

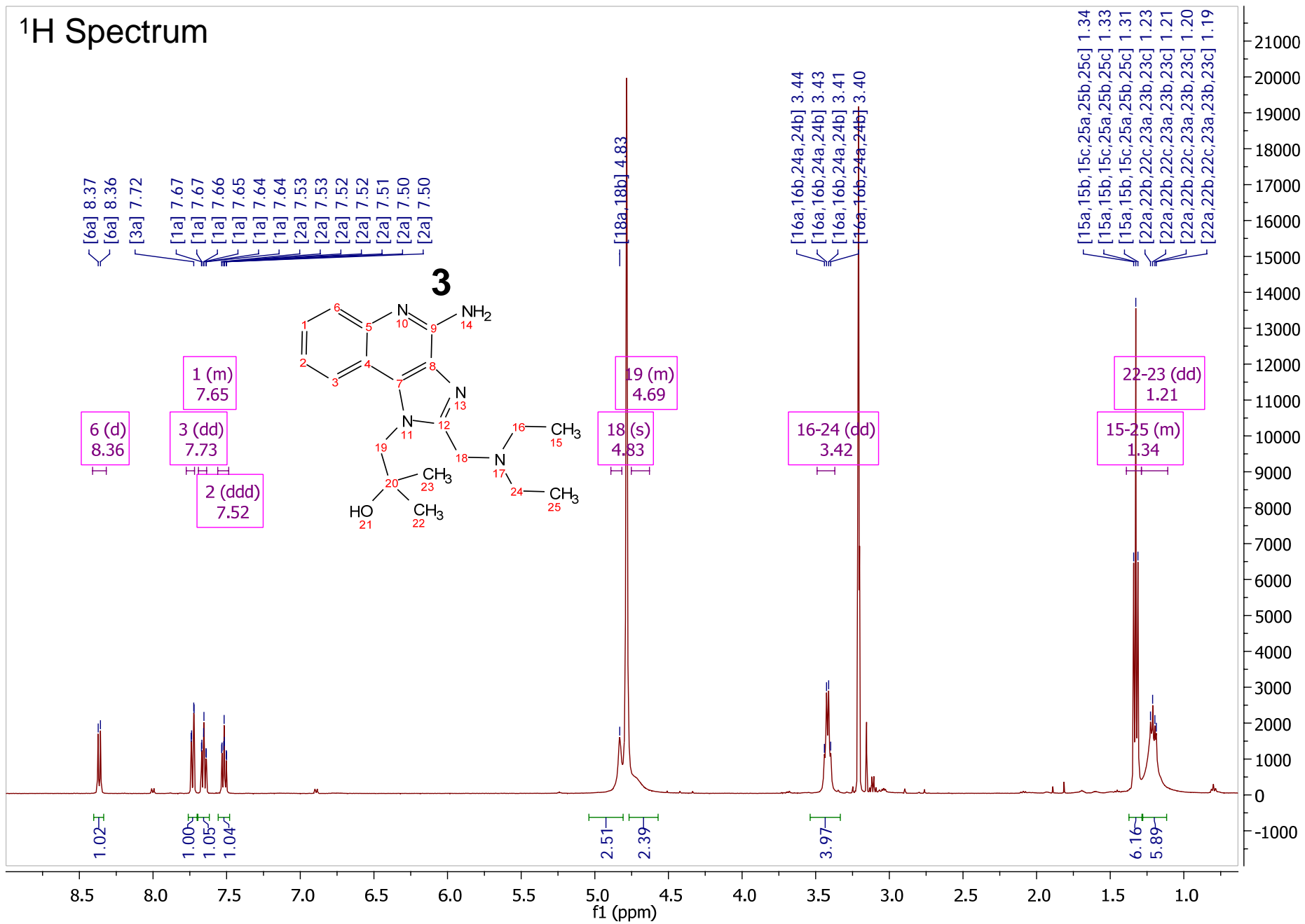
# Supporting Information

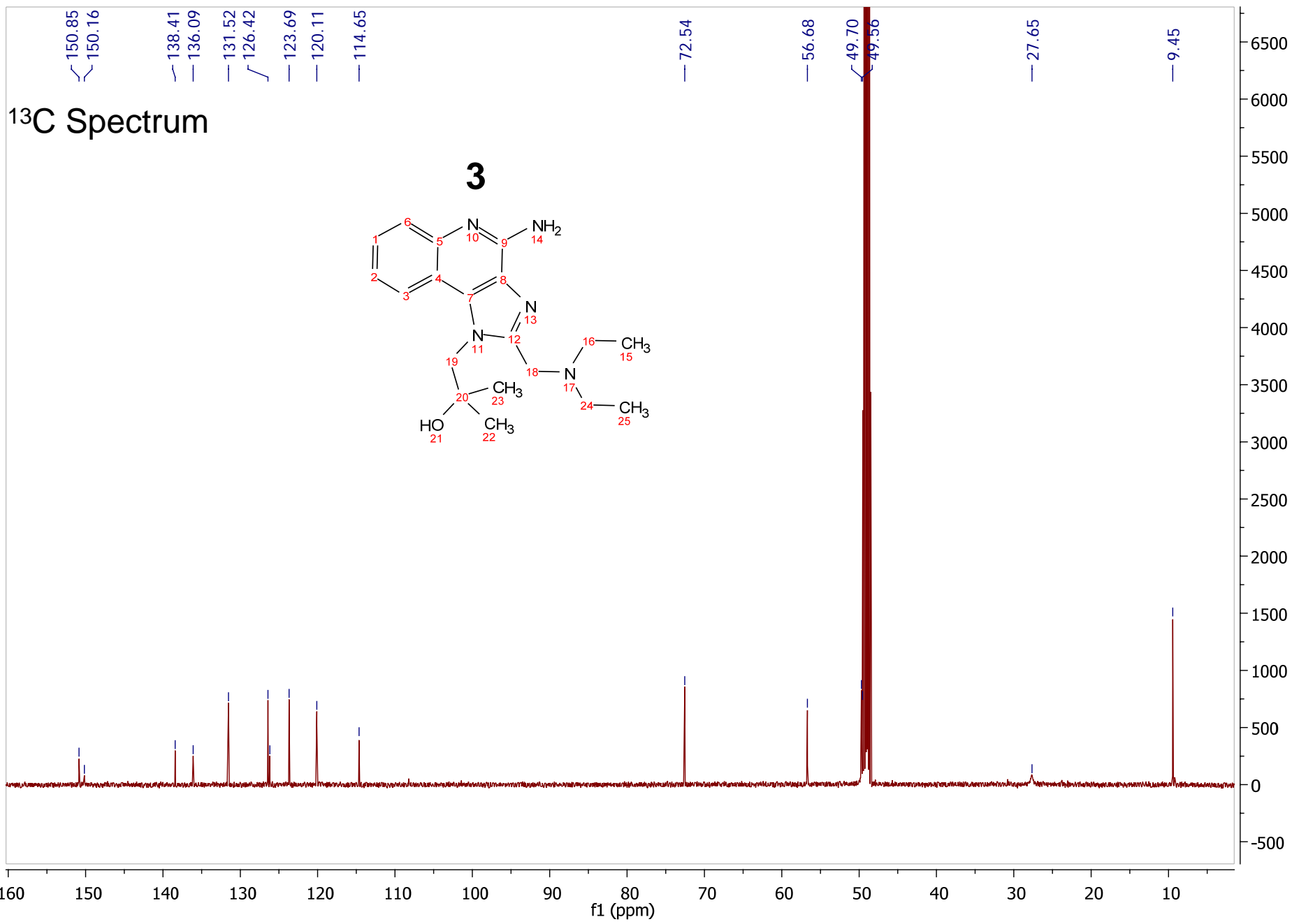
## **Structure-Activity Relationships in Human Toll-like Receptor 7-Active Imidazoquinoline Analogues**

**Nikunj M. Shukla, Subbalakshmi S. Malladi, Cole A. Mutz,  
Rajalakshmi Balakrishna, and Sunil A. David\***

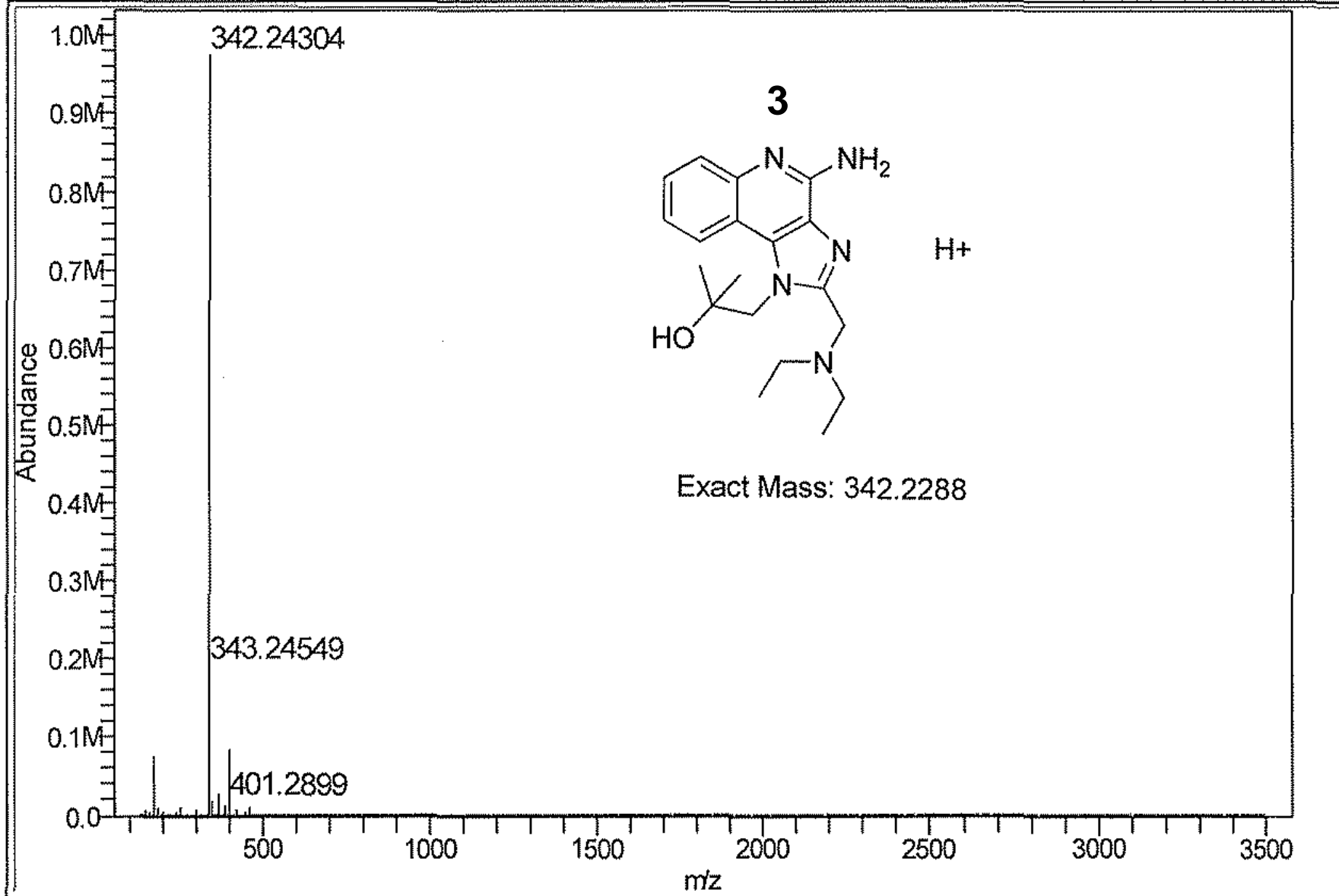
Department of Medicinal Chemistry,  
University of Kansas.

# <sup>1</sup>H Spectrum





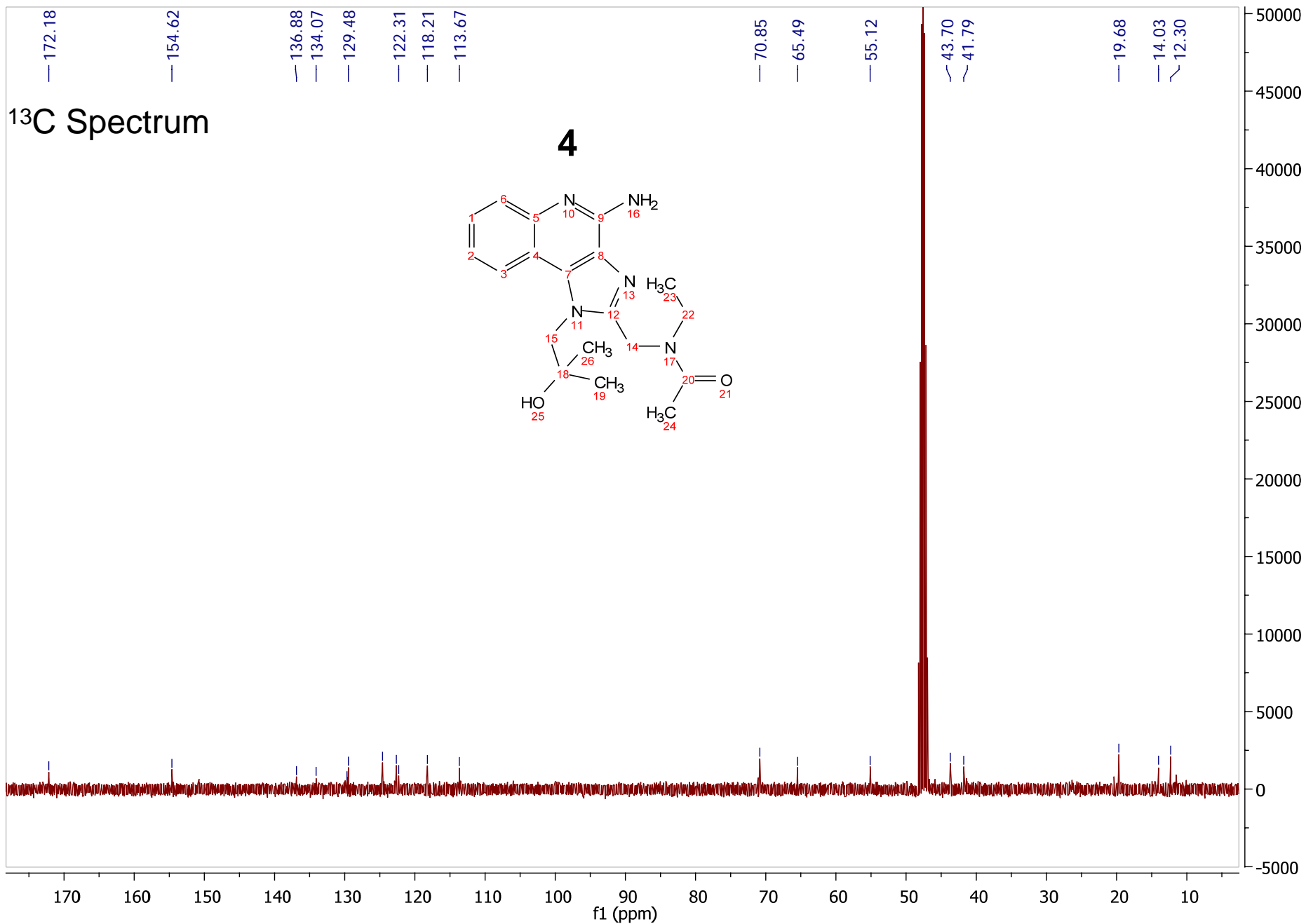
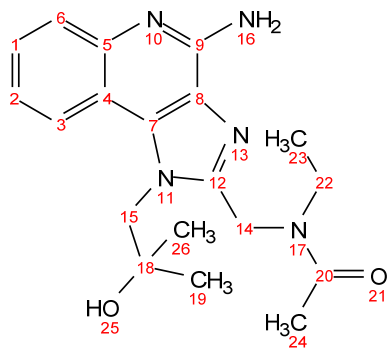
TOF Spectrum	TOF	Profile Spectrum at 9932.92 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 976201



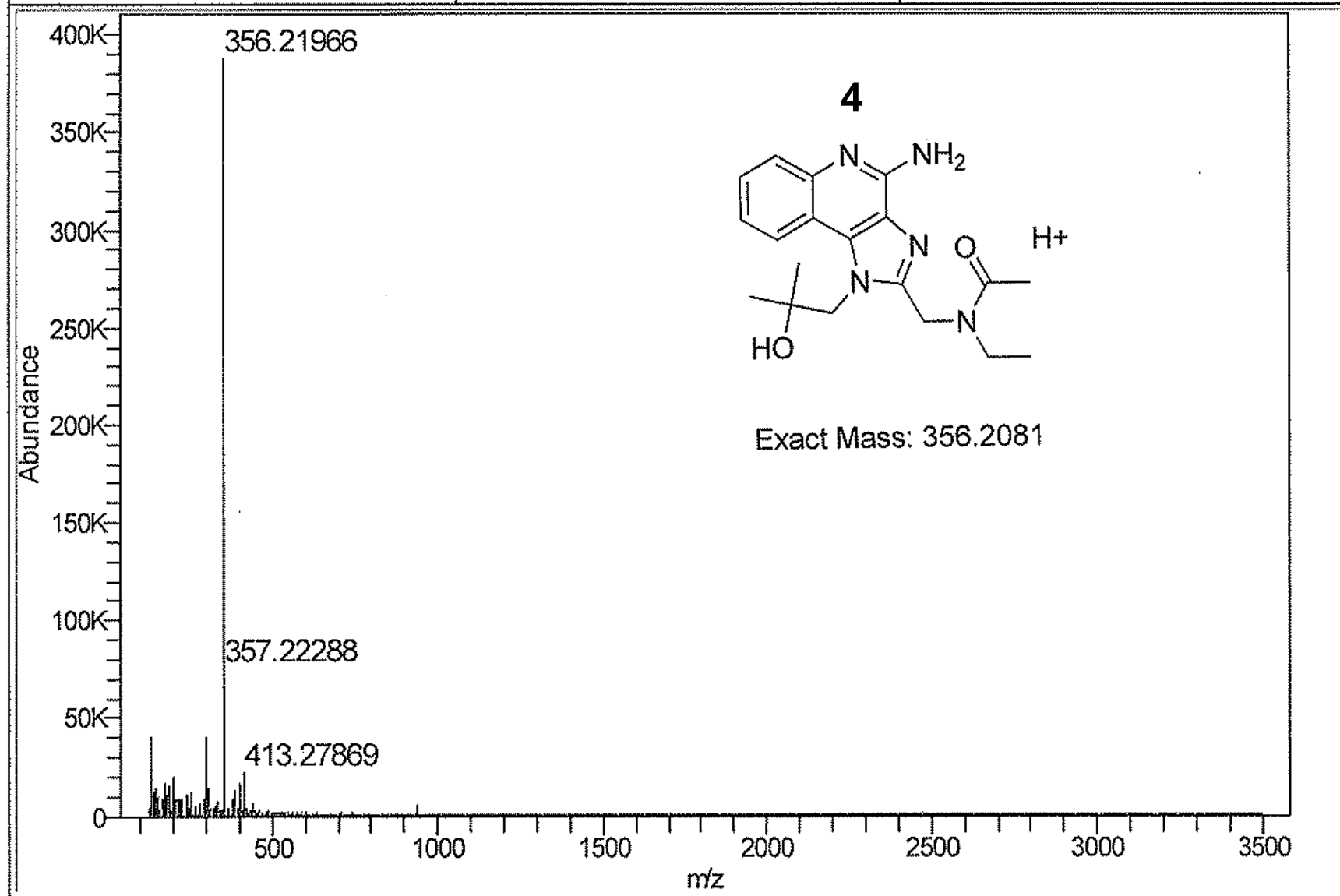


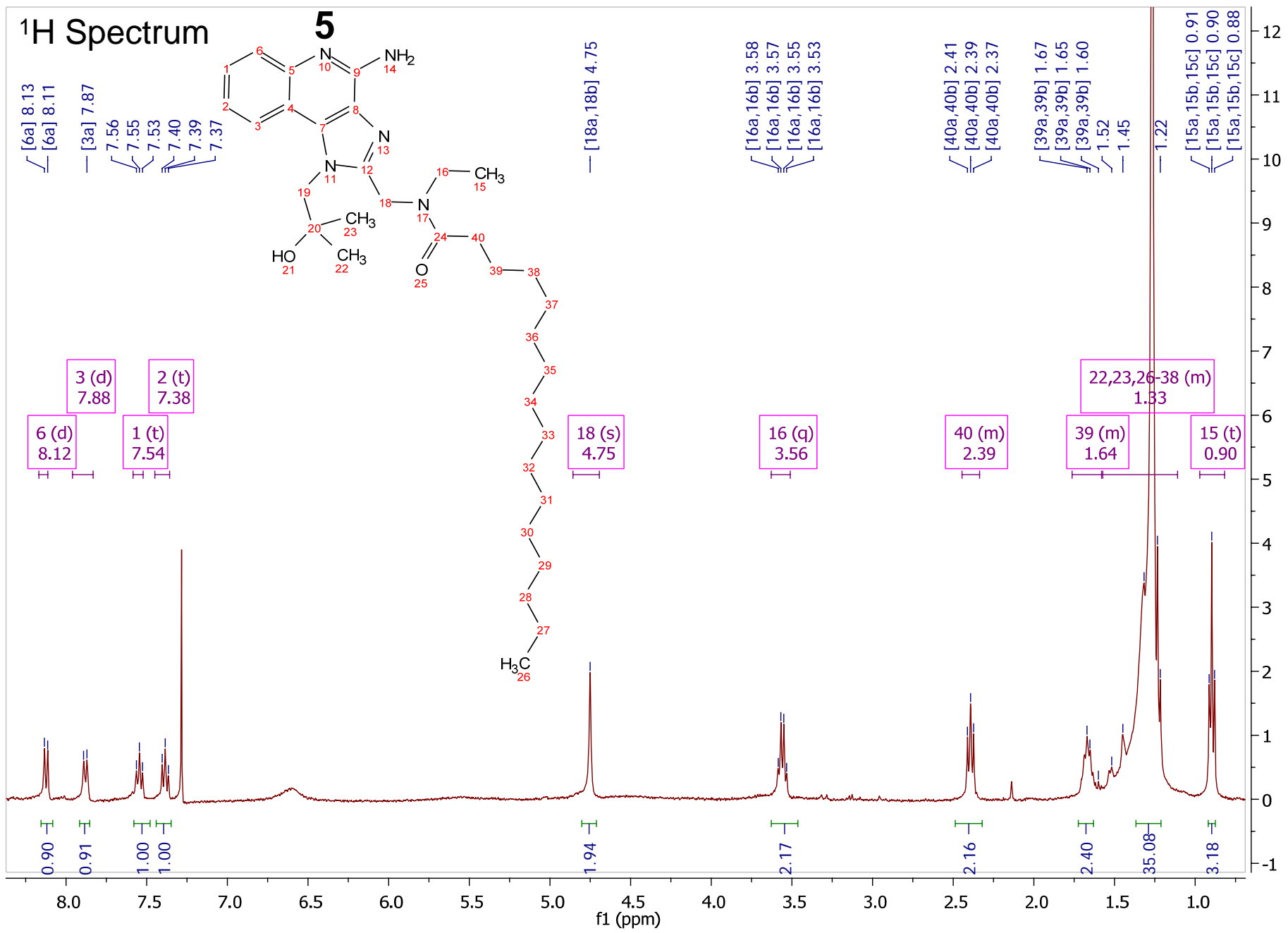
# <sup>13</sup>C Spectrum

4



TOF Spectrum	TOF	Profile Spectrum at 198.32 min (scan 1)
Baseline = 4.75398145947231E-02	Abundance Min = 0	Abundance Max = 388303

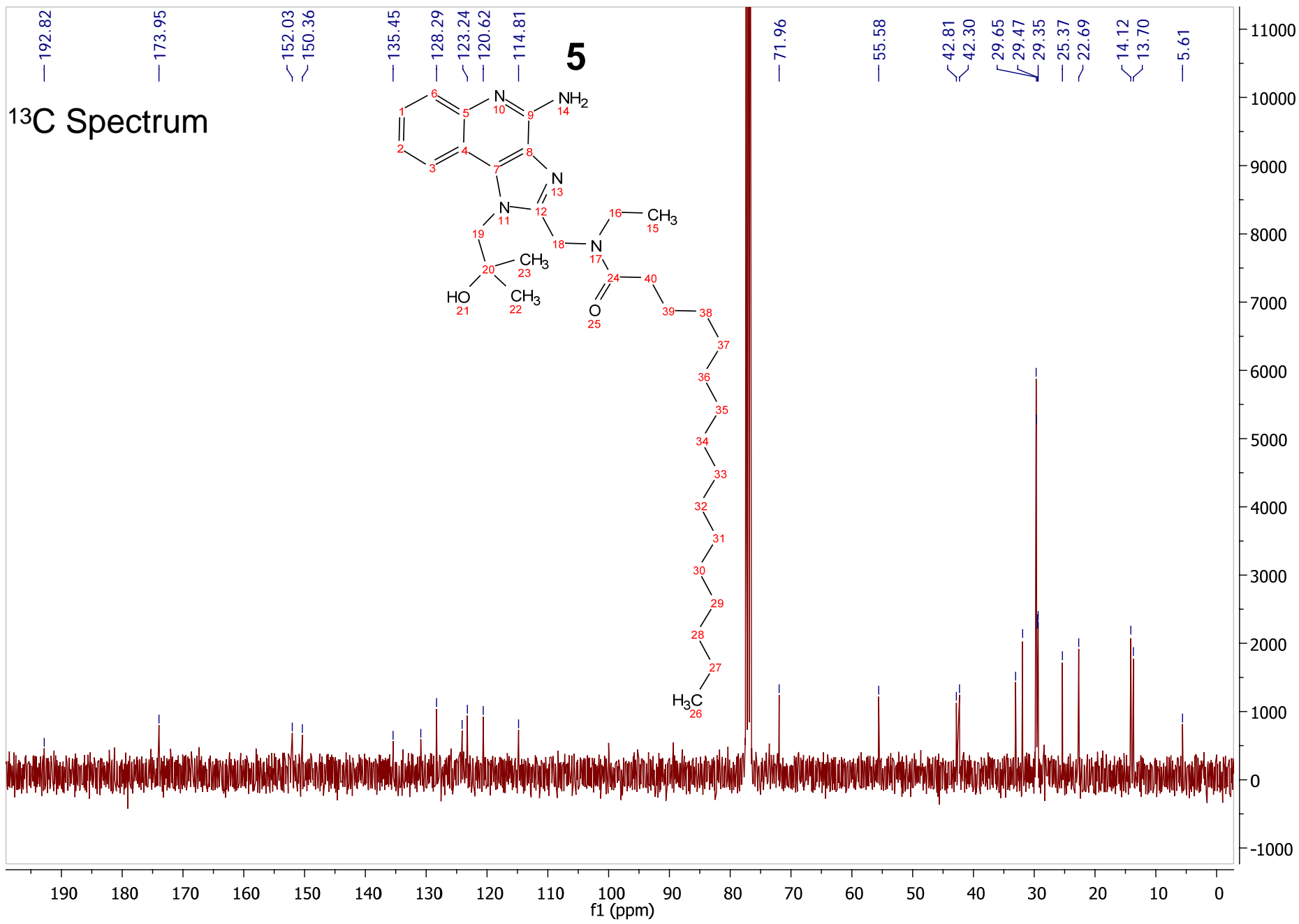
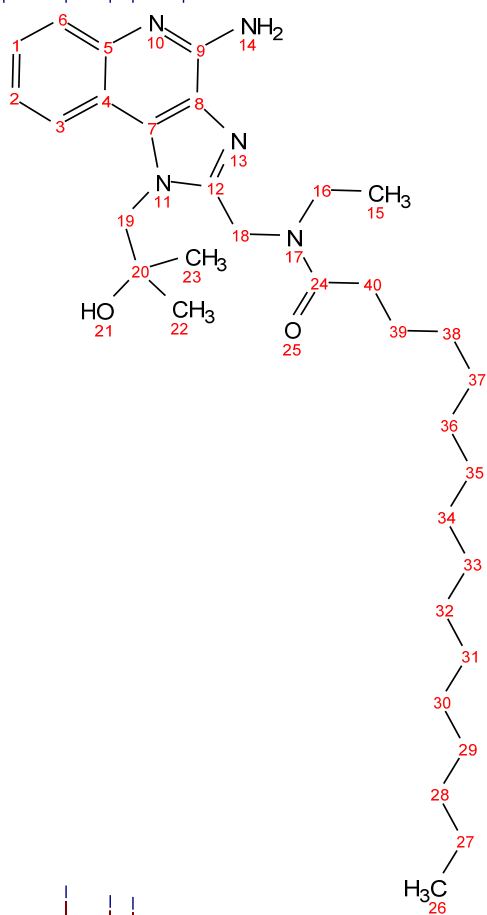


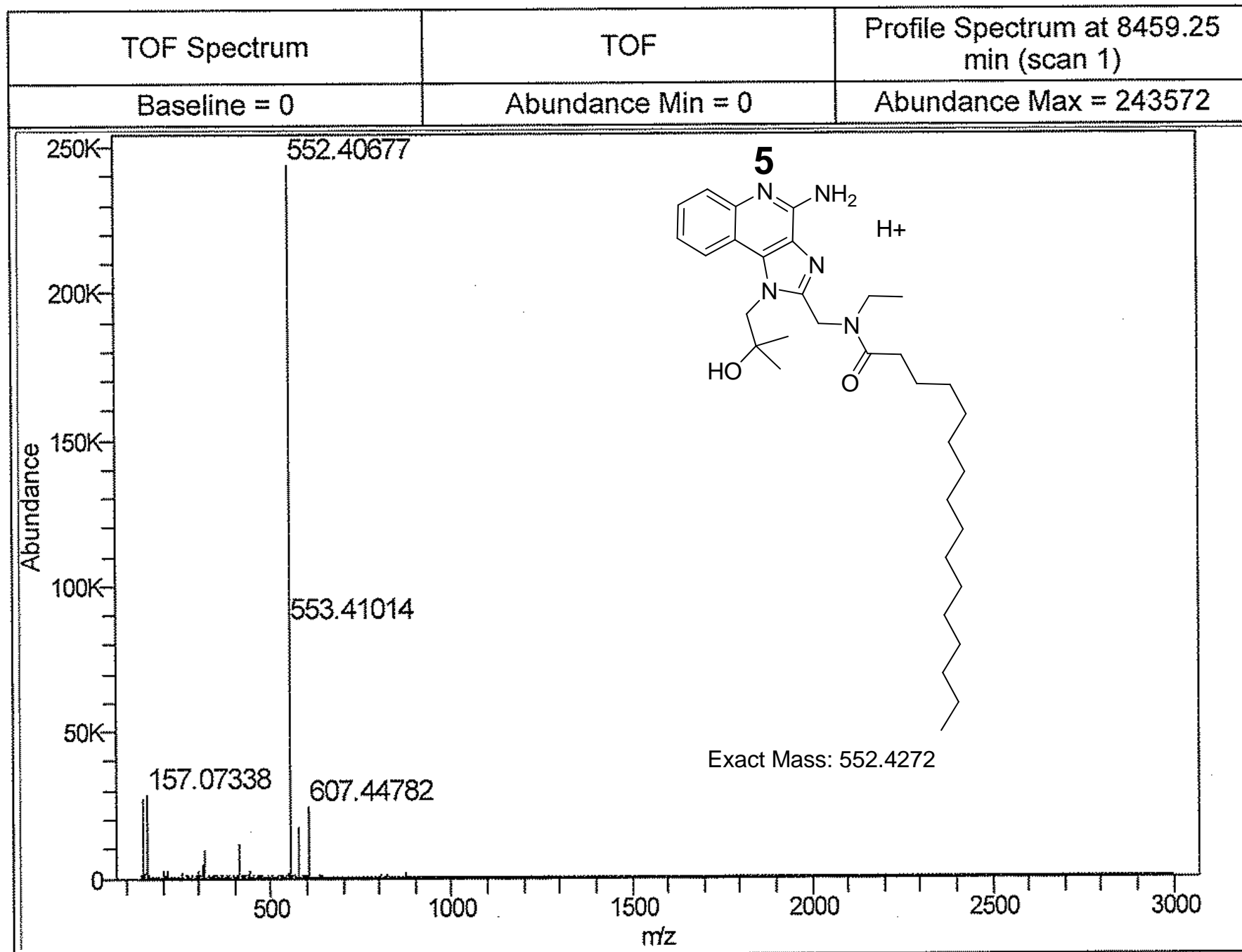




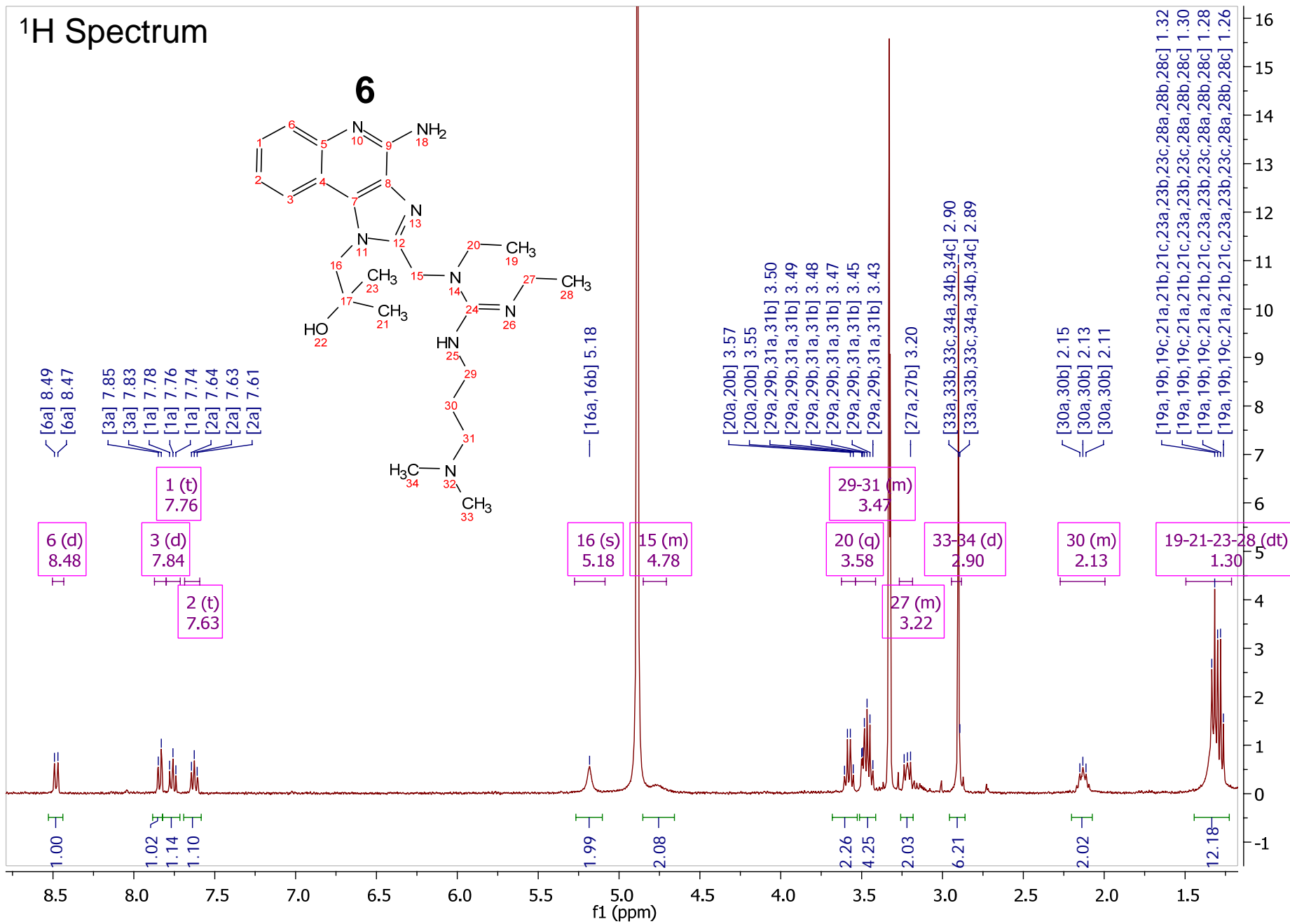
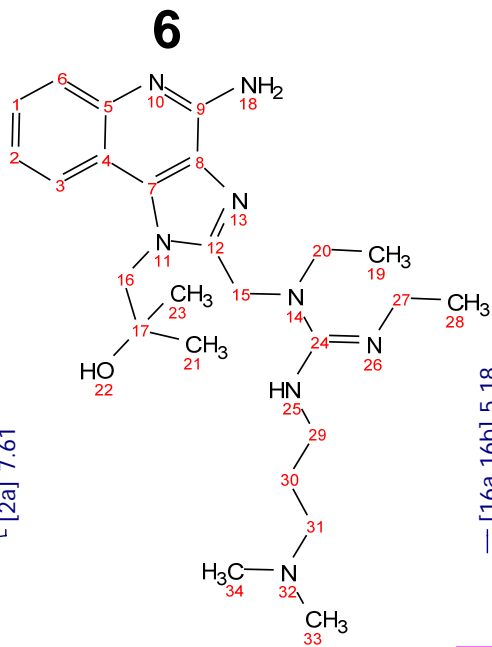
# <sup>13</sup>C Spectrum

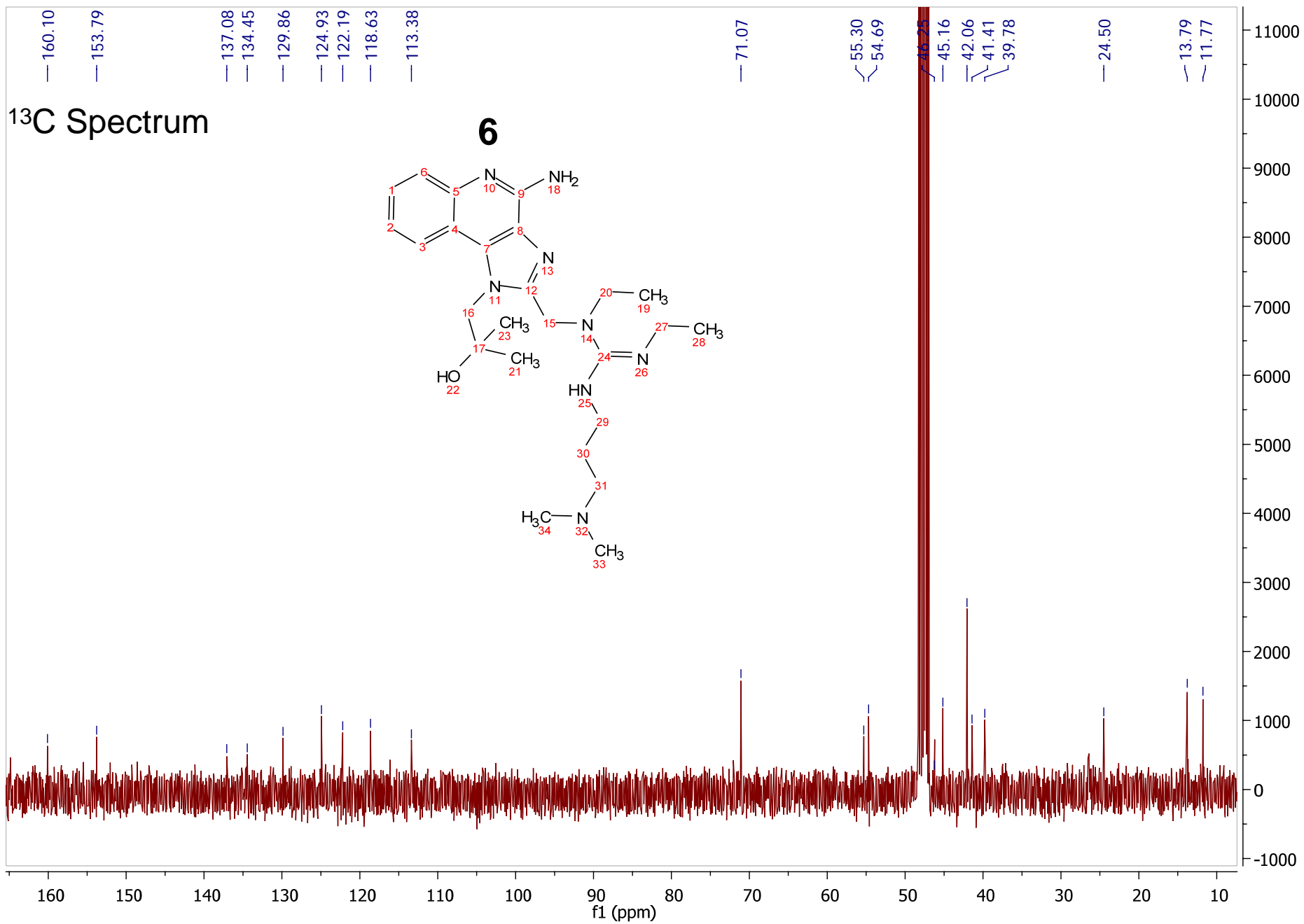
5



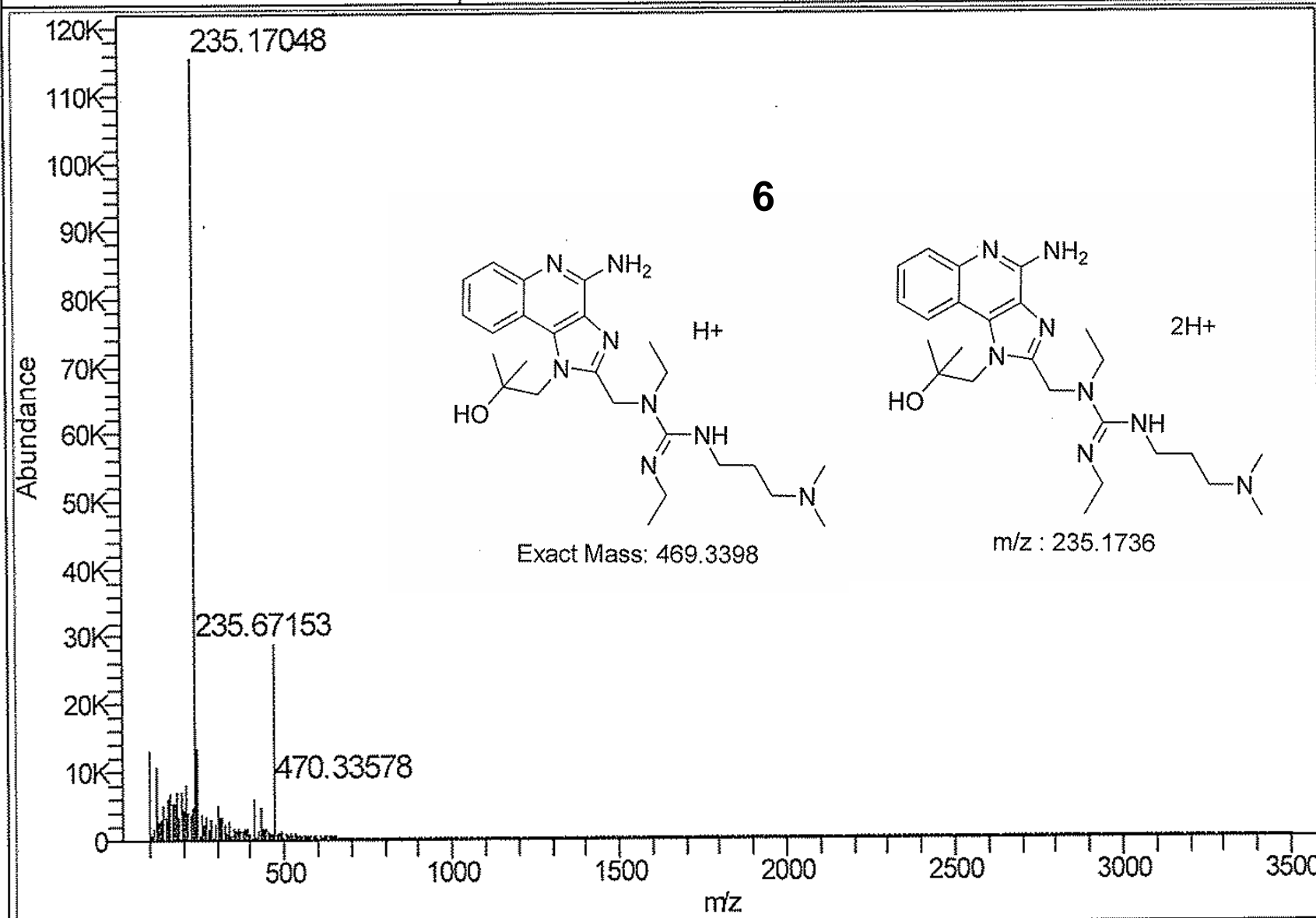


# <sup>1</sup>H Spectrum

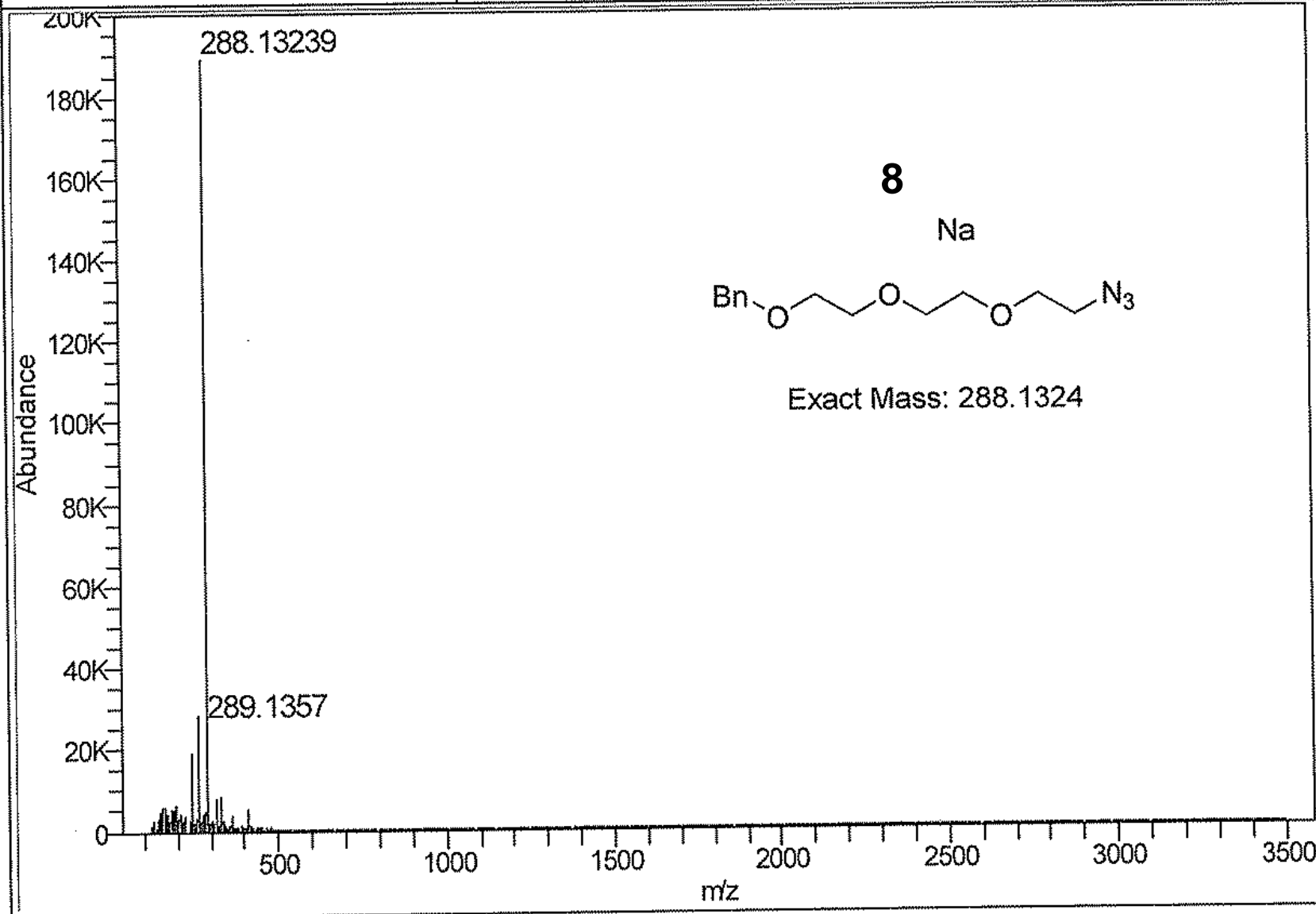




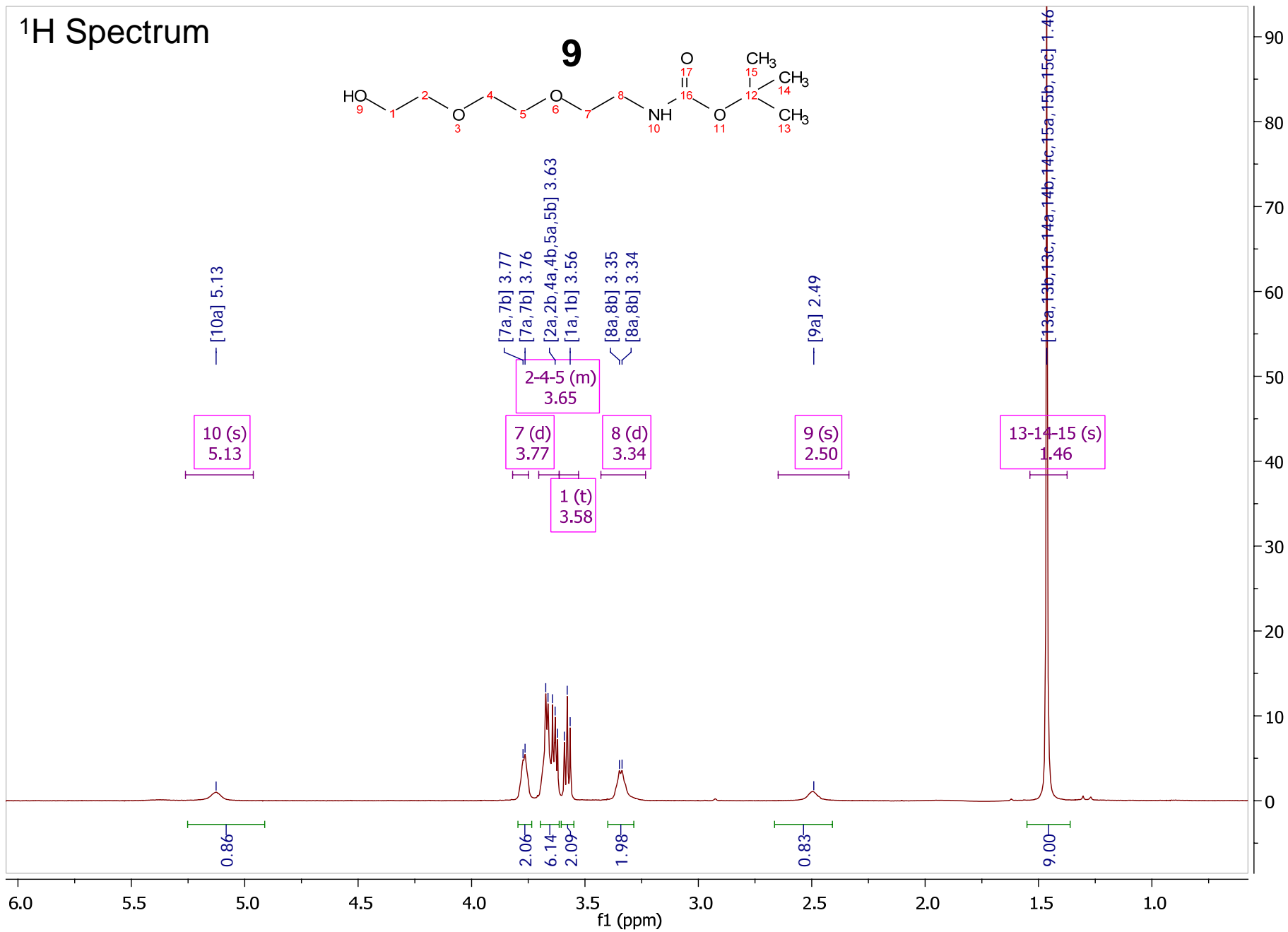
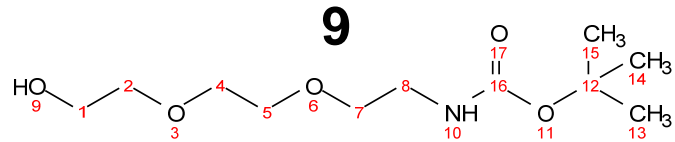
TOF Spectrum	TOF	Profile Spectrum at 3928.39 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 115884



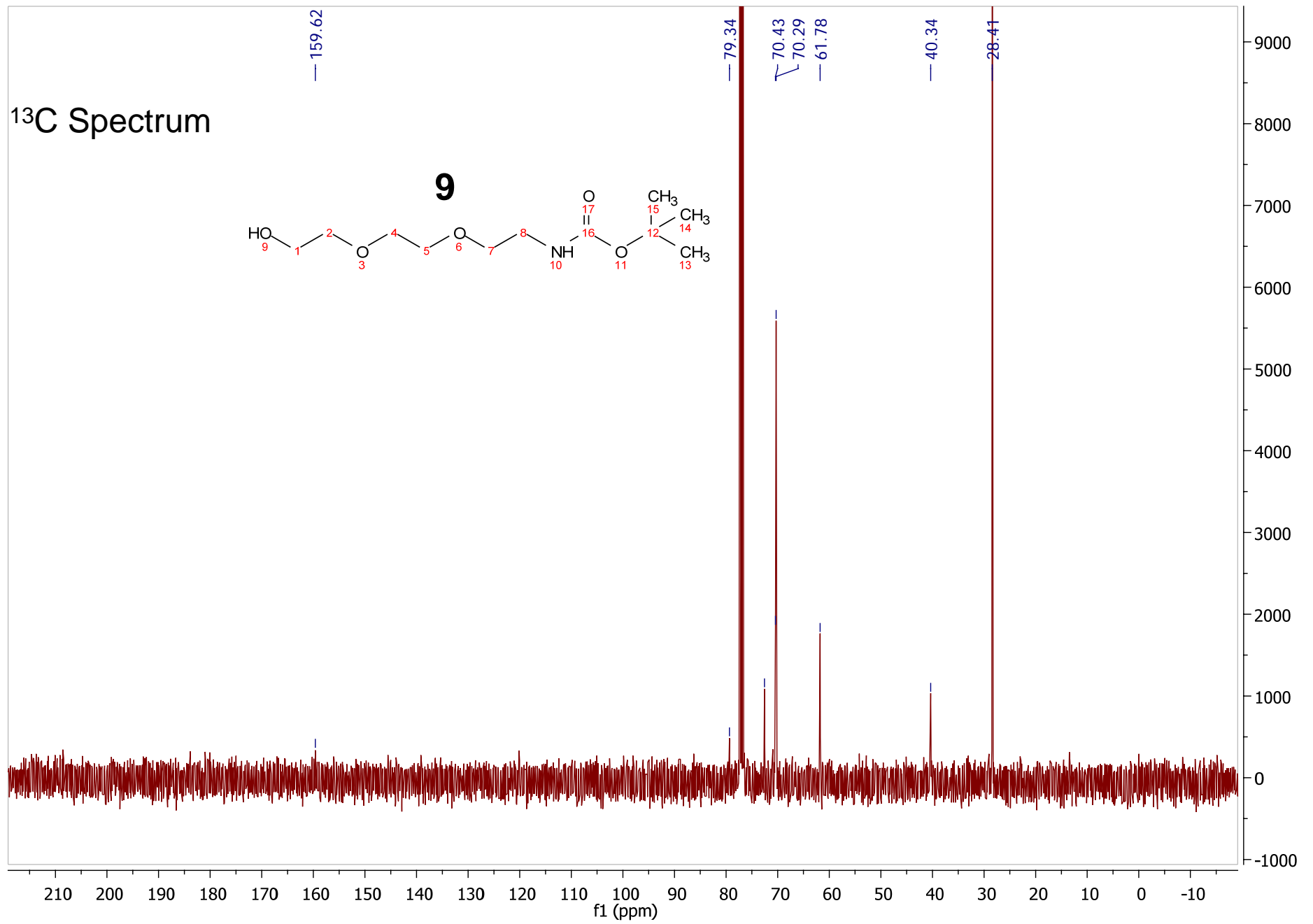
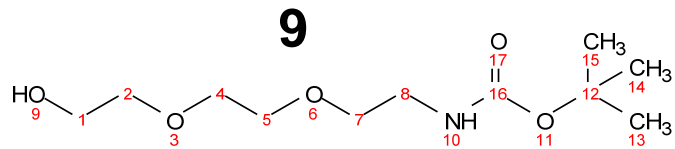
TOF Spectrum	TOF	Profile Spectrum at 202.33 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 189351



