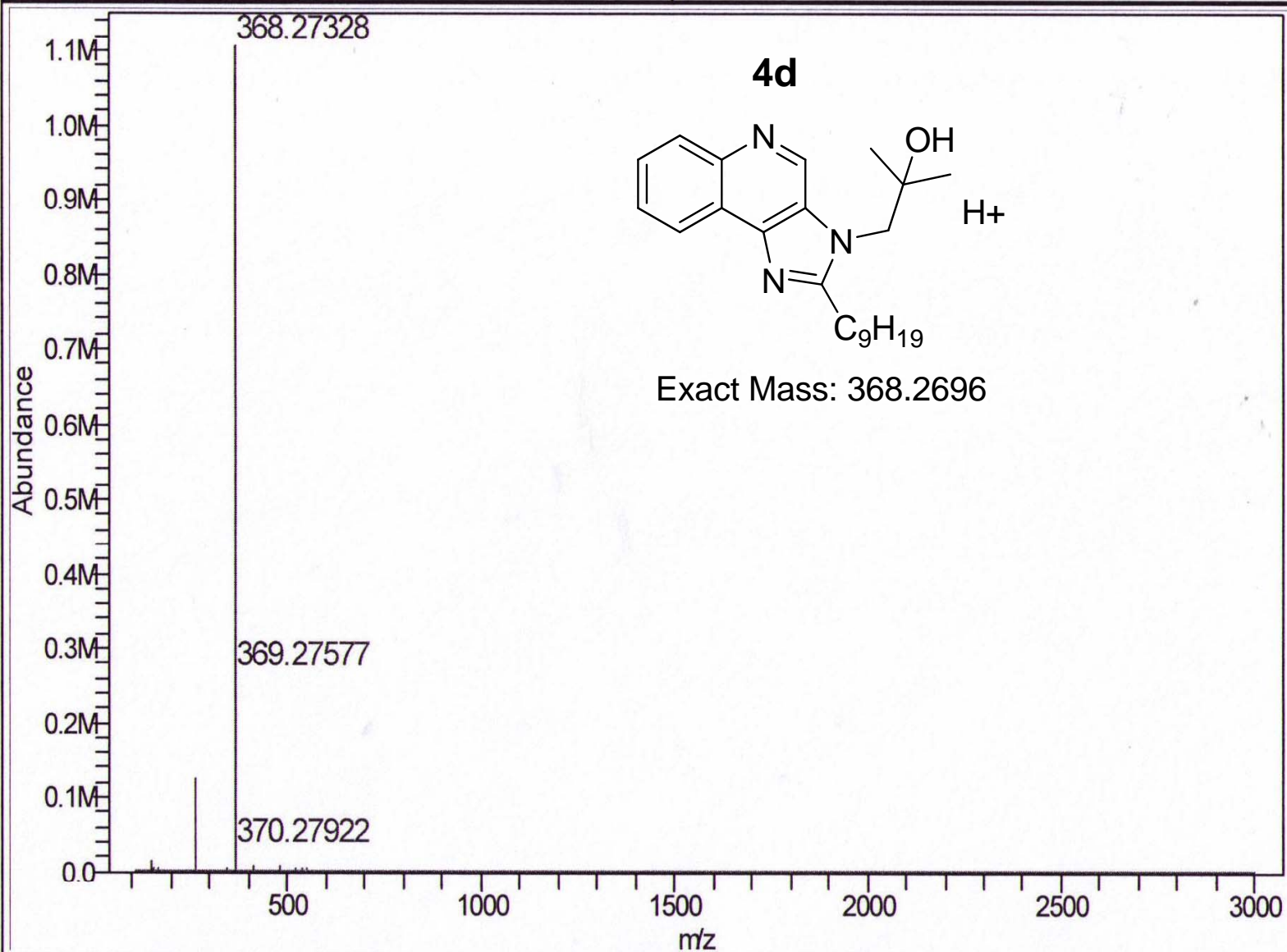
# <sup>13</sup>C Spectrum



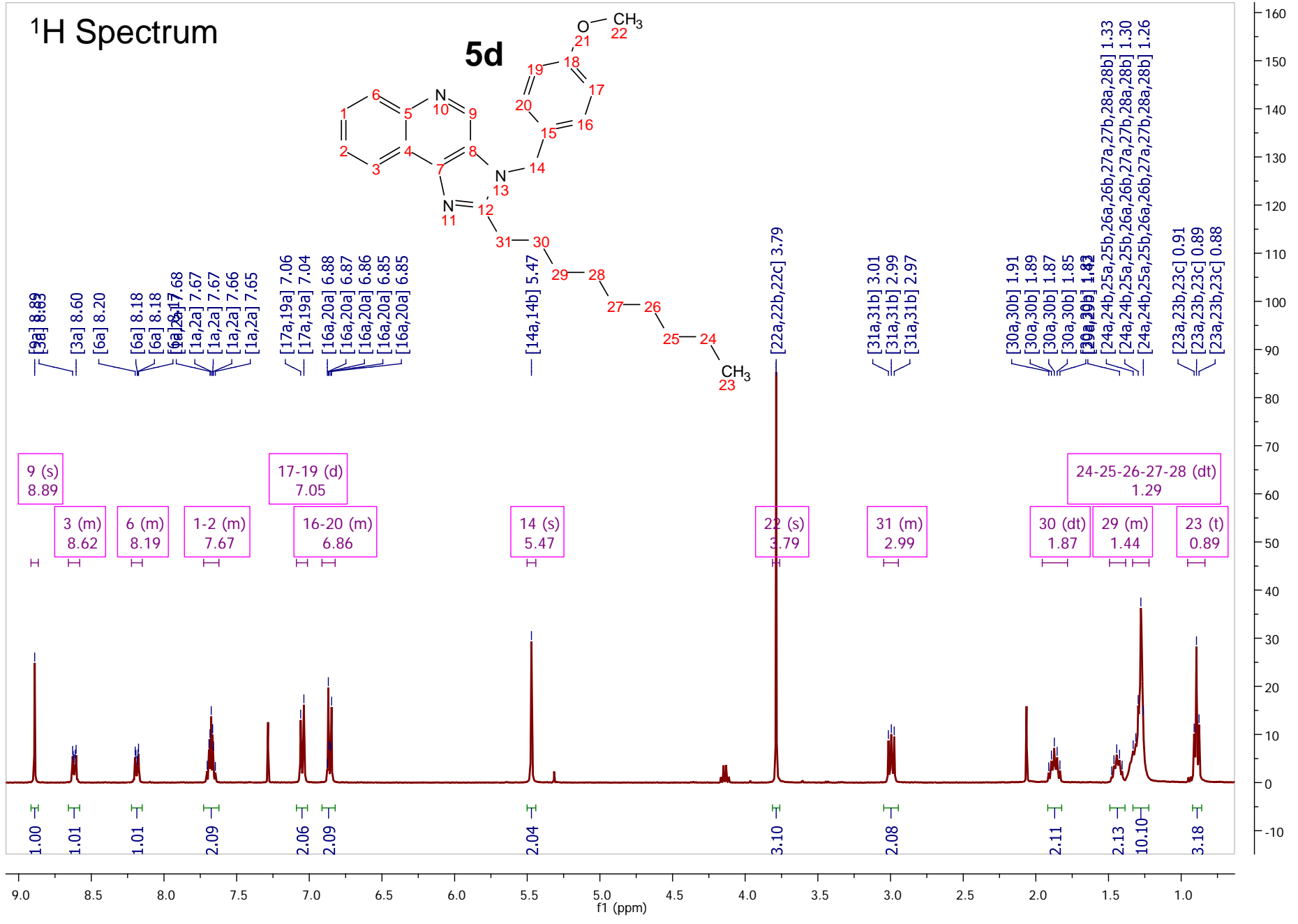
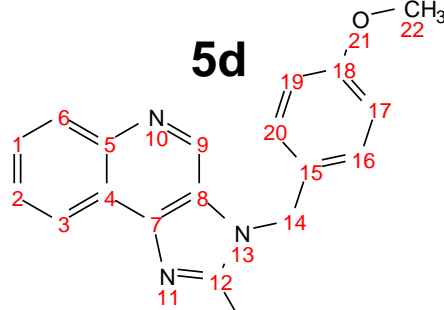


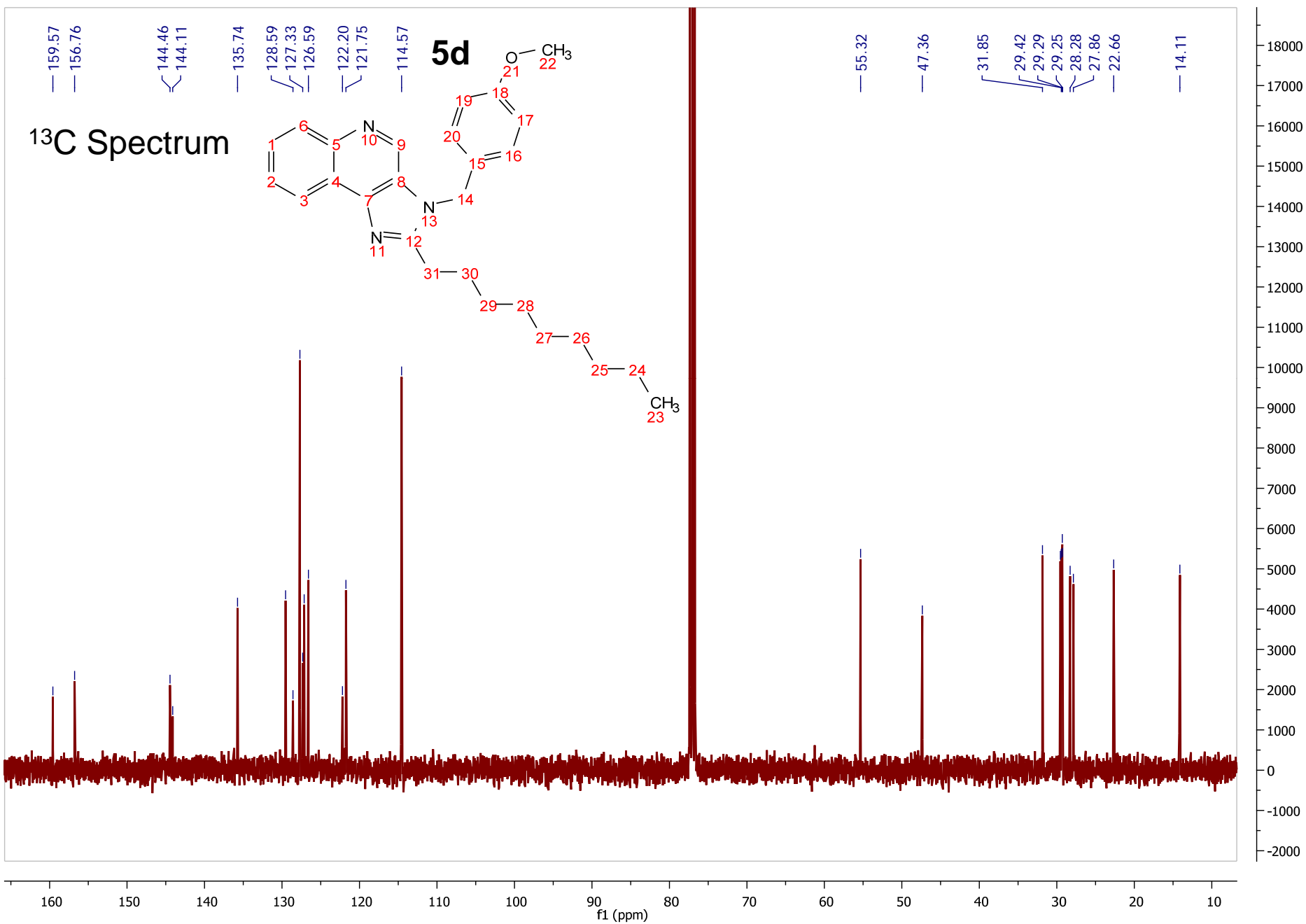
TOF Spectrum

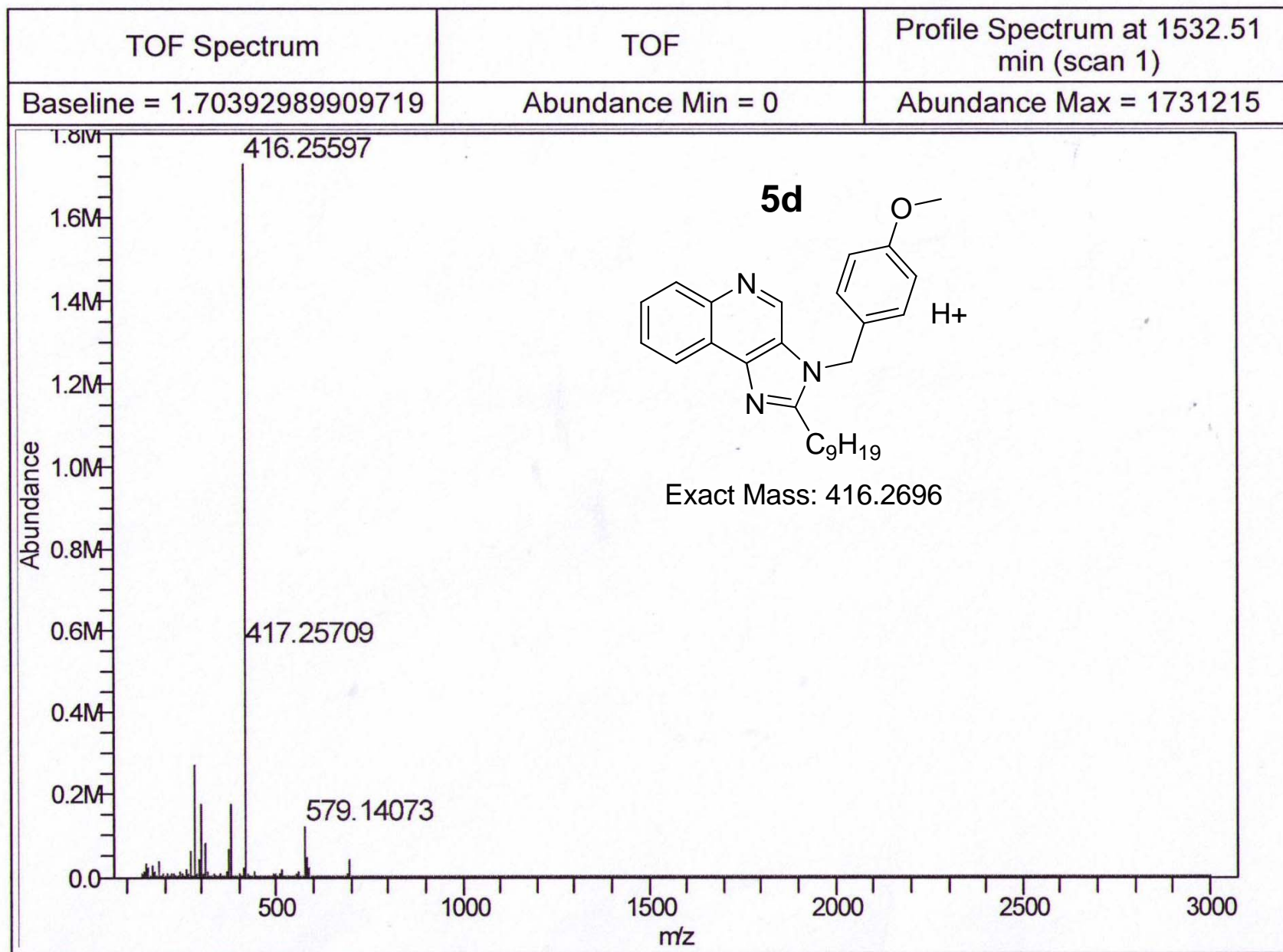
Profile Spectrum at 28.09 min (scan 1)



