

## SUPPORTING INFORMATION

### Synthesis of Diverse Annelated Pyridines with 6-Membered Functionalized Saturated Cycles for MedChem Investigations

Dmytro V. Yehorov,<sup>1,2</sup> Andrii I. Subota<sup>\*1,2</sup>

<sup>1</sup> *Institute of Organic Chemistry, National Academy of Sciences of Ukraine, 5 Akademik Kuhar str., 02660 Kyiv, Ukraine*

<sup>2</sup> *Enamine Ltd, 78 Winston Churchill str., 02094 Kyiv, Ukraine*

Corresponding Author E-mail: [andrii.subota@gmail.com](mailto:andrii.subota@gmail.com)

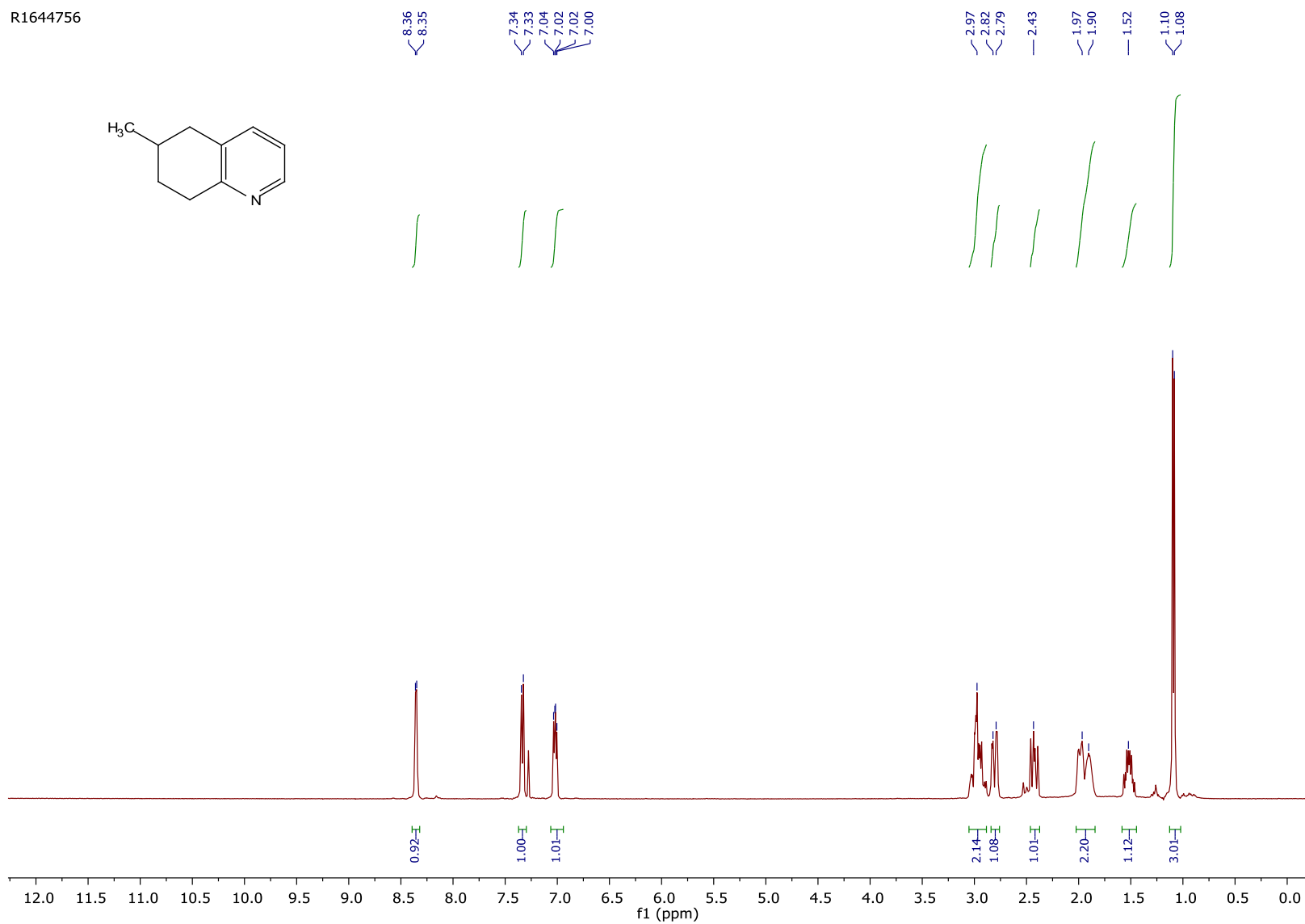
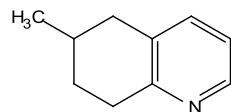
#### Table of Contents