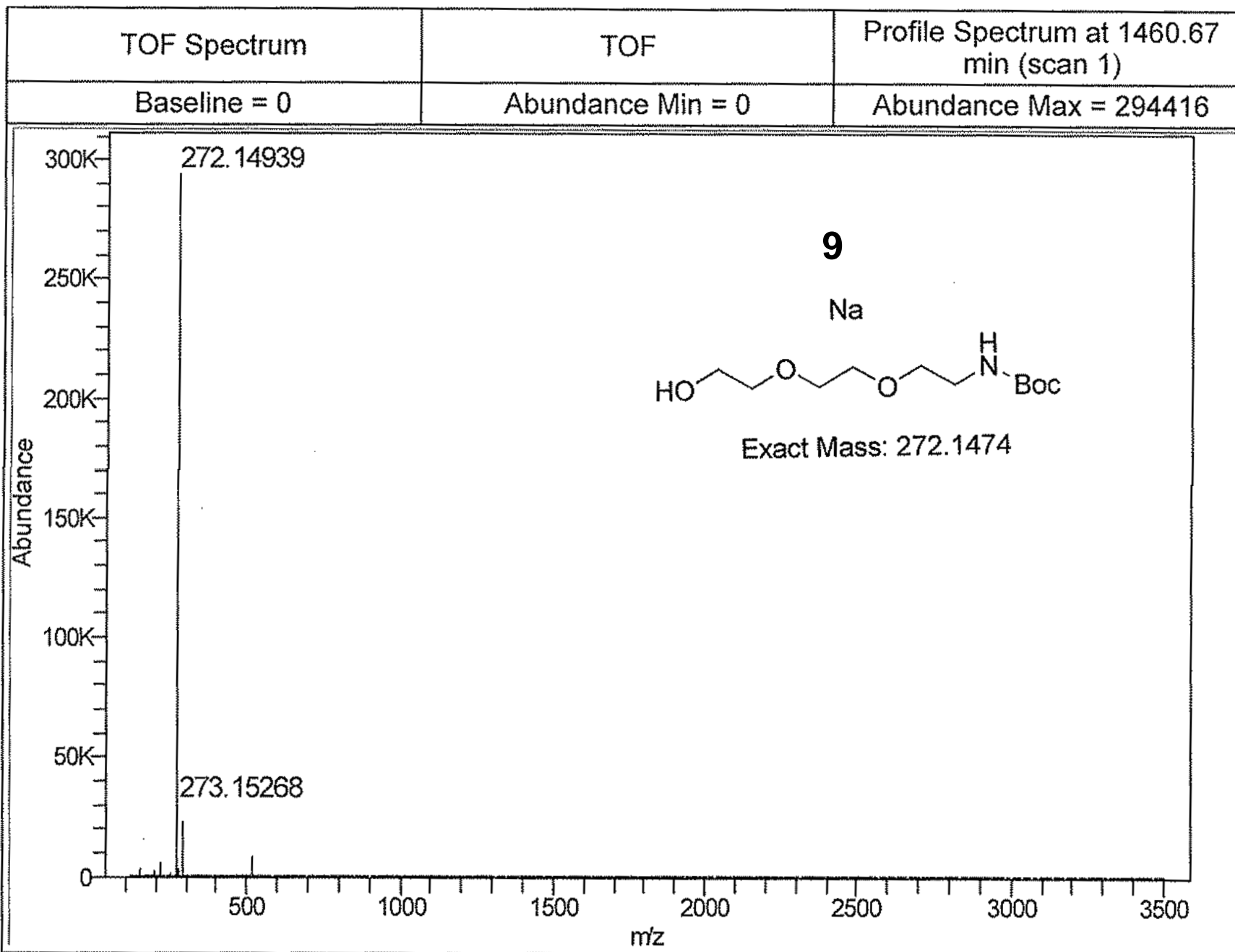
# <sup>1</sup>H Spectrum



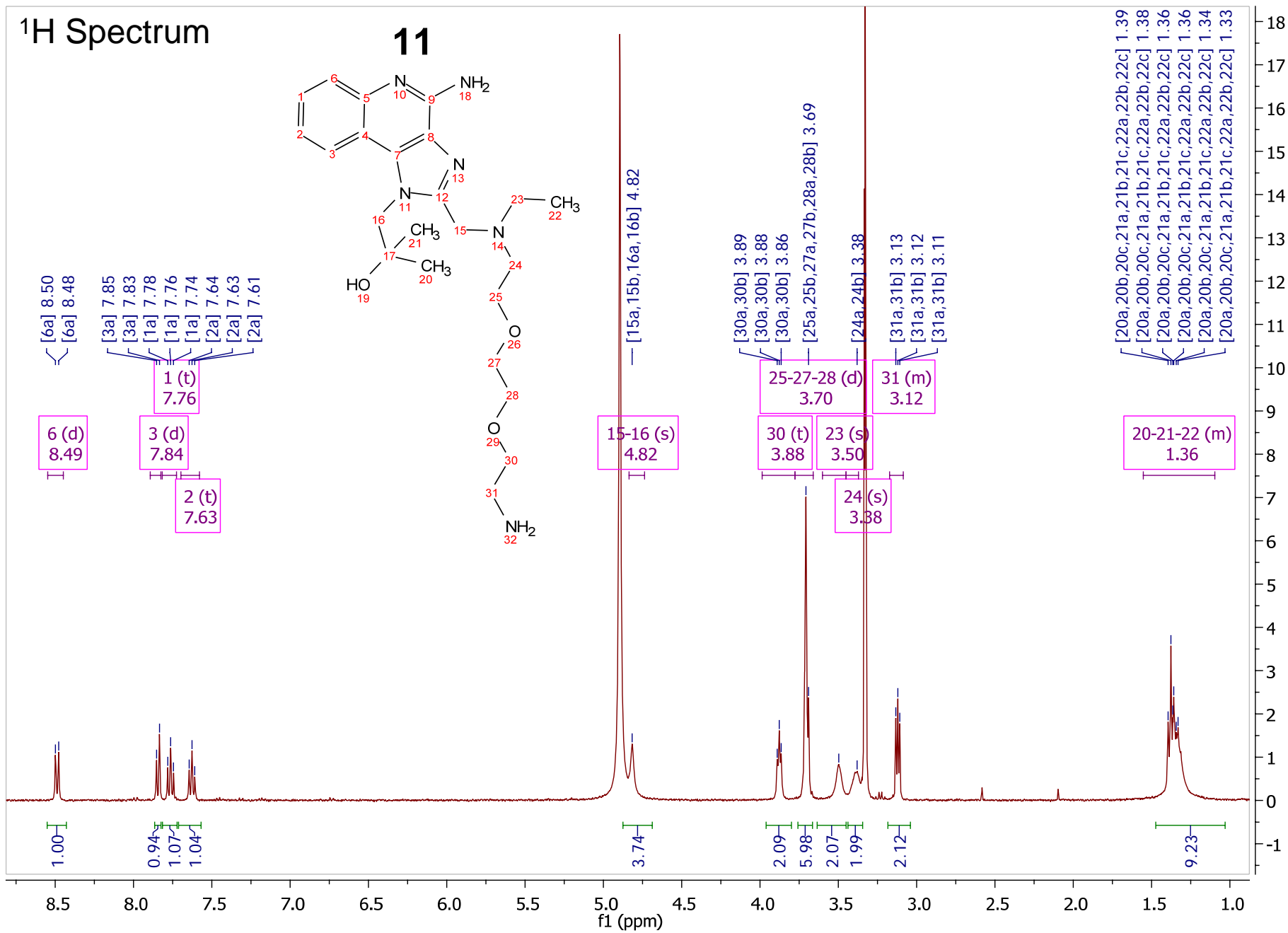
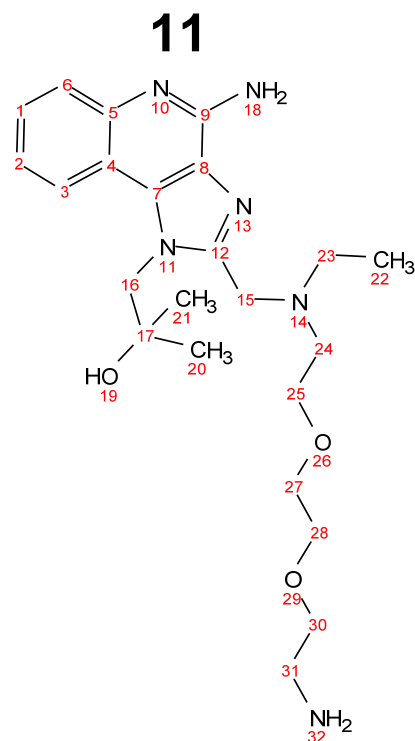
# <sup>13</sup>C Spectrum

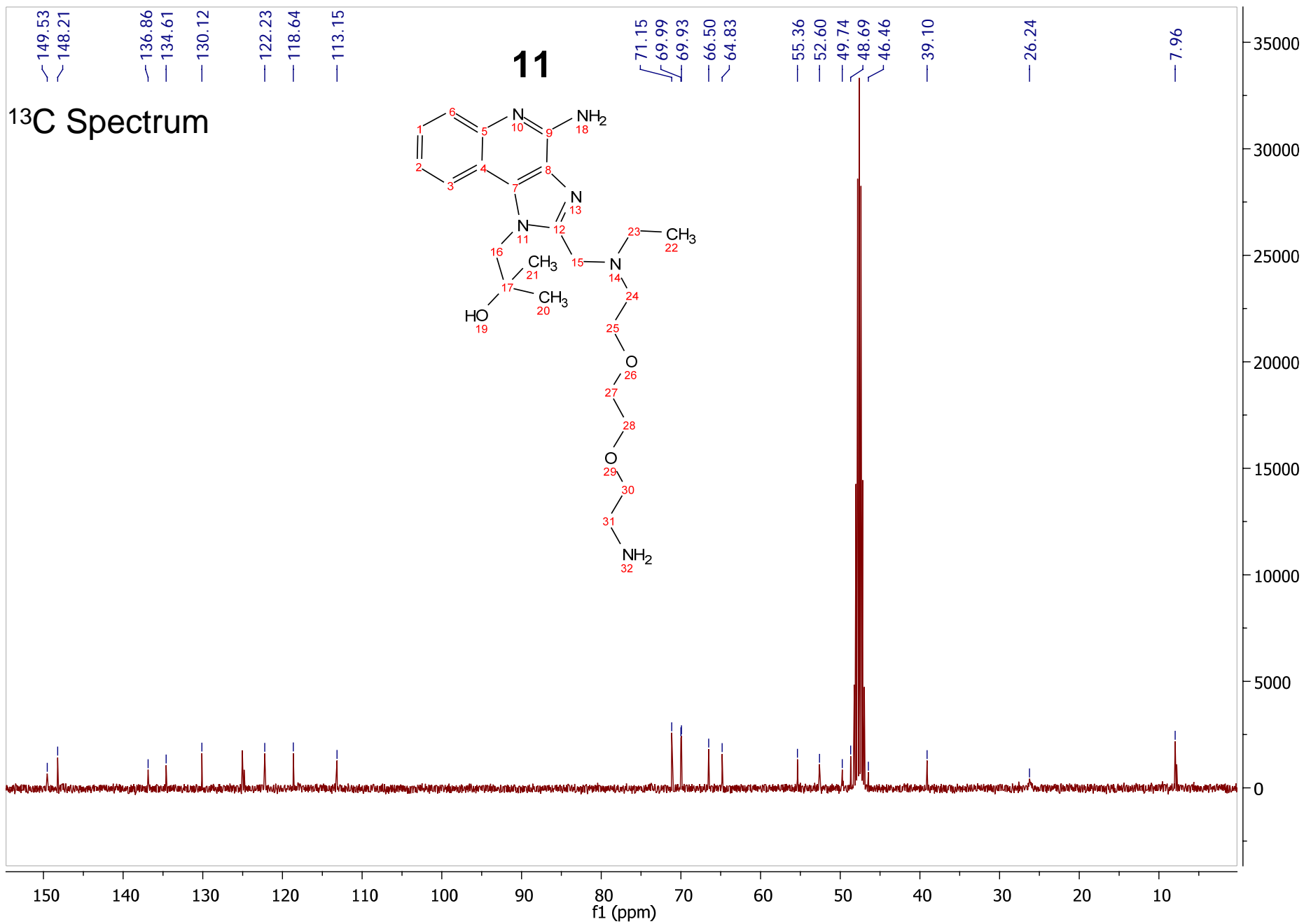




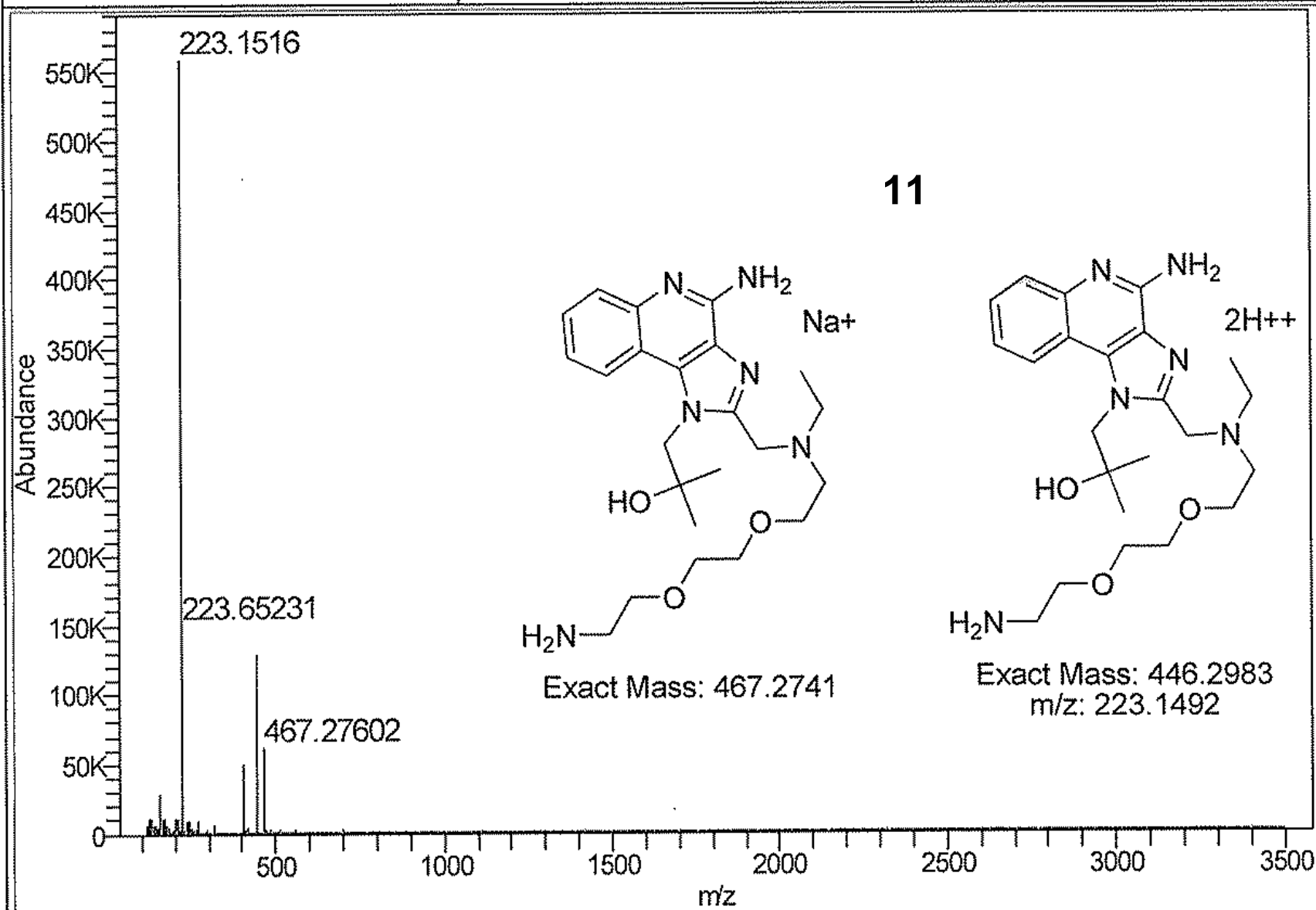


# <sup>1</sup>H Spectrum



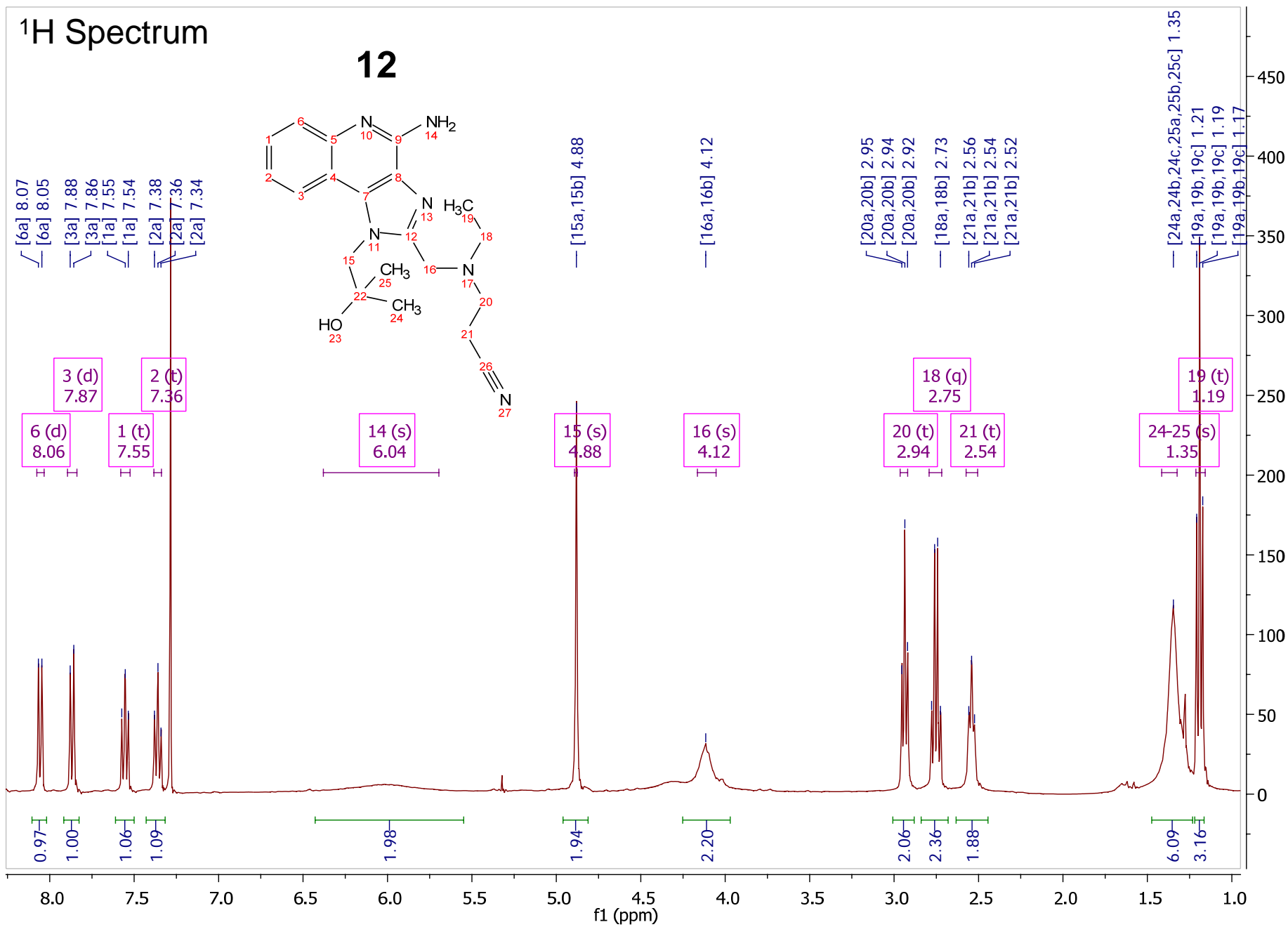
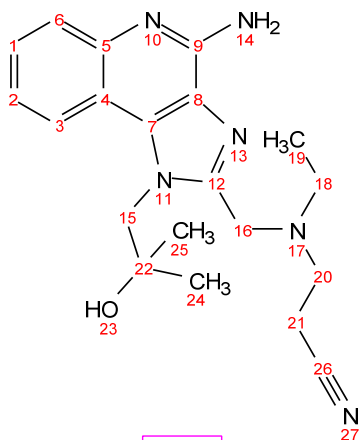


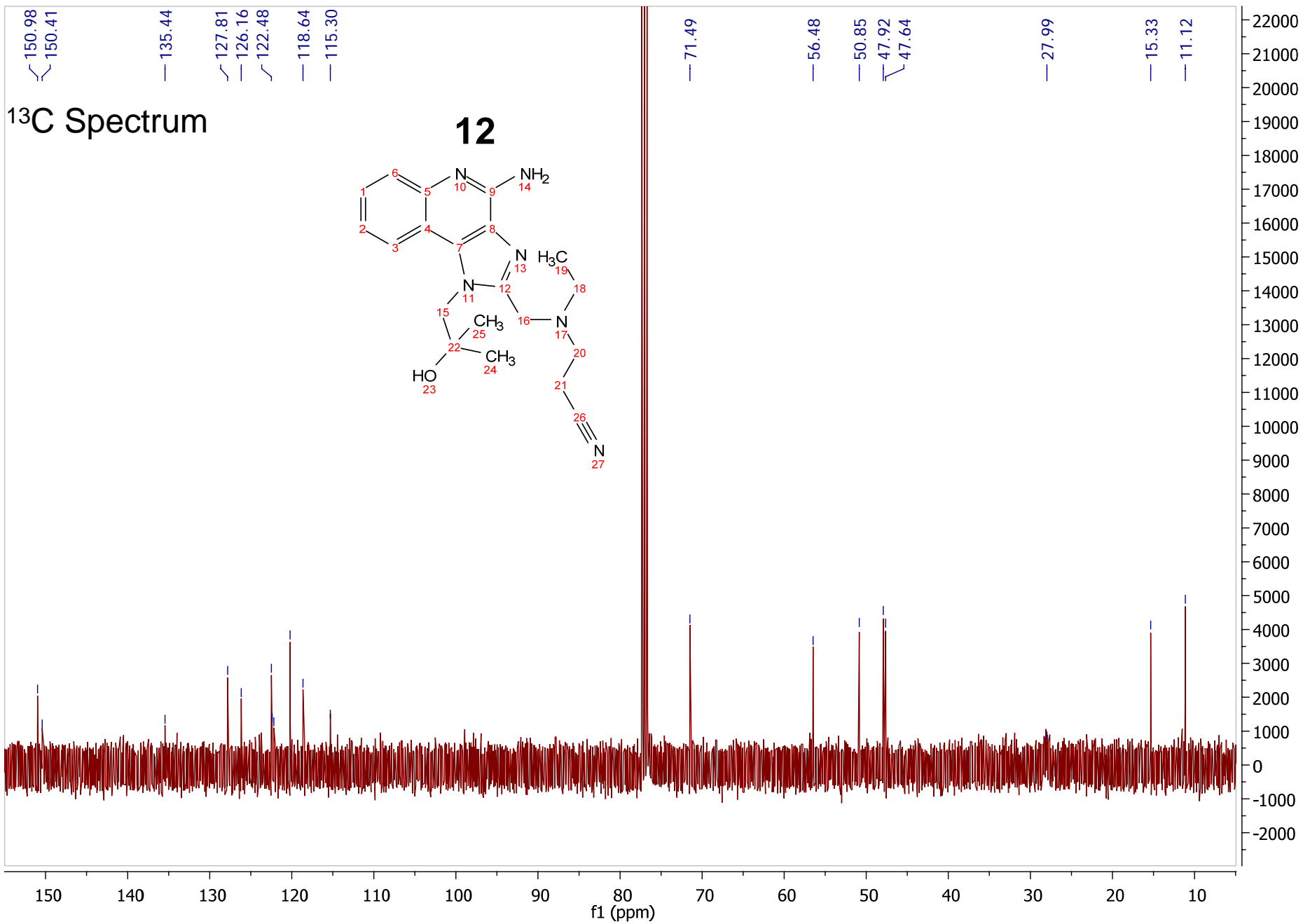
TOF Spectrum	TOF	Profile Spectrum at 3238.79 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 559102

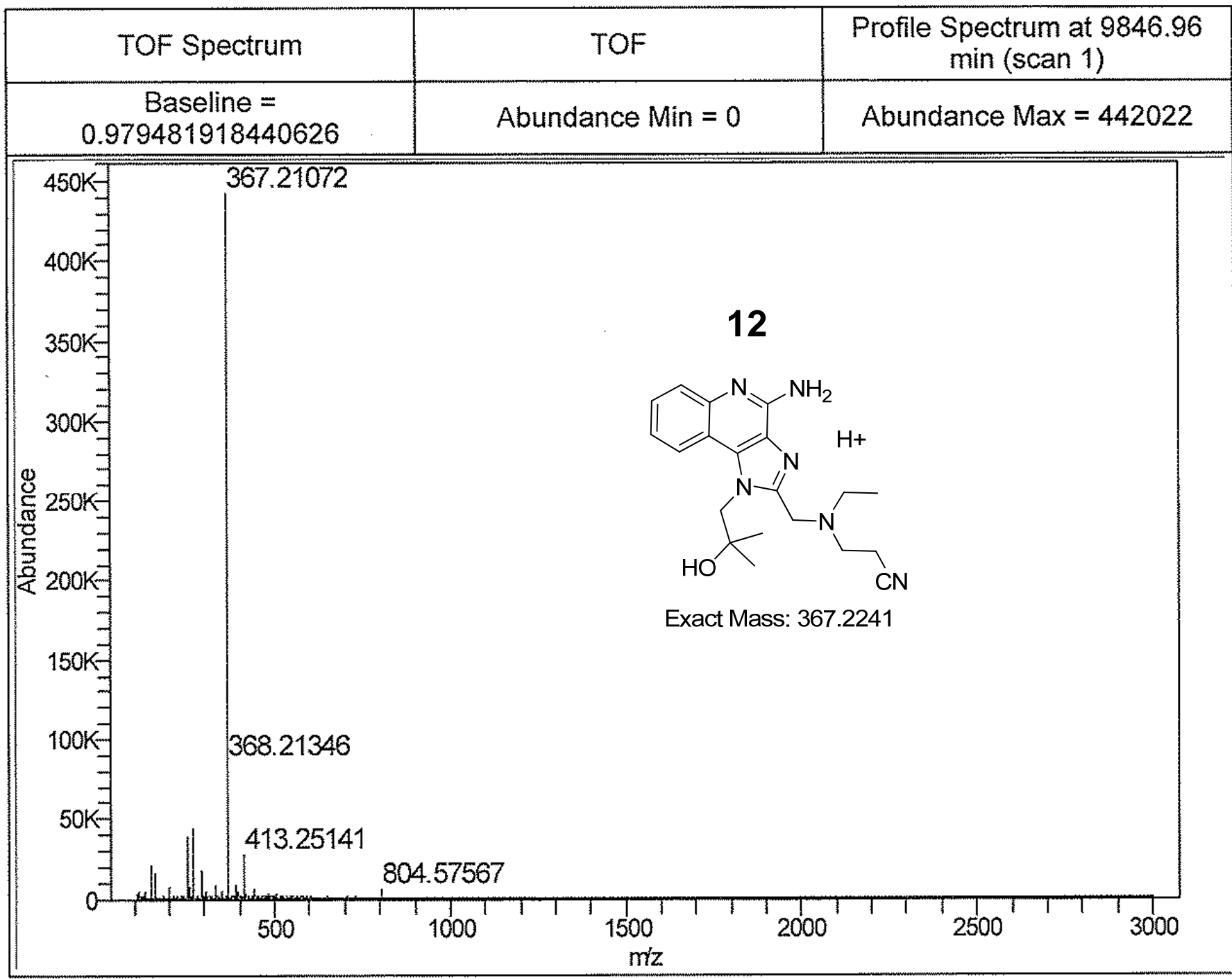


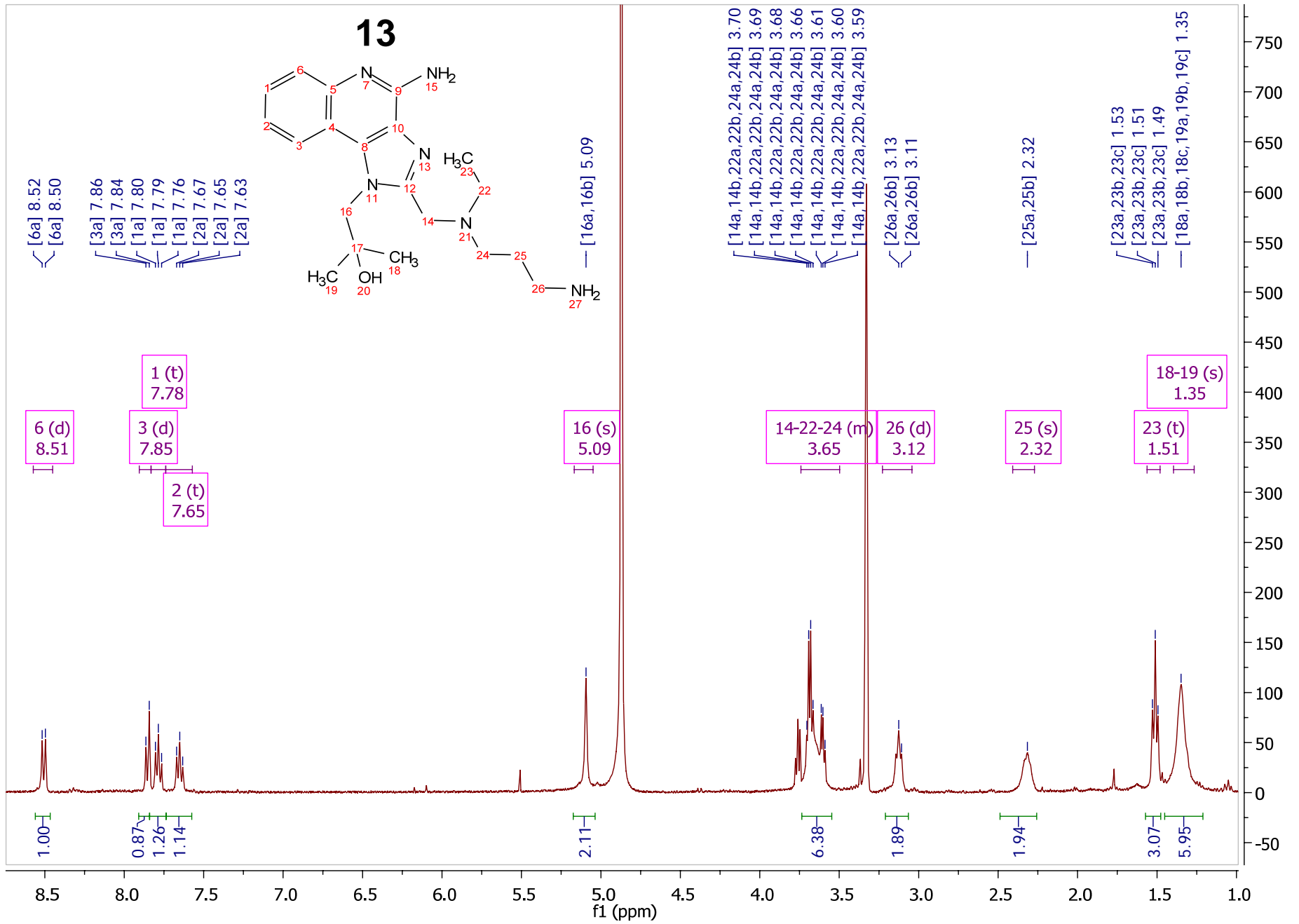
# <sup>1</sup>H Spectrum

## 12



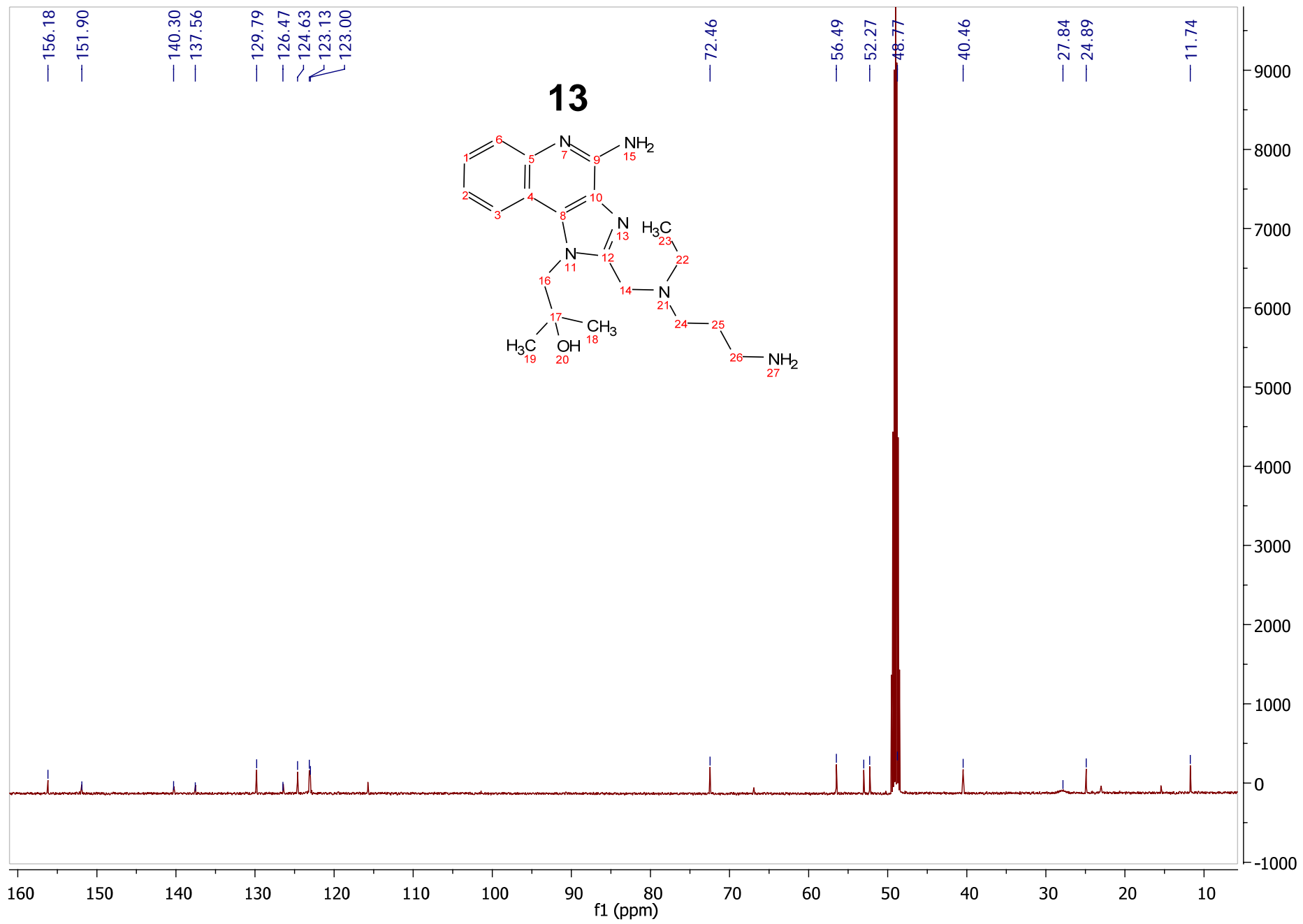
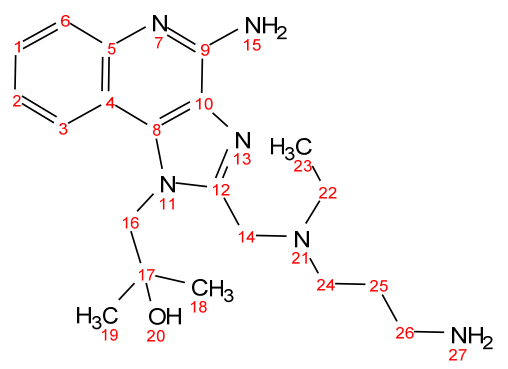


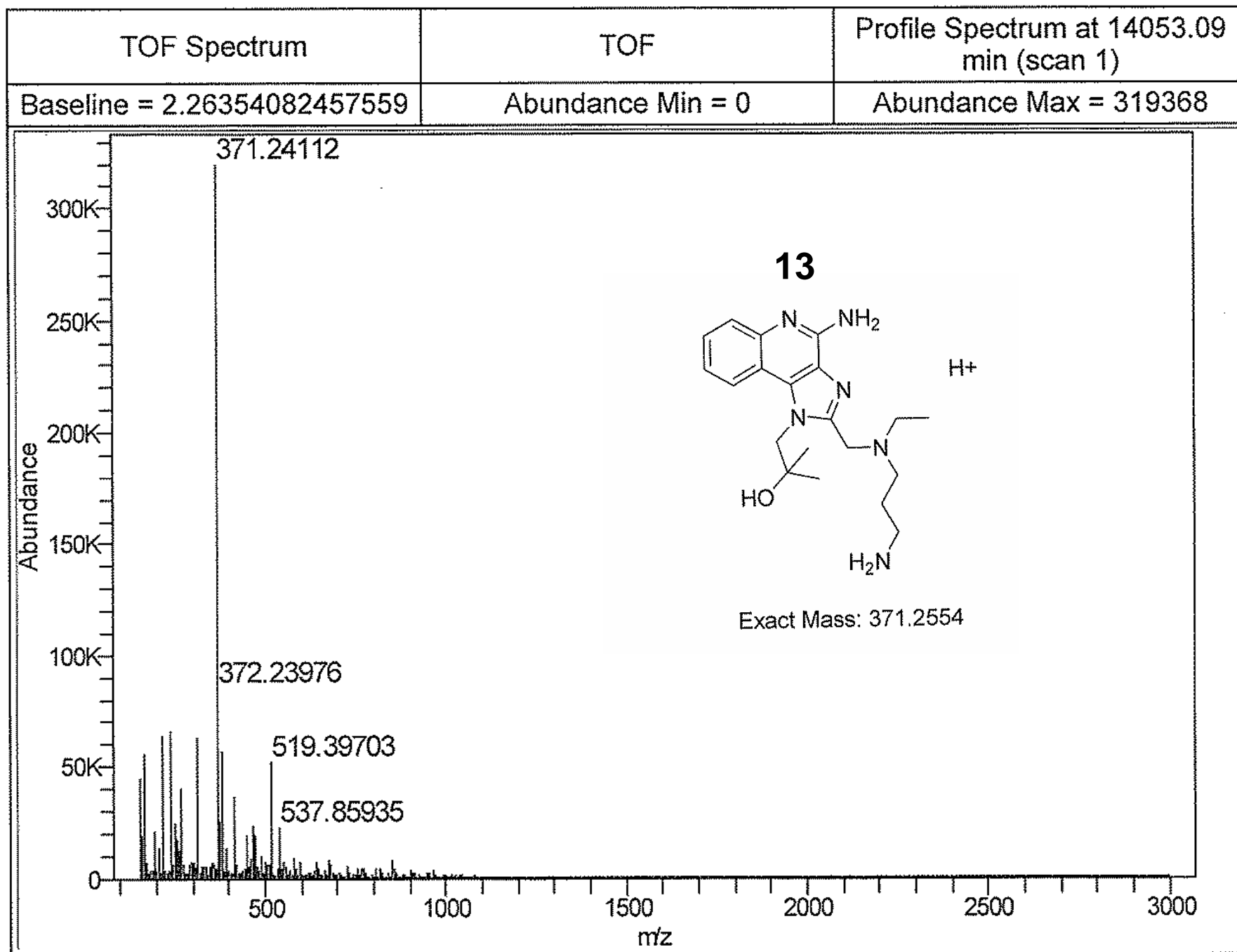


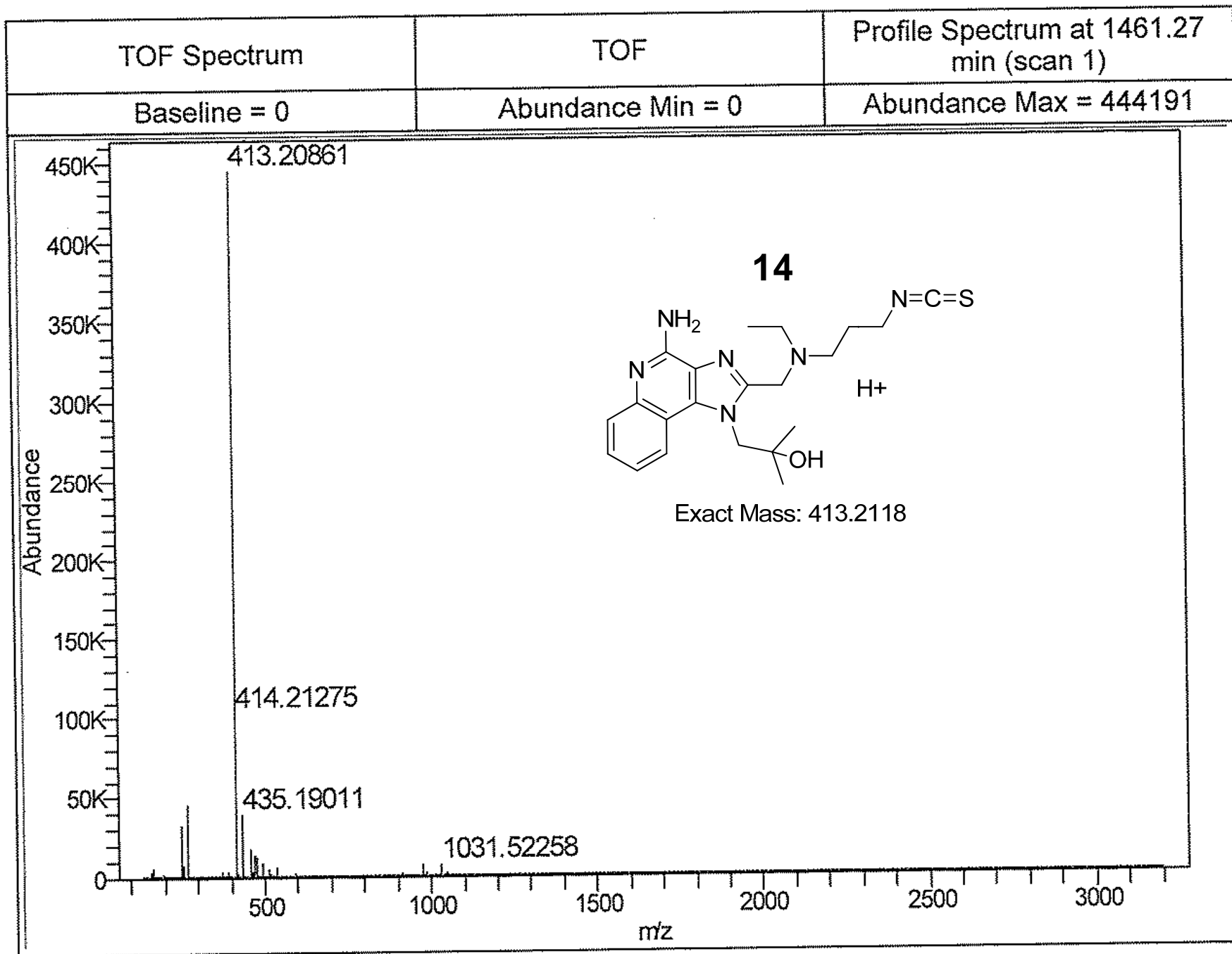




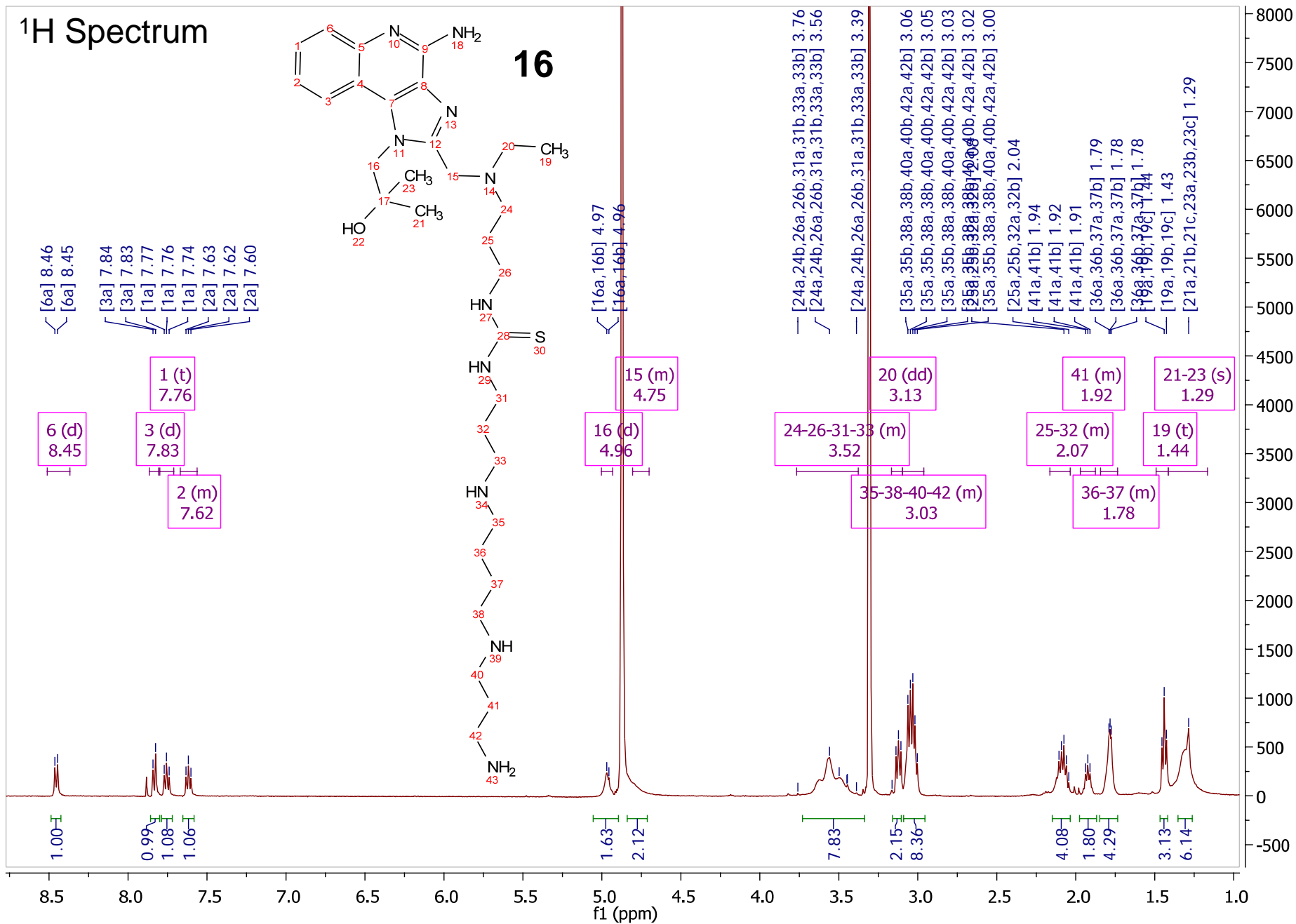
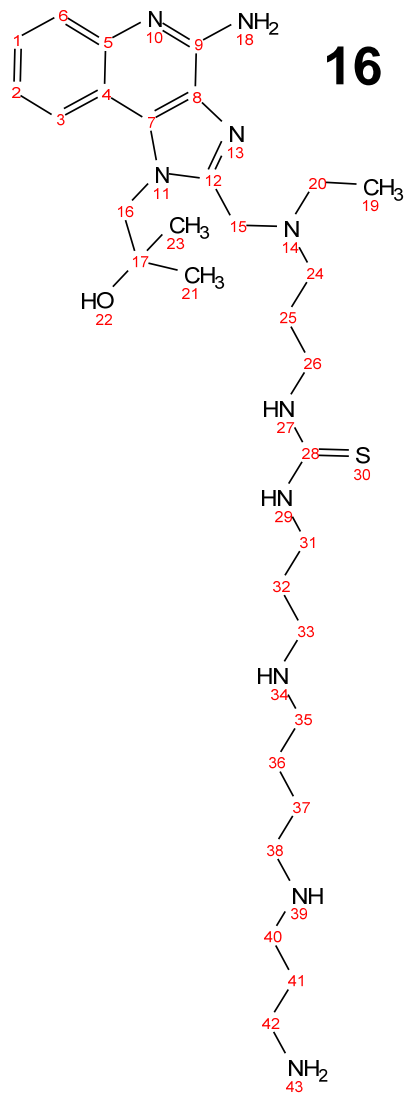
**13**