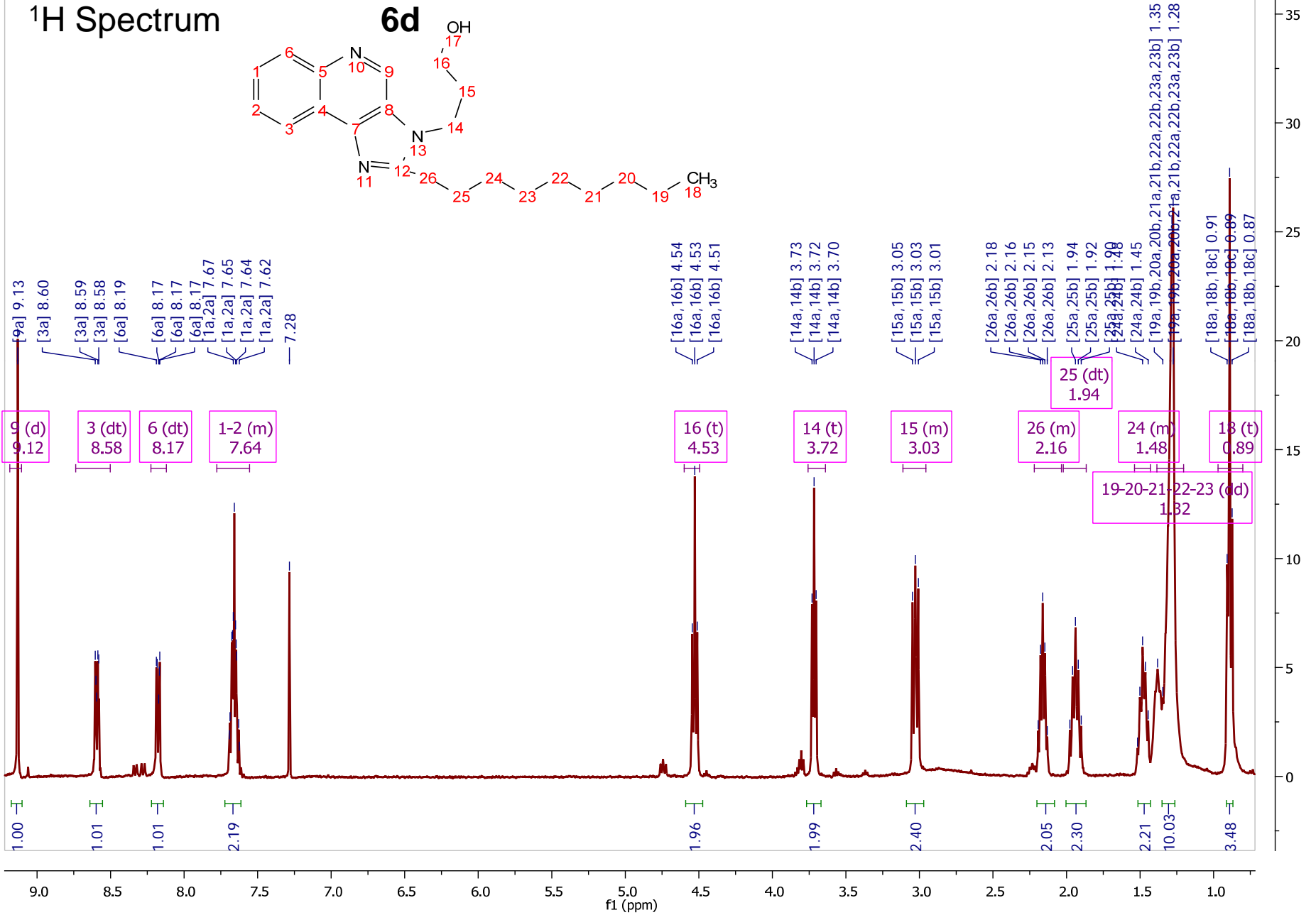
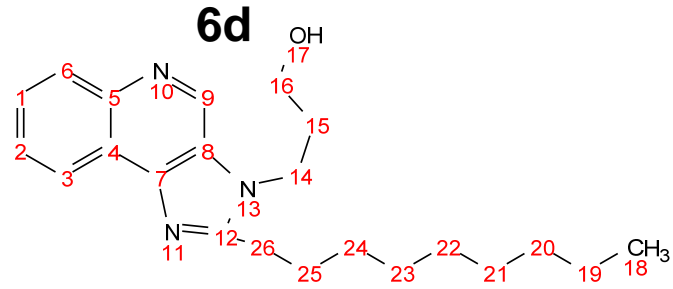
# <sup>1</sup>H Spectrum

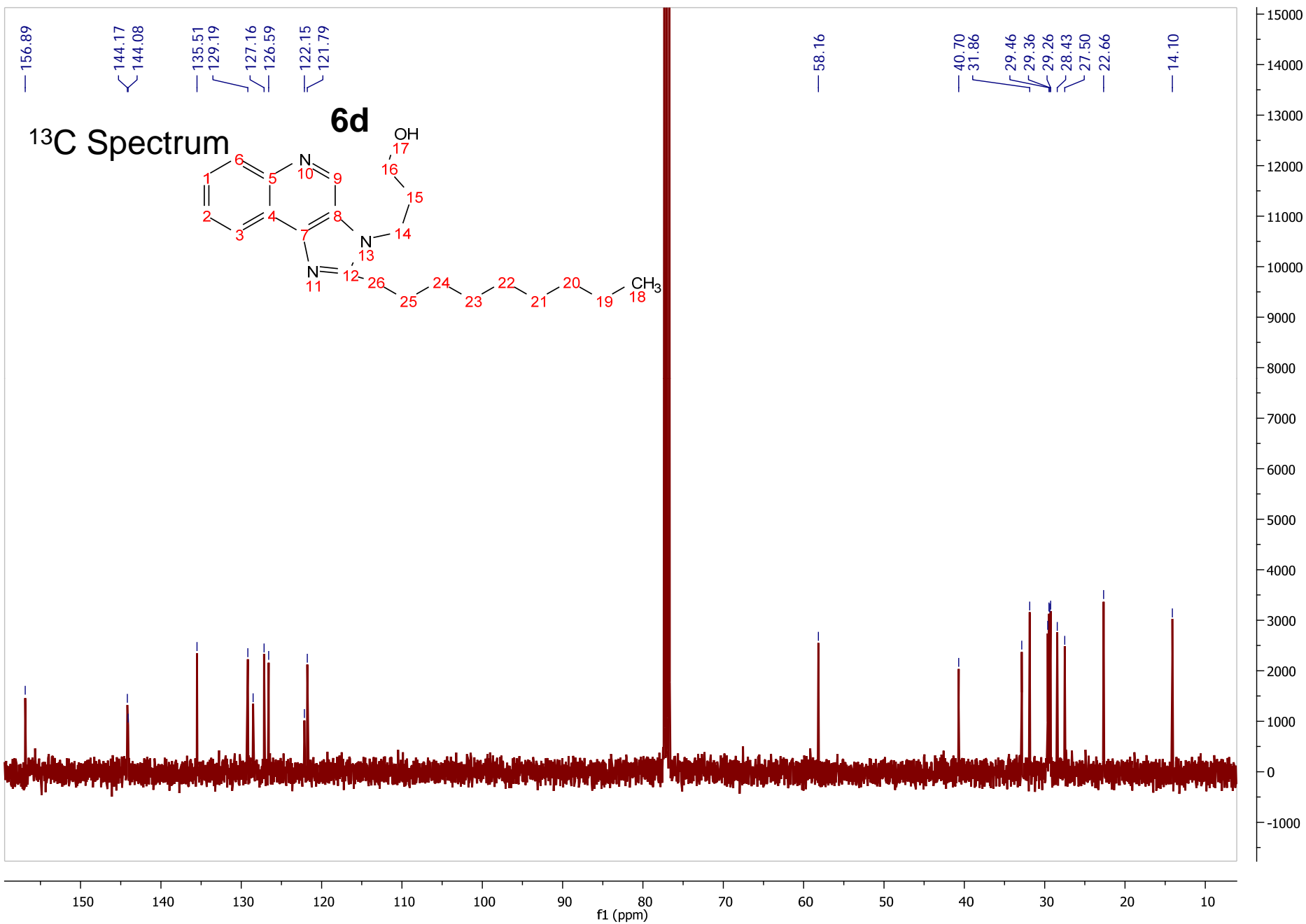


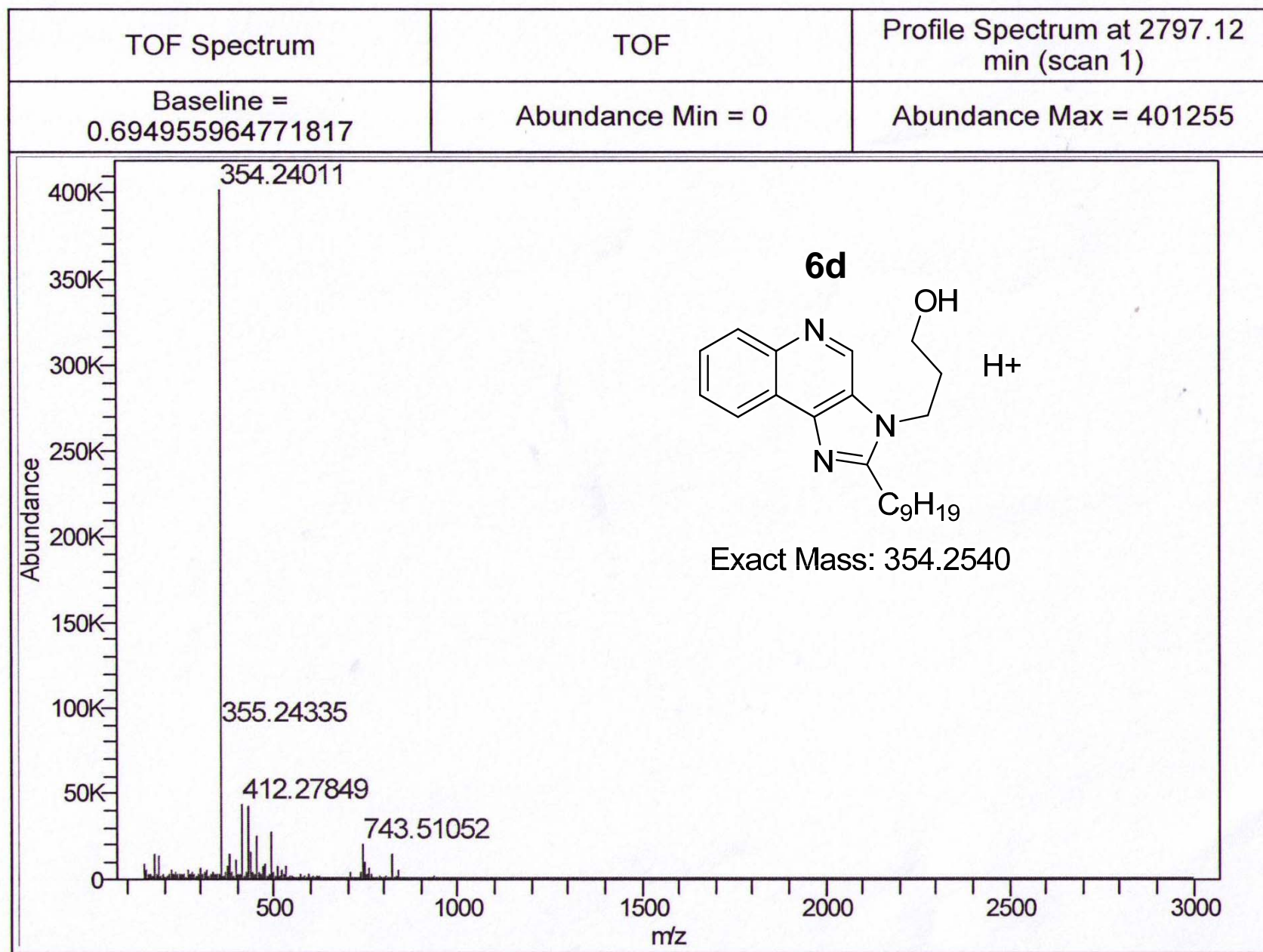




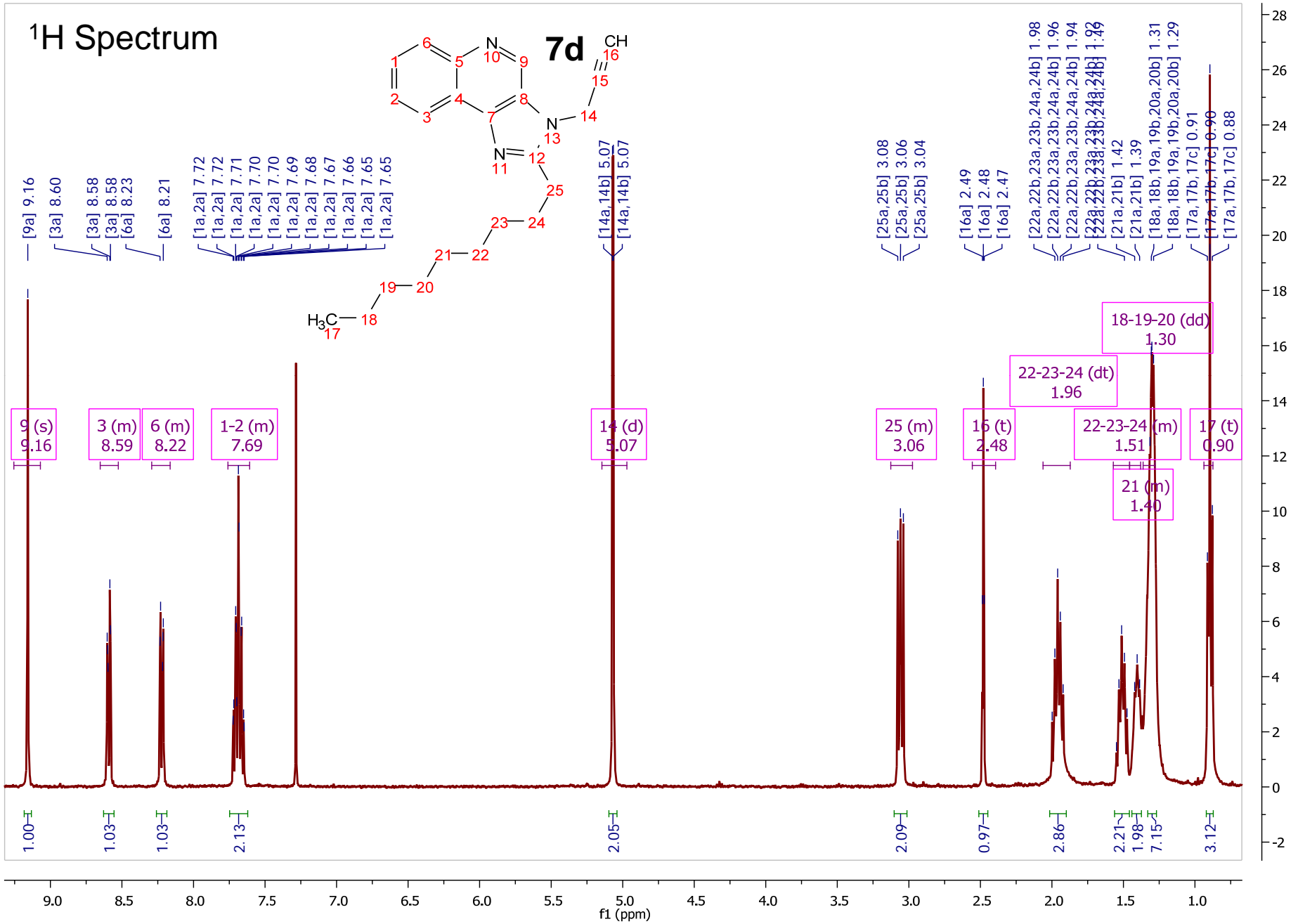
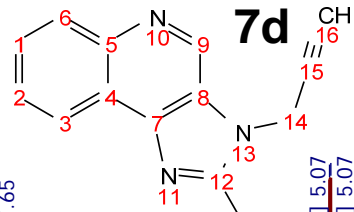
# <sup>1</sup>H Spectrum





