

Synthesis and Activity Evaluation of Vinpocetine-Derived Indole Alkaloids

Zhang-Chao Dong^{1,†}, Yang Shi^{1,†}, Liang-Liang Zheng¹, You-Ping Tian¹, Jian Yang³, Ying Wei¹, Ying Zhou^{1,*}
and Bo-Wen Pan^{1,2*}

Zhang-Chao Dong ^{1,†}, Yang Shi ^{1,†}, Liang-Liang Zheng ¹, You-Ping Tian ¹, Jian Yang ², Ying Wei ¹, Ying Zhou ^{1,*}
and Bo-Wen Pan ^{1,3,*}

¹ College of Pharmacy, Guizhou University of Traditional Chinese Medicine, Guiyang 550025, China; weiyang1969@126.com (Y.W.); dongzhangchao0824@163.com (Z.-C.D.); xiaoyewater@163.com (Y.S.); zxl5117508142@163.com (L.-L.Z.); nanshan-tia@163.com (Y.-P.T.); weiyang479@gzy.edu.cn (Y.W.)

² College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, SK S7N 5E5, Canada; jian.yang@usask.ca

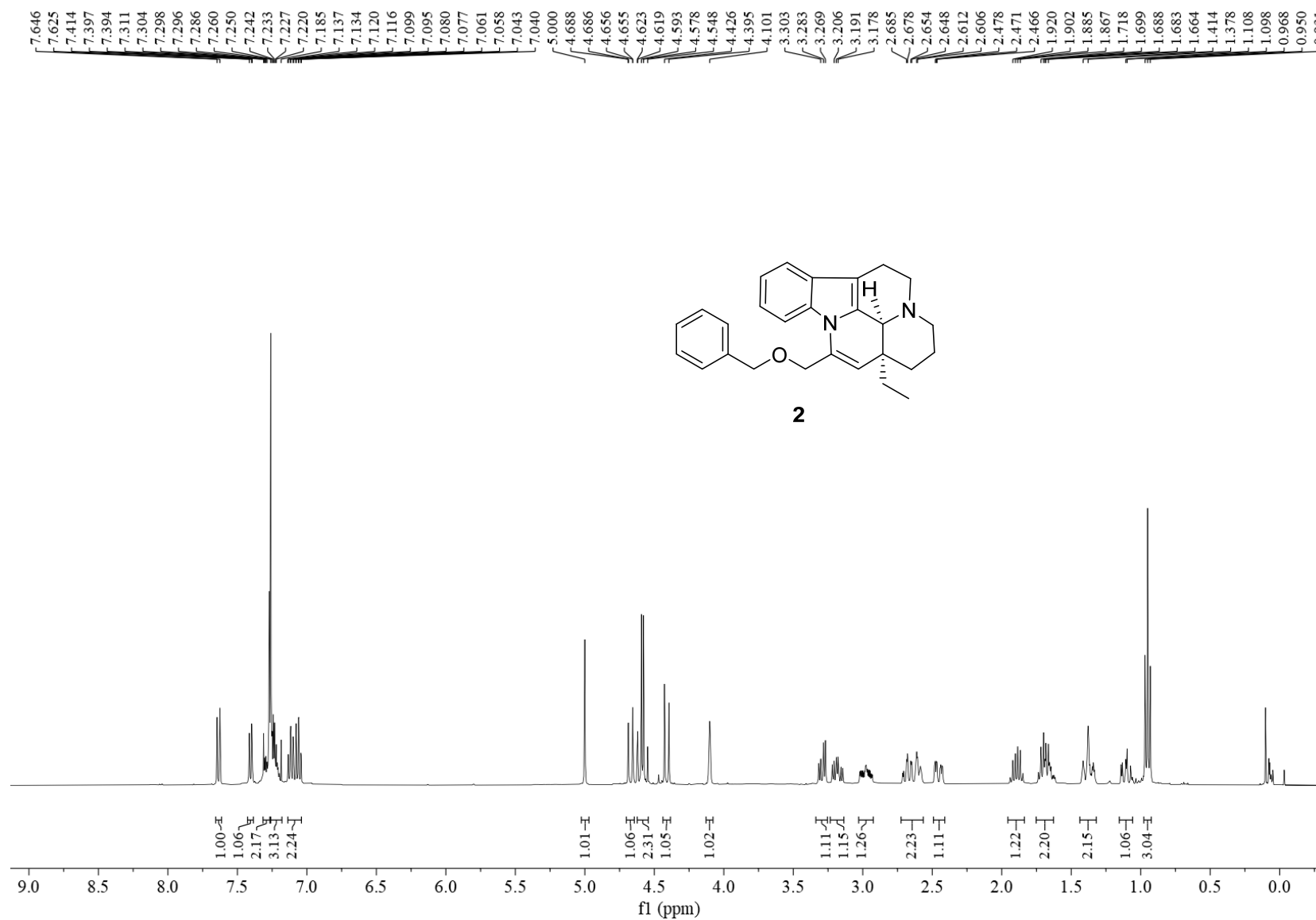
³ State Key Laboratory of Natural and Biomimetic Drugs, School of Pharmaceutical Sciences, Peking University, Beijing 100191, China

* Correspondence: bwpan@gzy.edu.cn (B.W.P.); zhouying067@gzy.edu.cn (Y.Z.); Tel.: +86-0851-88233090 (Y.Z.)

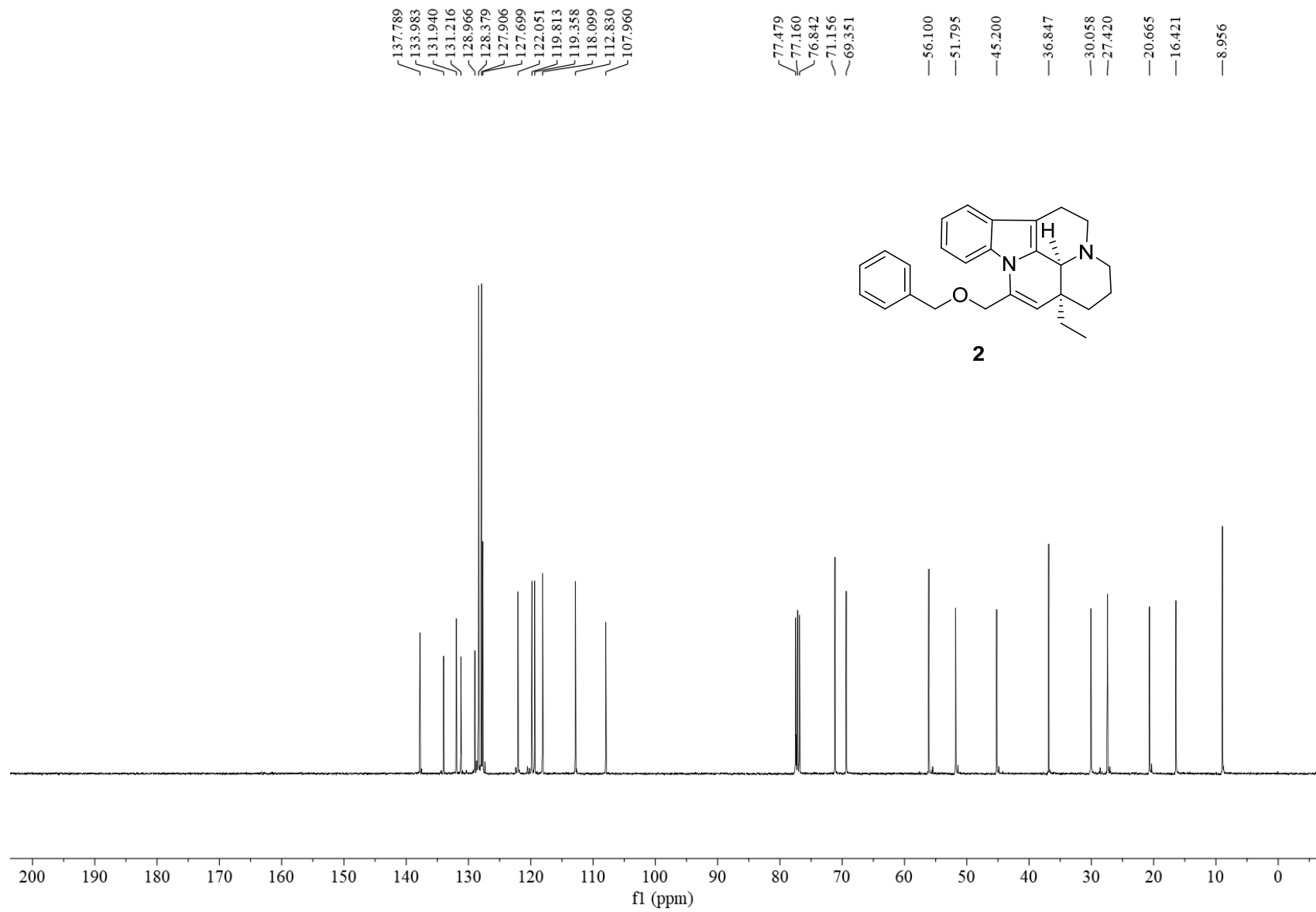
† These authors contributed equally to this work.

Contents	Page
1. NMR and HRMS spectra	2–79

1. NMR and HRMS spectra



^1H NMR of Compound **2** (400 MHz, CDCl_3)

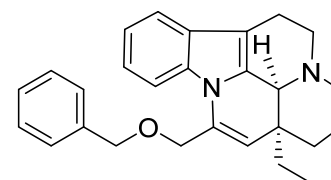
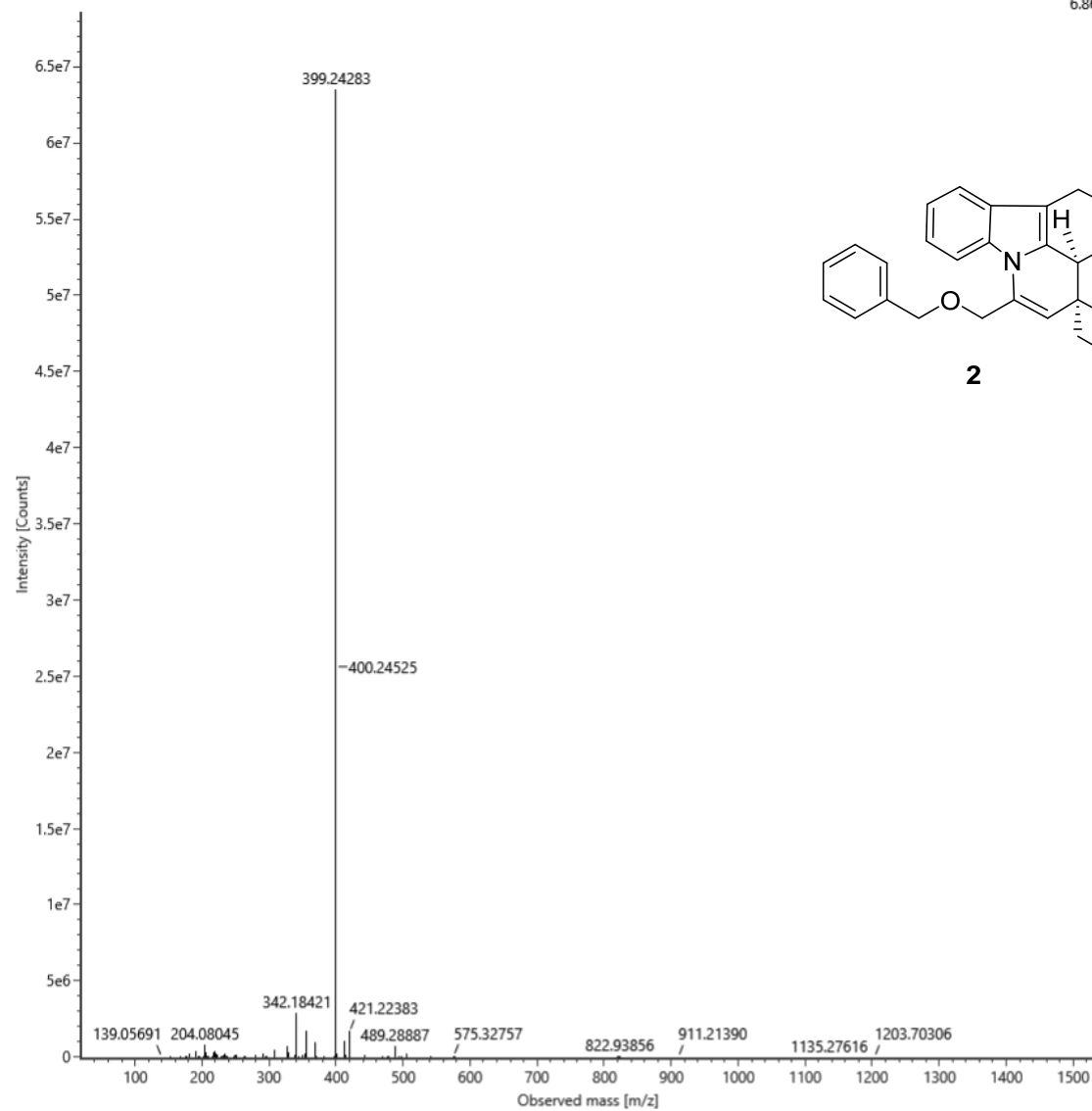


¹³C NMR of Compound **2** (100 MHz, CDCl₃)

Item name: DB-60-2
Item description:

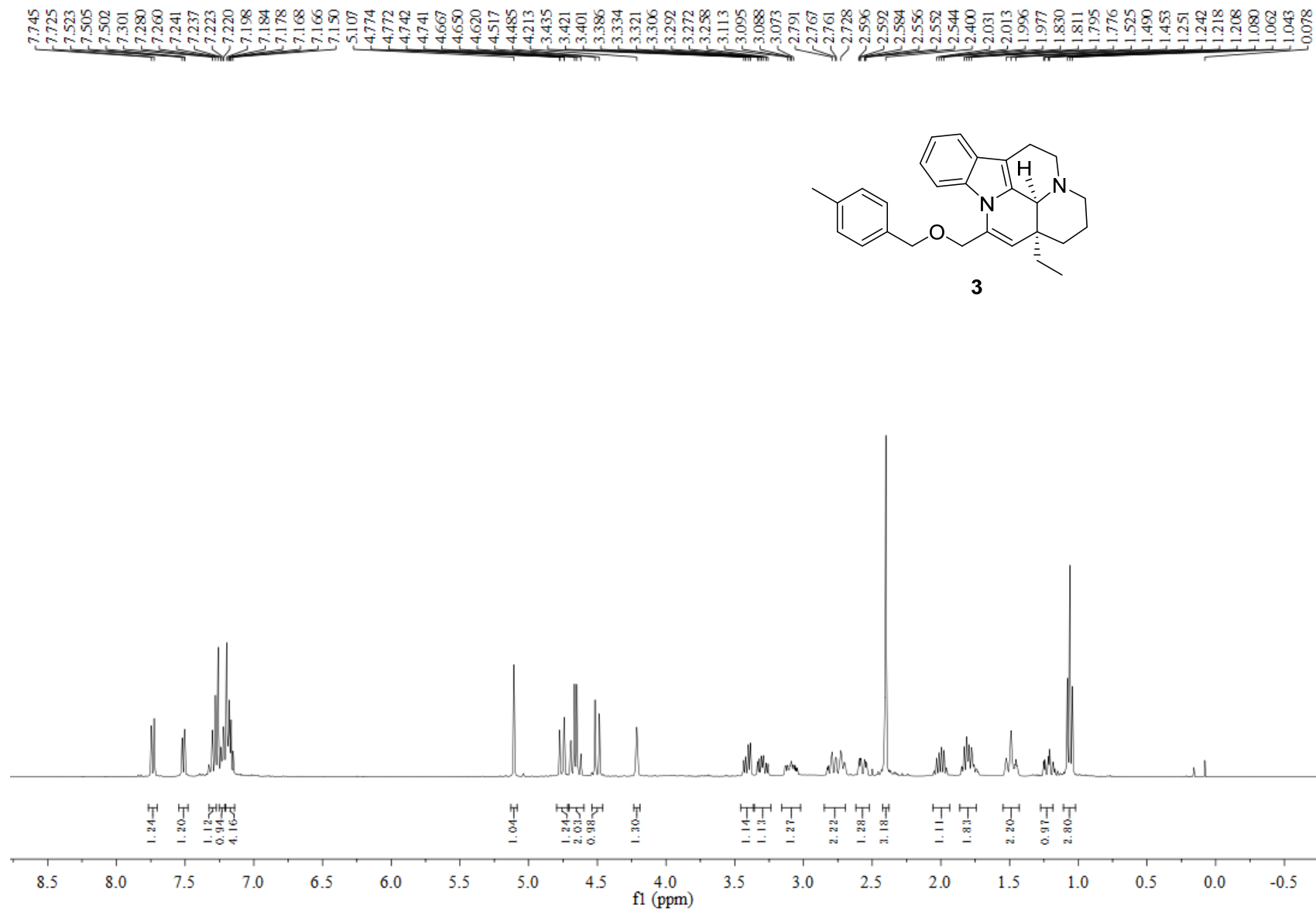
Channel name: 1: Average Time 0.0874 min : TOF MS (50-1500) ESI+ : Centroided : Combined

6.86e7

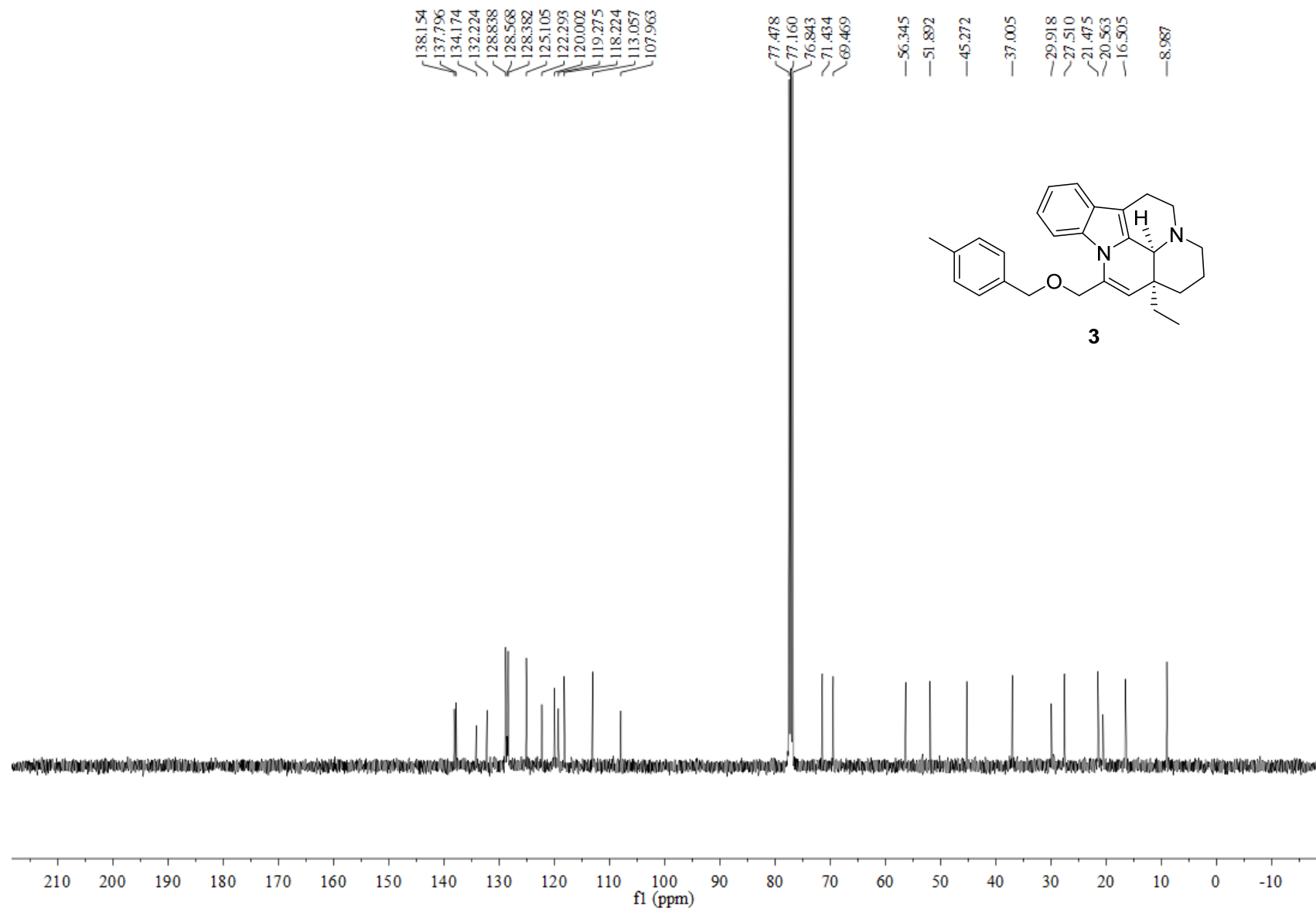


2

HRMS of Compound **2**



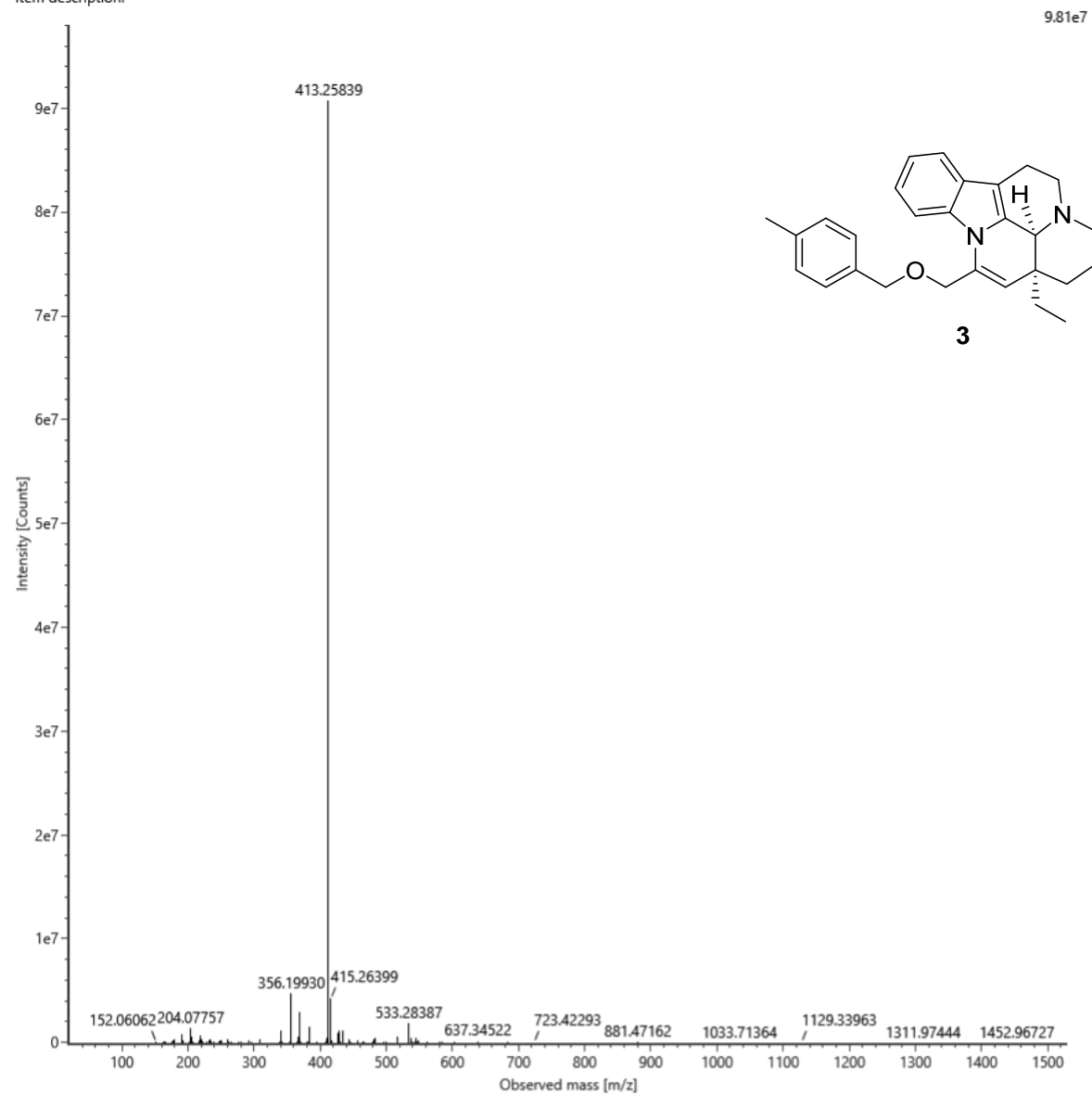
¹H NMR of Compound **3** (400 MHz, CDCl₃)



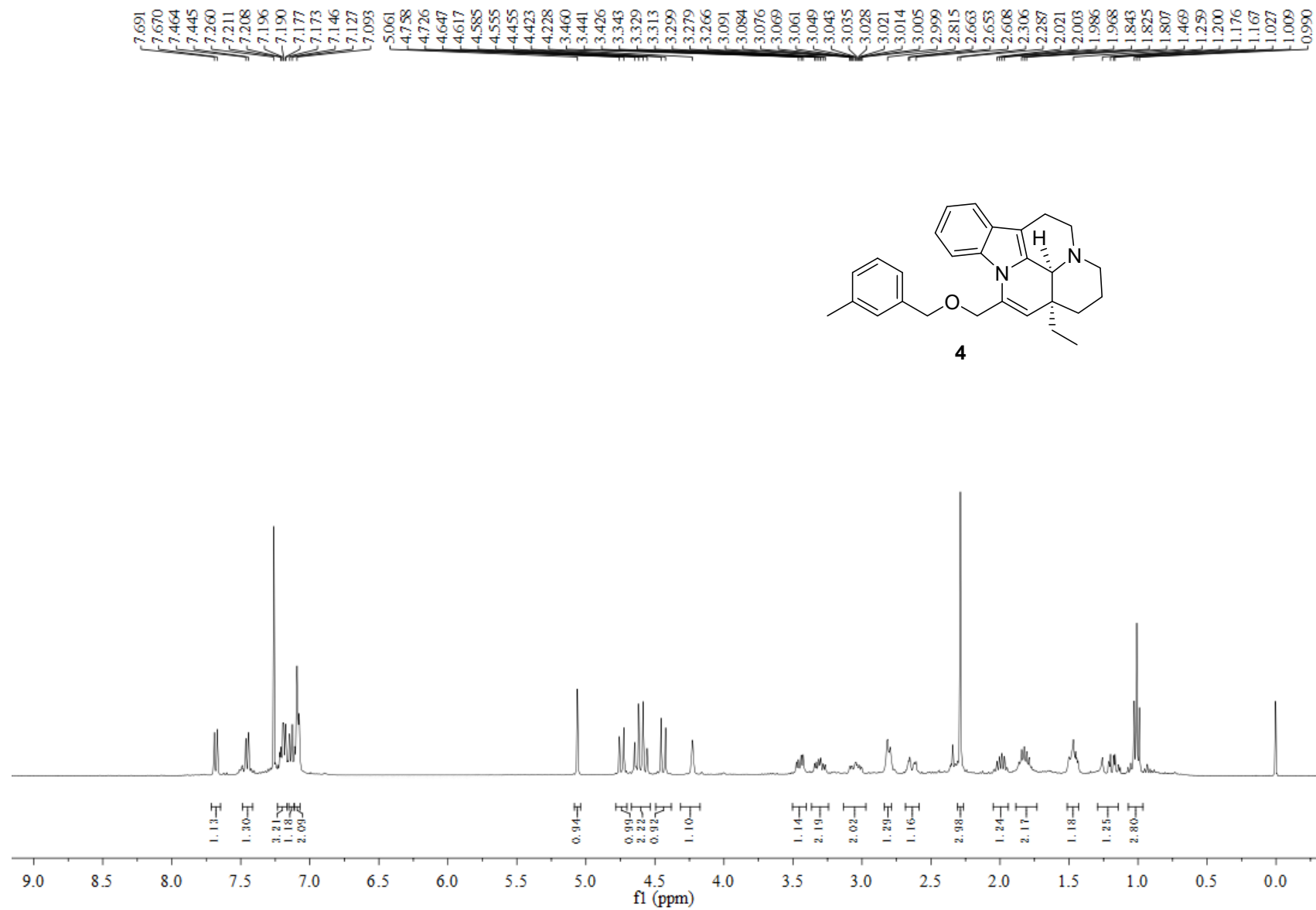
¹³C NMR of Compound **3** (100 MHz, CDCl₃)

Item name: DB-60-11
Item description:

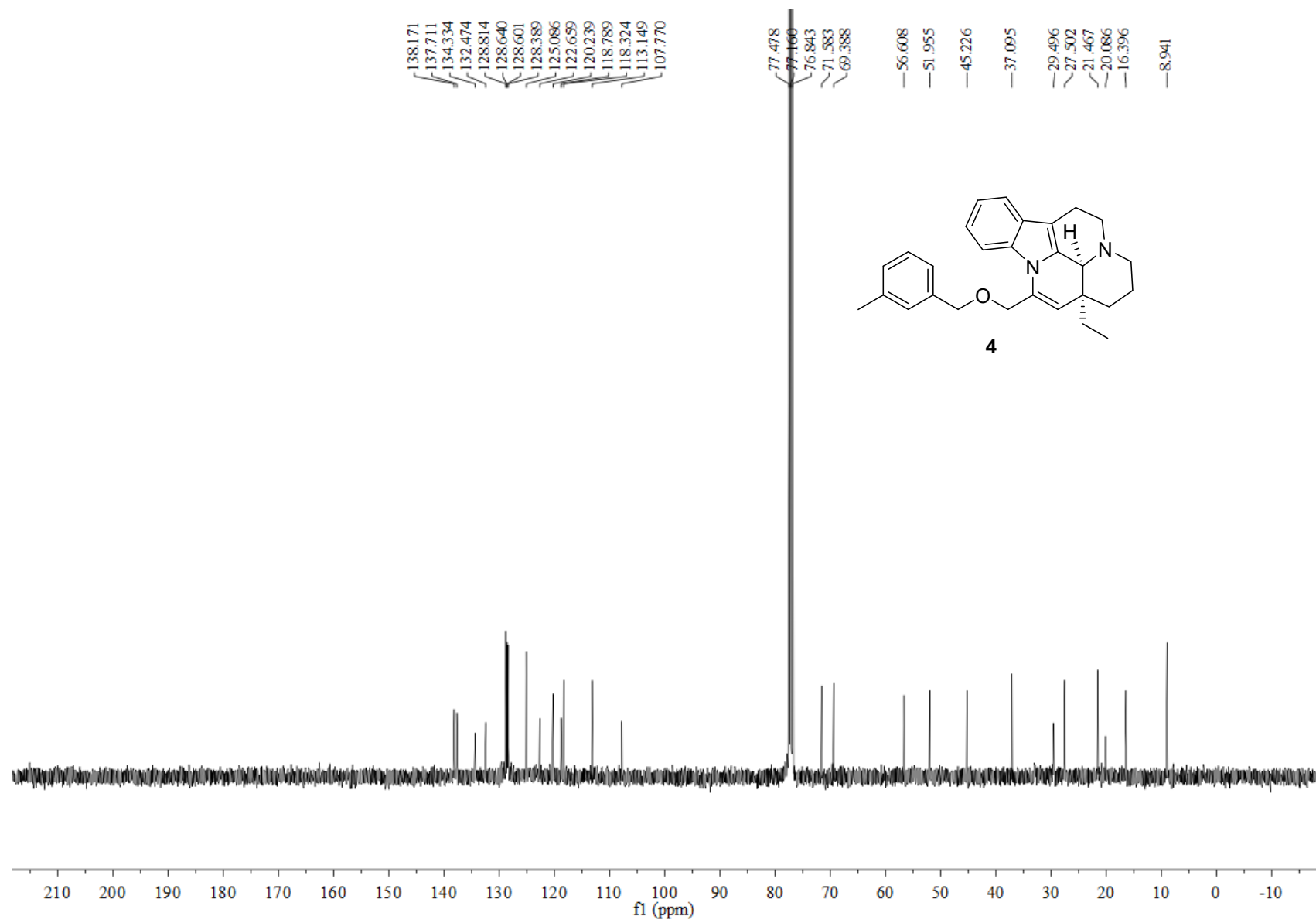
Channel name: 1: Average Time 0.1132 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **3**



¹H NMR of Compound 4 (400 MHz, CDCl₃)

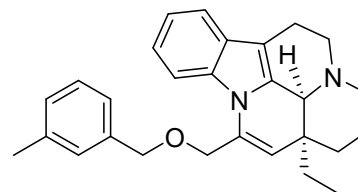
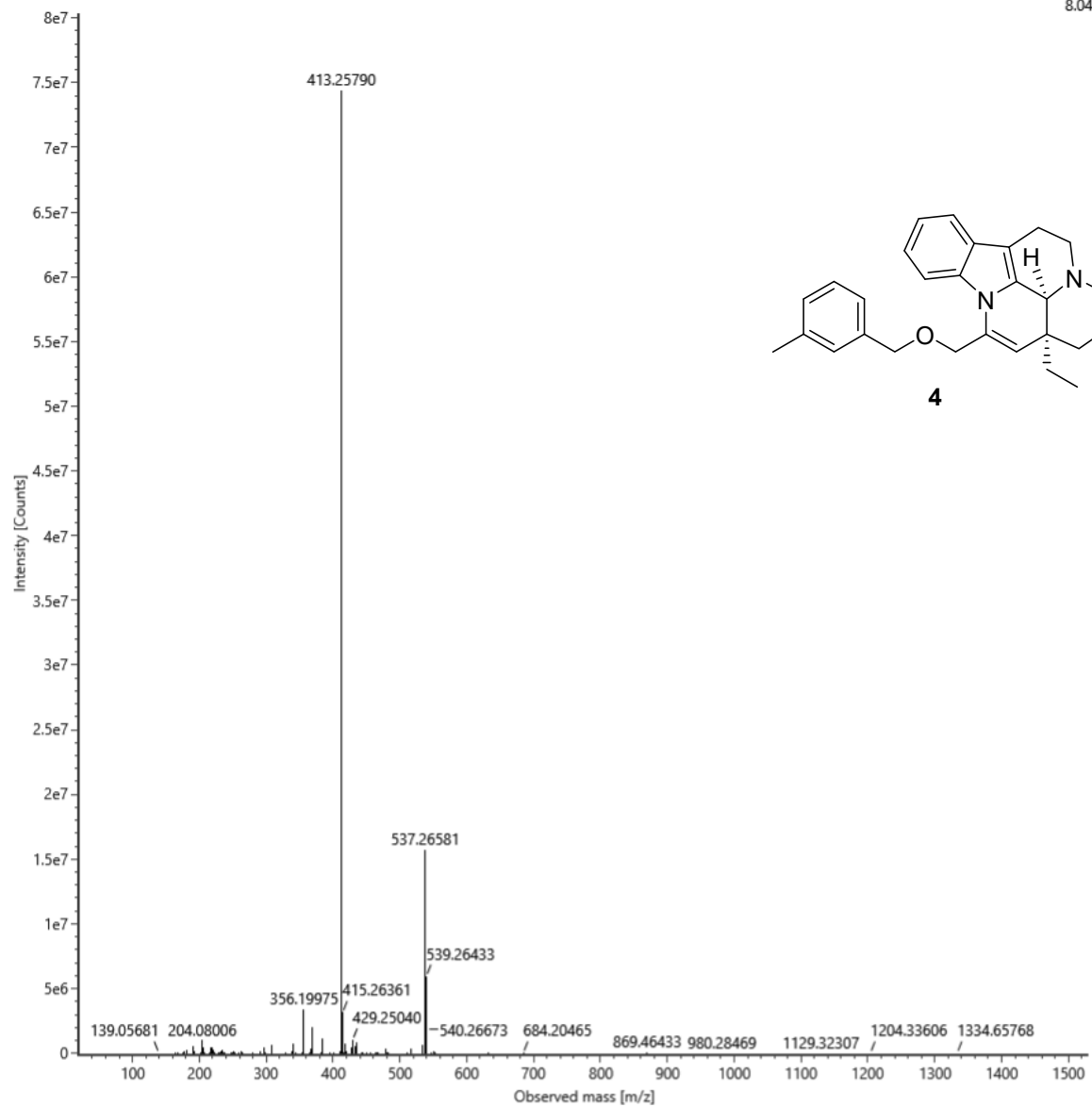


¹³C NMR of Compound **4** (100 MHz, CDCl₃)

Item name: DB-60-9
Item description:

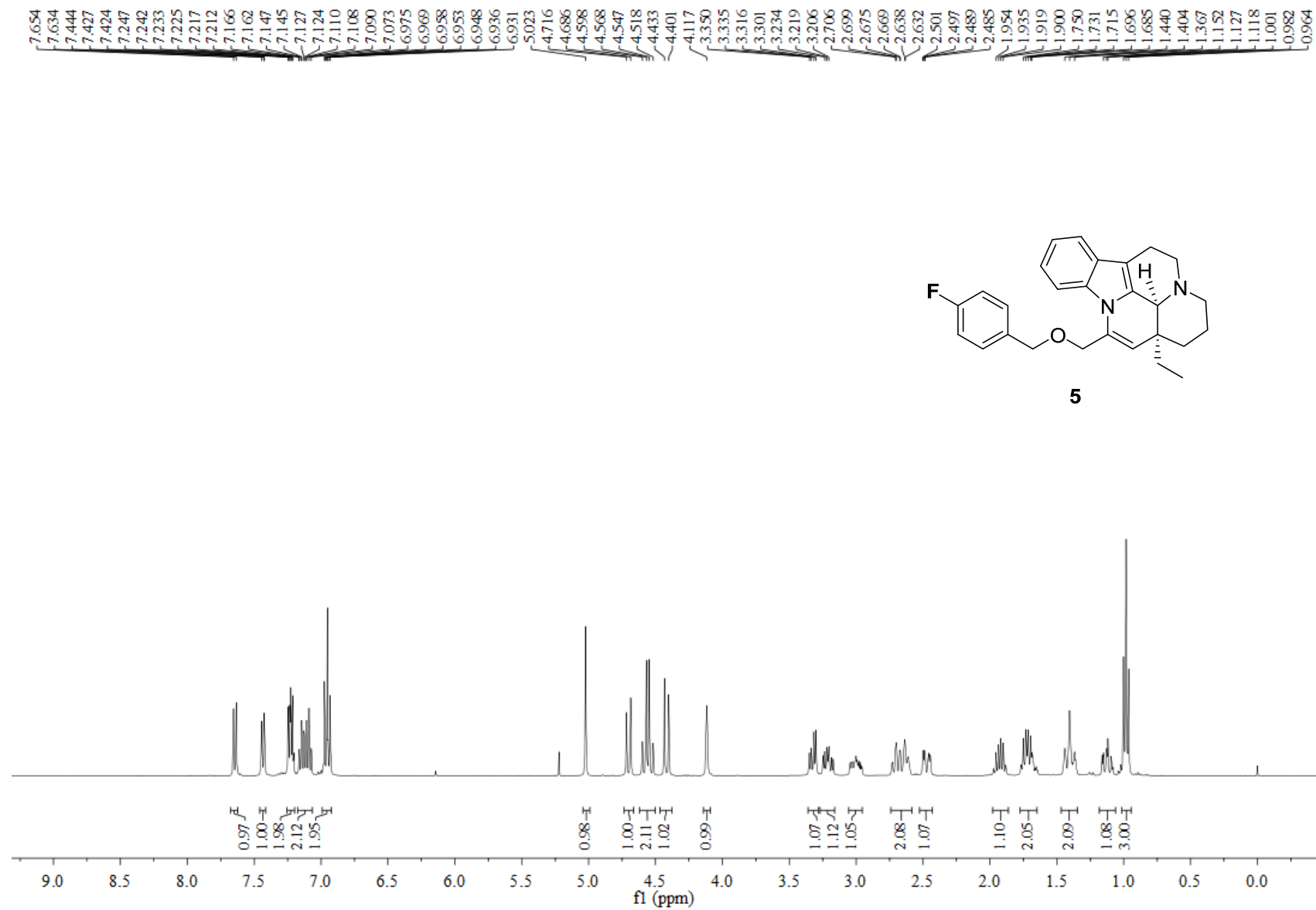
Channel name: 1: Average Time 0.1089 min : TOF MS (50-1500) ESI+ : Centroided : Combined

8.04e7

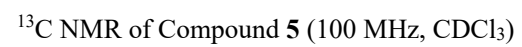


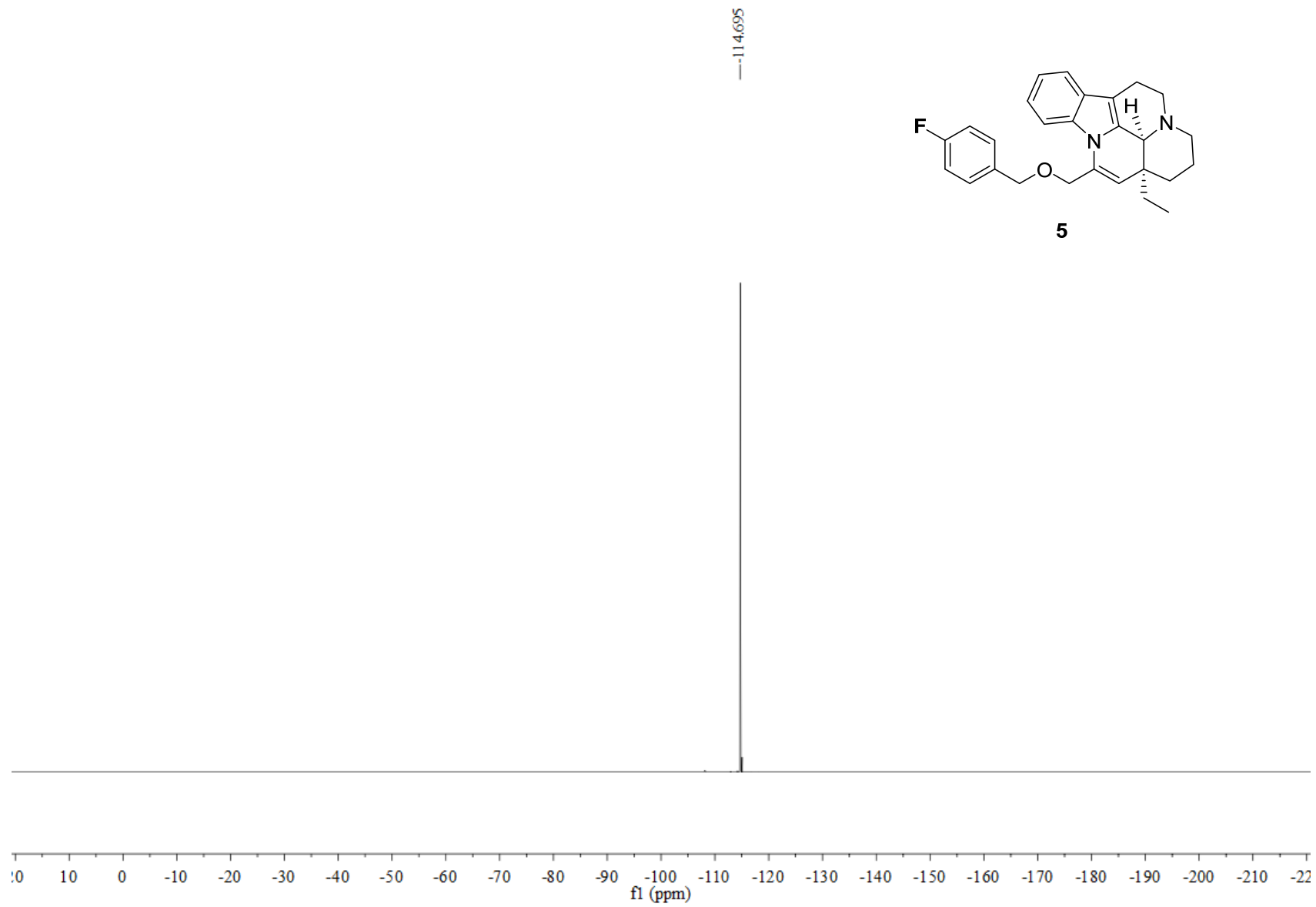
4

HRMS of Compound 4



¹H NMR of Compound **5** (400 MHz, CDCl₃)



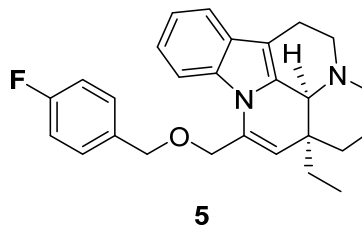
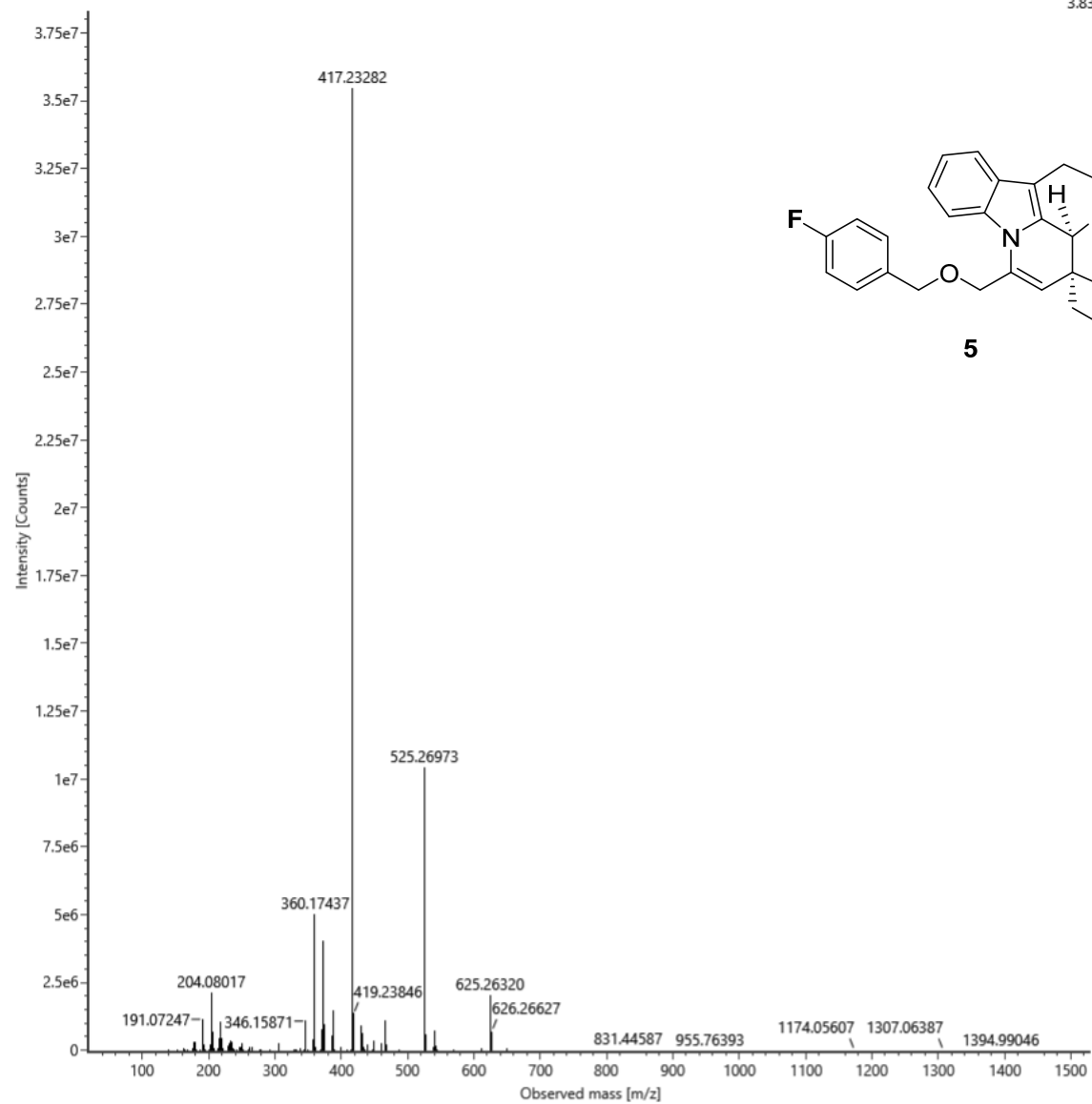


^{19}F NMR of Compound **5** (377 MHz, CDCl_3)

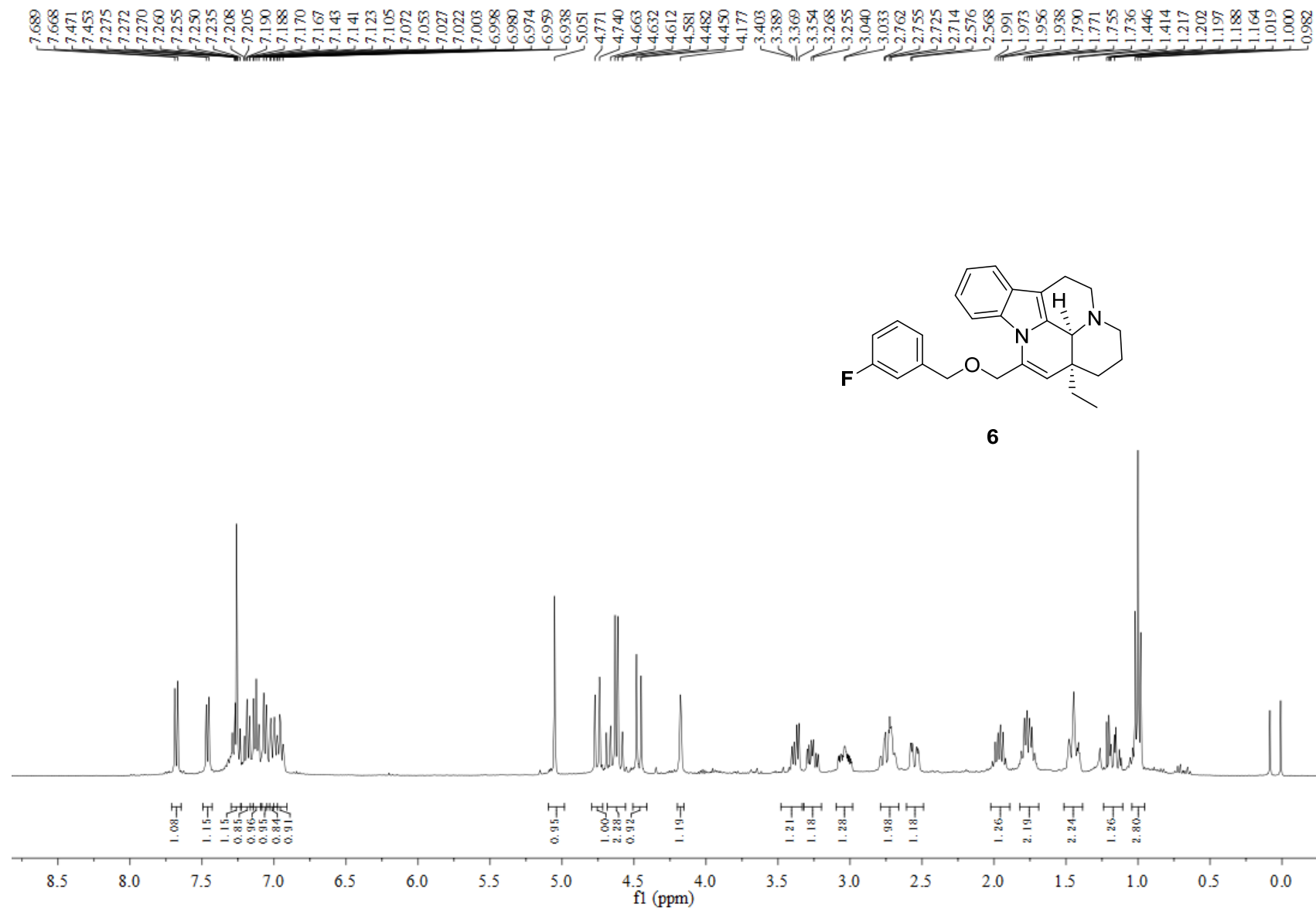
Item name: DB-60-28
Item description:

Channel name: 1: Average Time 0.0788 min : TOF MS (50-1500) ESI+ : Centroided : Combined

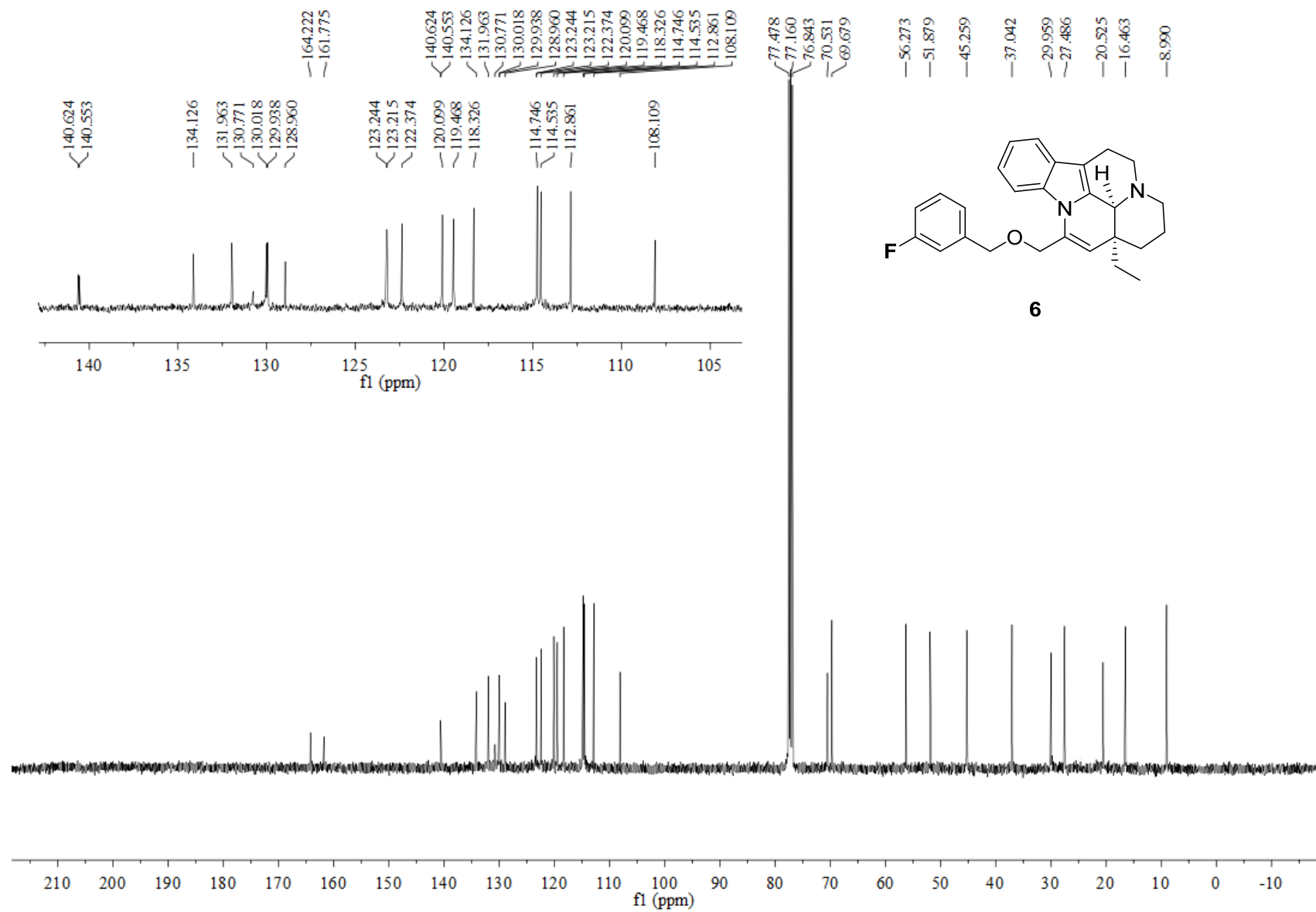
3.83e7



HRMS of Compound 5



¹H NMR of Compound 6 (400 MHz, CDCl₃)



¹³C NMR of Compound **6** (100 MHz, CDCl₃)

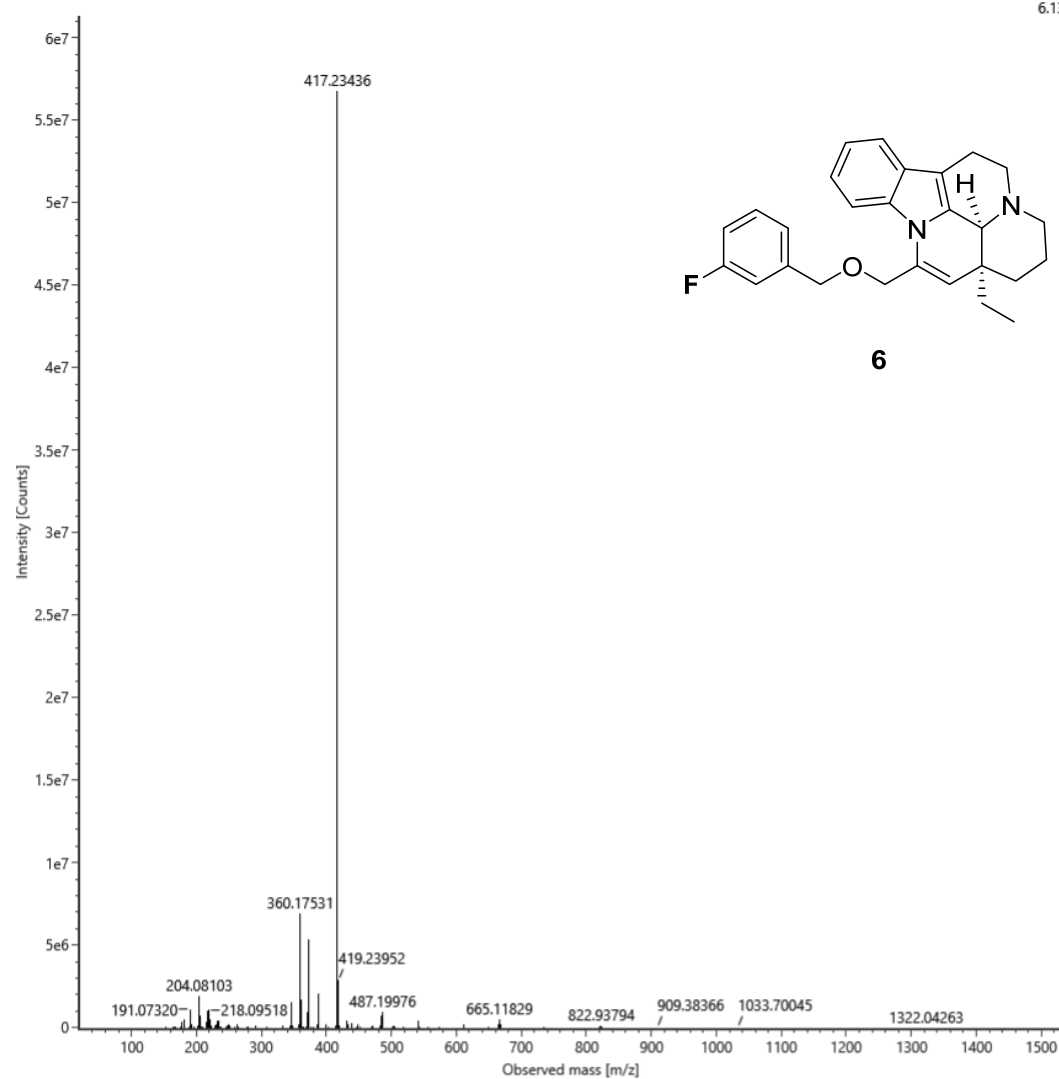


^{19}F NMR of Compound **6** (377 MHz, CDCl_3)

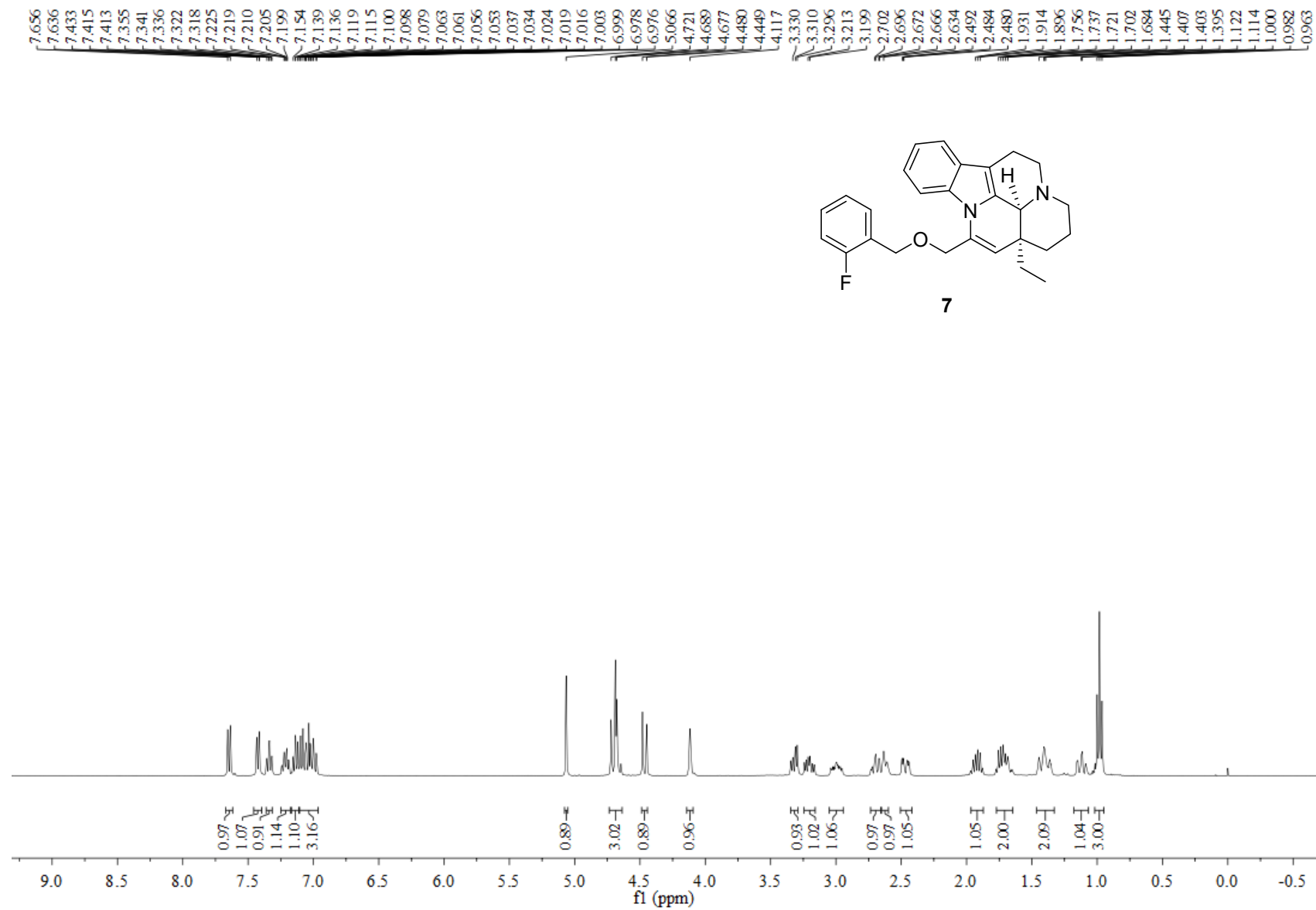
Item name: DB-60-6
Item description:

Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined

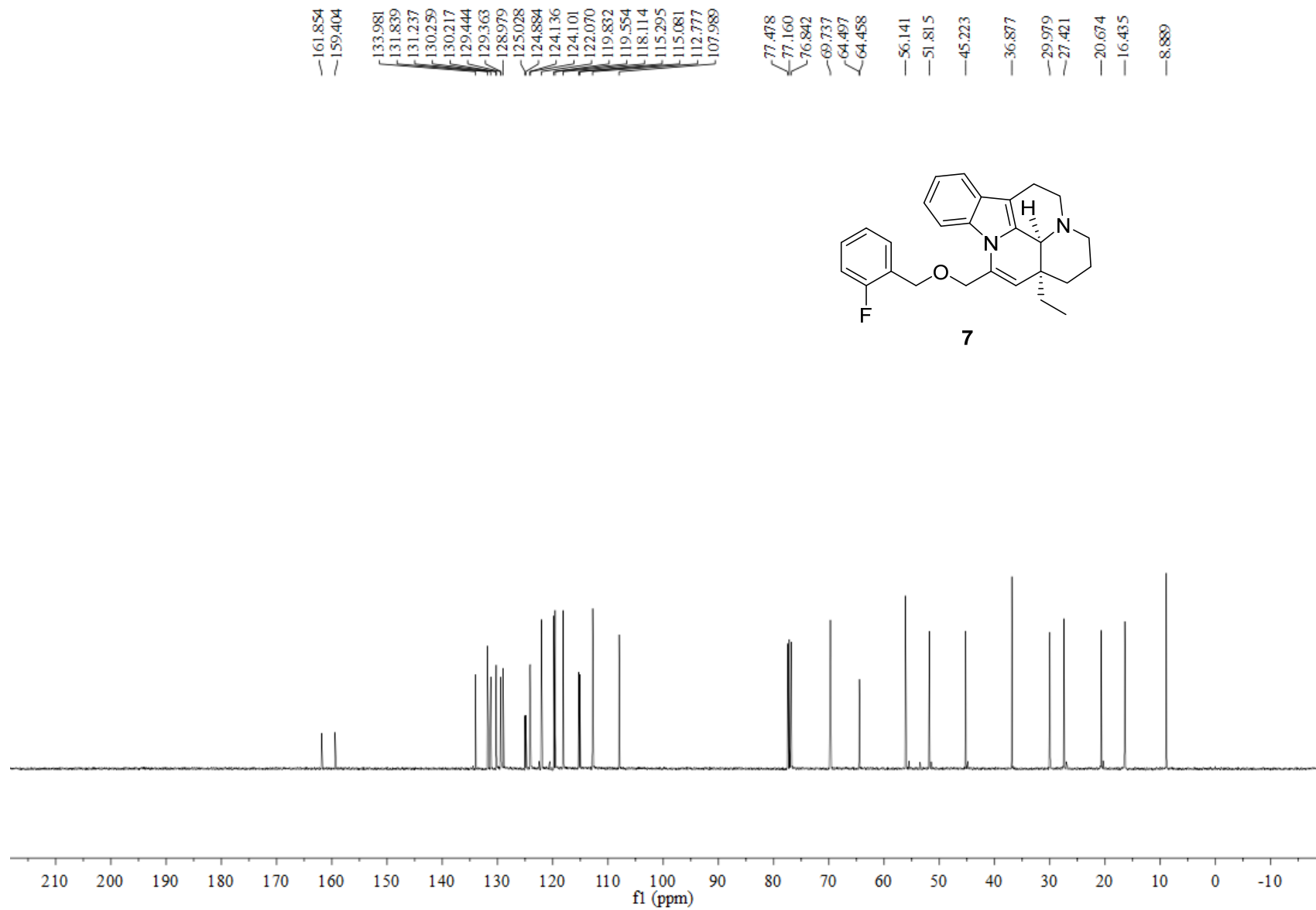
6.13e7



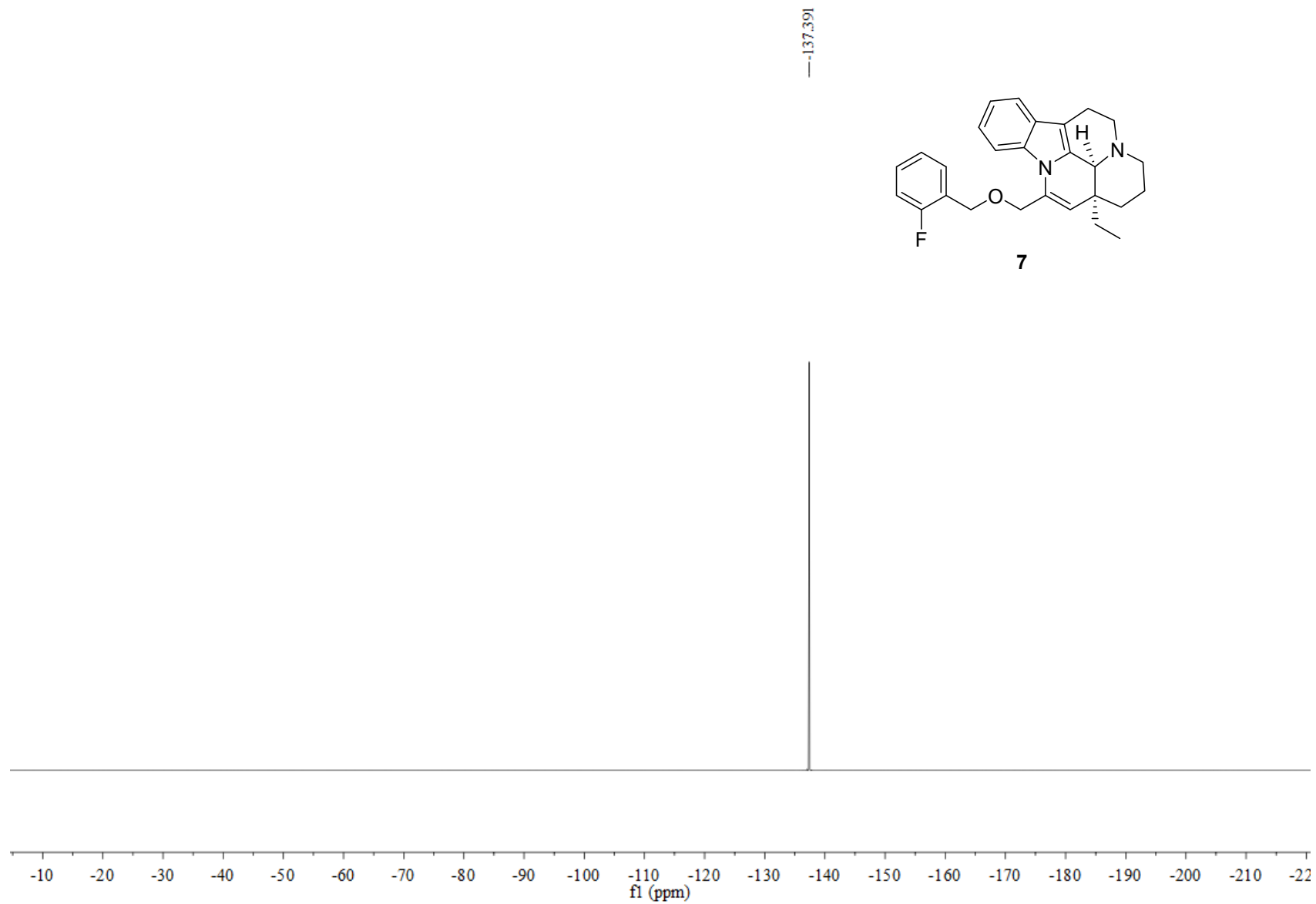
HRMS of Compound 6



¹H NMR of Compound 7 (400 MHz, CDCl₃)