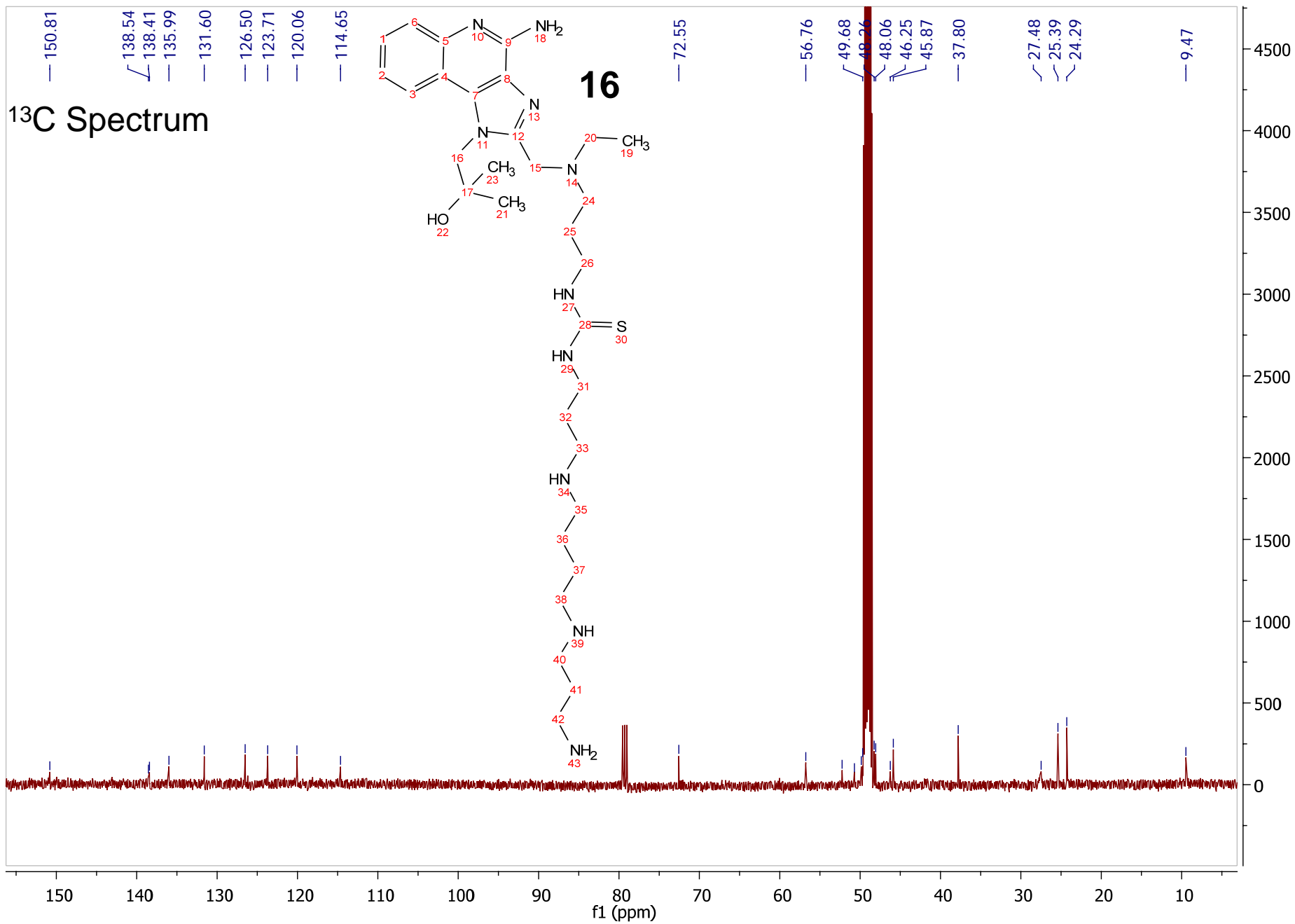




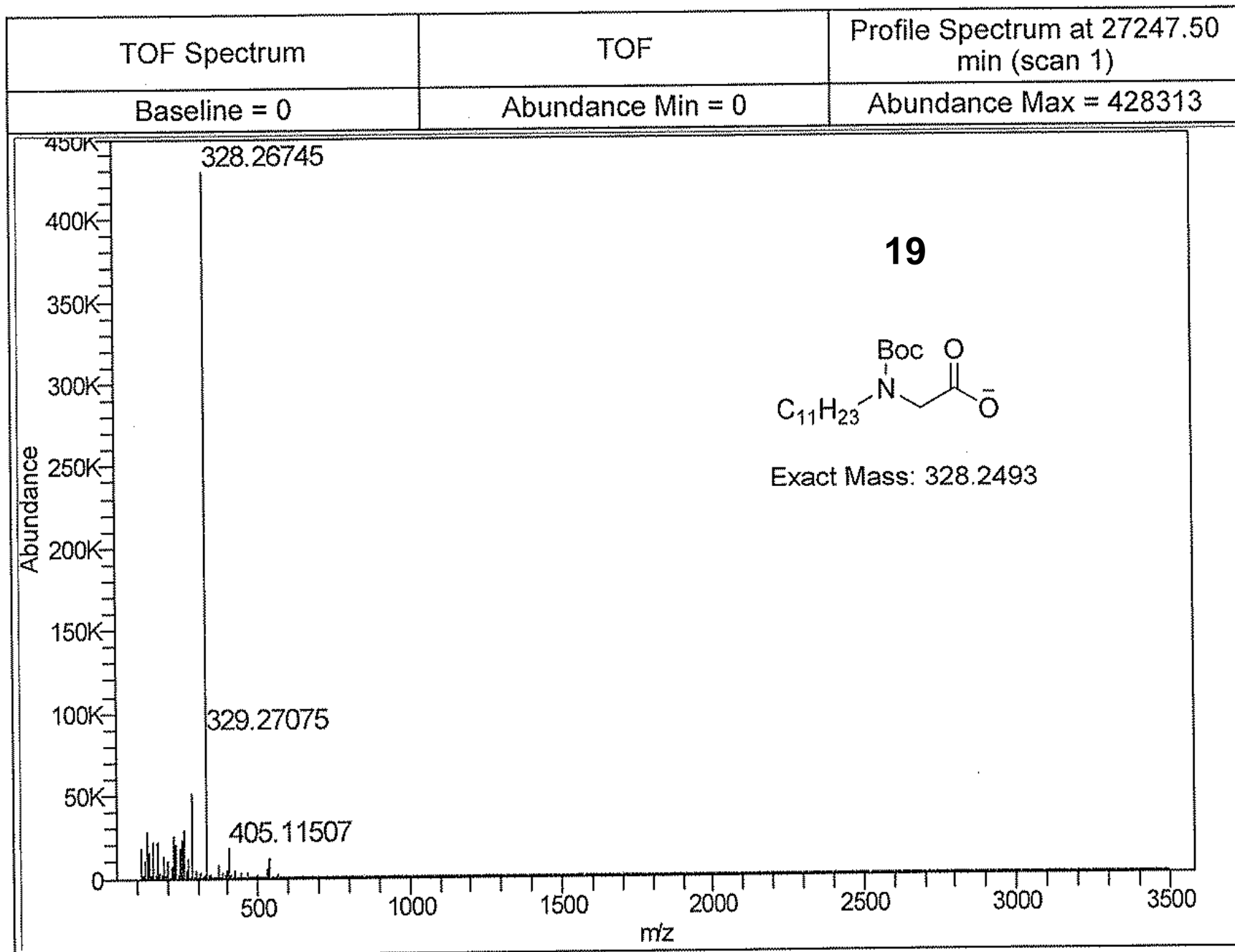
# <sup>1</sup>H Spectrum

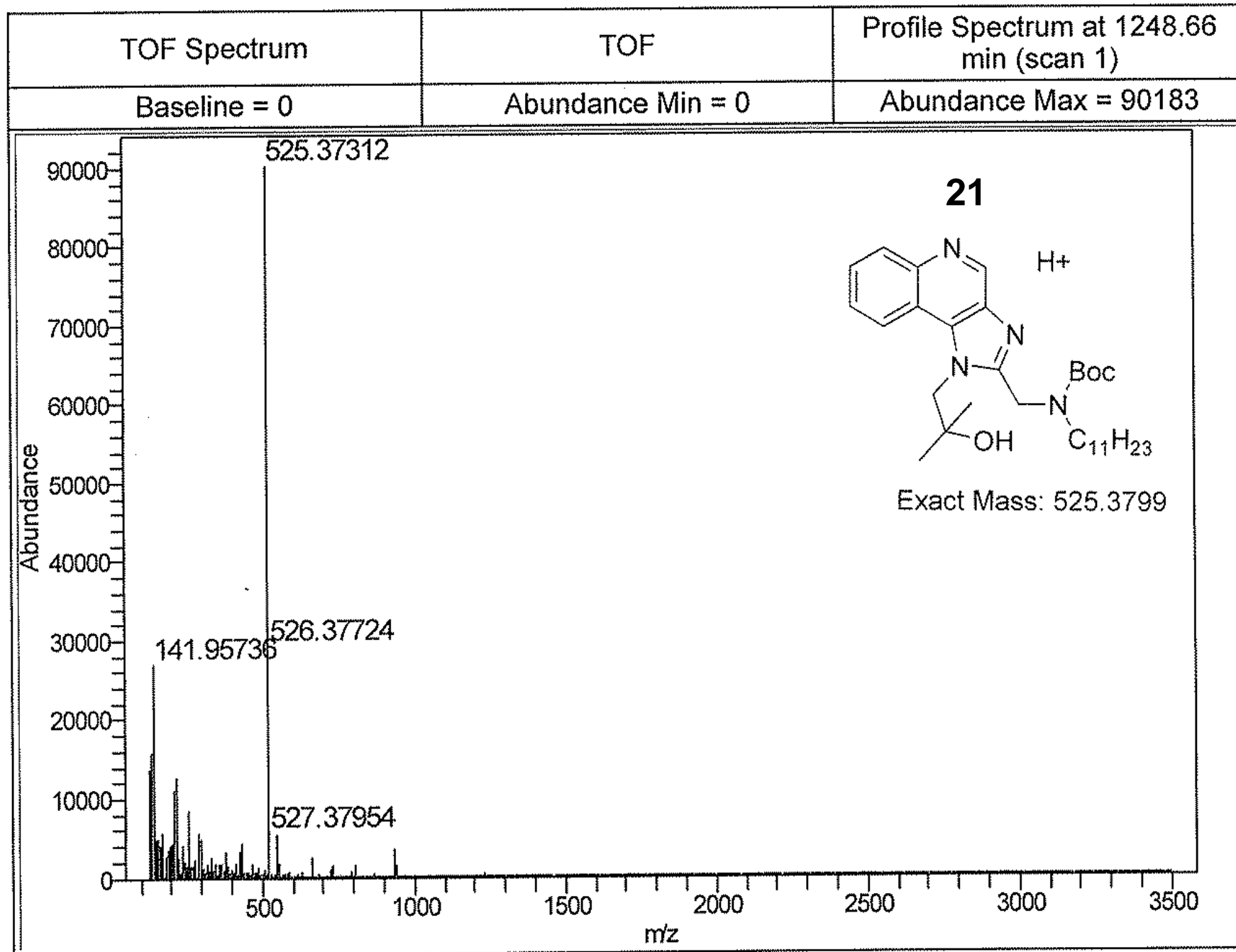


# <sup>13</sup>C Spectrum

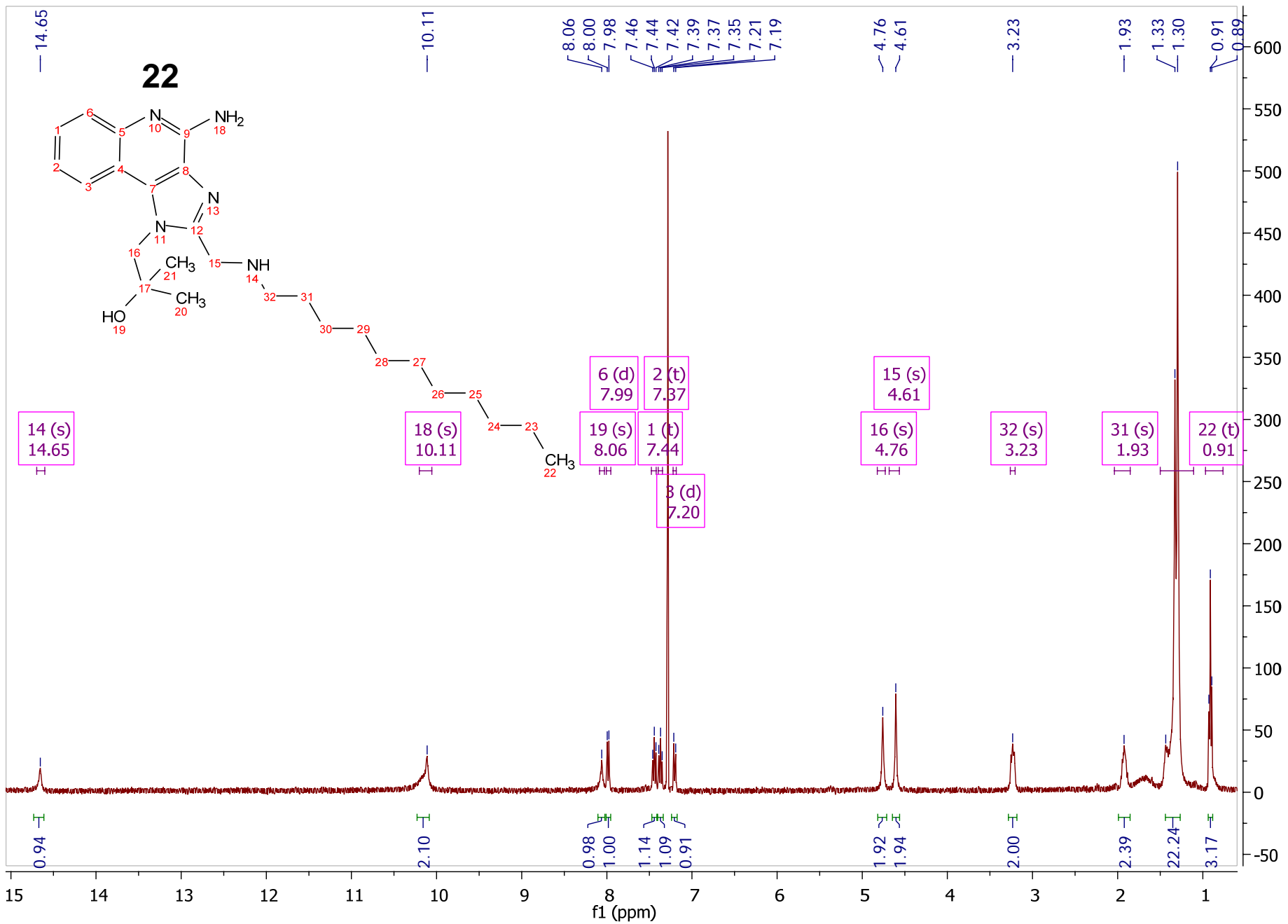


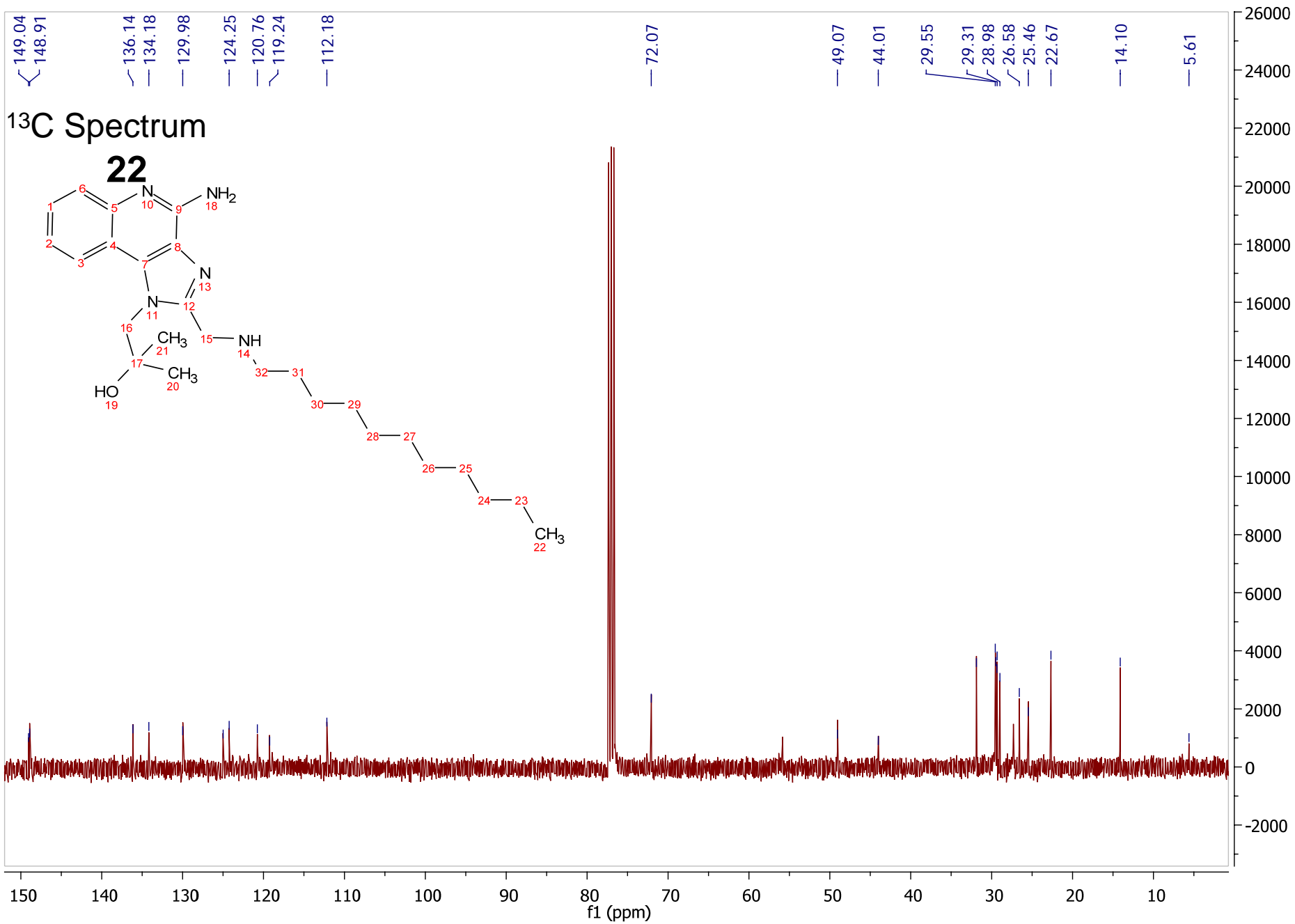




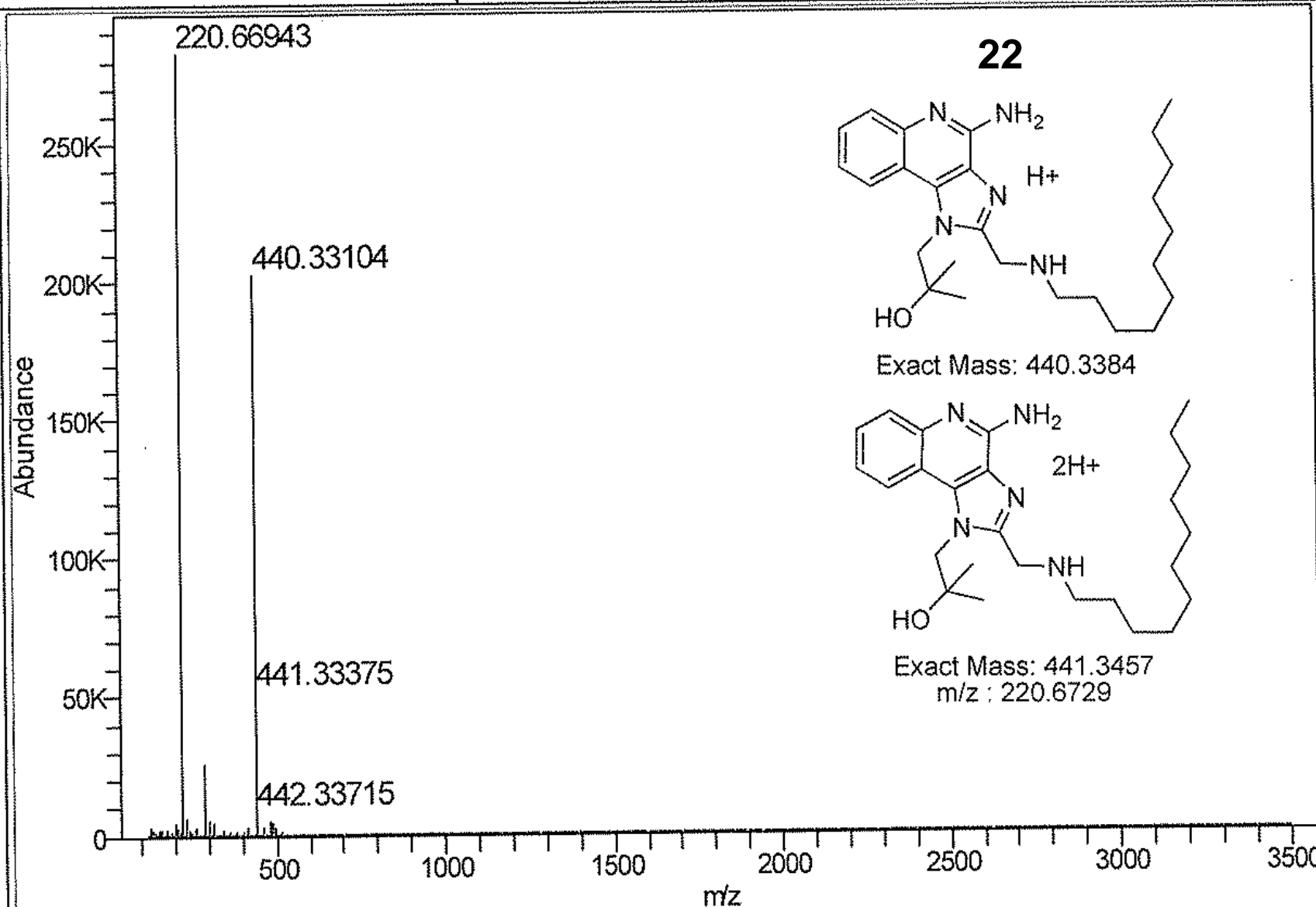




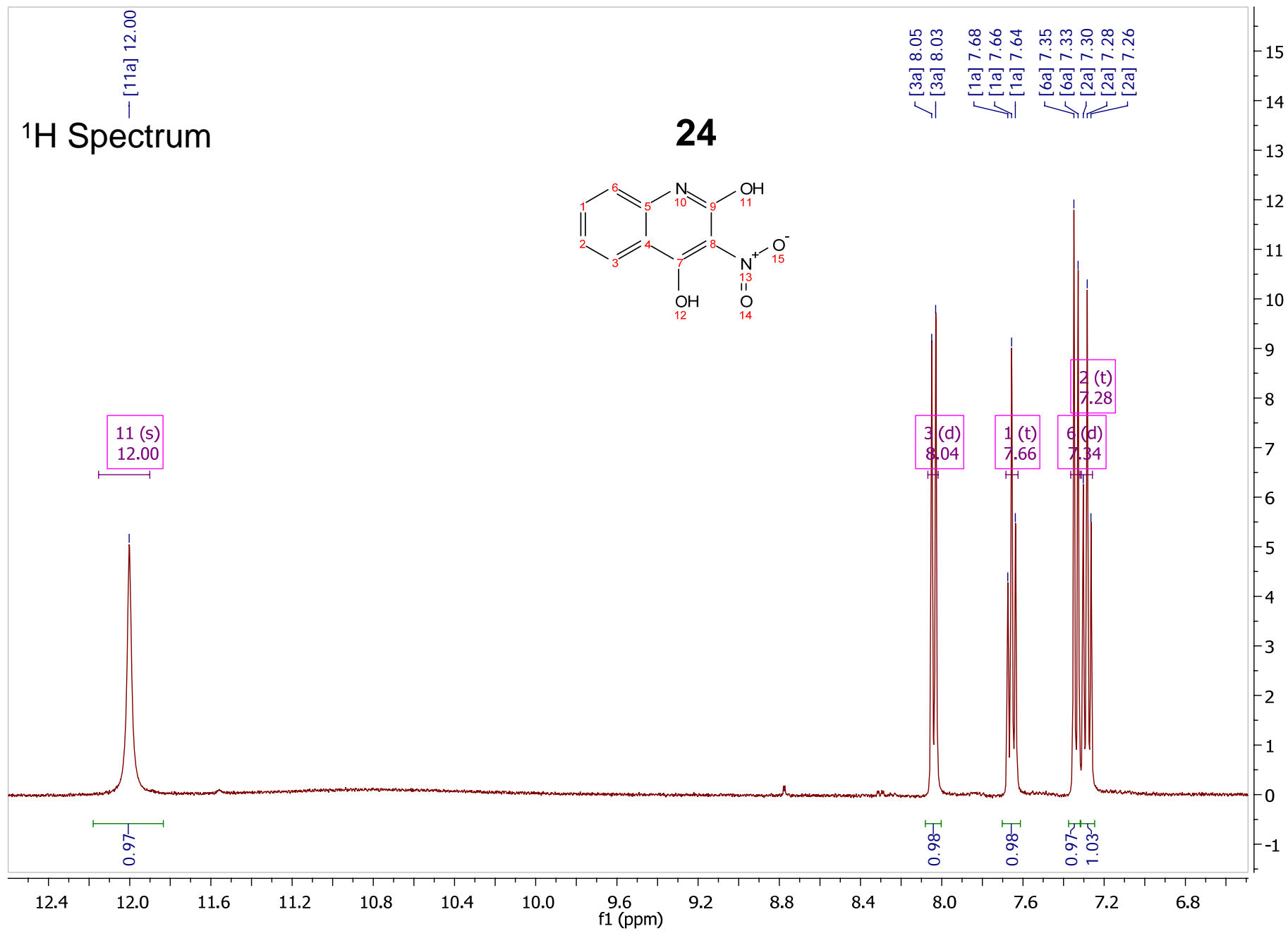


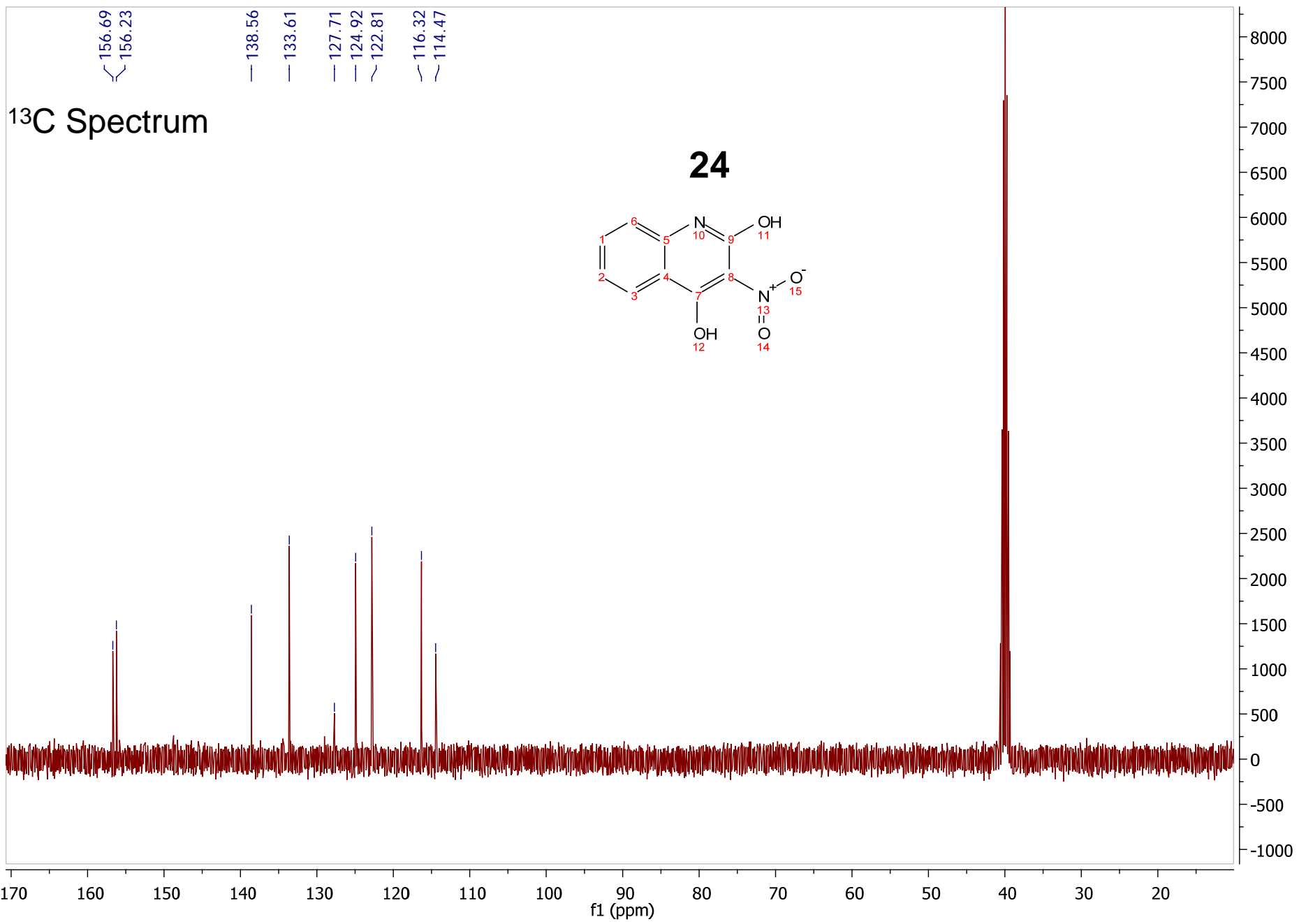


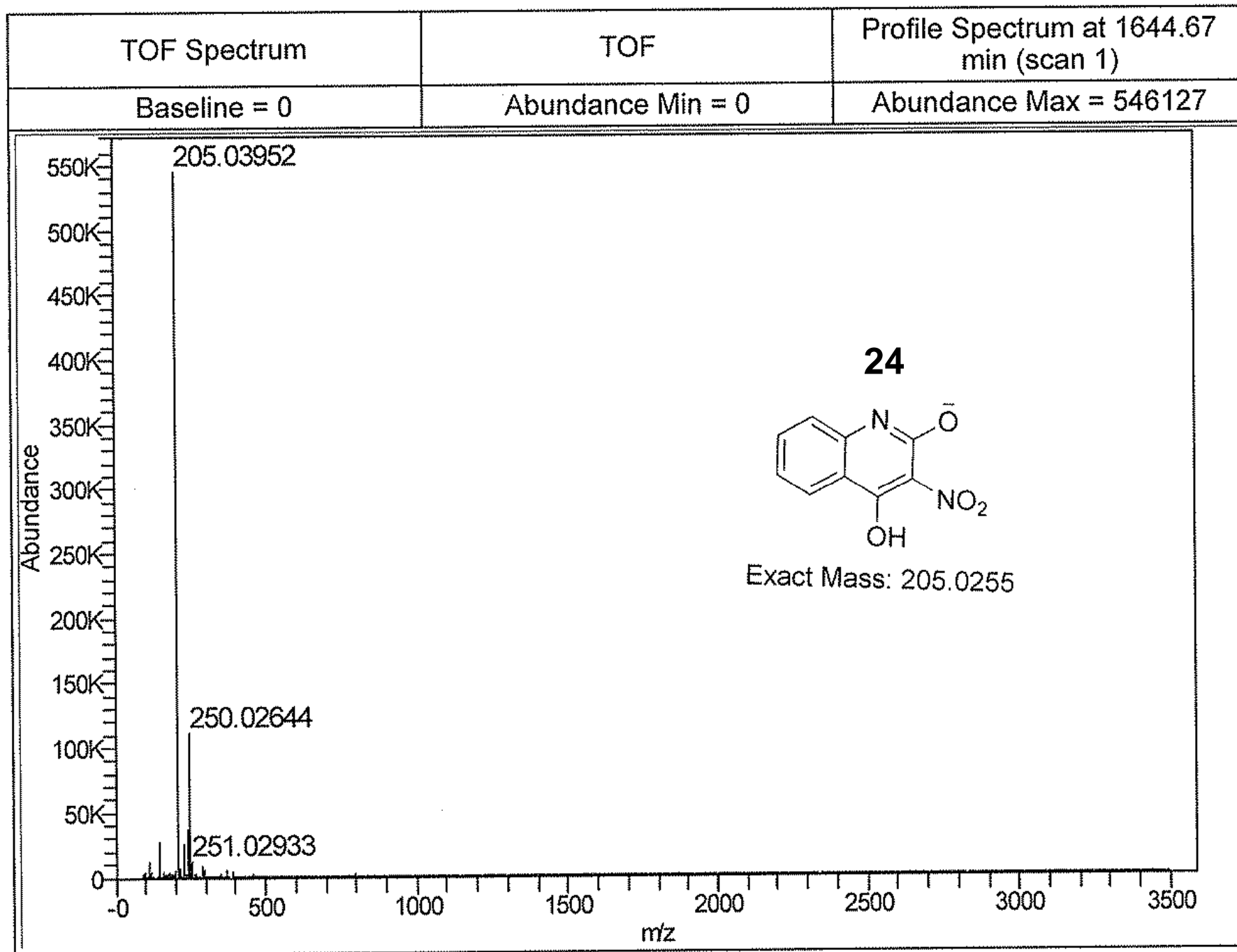
TOF Spectrum	TOF	Profile Spectrum at 1454.44 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 282837

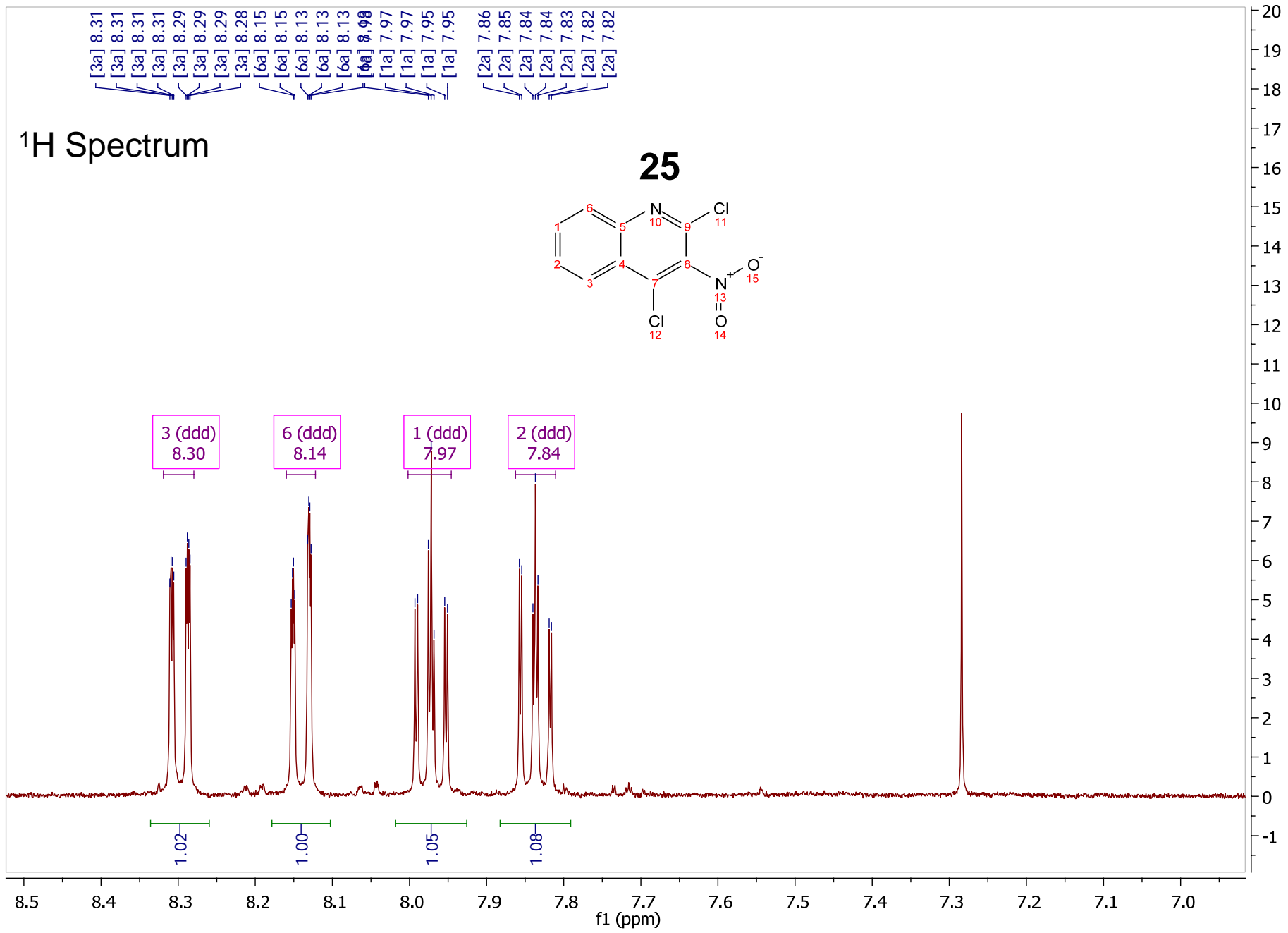


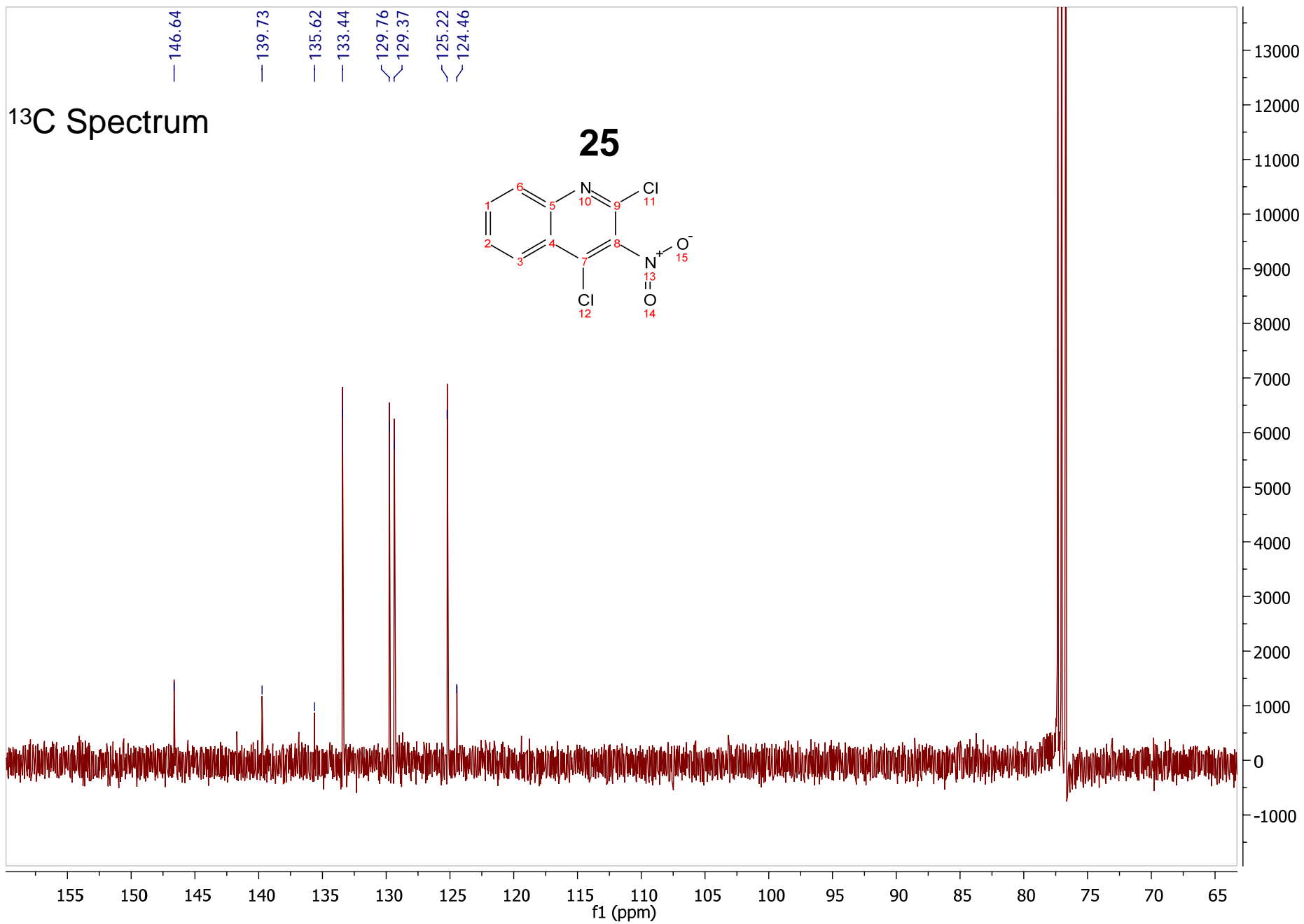
# <sup>1</sup>H Spectrum





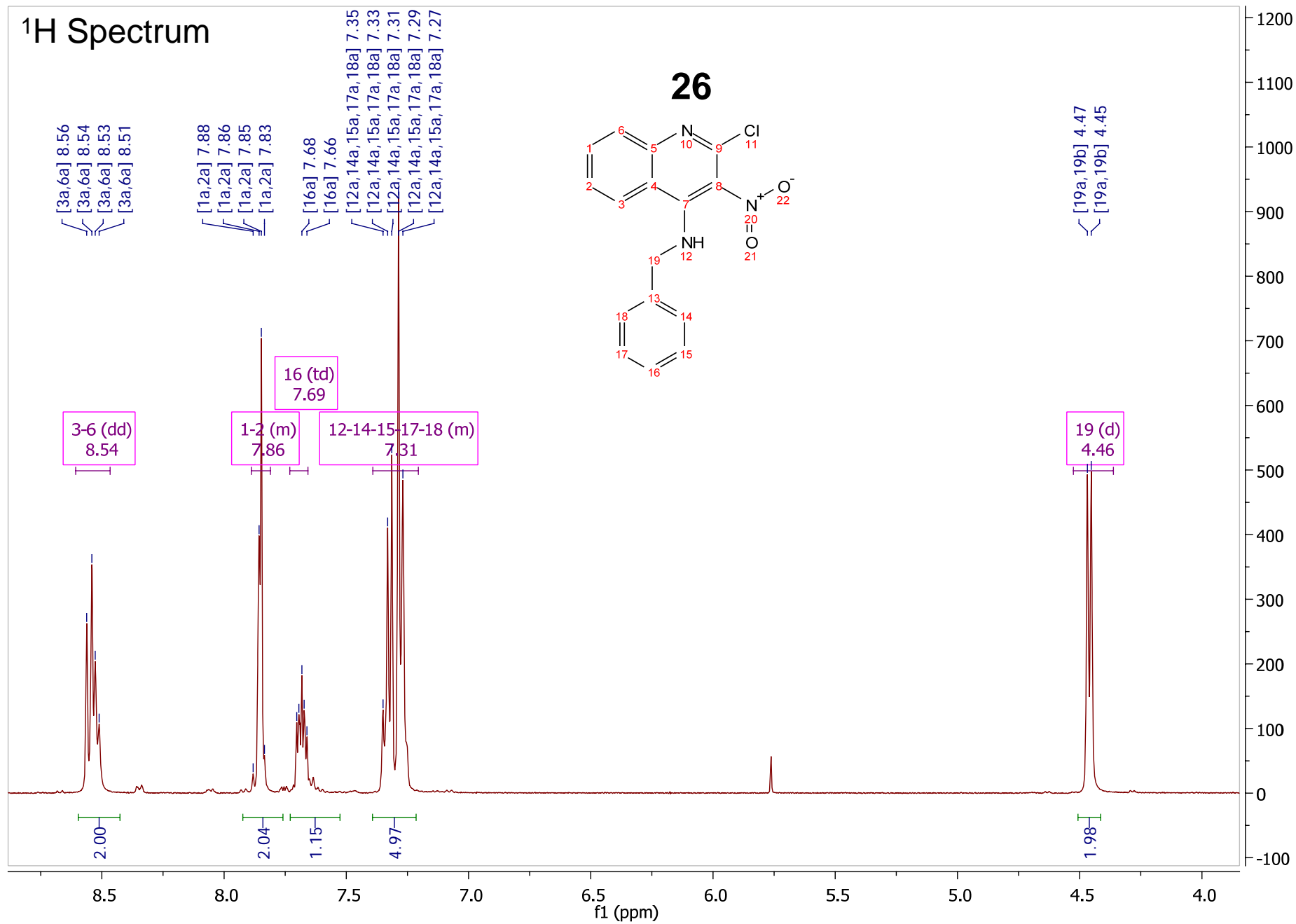




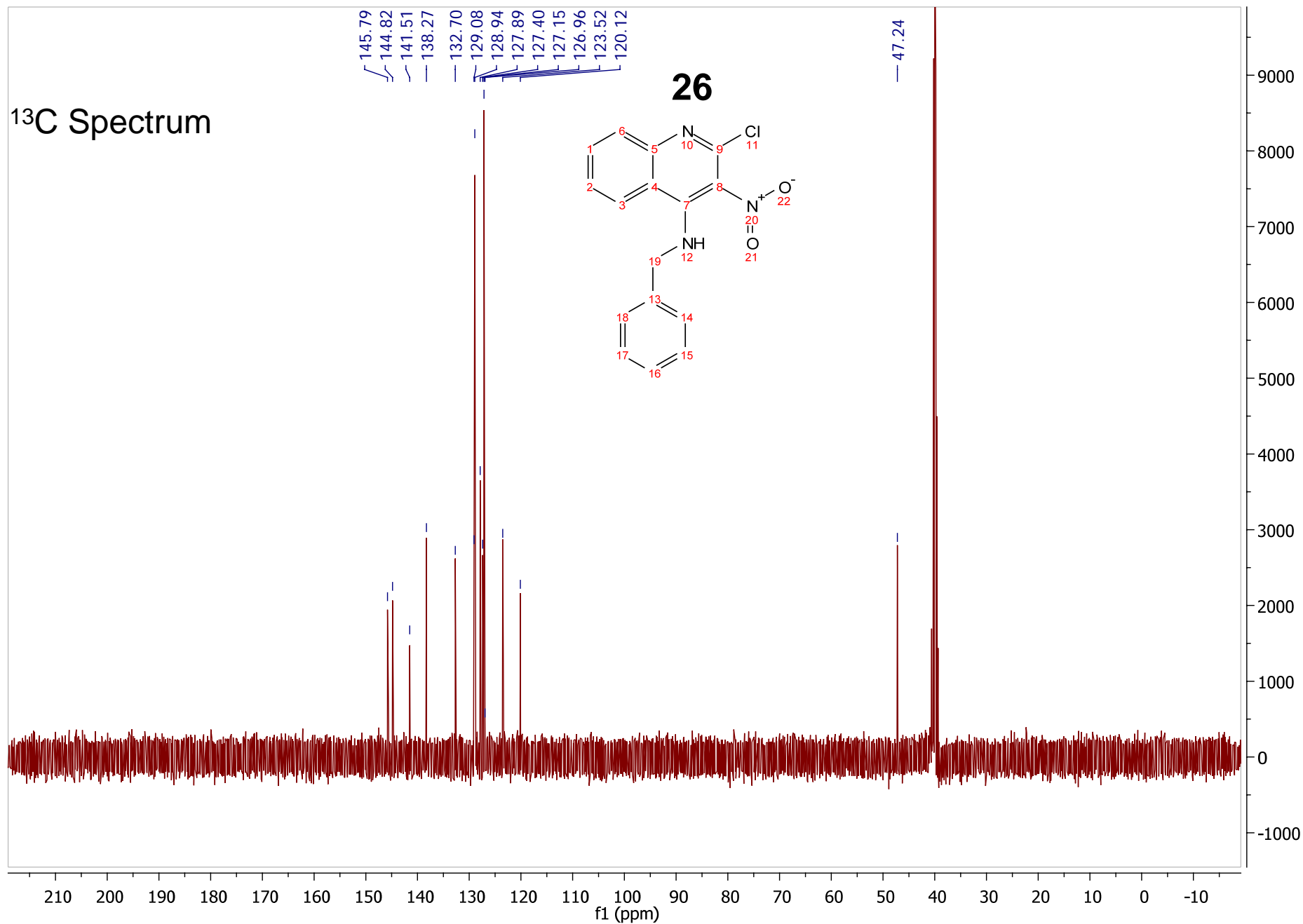


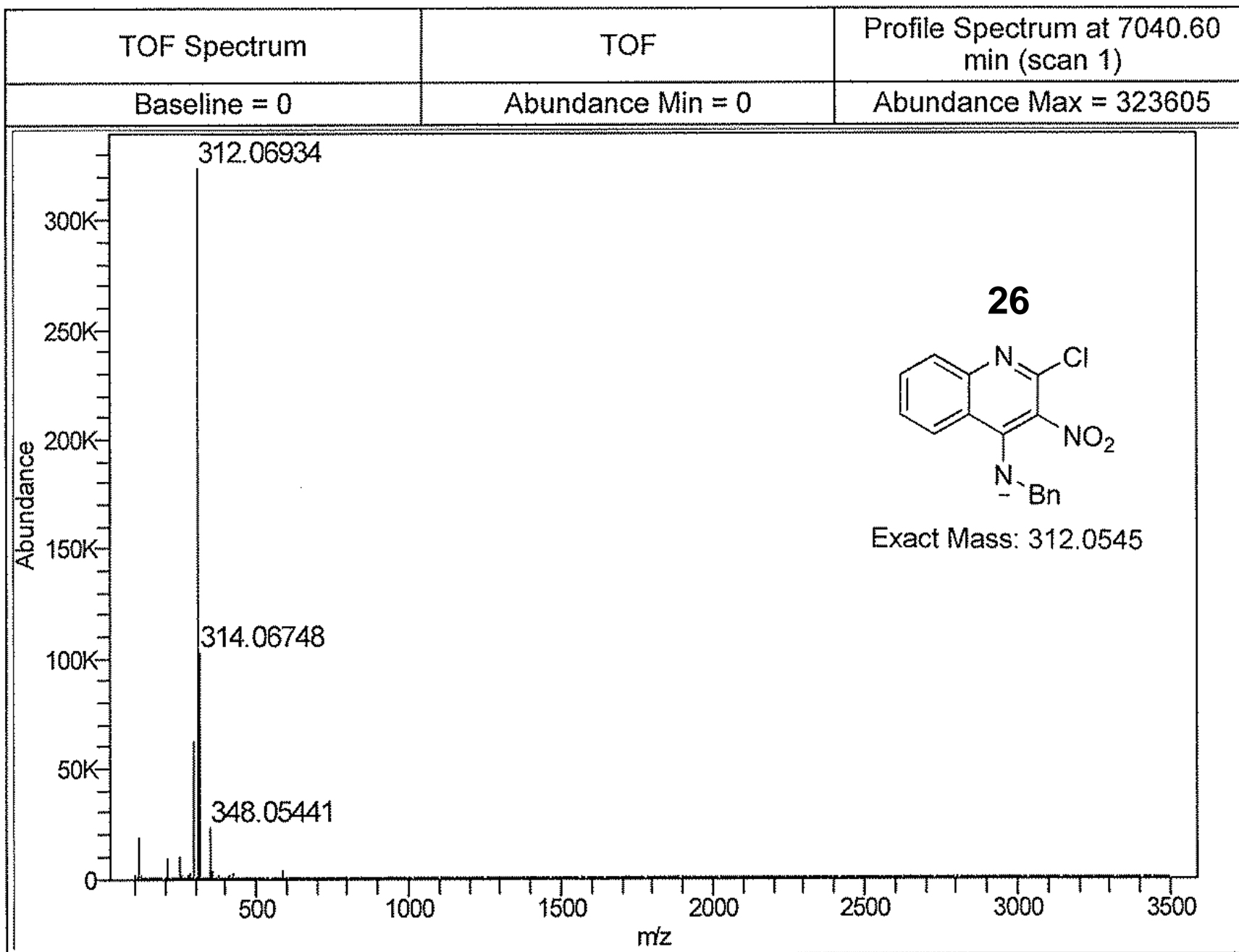


# <sup>1</sup>H Spectrum



# <sup>13</sup>C Spectrum

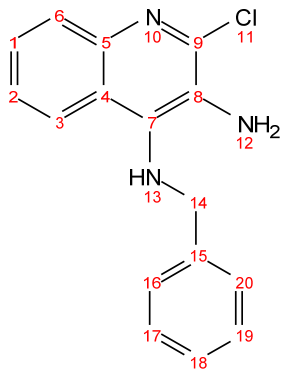




# <sup>1</sup>H Spectrum

[6a] 7.91  
[6a] 7.88  
[3a] 7.69  
[1a] 7.45  
[1a] 7.43  
[1a] 7.41  
[2a, 16a, 20a] 7.37  
[2a, 16a, 20a] 7.35  
[2a, 16a, 20a] 7.33  
[17a, 19a] 7.27  
[17a, 19a] 7.26  
[17a, 19a] 7.24  
[18a] 7.21  
[18a] 7.19

**27**



2-16-20 (m)  
7.35  
3 (d)  
7.70  
17-19 (t)  
7.25  
6 (d)  
7.90  
1 (t)  
7.43  
18 (d)  
7.20

[14a, 14b] 4.51

14 (s)  
4.51

1.04

1.00

1.01

3.07

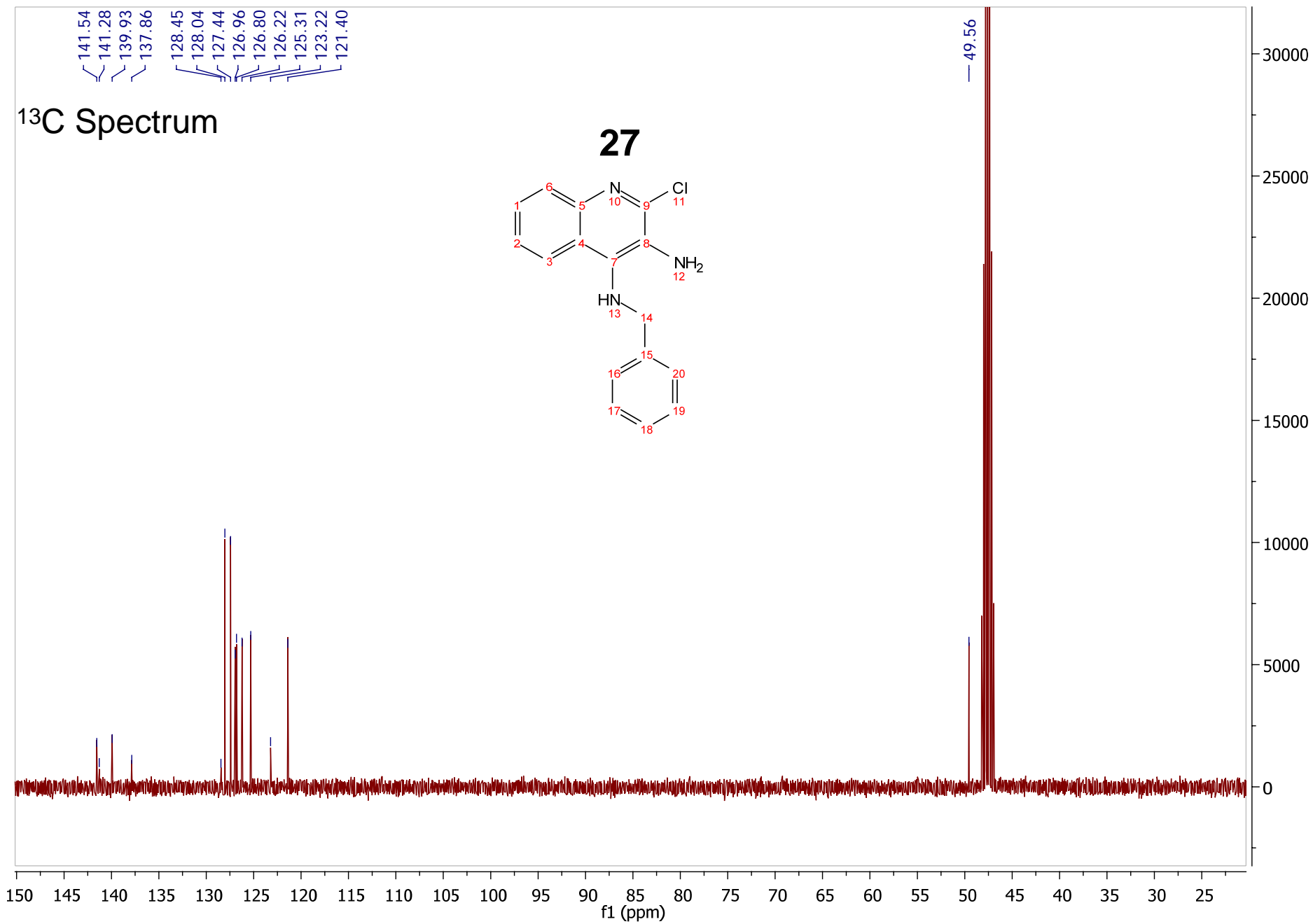
2.09

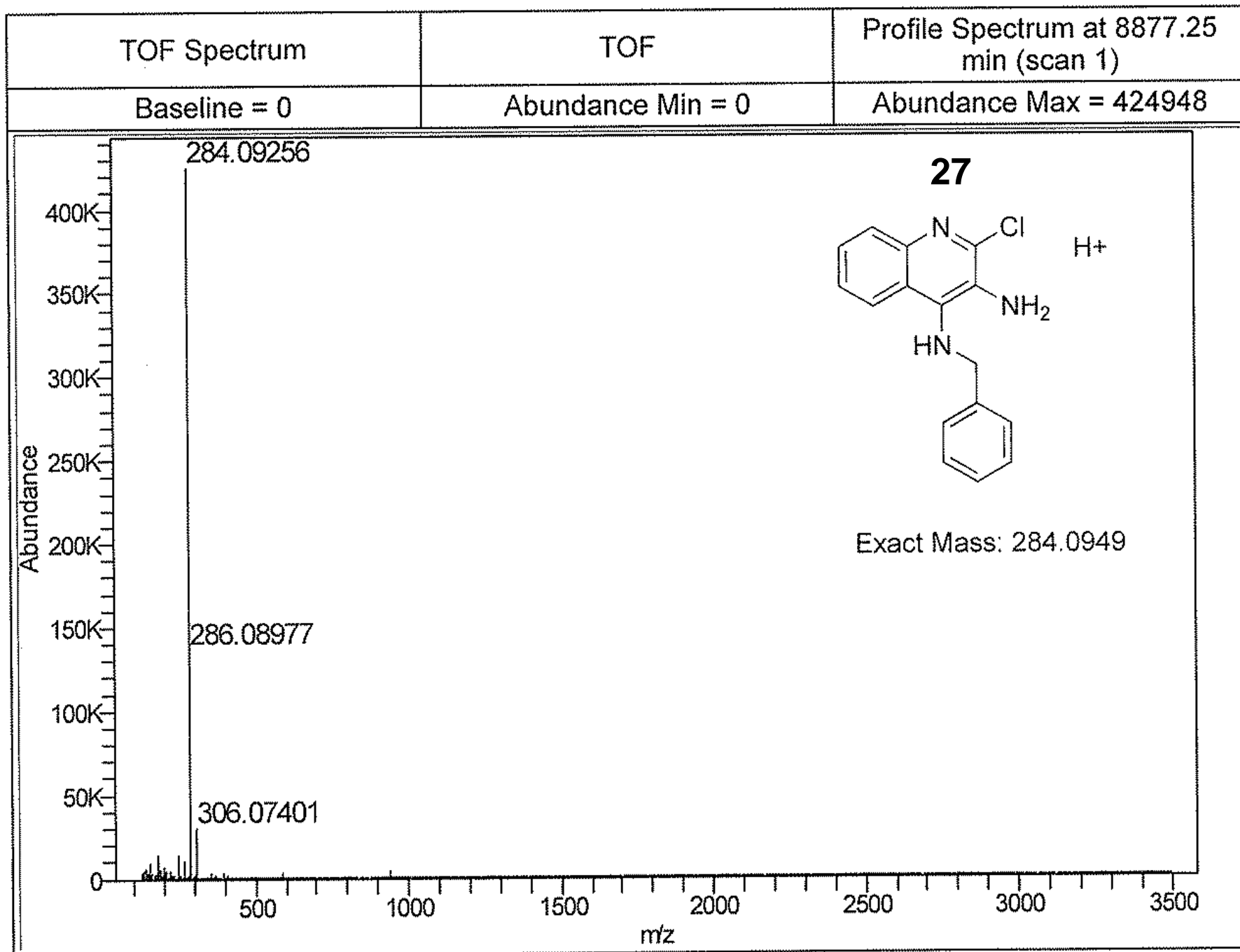
1.11

2.13

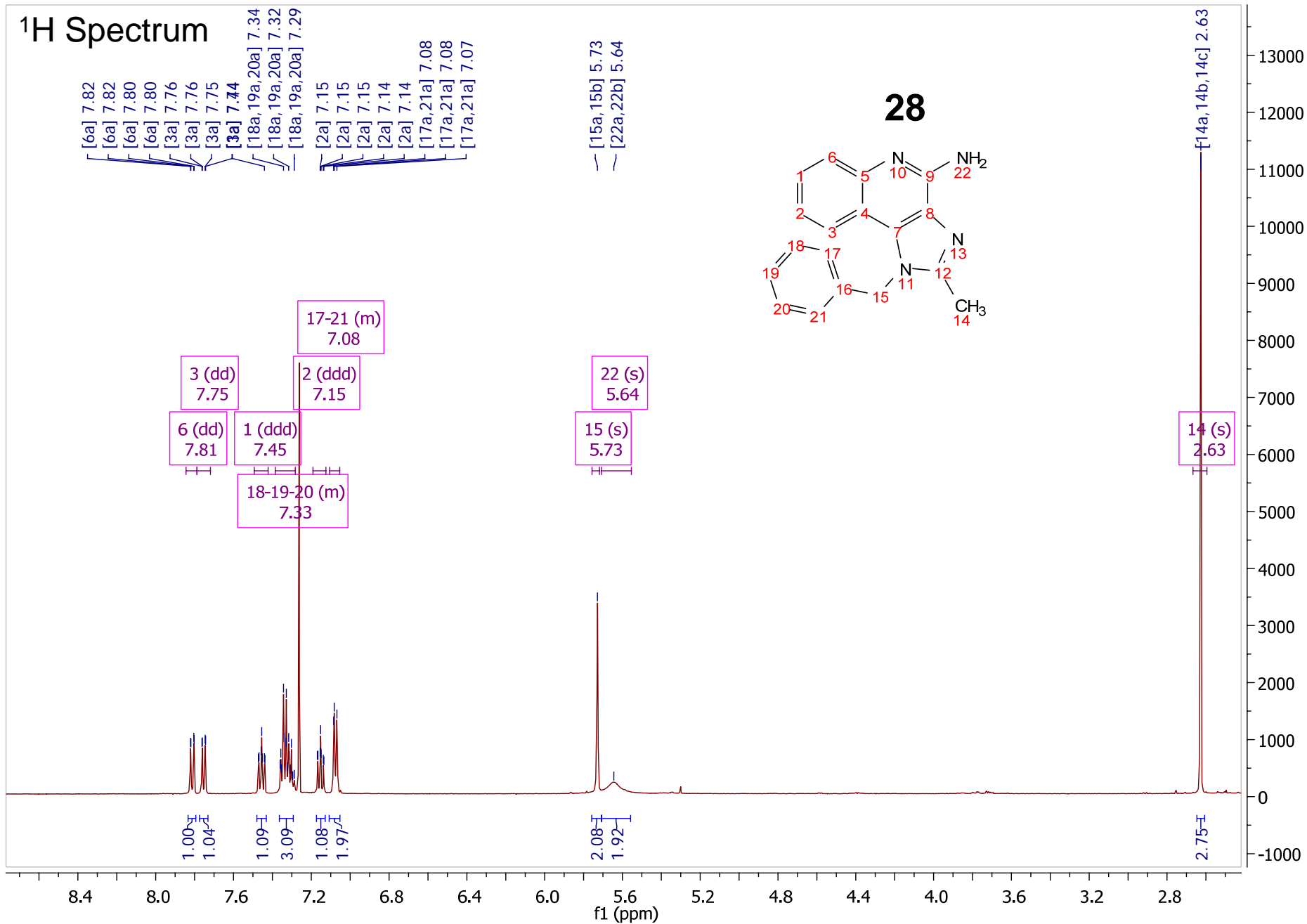
8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6  
f1 (ppm)

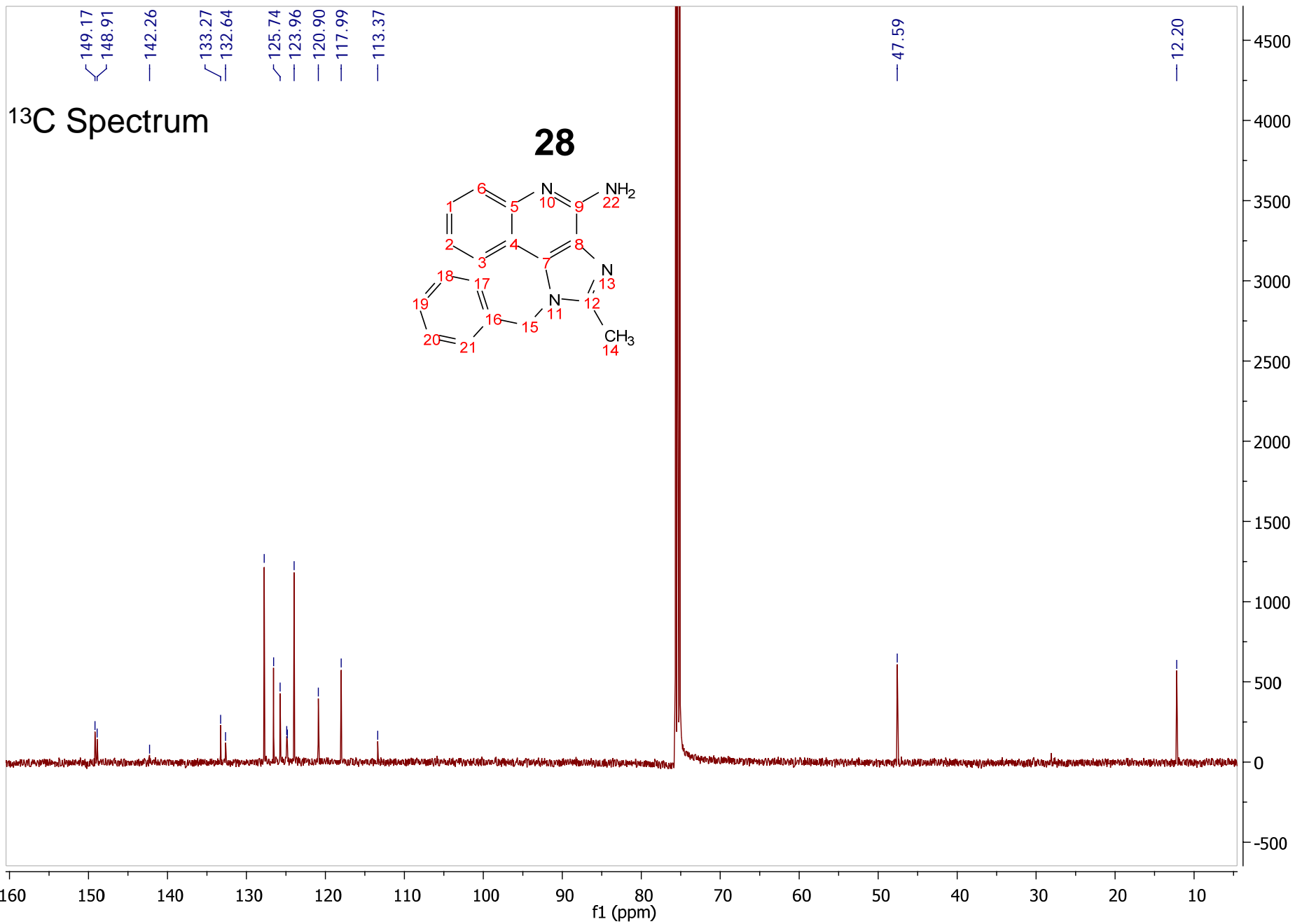
50  
45  
40  
35  
30  
25  
20  
15  
10  
5  
0