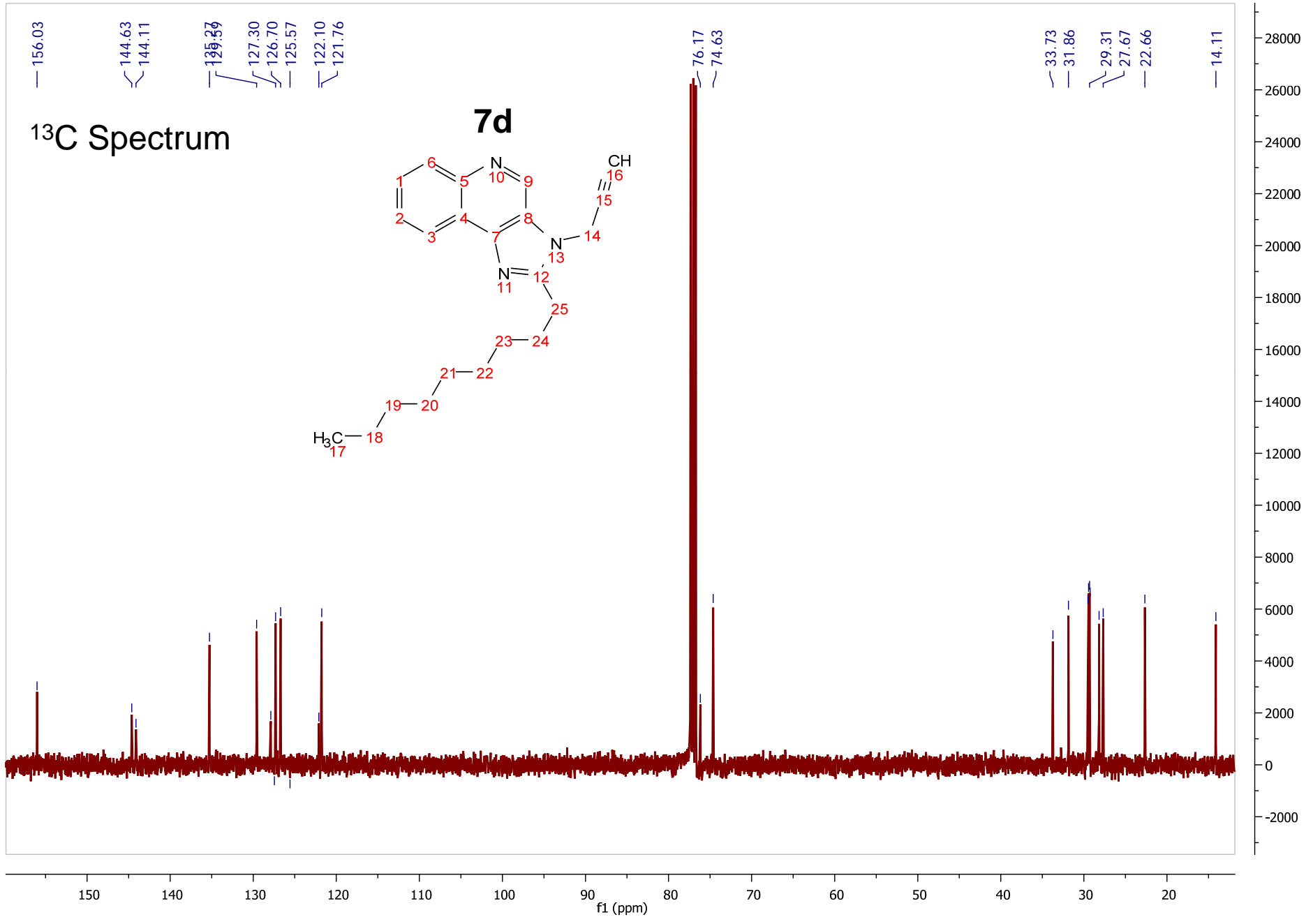
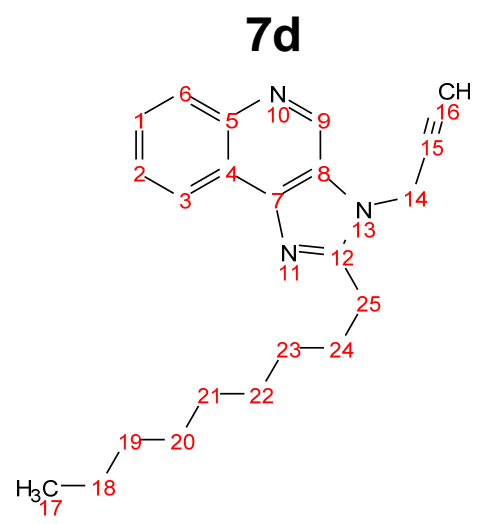


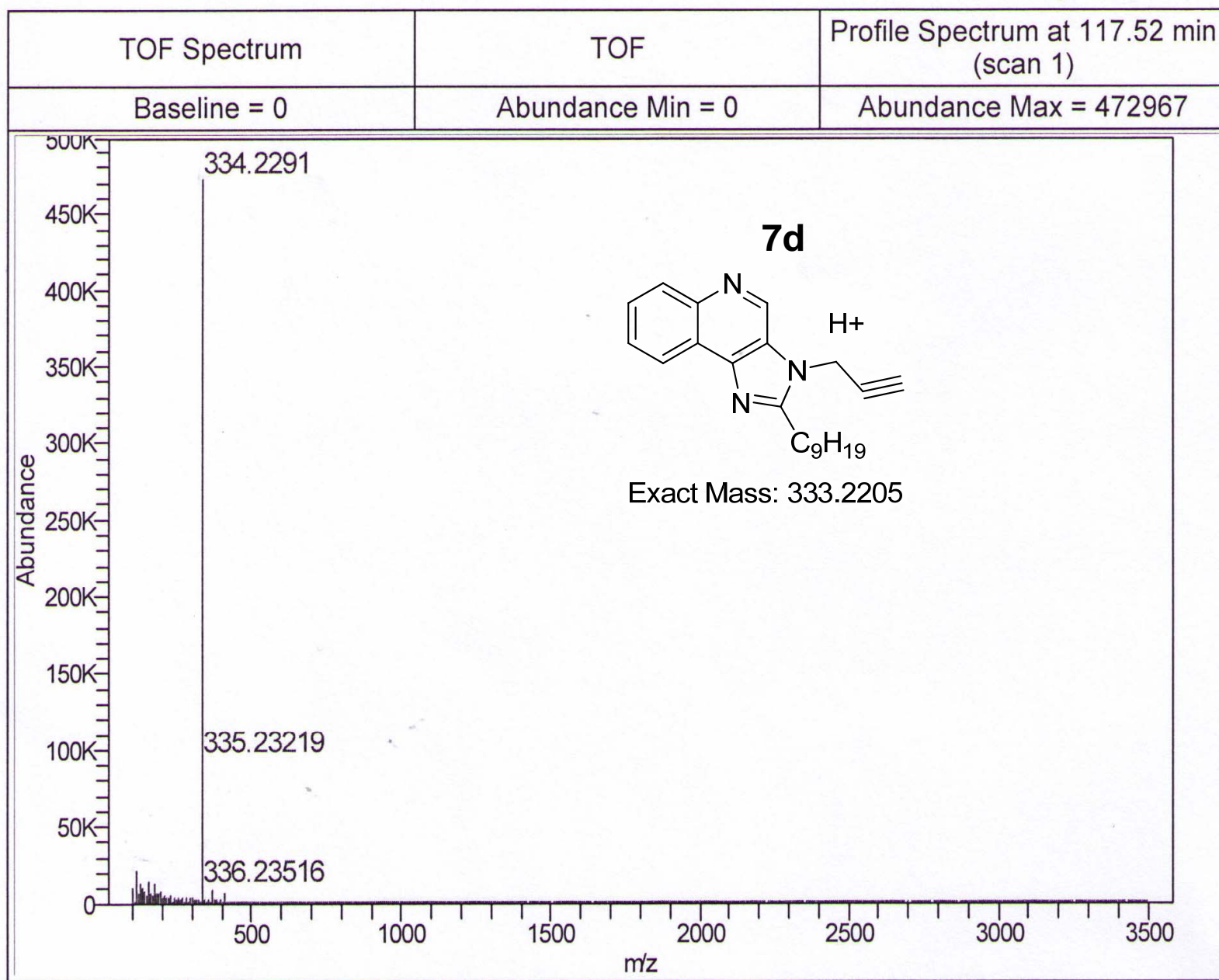
# <sup>1</sup>H Spectrum



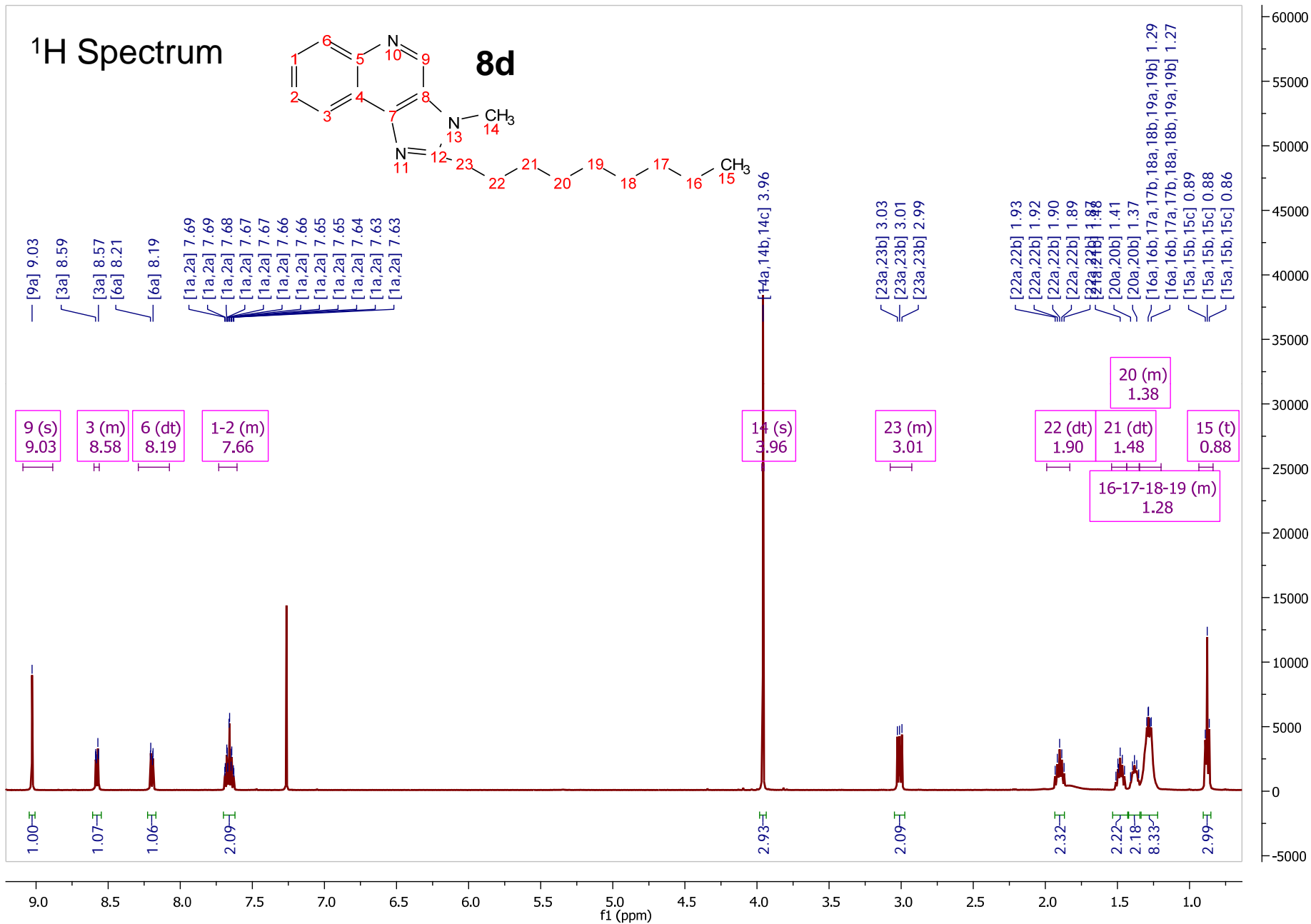
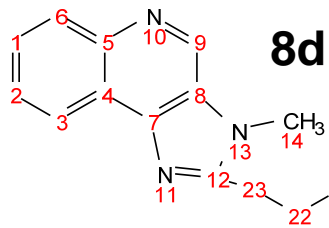