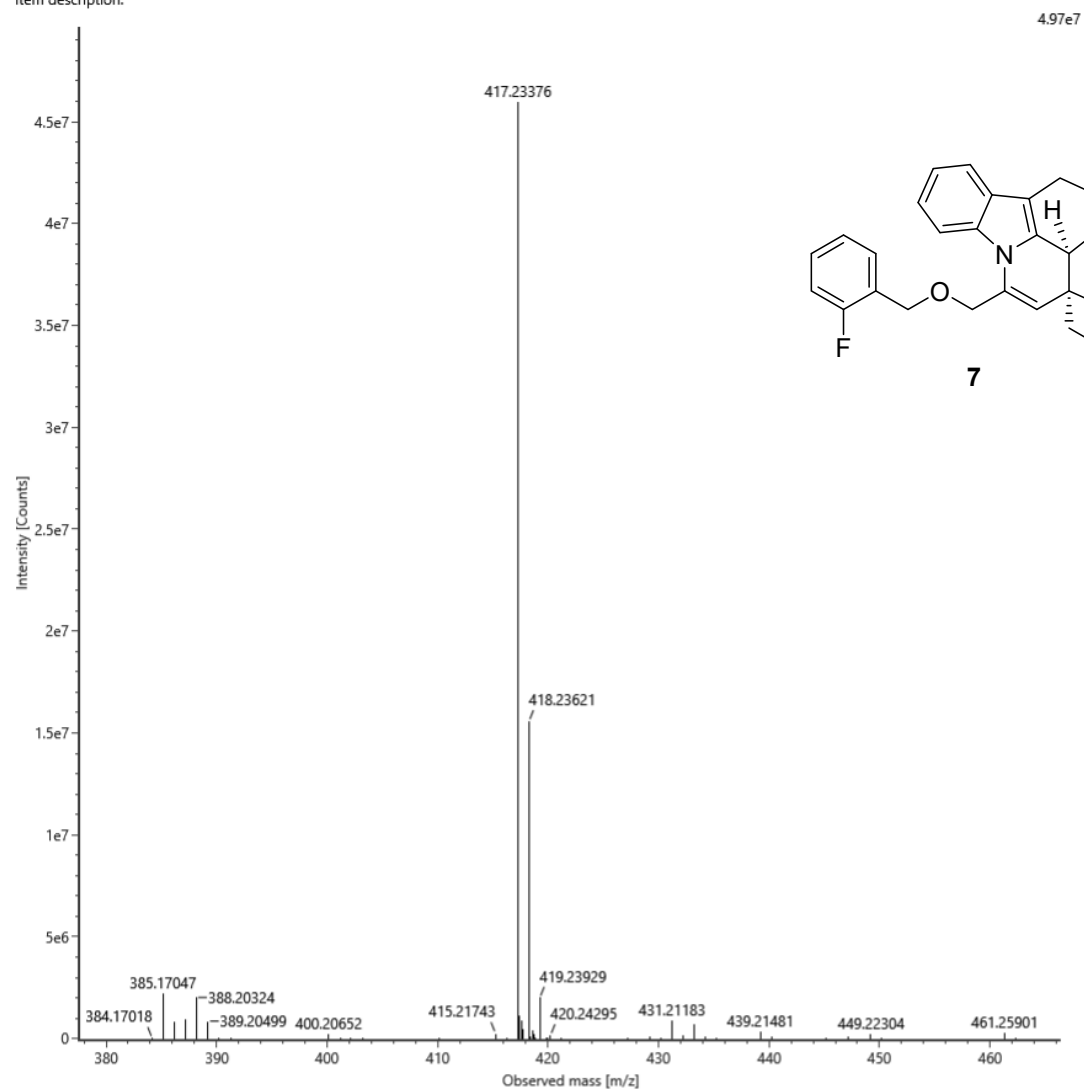
¹³C NMR of Compound 7 (100 MHz, CDCl₃)



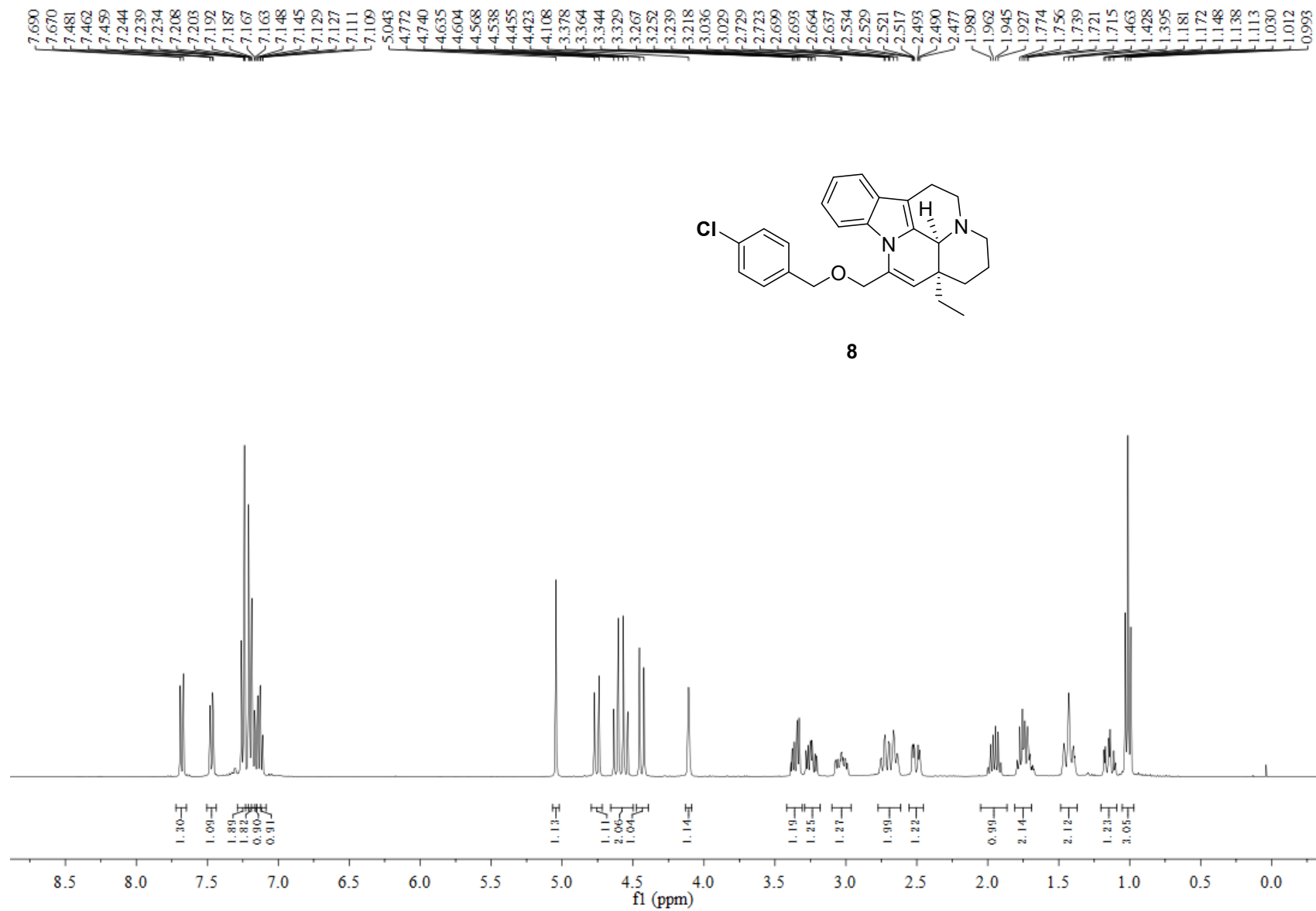
^{19}F NMR of Compound 7 (377 MHz, CDCl_3)

Item name: DB-60-25
Item description:

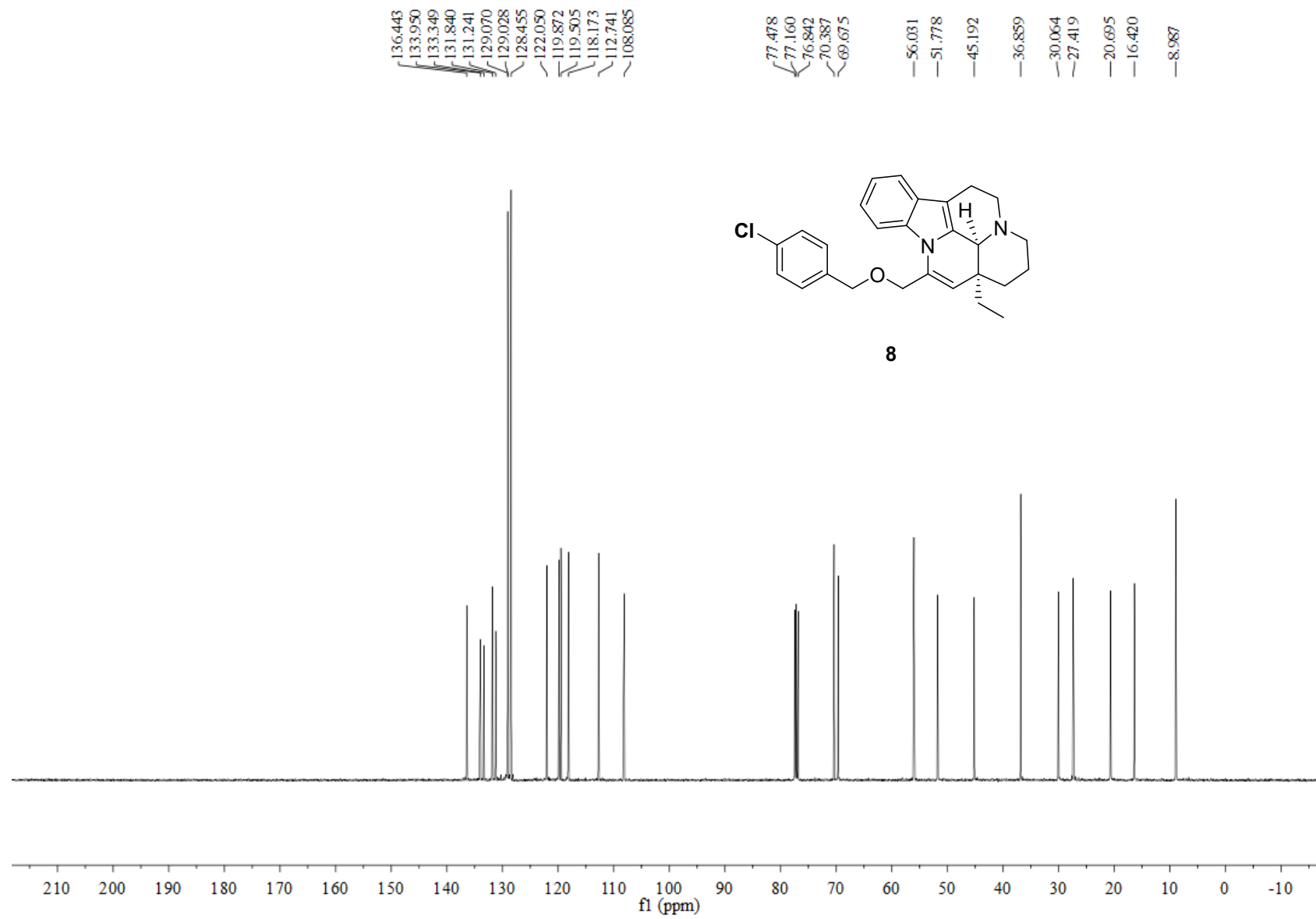
Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound 7



¹H NMR of Compound **8** (400 MHz, CDCl₃)

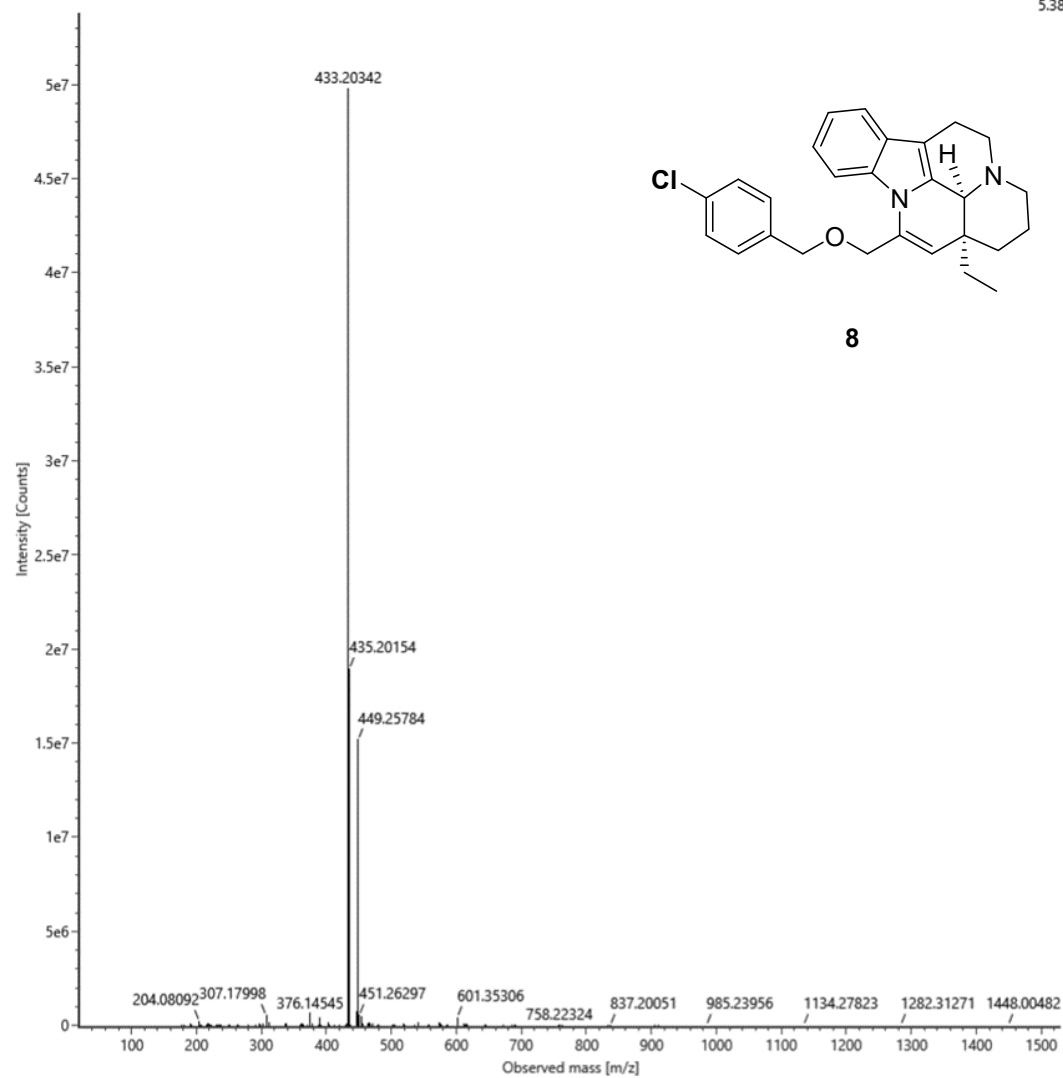


¹³C NMR of Compound 8 (100 MHz, CDCl₃)

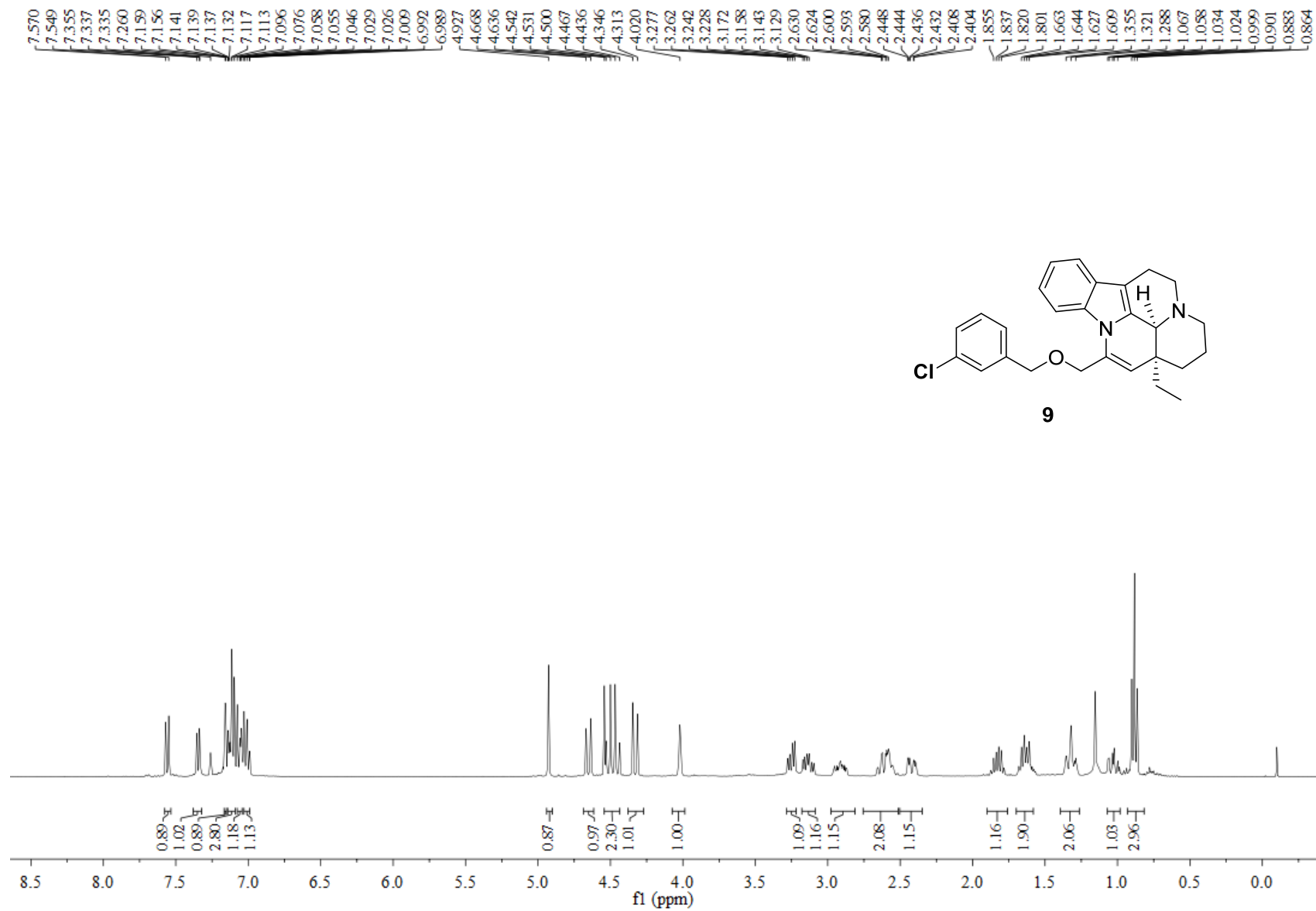
Item name: DA-5-16
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined

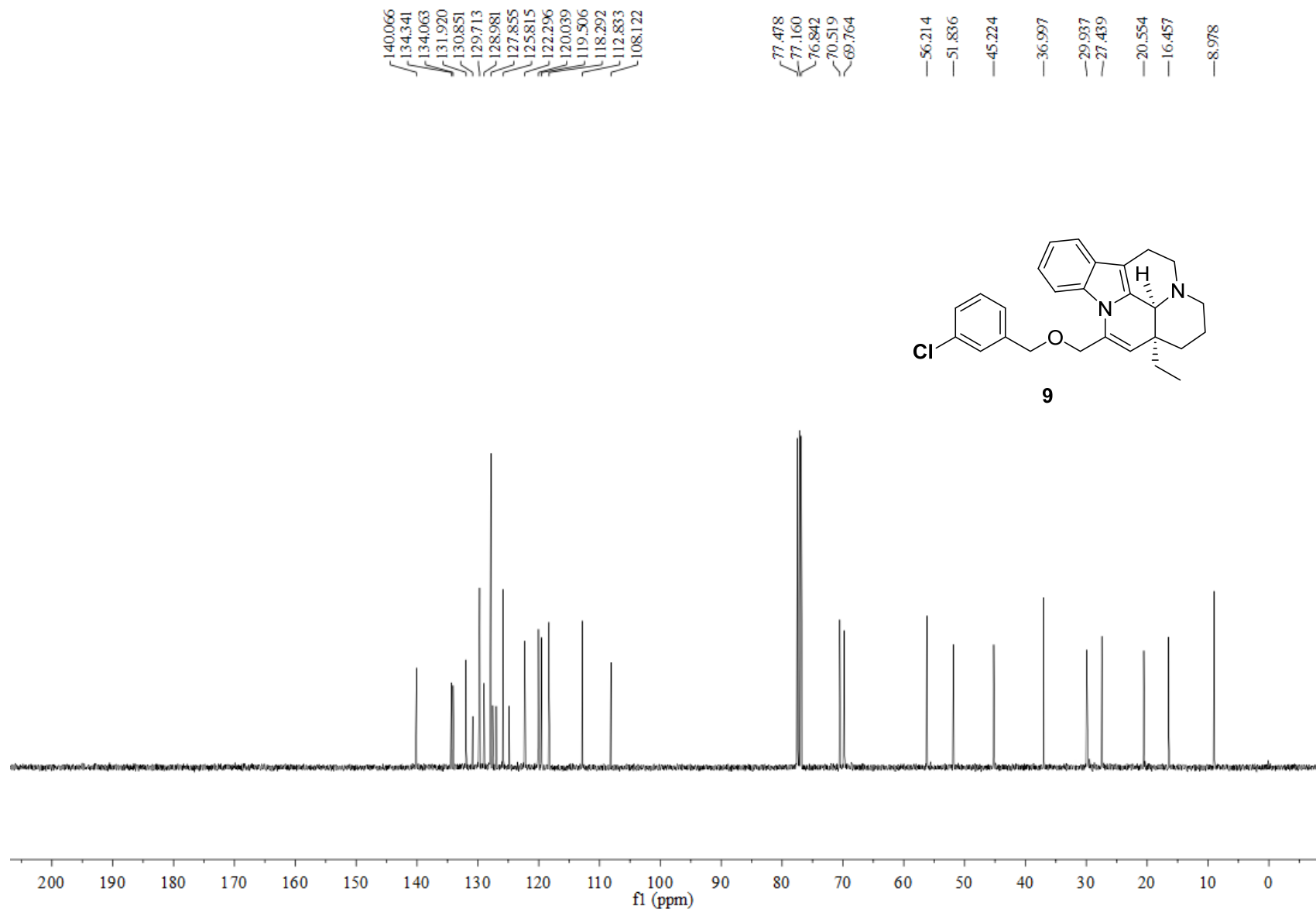
5.38e7



HRMS of Compound 8



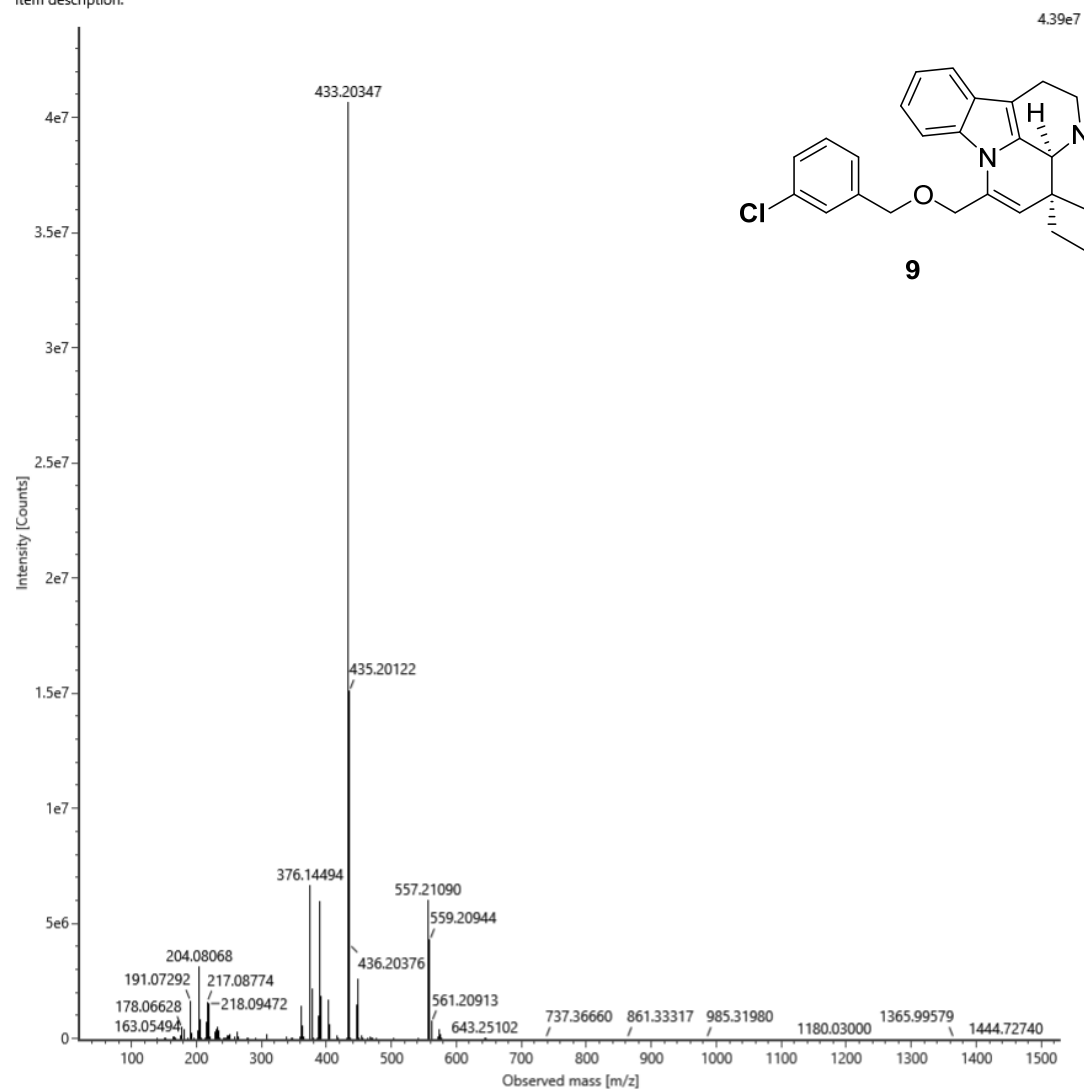
¹H NMR of Compound **9** (400 MHz, CDCl₃)



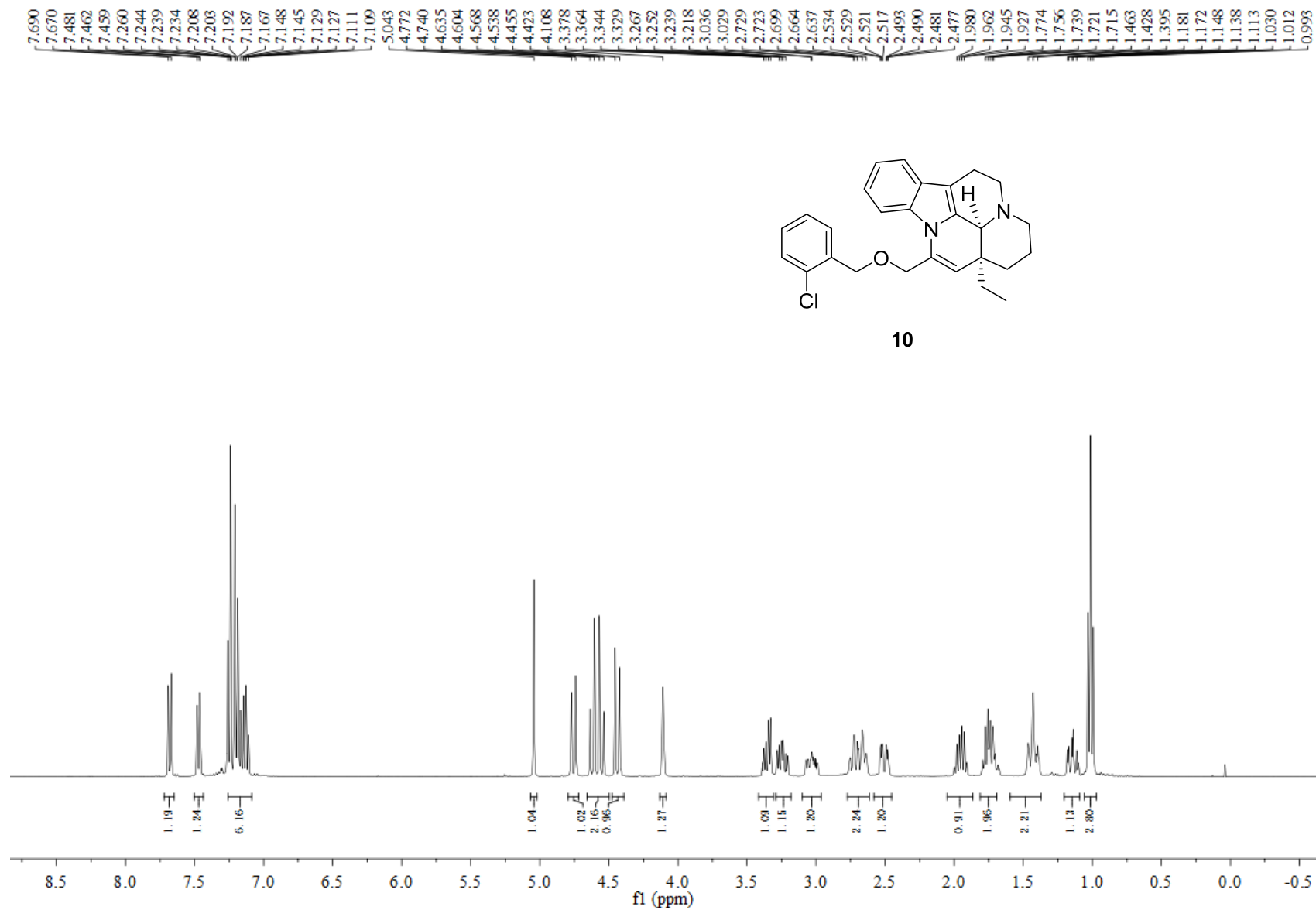
¹³C NMR of Compound **9** (100 MHz, CDCl₃)

Item name: DB-60-30
Item description:

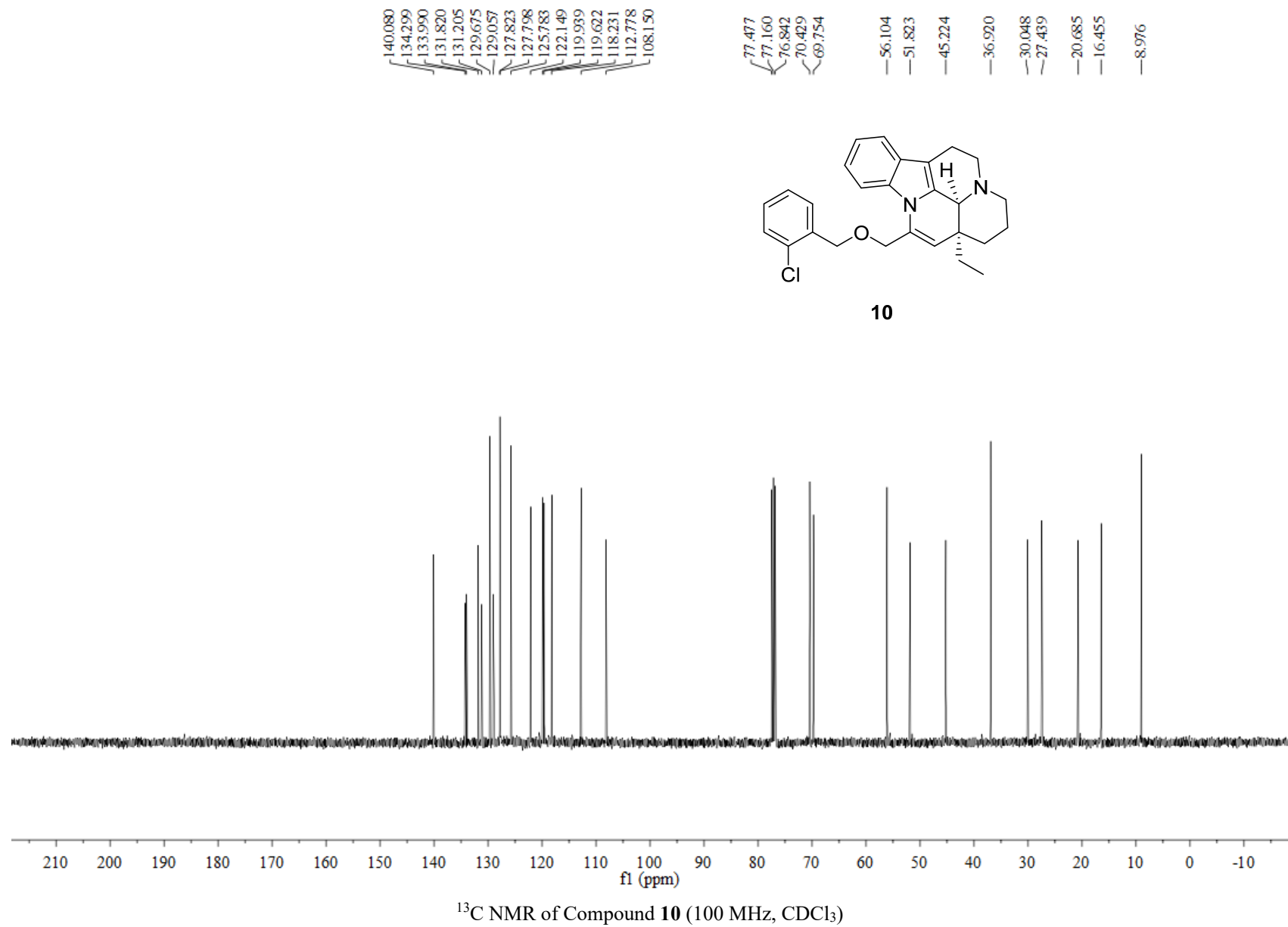
Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **9**



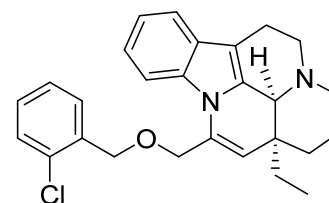
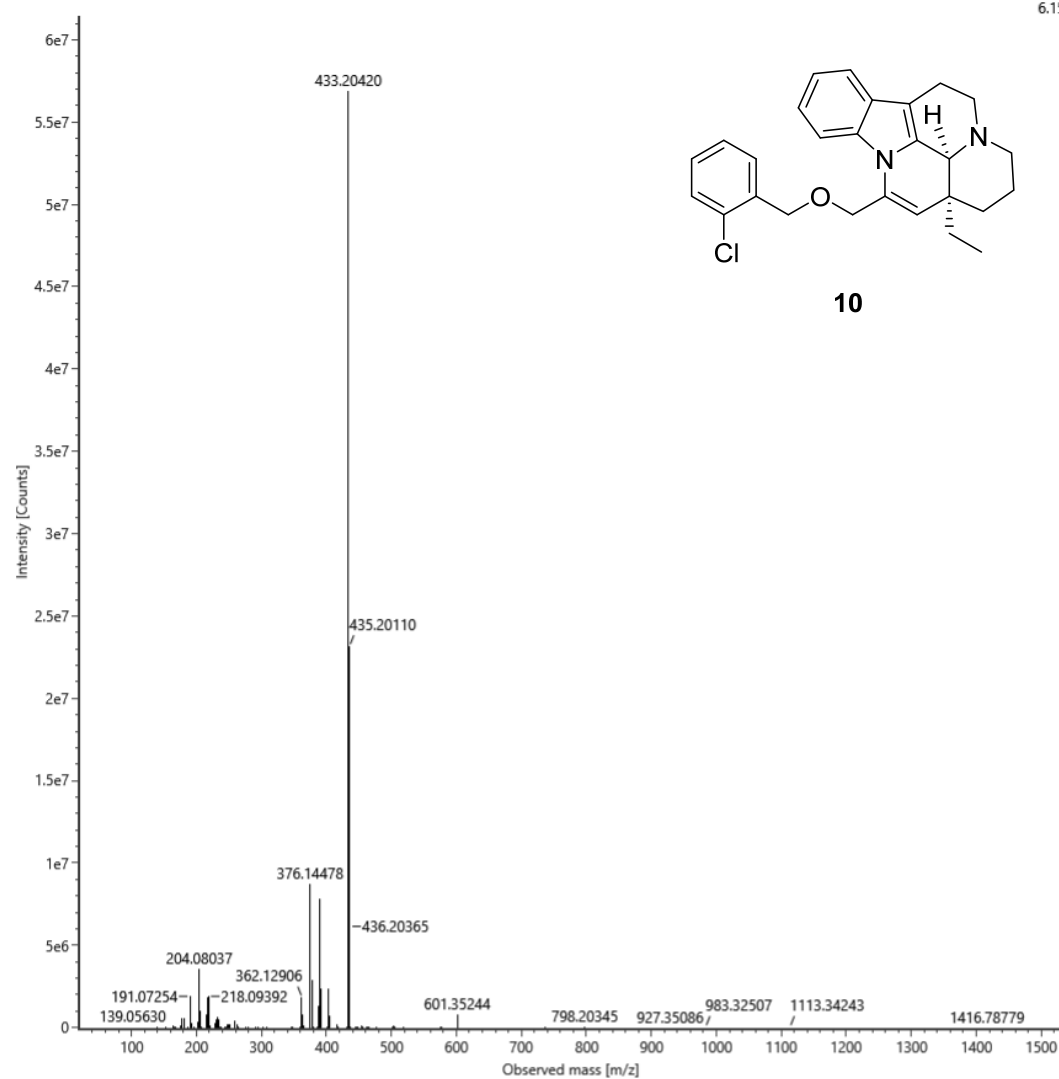
¹H NMR of Compound **10** (400 MHz, CDCl₃)



Item name: DB-60-14
Item description:

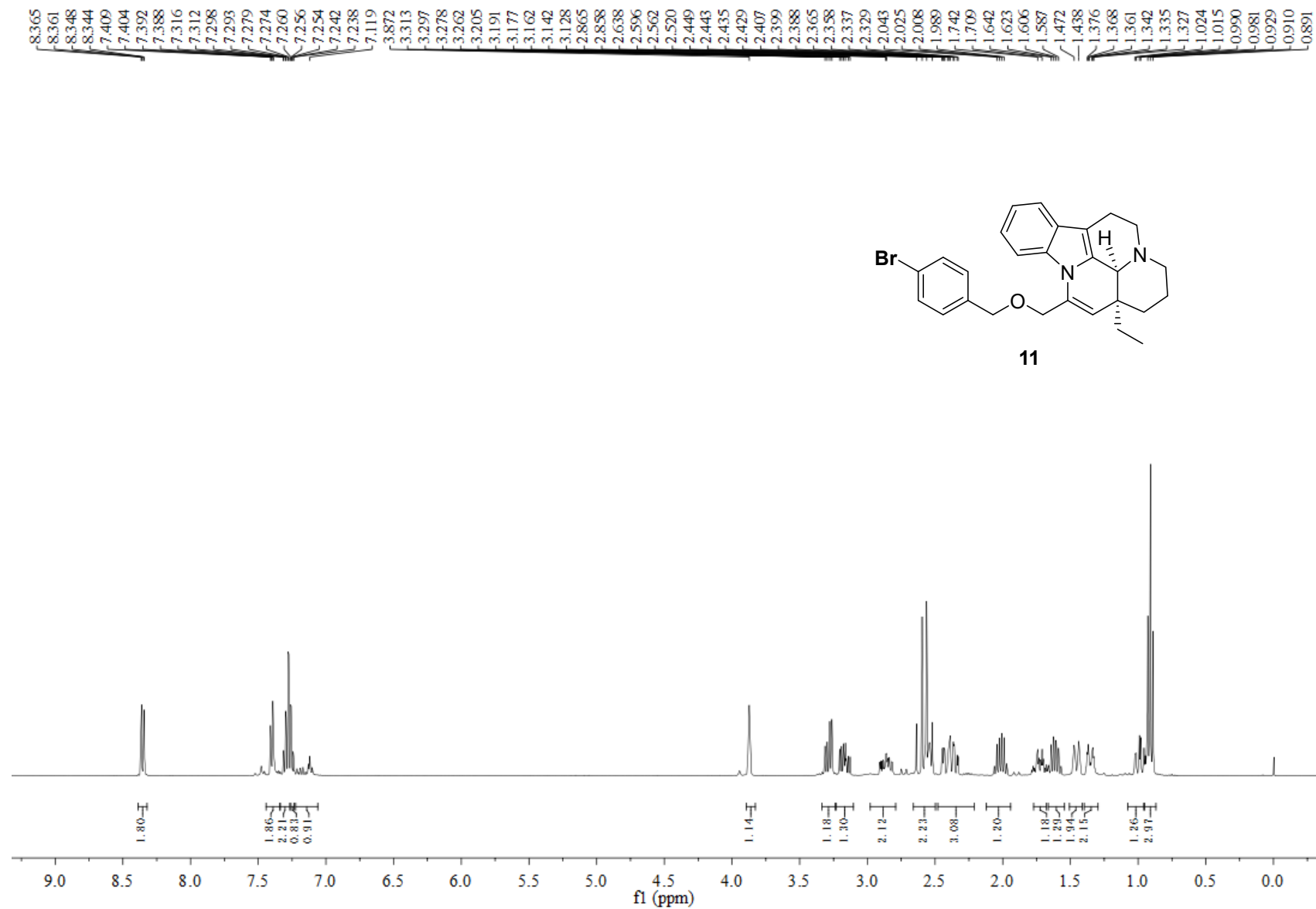
Channel name: 1: Average Time 0.0874 min : TOF MS (50-1500) ESI+ : Centroided : Combined

6.15e7

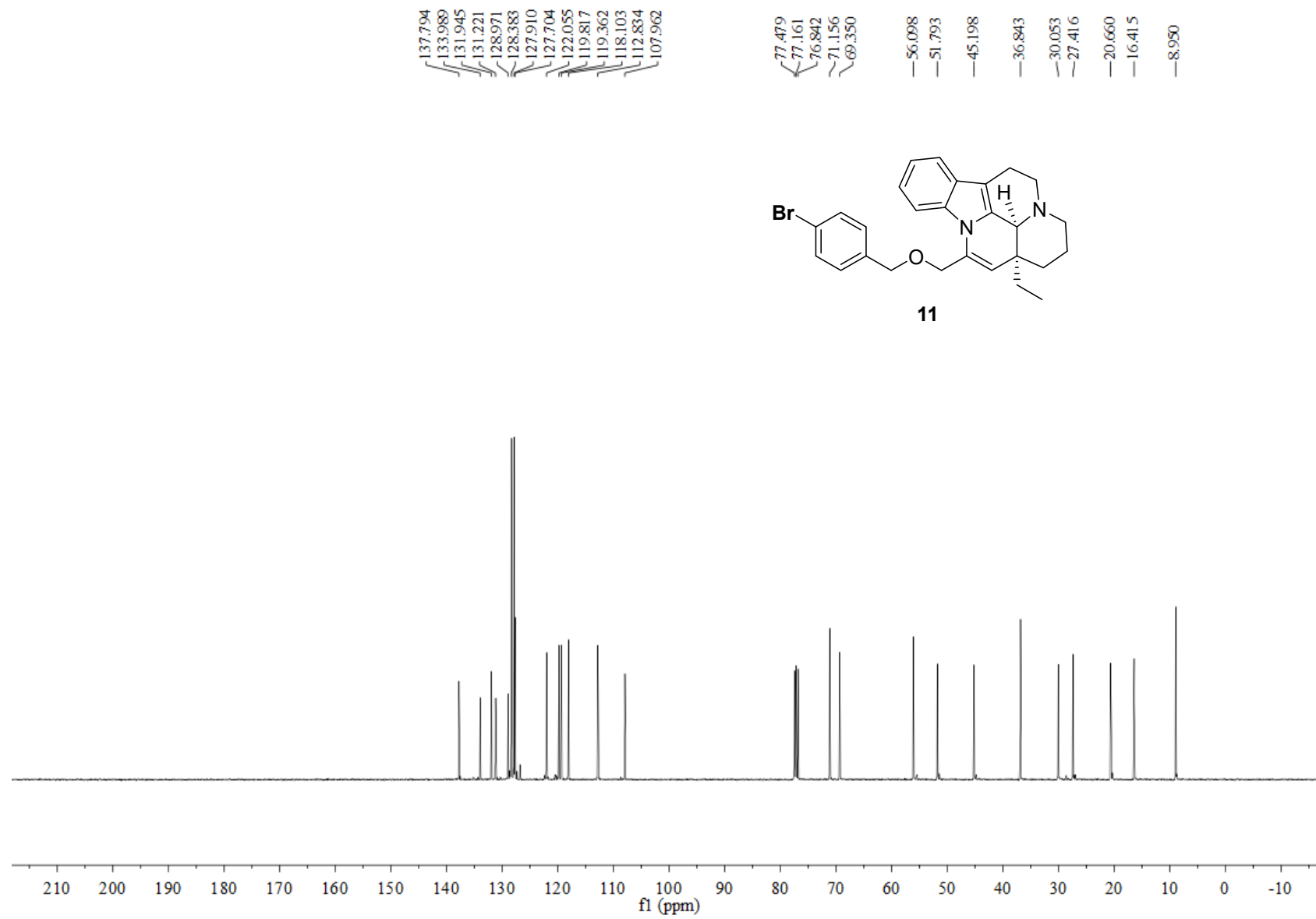


10

HRMS of Compound **10**



^1H NMR of Compound **11** (400 MHz, CDCl_3)

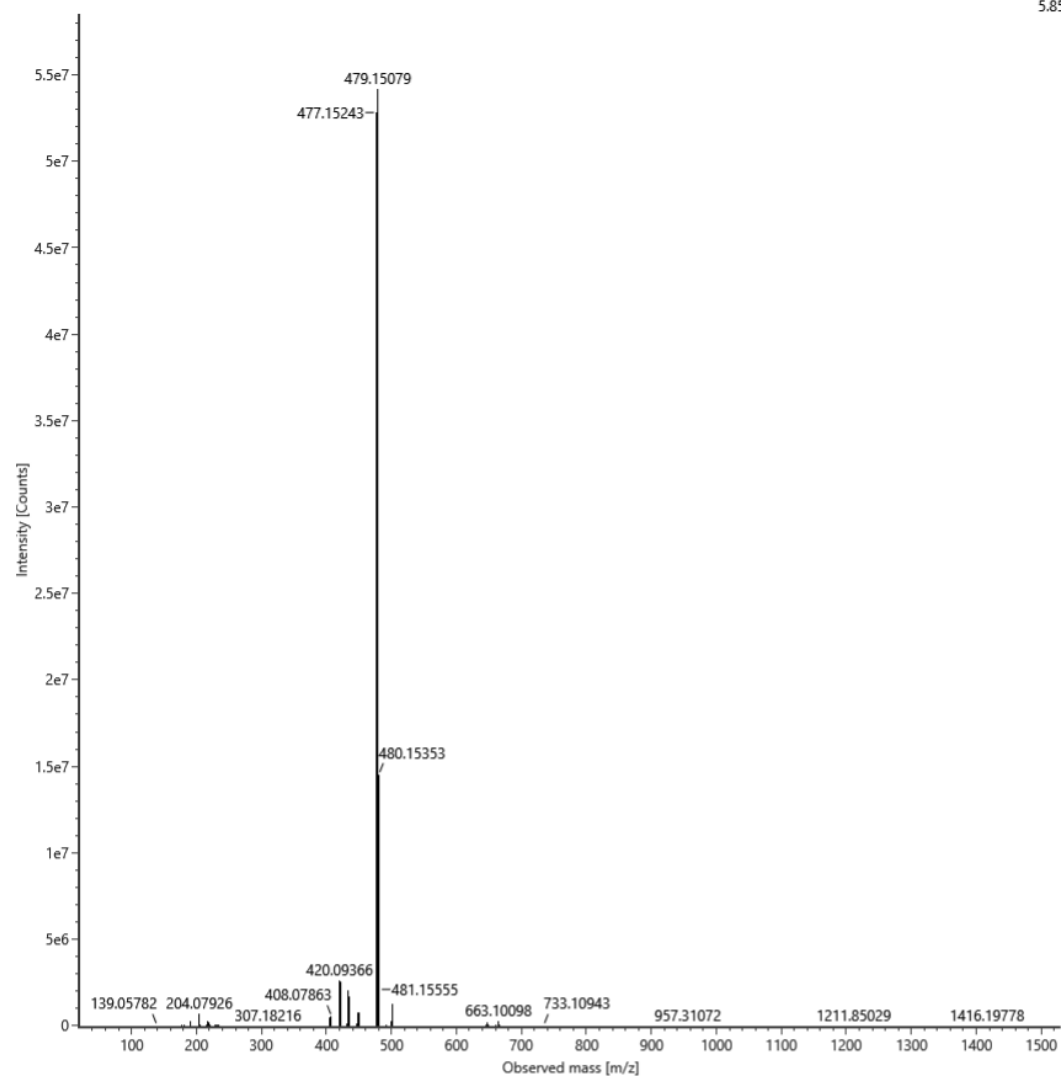


¹³C NMR of Compound **11** (100 MHz, CDCl₃)

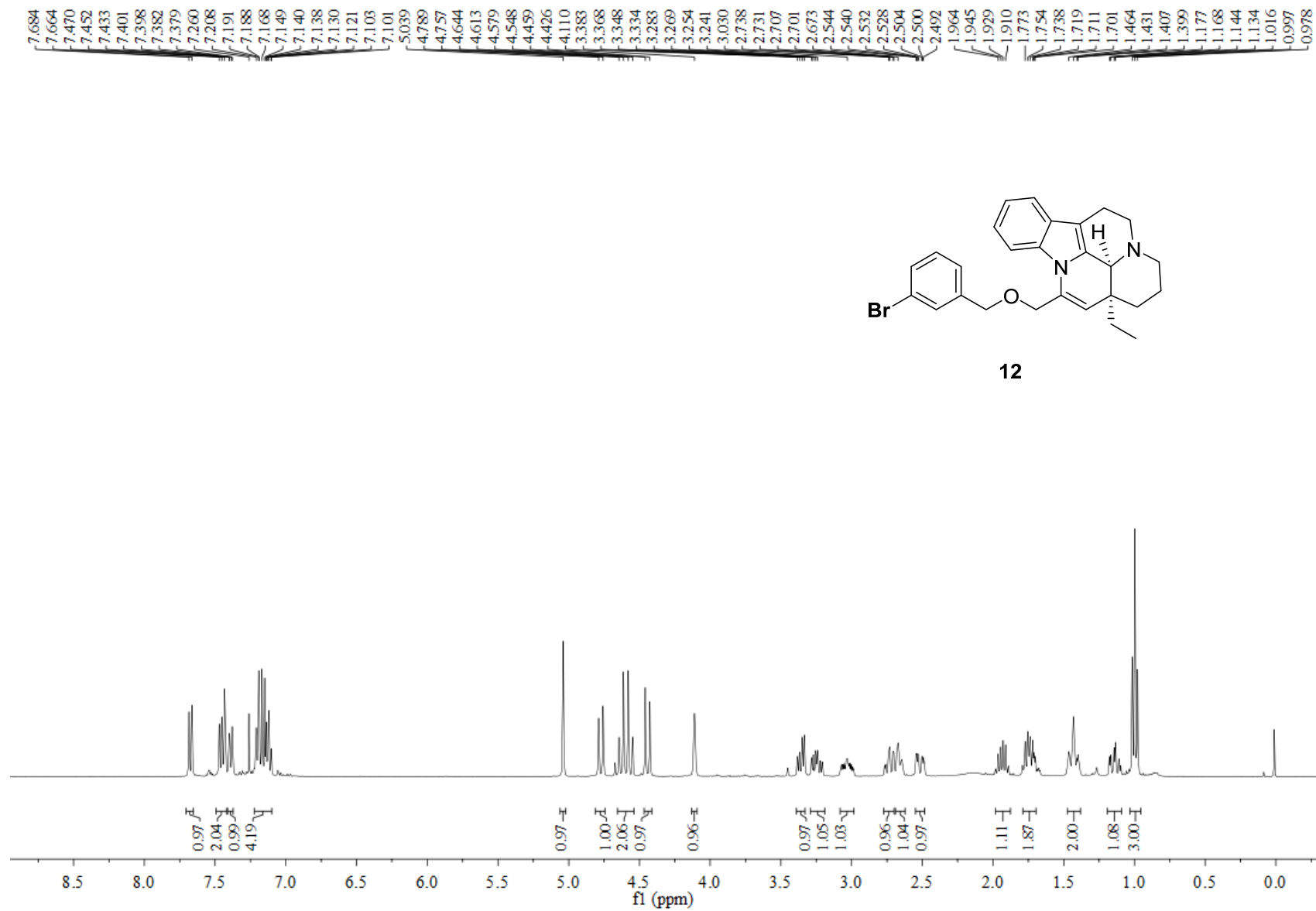
Item name: DB-60-5-1
Item description:

Channel name: 1: Average Time 0.1089 min : TOF MS (50-1500) ESI+ : Centroided : Combined

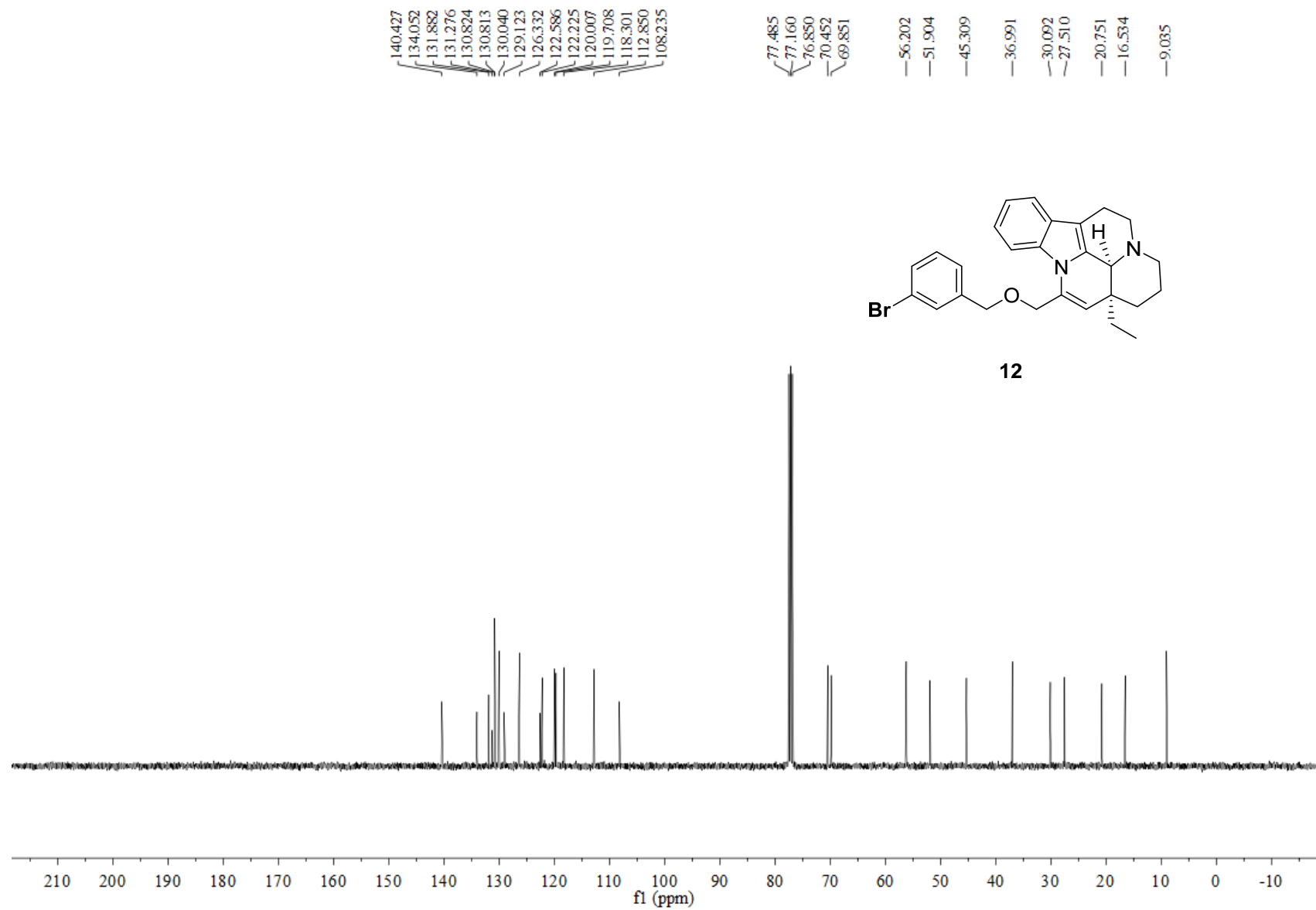
5.85e7



HRMS of Compound **11**



¹H NMR of Compound 12 (400 MHz, CDCl₃)

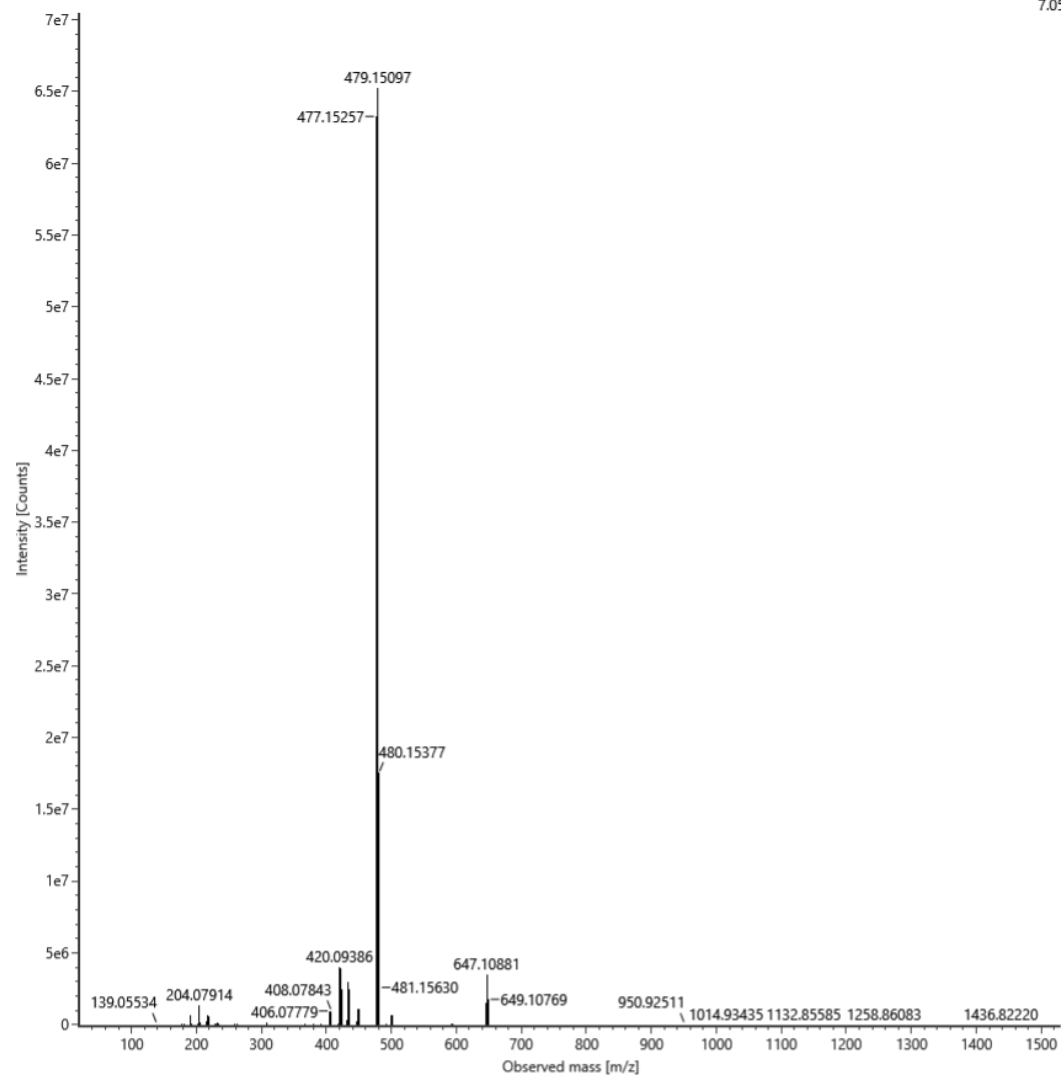


¹³C NMR of Compound **12** (100 MHz, CDCl₃)

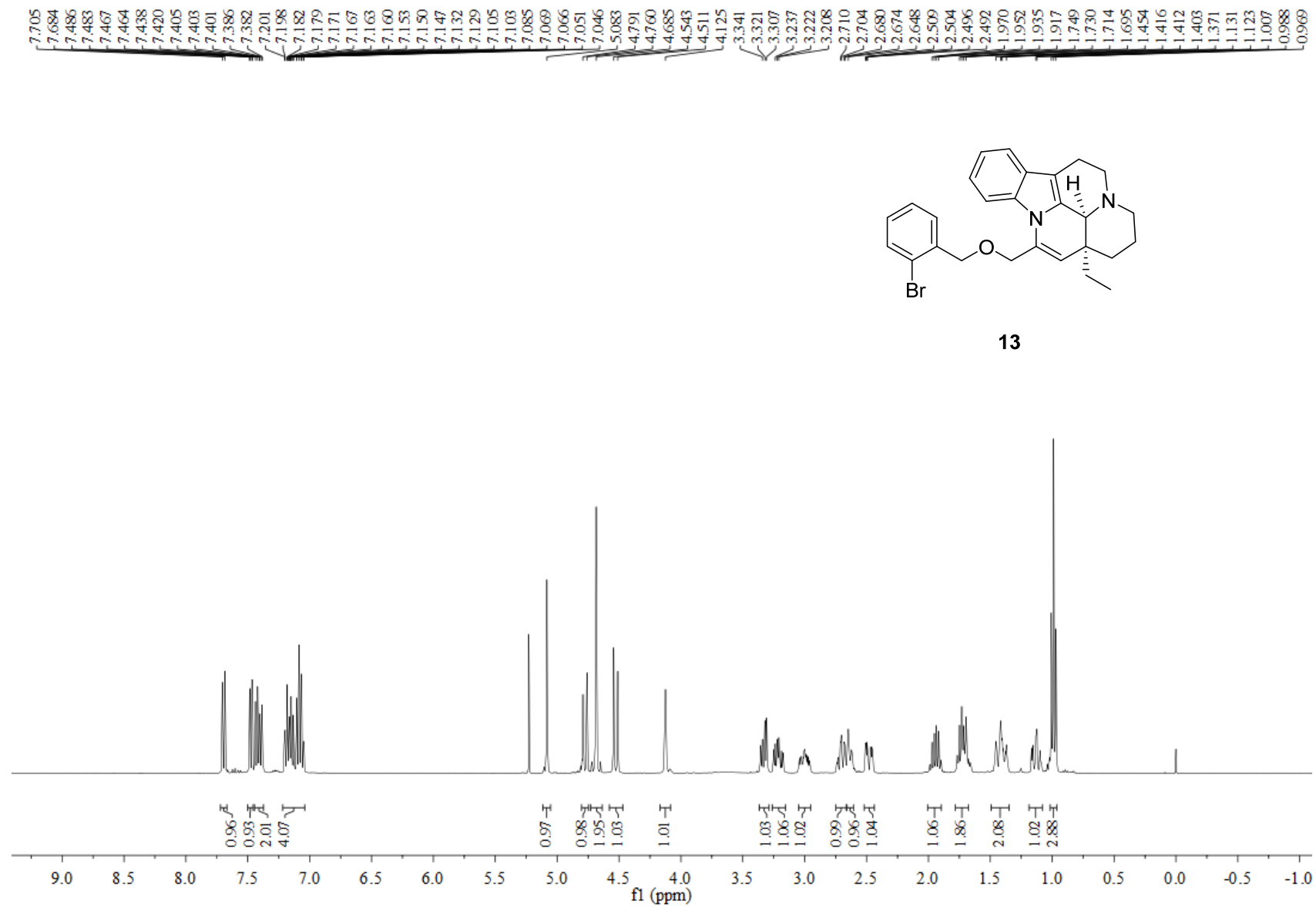
Item name: DB-60-3-1
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

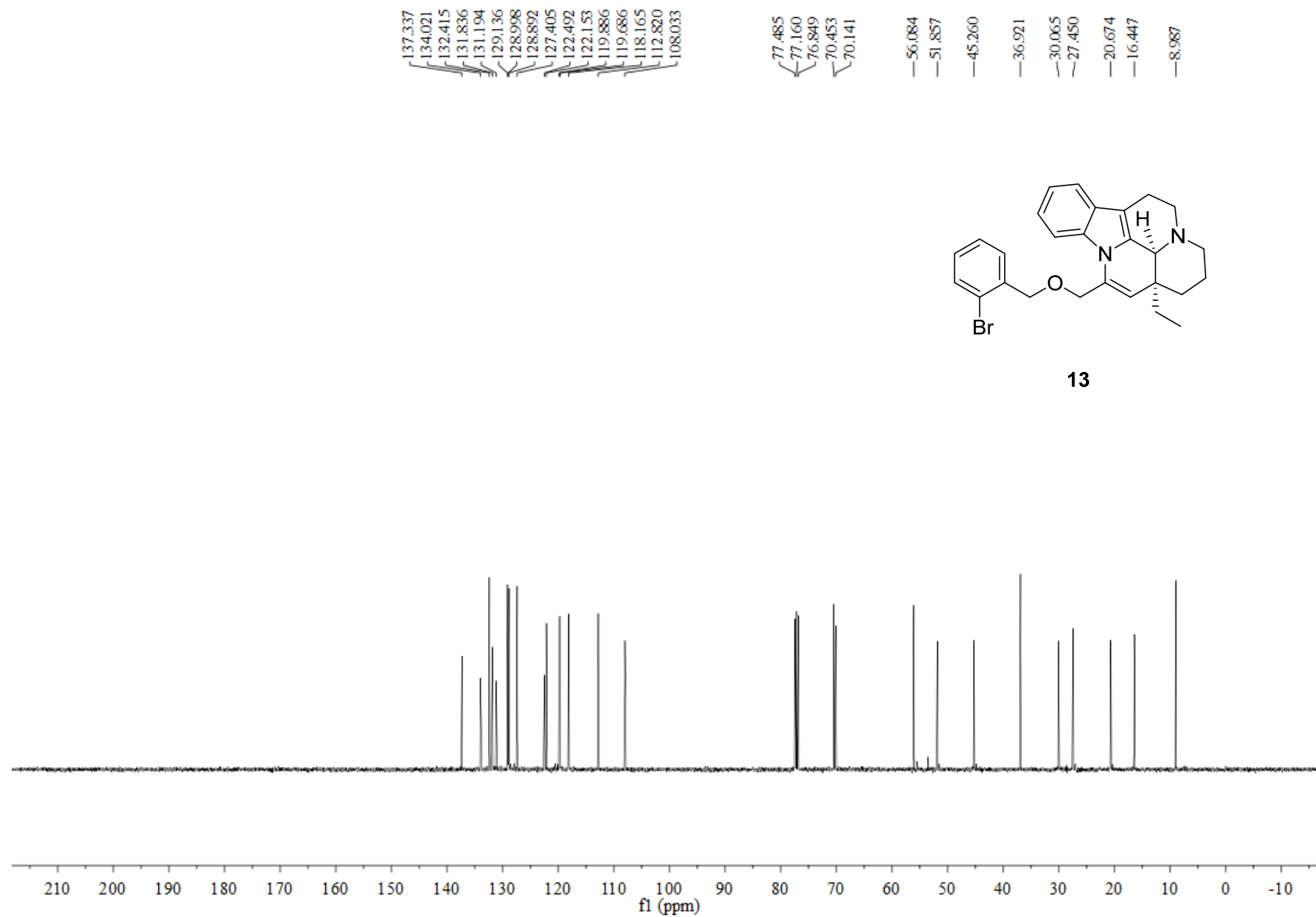
7.05e7



HRMS of Compound 12



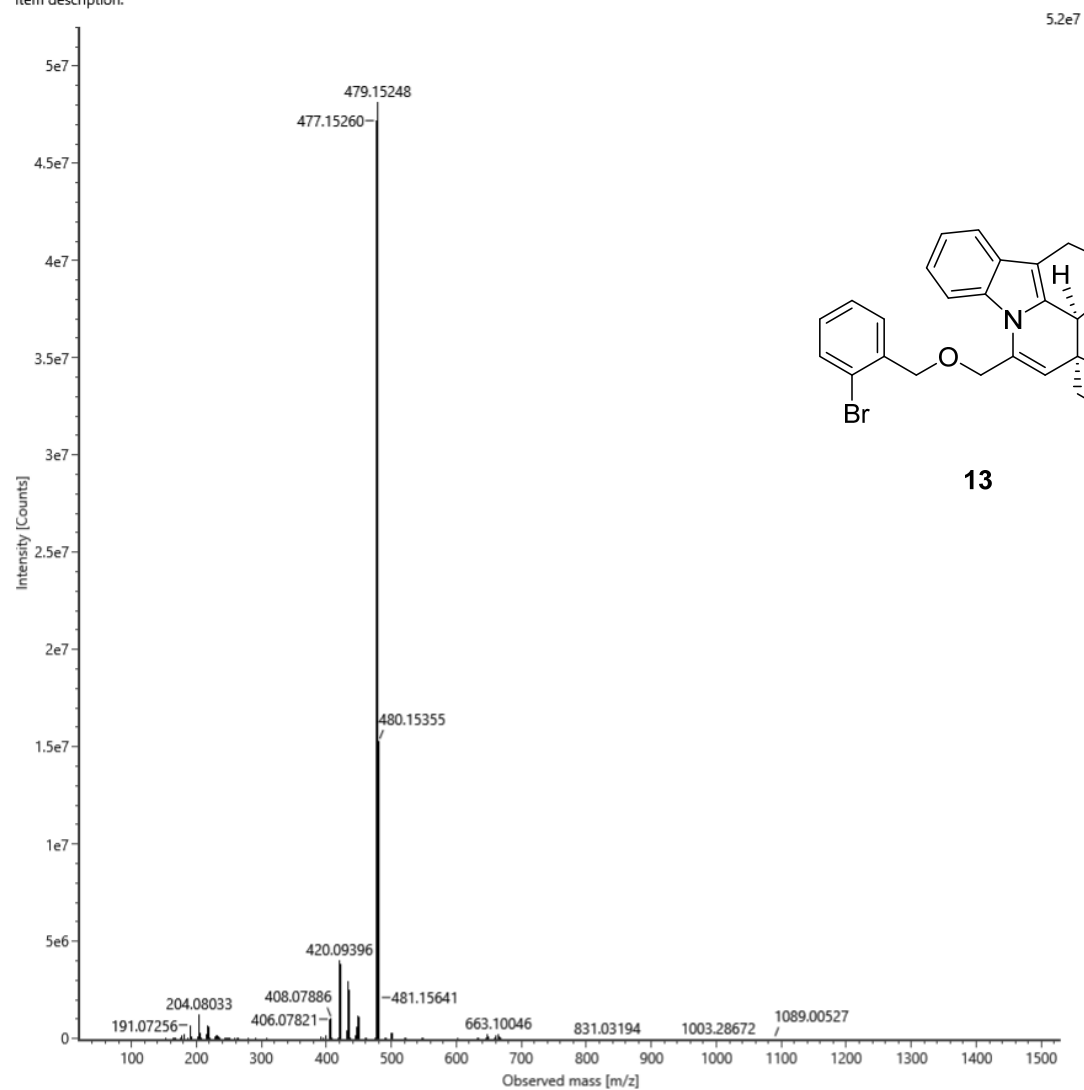
¹H NMR of Compound **13** (400 MHz, CDCl₃)



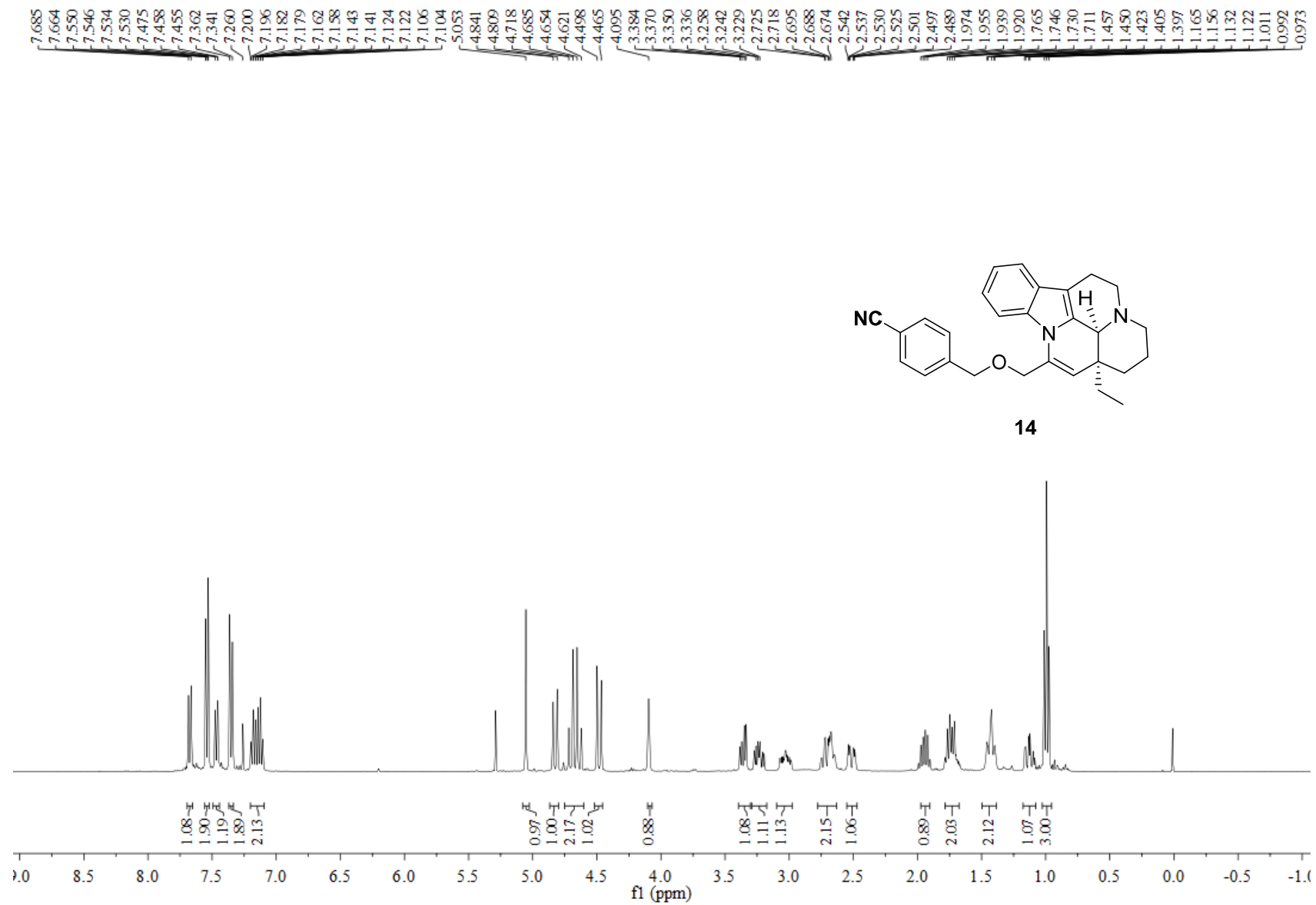
¹³C NMR of Compound **13** (100 MHz, CDCl₃)