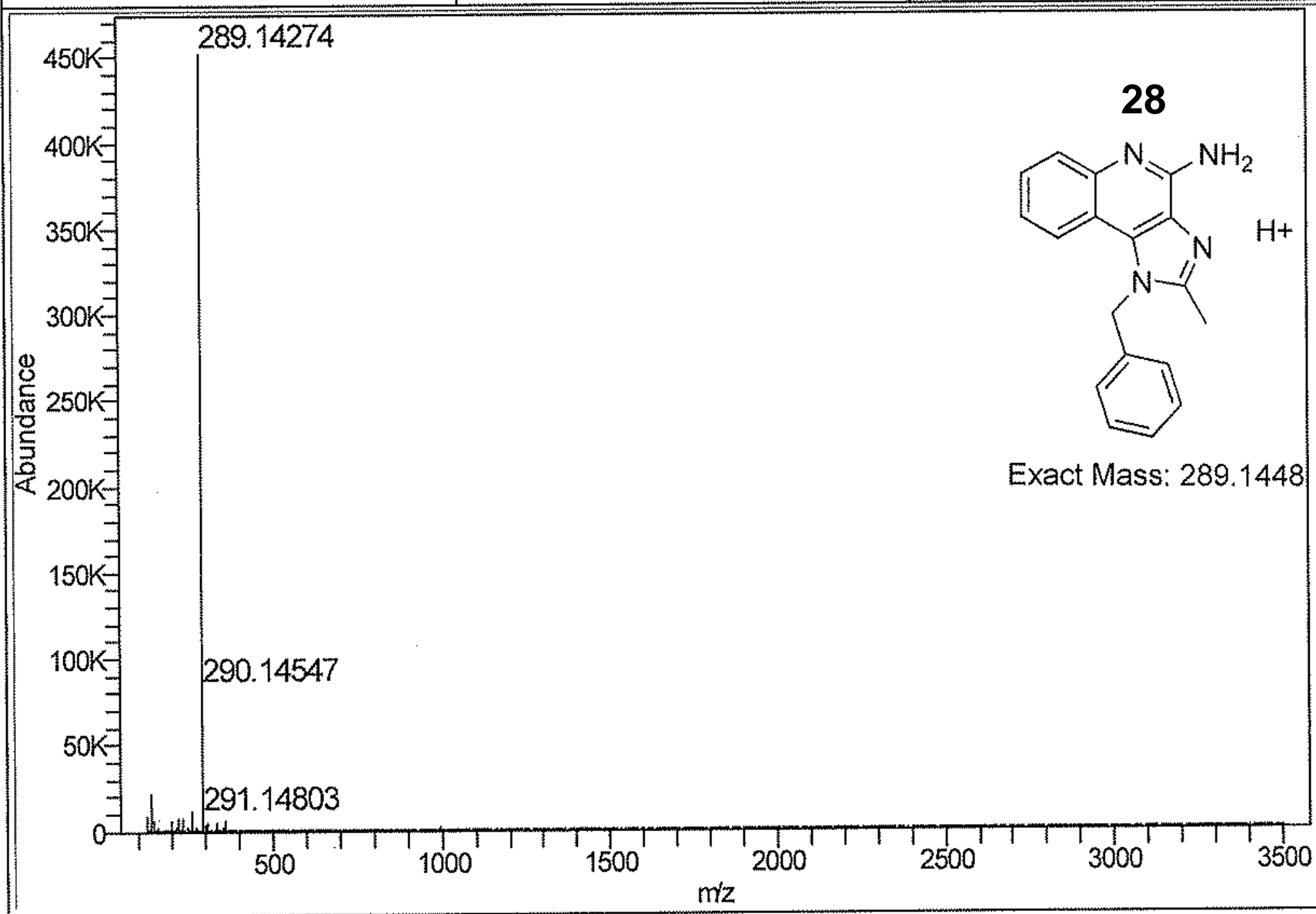
# <sup>1</sup>H Spectrum

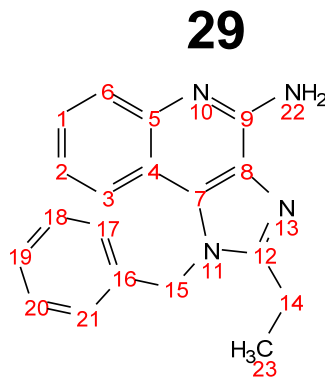




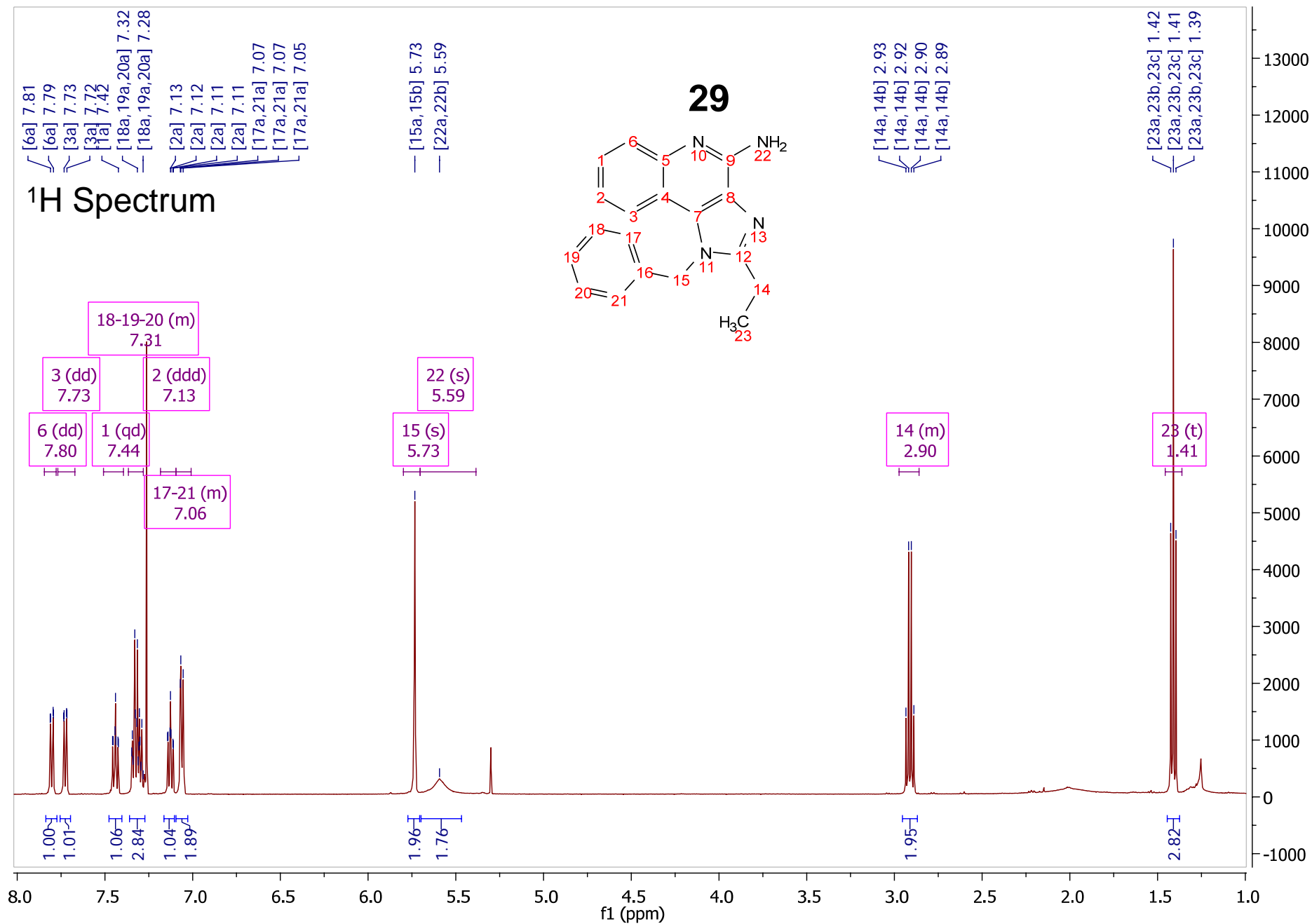


TOF Spectrum	TOF	Profile Spectrum at 21888.19 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 452516

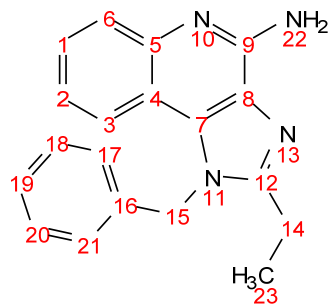




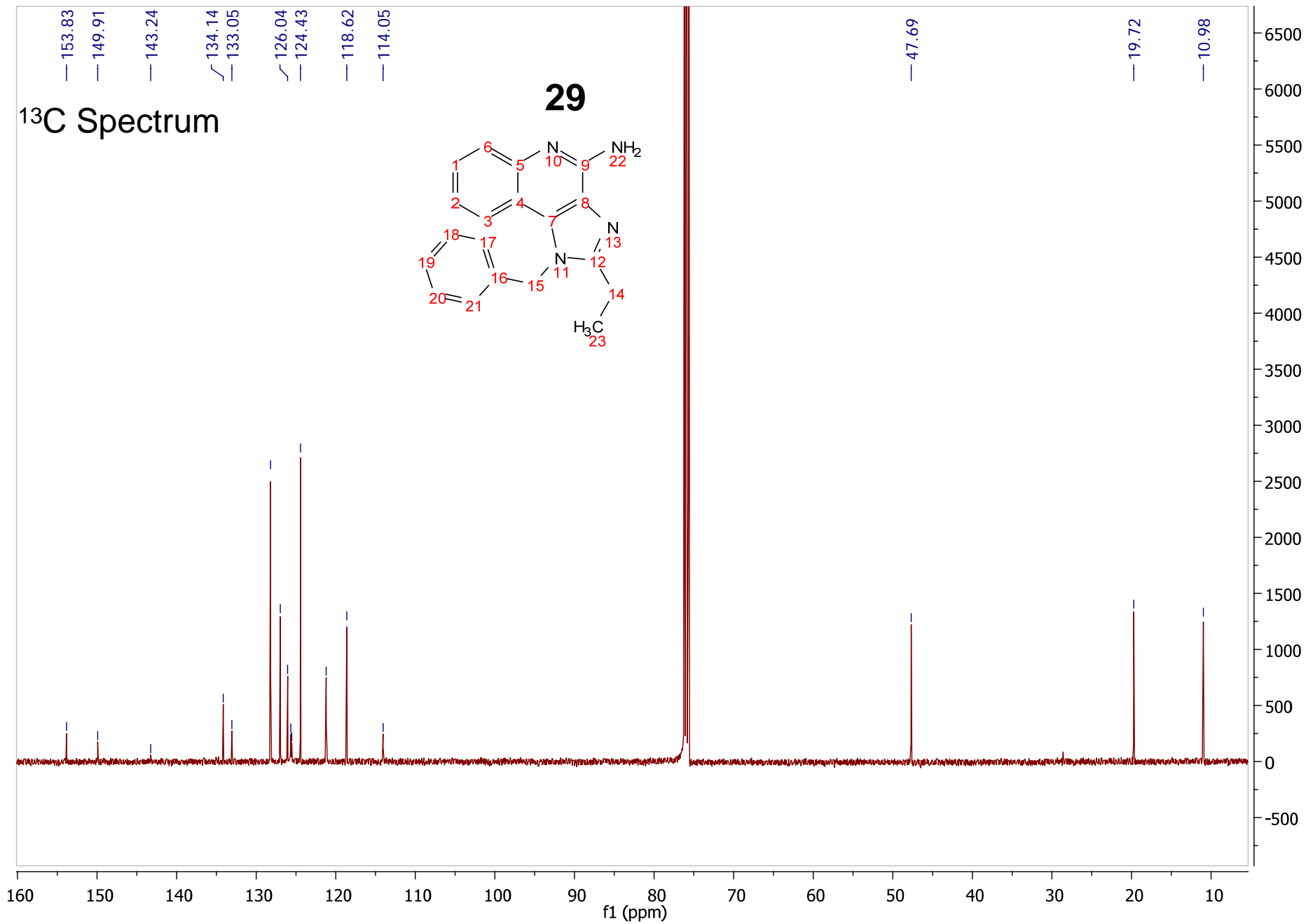
# <sup>1</sup>H Spectrum



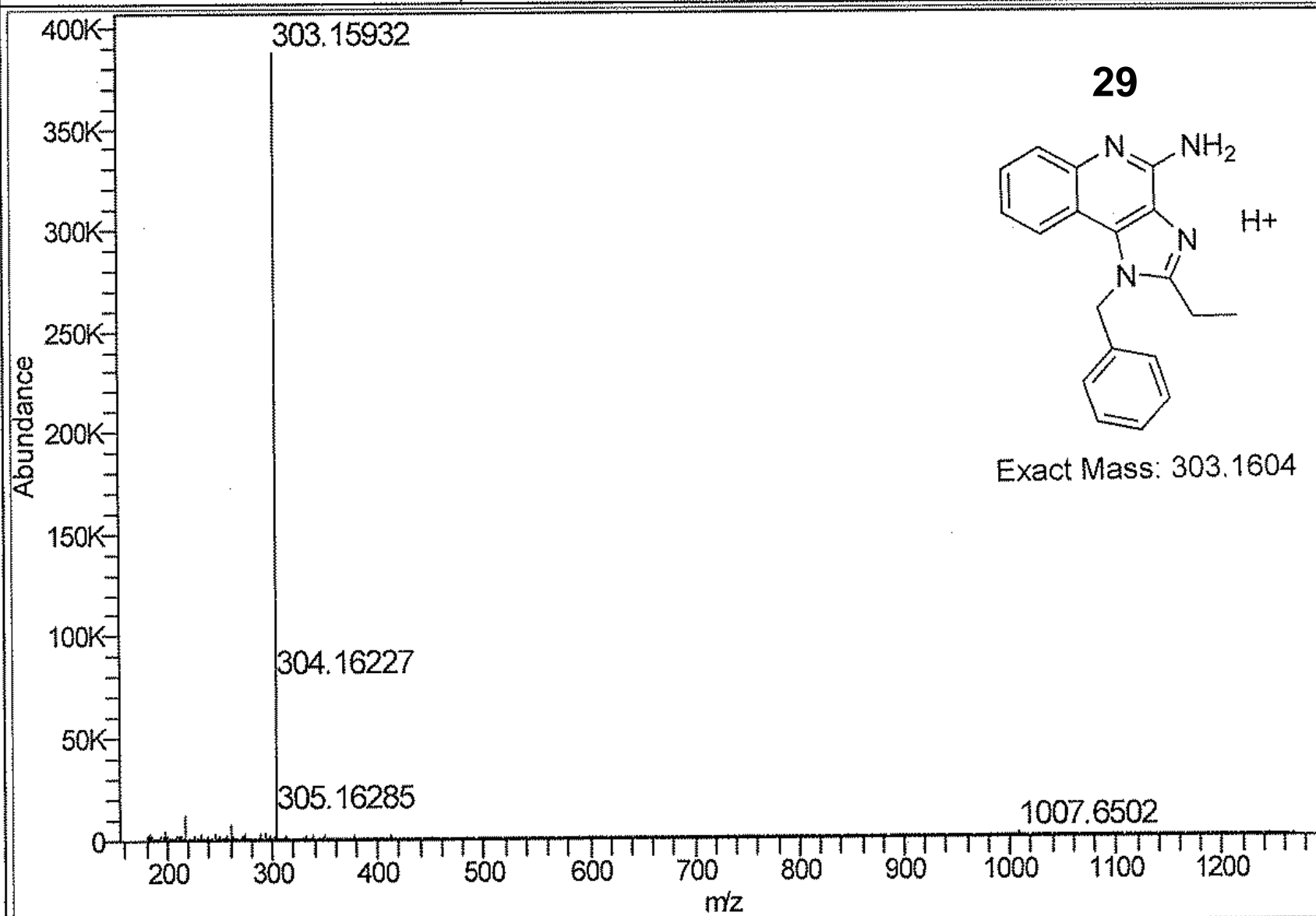
29

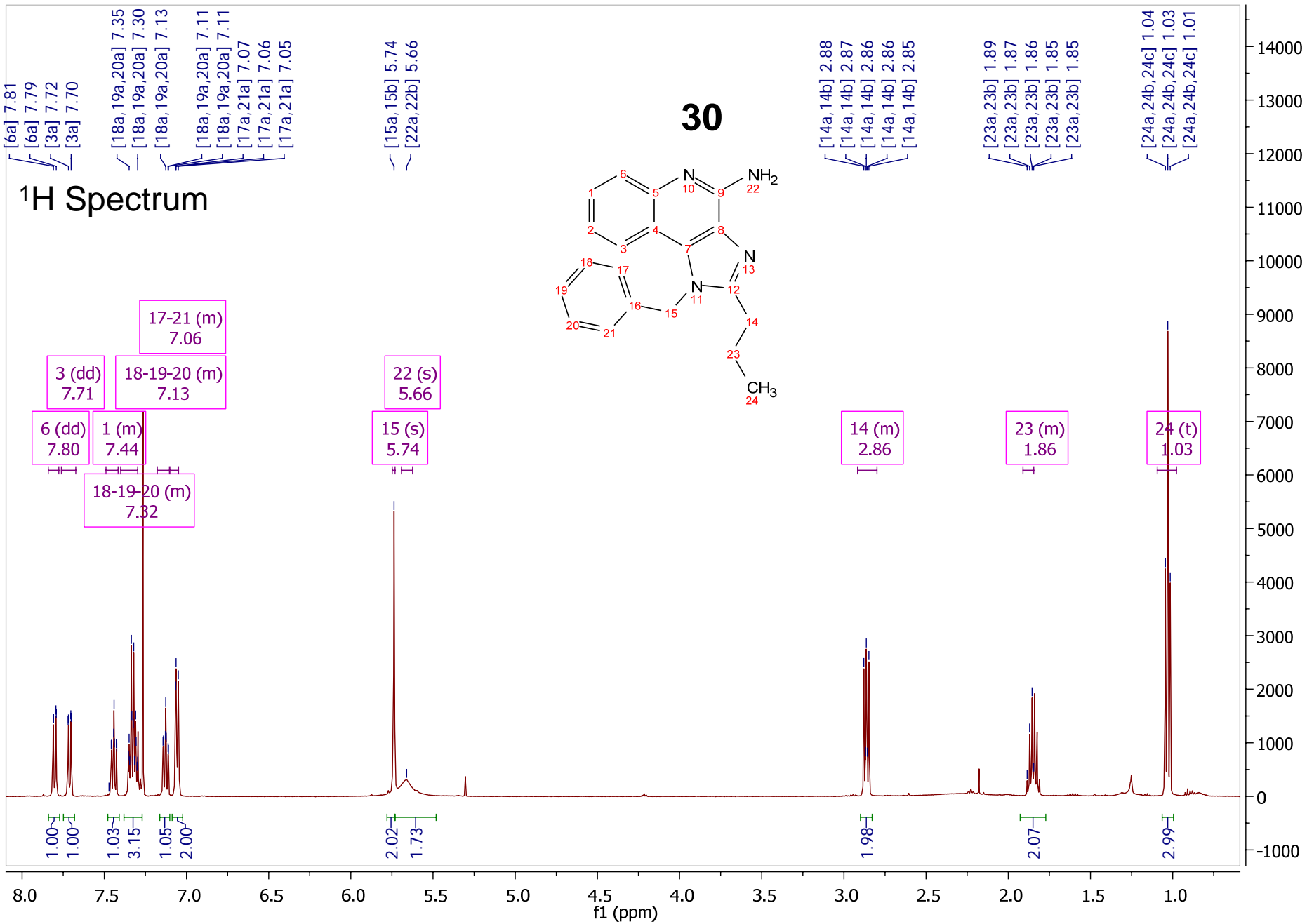


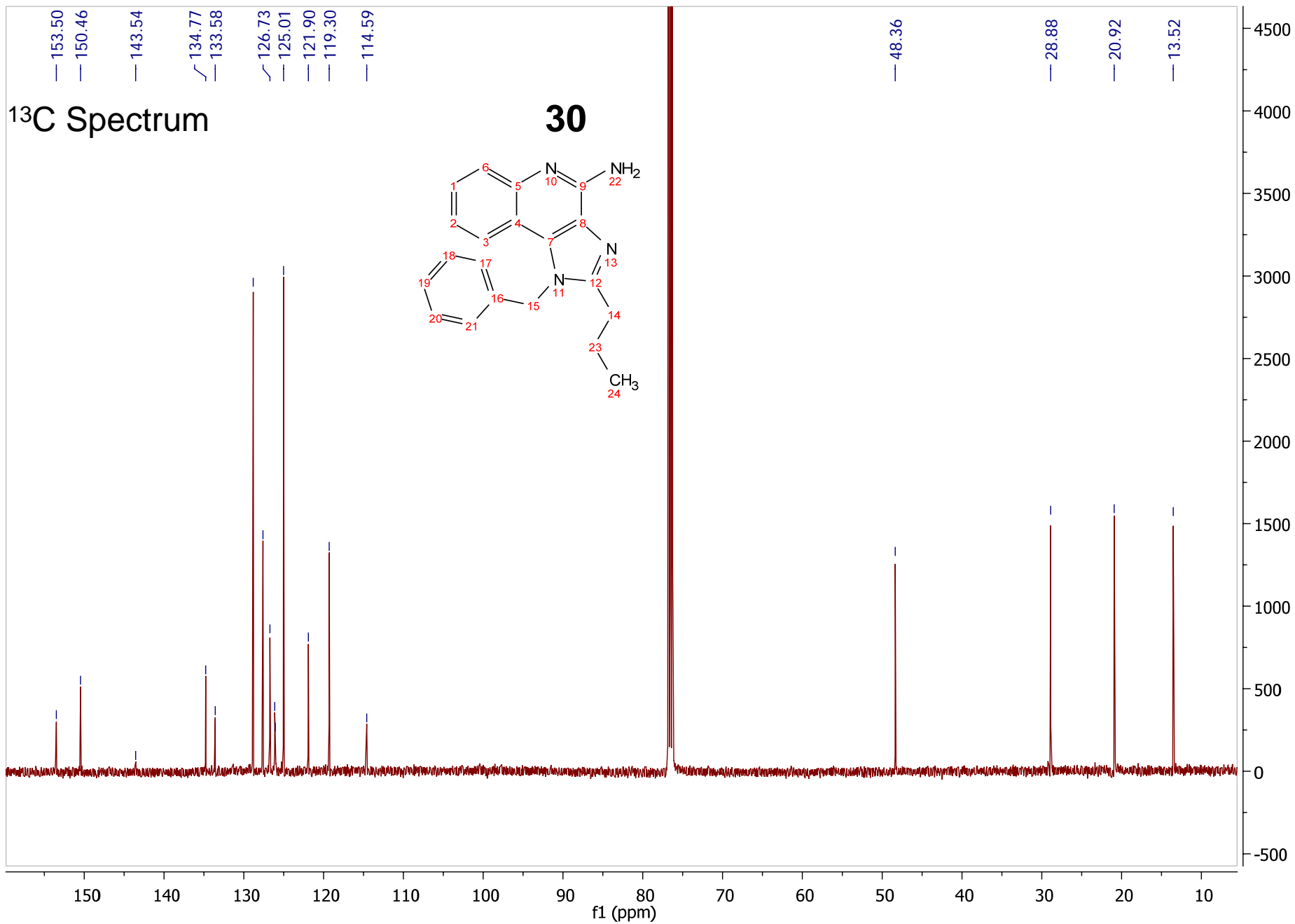
<sup>13</sup>C Spectrum

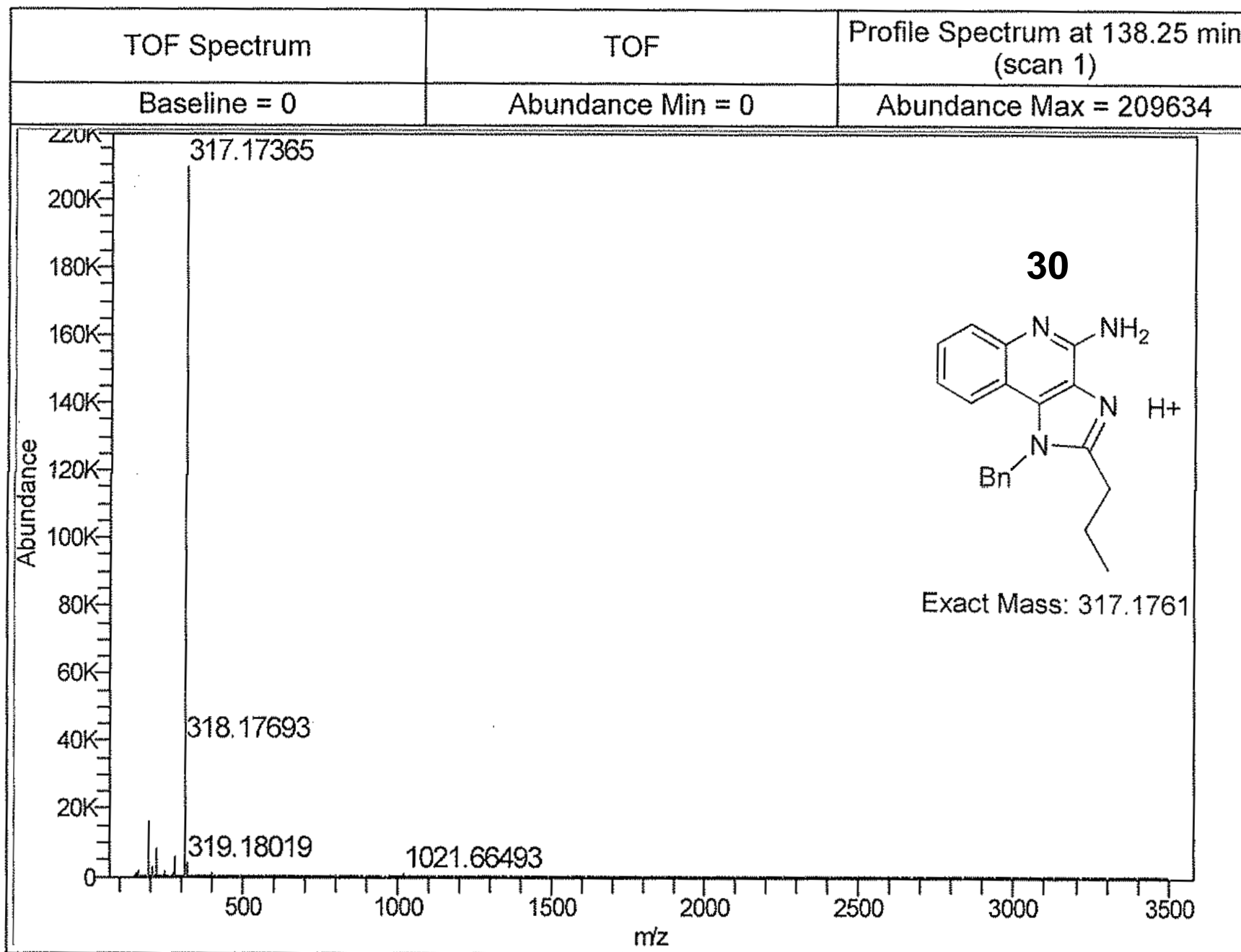


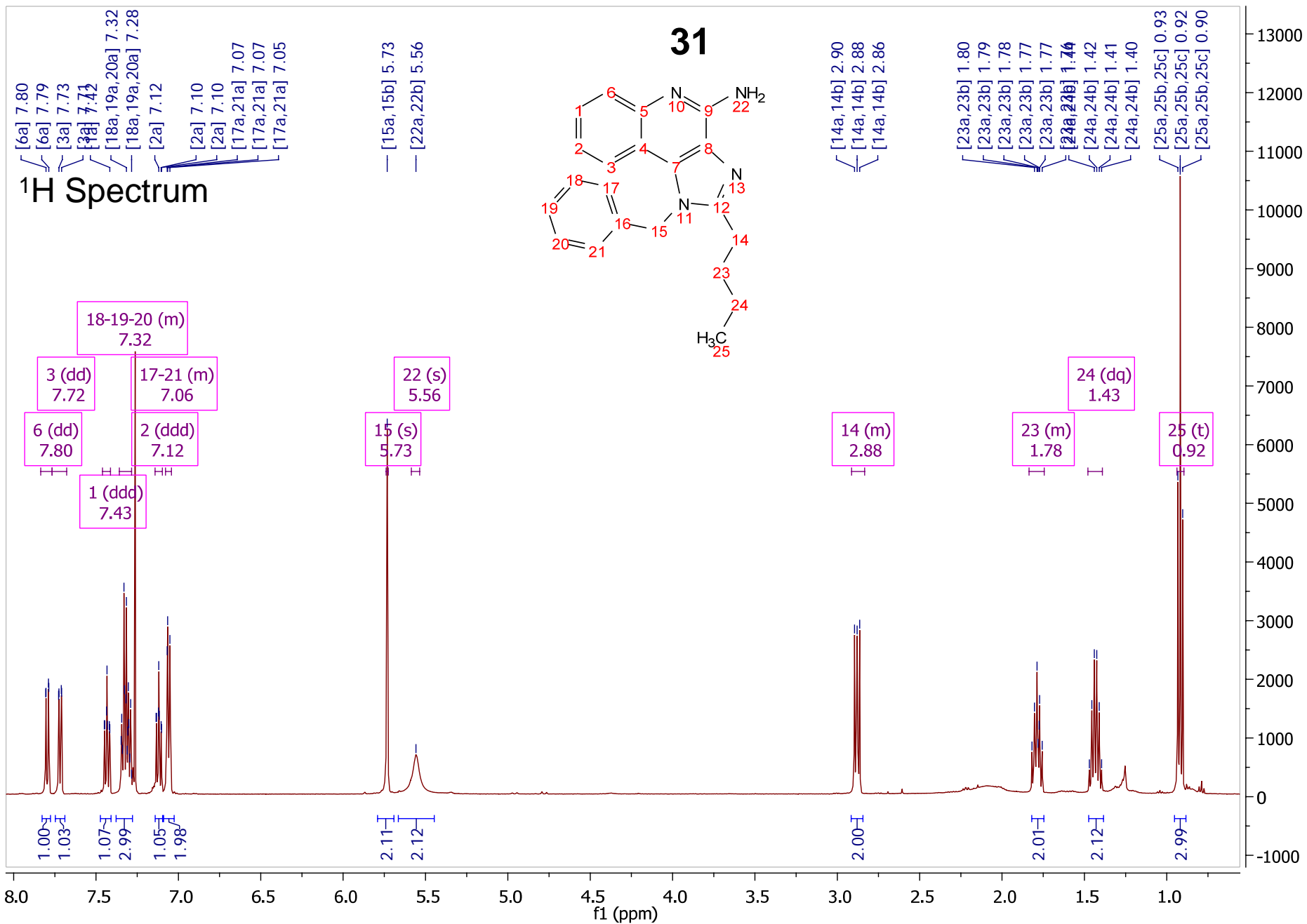
TOF Spectrum	TOF	Profile Spectrum at 21800.80 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 388055



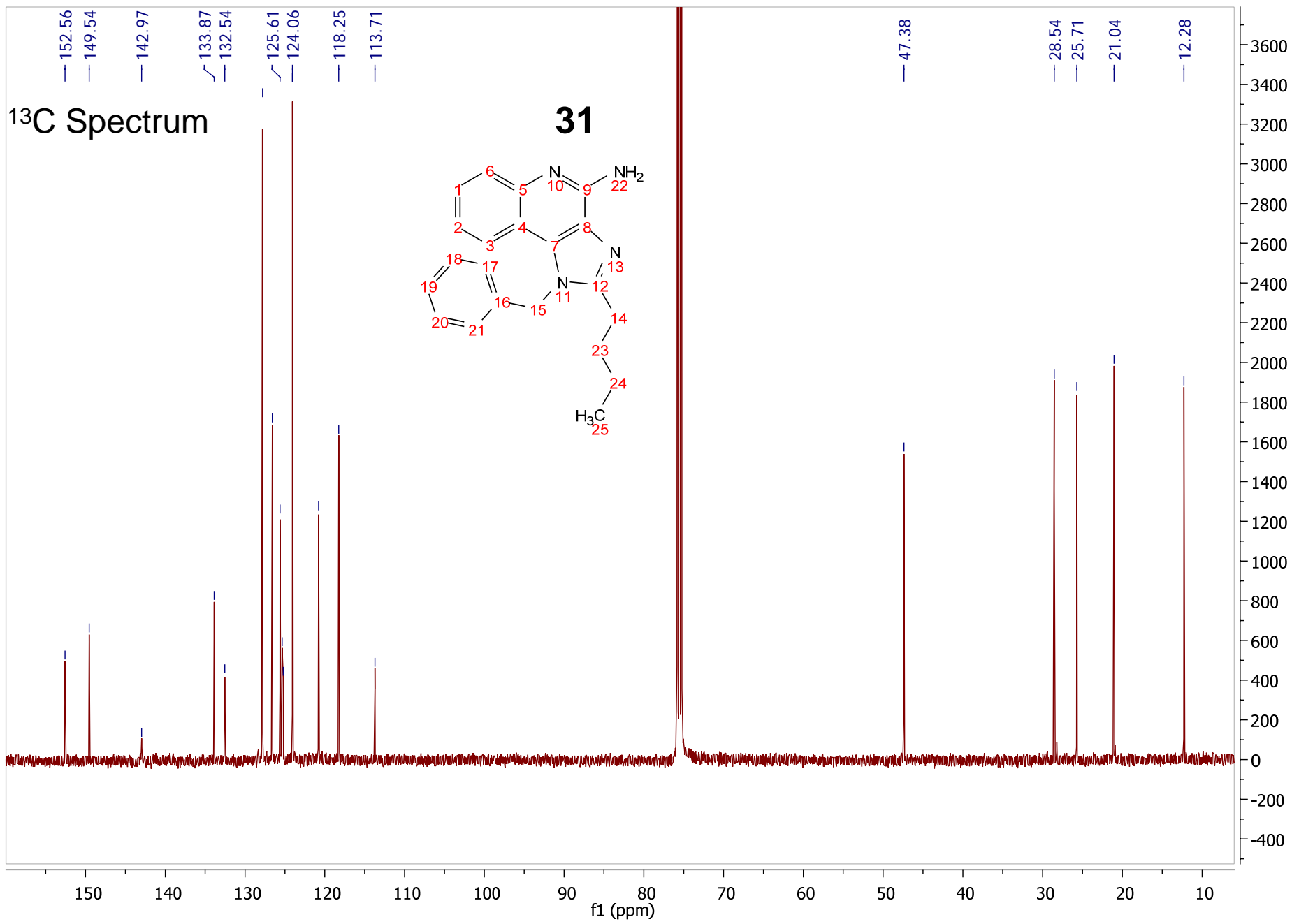




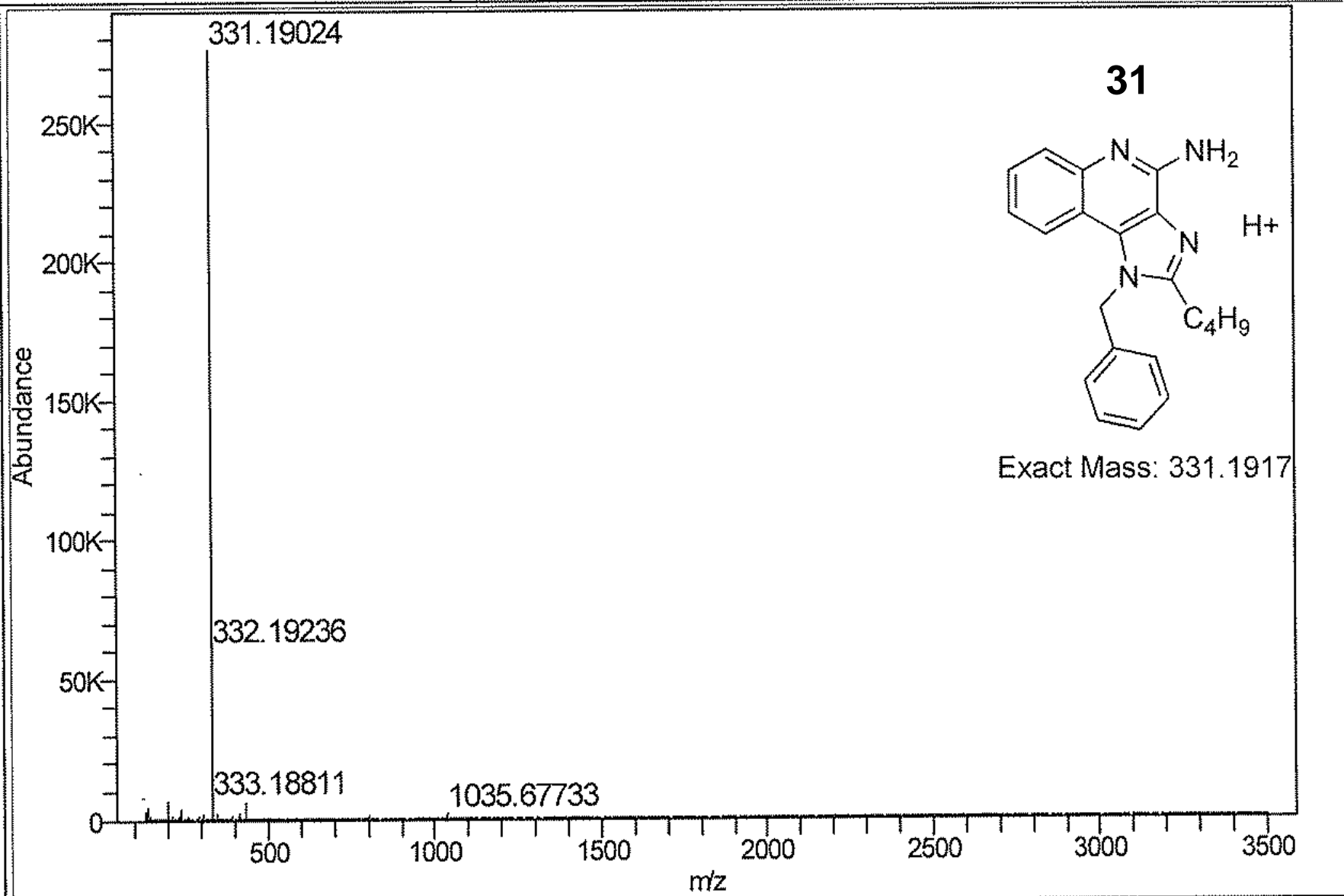




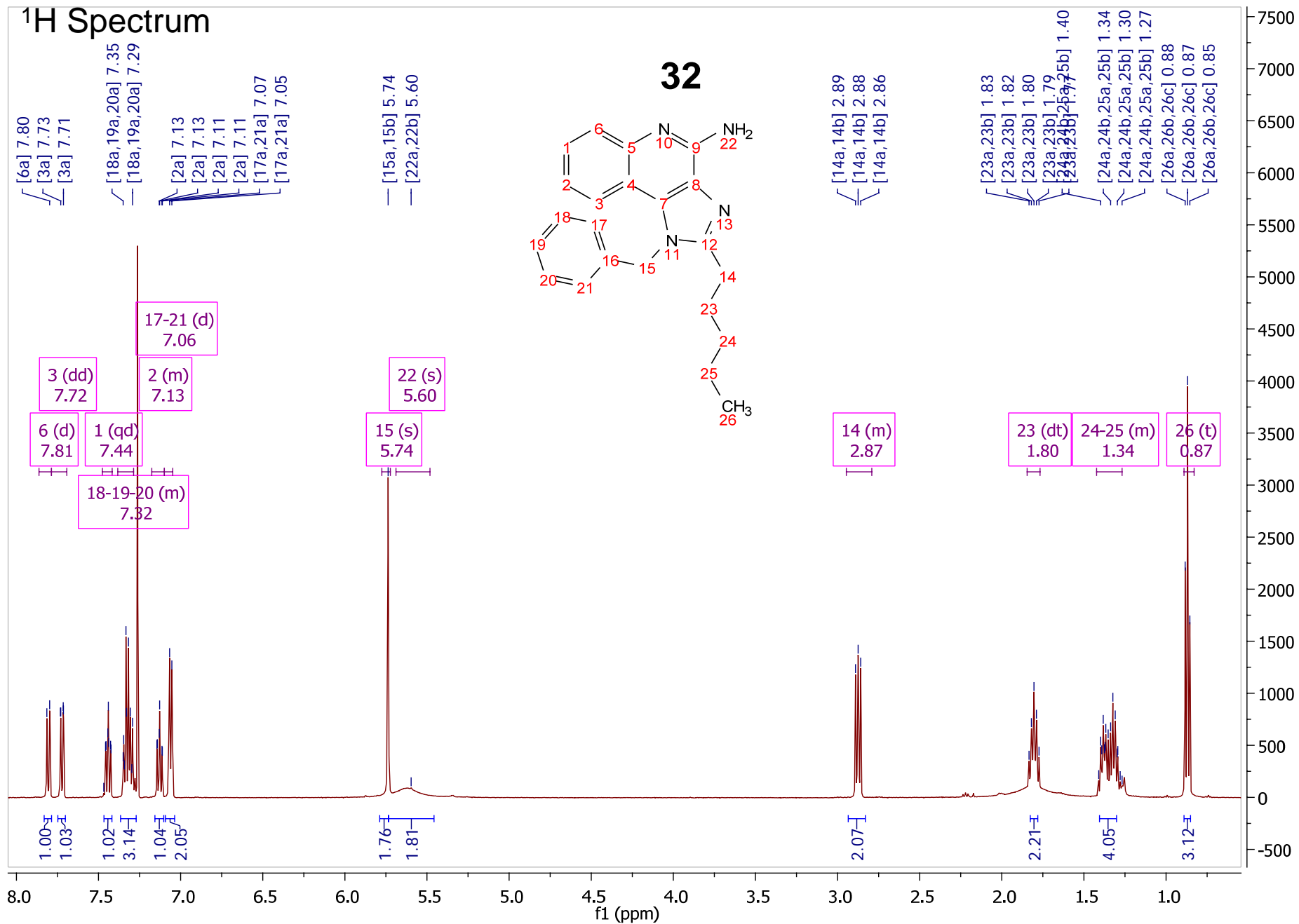


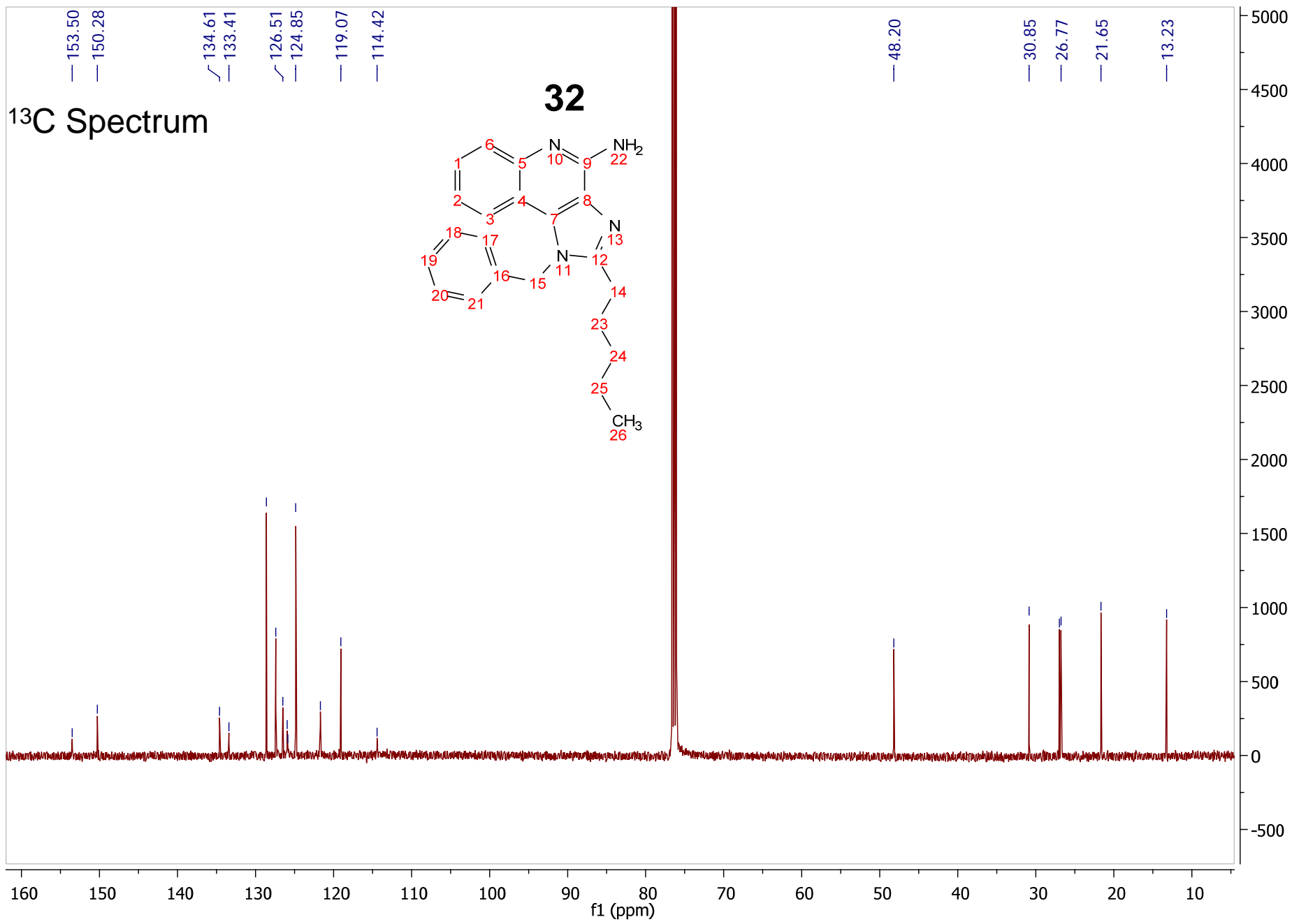


TOF Spectrum	TOF	Profile Spectrum at 21824.52 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 276688

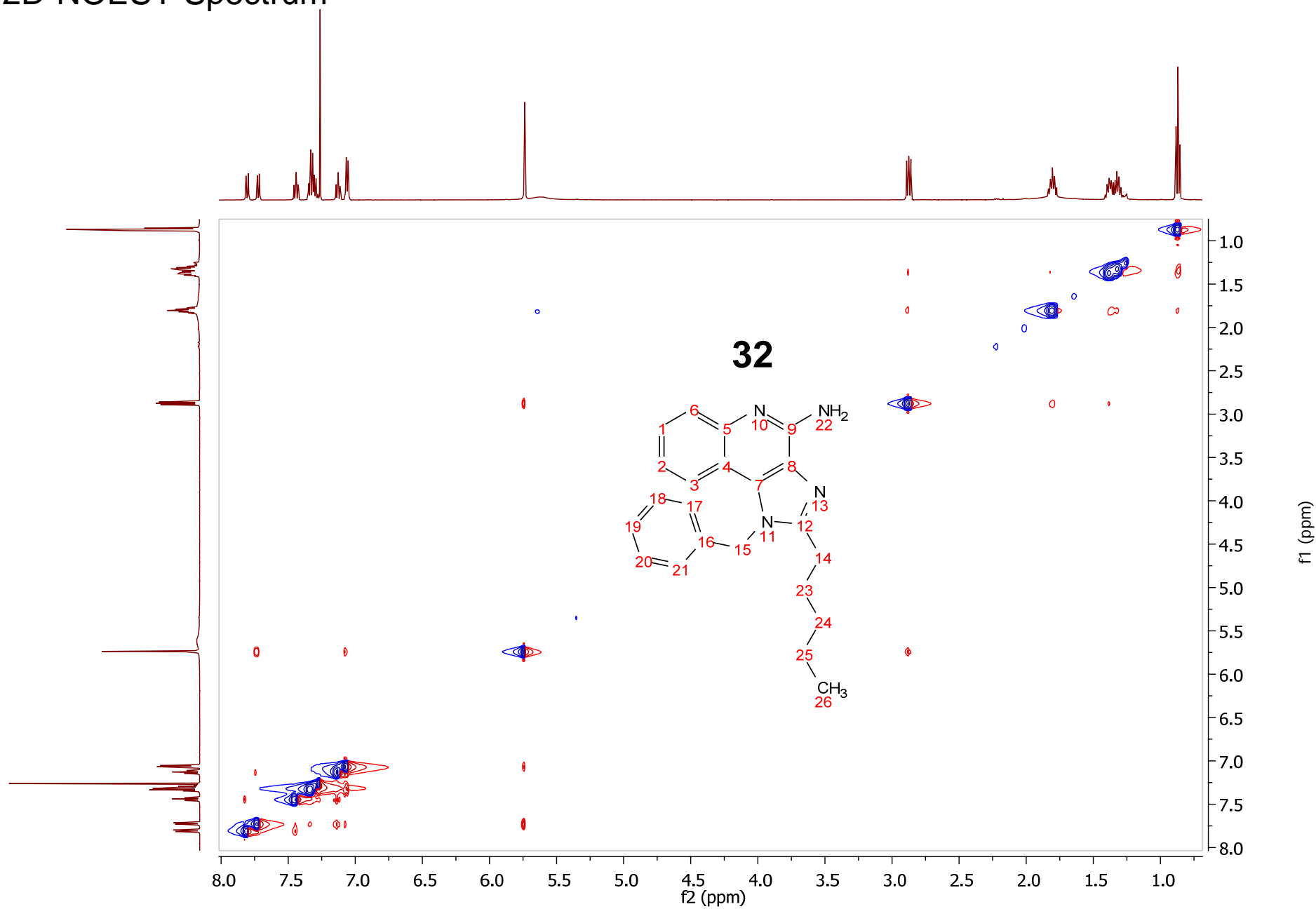


# <sup>1</sup>H Spectrum

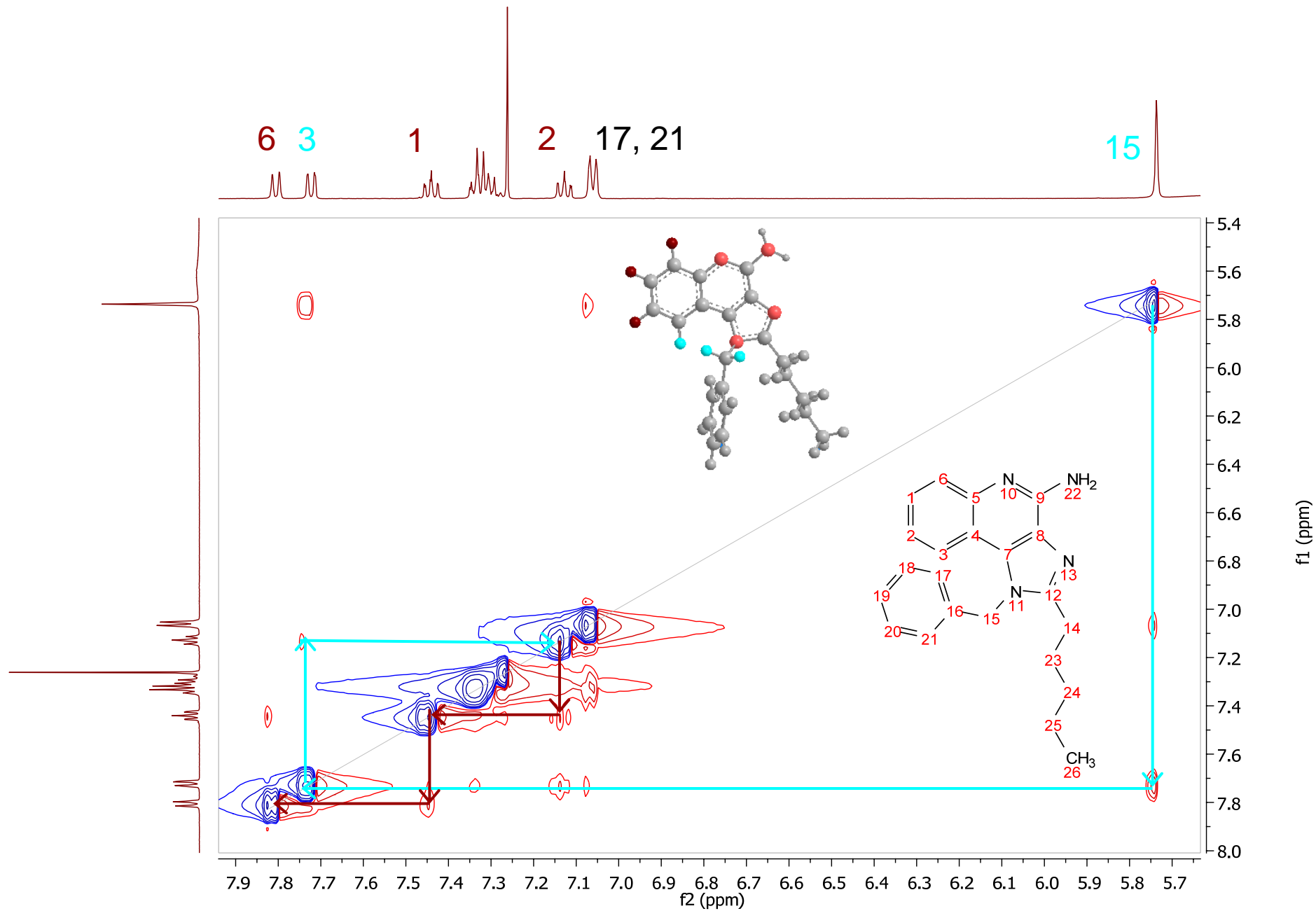




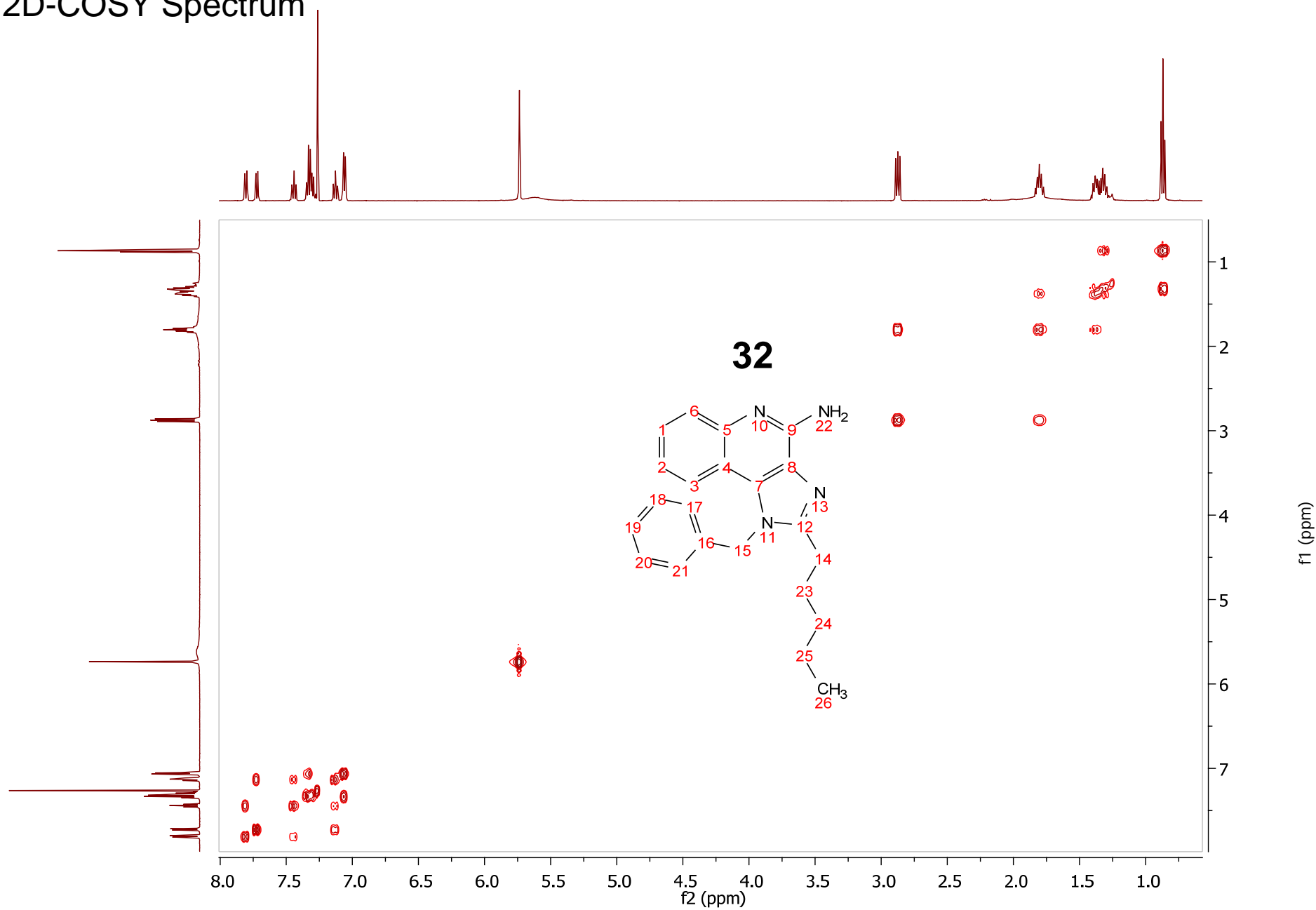
# 2D-NOESY Spectrum



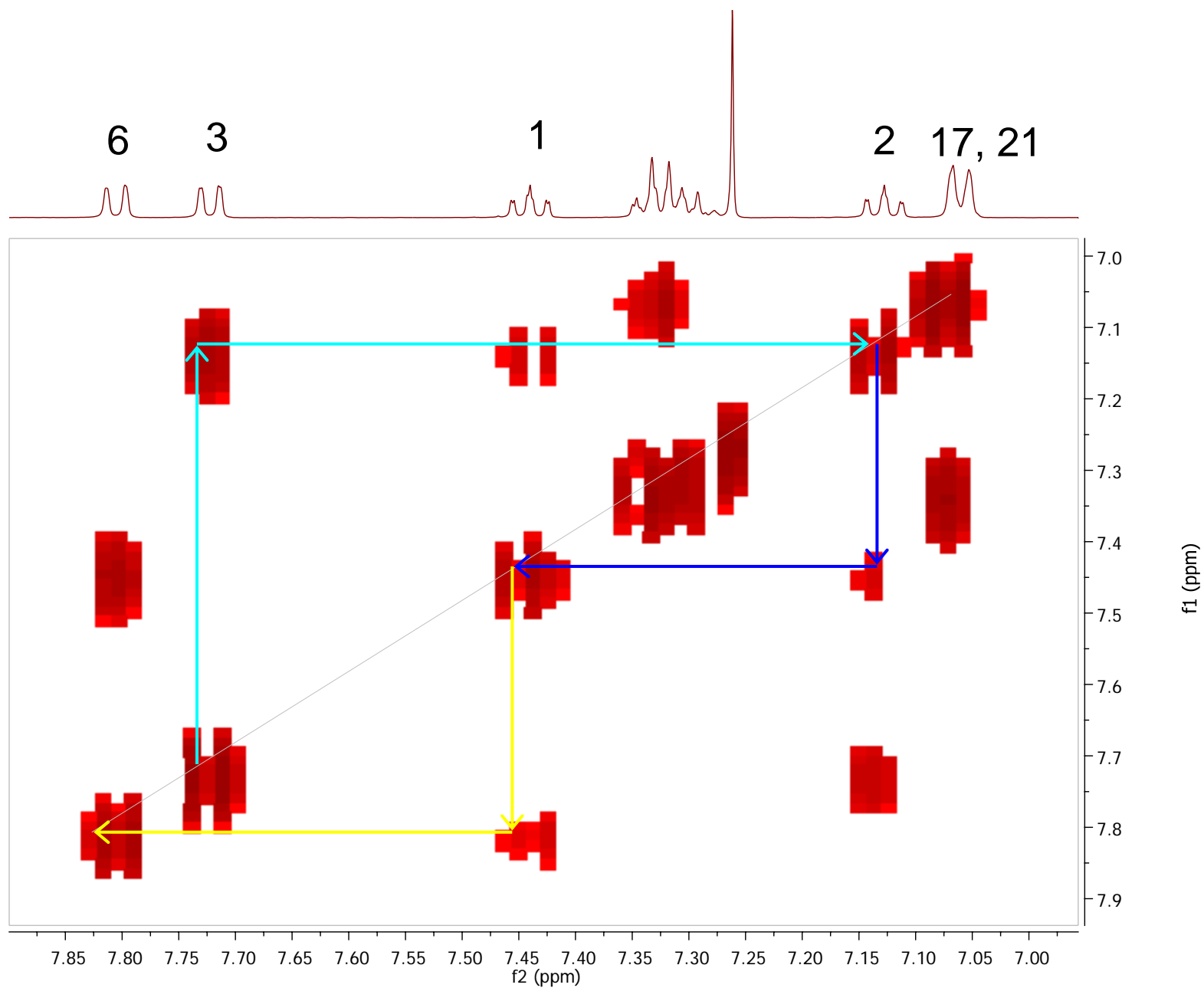
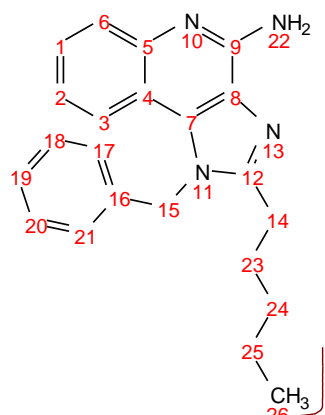
# Aromatic Region of the 2D-NOESY Spectrum of the Compound **32**