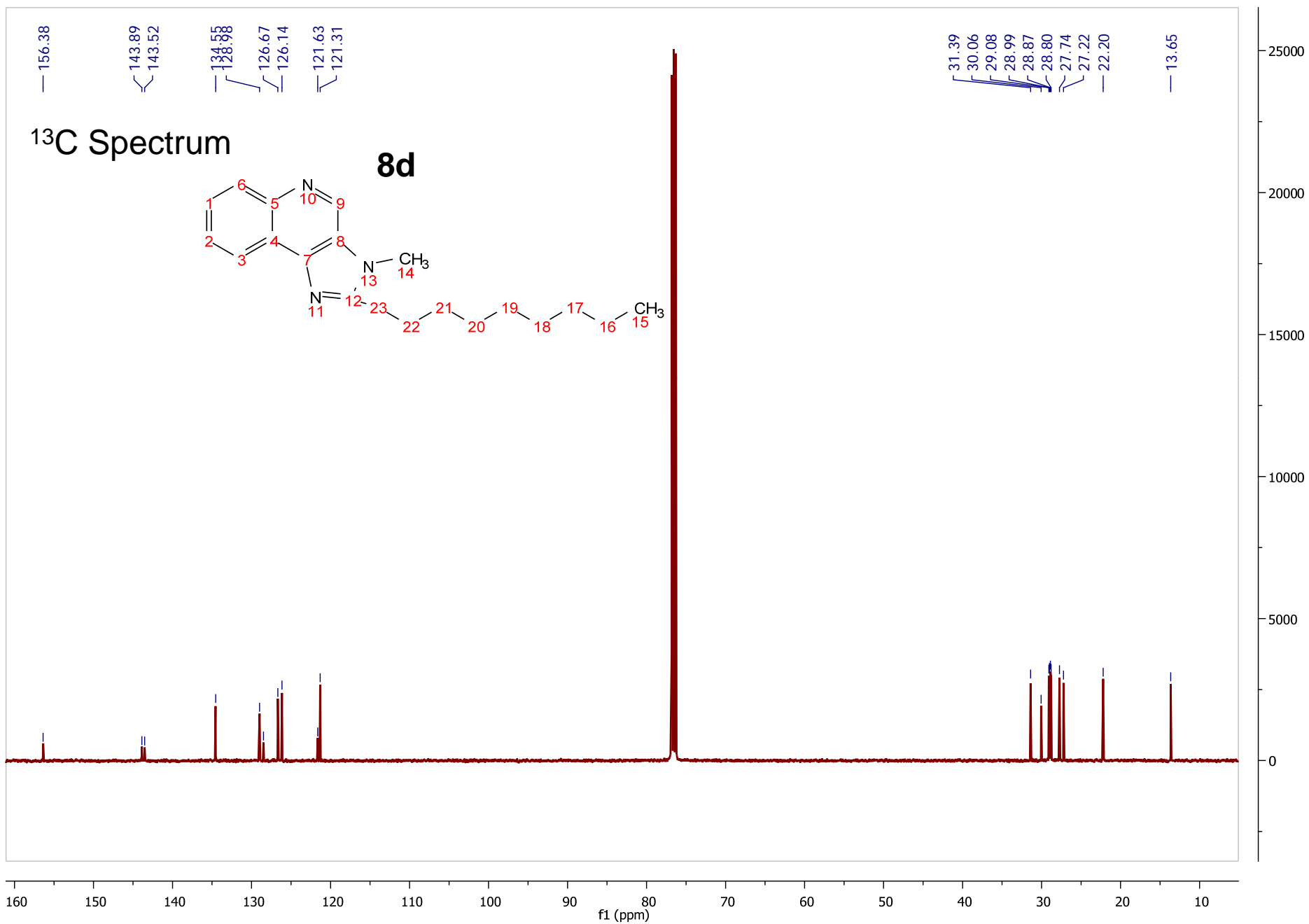
# <sup>13</sup>C Spectrum

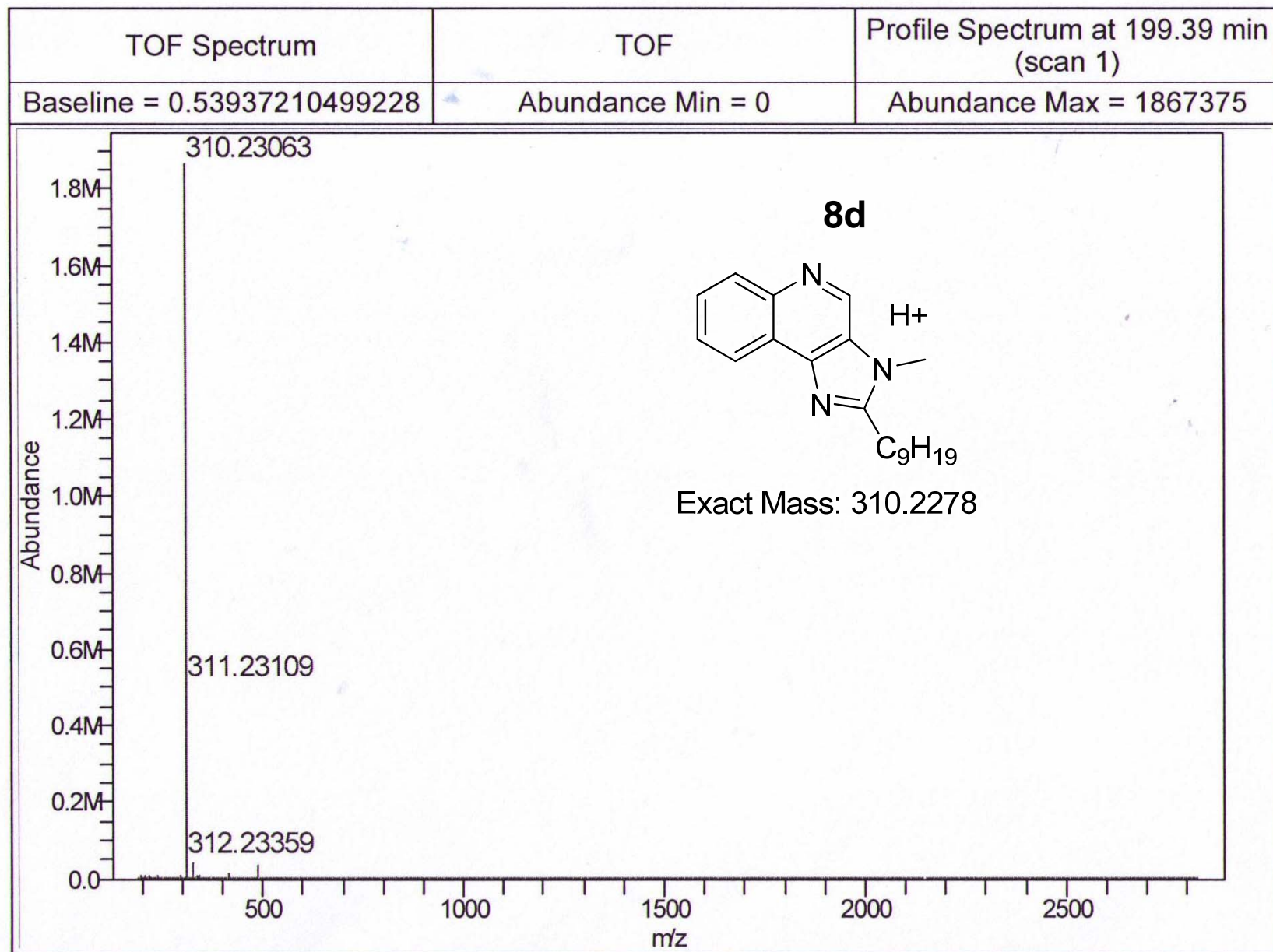




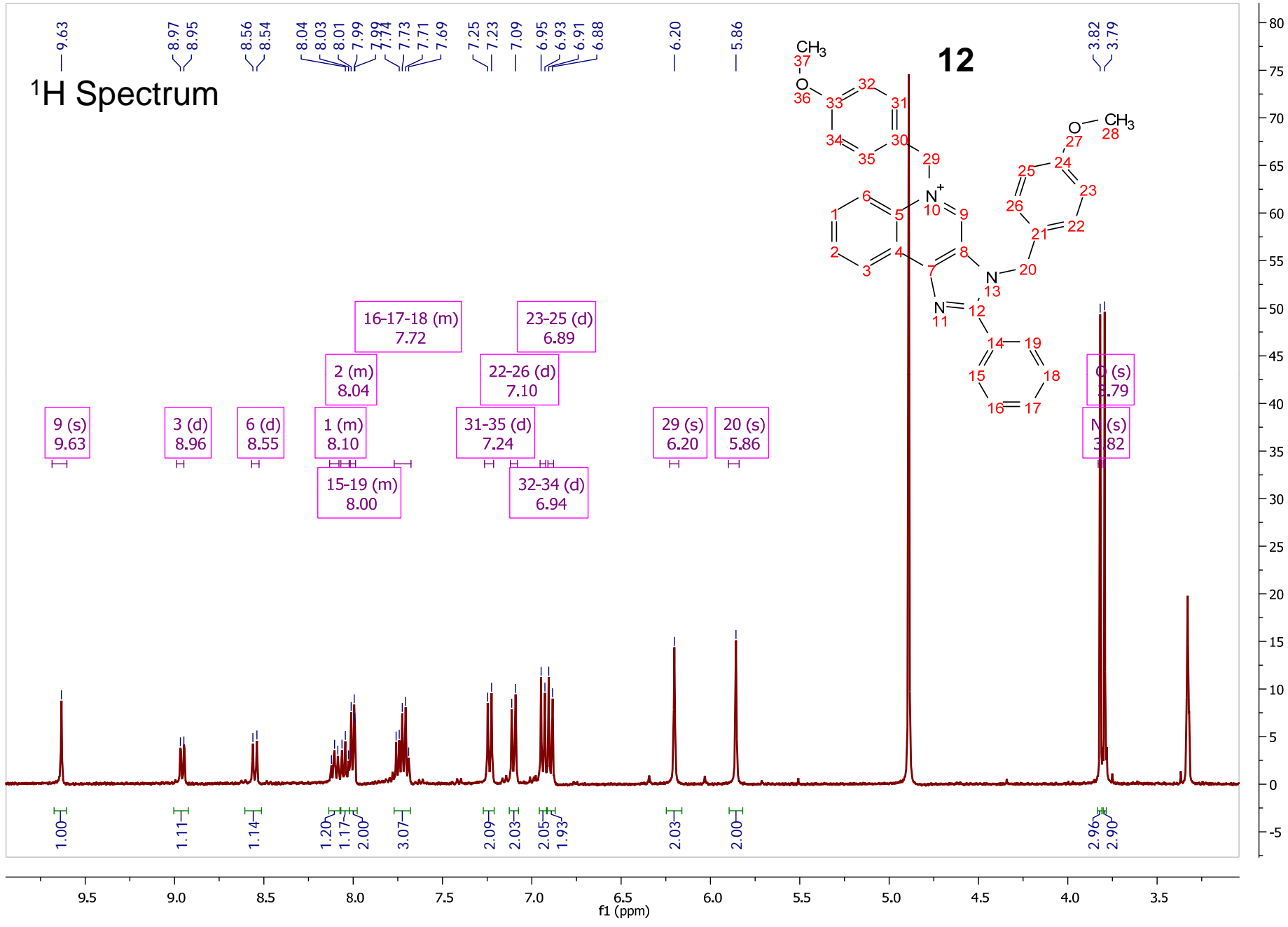
# <sup>1</sup>H Spectrum





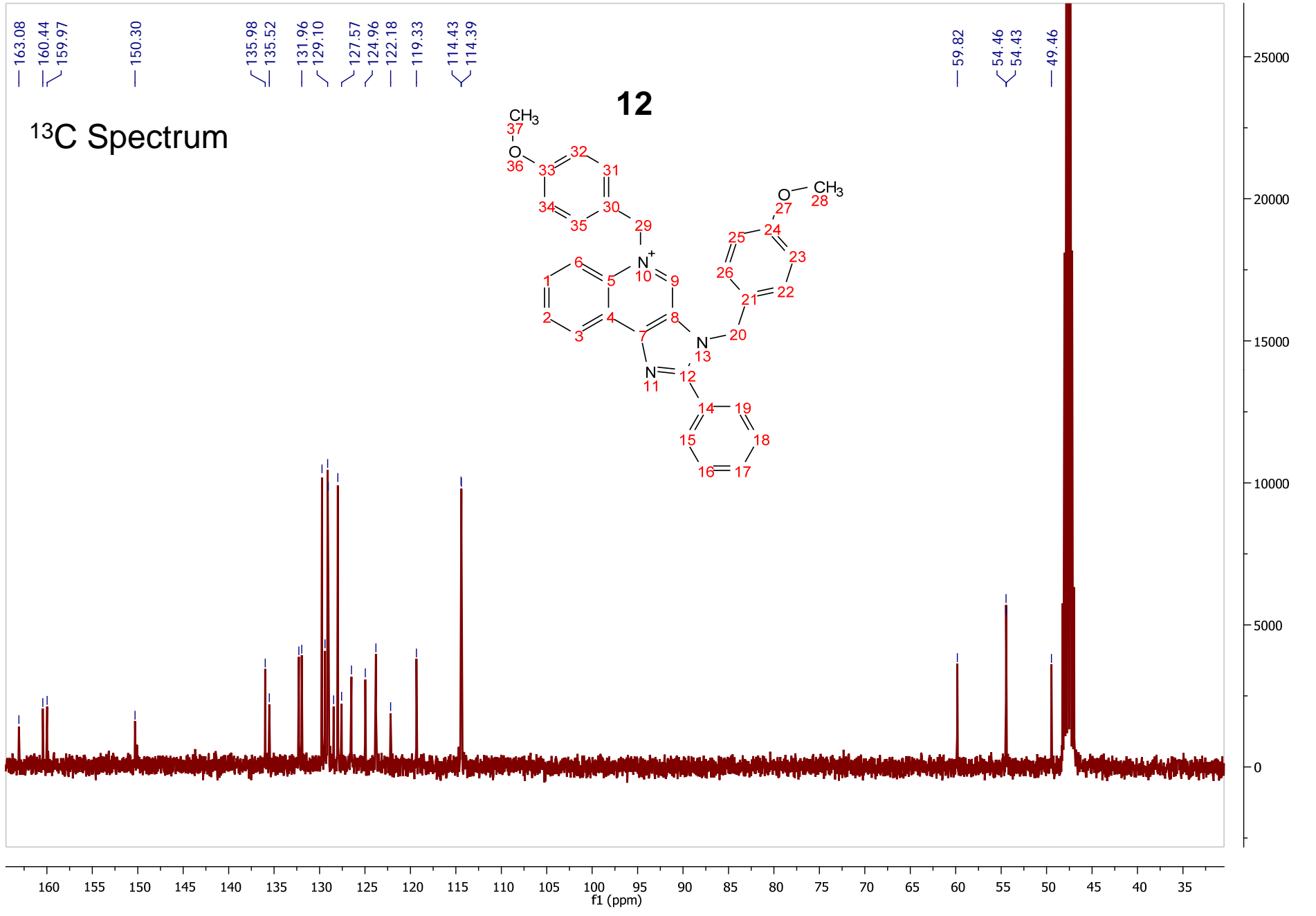
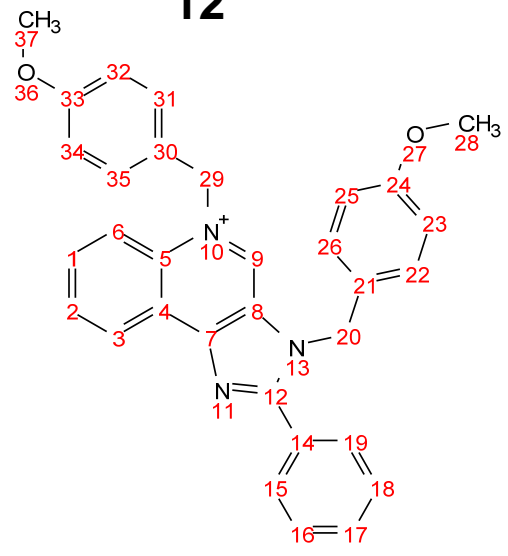