Item name: DB-60-24
Item description:

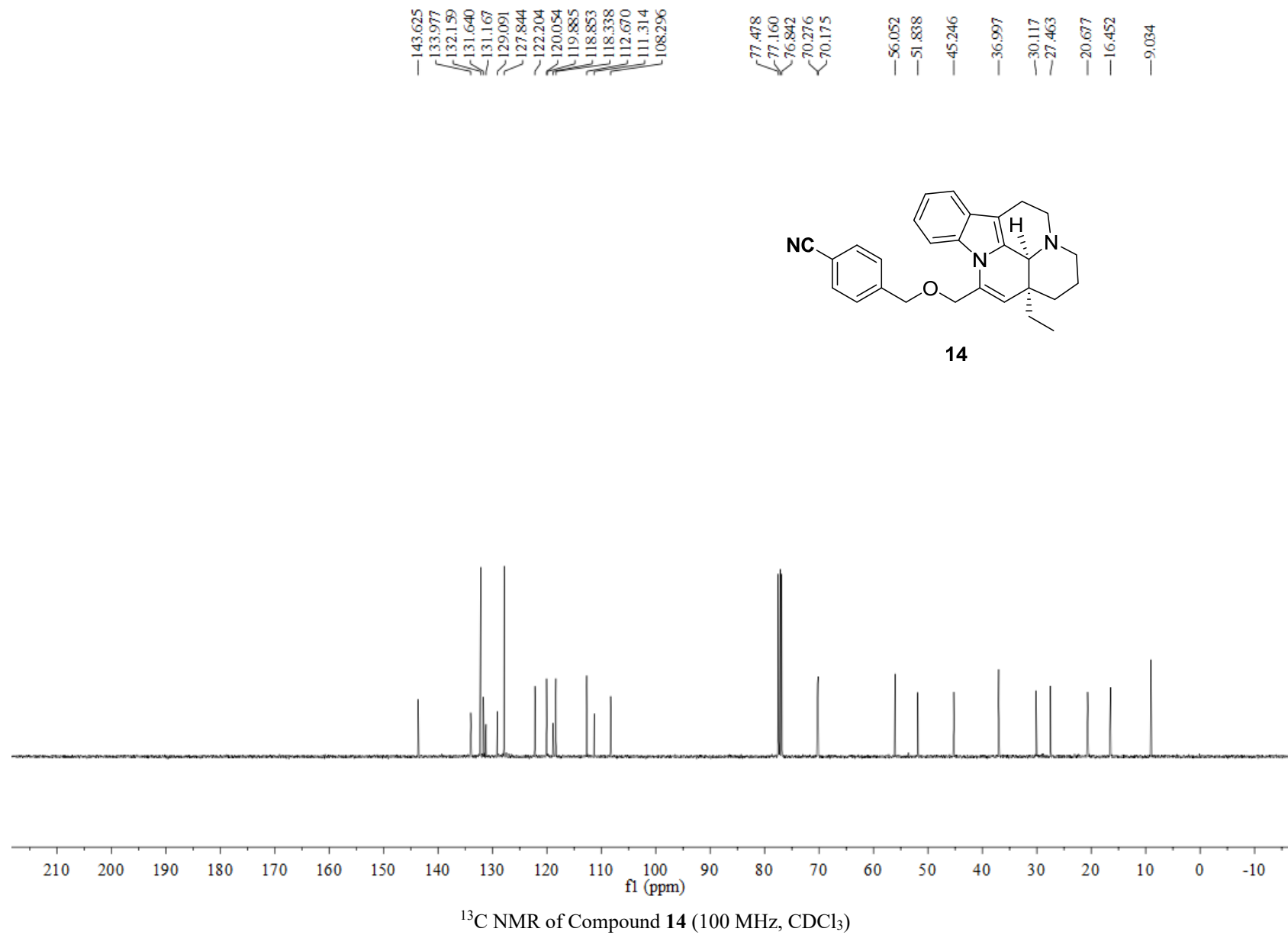
Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **13**



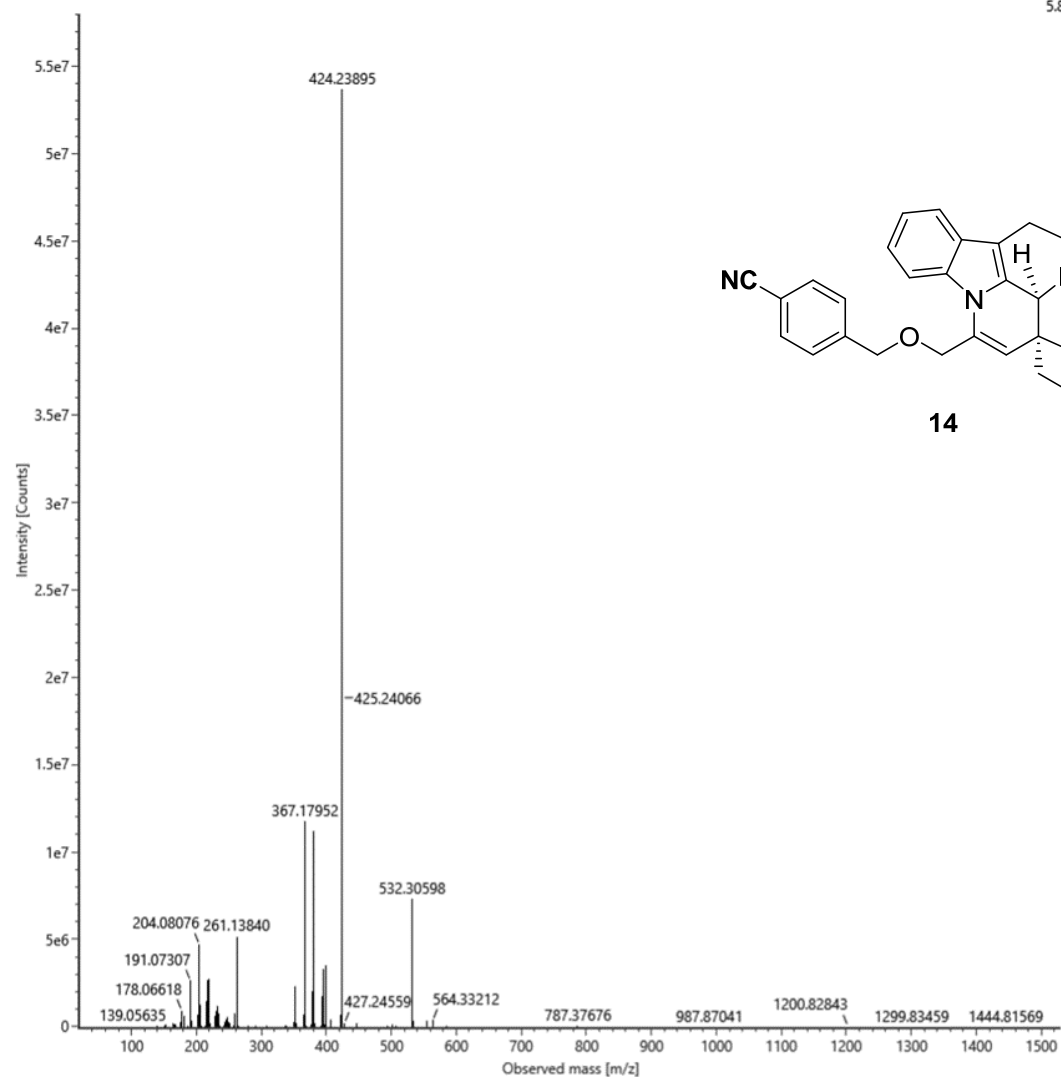
¹H NMR of Compound **14** (400 MHz, CDCl₃)



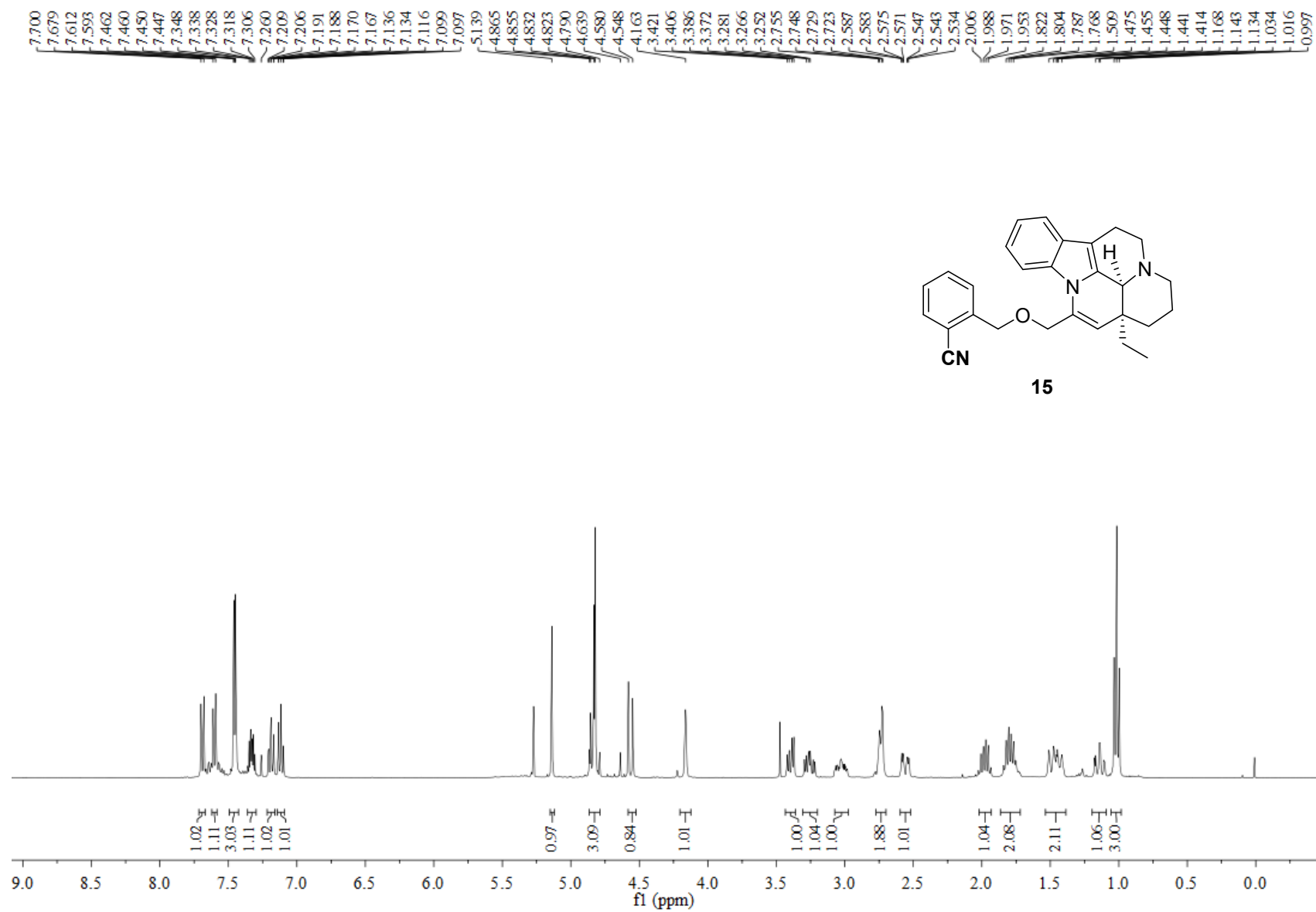
Item name: DB-60-31
Item description:

Channel name: 1: Average Time 0.0874 min : TOF MS (50-1500) ESI+ : Centroided : Combined

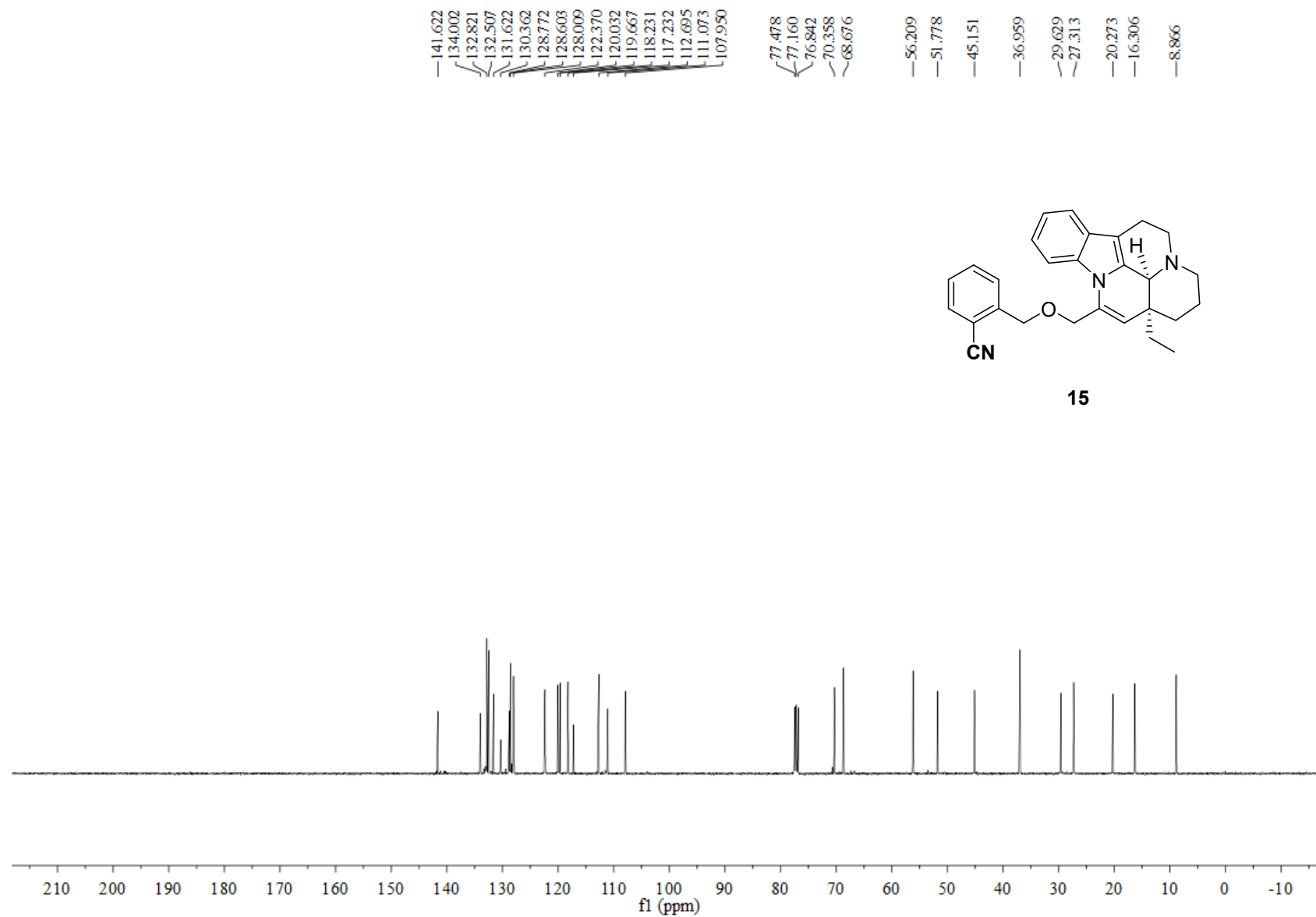
5.8e7



HRMS of Compound 14



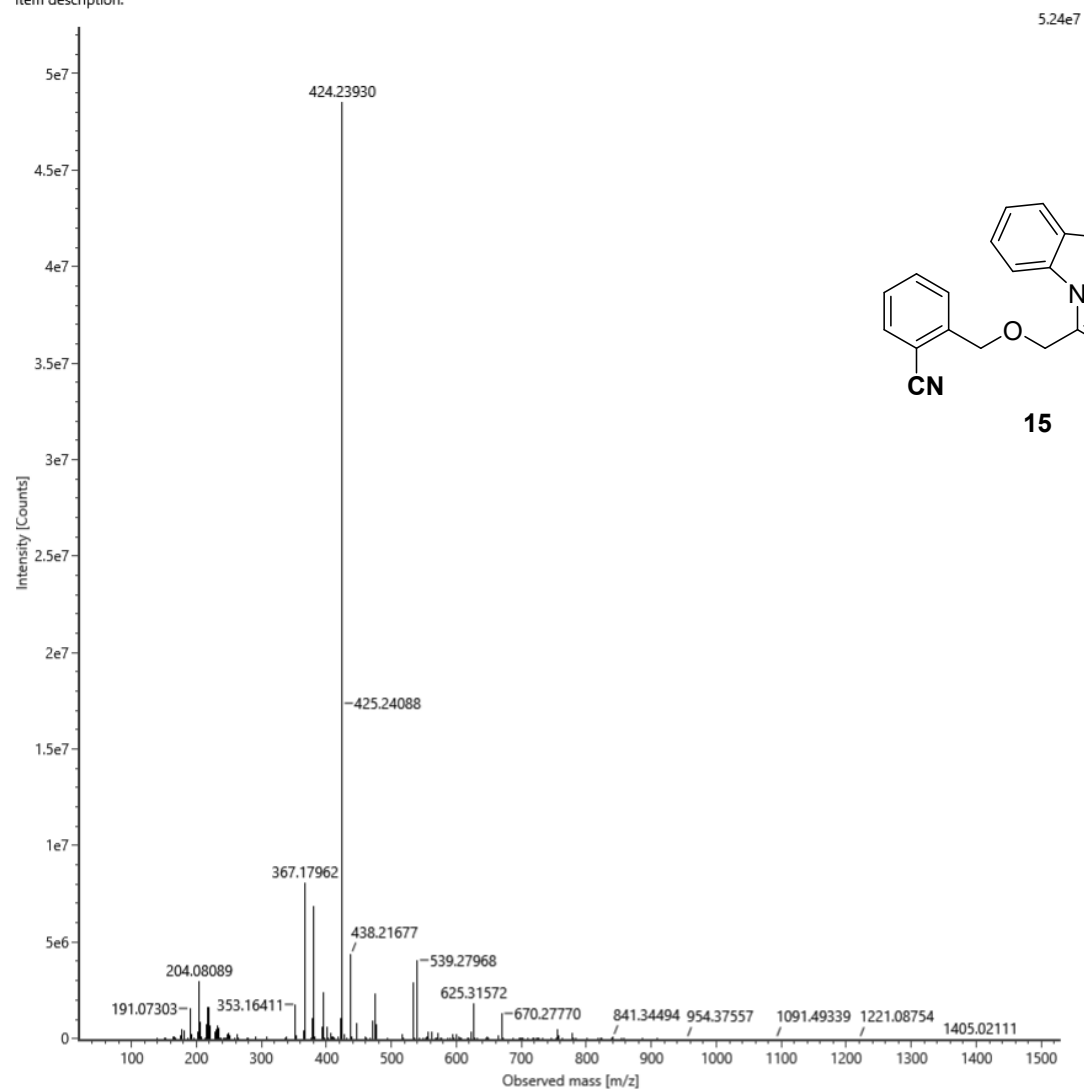
¹H NMR of Compound **15** (400 MHz, CDCl₃)



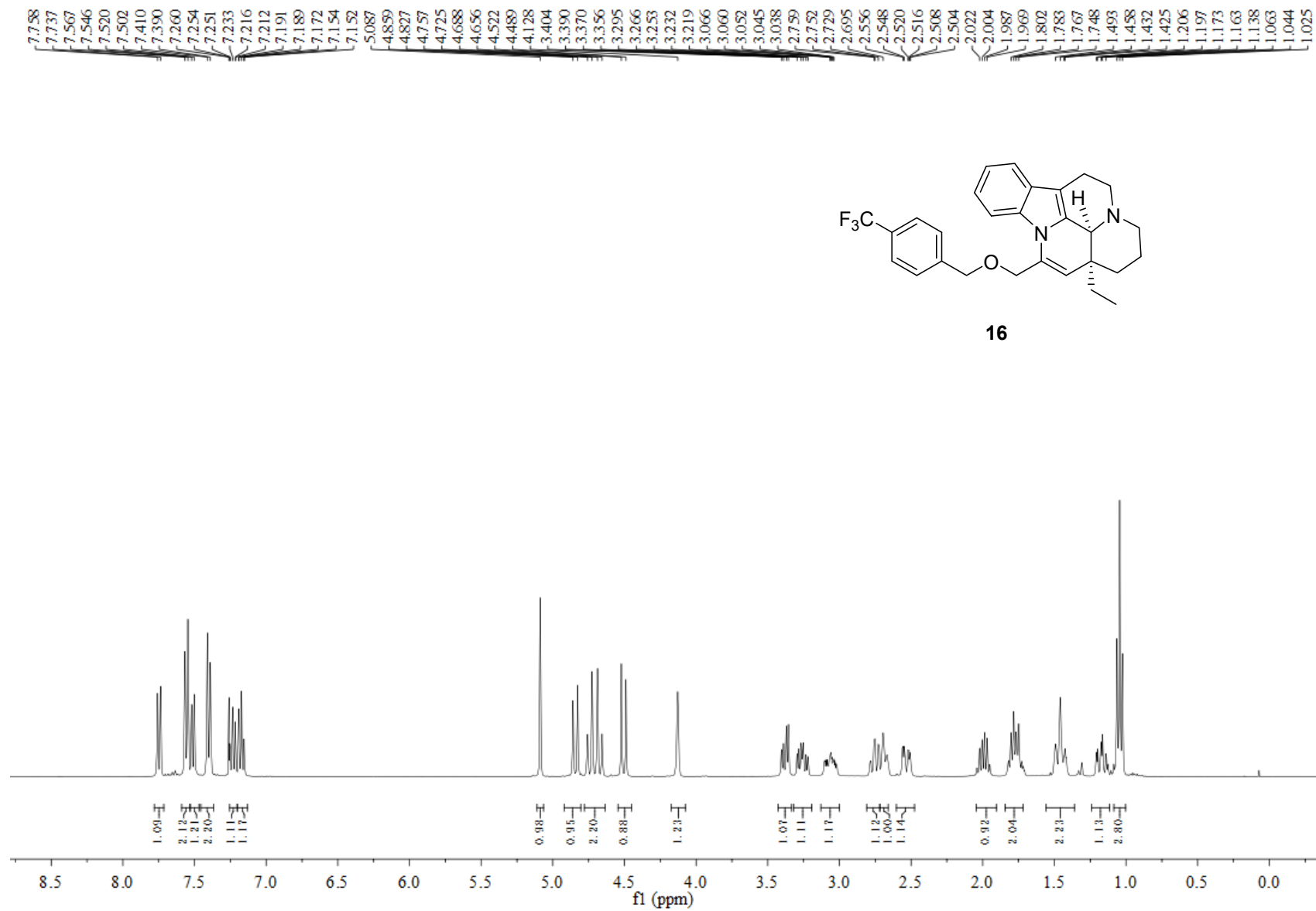
¹³C NMR of Compound **15** (100 MHz, CDCl₃)

Item name: DB-60-8
Item description:

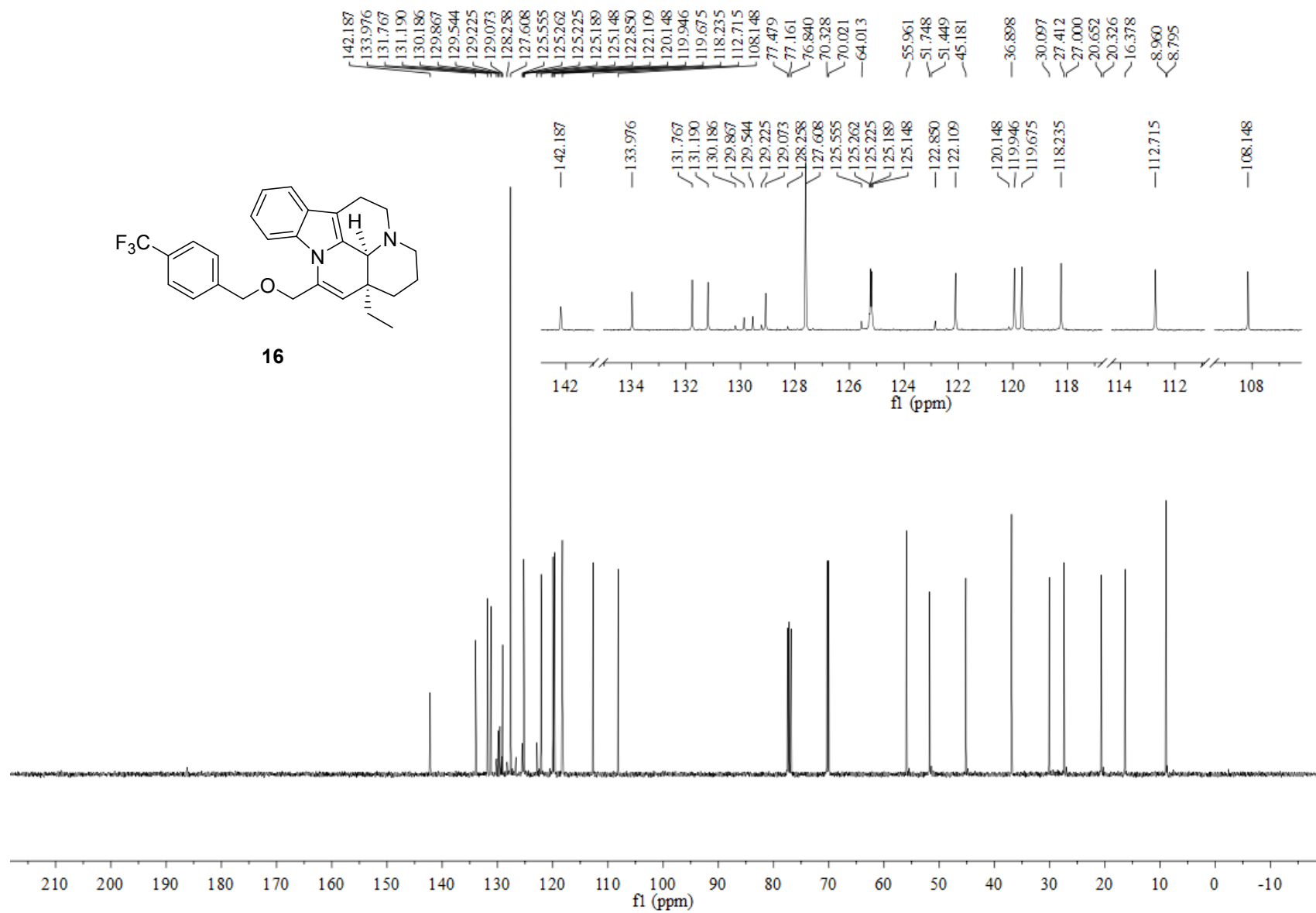
Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined

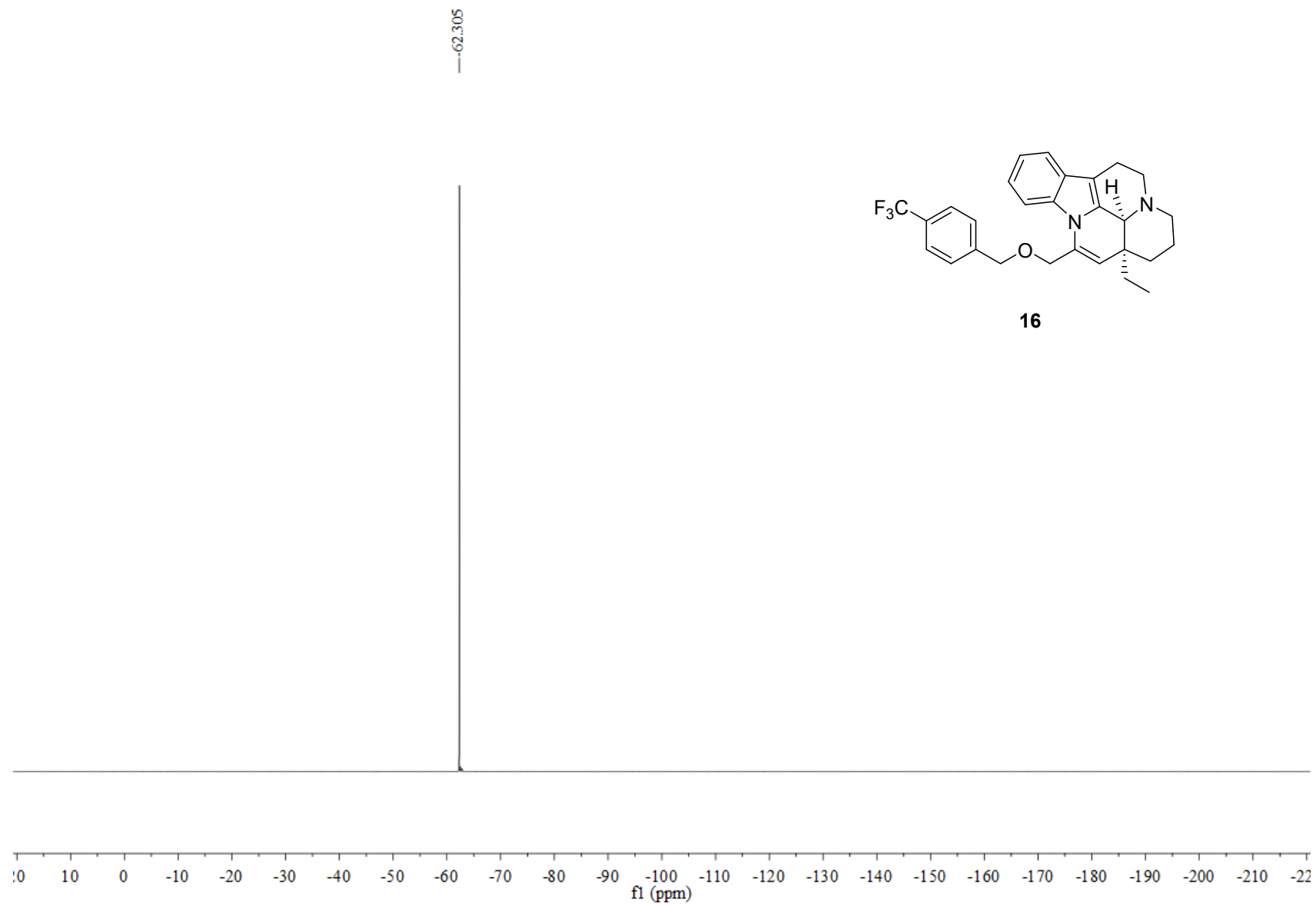


HRMS of Compound **15**



¹H NMR of Compound **16**(400 MHz, CDCl₃)

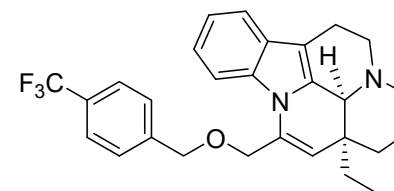
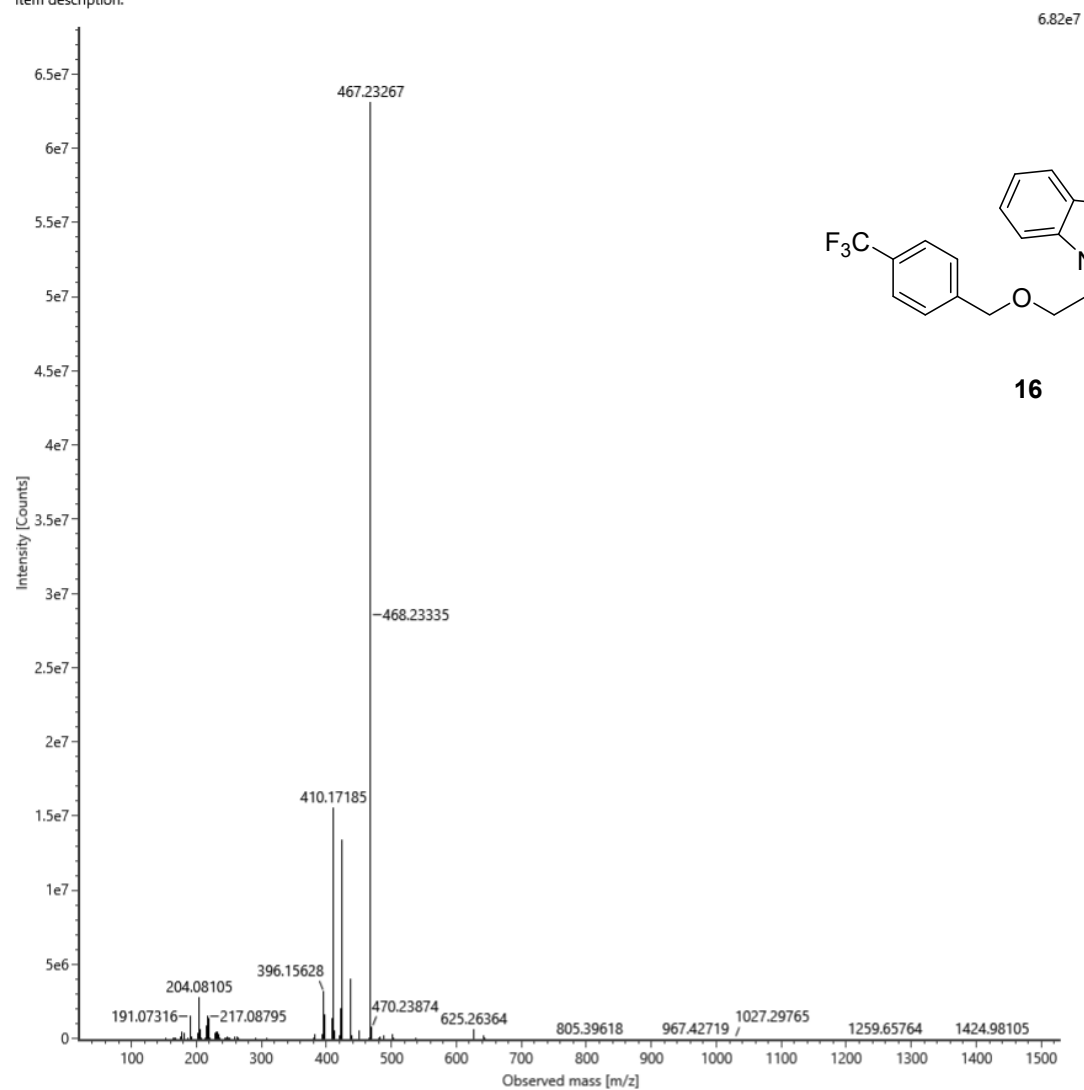




^{19}F NMR of Compound **16** (377 MHz, CDCl_3)