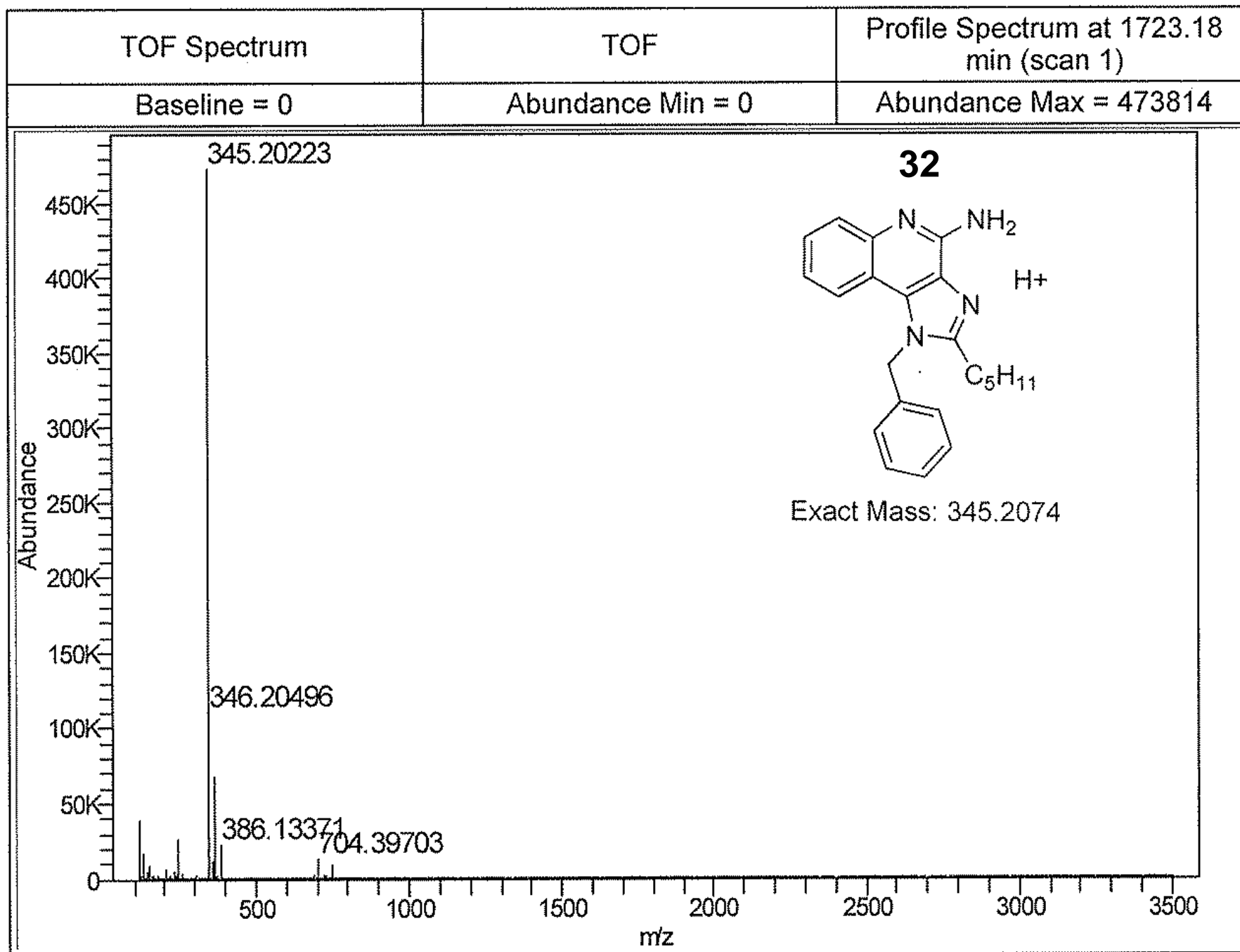
# 2D-COSY Spectrum



# Aromatic Region of the 2D-COSY Spectrum of the Compound **32**

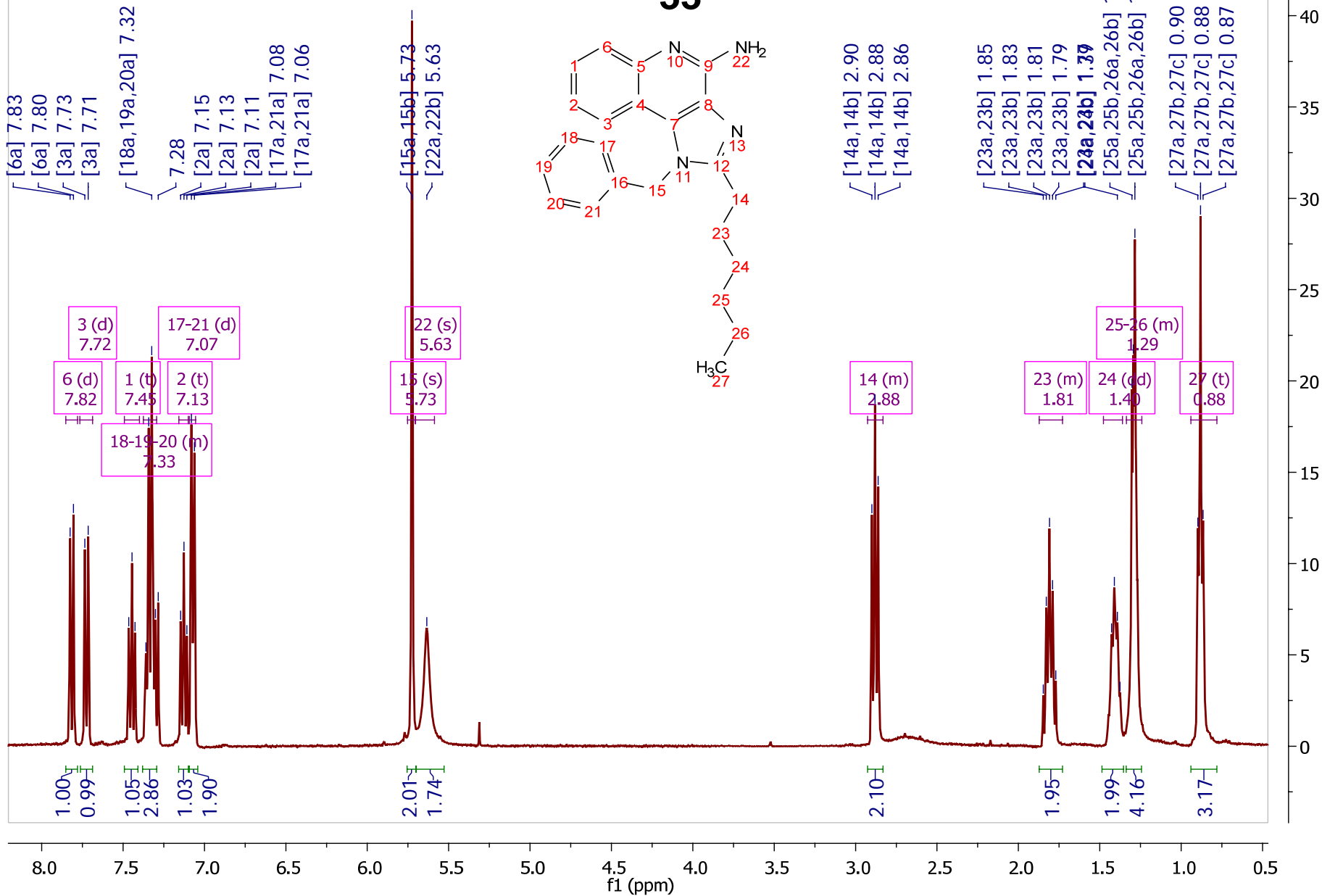
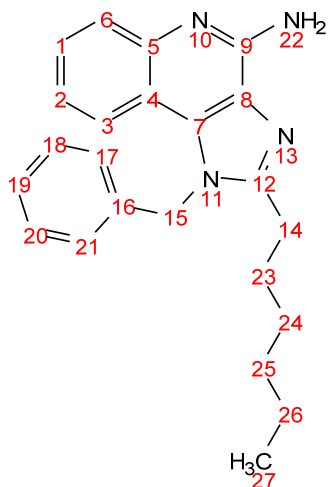






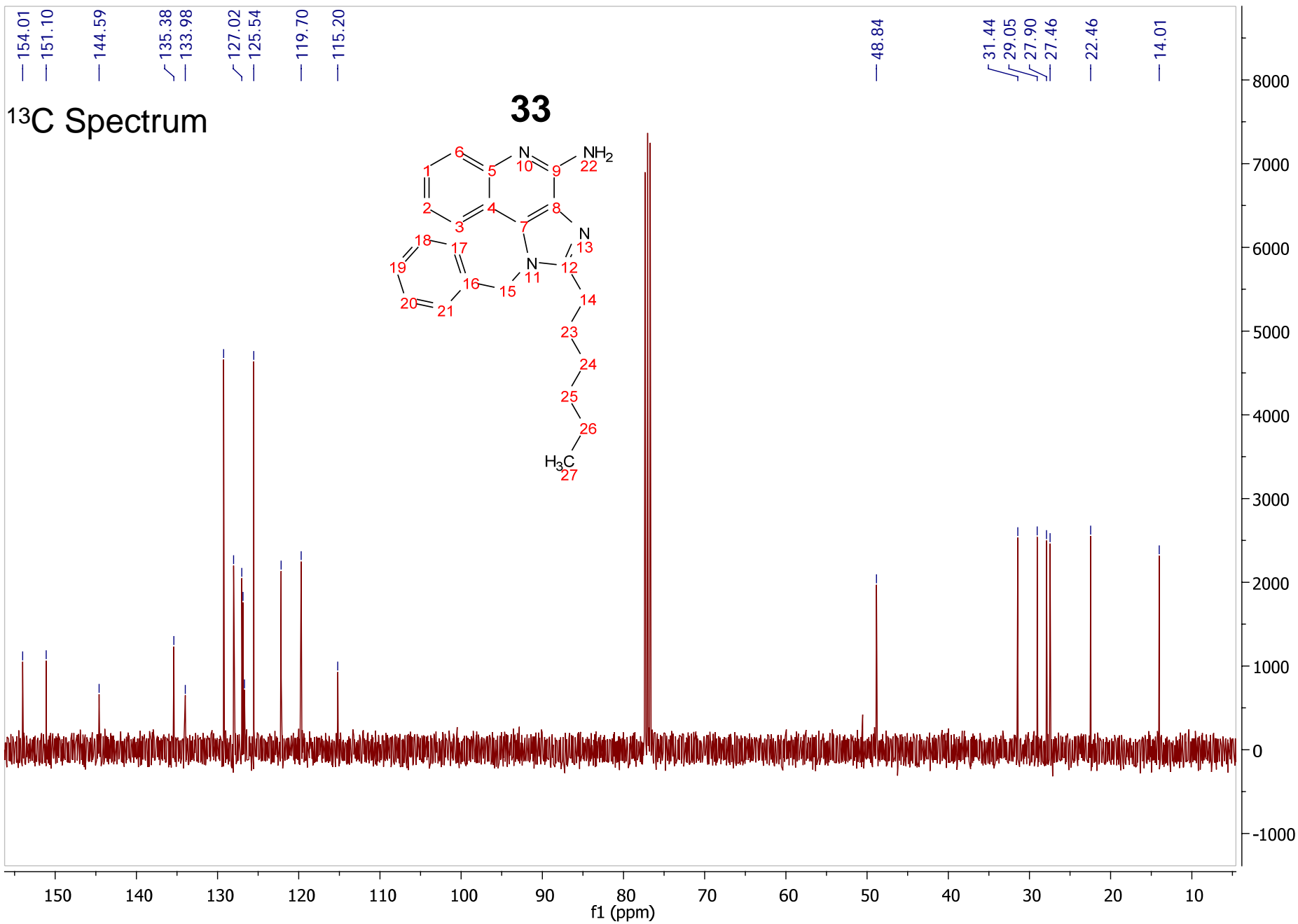
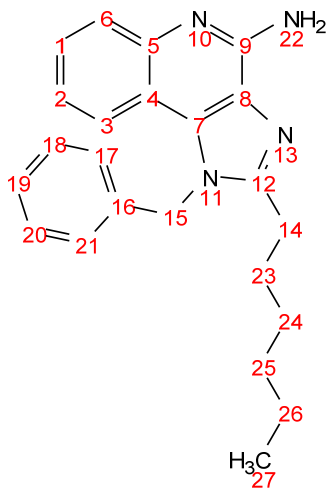
# <sup>1</sup>H Spectrum

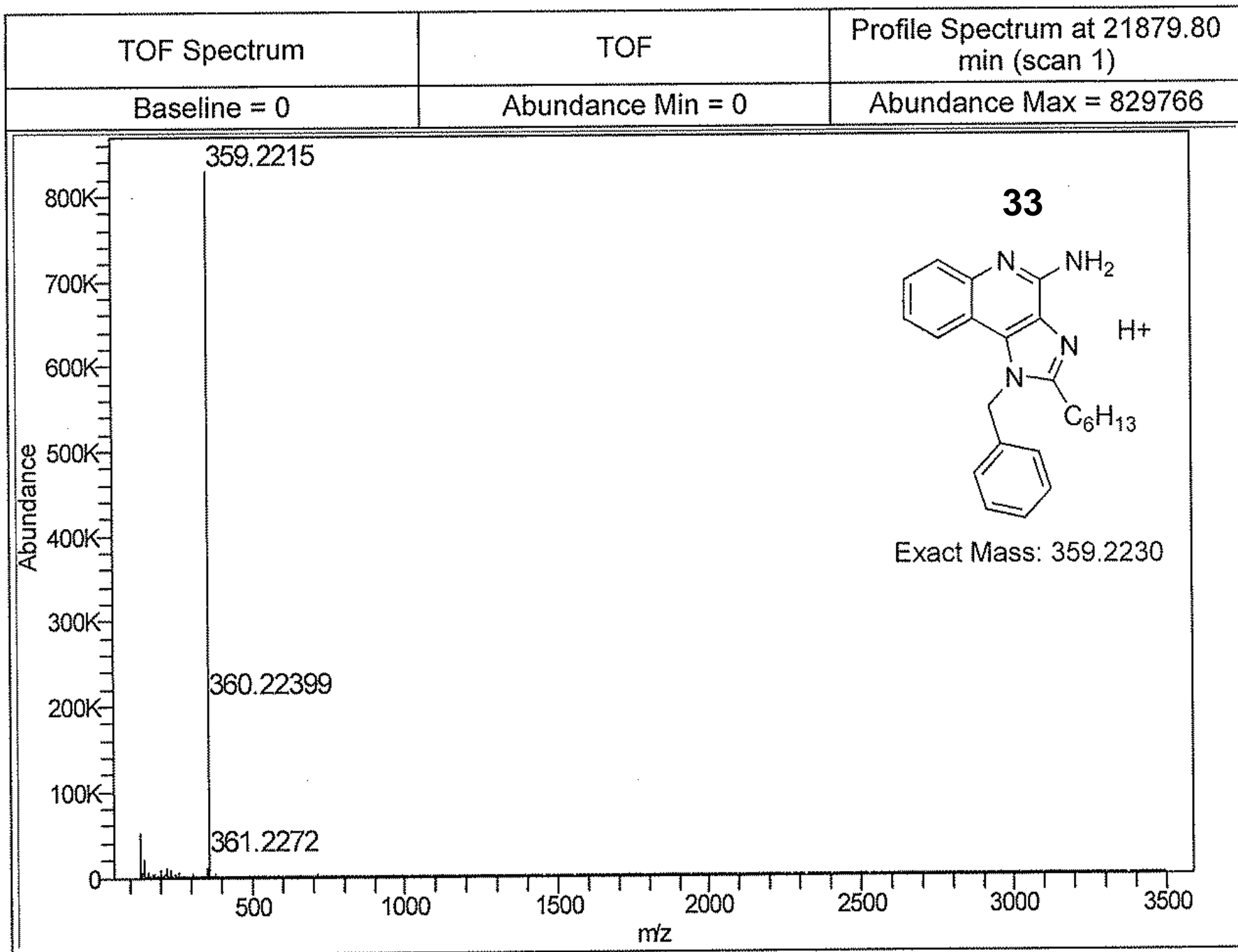
**33**



# <sup>13</sup>C Spectrum

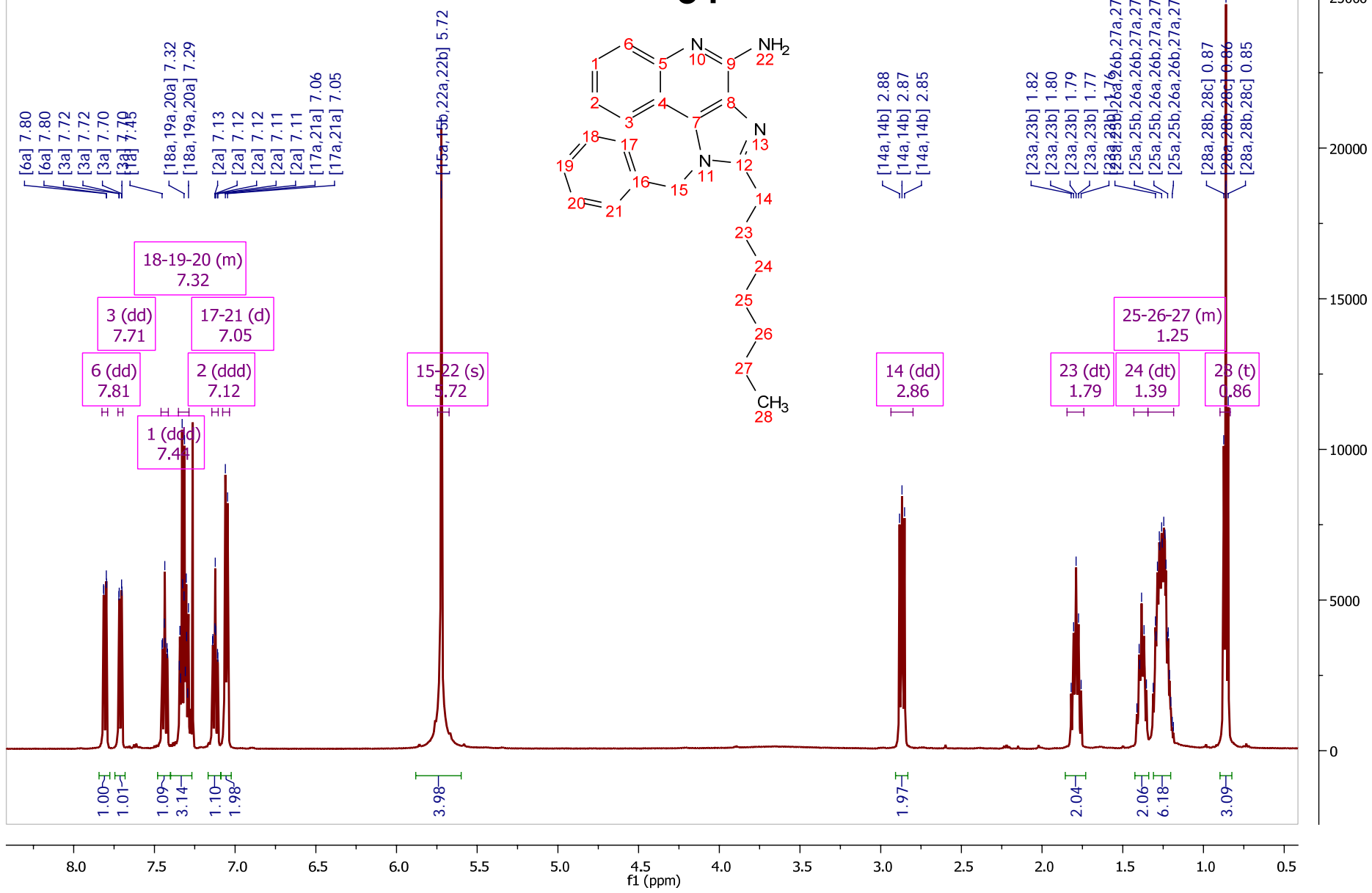
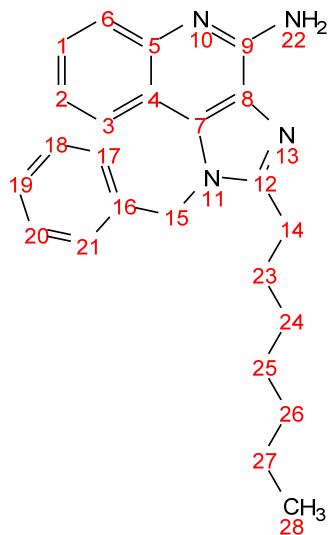
**33**





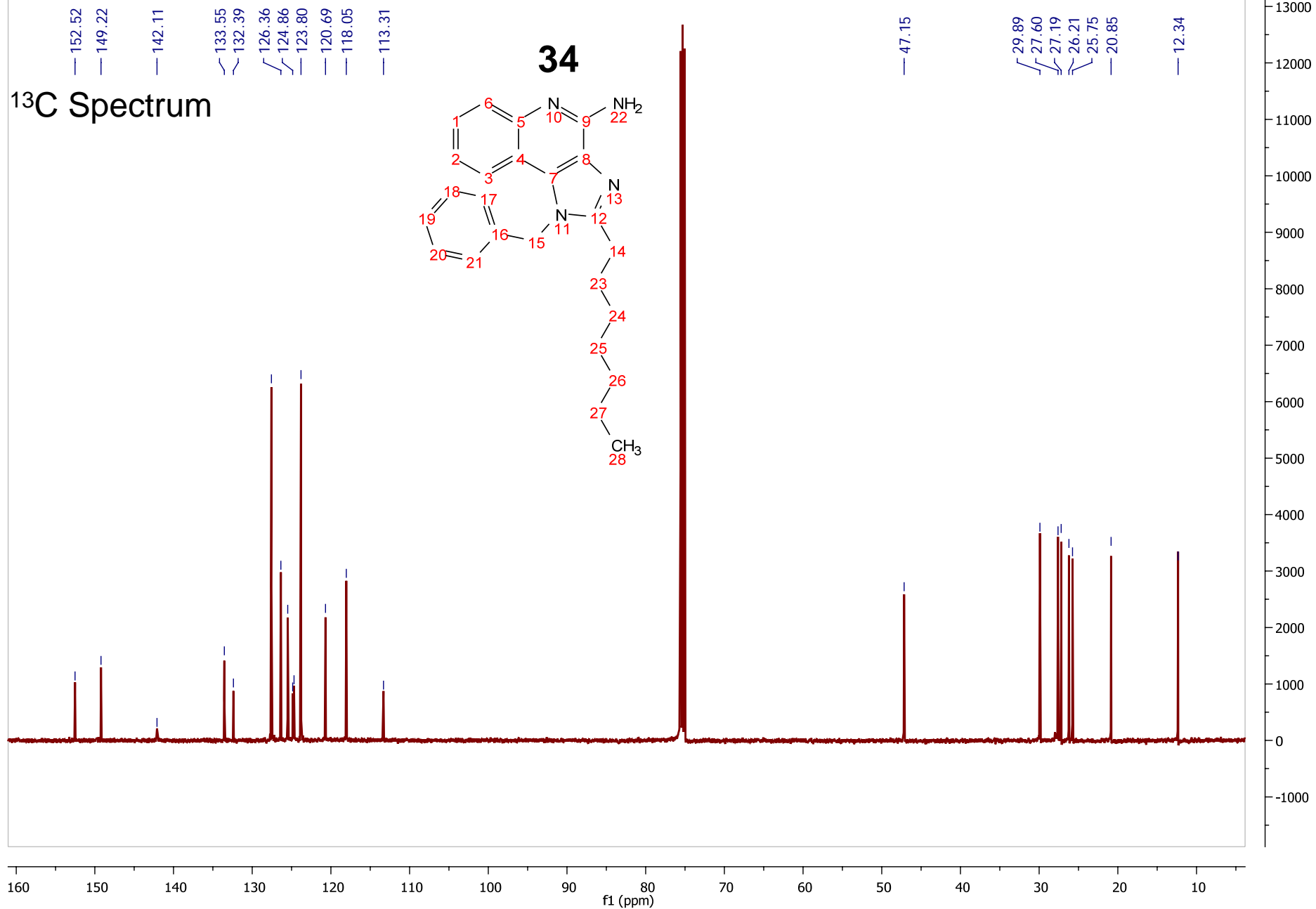
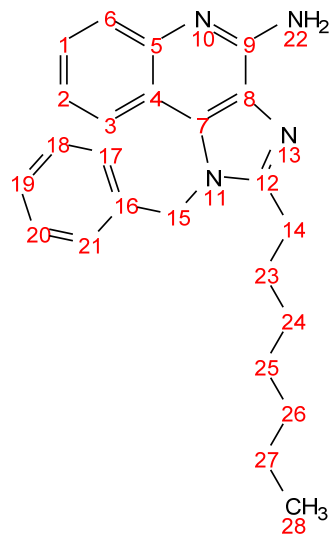
# <sup>1</sup>H Spectrum

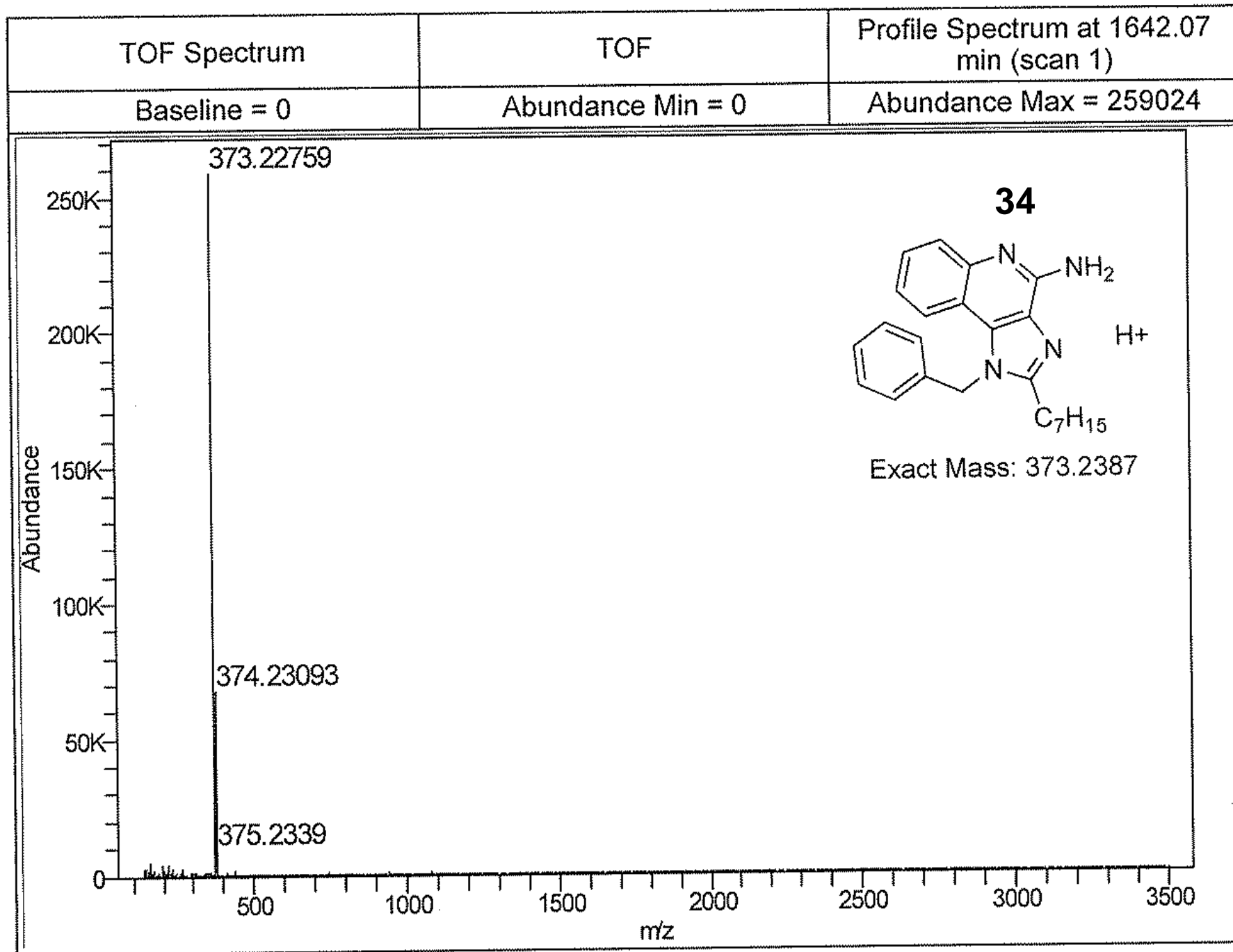
34



# <sup>13</sup>C Spectrum

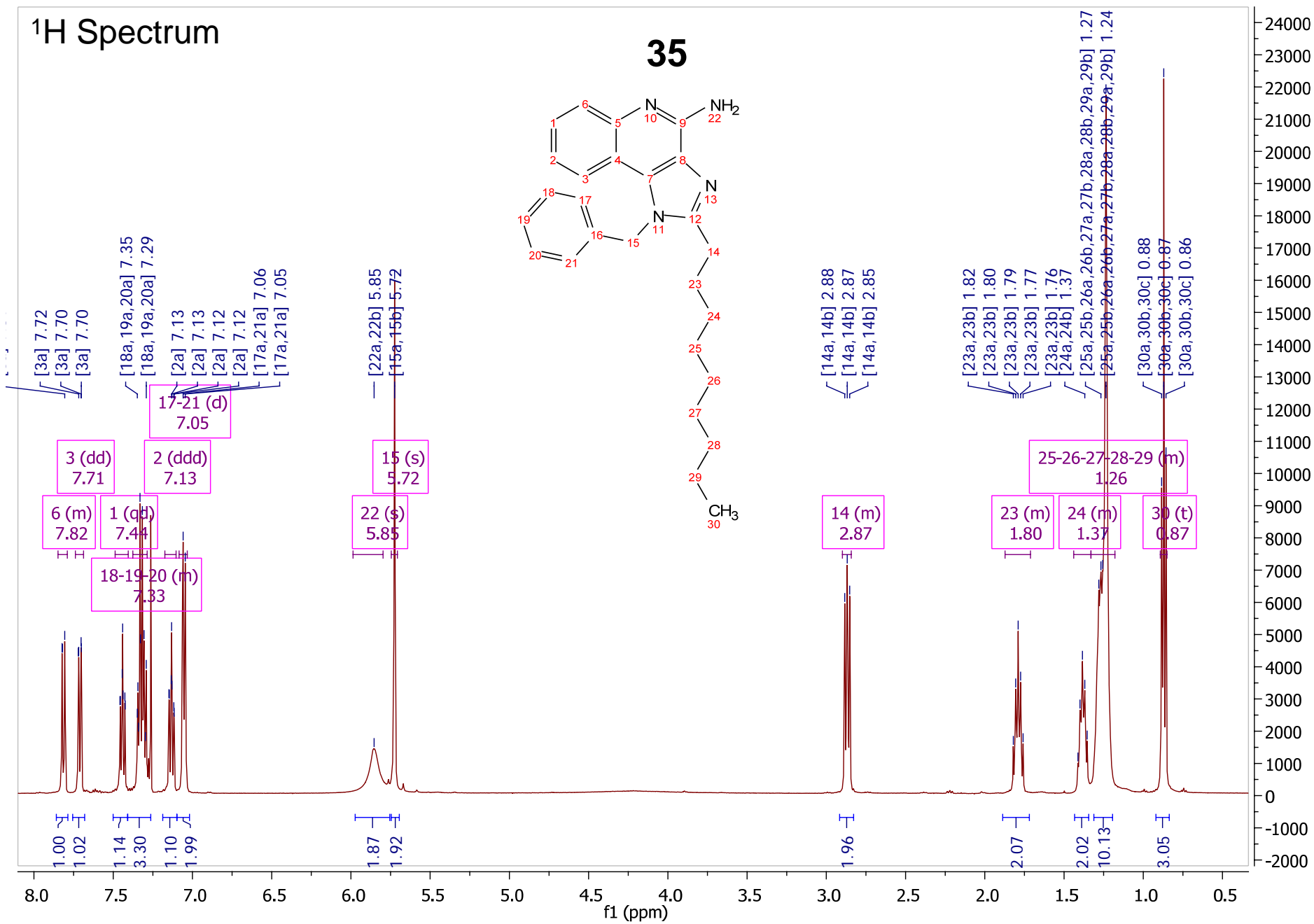
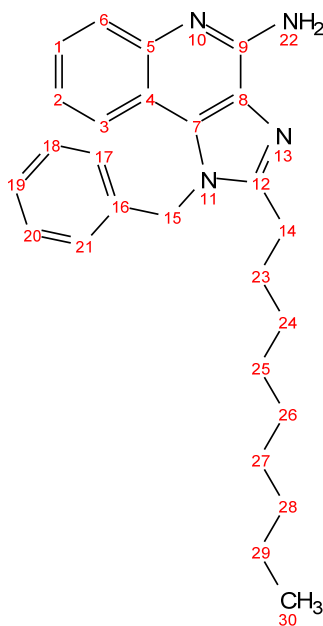
**34**



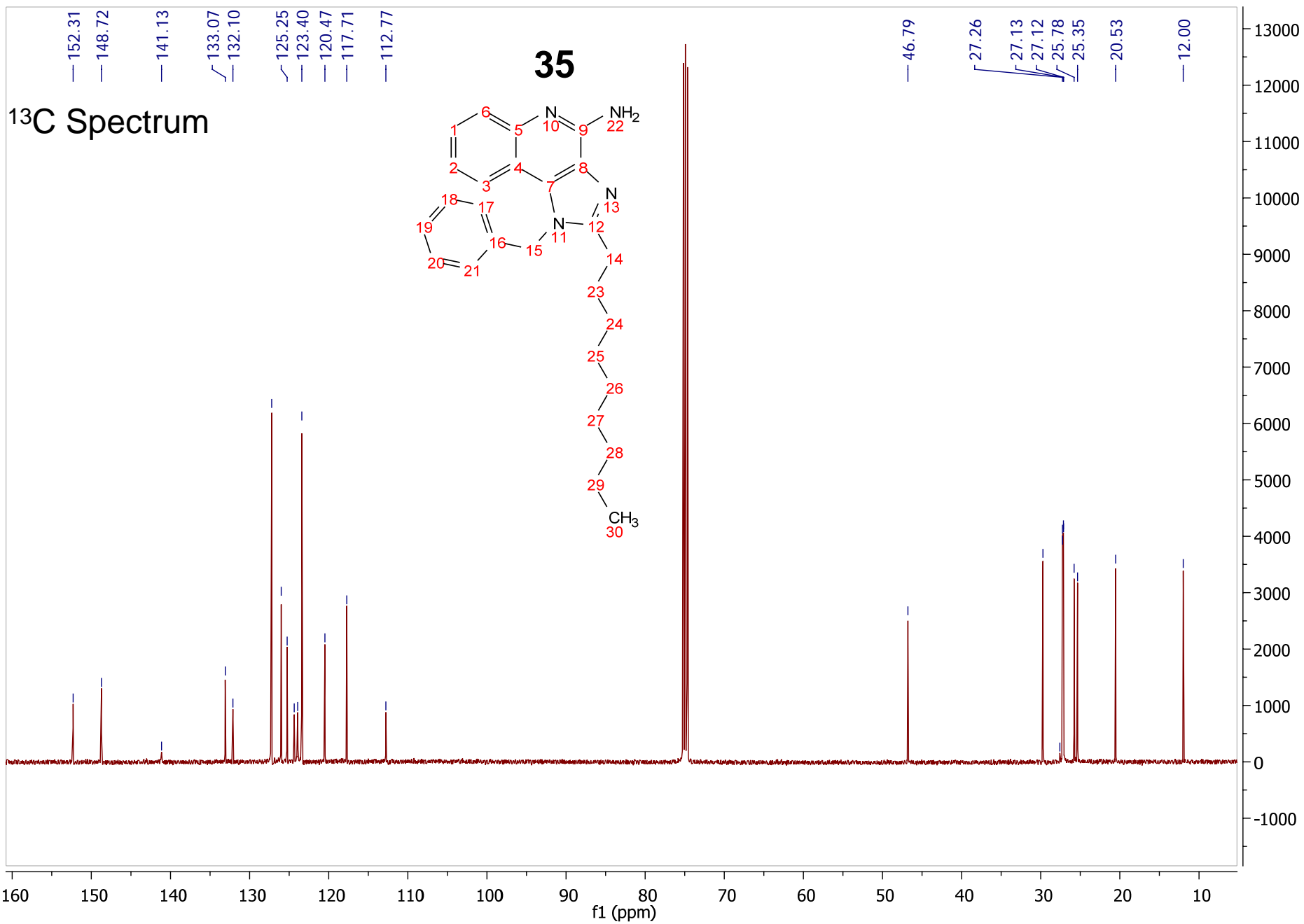


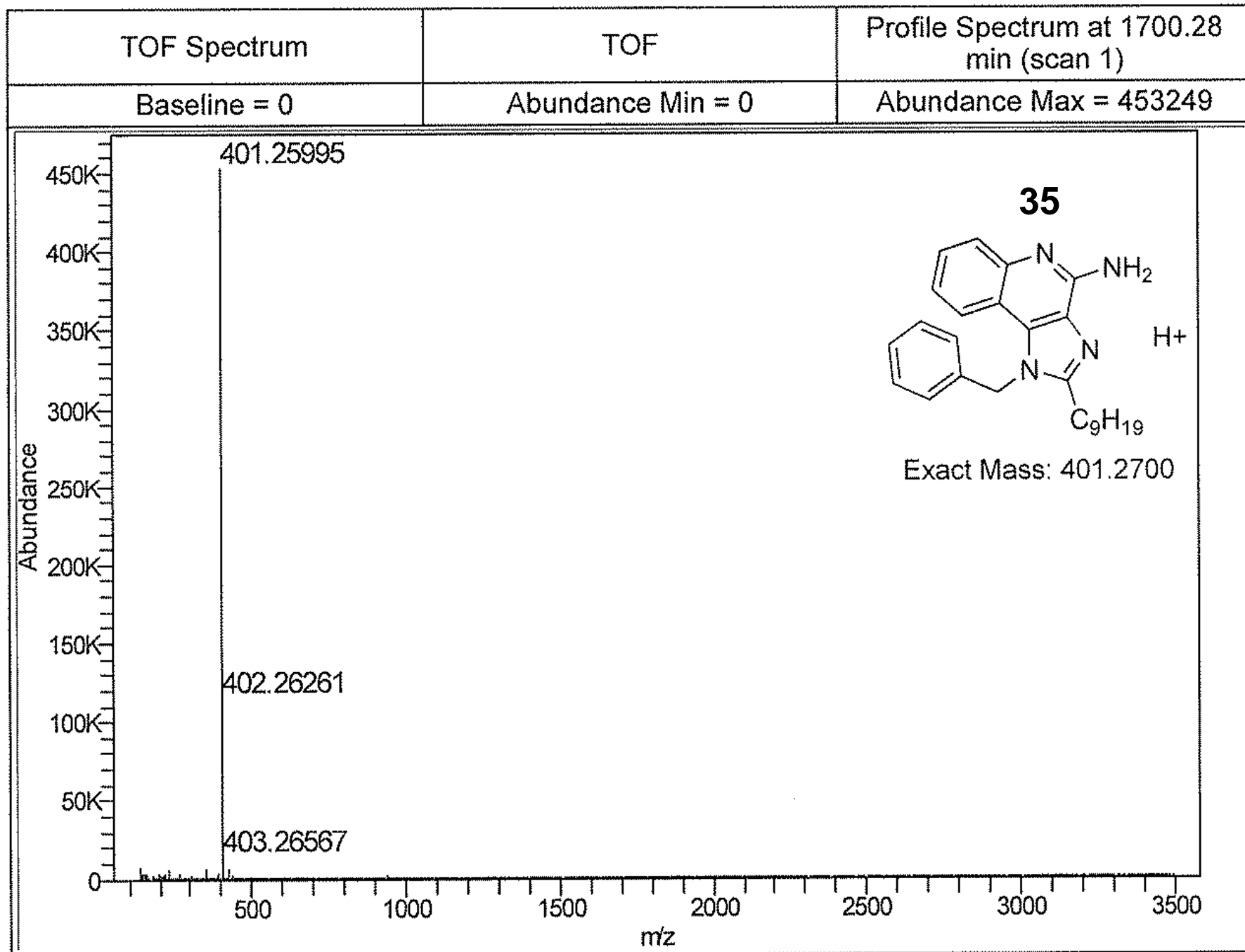
# <sup>1</sup>H Spectrum

35



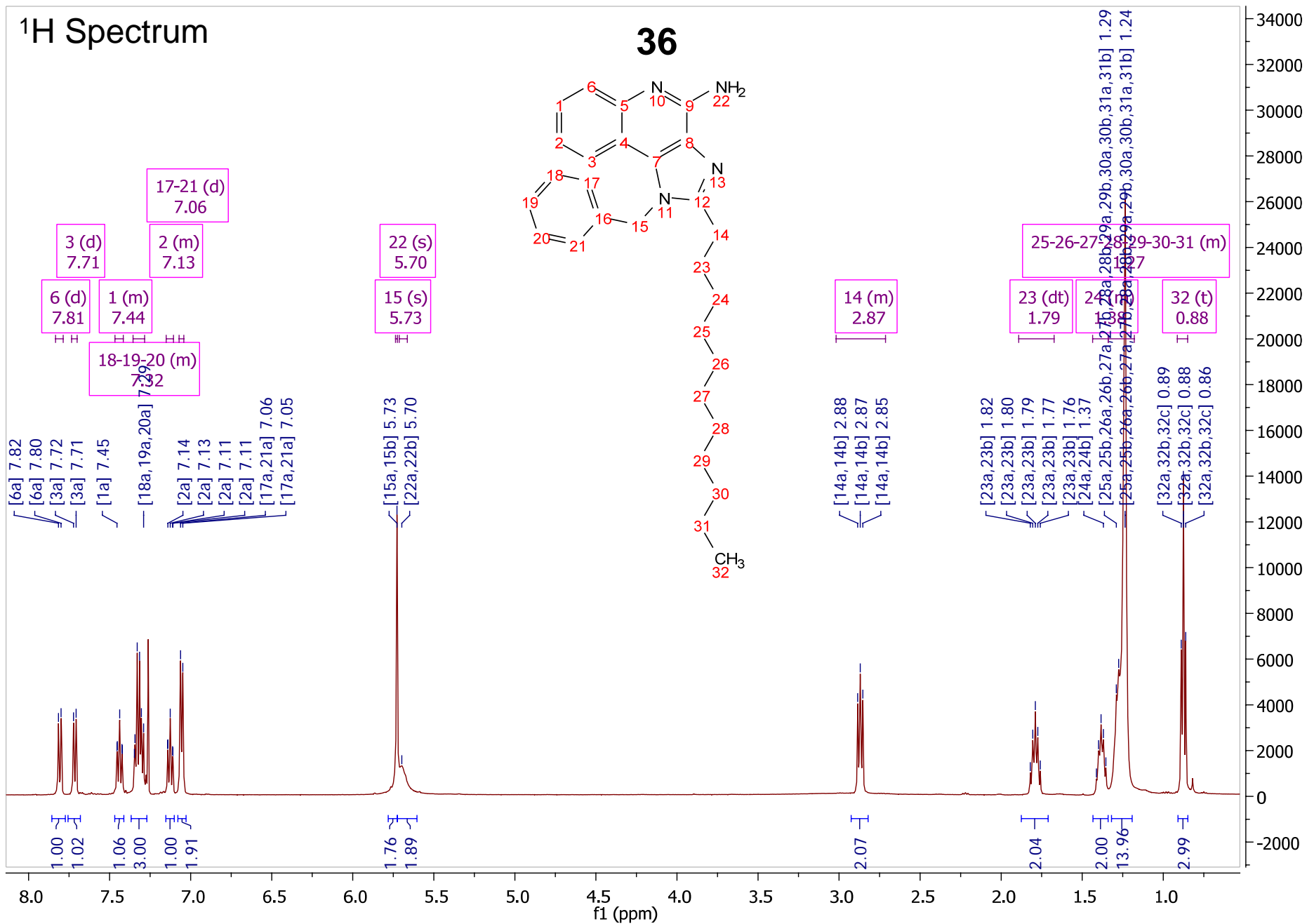
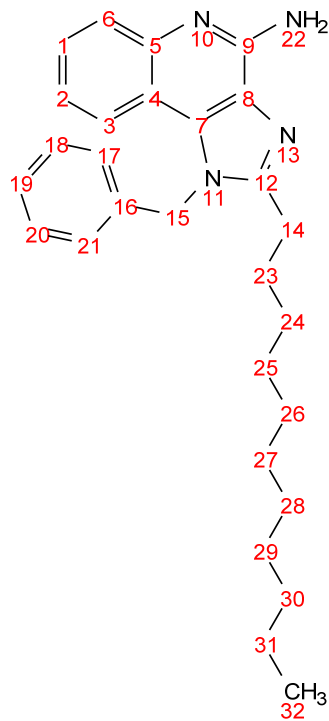


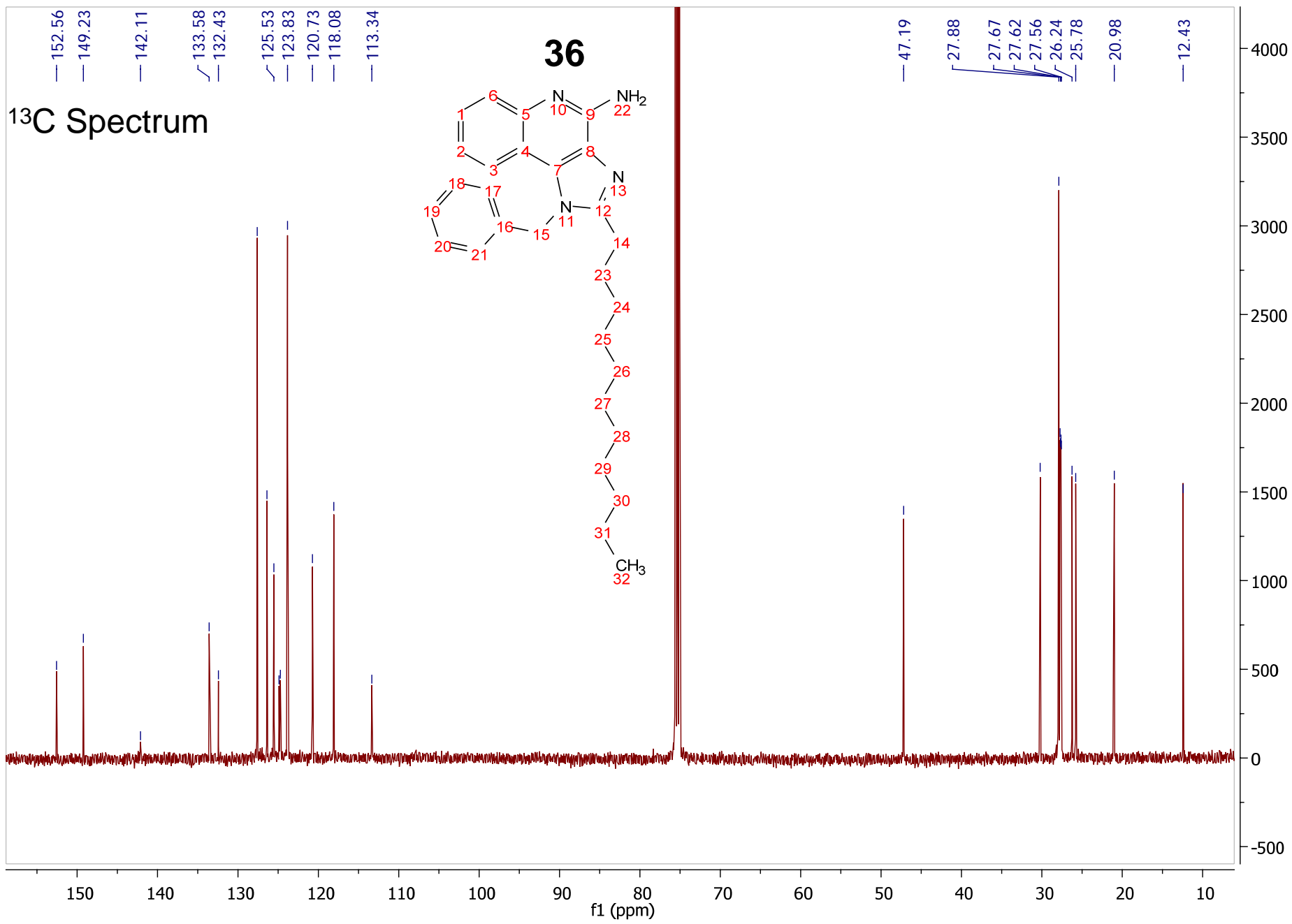


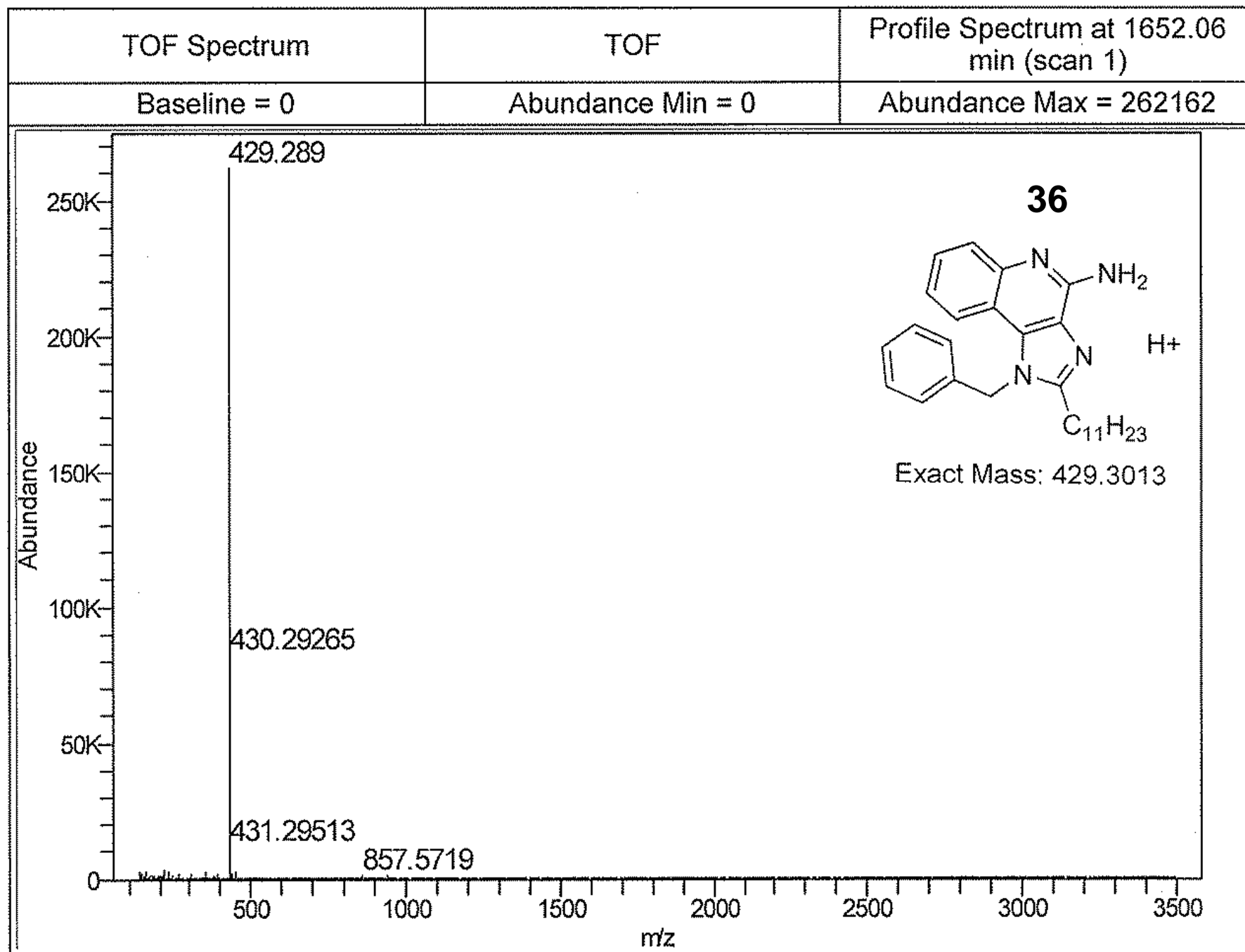


# <sup>1</sup>H Spectrum

36

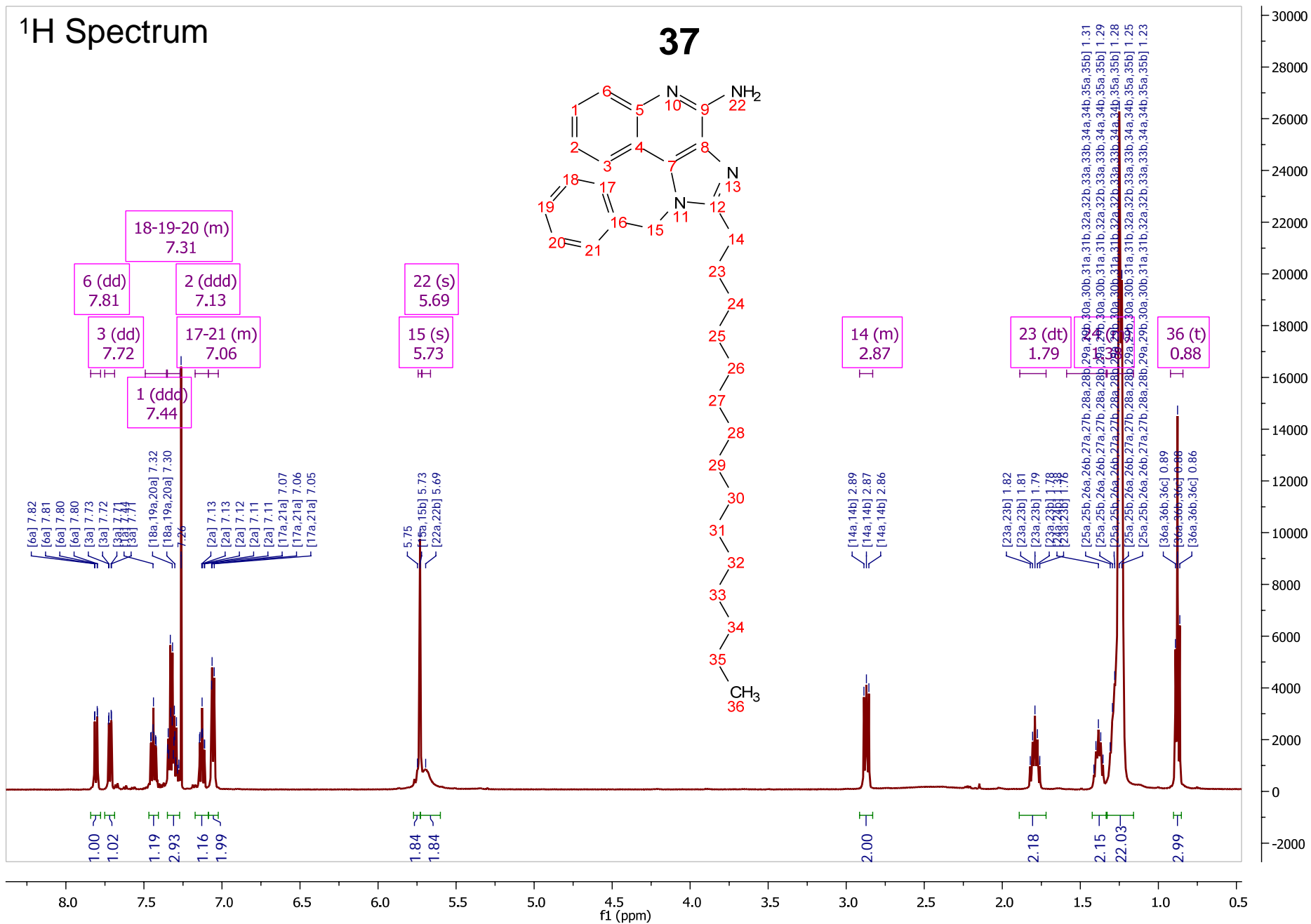
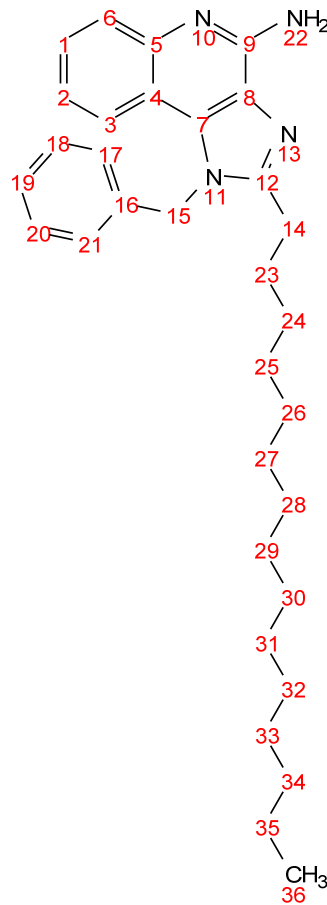