# <sup>1</sup>H Spectrum



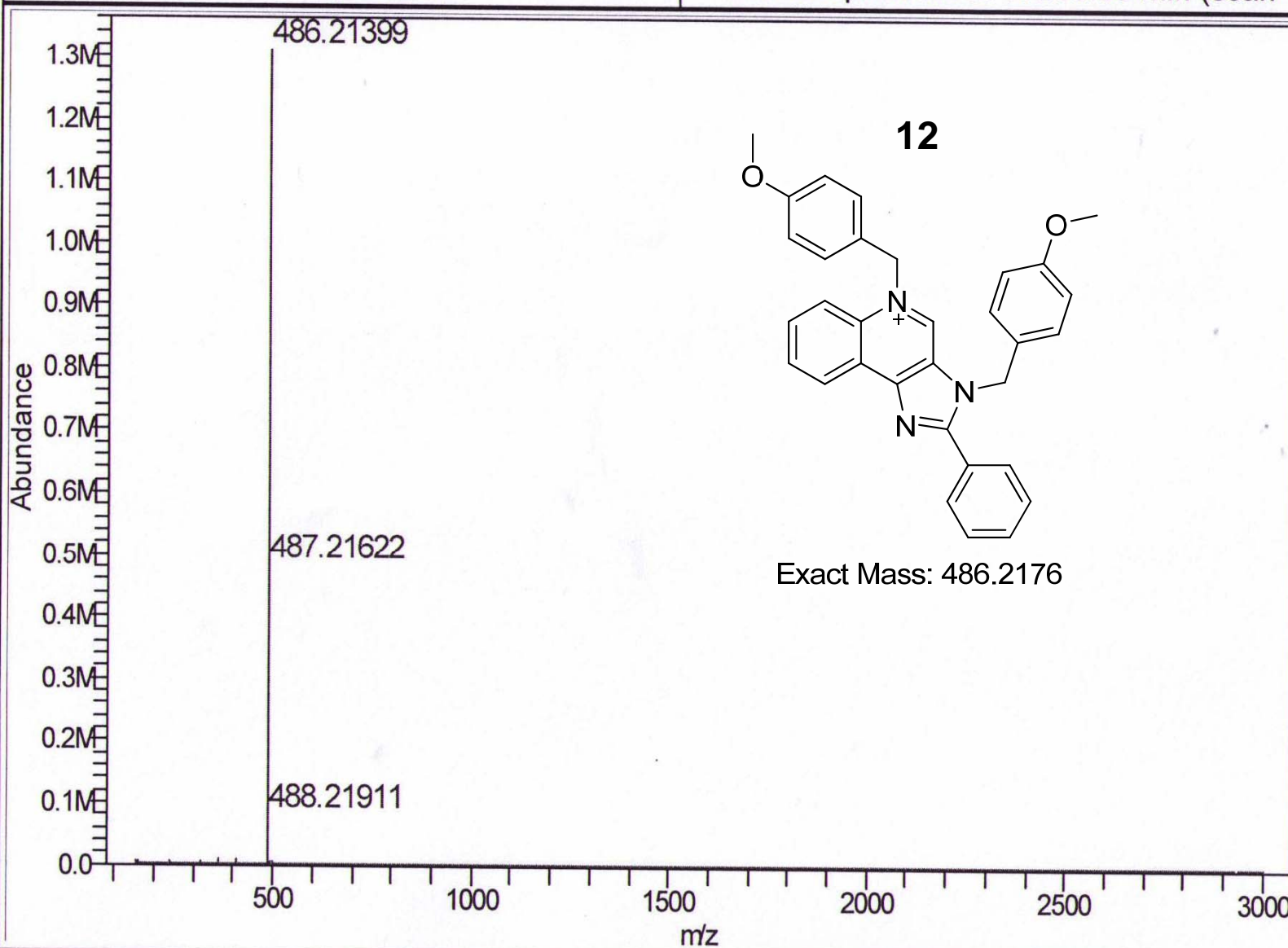
# <sup>13</sup>C Spectrum

**12**



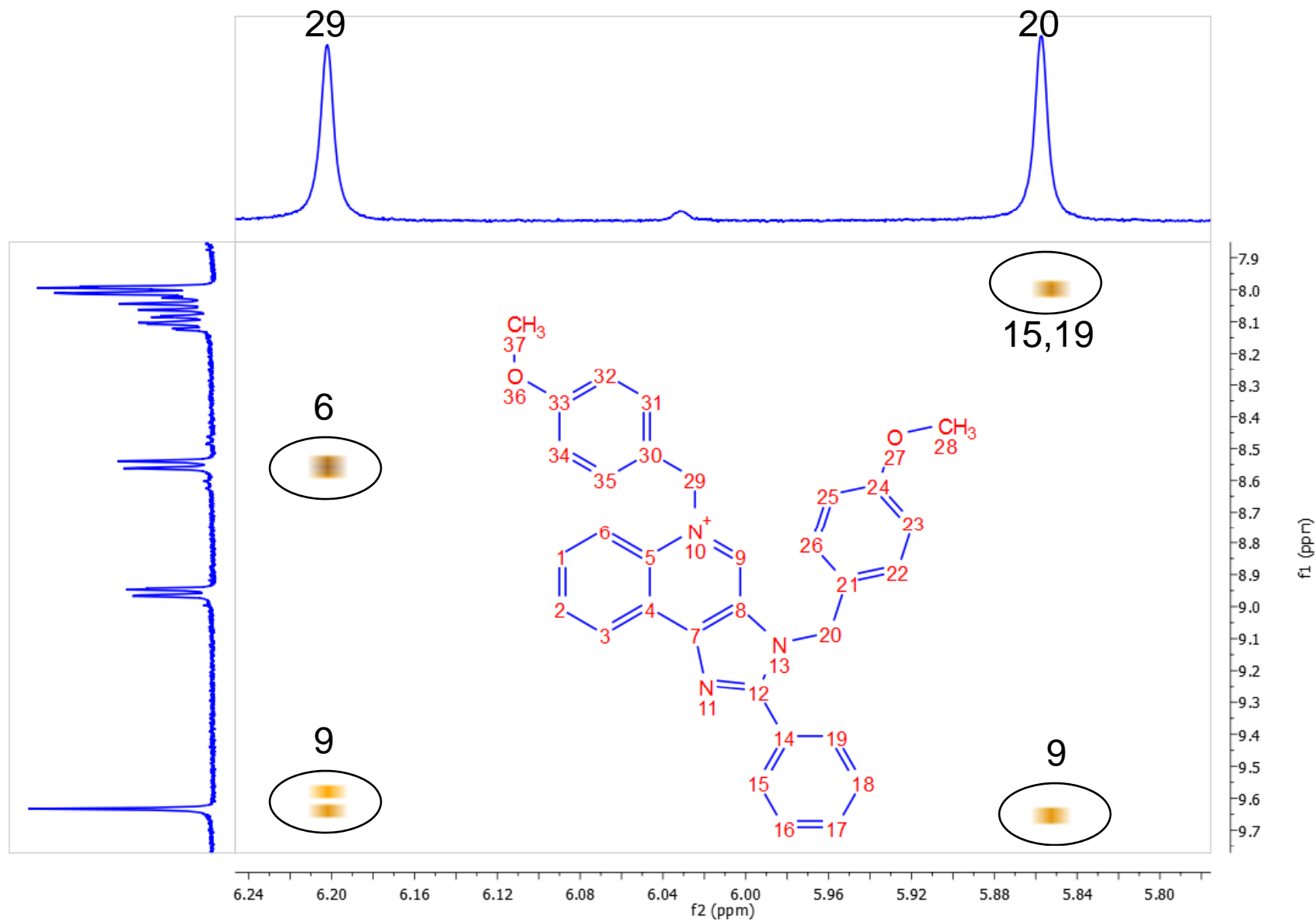
TOF Spectrum

Profile Spectrum at 17250.58 min (scan 1)