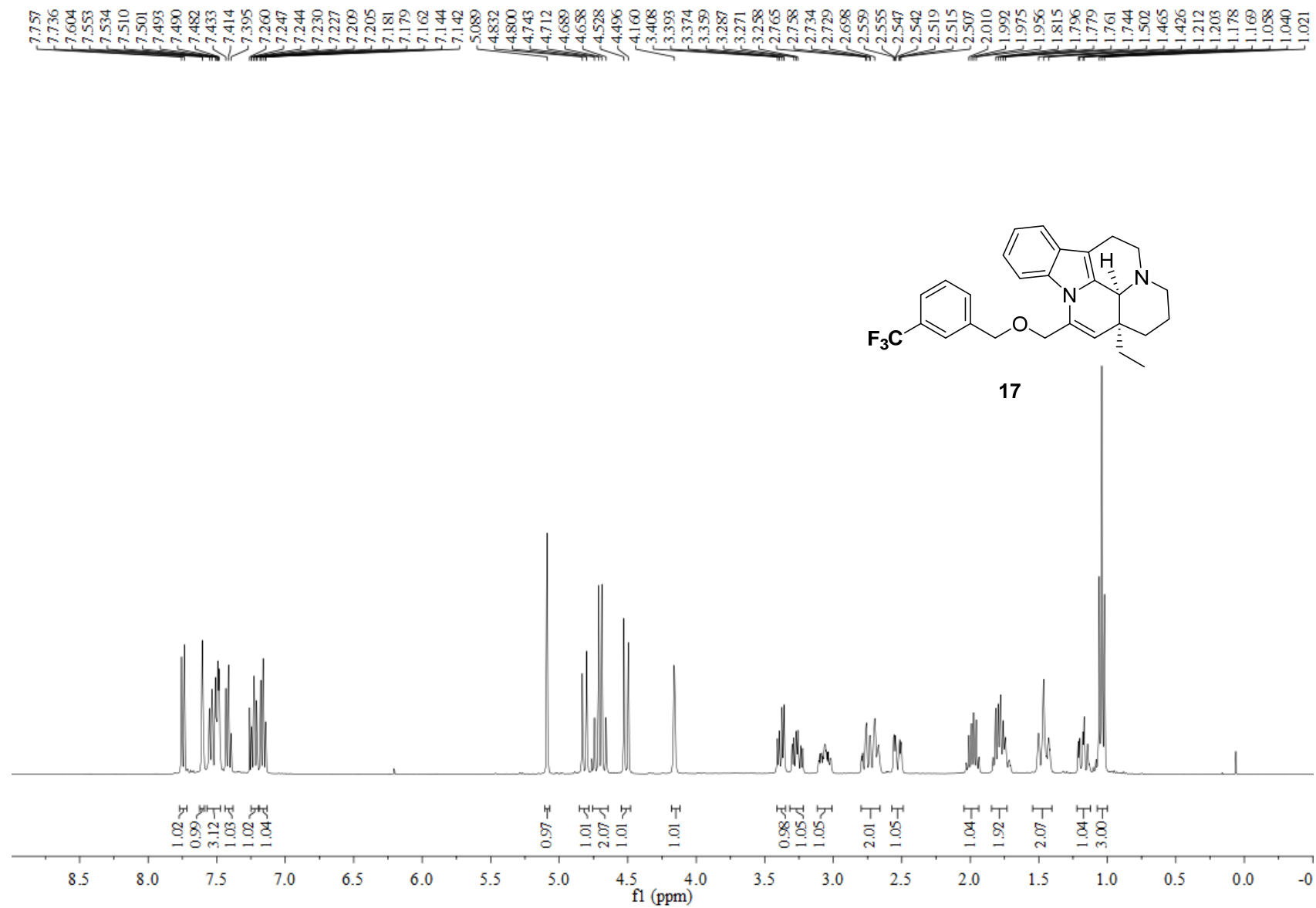
Item name: DB-60-12
Item description:

Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined

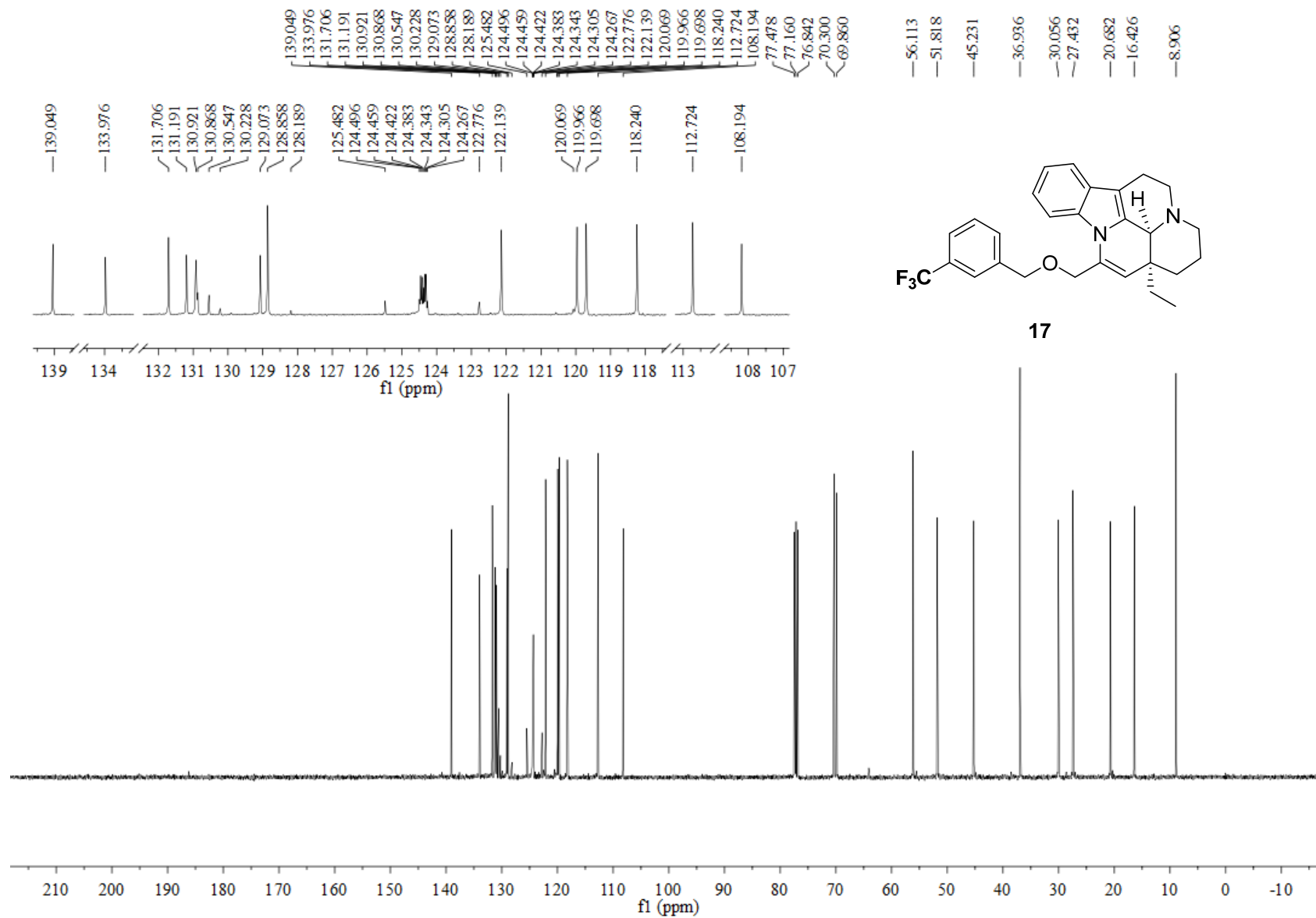


16

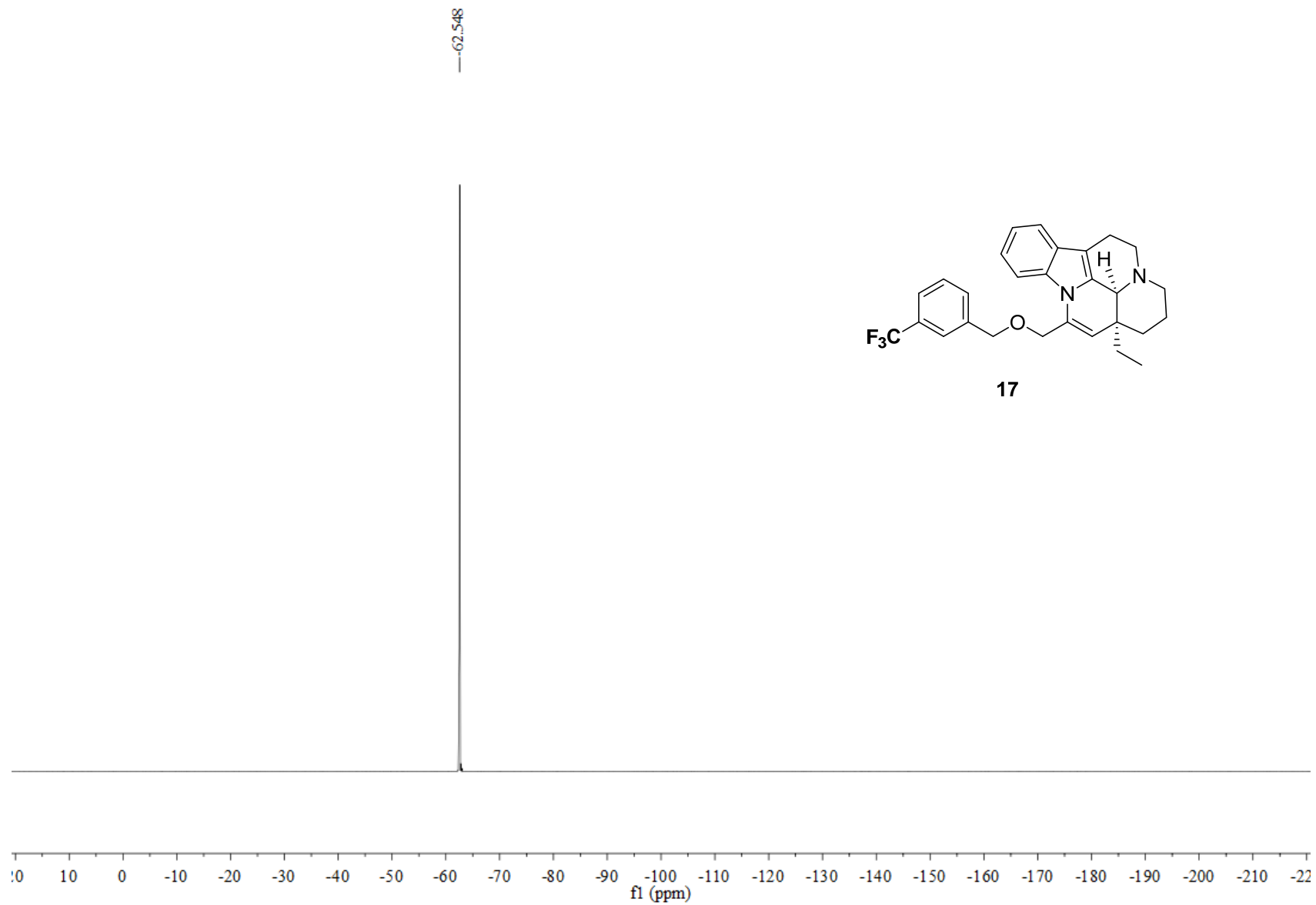
HRMS of Compound **16**



¹H NMR of Compound **17** (400 MHz, CDCl₃)



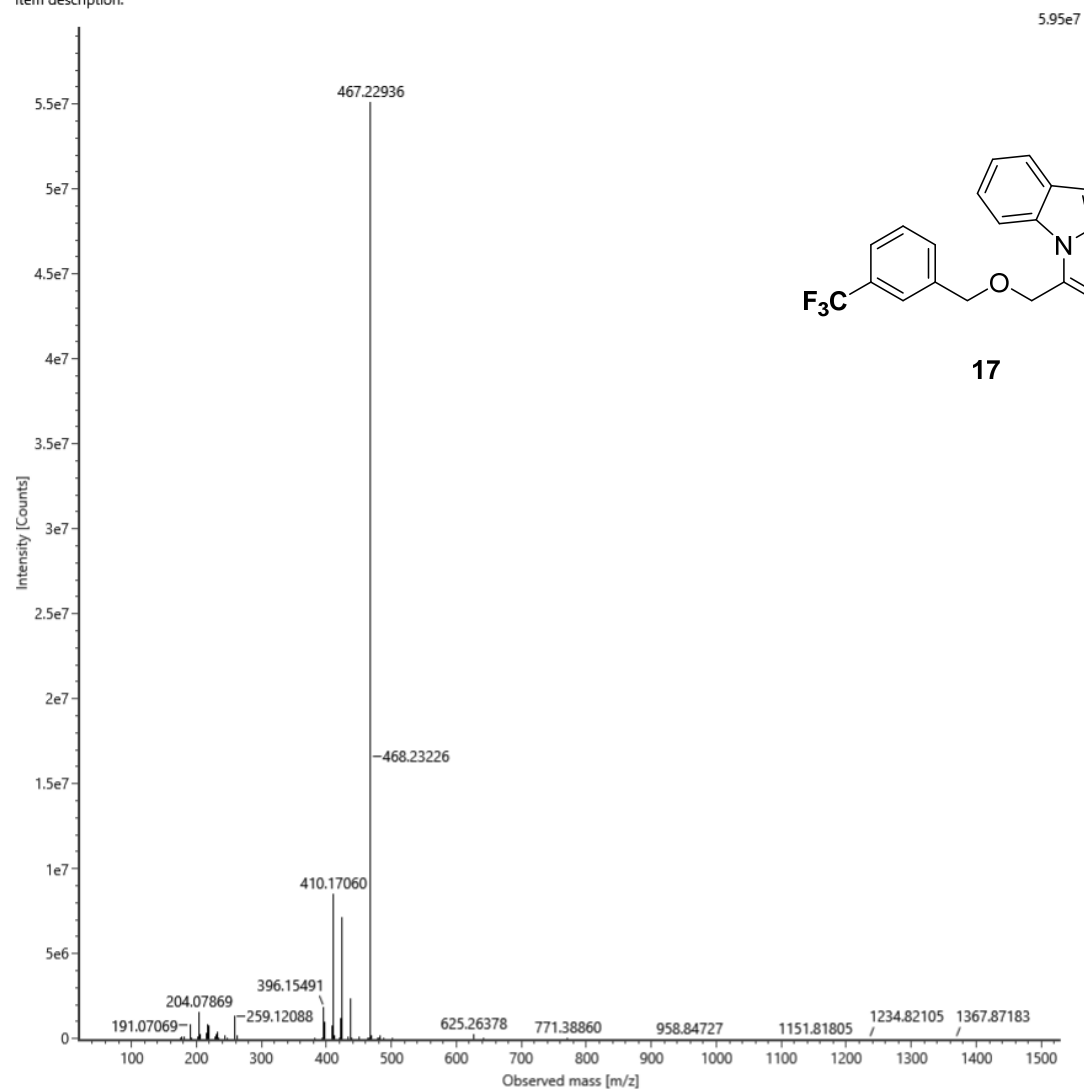
¹³C NMR of Compound **17** (100 MHz, CDCl₃)



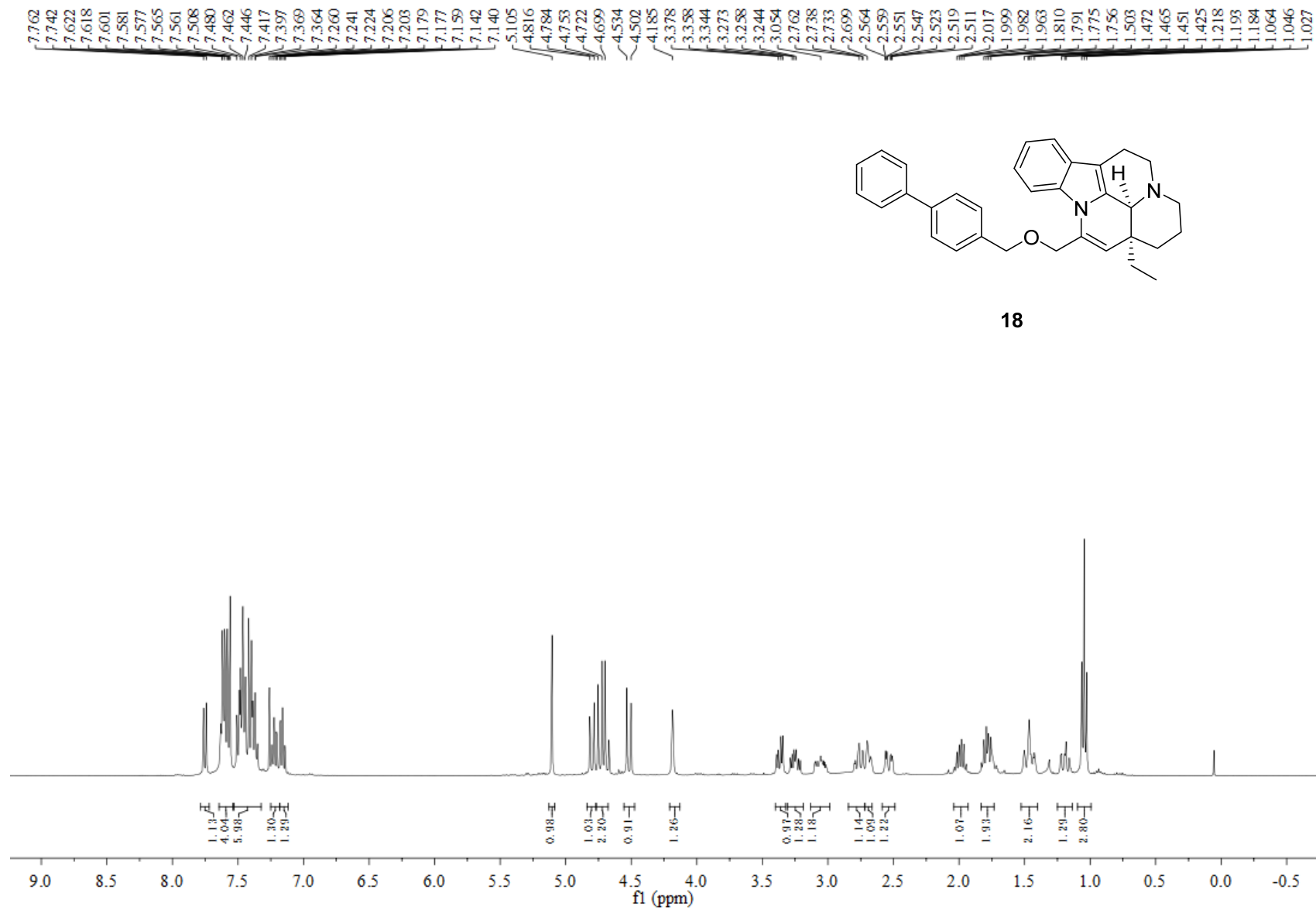
^{19}F NMR of Compound **17** (377 MHz, CDCl_3)

Item name: DB-60-12
Item description:

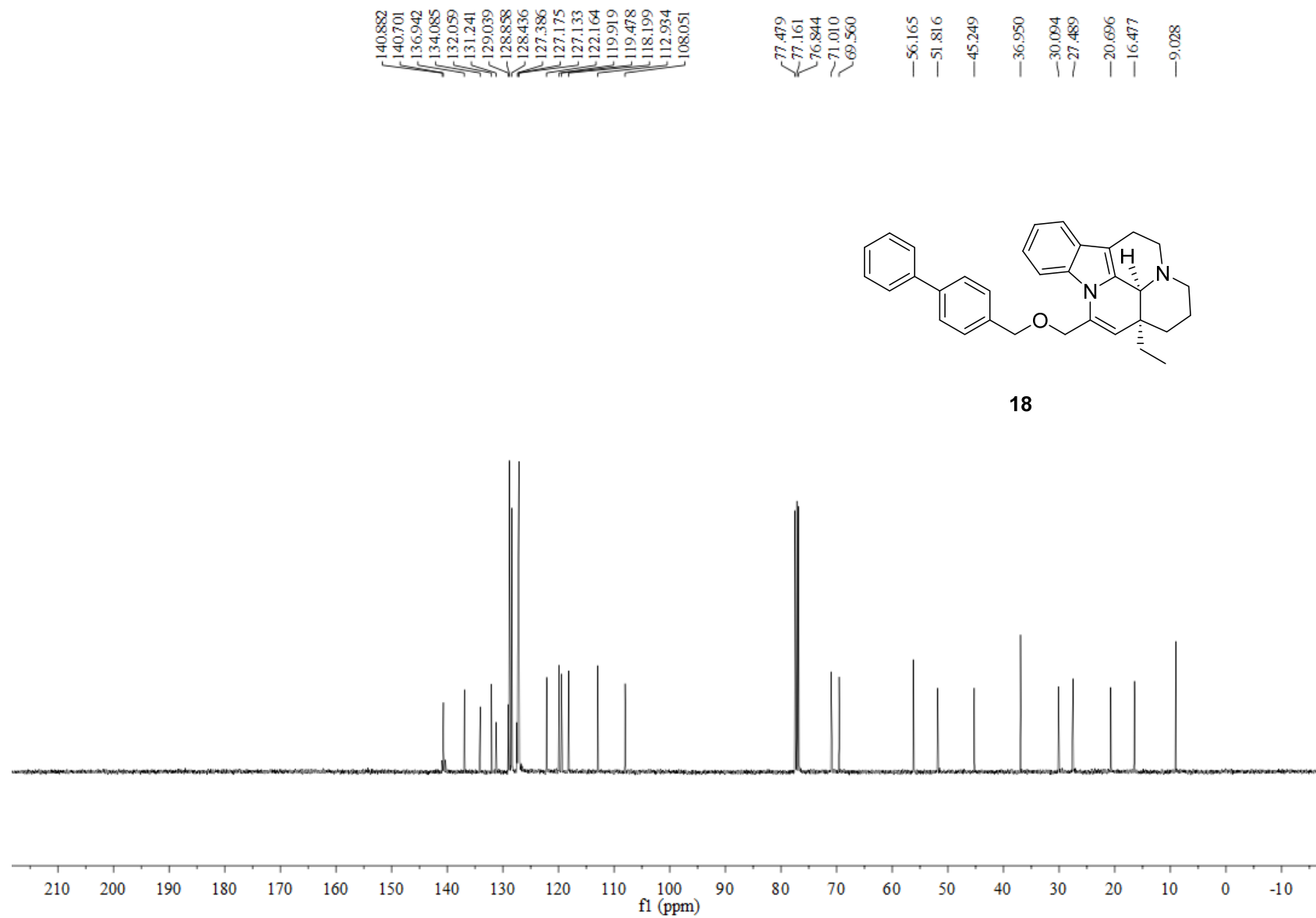
Channel name: 1: Average Time 0.0917 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **17**



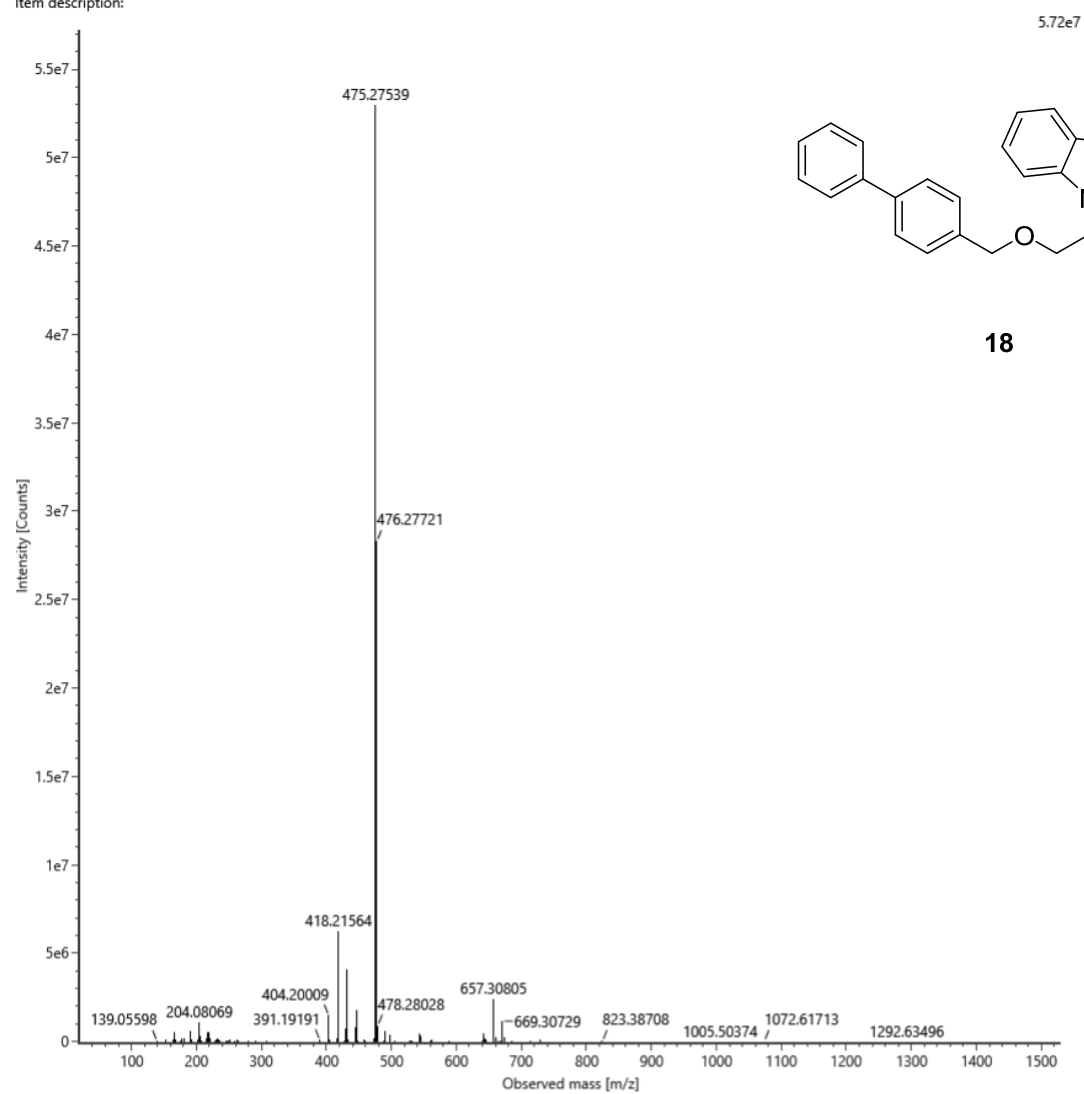
¹H NMR of Compound 18 (400 MHz, CDCl₃)



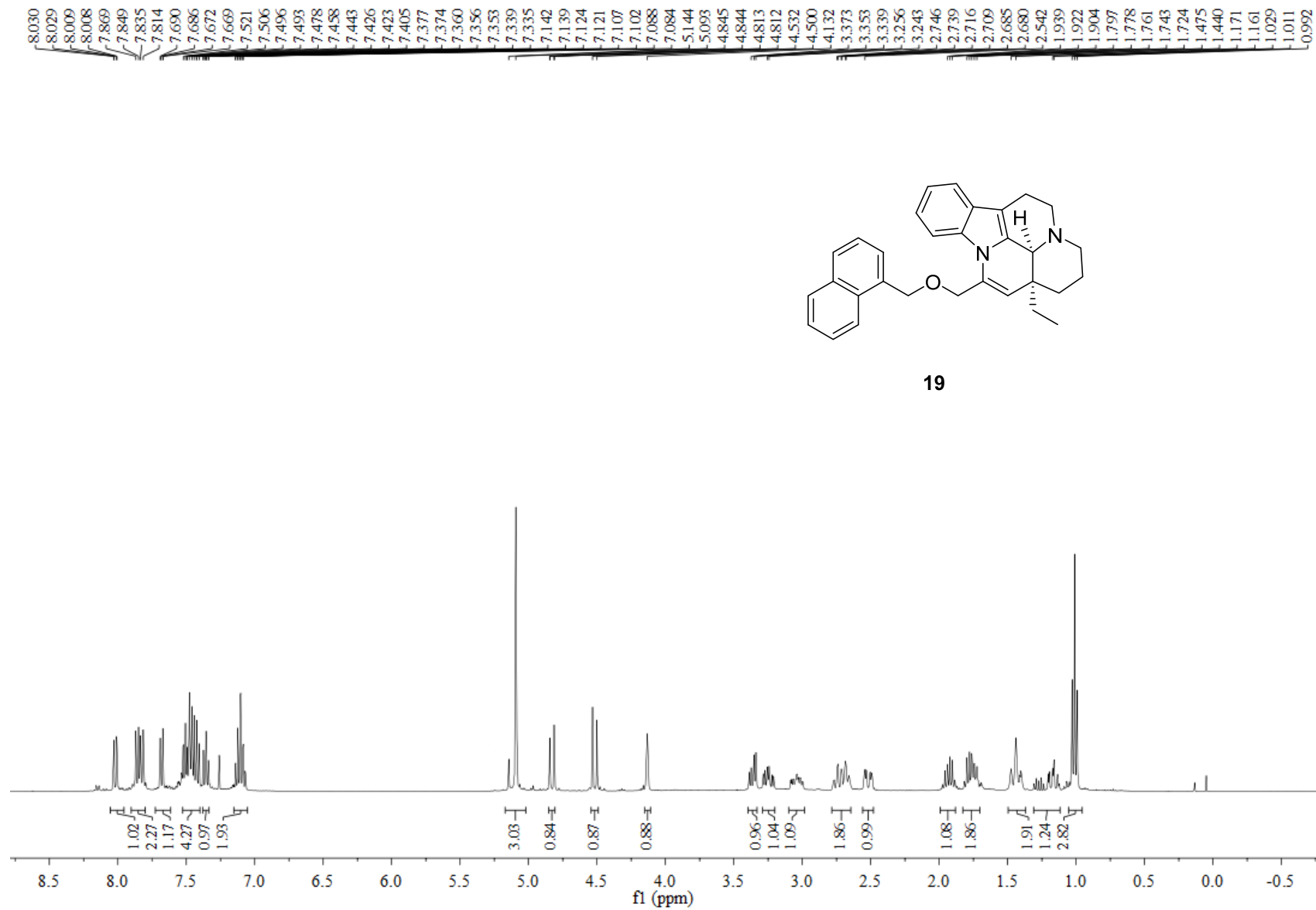
^{13}C NMR of Compound **18** (100 MHz, CDCl_3)

Item name: DB-60-7
Item description:

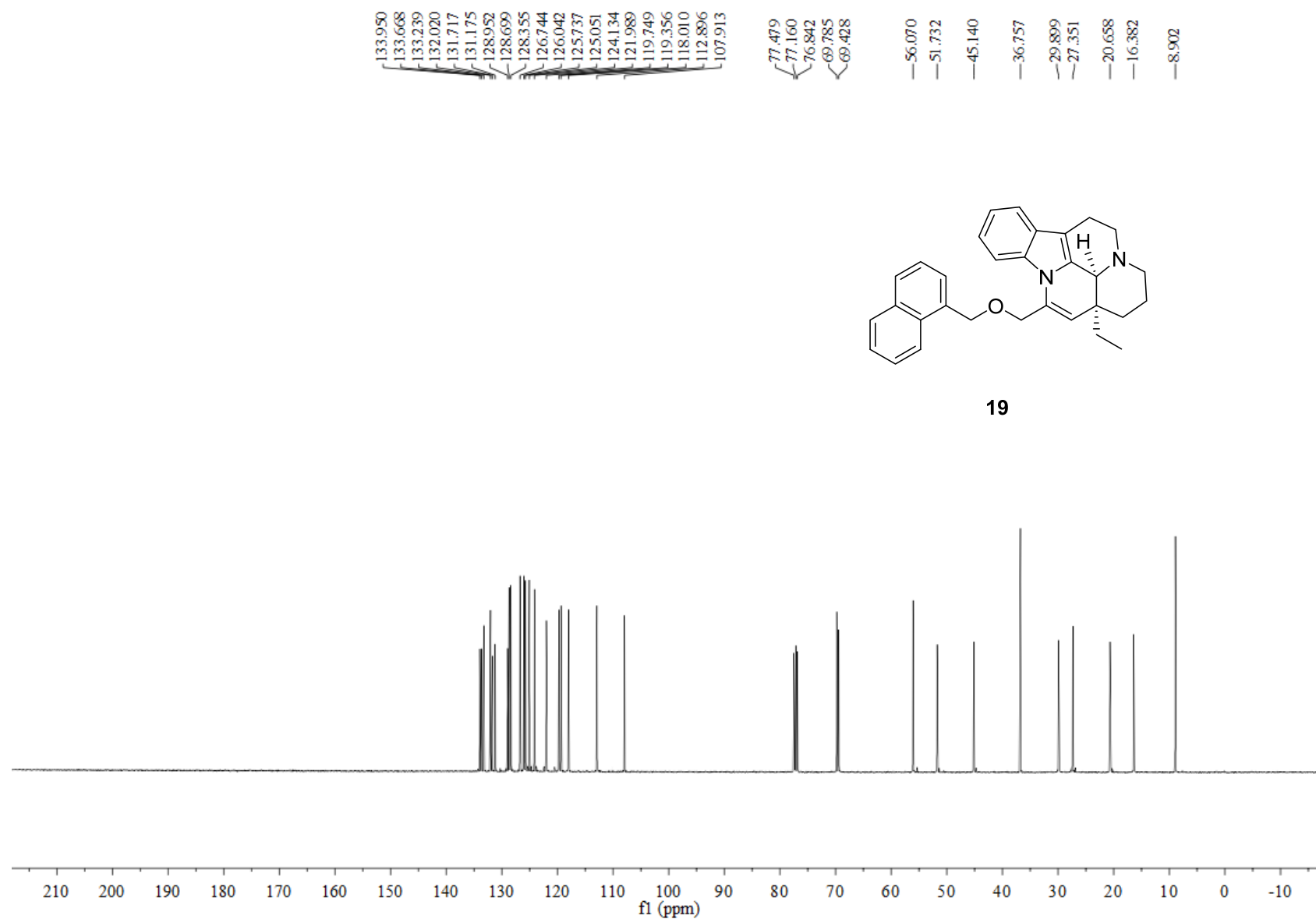
Channel name: 1: Average Time 0.0788 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **18**



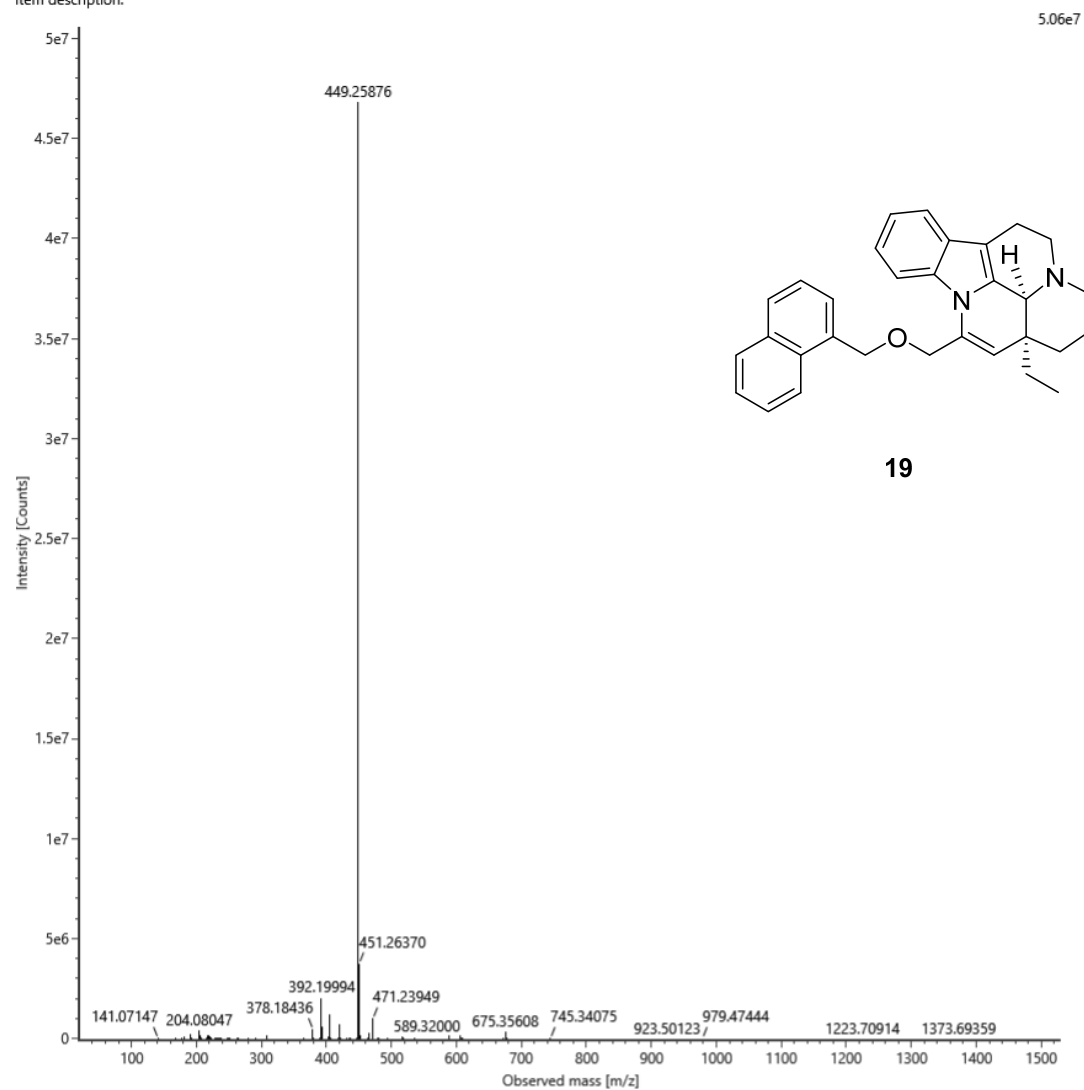
¹H NMR of Compound 19 (400 MHz, CDCl₃)