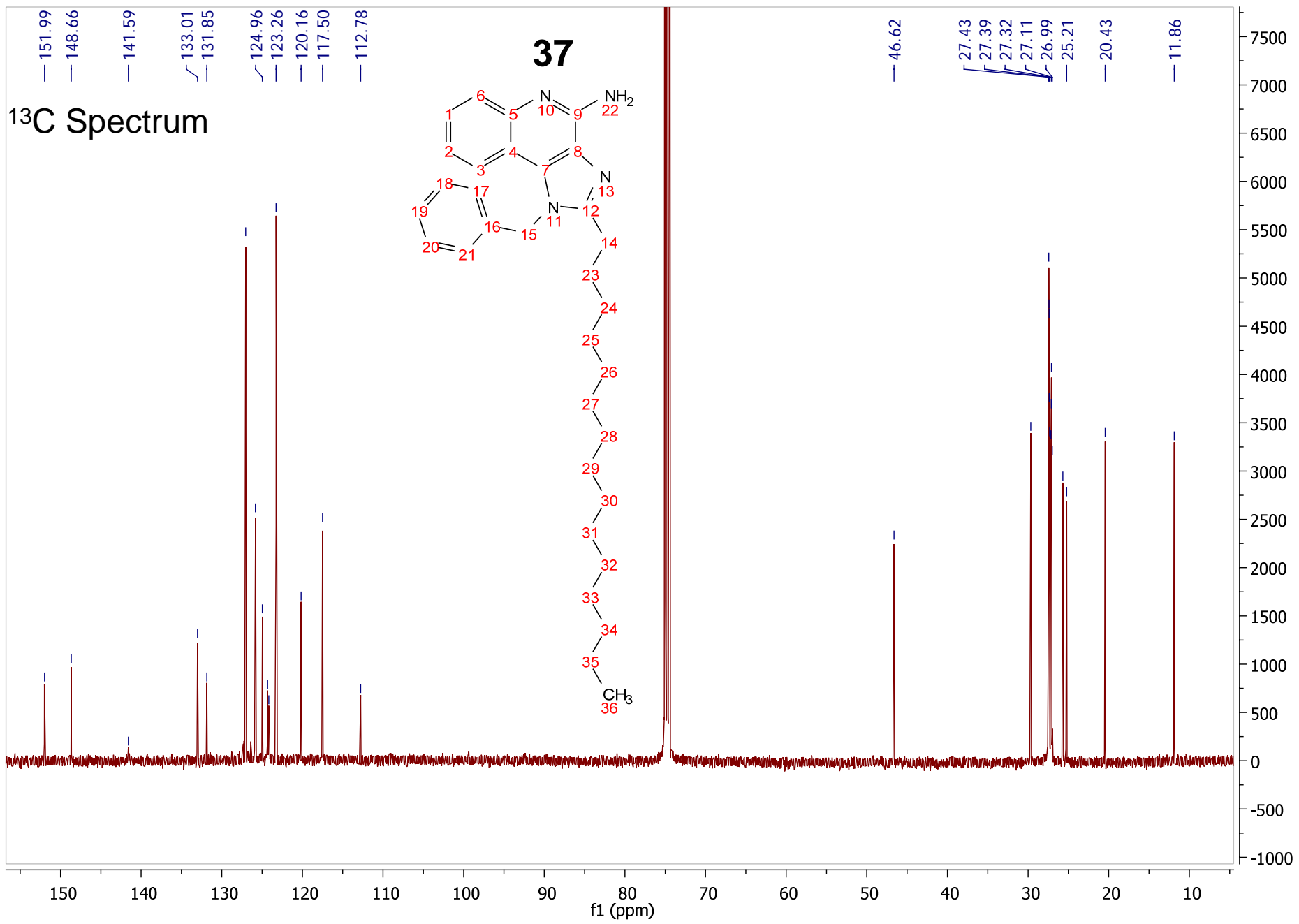




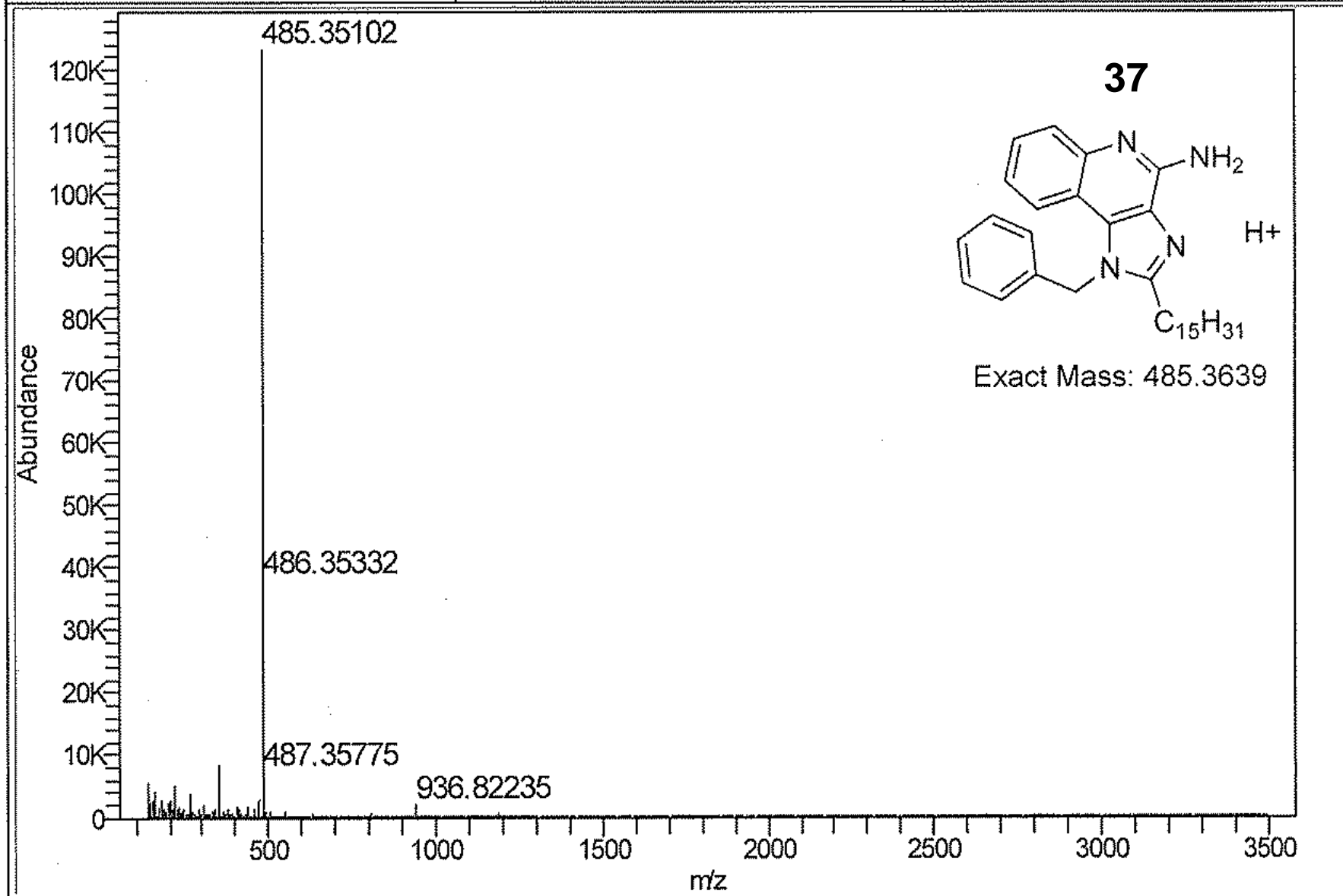
# <sup>1</sup>H Spectrum

## 37

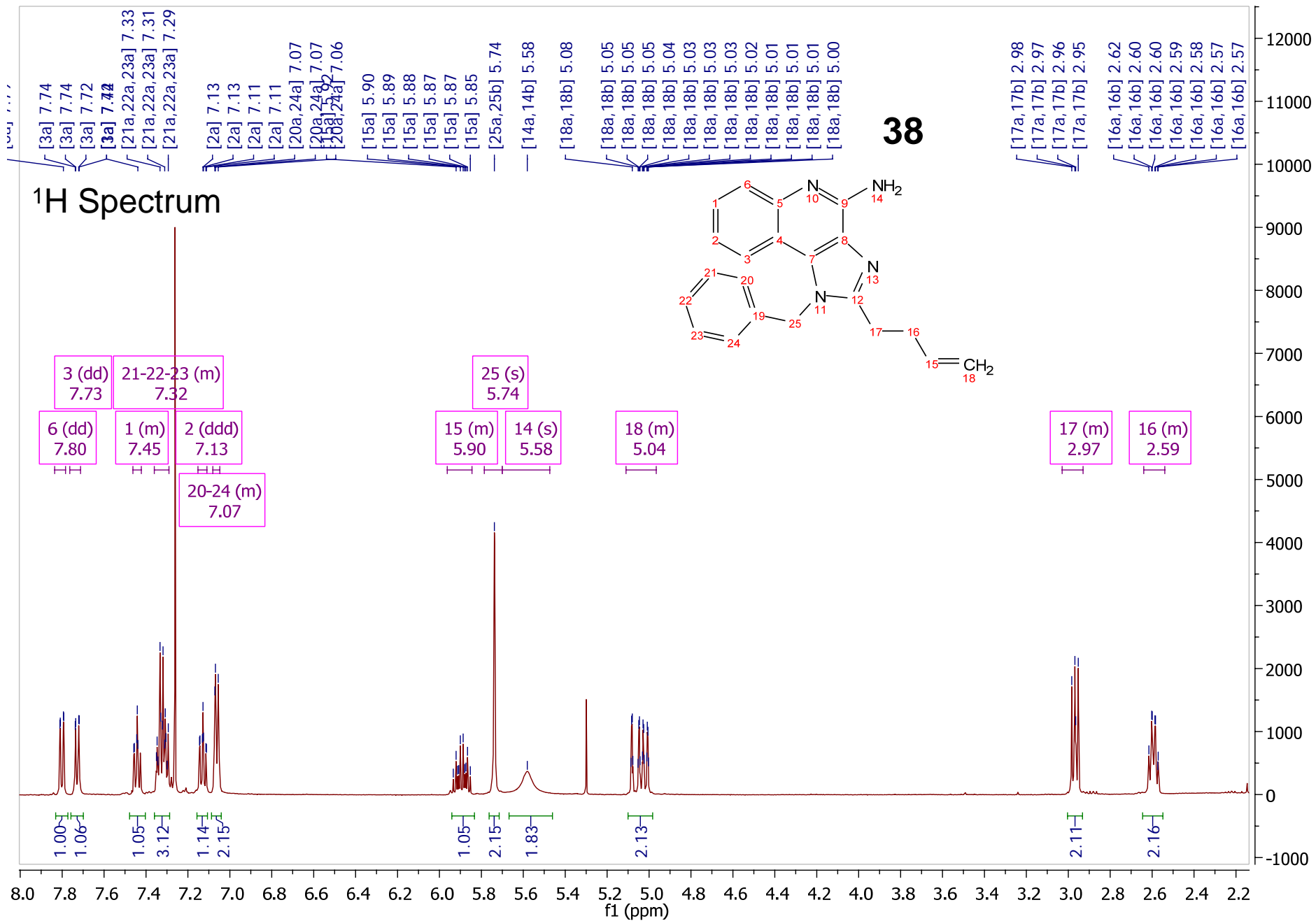


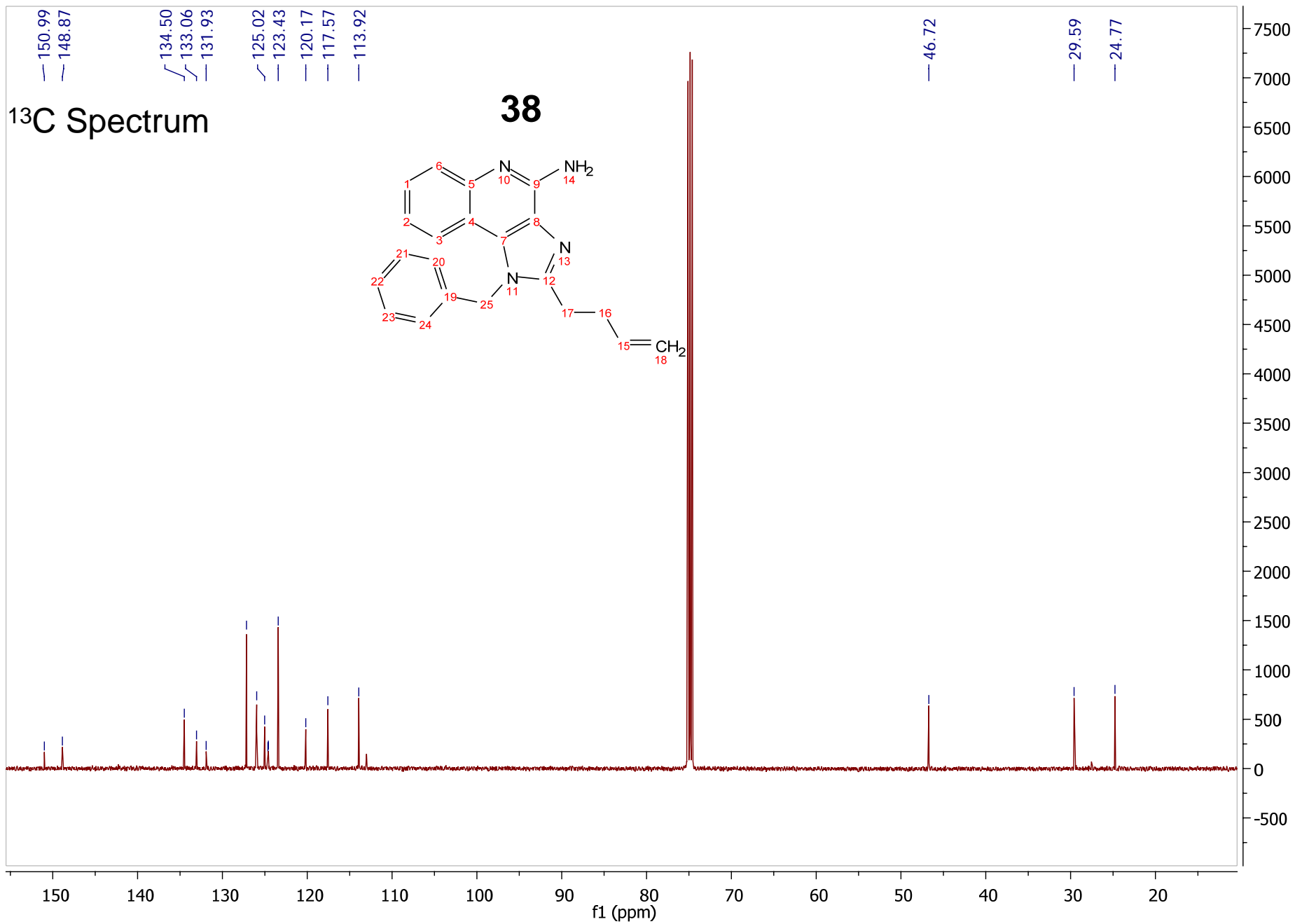


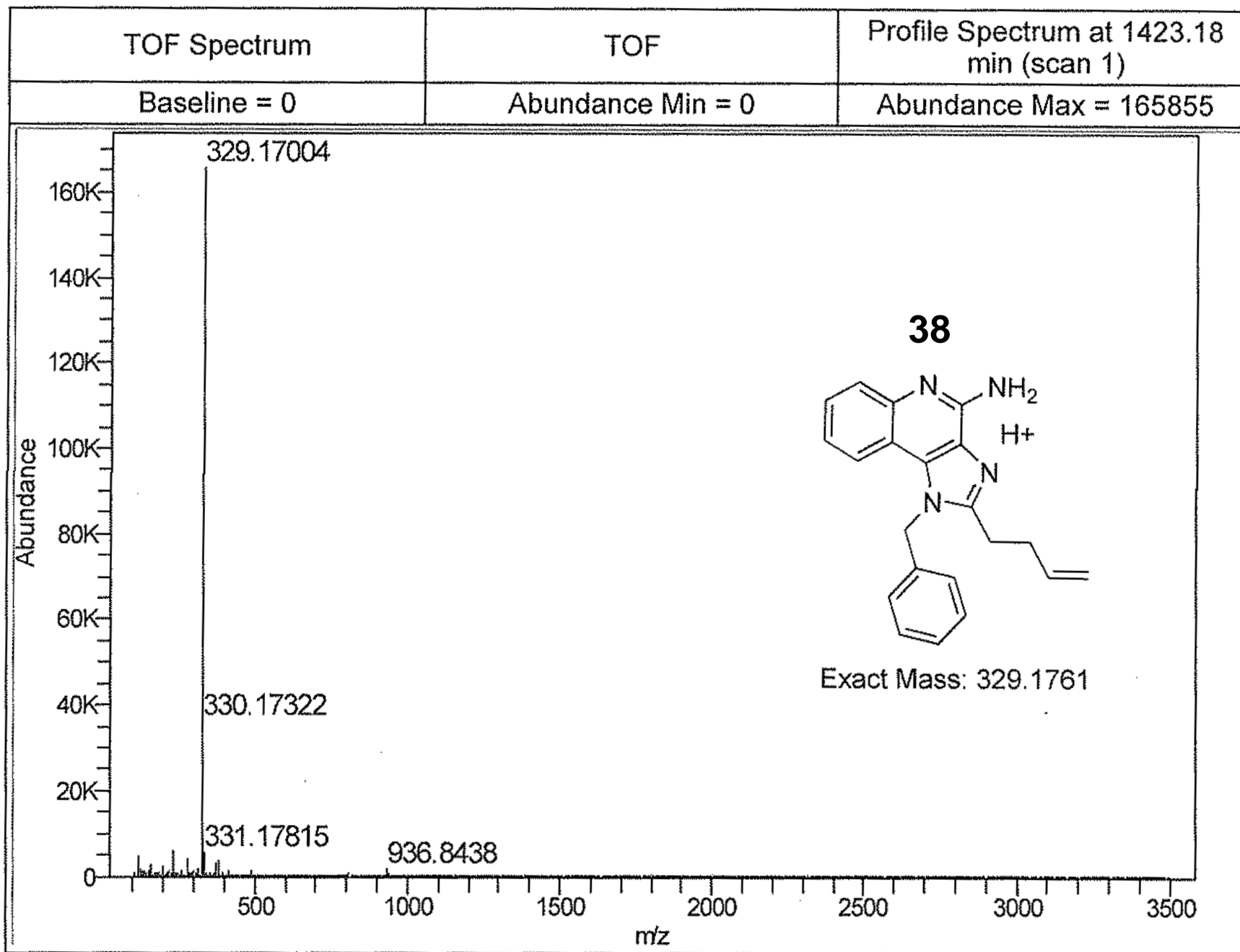
TOF Spectrum	TOF	Profile Spectrum at 1705.20 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 123388



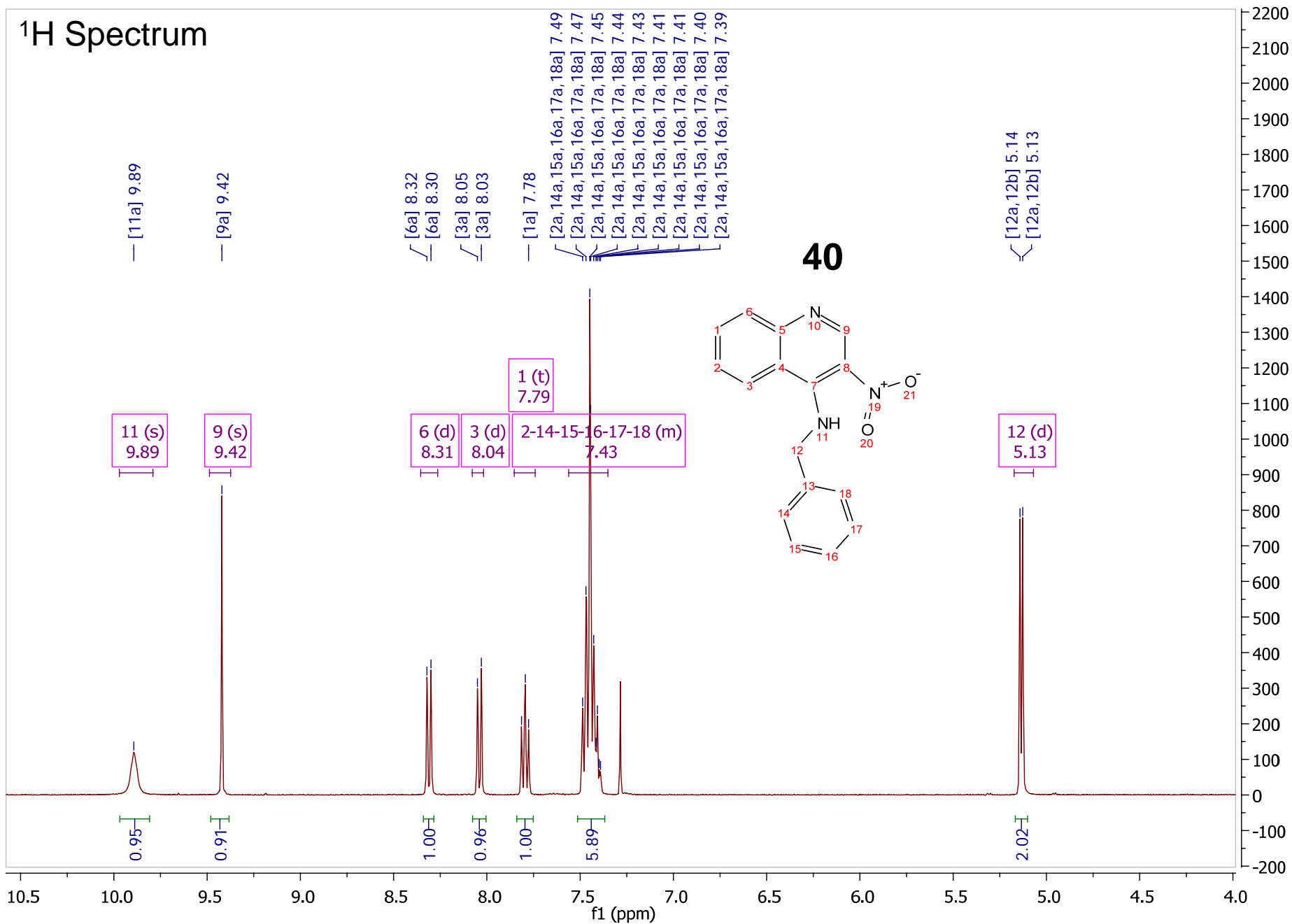


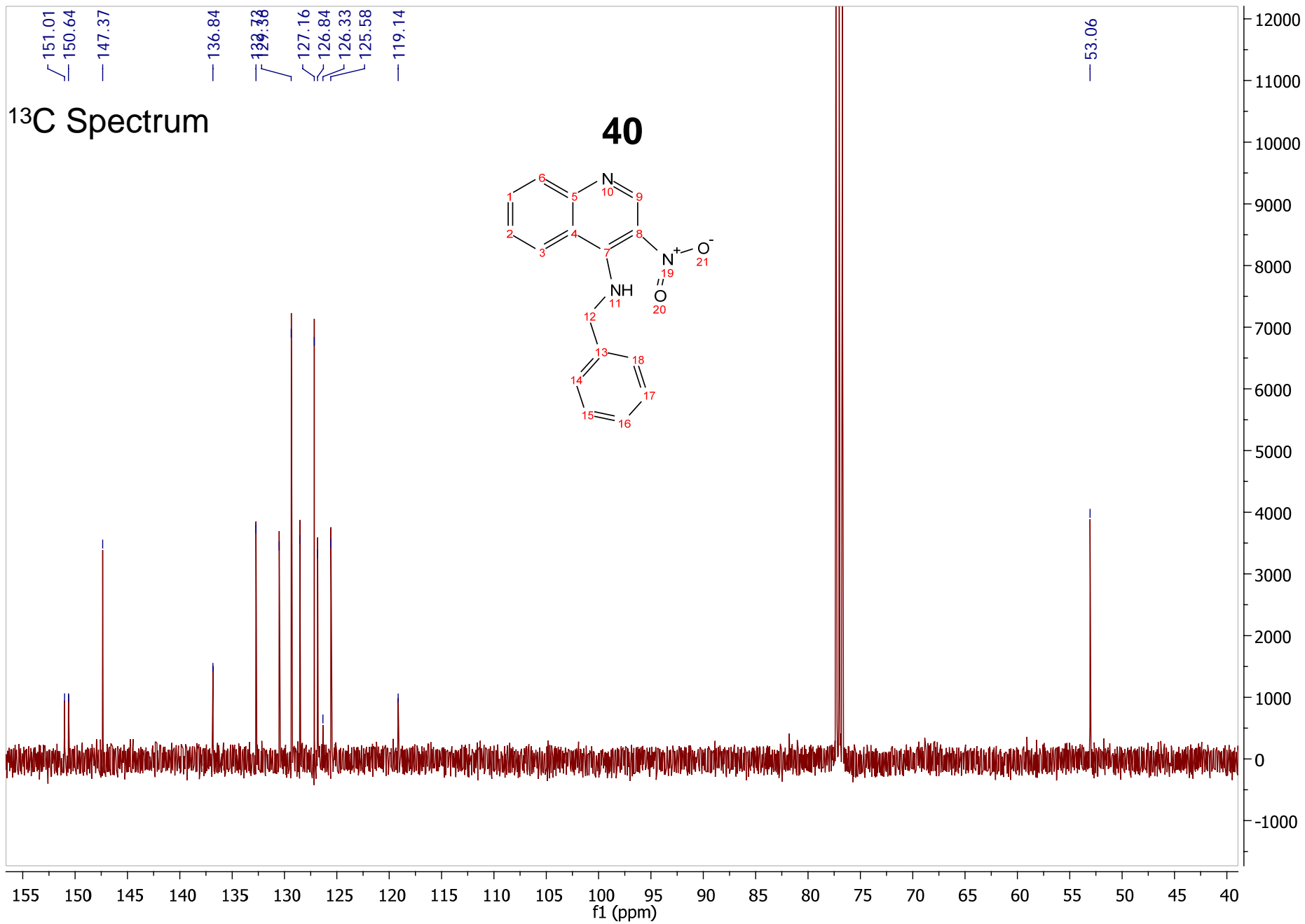


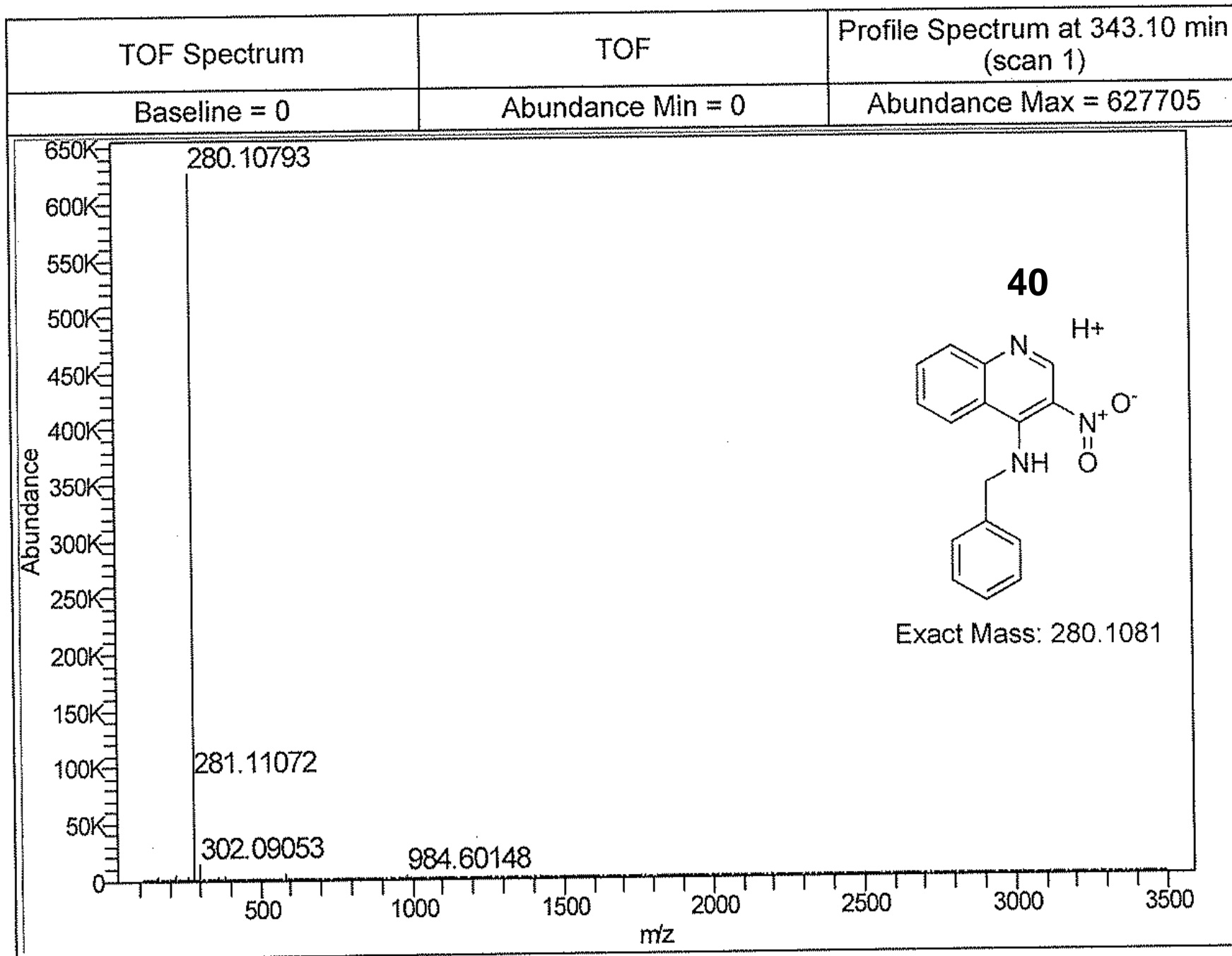




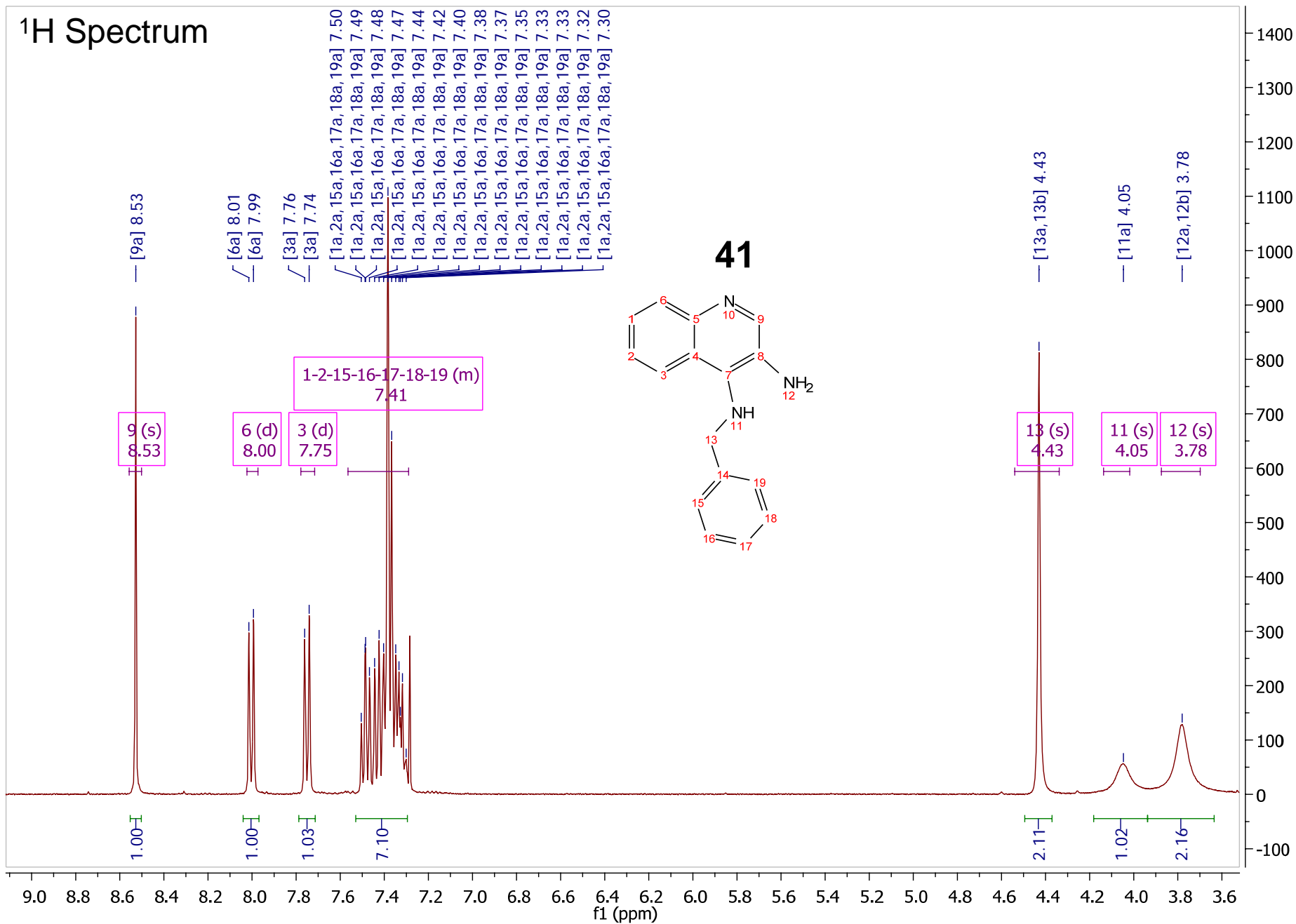
# <sup>1</sup>H Spectrum

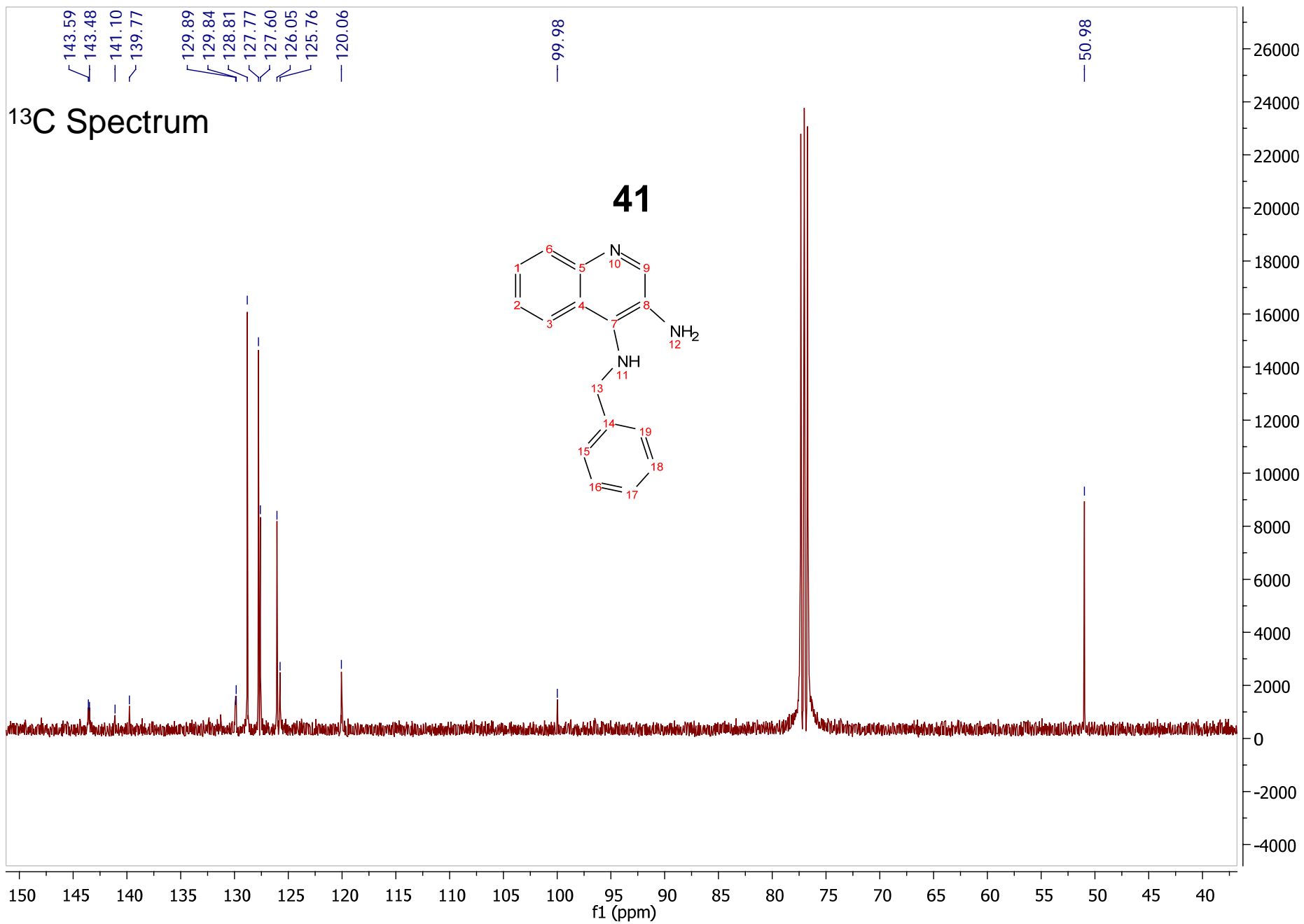




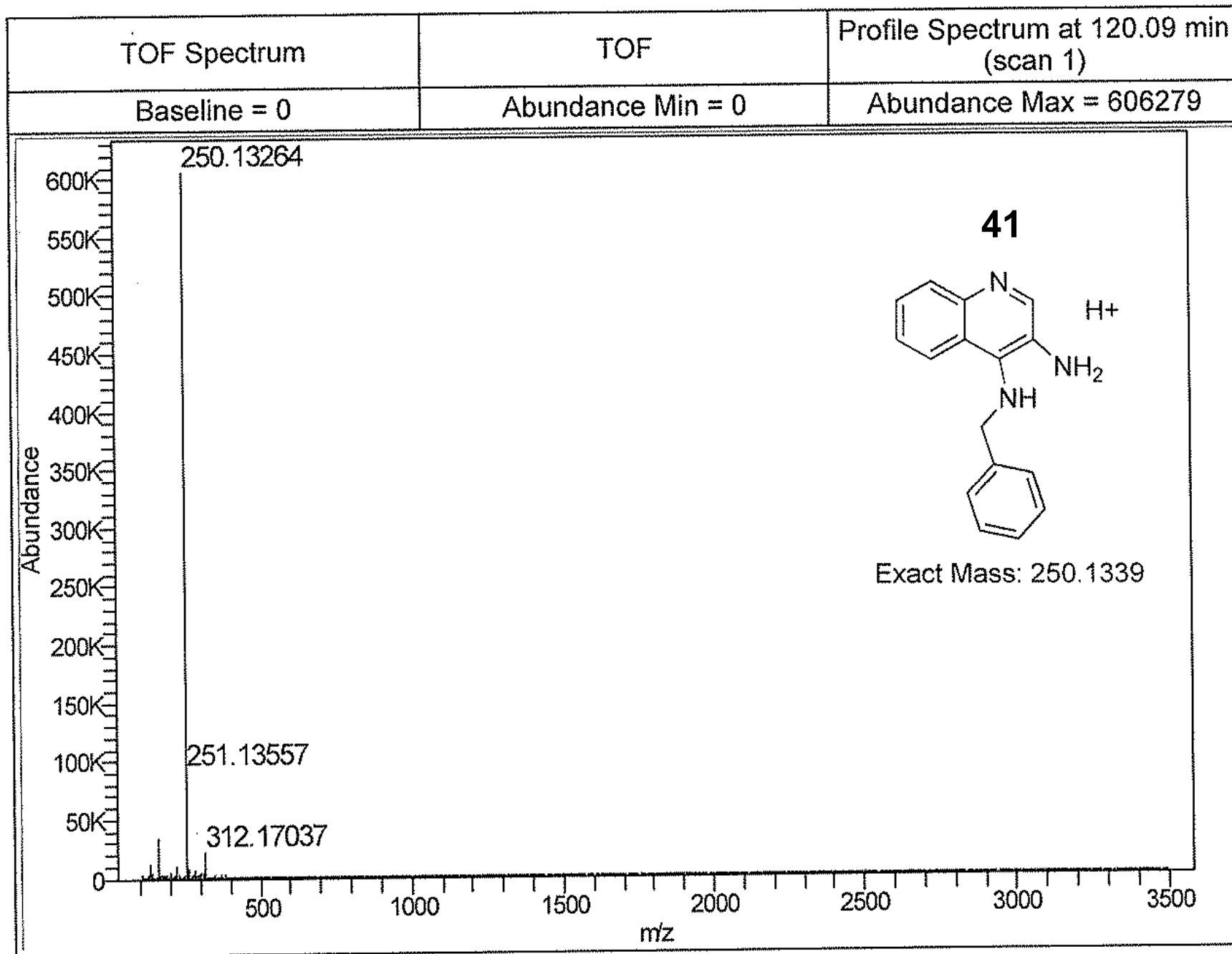


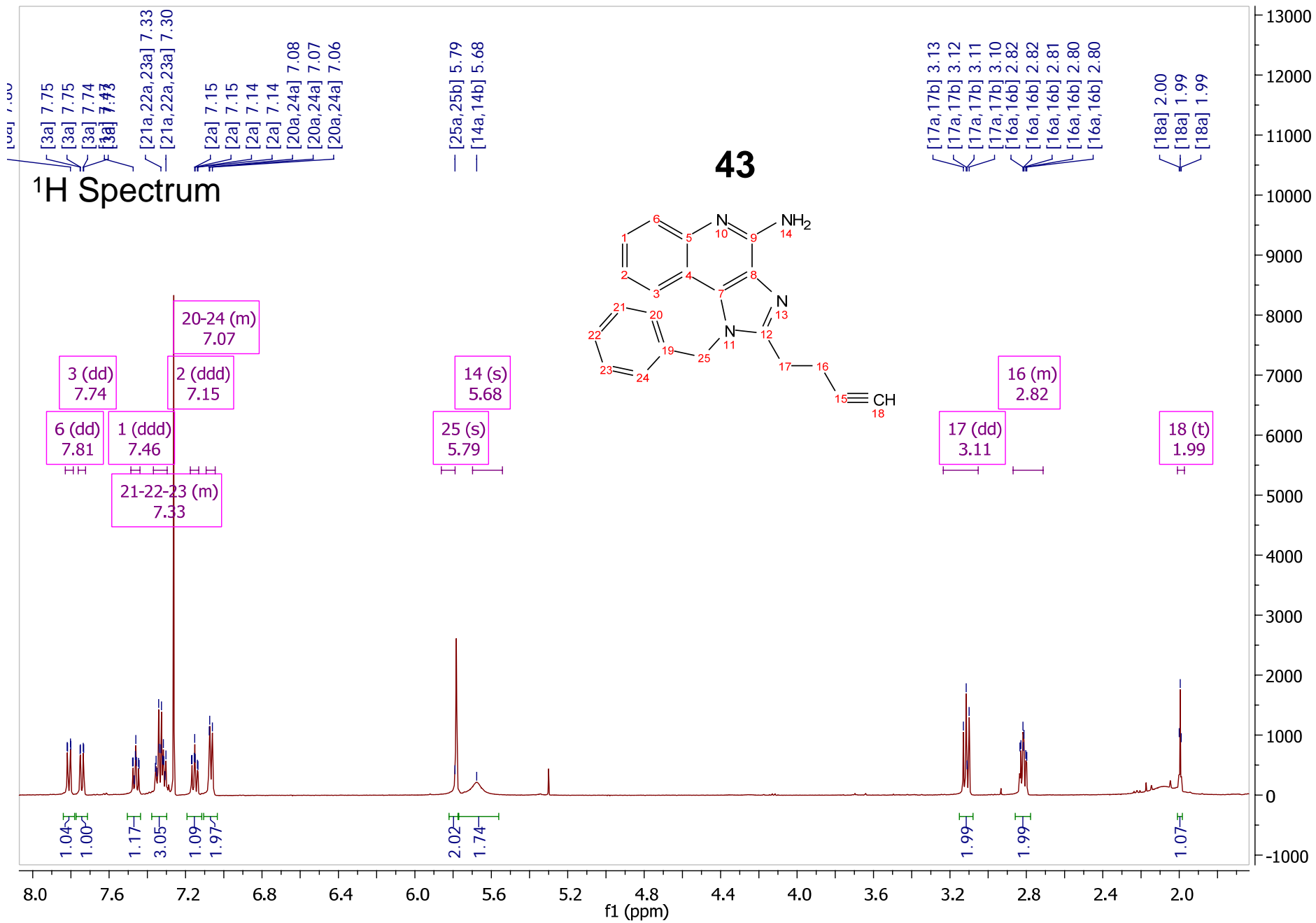
# <sup>1</sup>H Spectrum

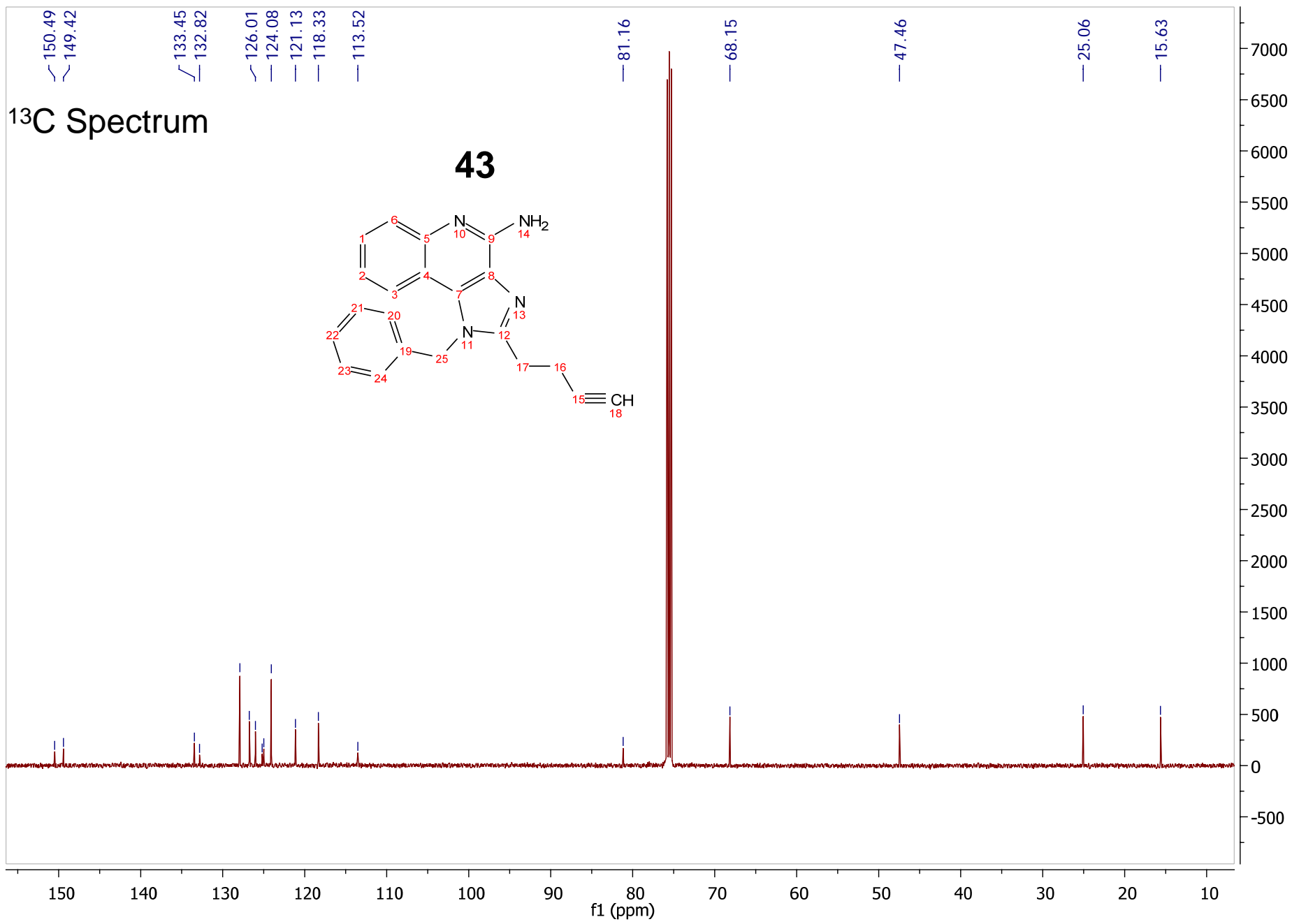


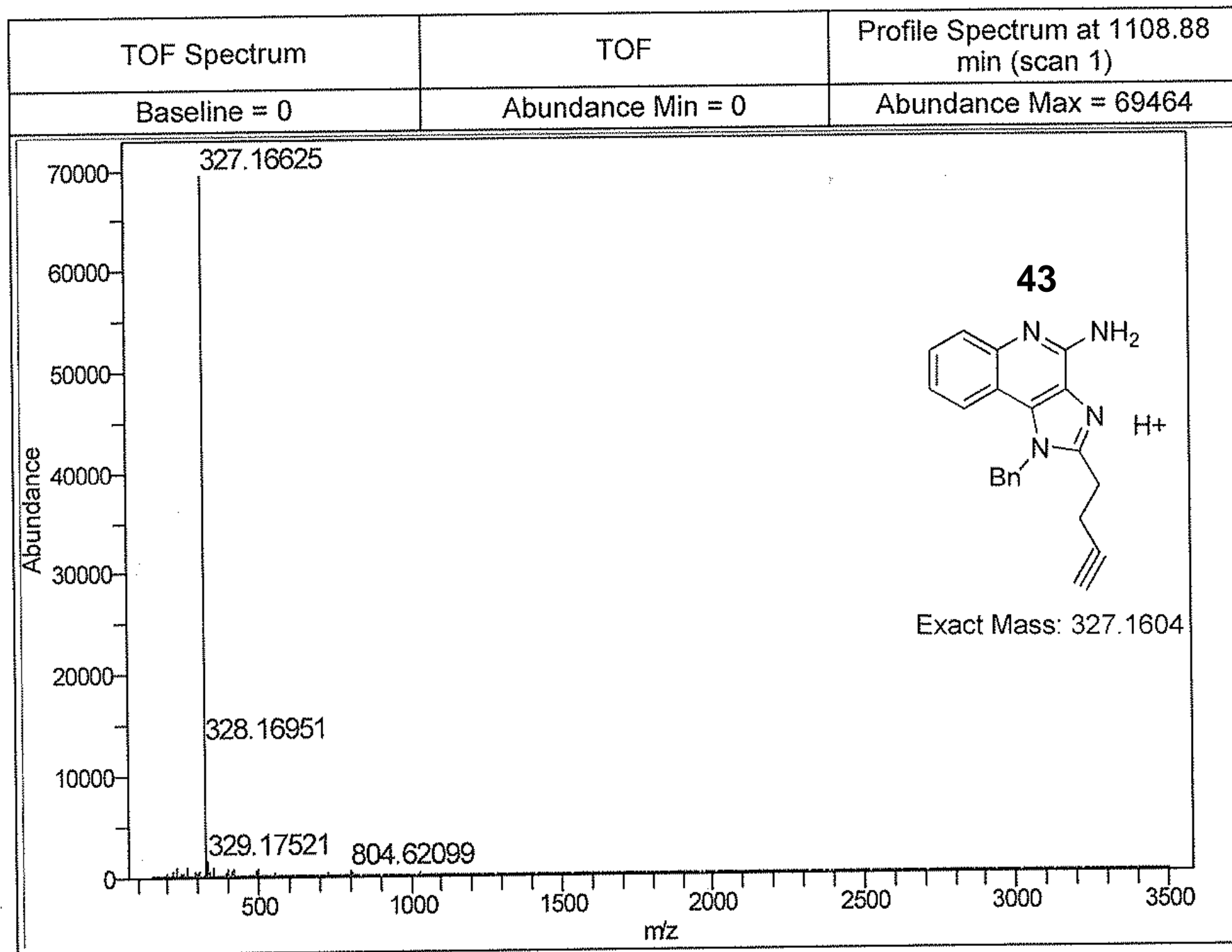






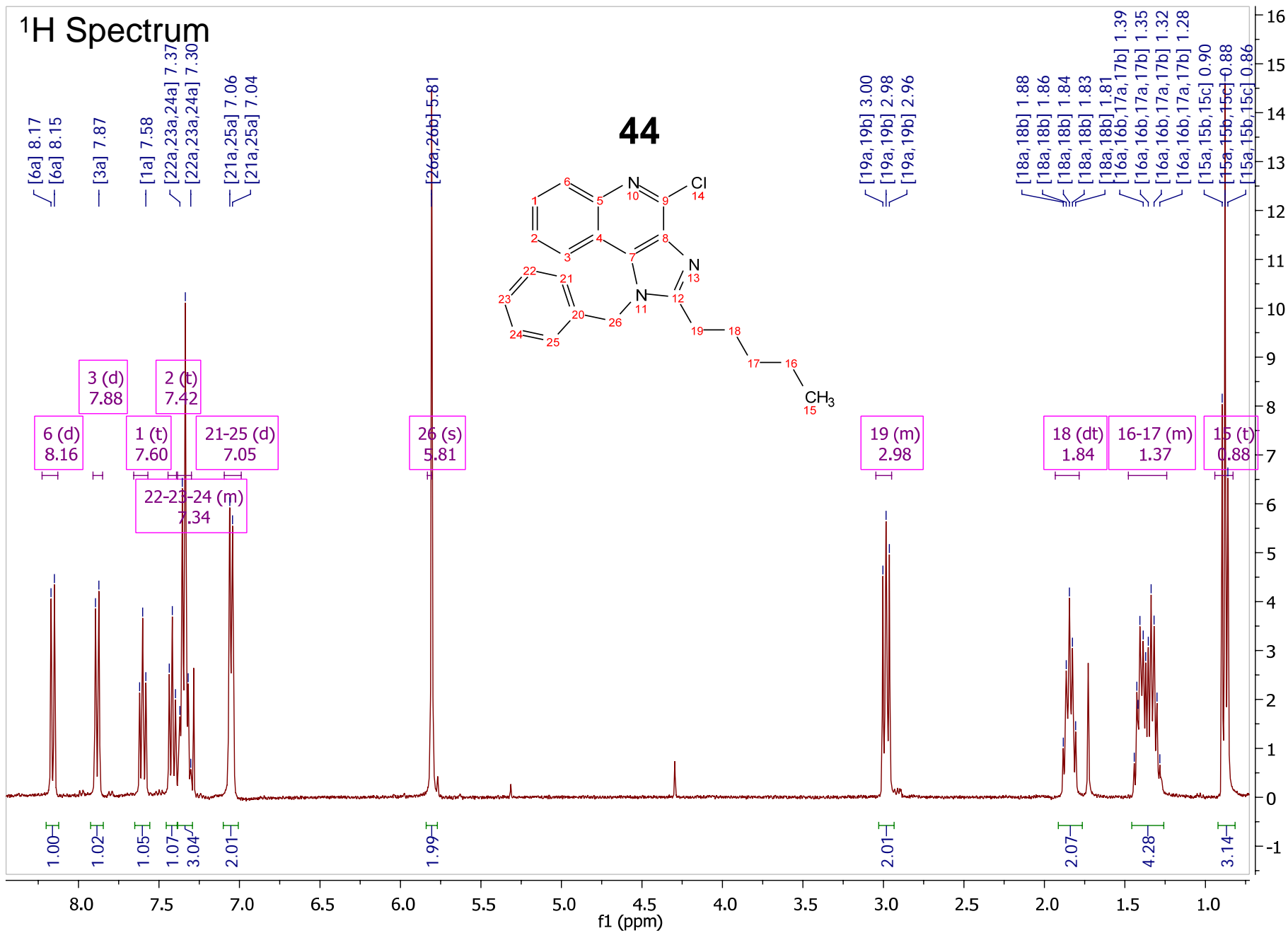
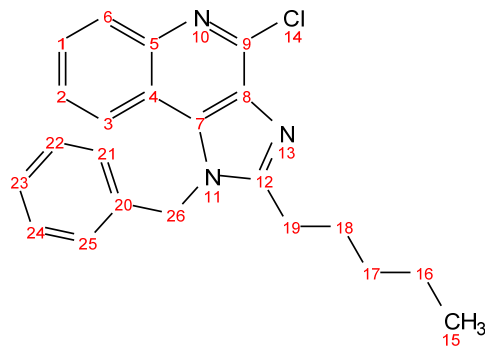