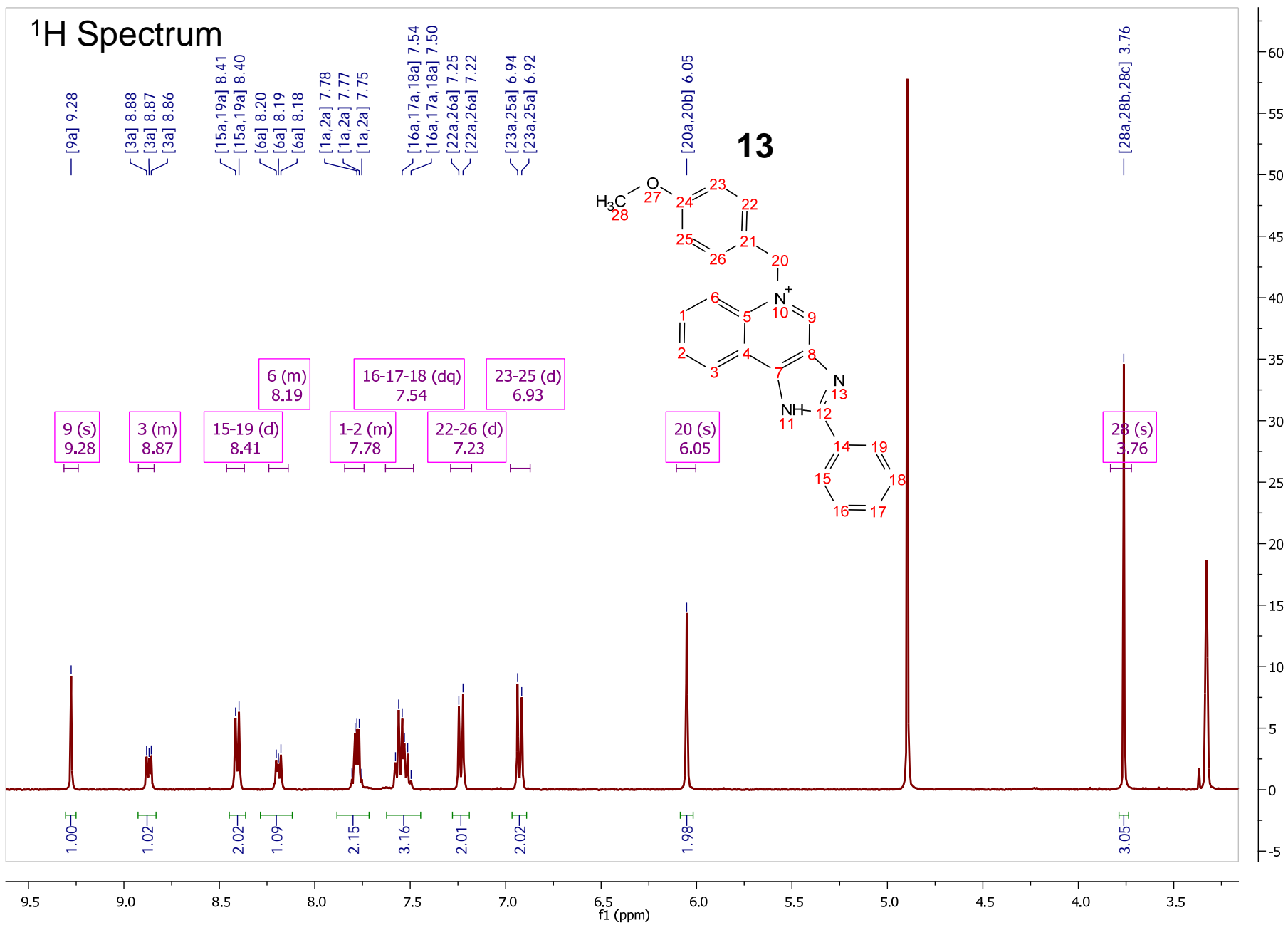




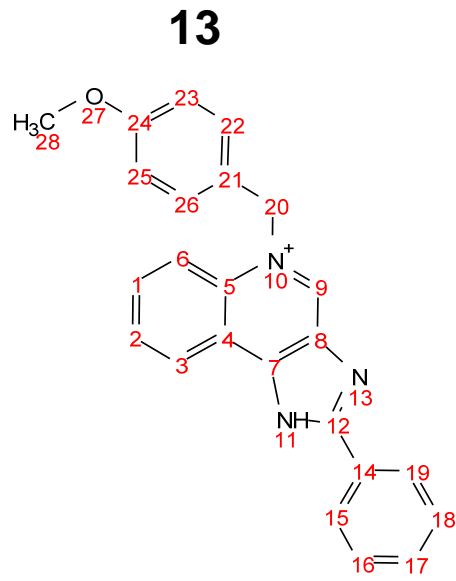
# 2D-NOESY Spectrum of Compound 12



# <sup>1</sup>H Spectrum



# <sup>13</sup>C Spectrum



— 159.99

— 138.62

— 137.14

— 133.69

— 128.37

— 126.66

— 123.91

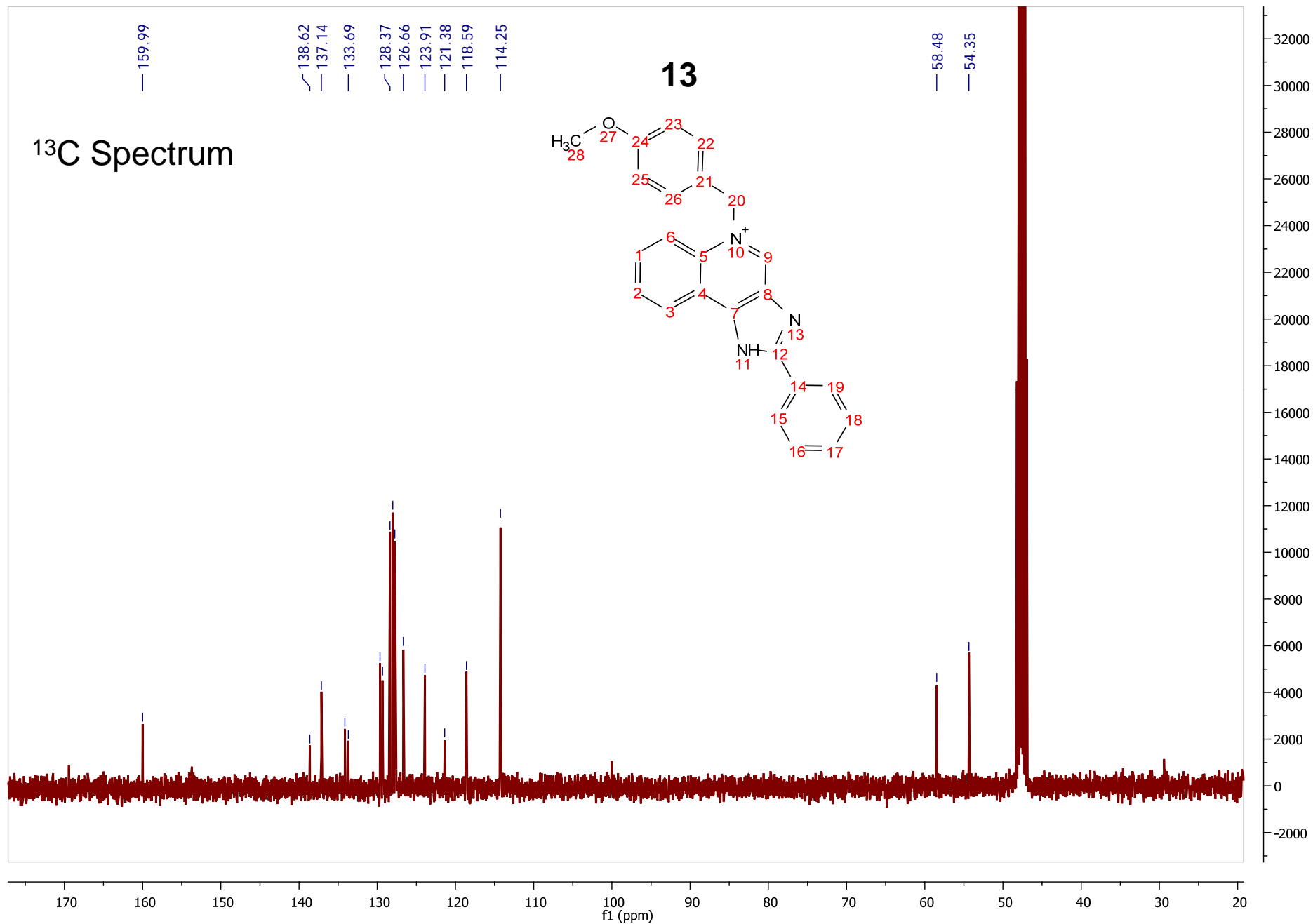
— 121.38

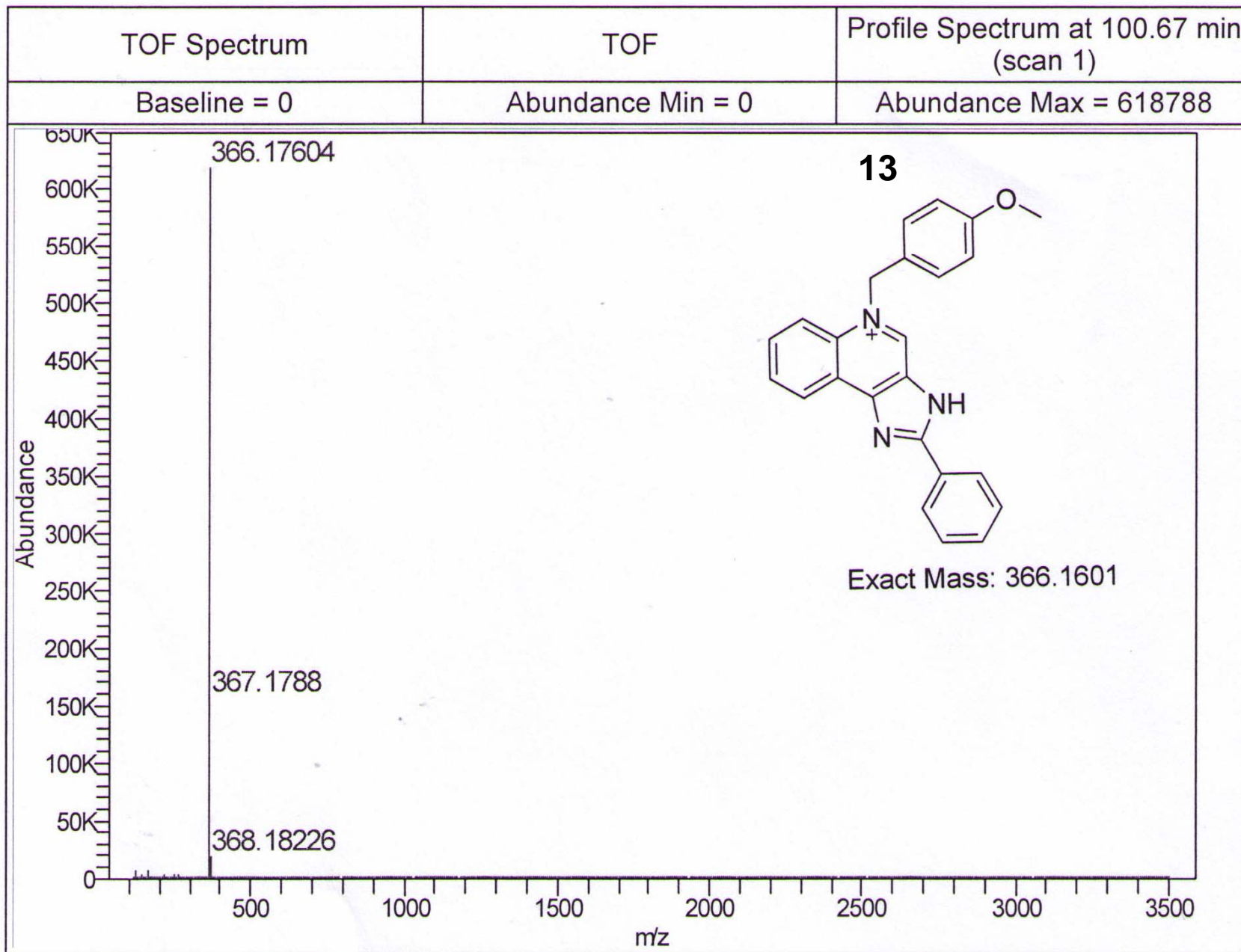
— 118.59

— 114.25

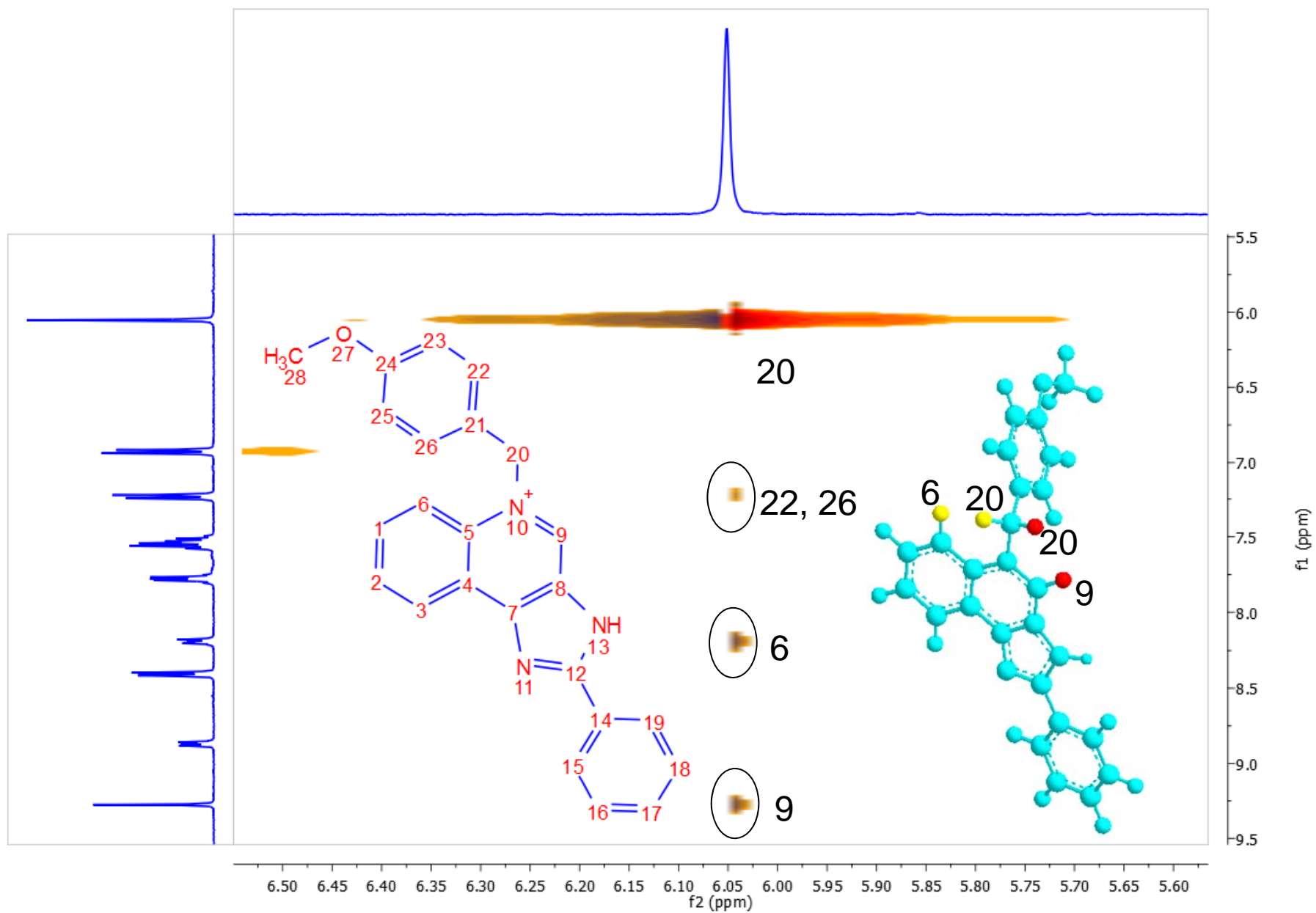
— 58.48

— 54.35

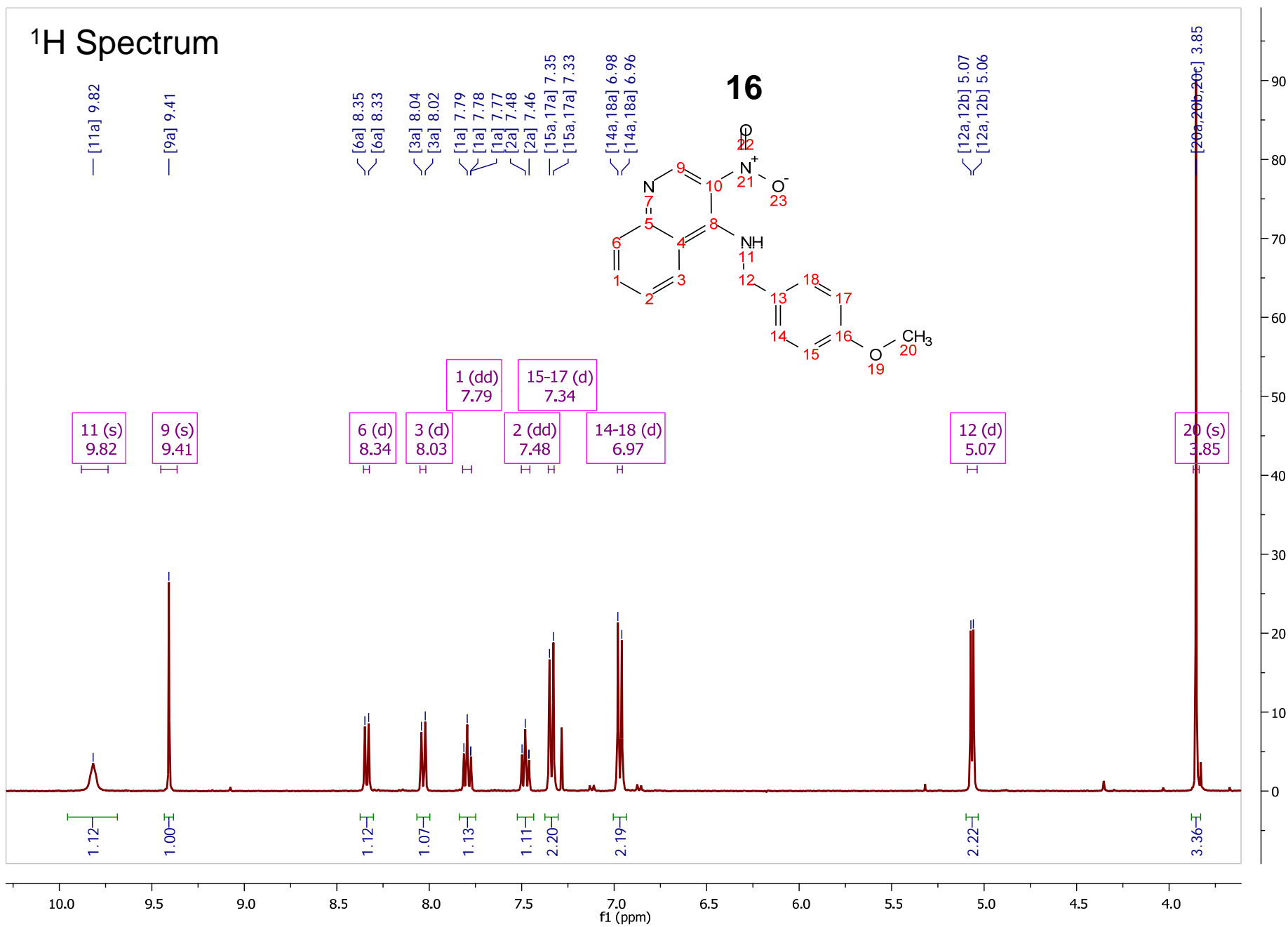




# 2D-NOESY Spectrum of Compound 13

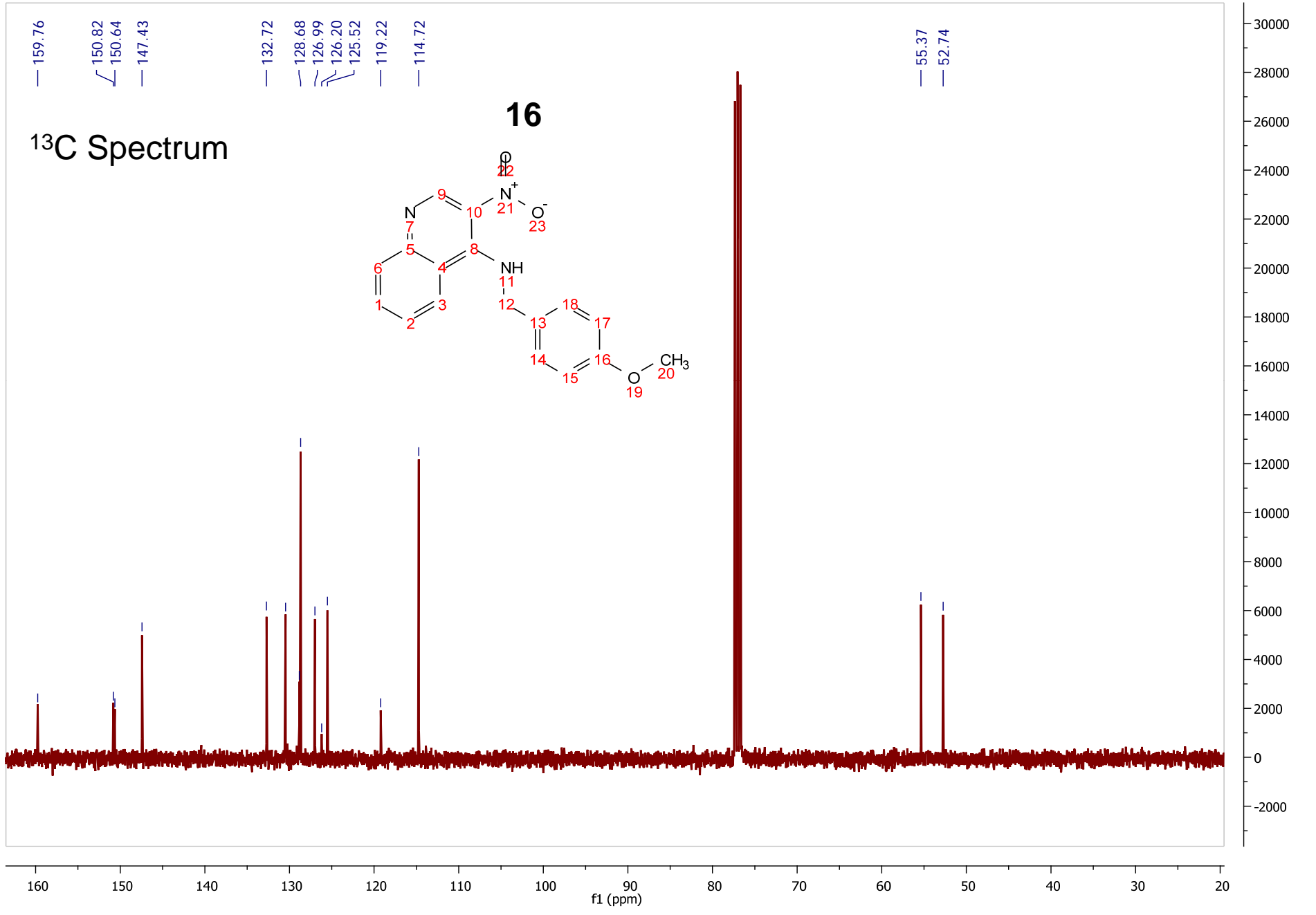
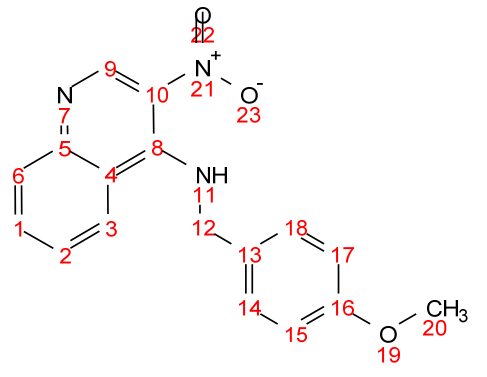