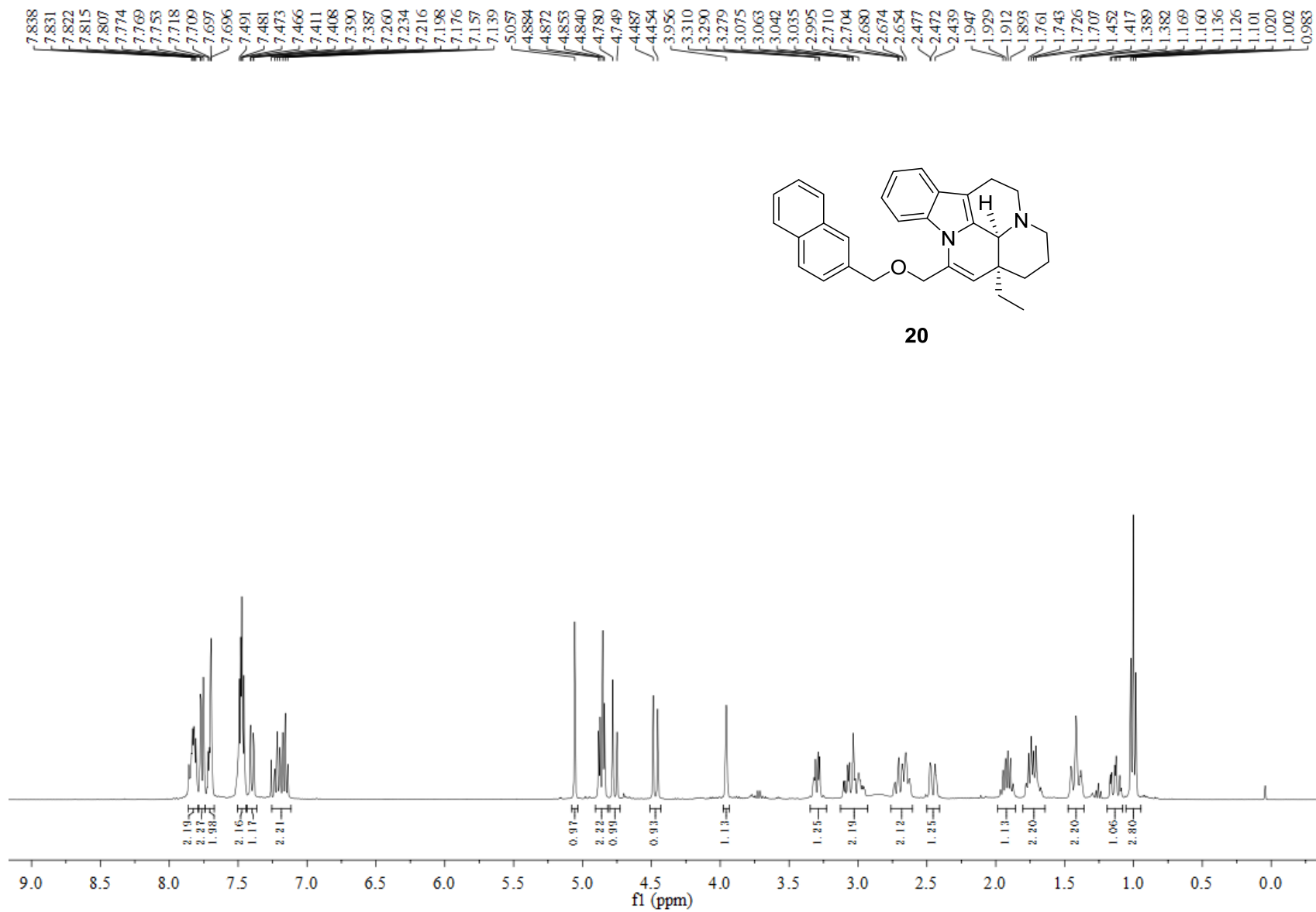
¹³C NMR of Compound **19** (100 MHz, CDCl₃)

Item name: DA-111
Item description:

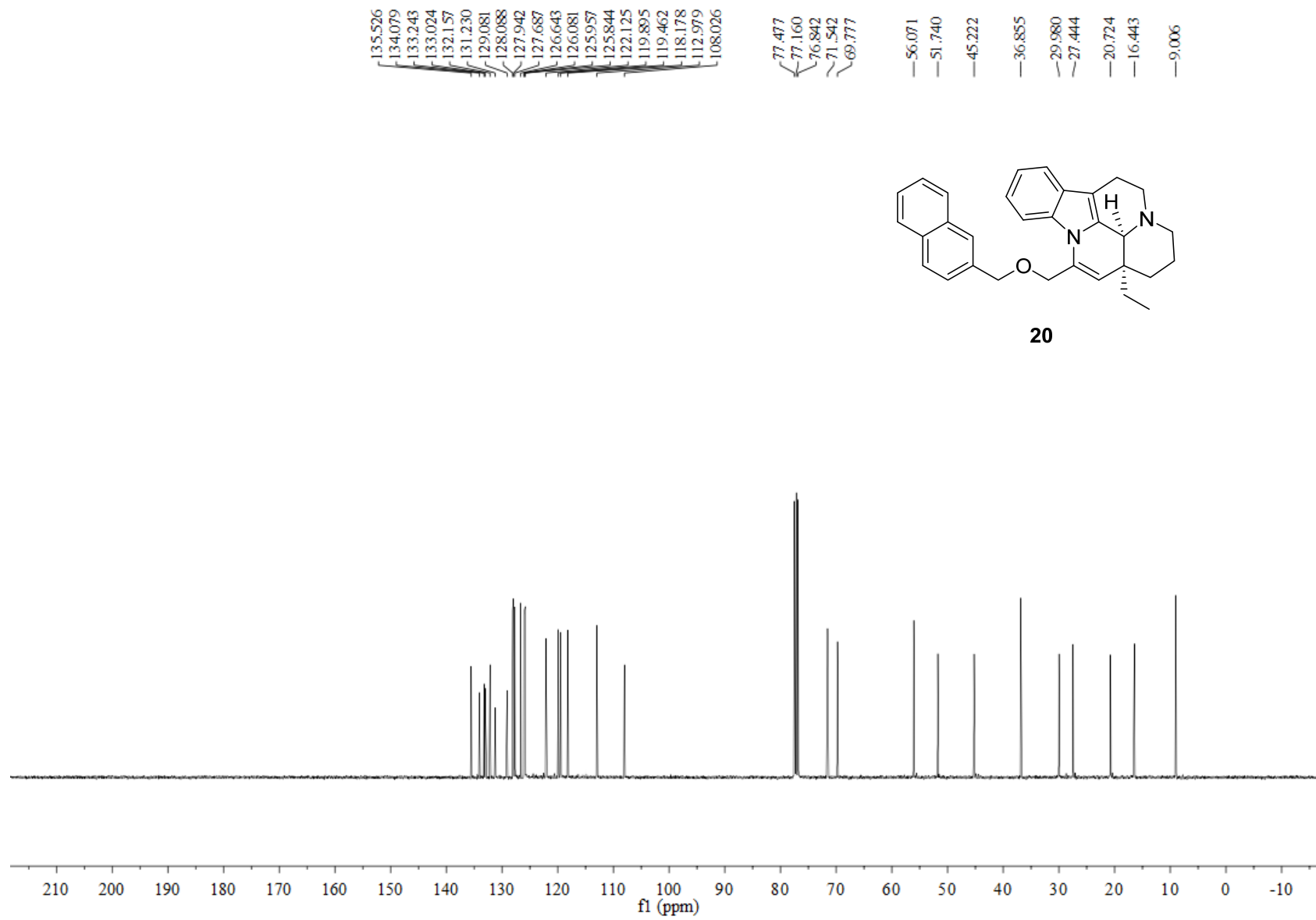
Channel name: 1: Average Time 0.0788 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **19**



¹H NMR of Compound **20** (400 MHz, CDCl₃)

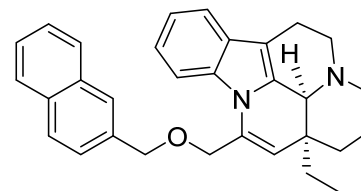
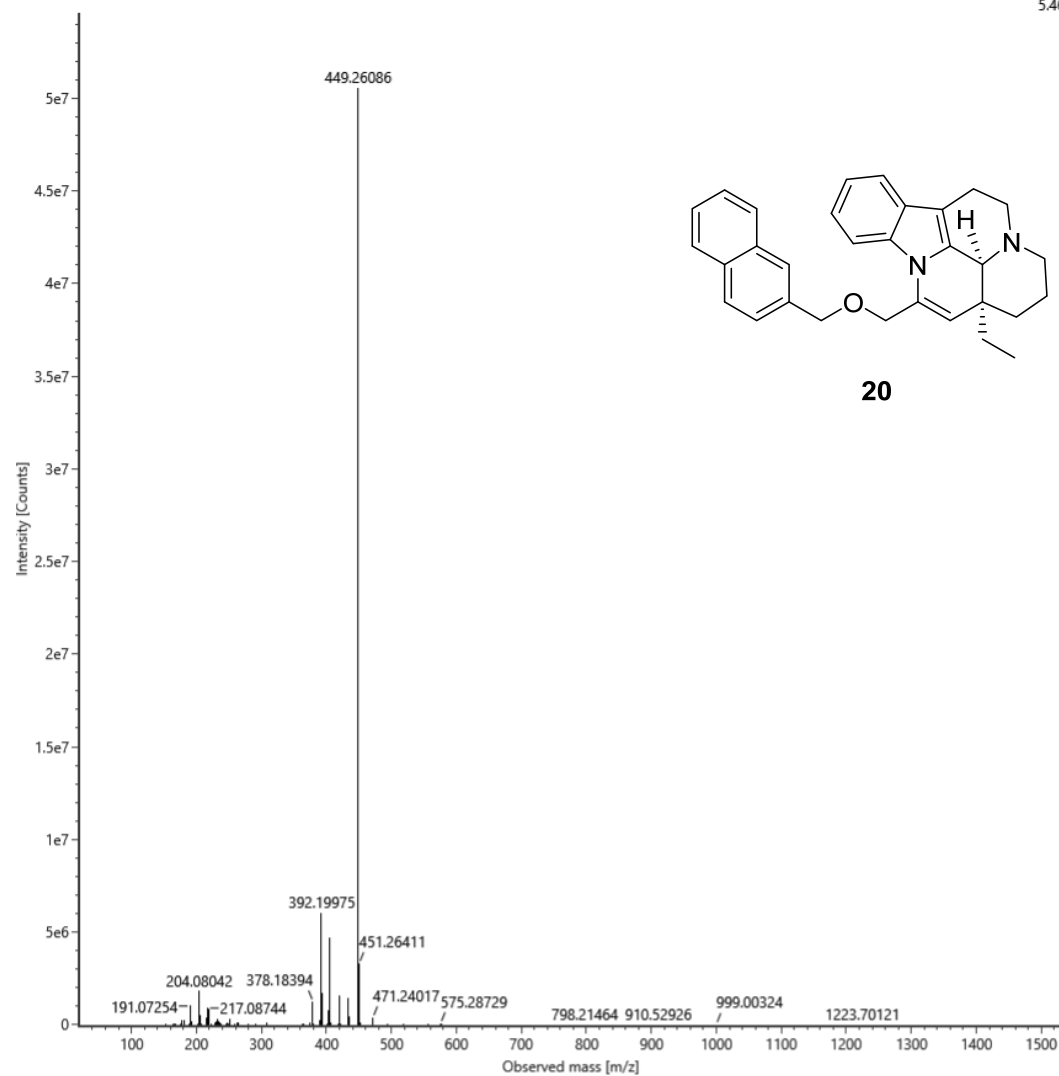


¹³C NMR of Compound **20** (100 MHz, CDCl₃)

Item name: DB-60-29
Item description:

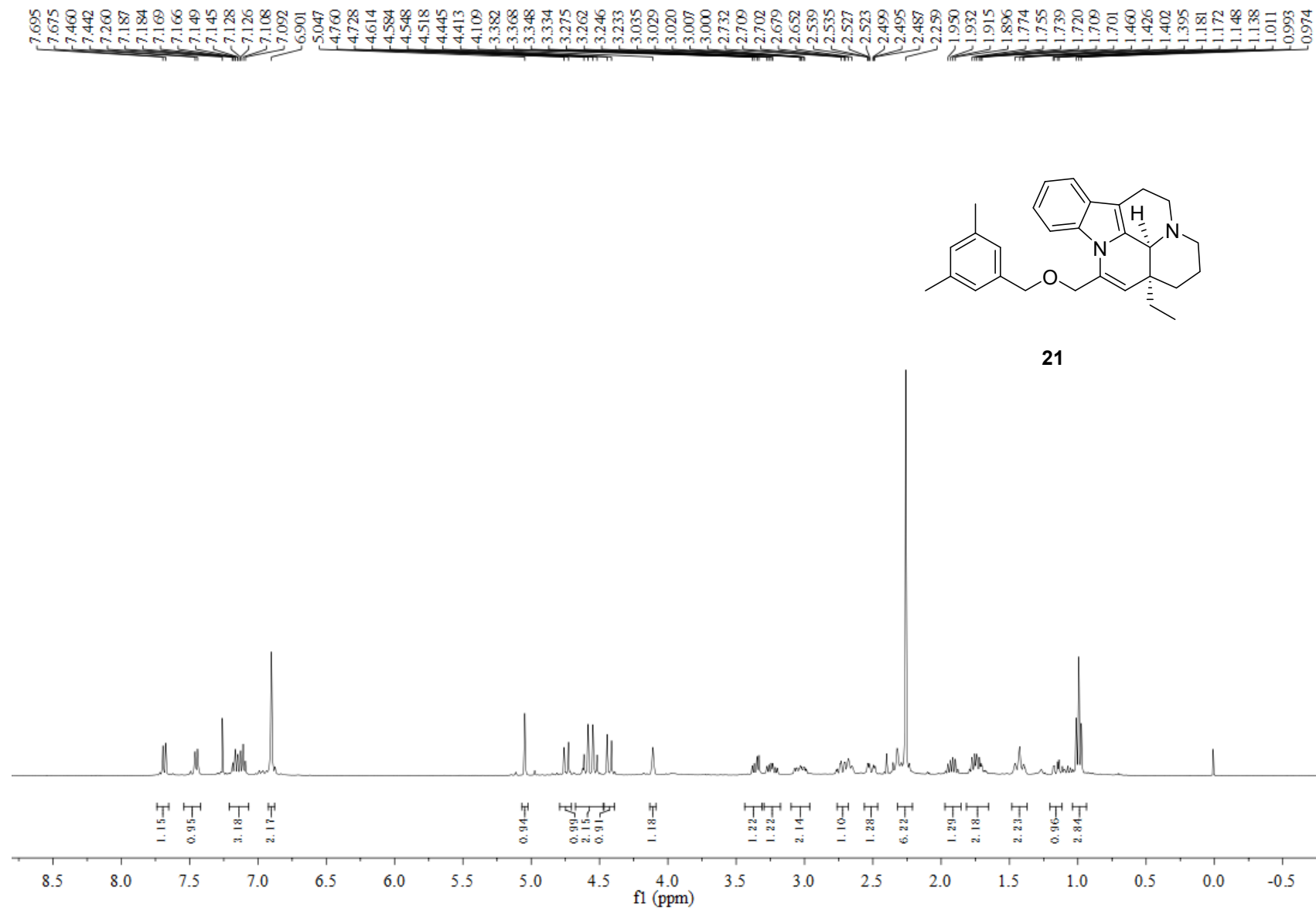
Channel name: 1: Average Time 0.0788 min : TOF MS (50-1500) ESI+ : Centroided : Combined

5.46e7



20

HRMS of Compound **20**



¹H NMR of Compound **21** (400 MHz, CDCl₃)

137.813
137.720
133.997
132.090
131.246
129.254
128.964
125.801
121.990
119.775
119.261
118.039
112.957
107.871

77.478
77.160
76.842
71.338
69.427

56.149
51.816

45.192

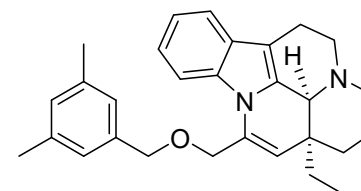
36.788

29.940
27.411

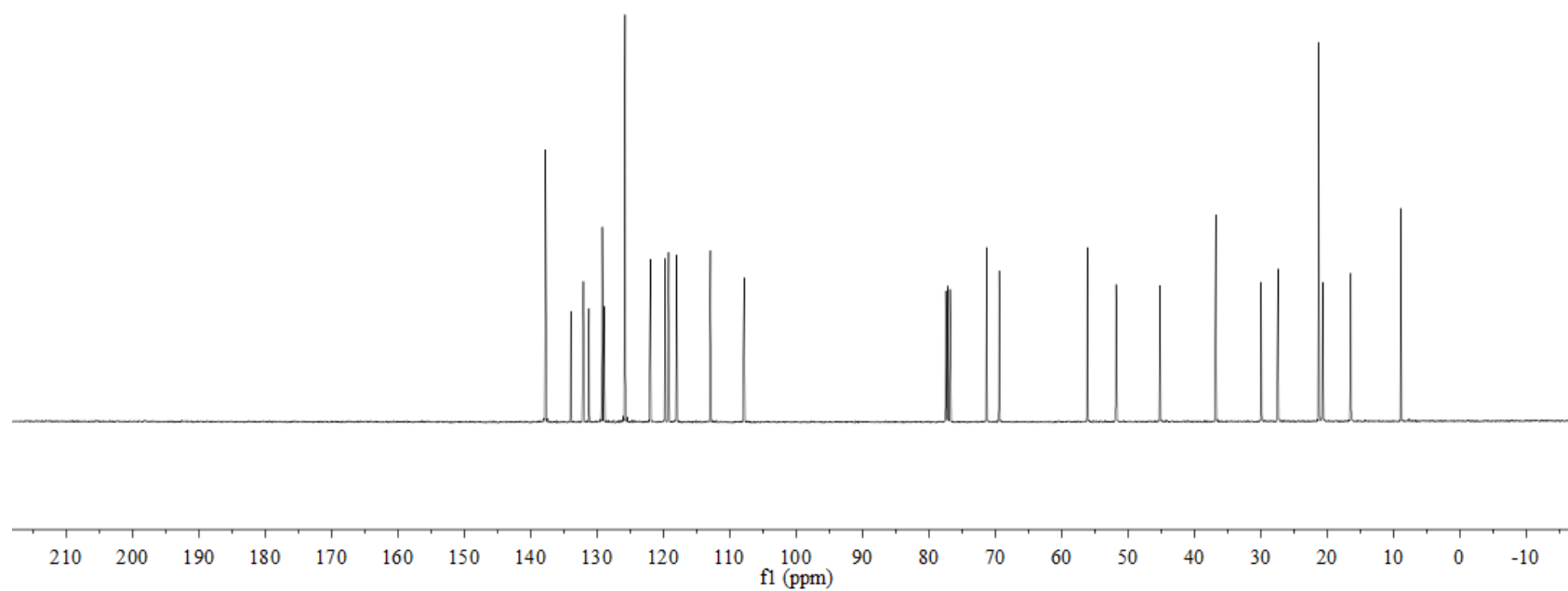
21.253
20.683

16.439

8.896



21

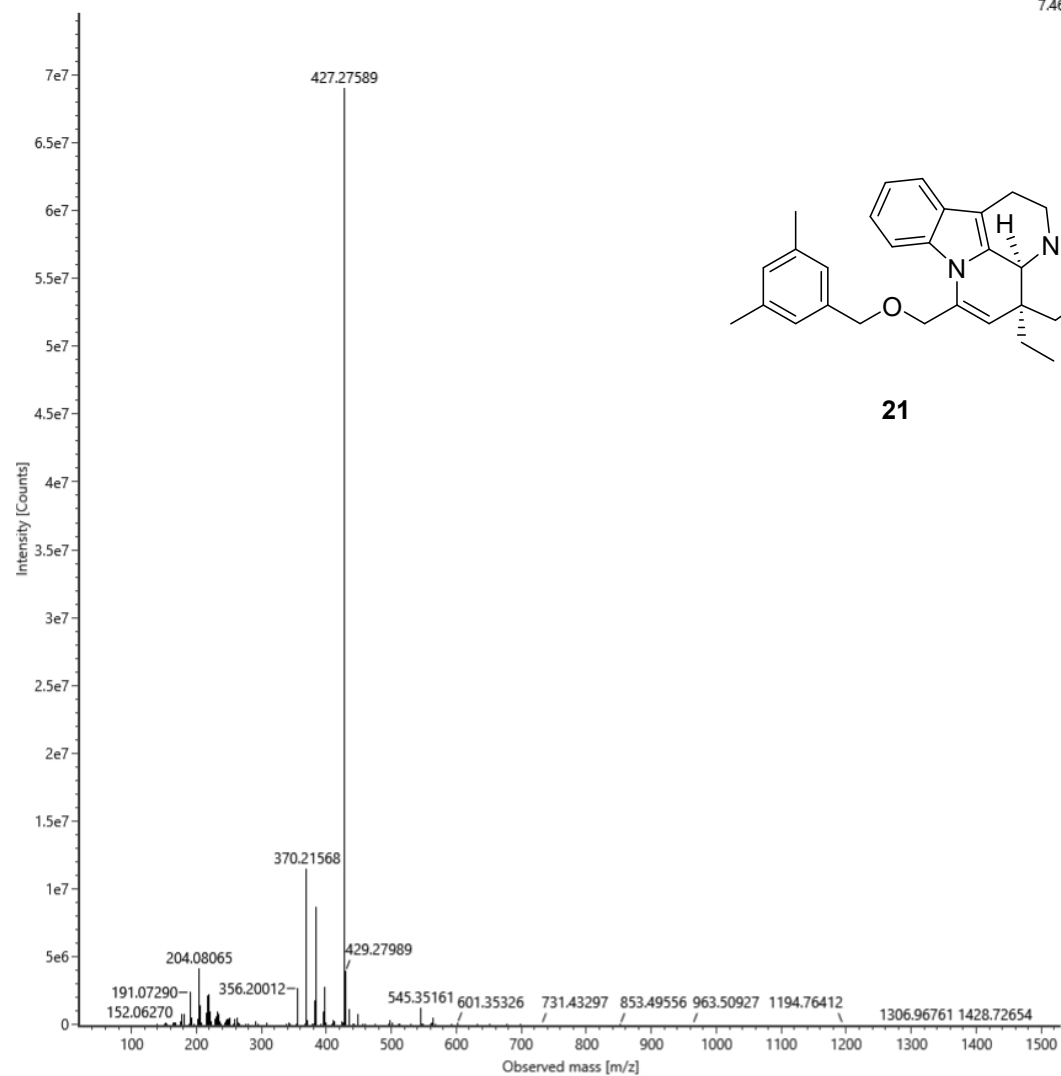


¹³C NMR of Compound **21** (100 MHz, CDCl₃)

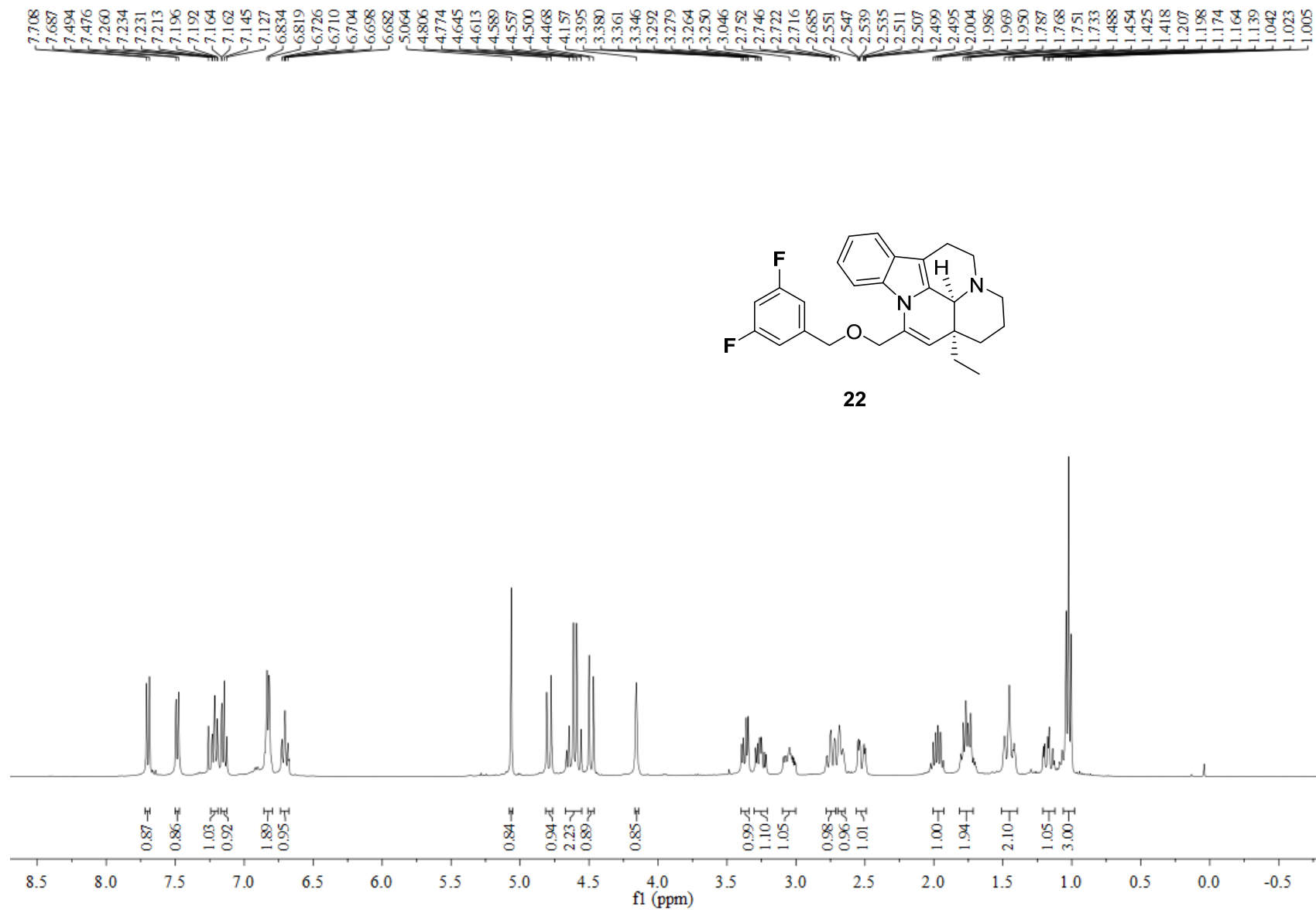
Item name: DB-60-19
Item description:

Channel name: 1: Average Time 0.0874 min : TOF MS (50-1500) ESI+ : Centroided : Combined

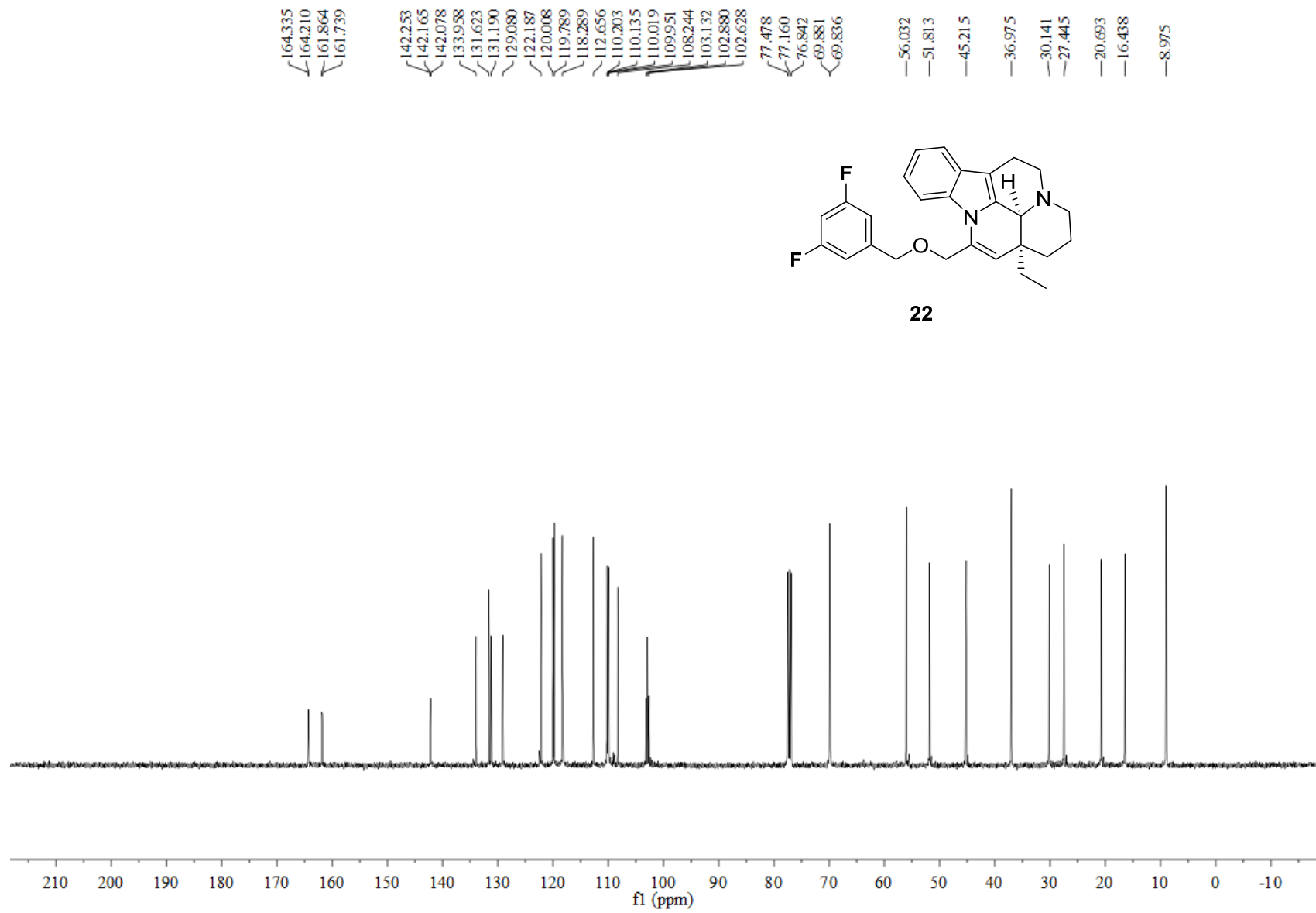
7.46e7



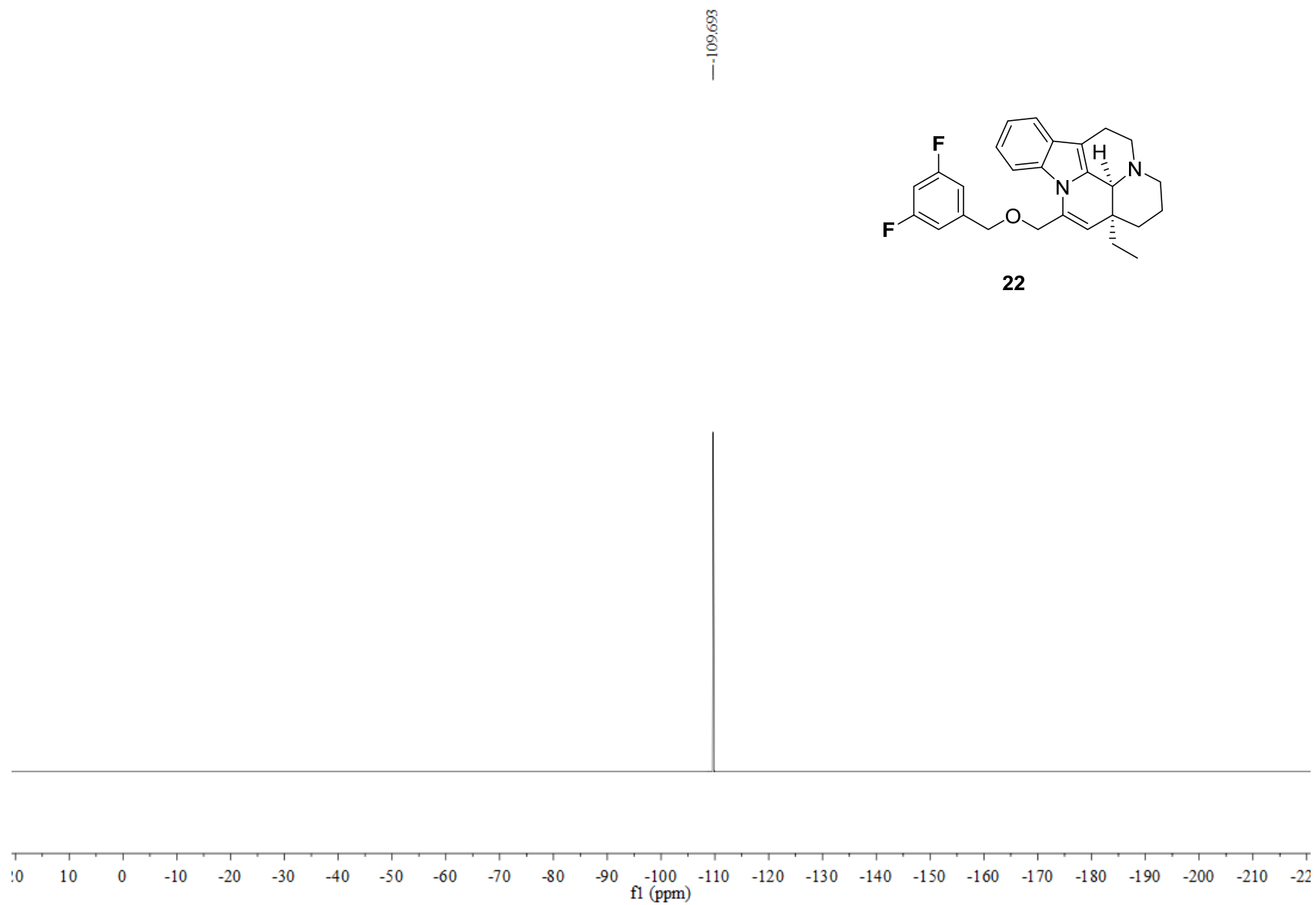
HRMS of Compound **21**



¹H NMR of Compound **22** (400 MHz, CDCl₃)