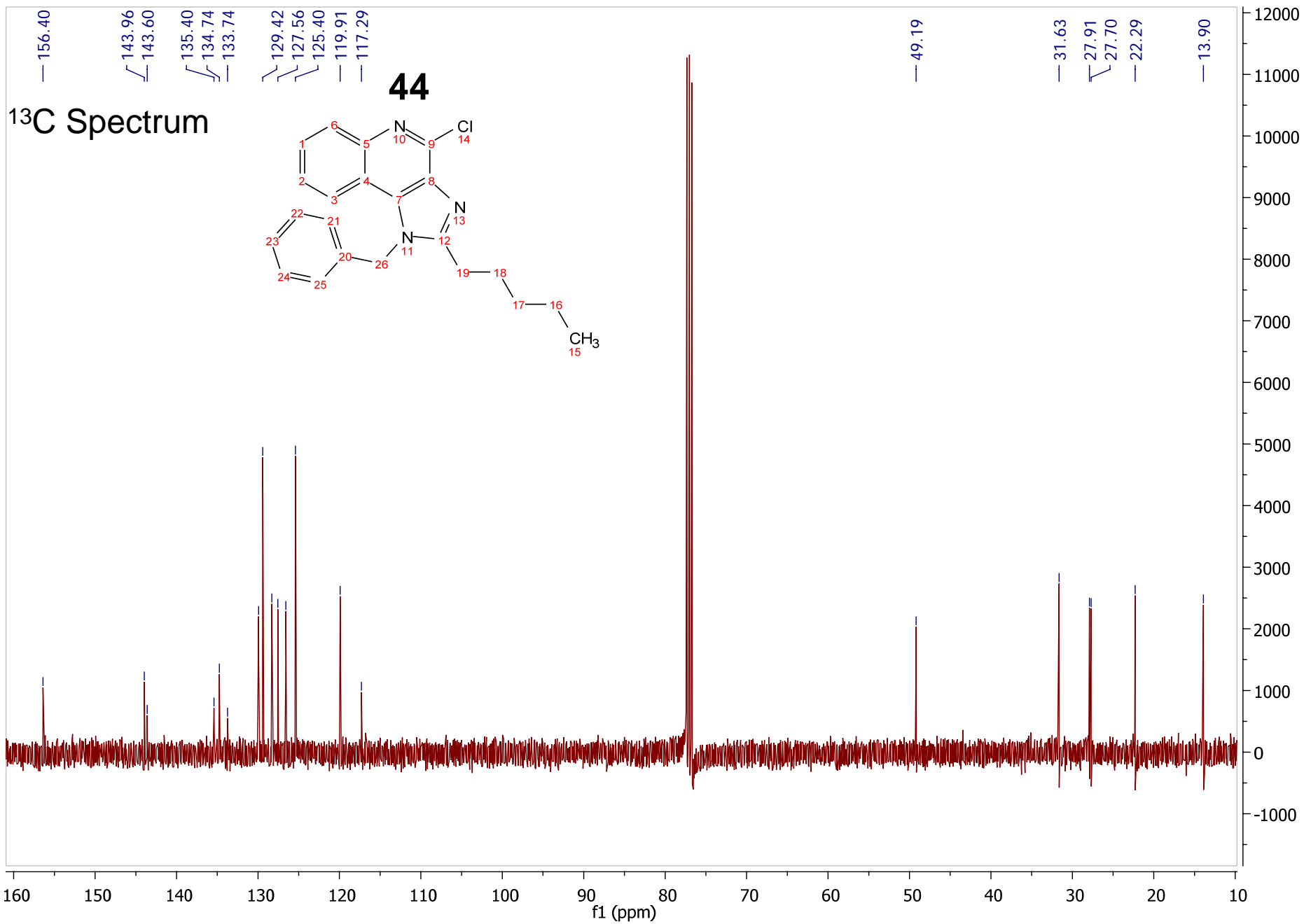


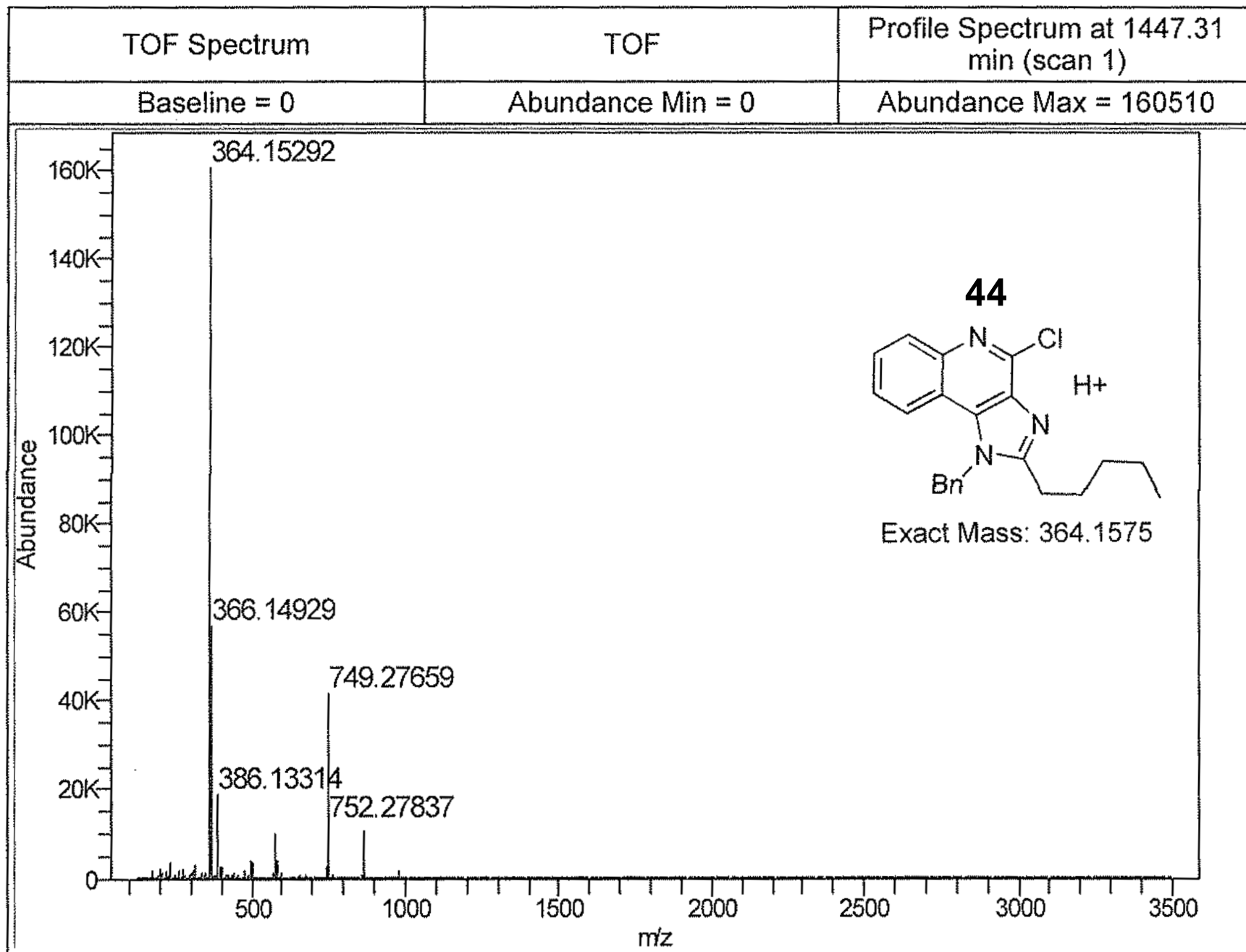


# <sup>1</sup>H Spectrum

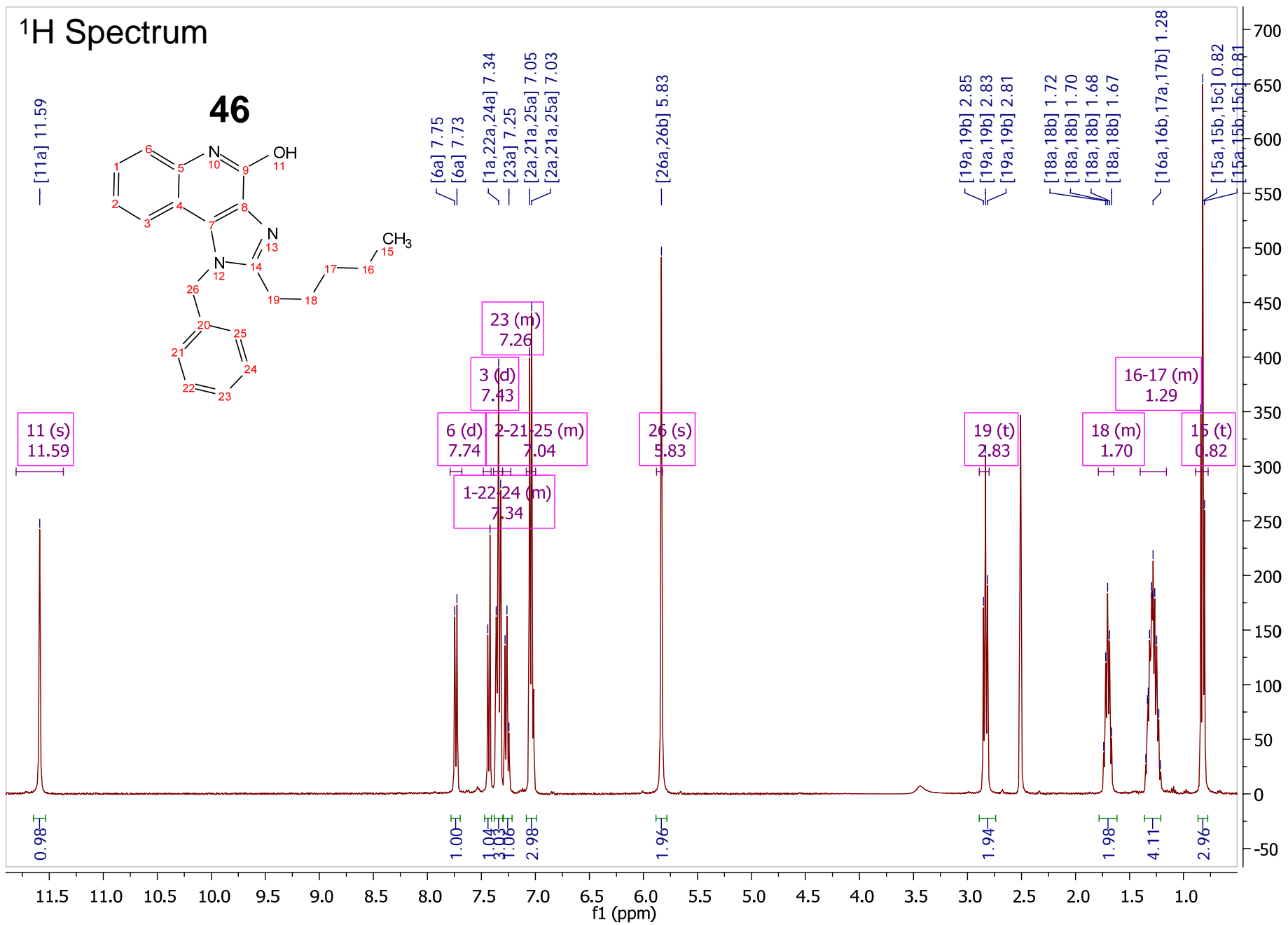
44



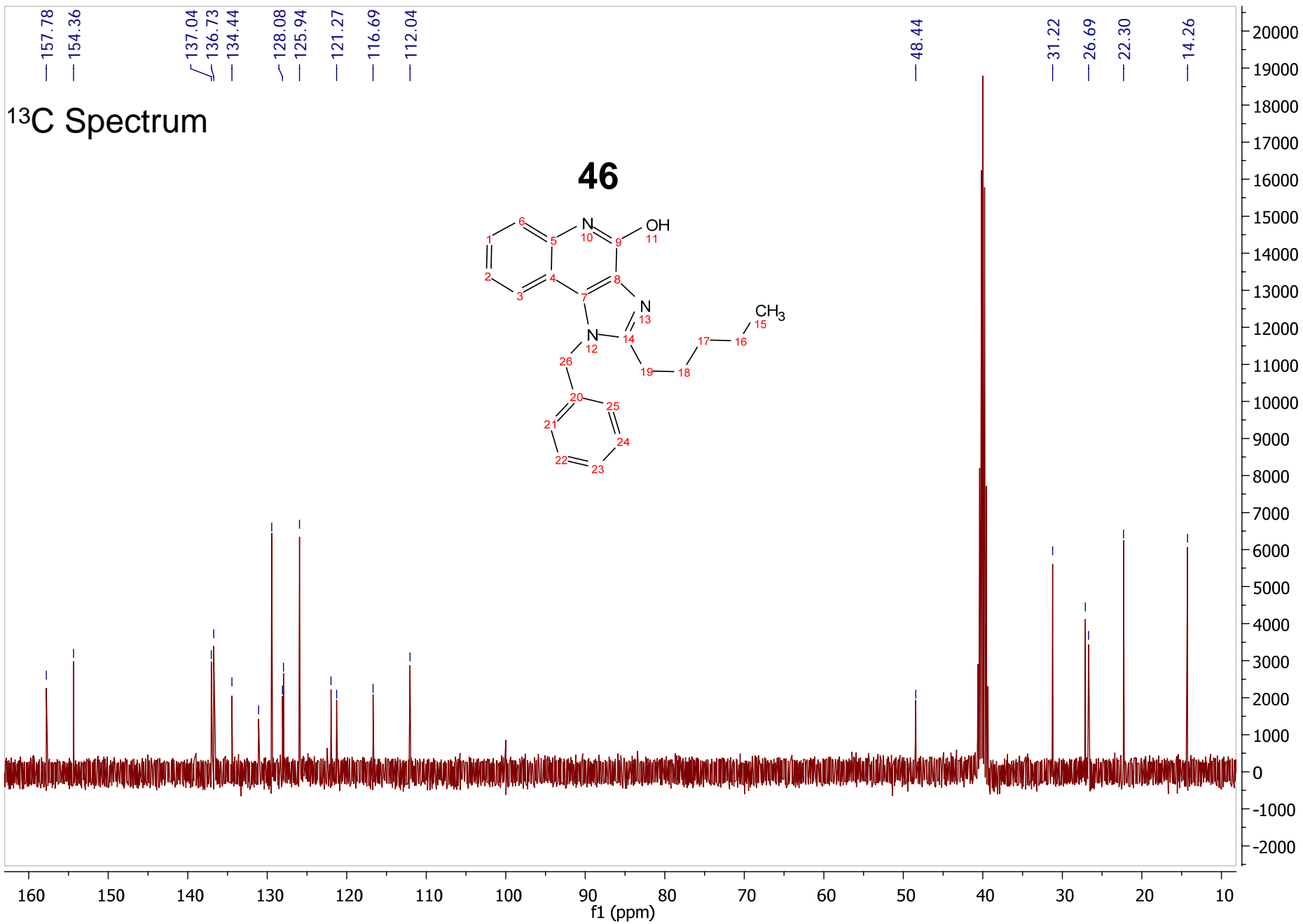




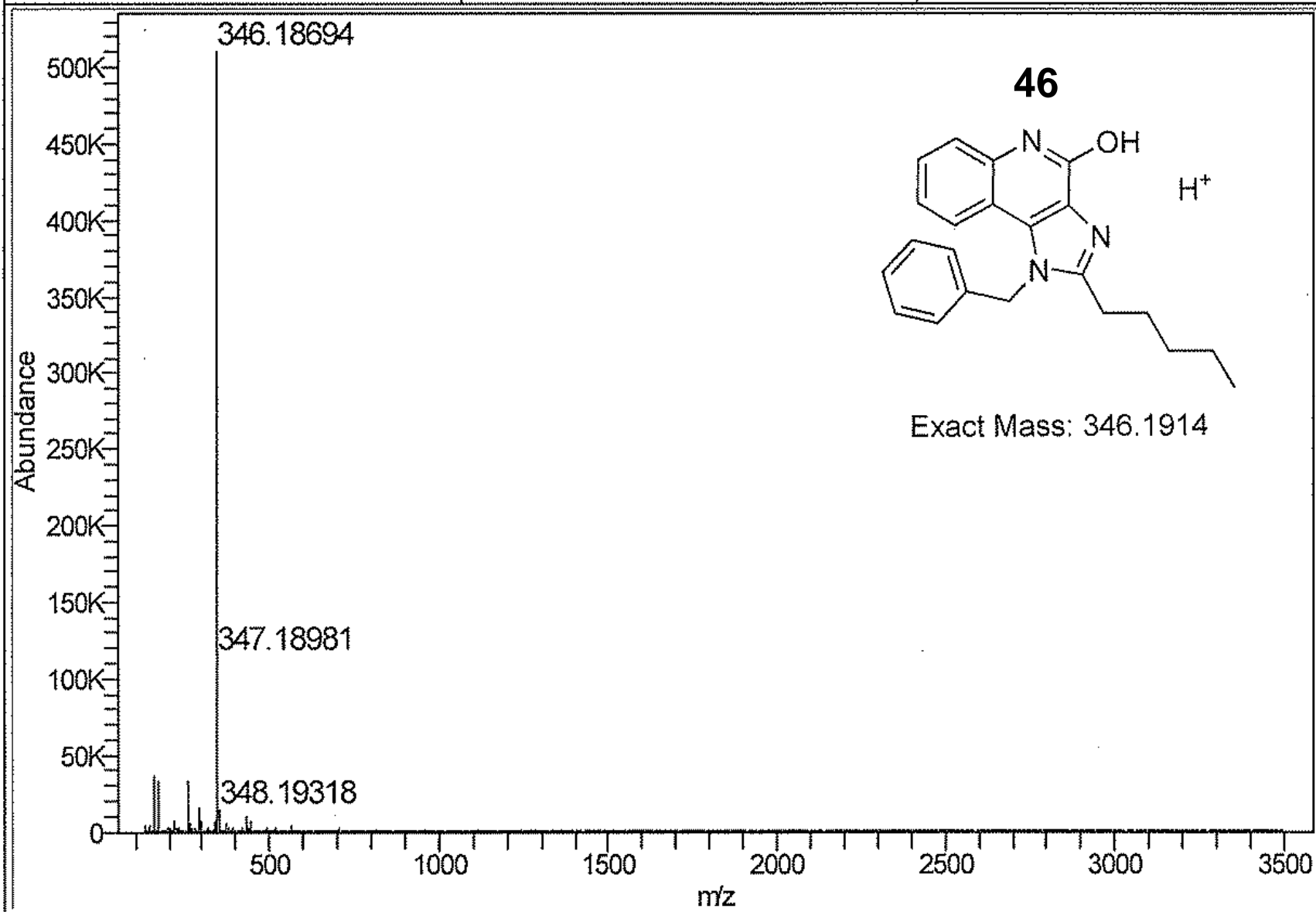
# <sup>1</sup>H Spectrum



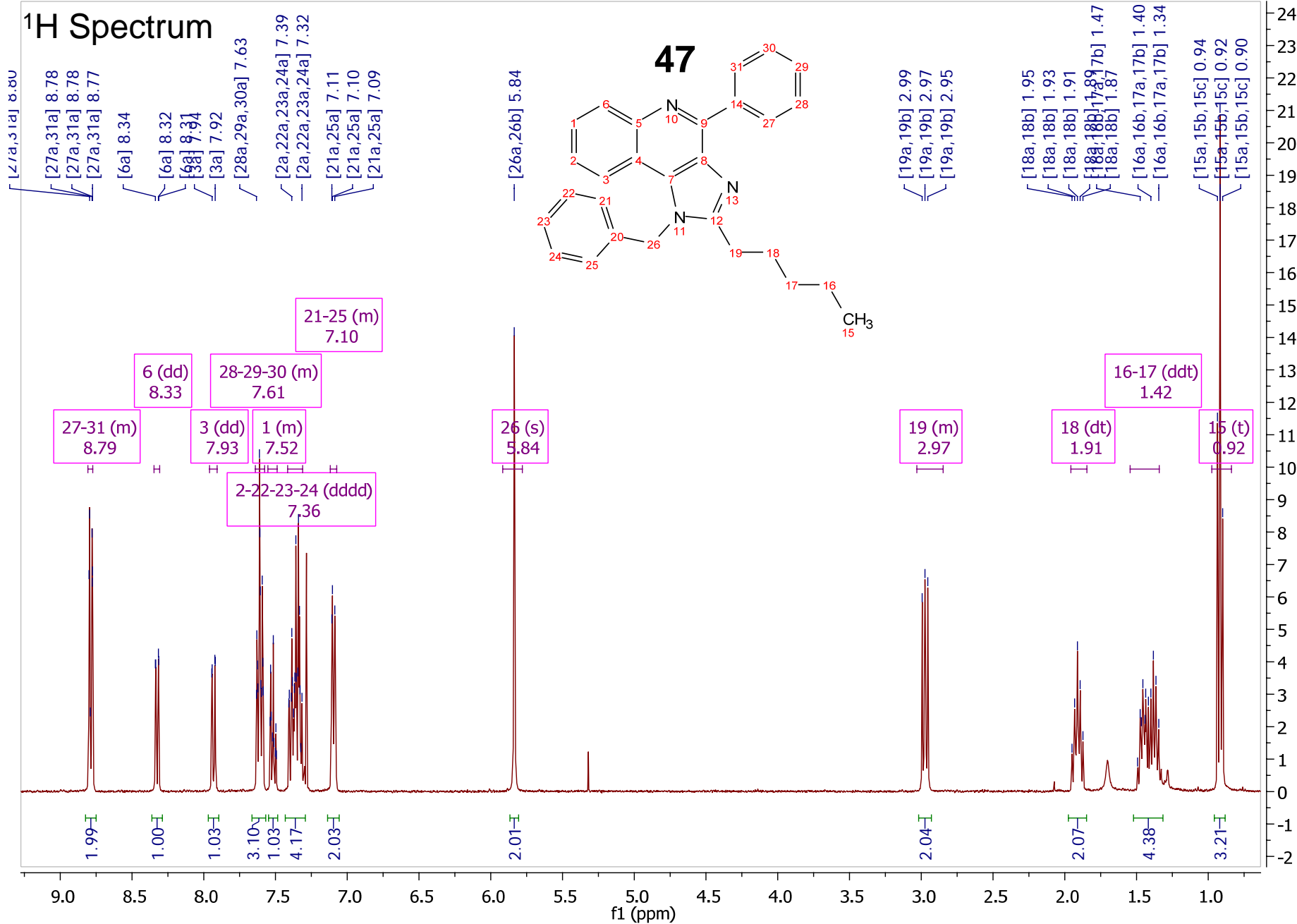


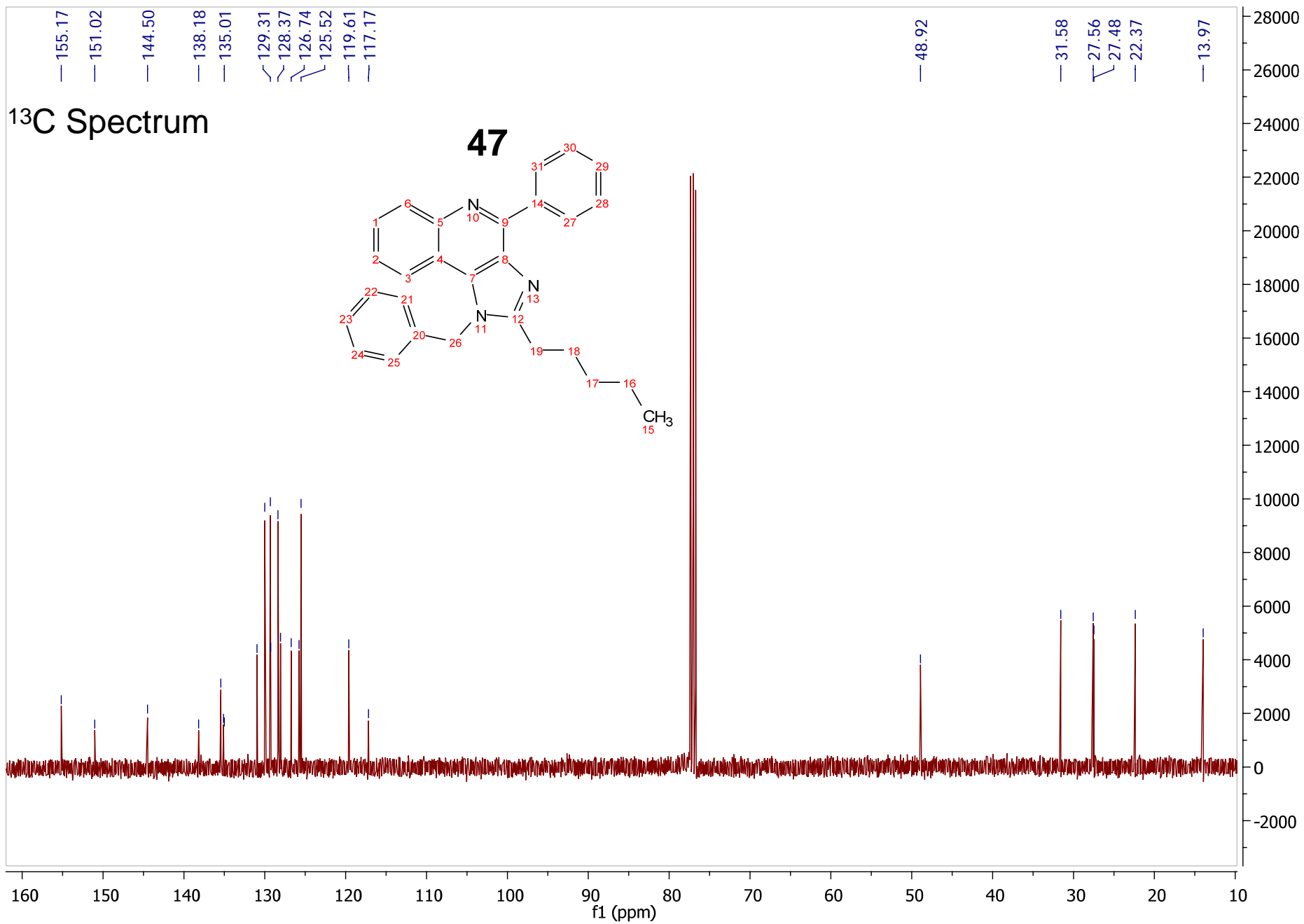


TOF Spectrum	TOF	Profile Spectrum at 171.60 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 510998

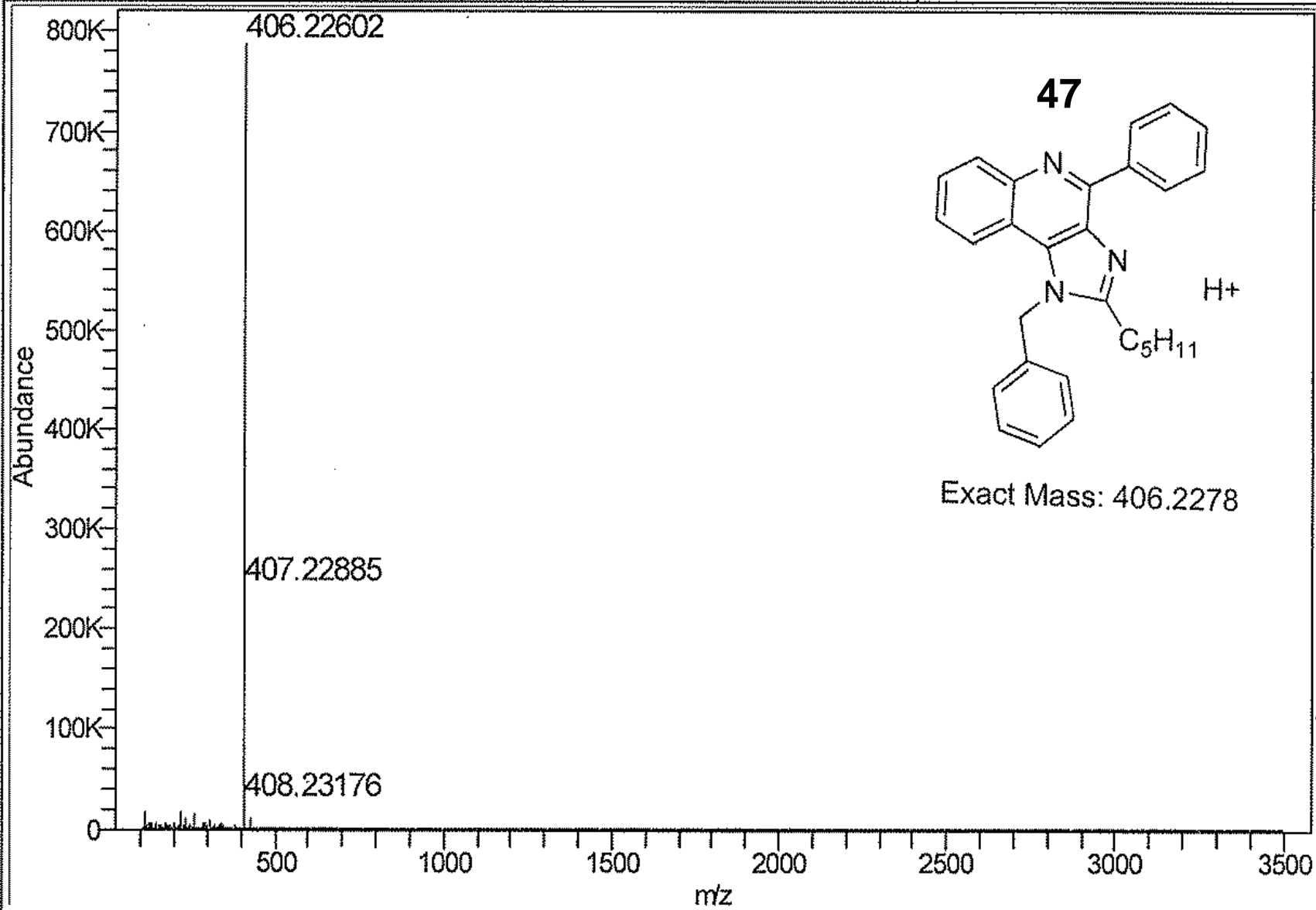


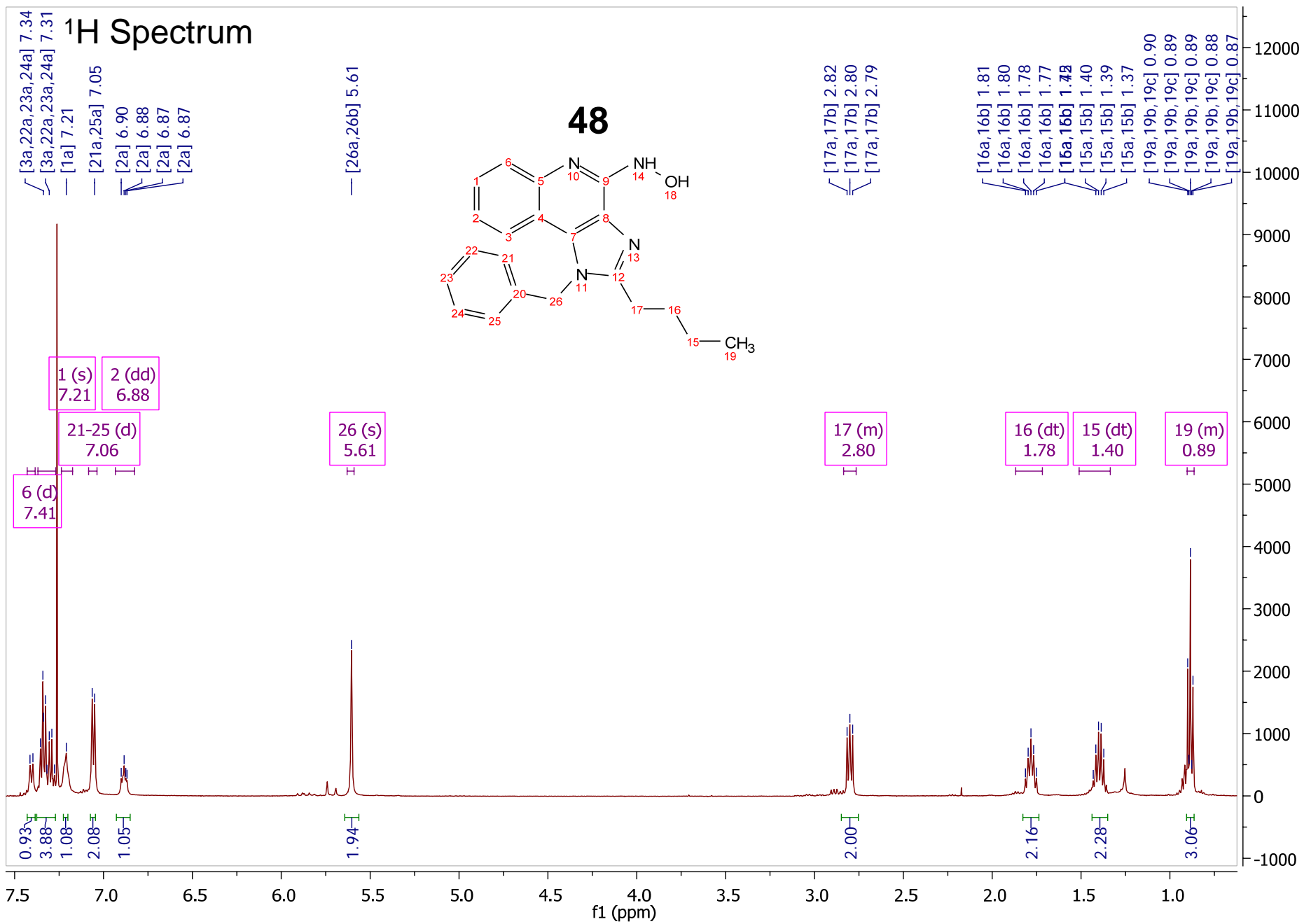
# <sup>1</sup>H Spectrum

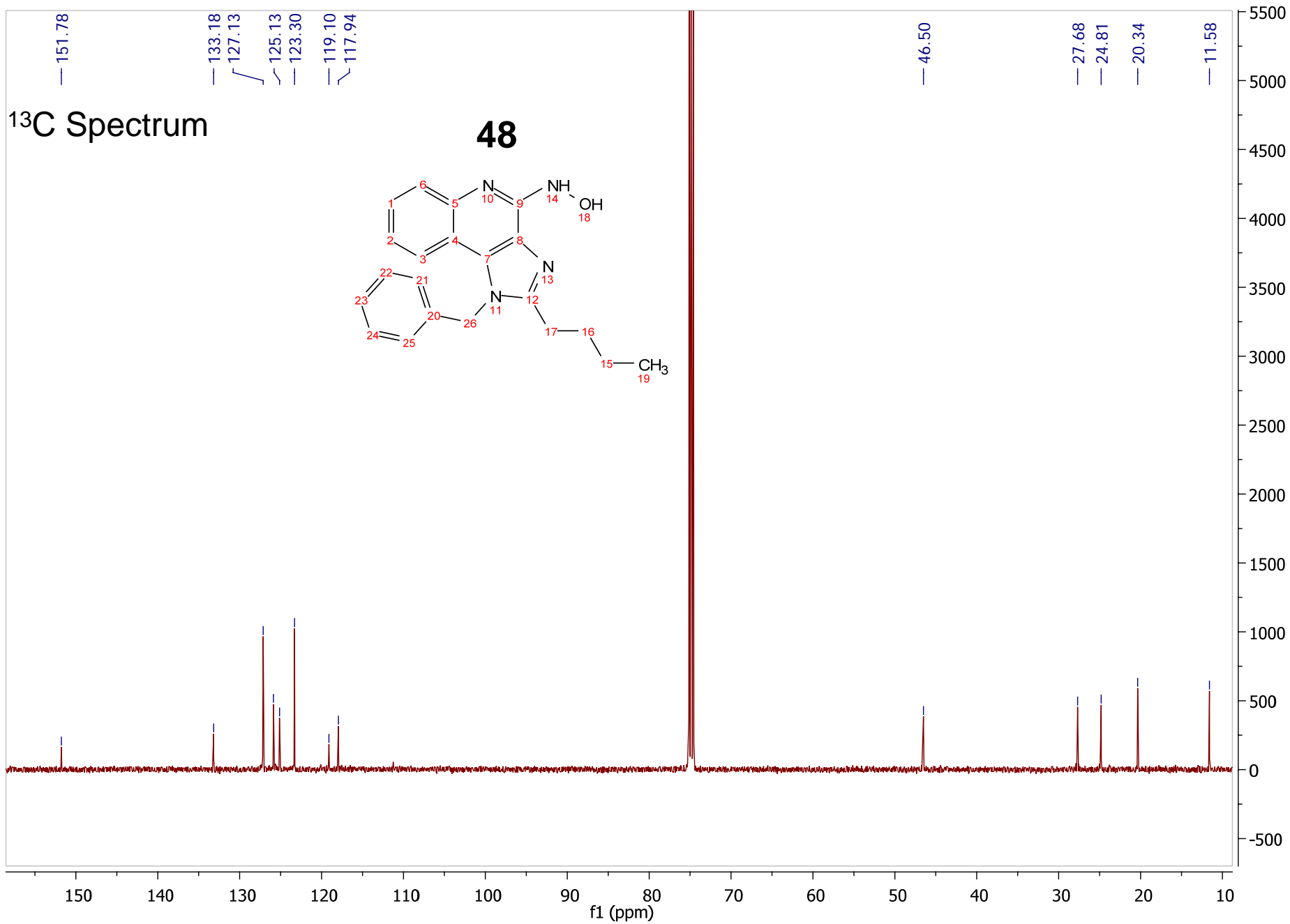




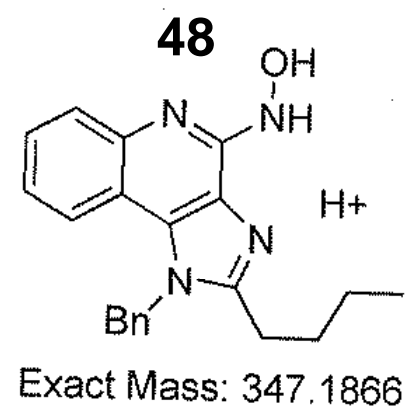
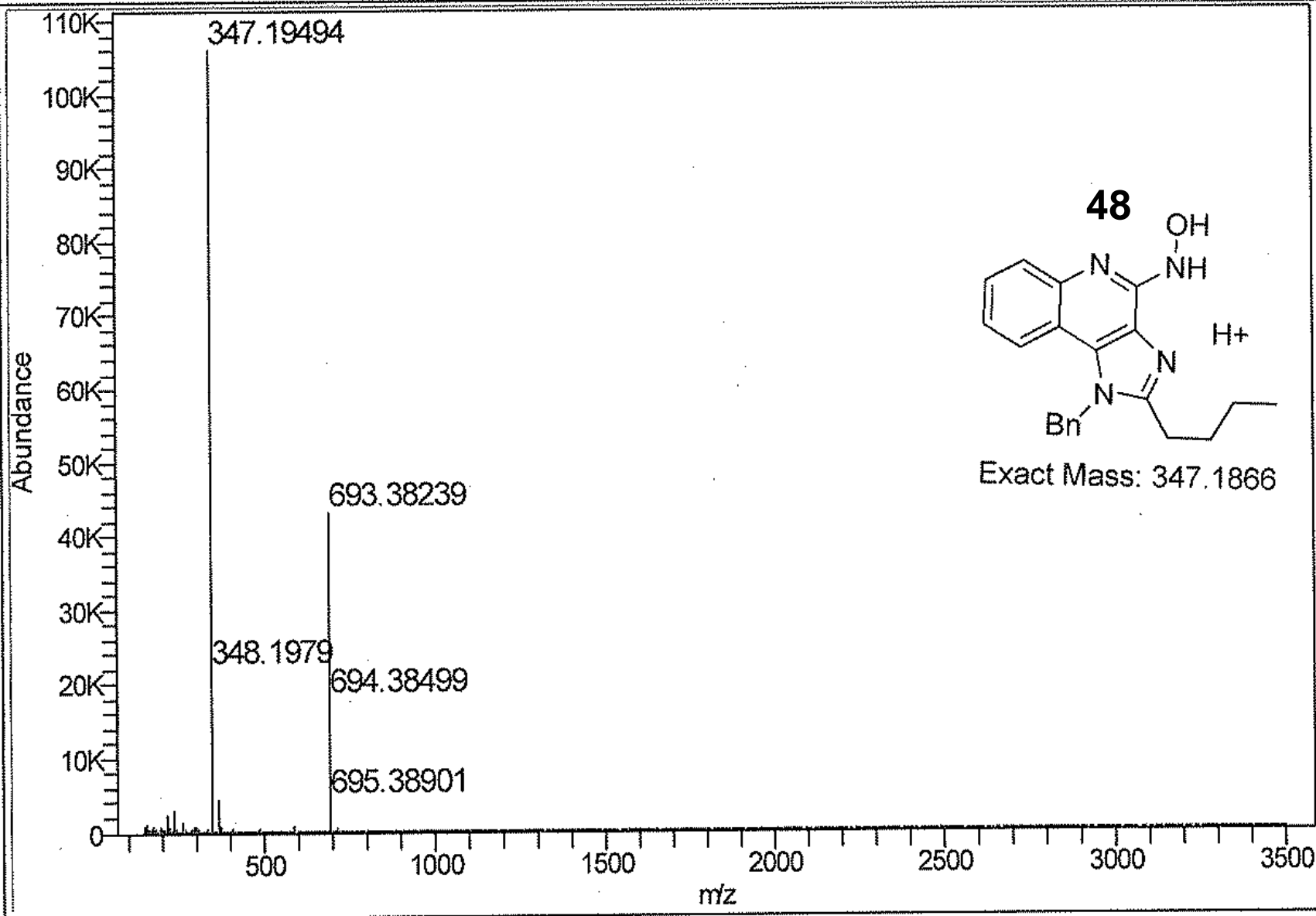
TOF Spectrum	TOF	Profile Spectrum at 33288.63 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 786367



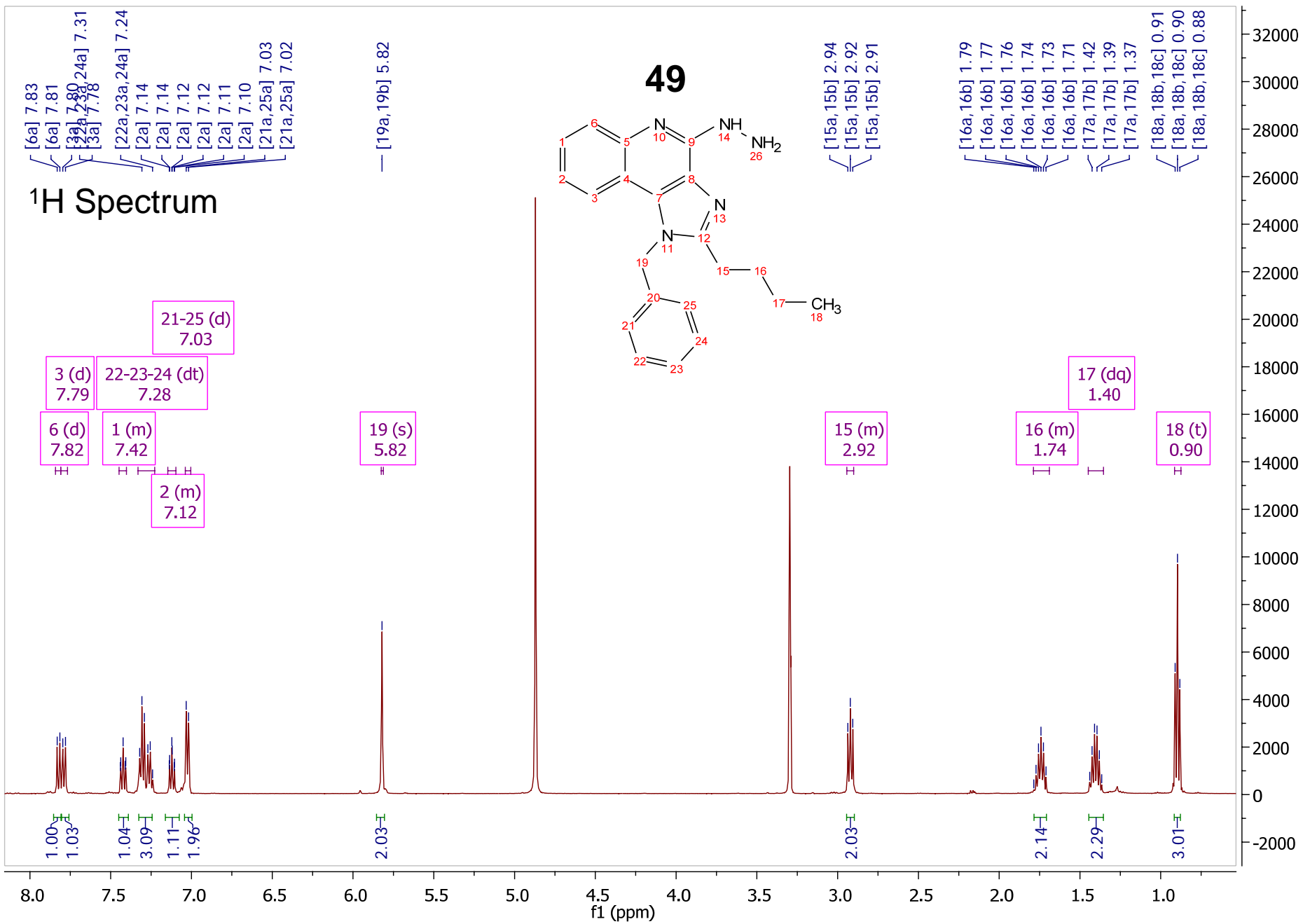




TOF Spectrum	TOF	Profile Spectrum at 2352.98 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 105988

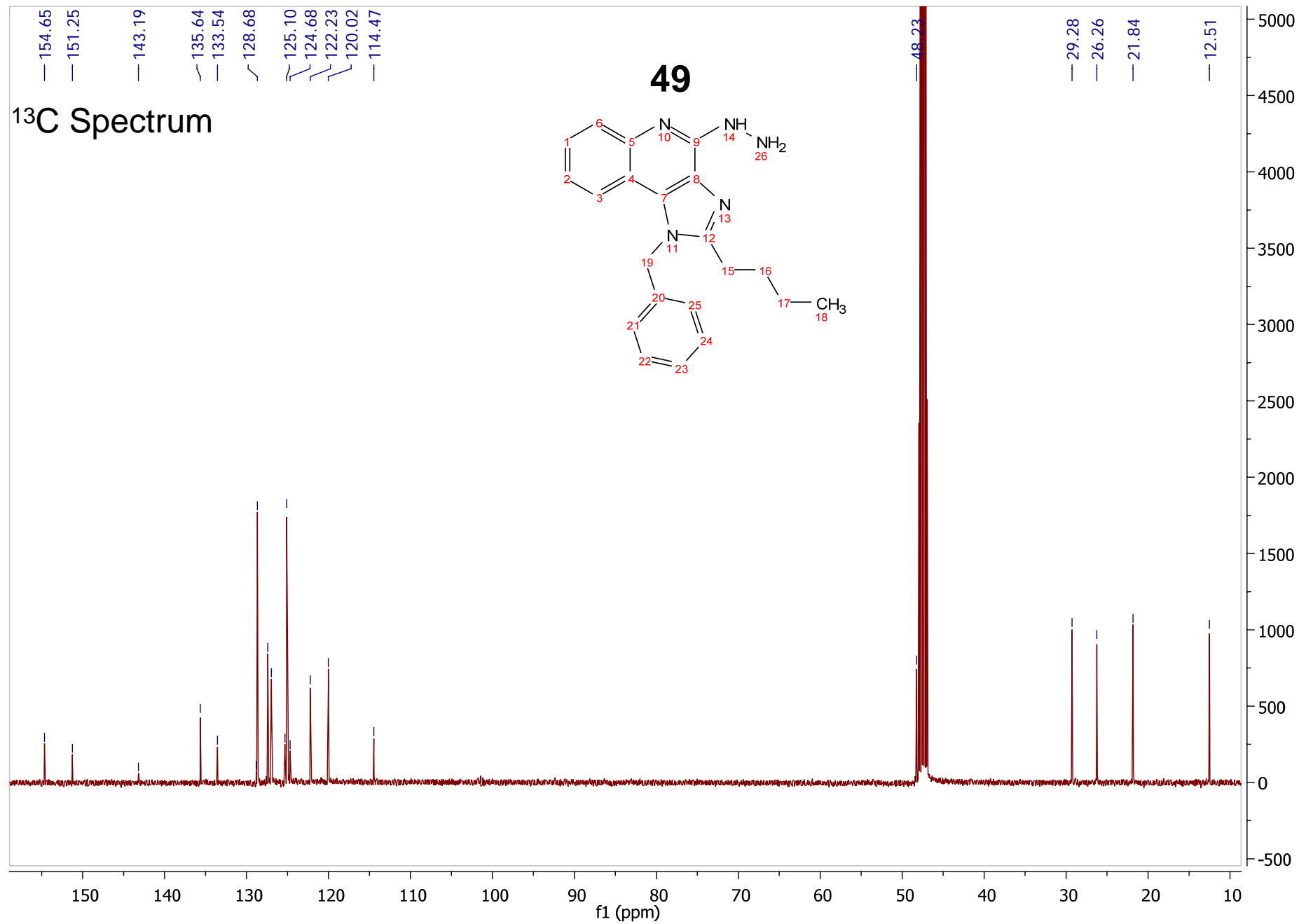
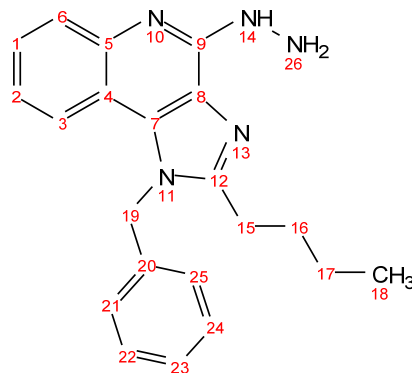


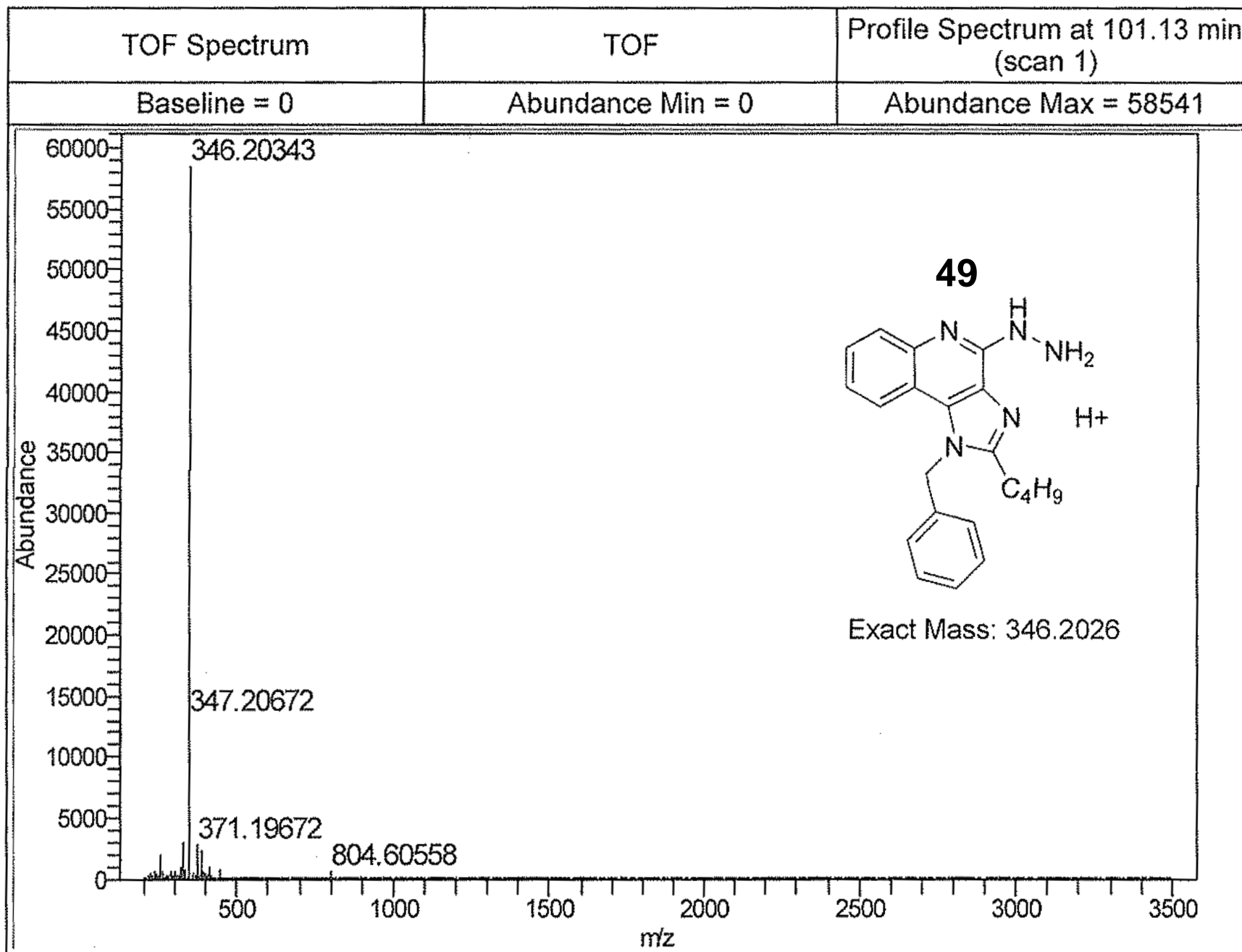




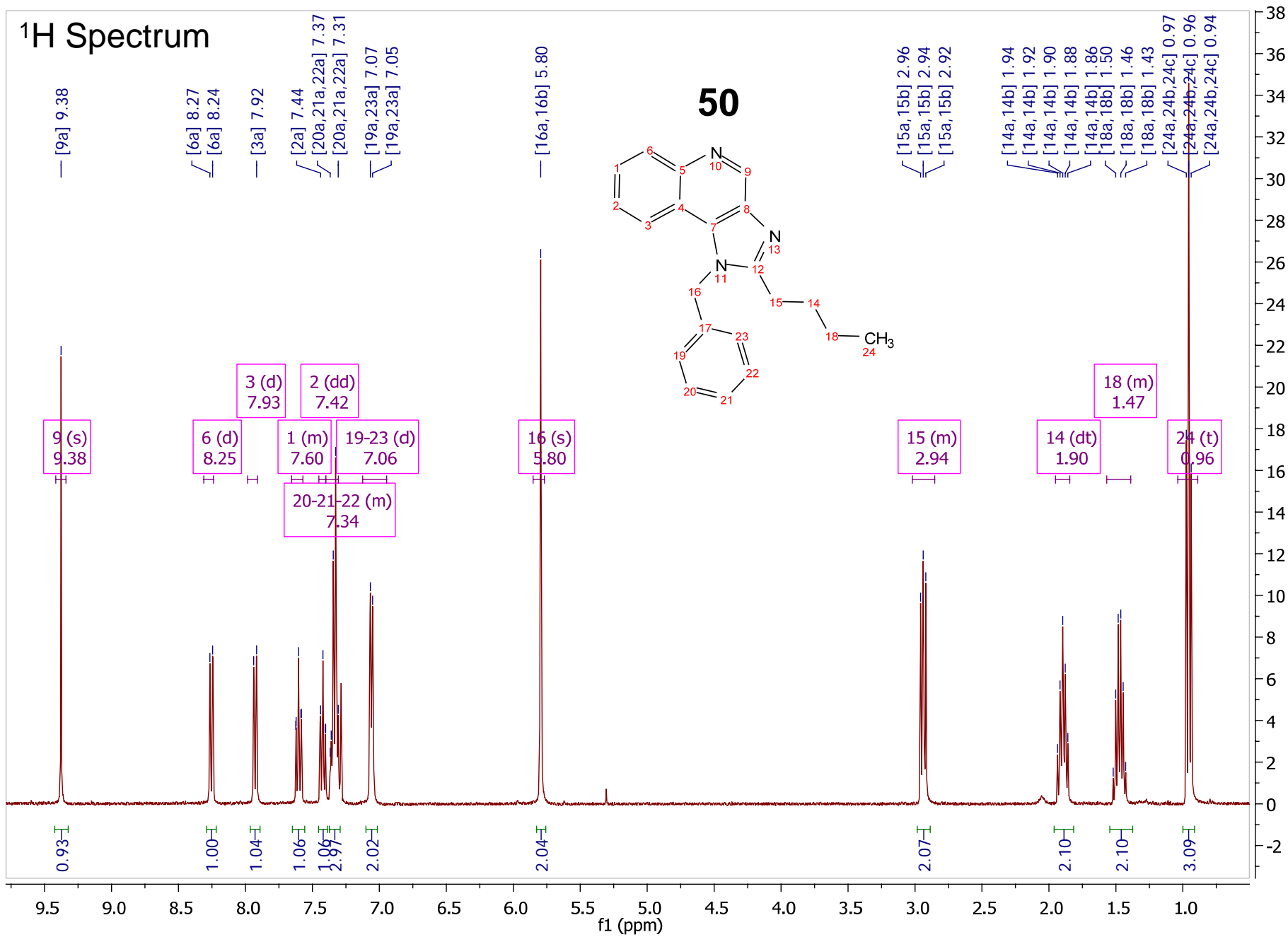
# <sup>13</sup>C Spectrum

49



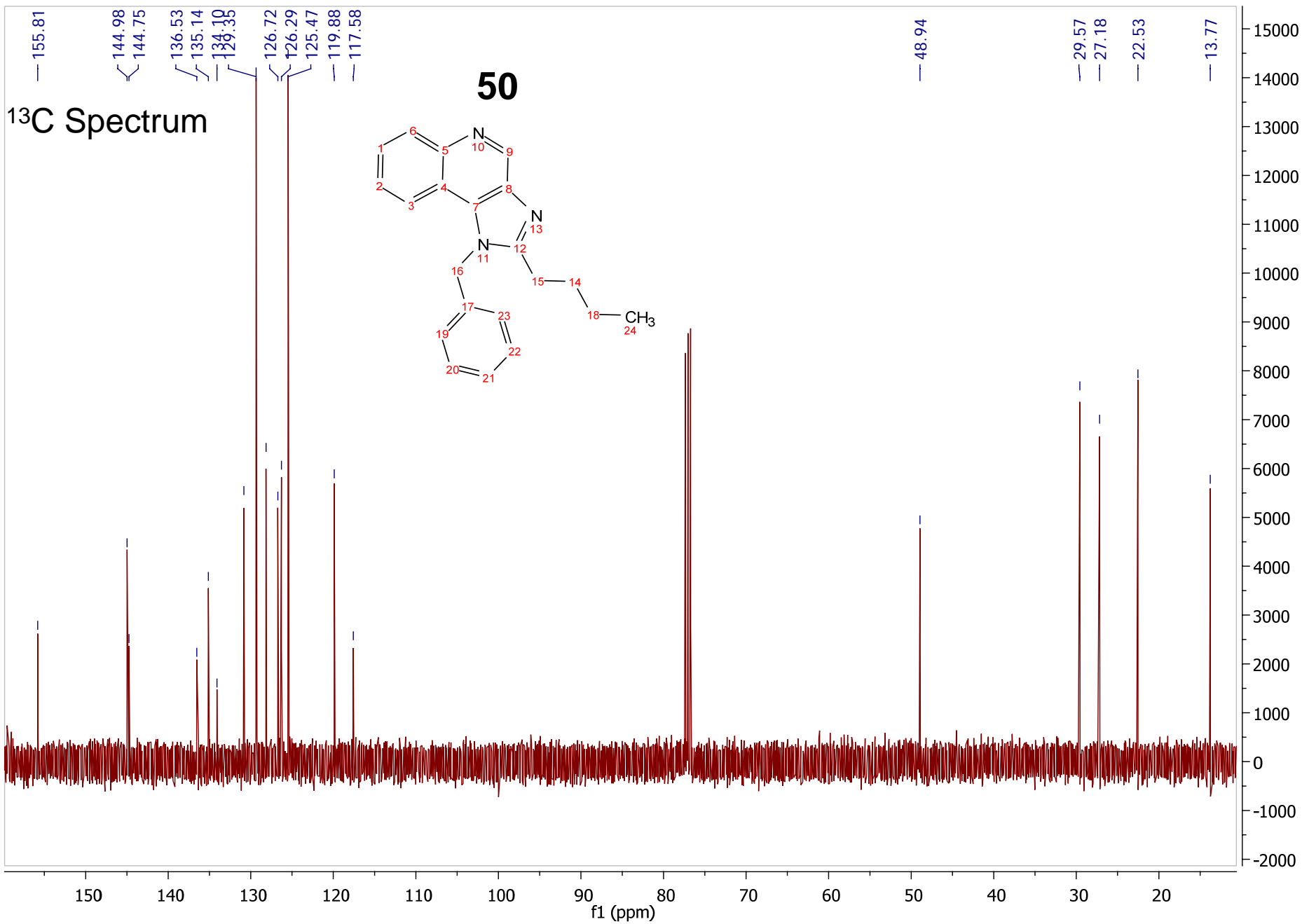
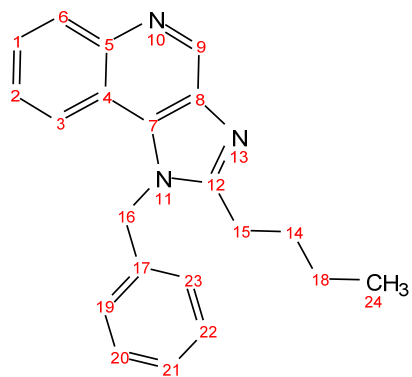