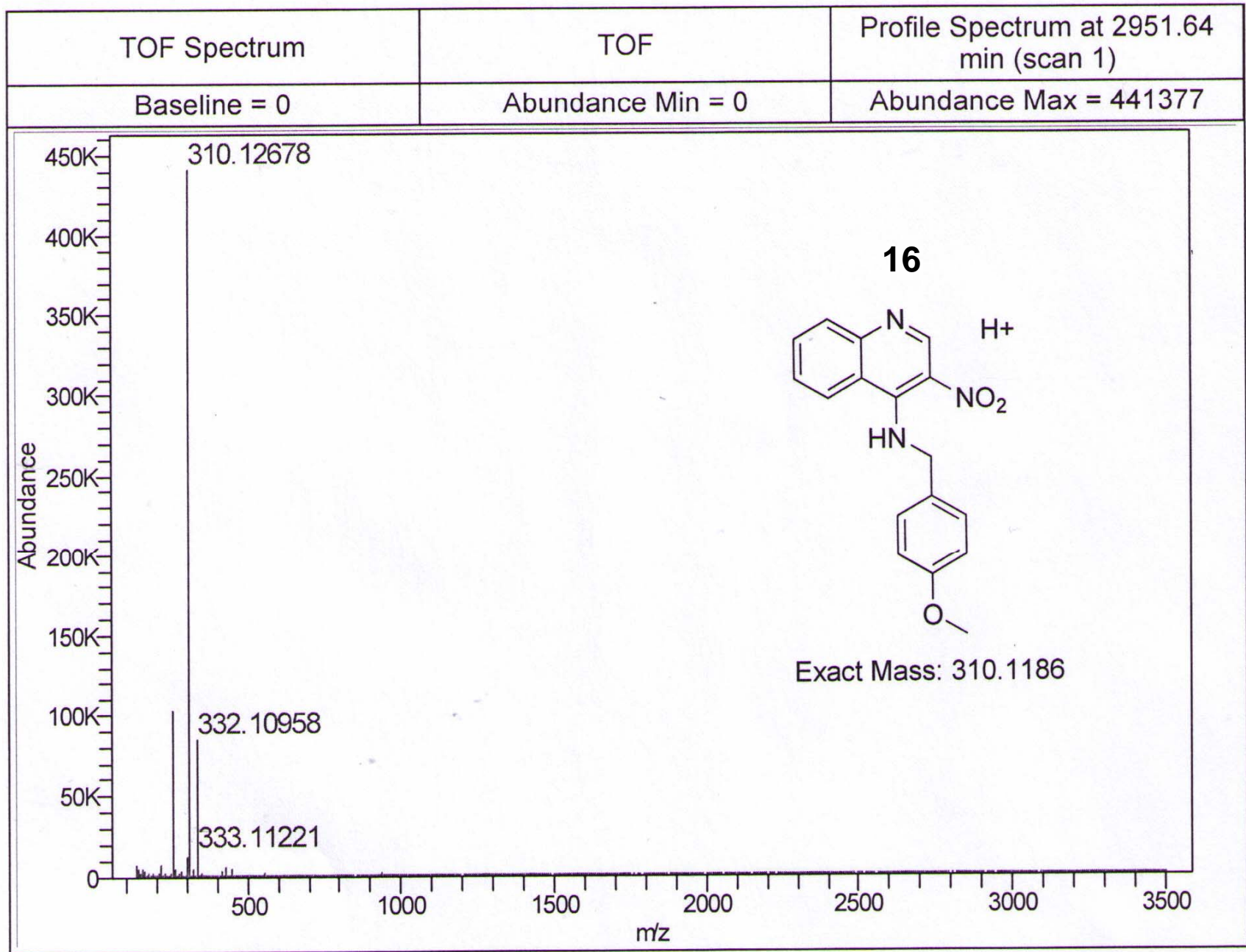
# <sup>1</sup>H Spectrum



# <sup>13</sup>C Spectrum

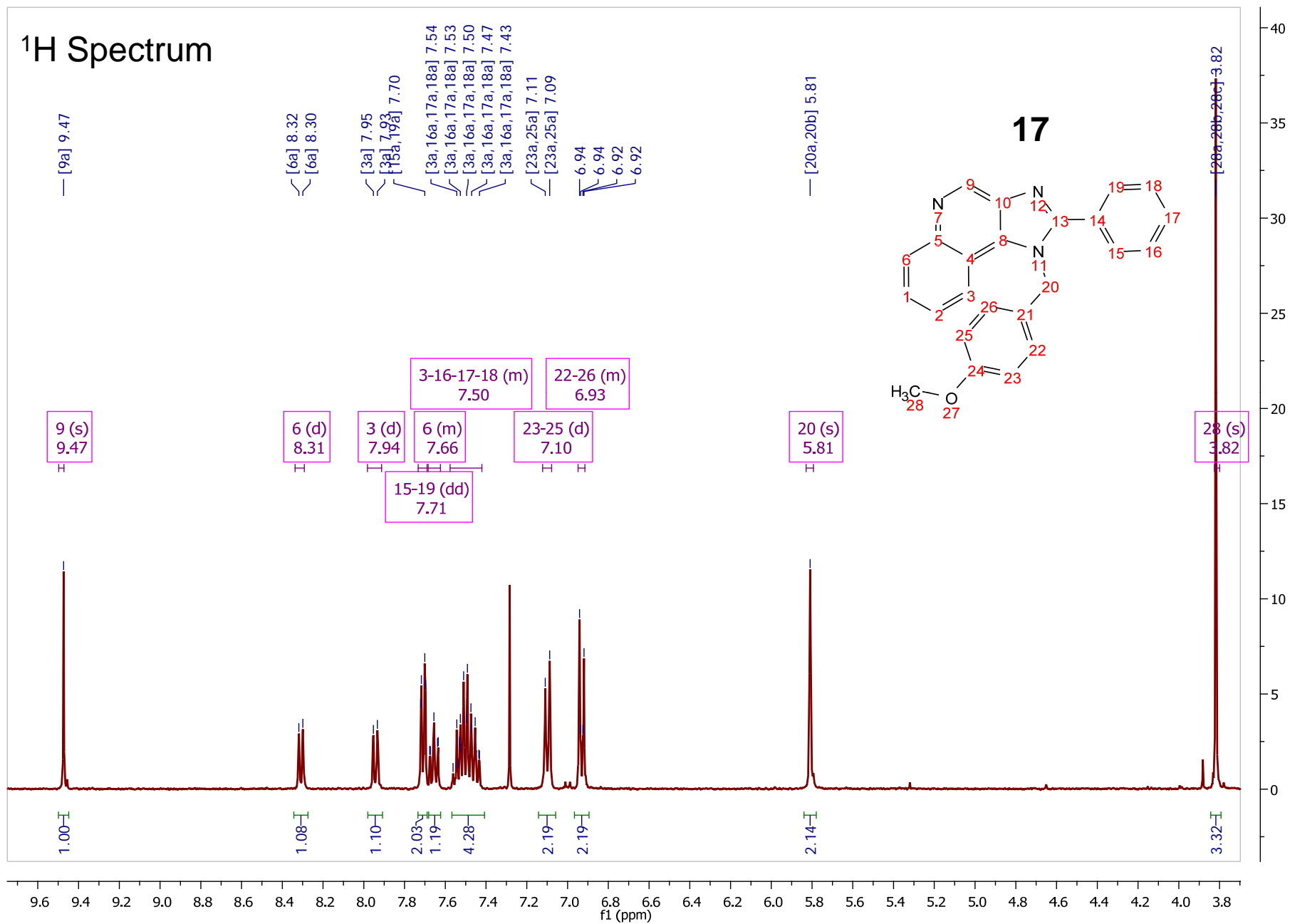
**16**





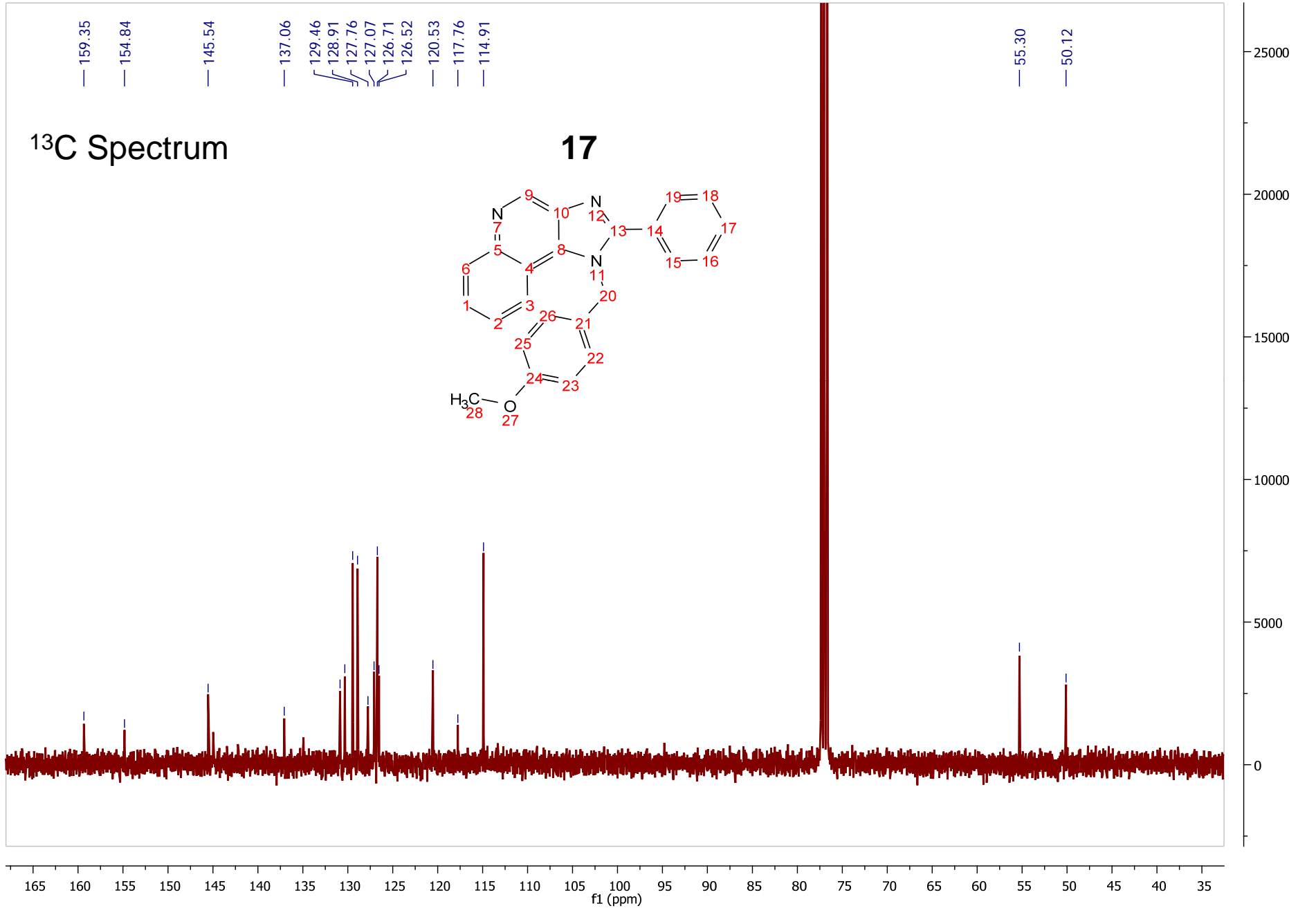
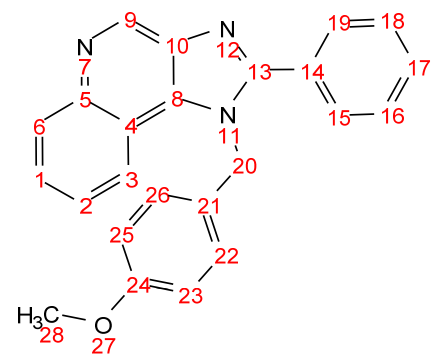


# <sup>1</sup>H Spectrum

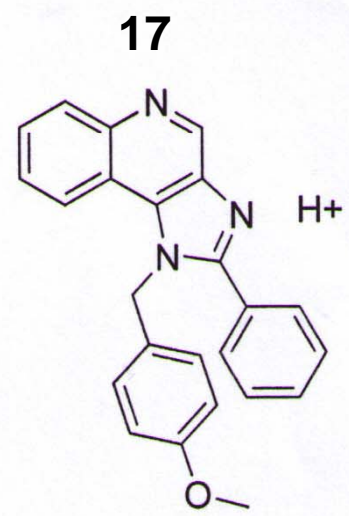
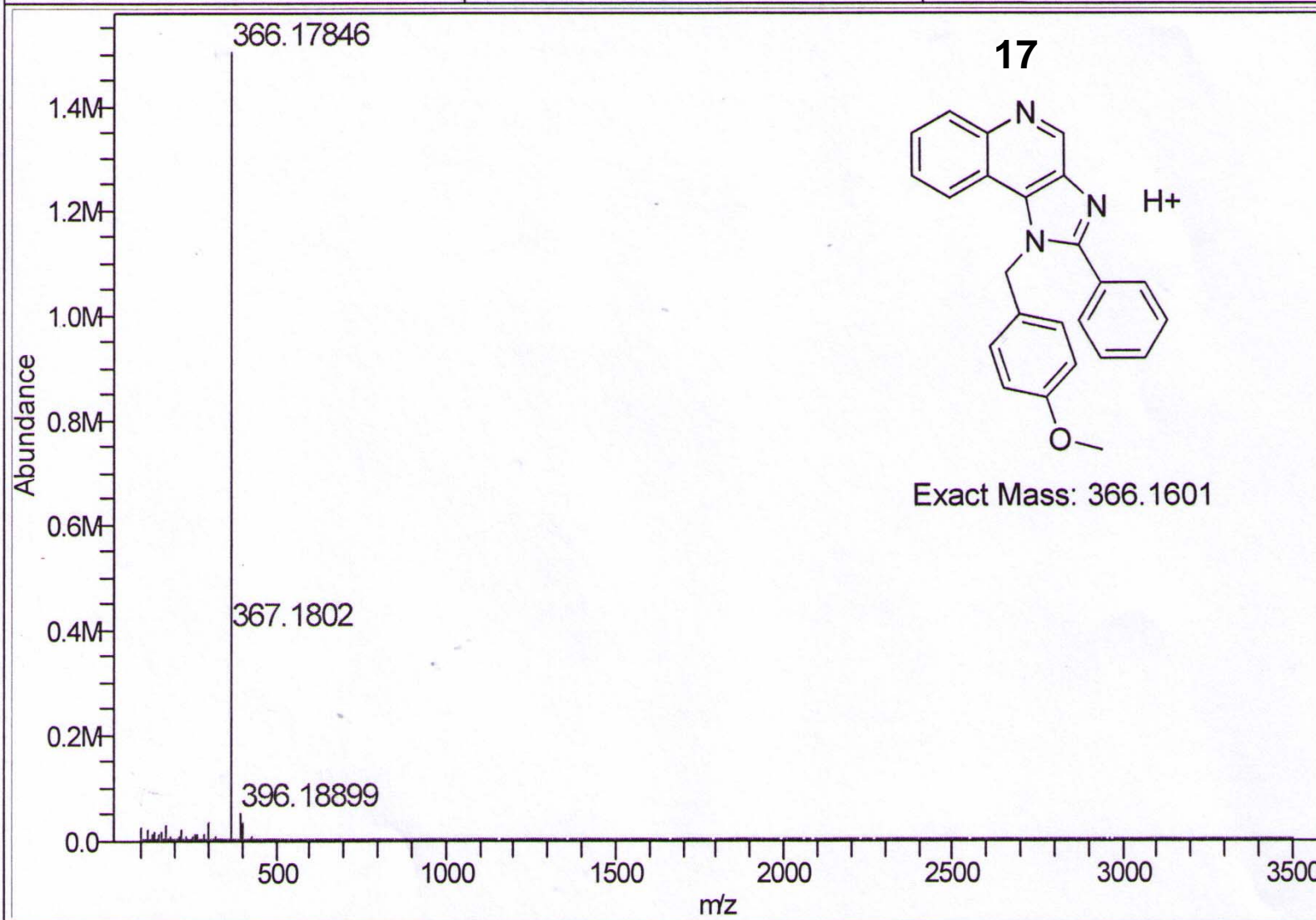


# <sup>13</sup>C Spectrum

## 17

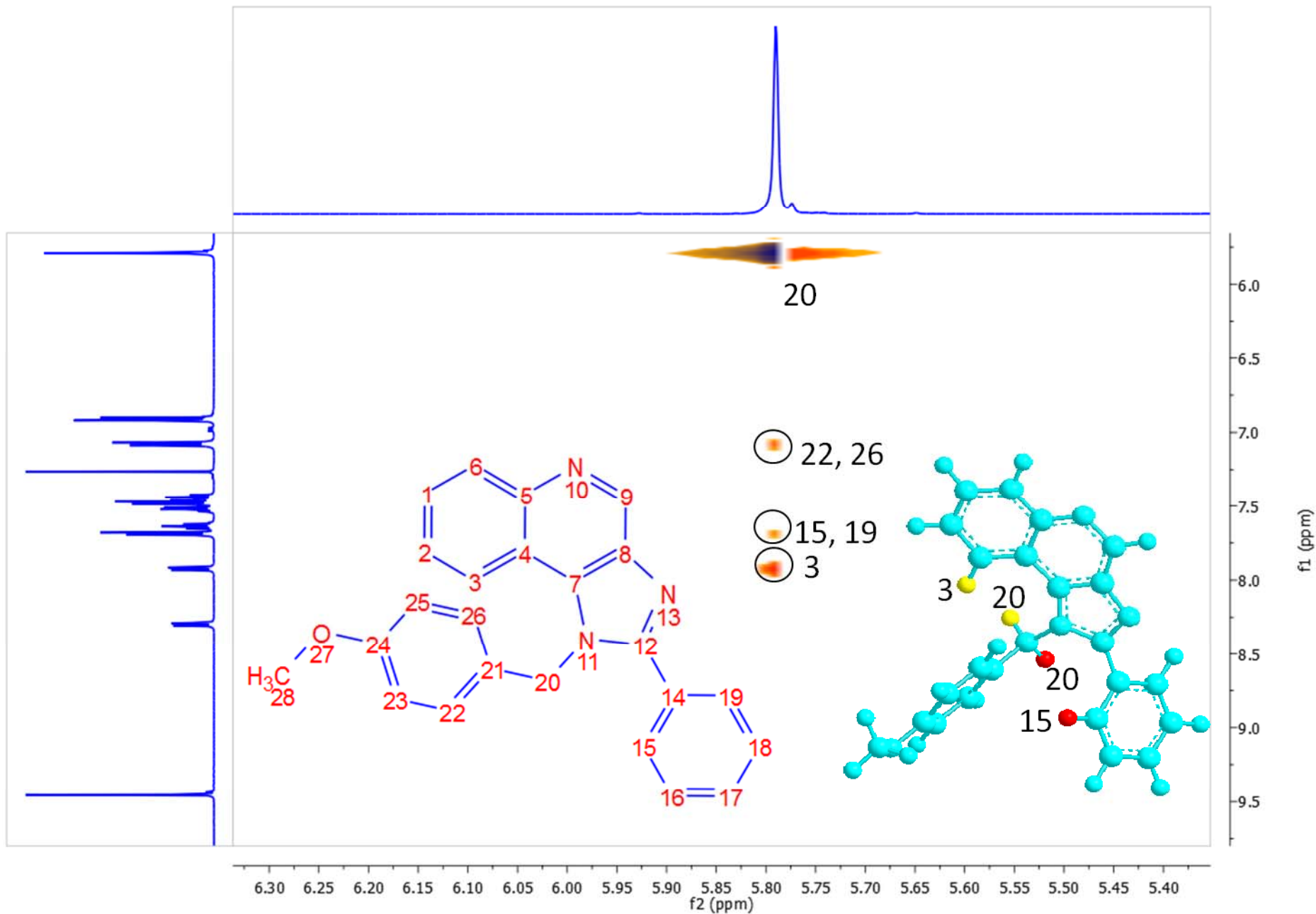


TOF Spectrum	TOF	Profile Spectrum at 132.53 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 1505805