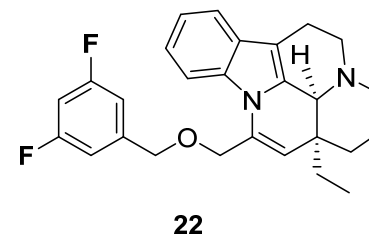
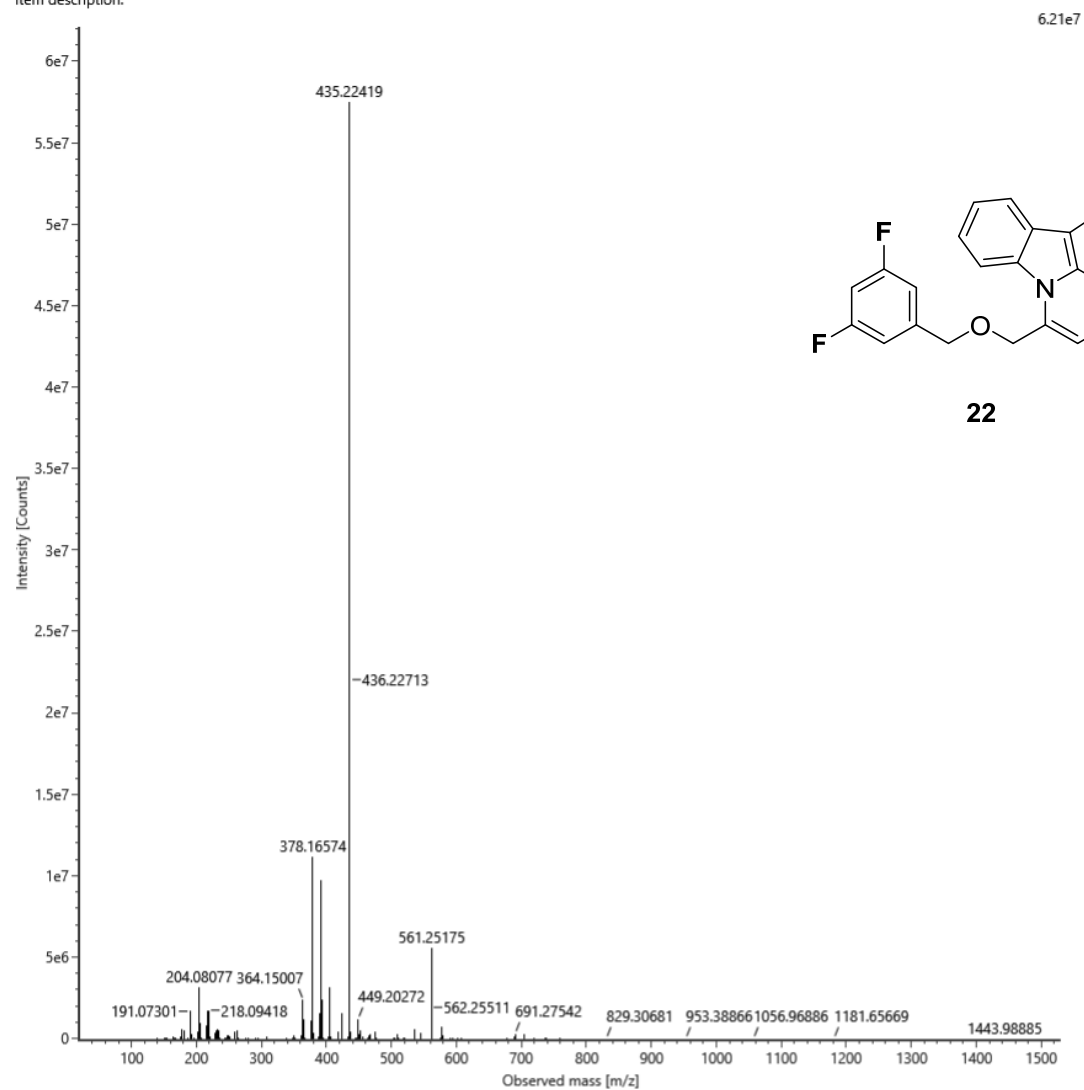


¹³C NMR of Compound **22** (100 MHz, CDCl₃)

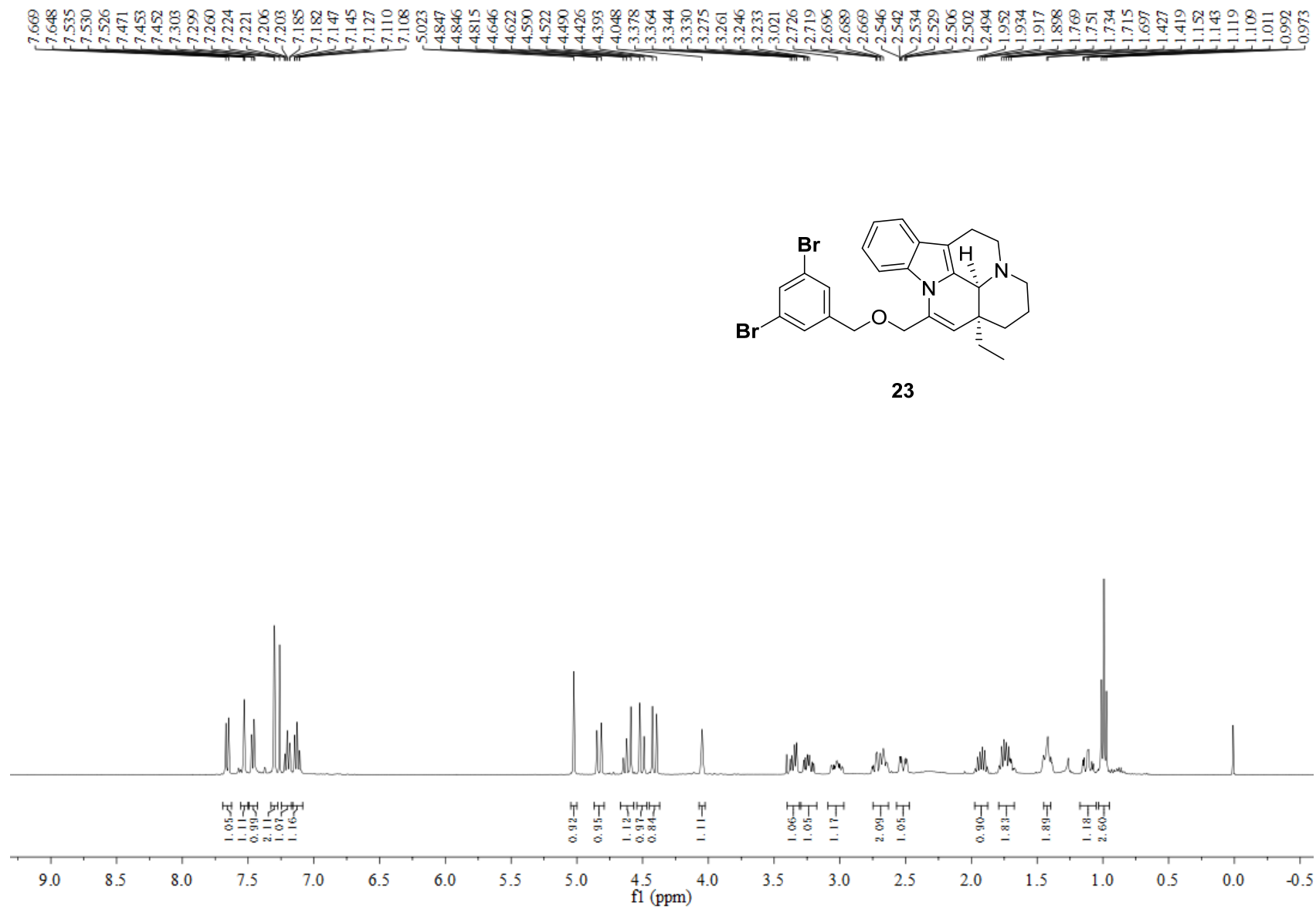


Item name: DB-60-18
Item description:

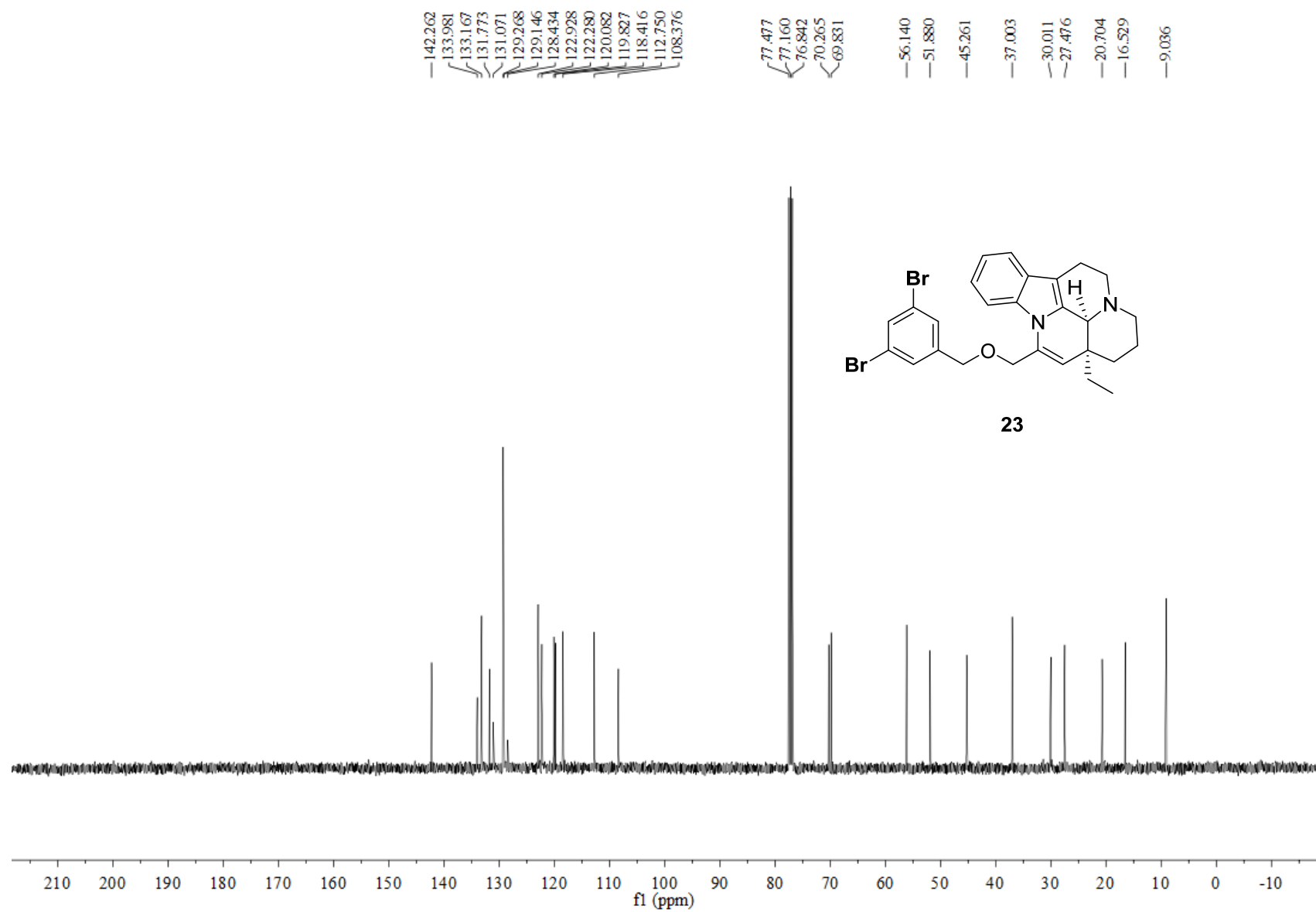
Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **22**



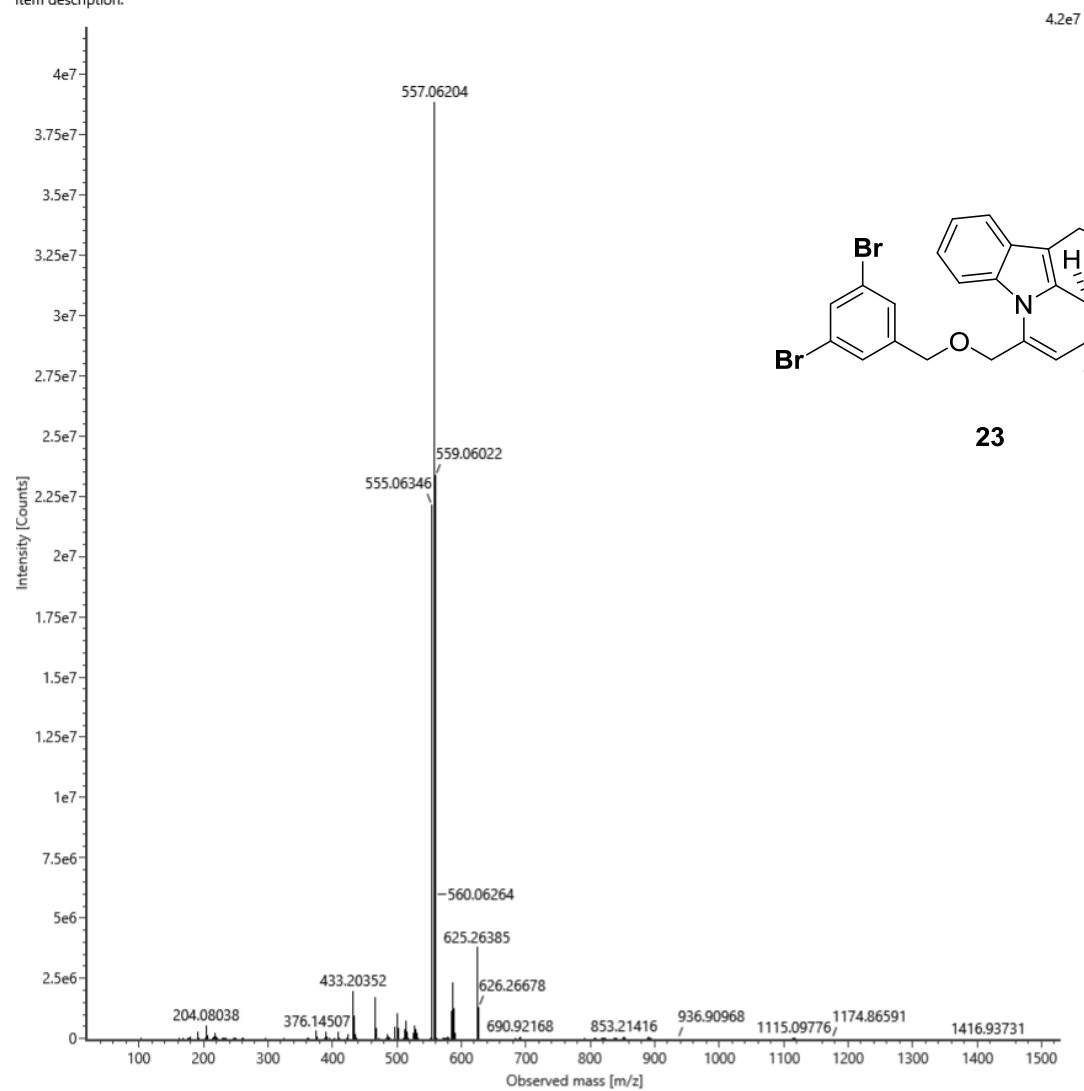
¹H NMR of Compound **23** (400 MHz, CDCl₃)



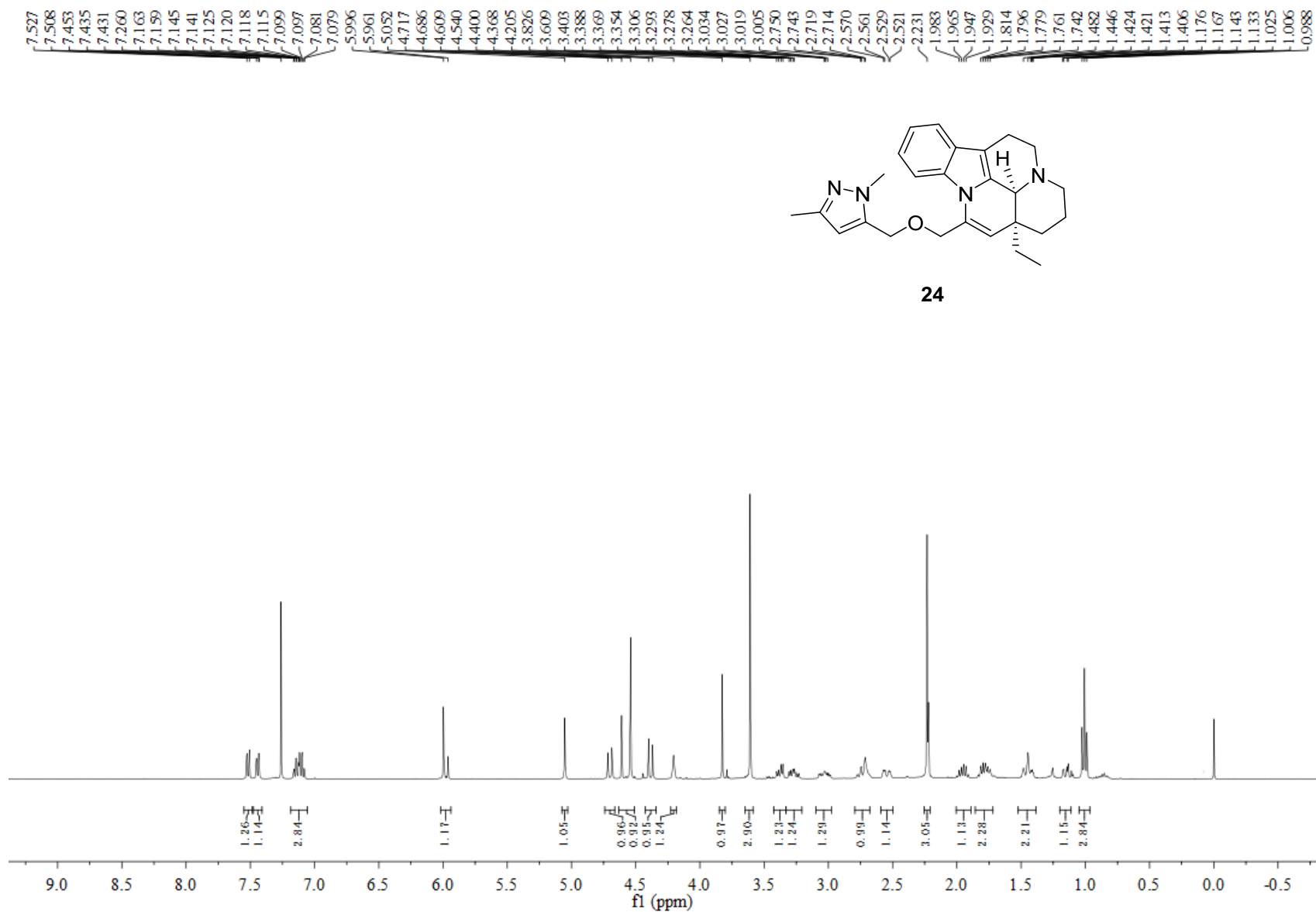
¹³C NMR of Compound **23** (100 MHz, CDCl₃)

Item name: DB-60-16
Item description:

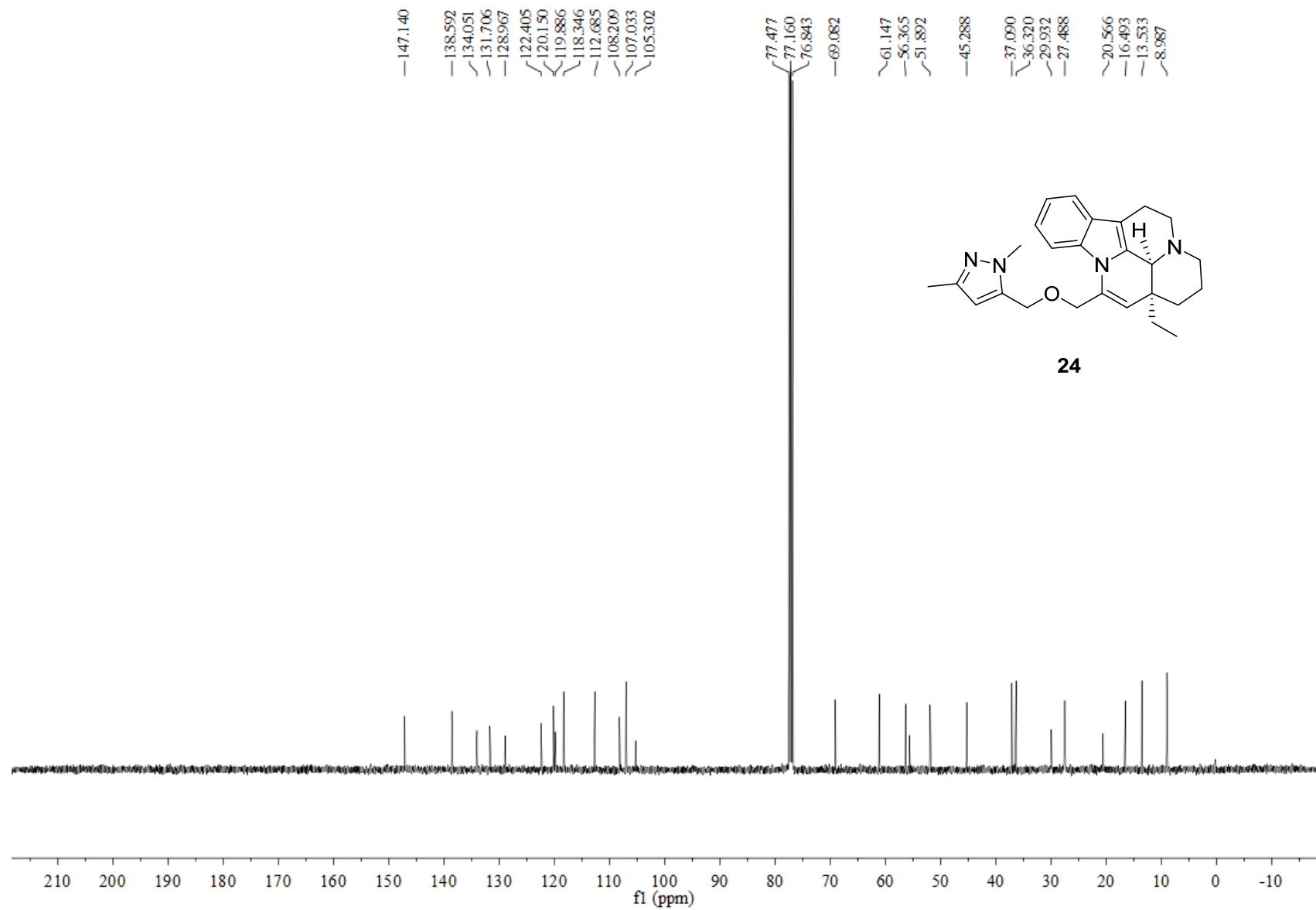
Channel name: 1: Average Time 0.0788 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **23**



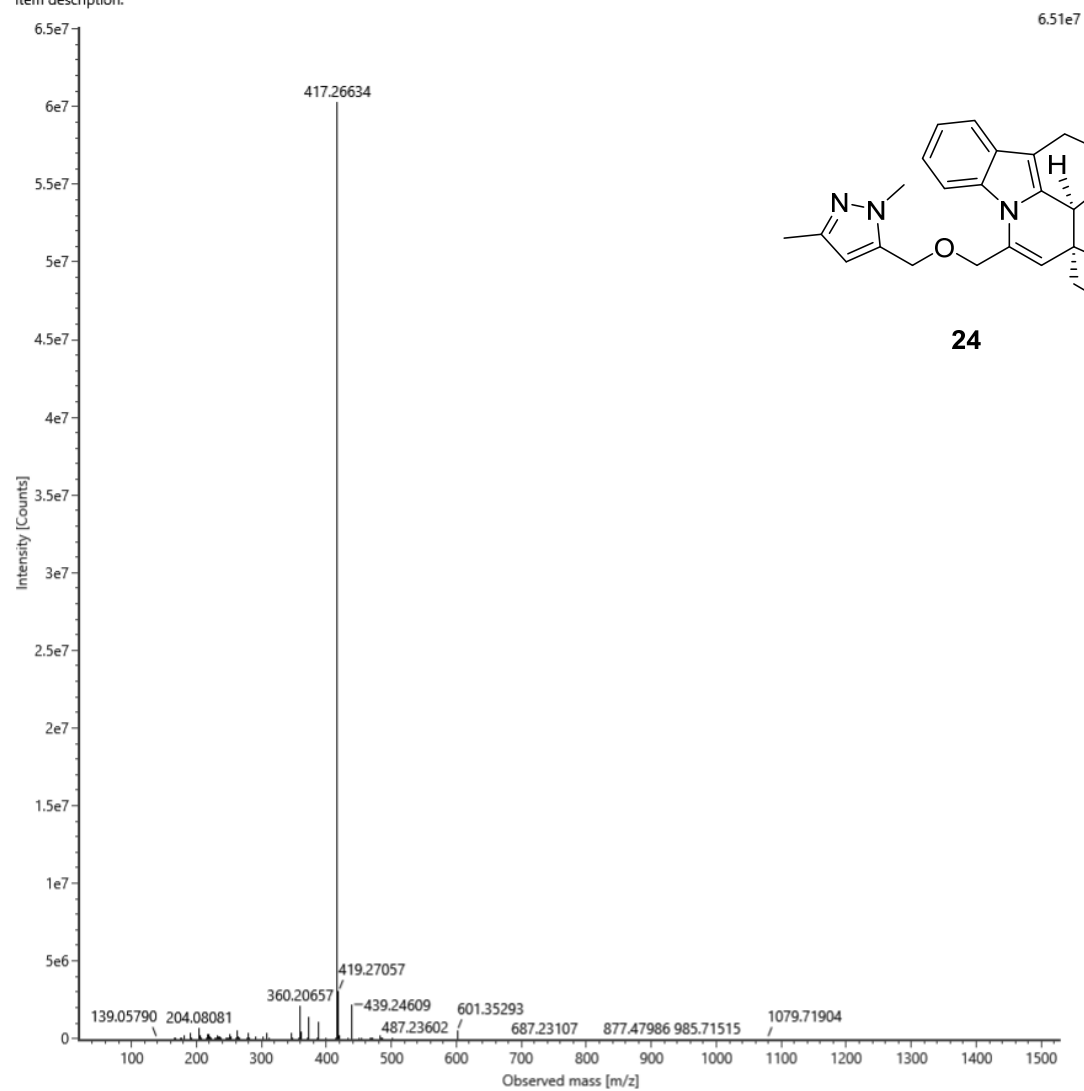
¹H NMR of Compound 24 (400 MHz, CDCl₃)



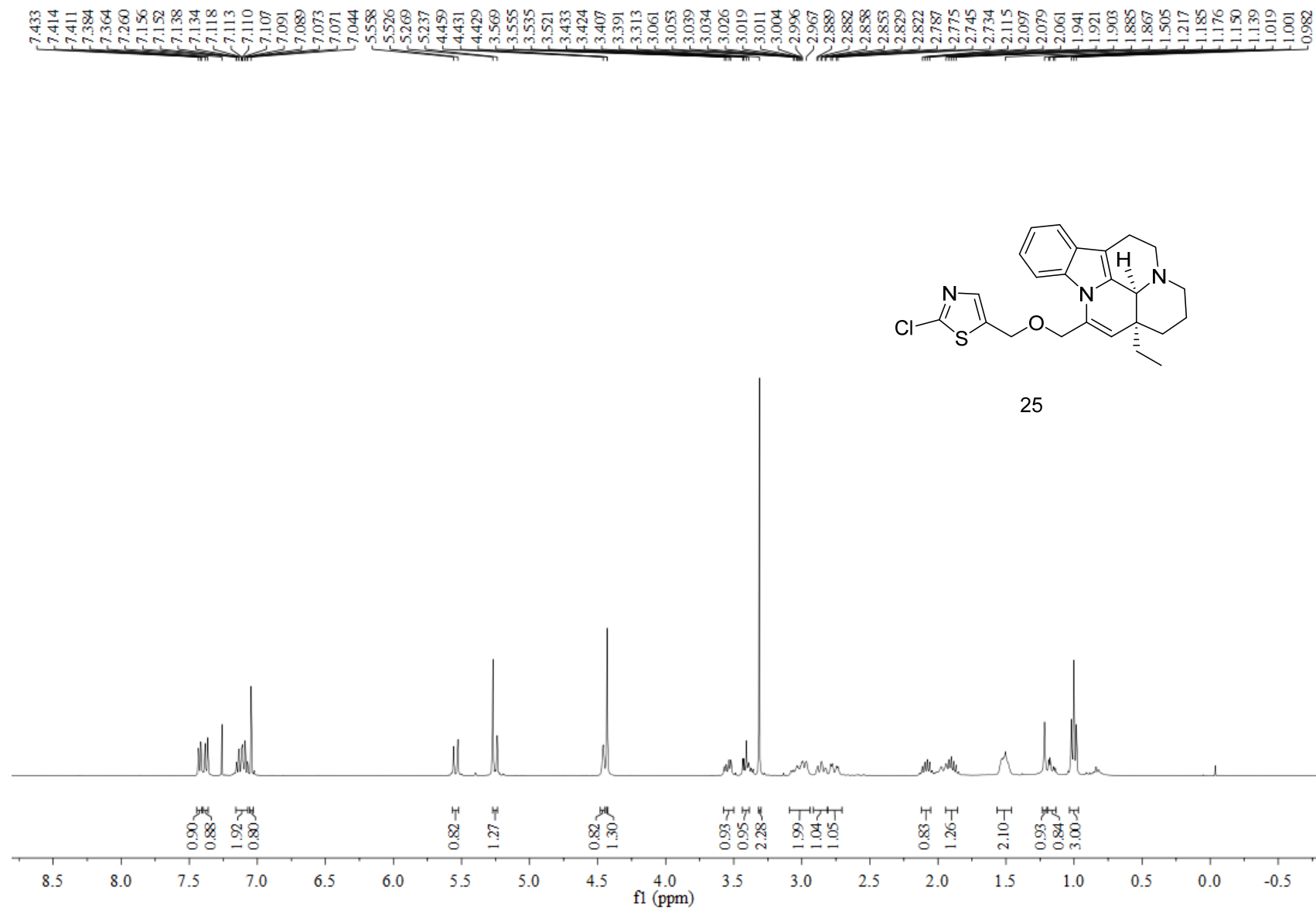
¹³C NMR of Compound **24** (100 MHz, CDCl₃)

Item name: DB-60-21
Item description:

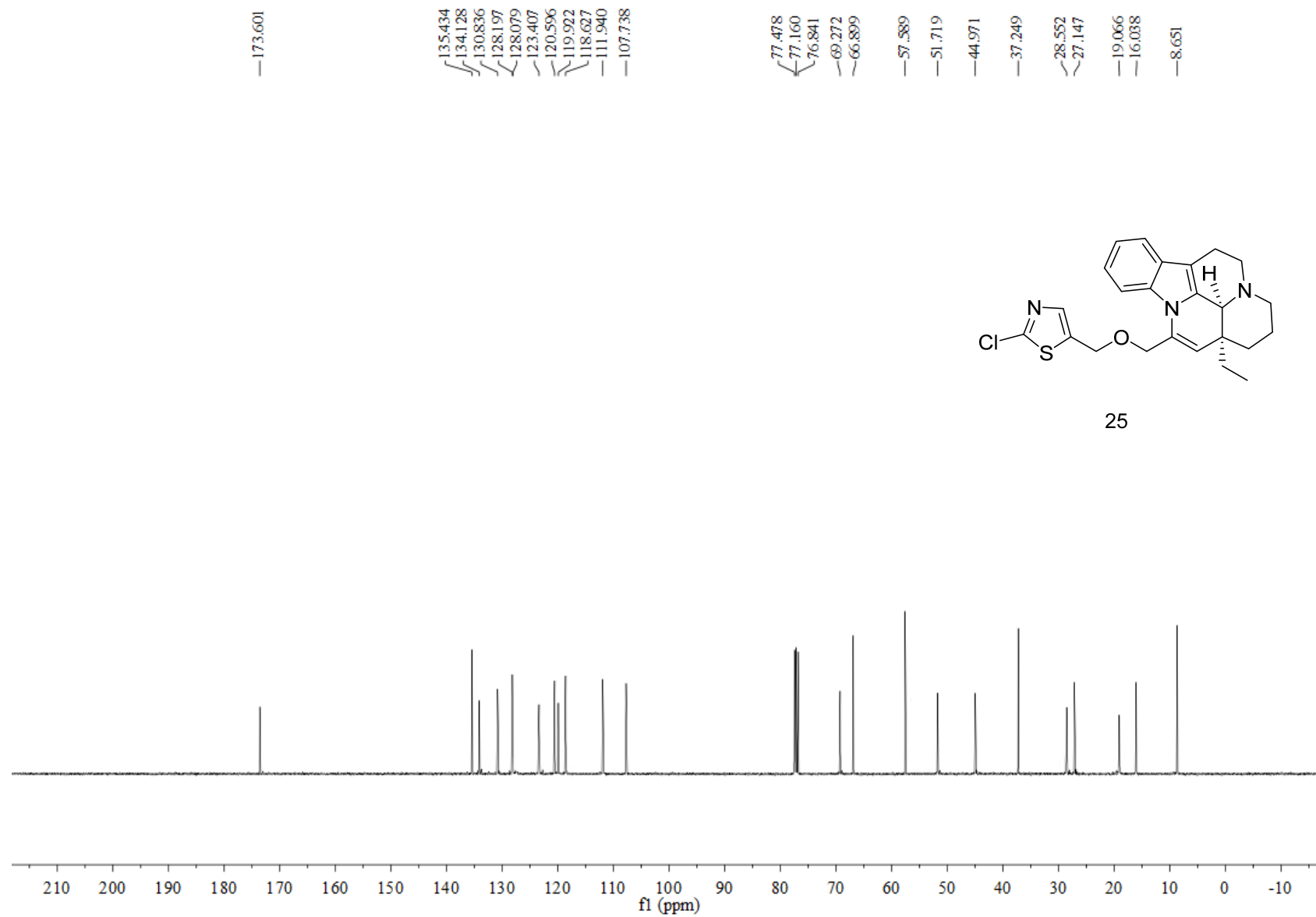
Channel name: 1: Average Time 0.0831 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **24**



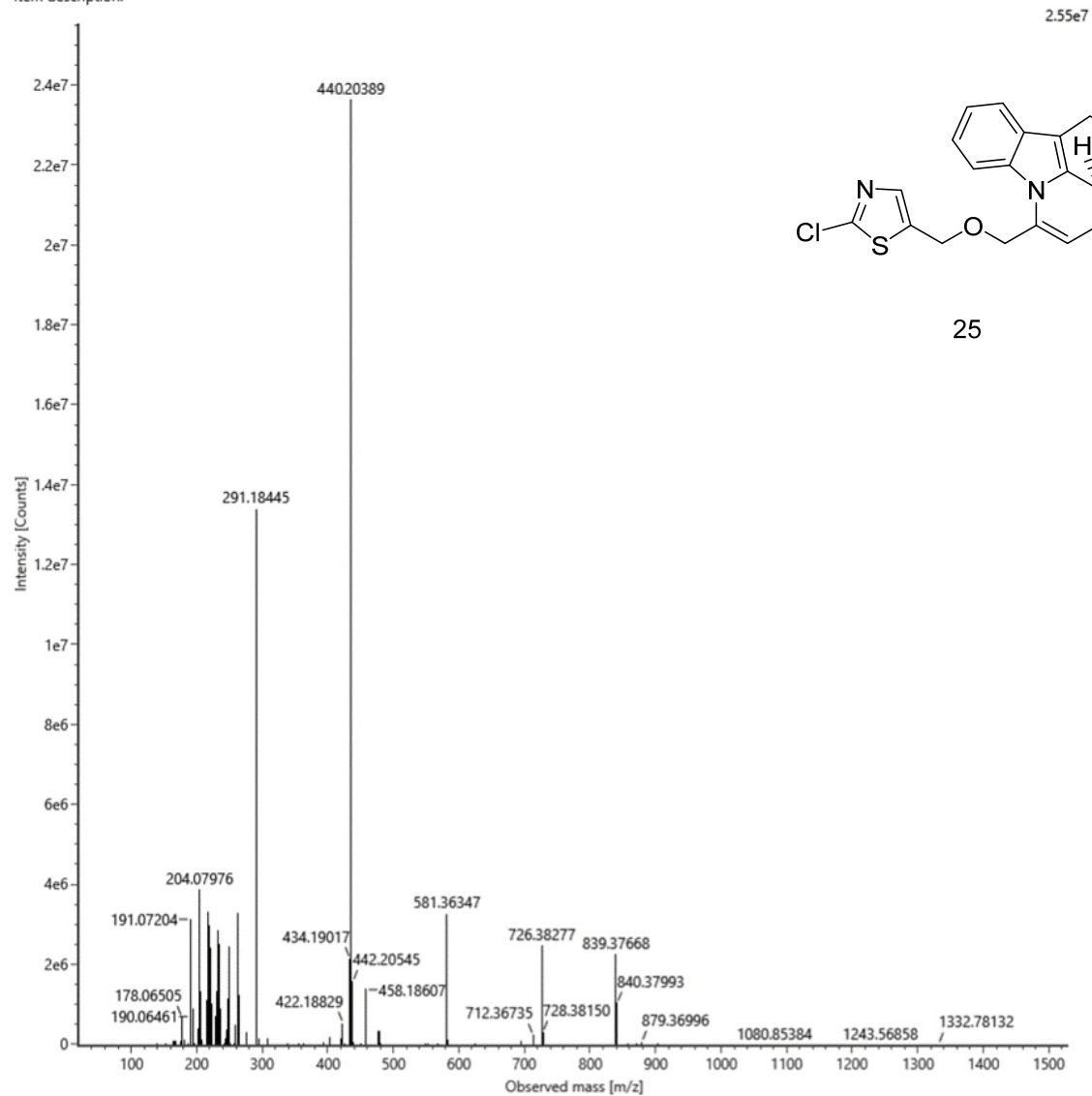
¹H NMR of Compound **25** (400 MHz, CDCl₃)



¹³C NMR of Compound **25** (100 MHz, CDCl₃)

Item name: DB-60-17-2
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound 25