# <sup>1</sup>H Spectrum

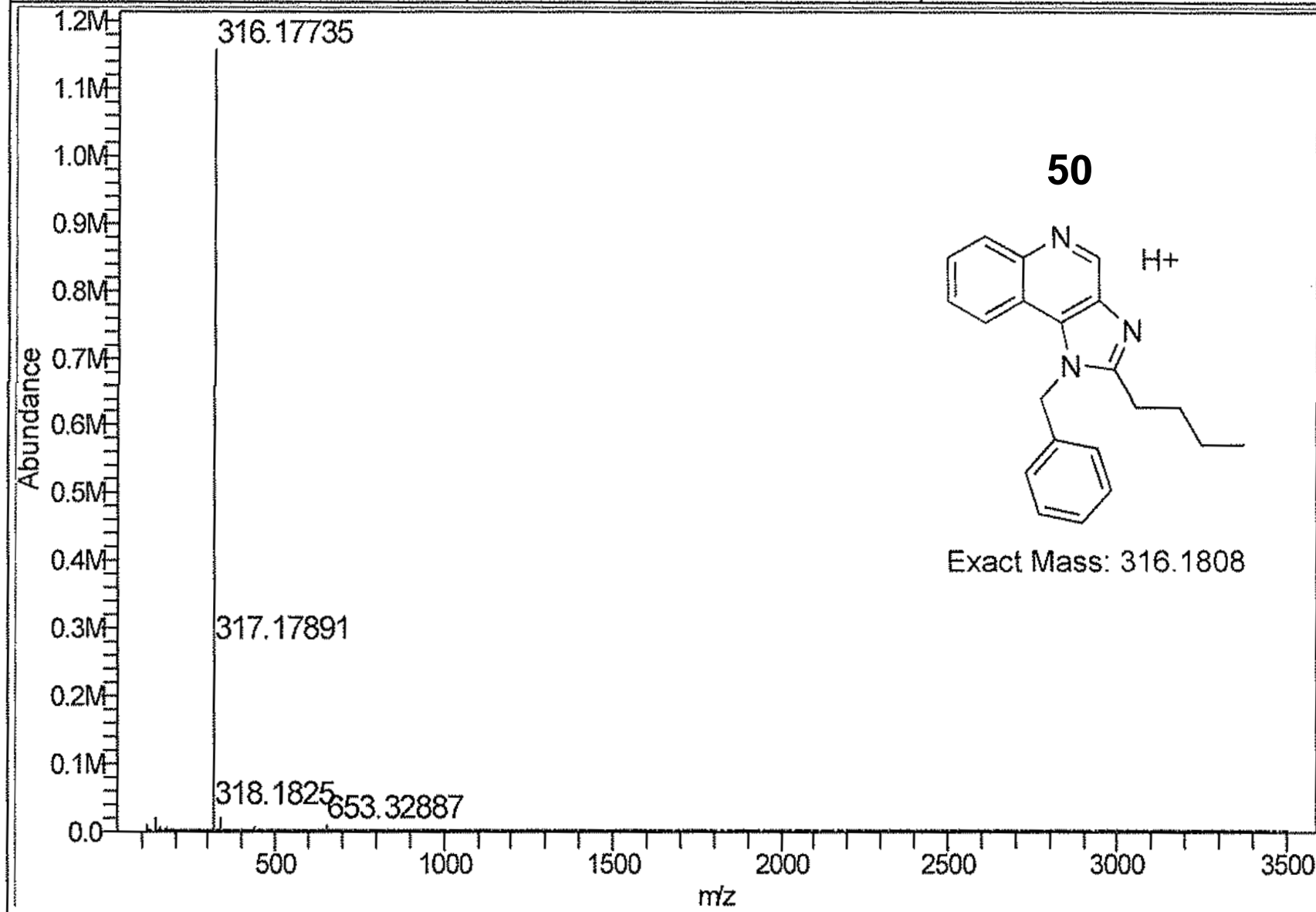


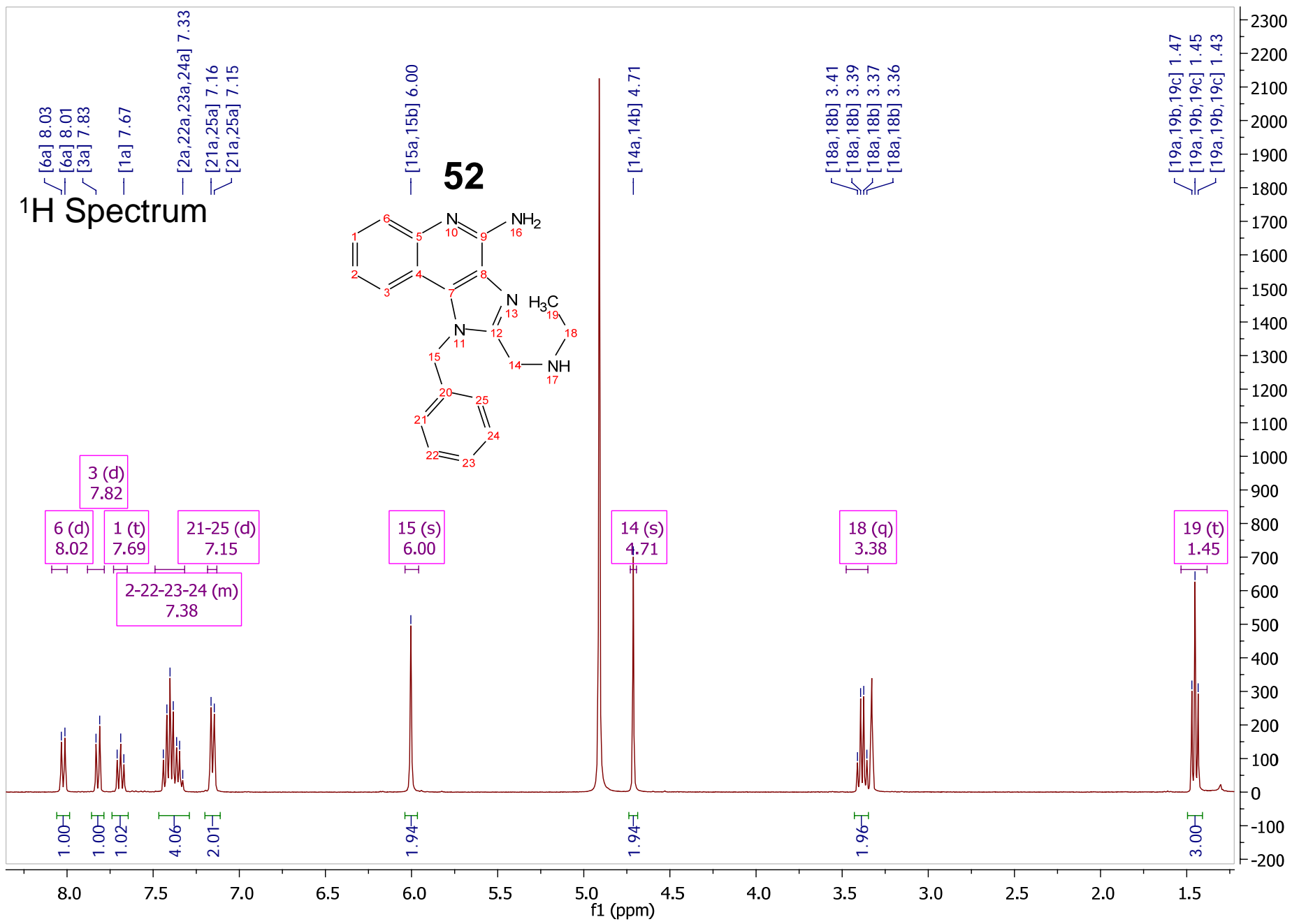
# <sup>13</sup>C Spectrum

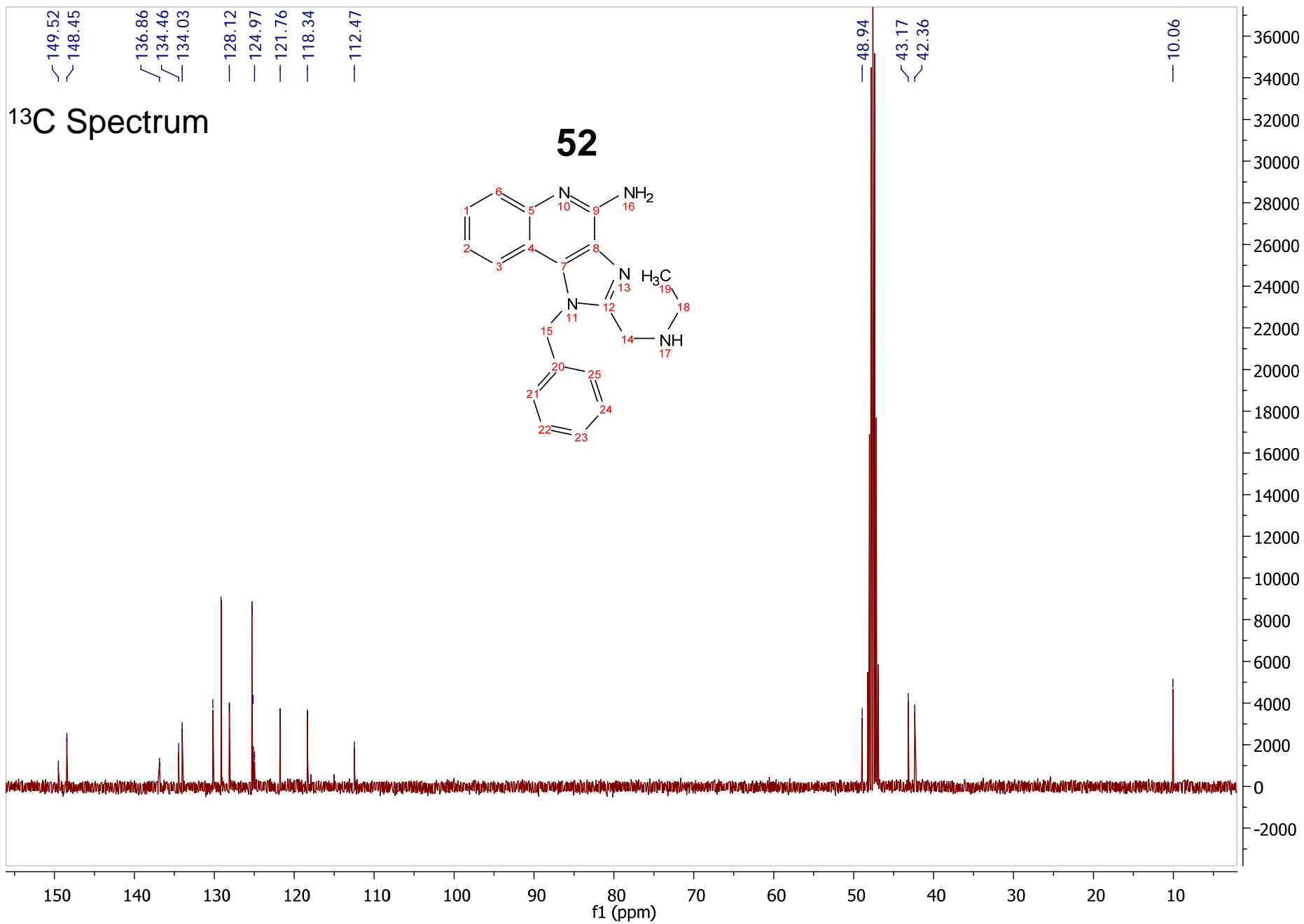
50



TOF Spectrum	TOF	Profile Spectrum at 57.33 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 1157019

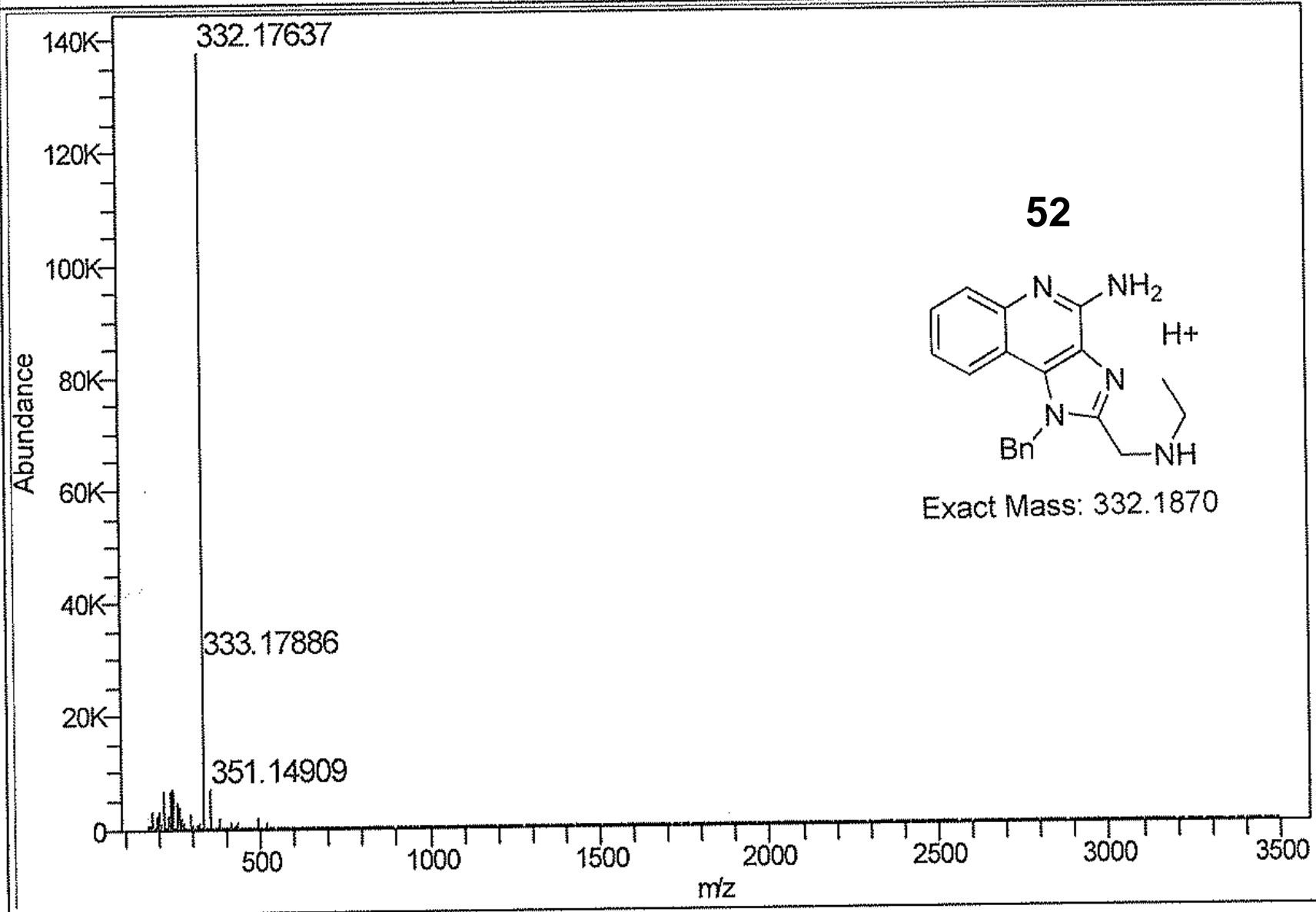




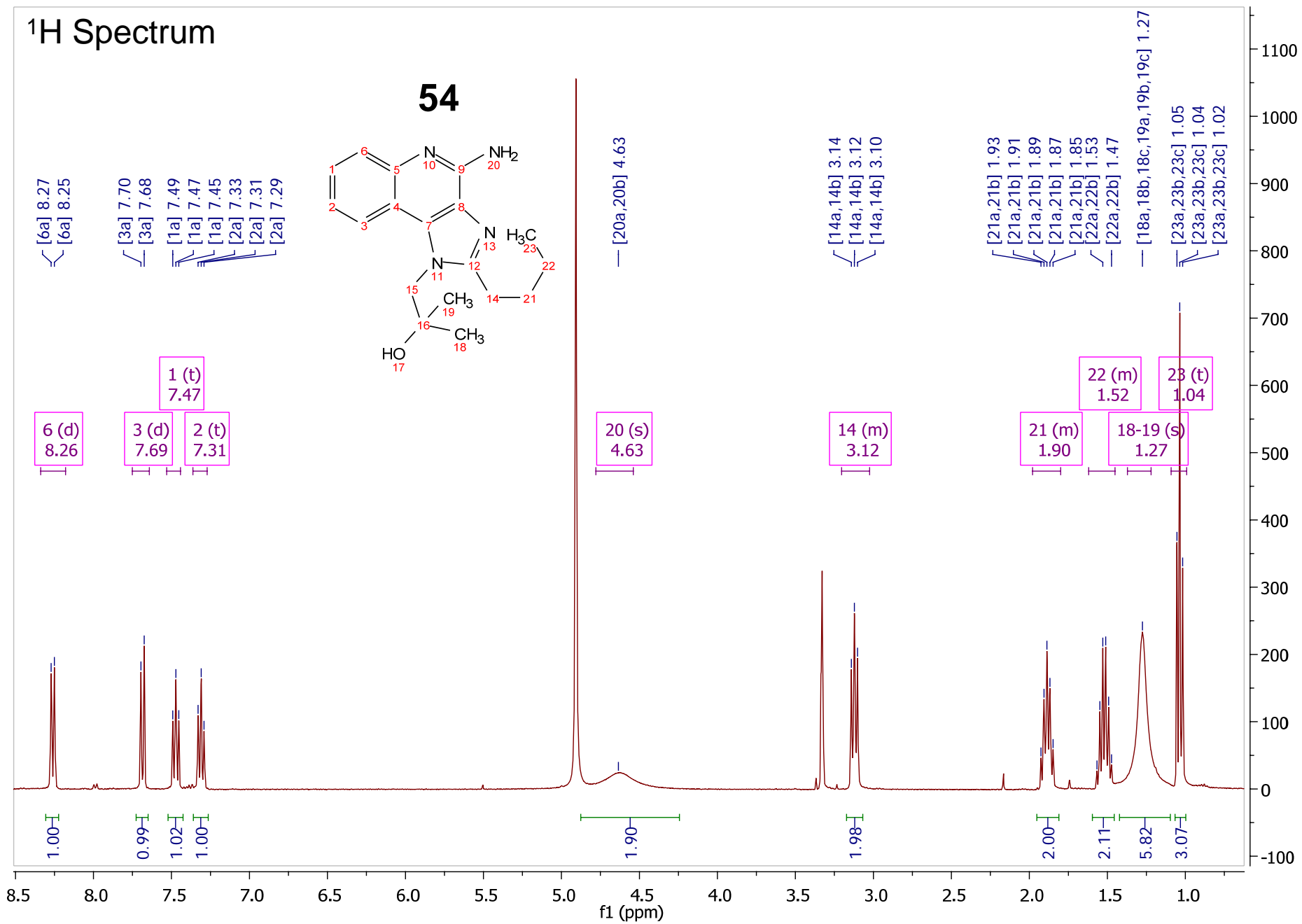


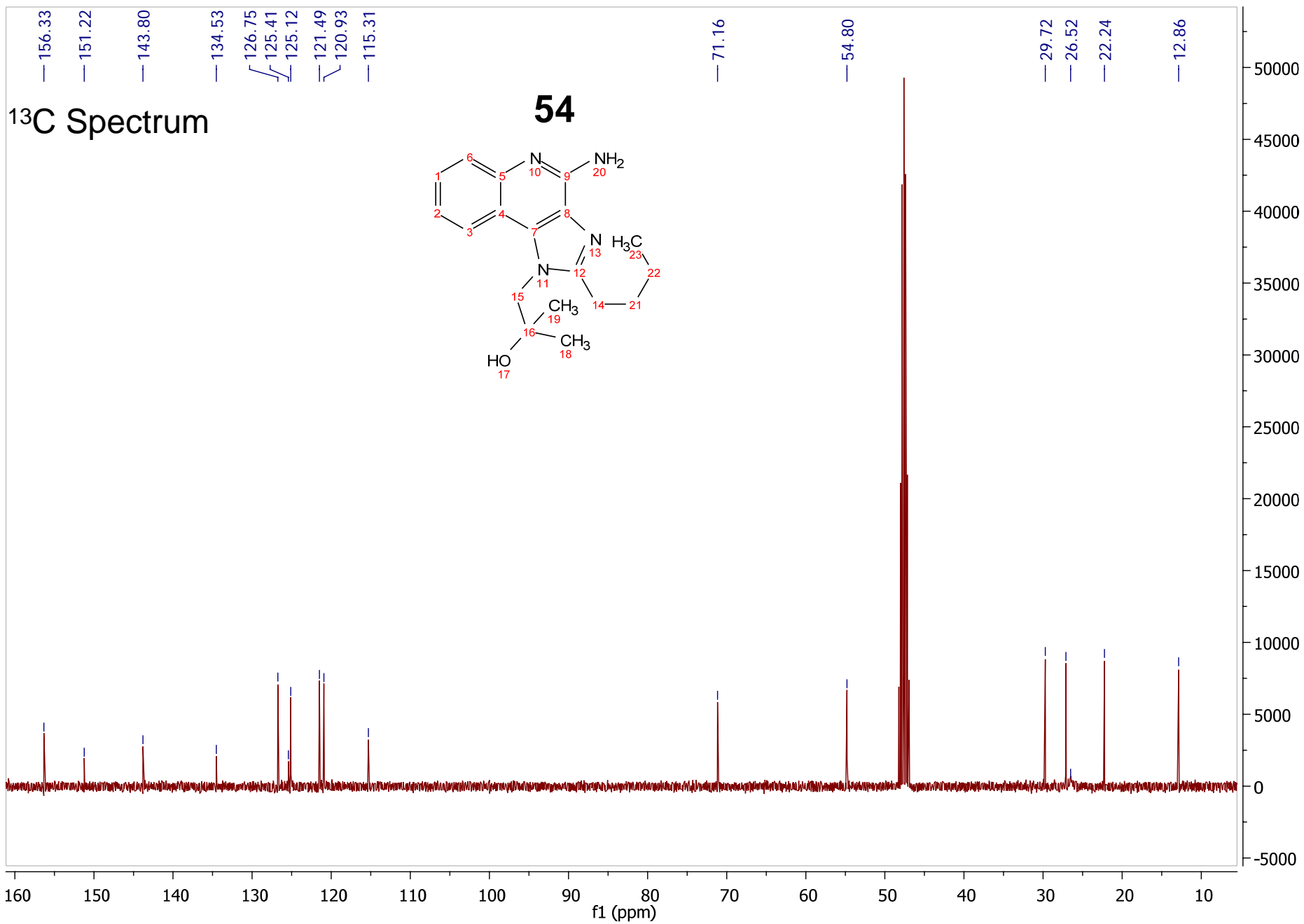


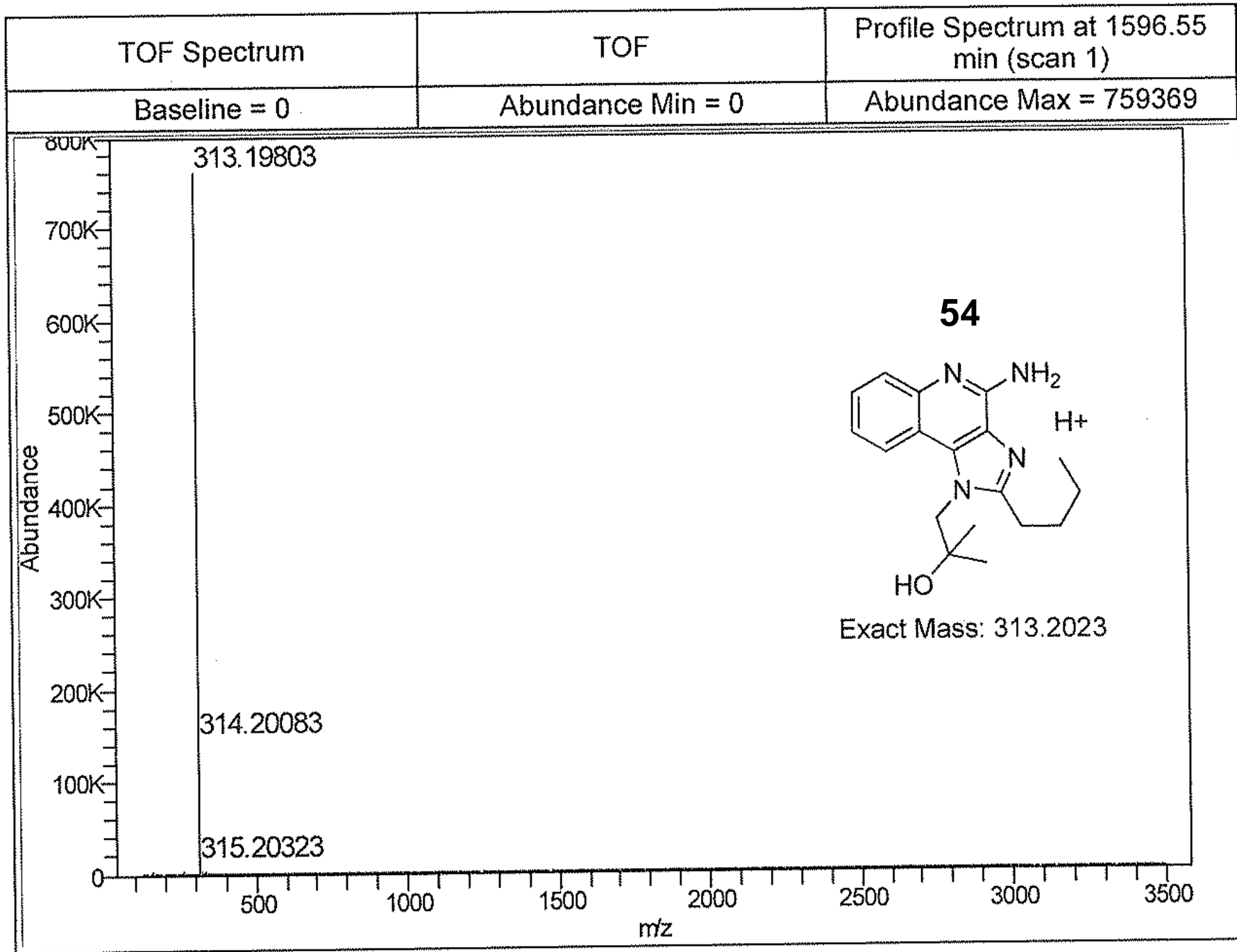
TOF Spectrum	TOF	Profile Spectrum at 1263.93 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 137658



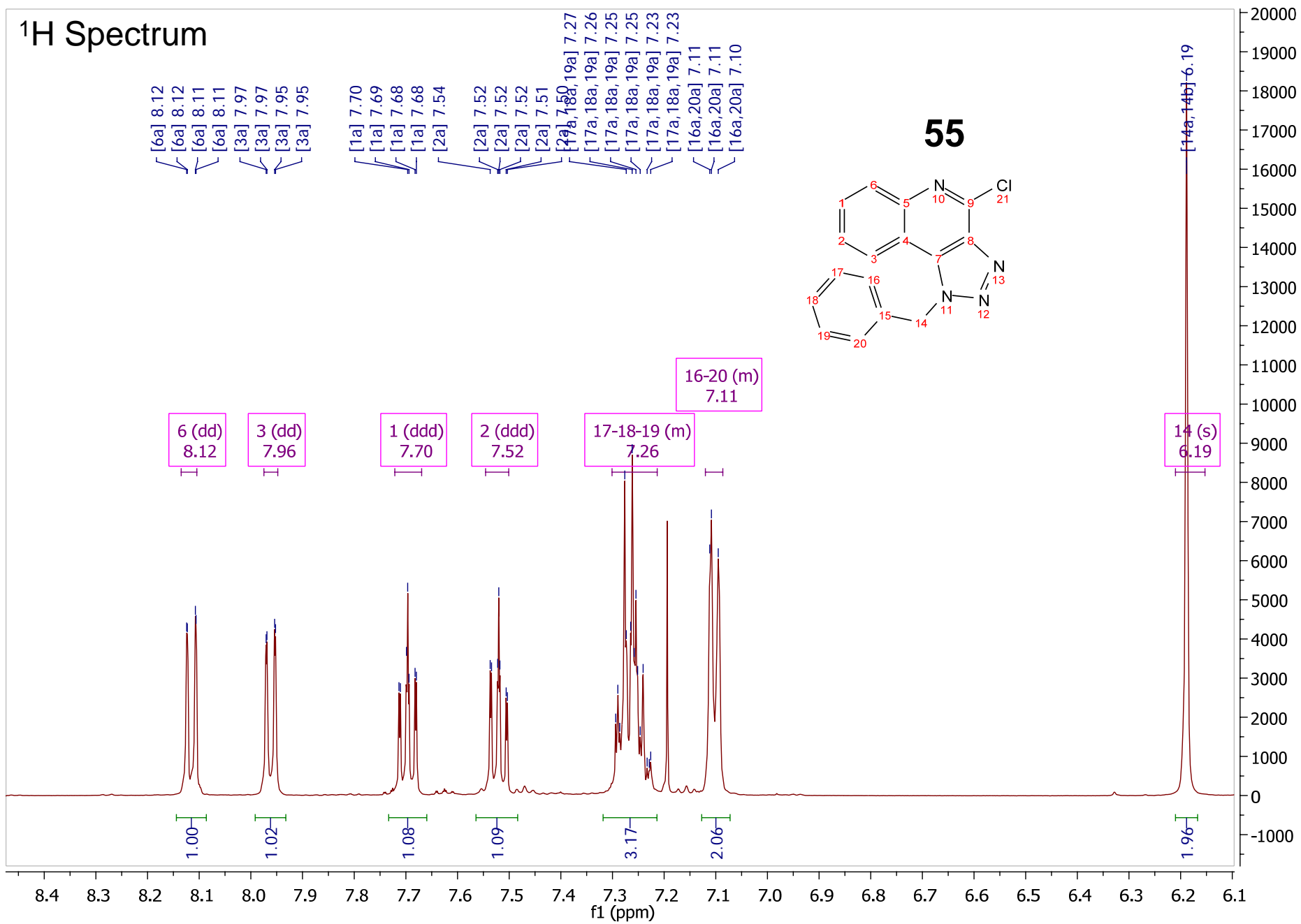
# <sup>1</sup>H Spectrum

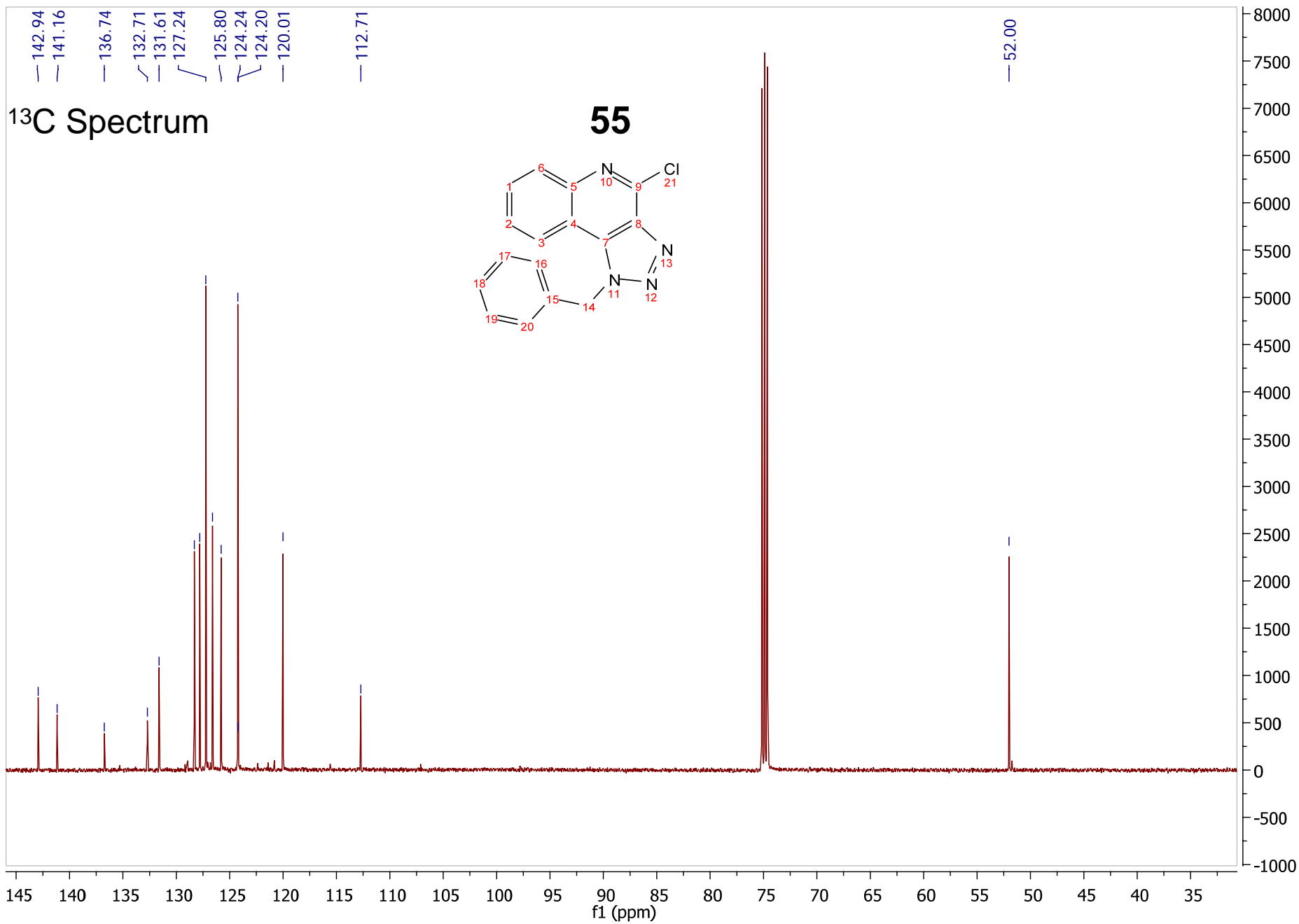


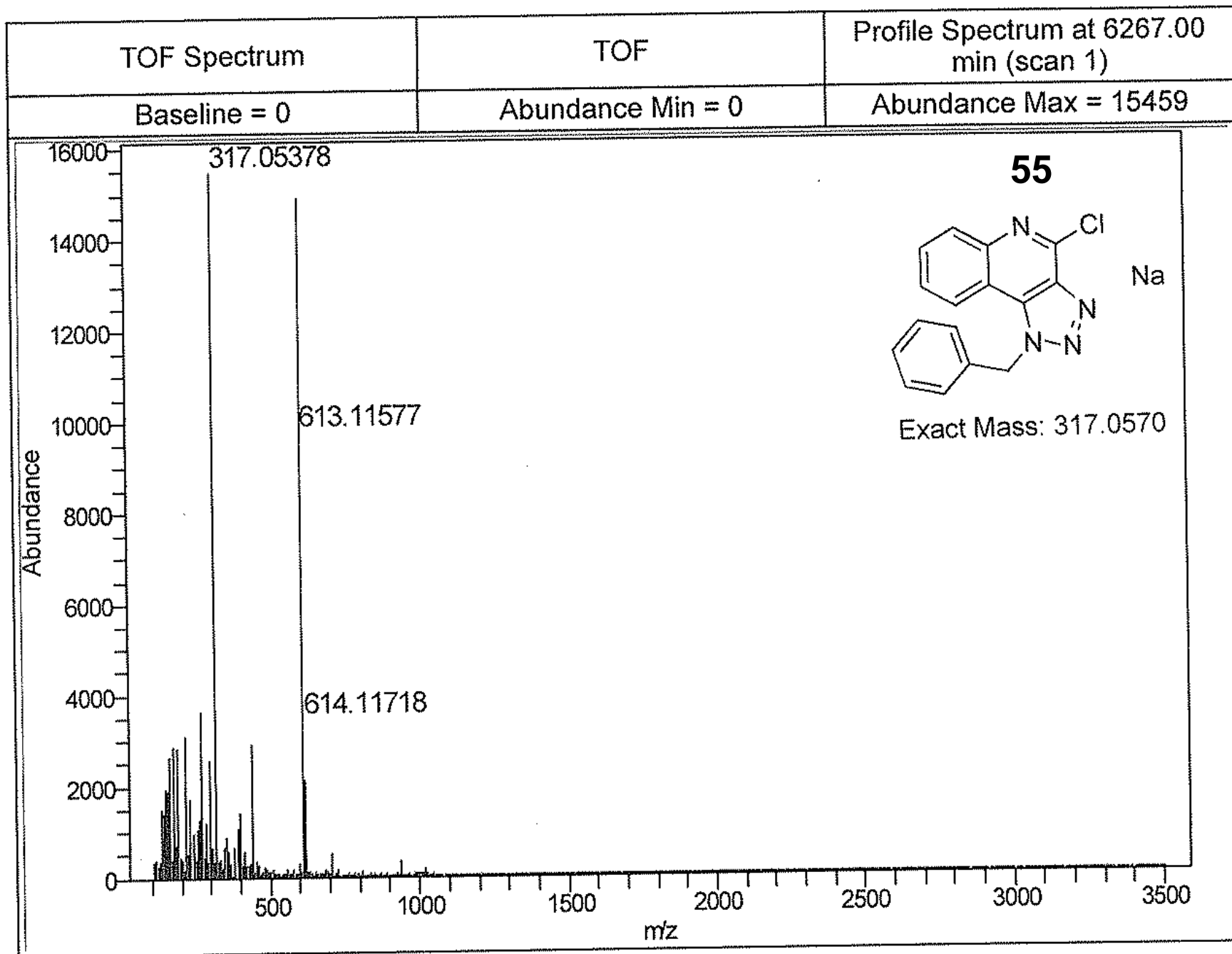




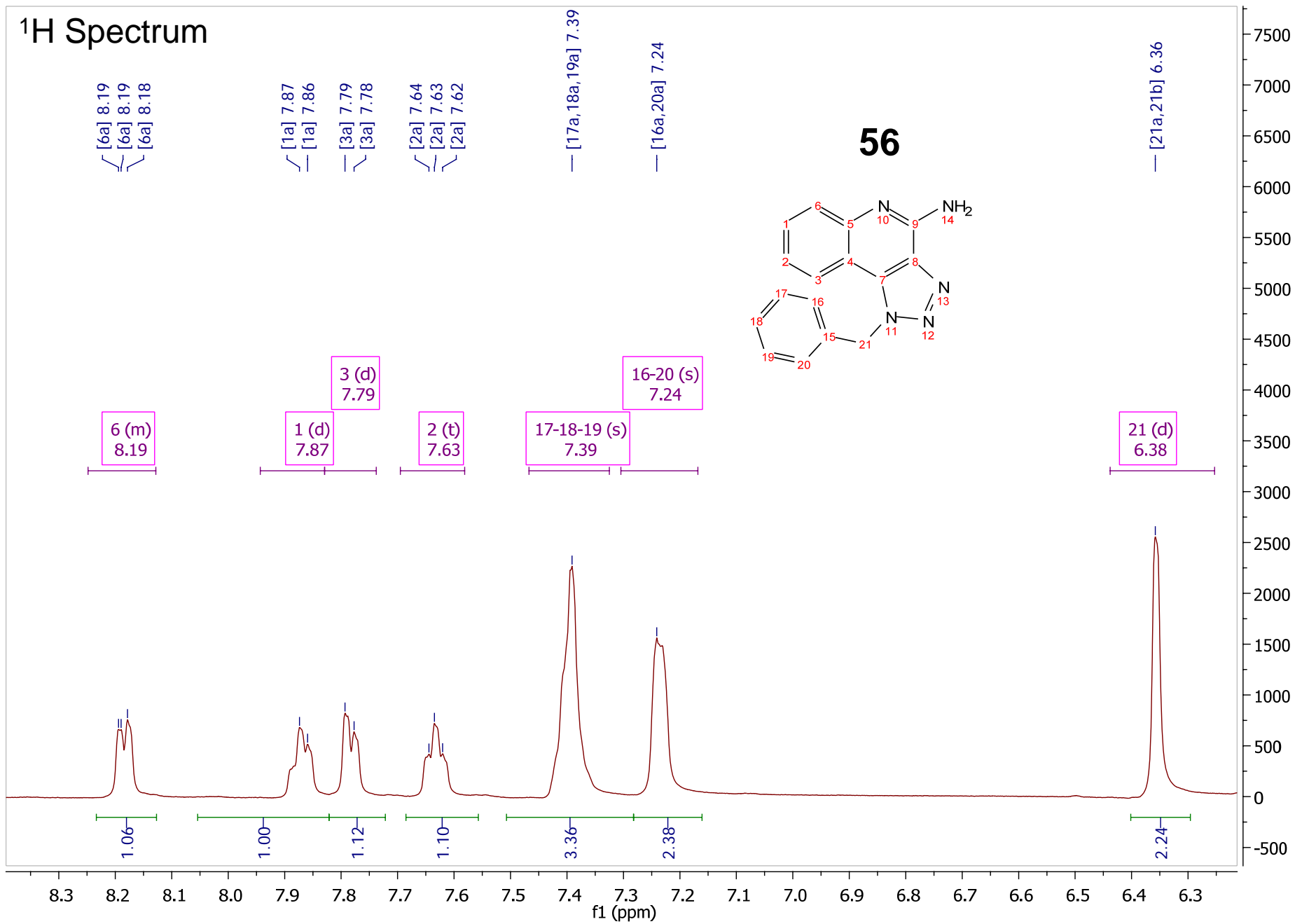
# <sup>1</sup>H Spectrum



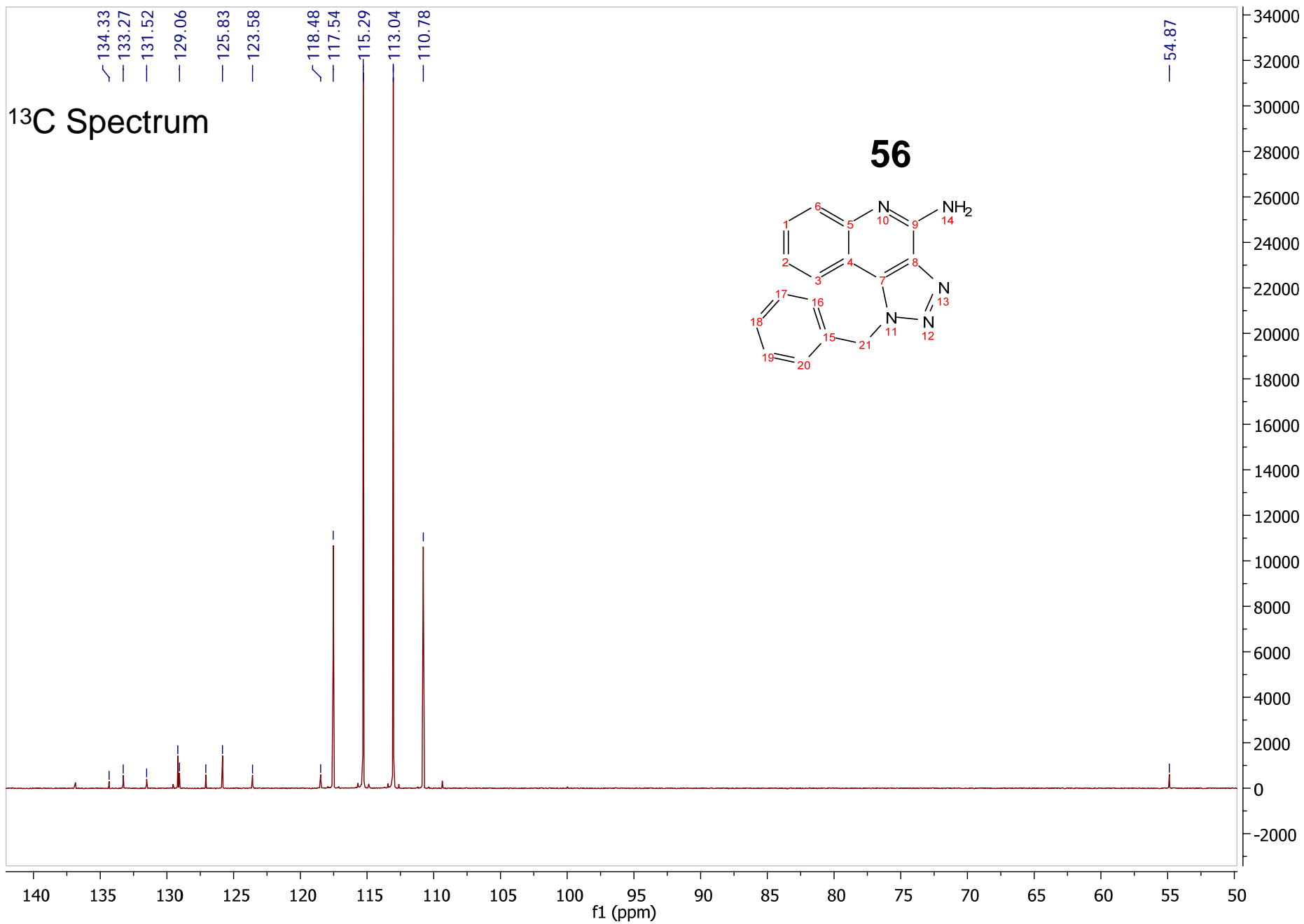




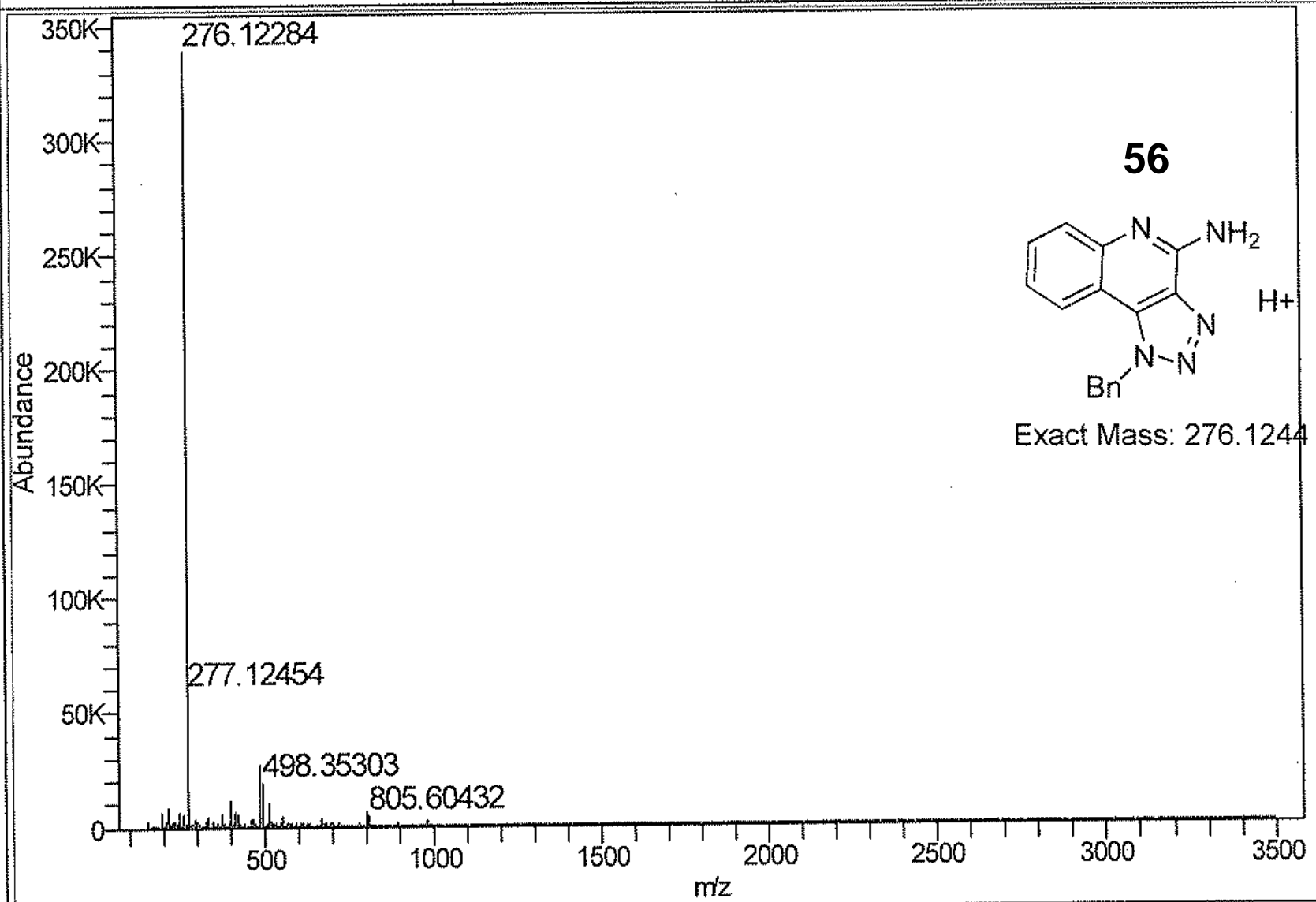
# <sup>1</sup>H Spectrum



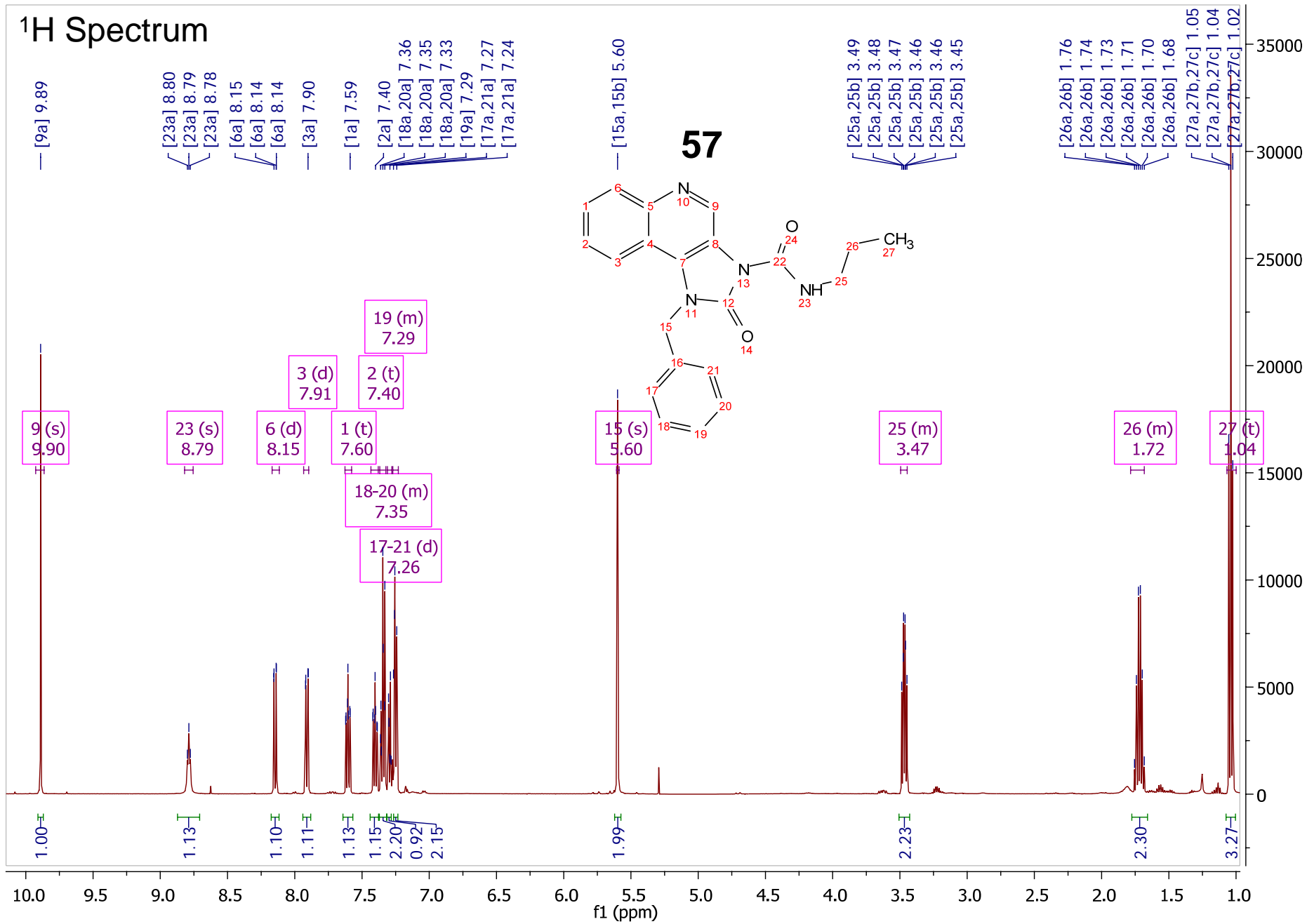


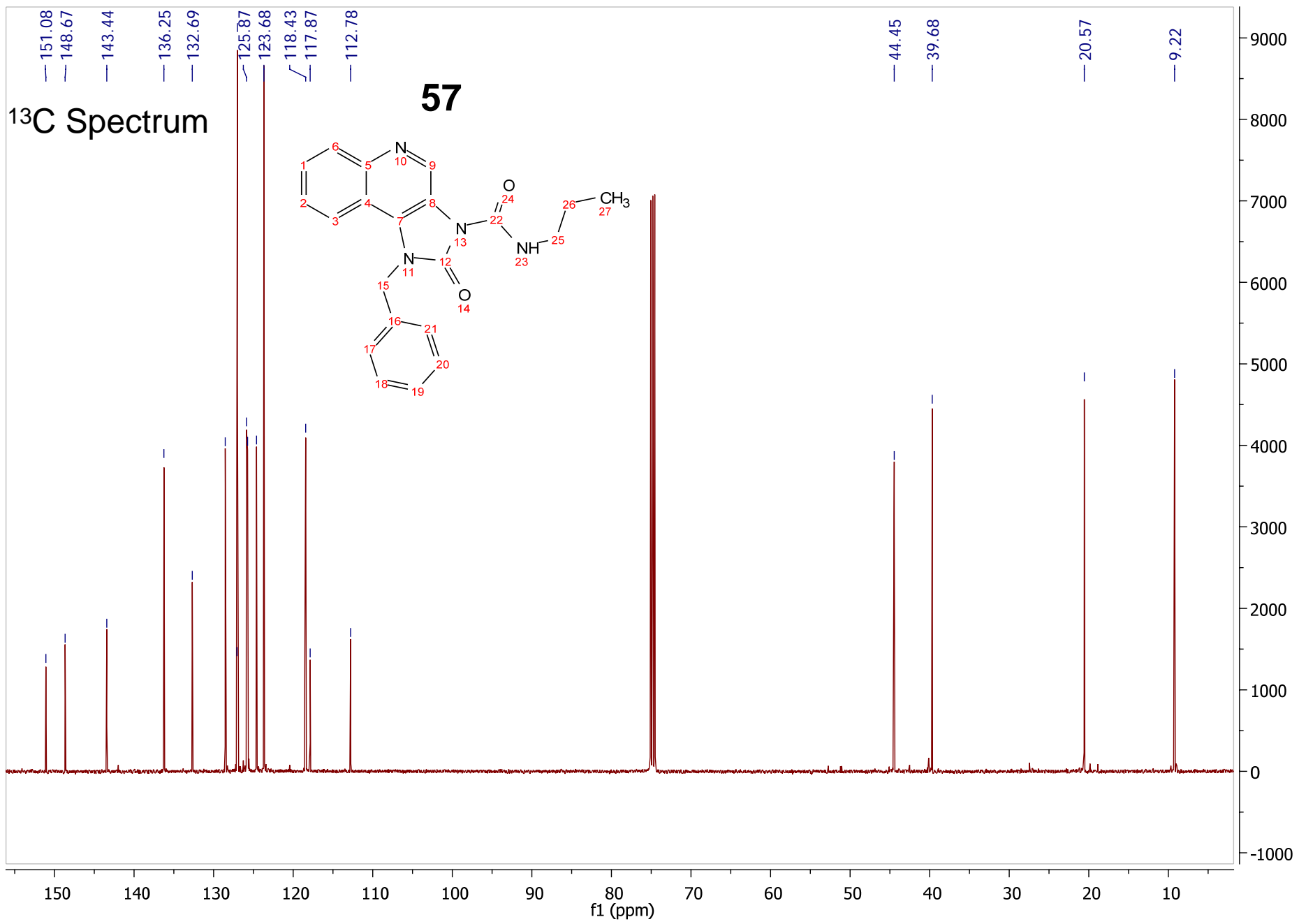


TOF Spectrum	TOF	Profile Spectrum at 1141.47 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 339392



# <sup>1</sup>H Spectrum





TOF Spectrum	TOF	Profile Spectrum at 8610.58 min (scan 1)
Baseline = 0	Abundance Min = 0	Abundance Max = 1076677