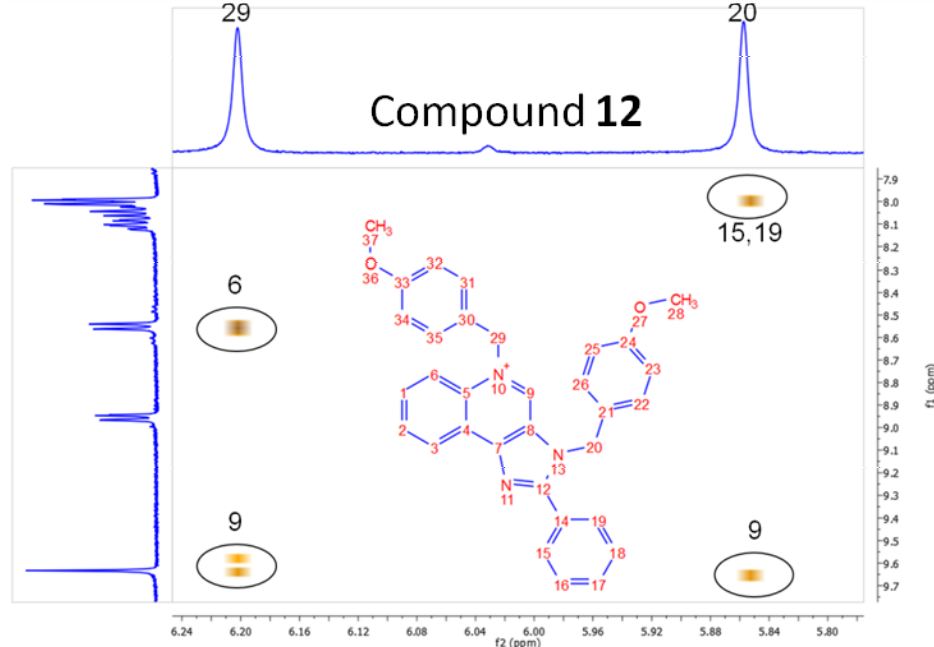
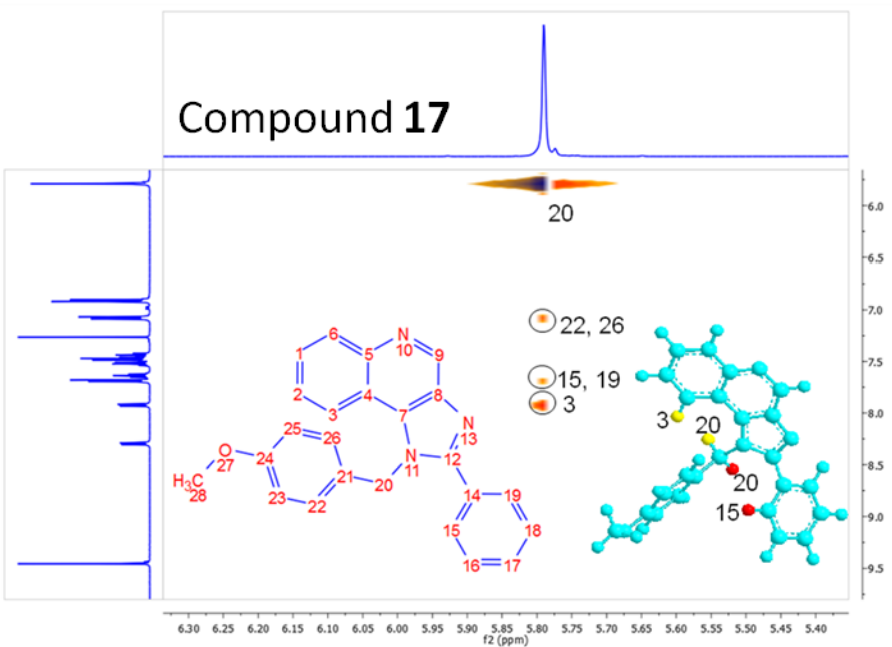
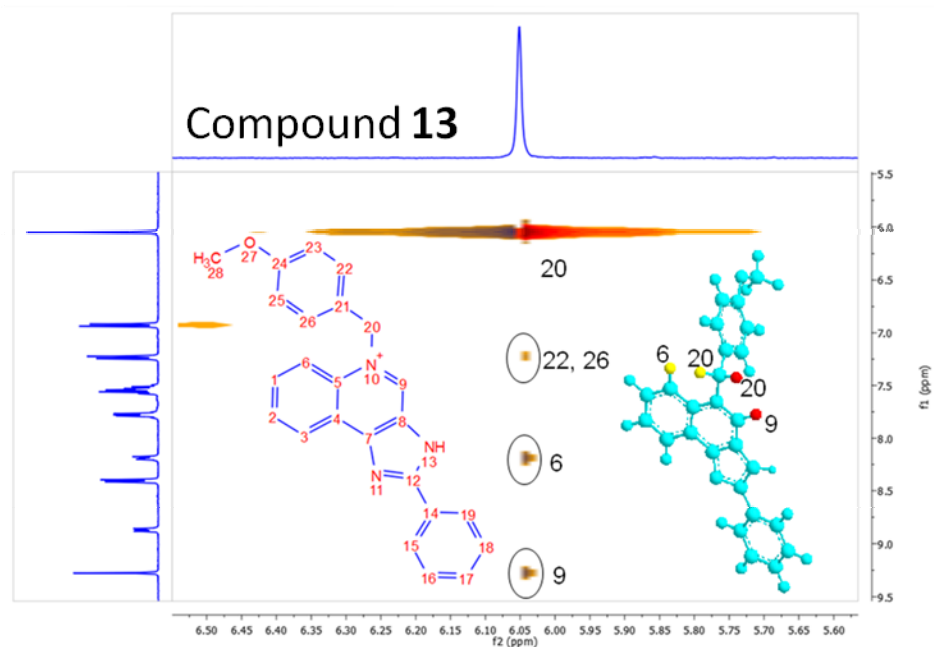
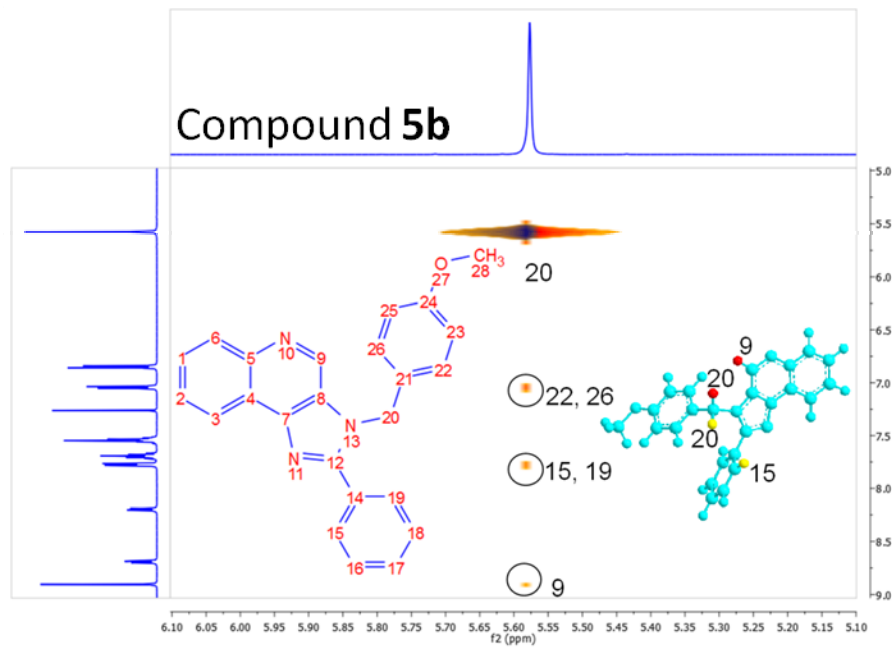


Exact Mass: 366.1601

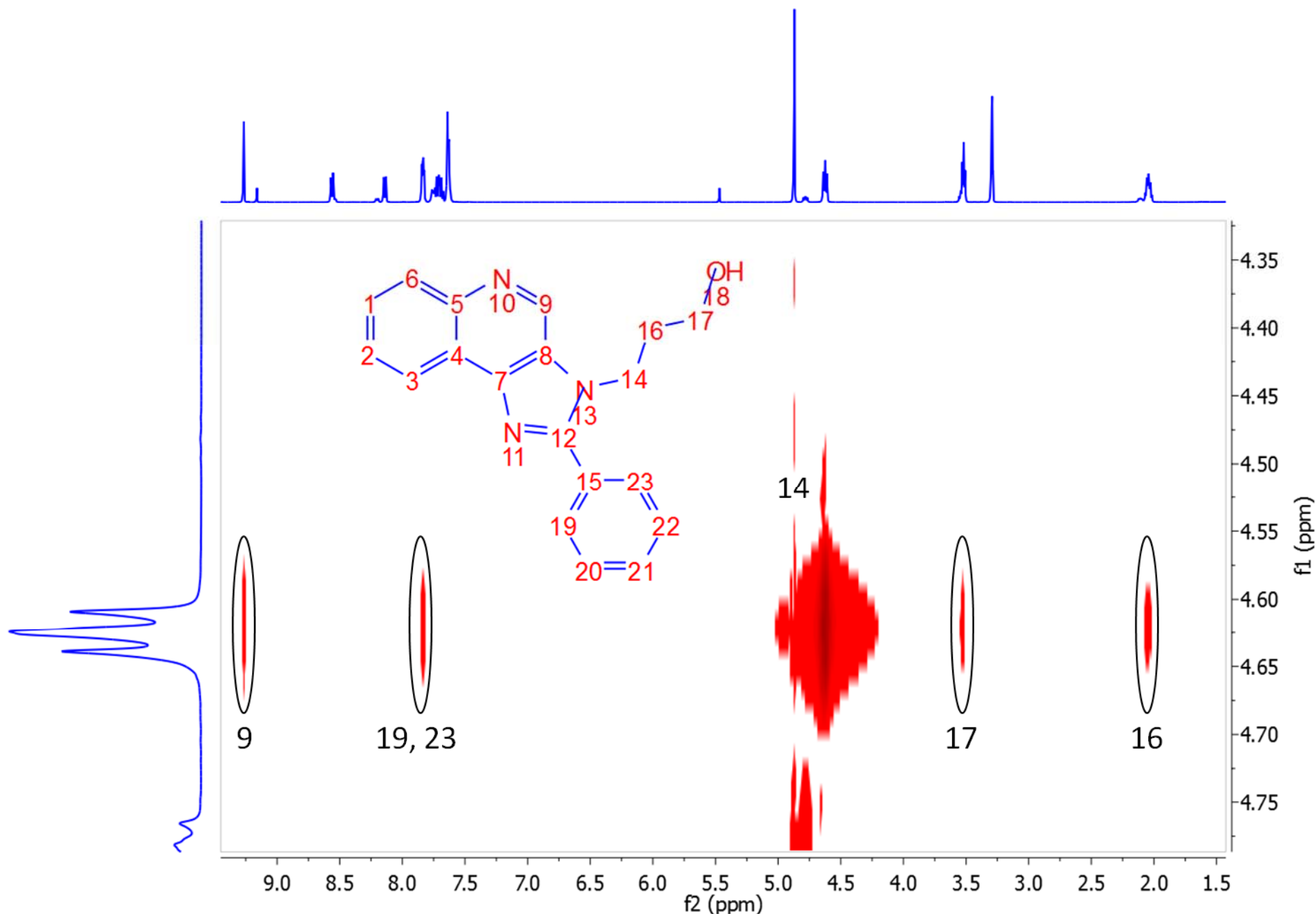
# 2D-NOESY Spectrum of Compound 17



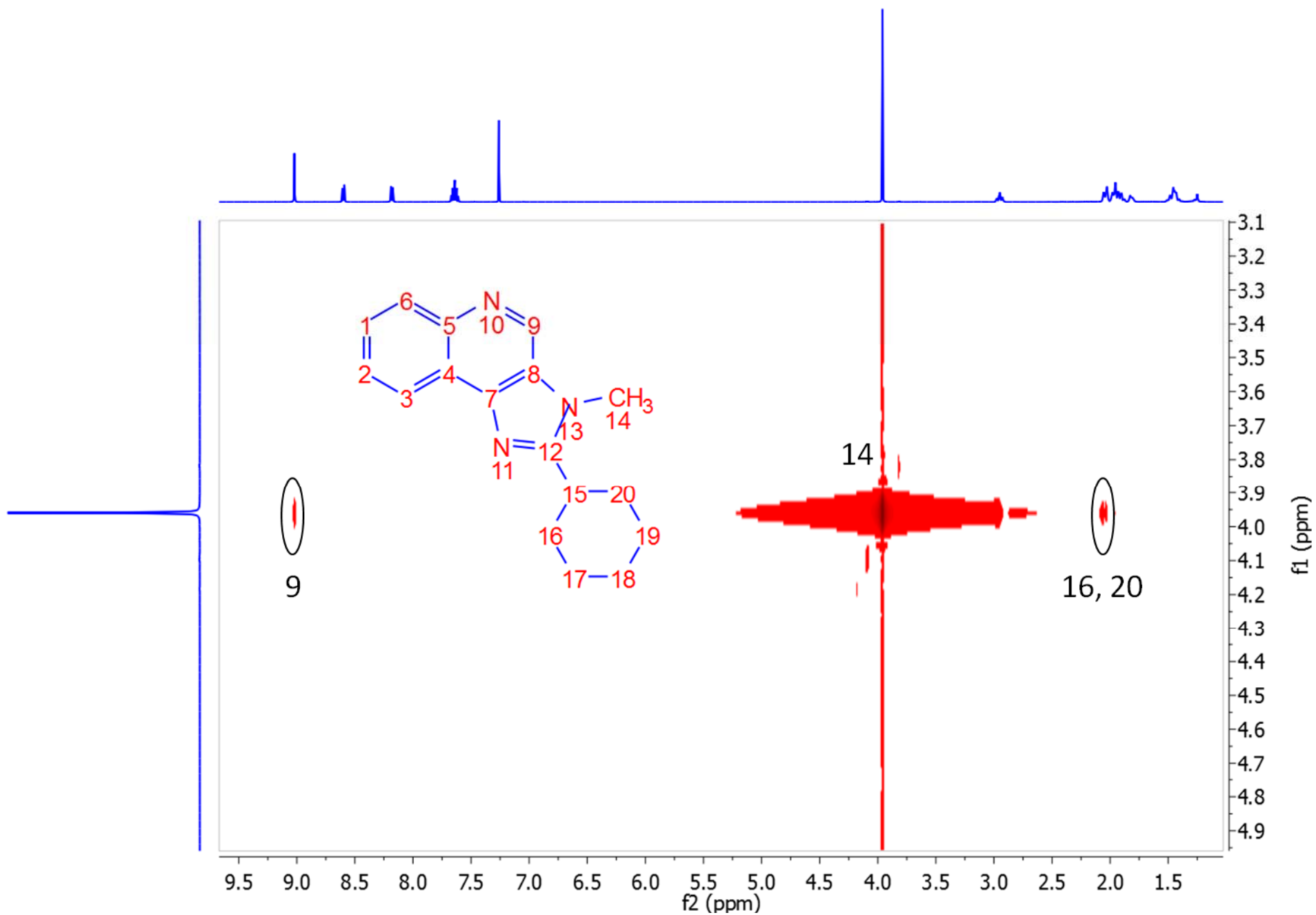
## 2D-NOESY Spectra of Compounds 5b, 13, 17 and 12



# 2D-NOESY Spectrum of Compound **6b**



# 2D-NOESY Spectrum of Compound **8c**



# 2D-NOESY Spectrum of Compound 7d