<sup>1</sup> H and LCMS spectra of <b>2</b> .....	2
<sup>1</sup> H and LCMS spectra of <b>3</b> .....	4
<sup>1</sup> H, <sup>19</sup> F and LCMS spectra of <b>4</b> .....	6
<sup>1</sup> H and LCMS spectra of <b>5</b> .....	9
<sup>1</sup> H and LCMS spectra of <b>6b</b> .....	11
<sup>1</sup> H and LCMS spectra of <b>7a·HCl</b> .....	13
<sup>1</sup> H and LCMS spectra of <b>9c·2HCl</b> .....	15
<sup>1</sup> H and LCMS spectra of <b>9d</b> .....	17
<sup>1</sup> H and LCMS spectra of <b>10c</b> .....	19

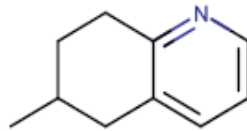
<sup>1</sup> H and LCMS spectra of <b>21</b> .....	21
<sup>1</sup> H and LCMS spectra of <b>22</b> .....	23
<sup>1</sup> H and LCMS spectra of <b>24</b> .....	25

# <sup>1</sup>H and LCMS spectra of **2**

R1644756



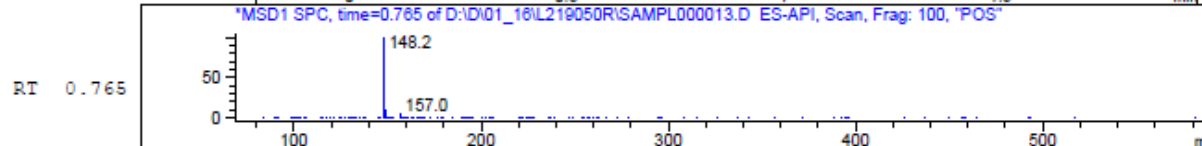
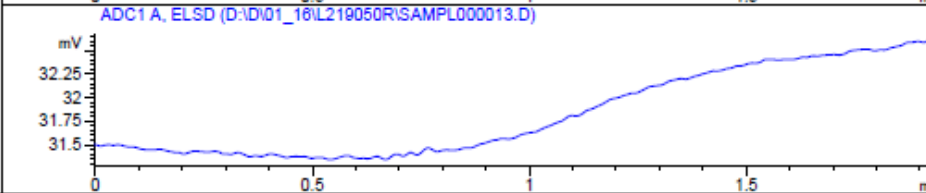
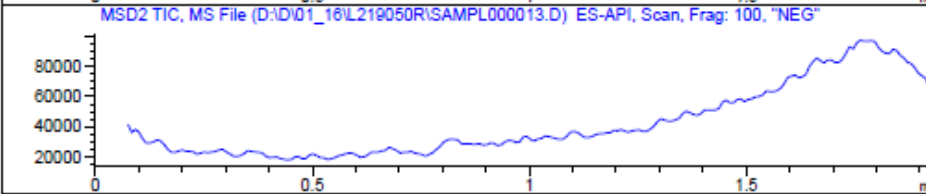
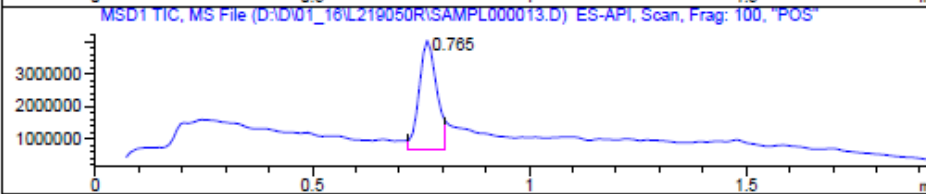
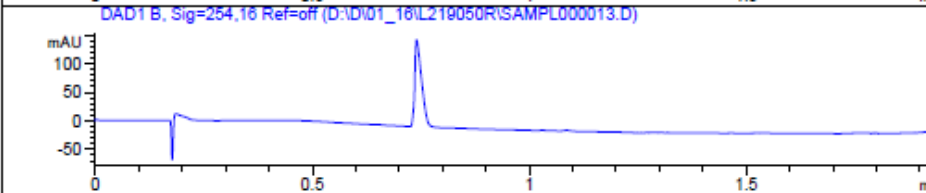
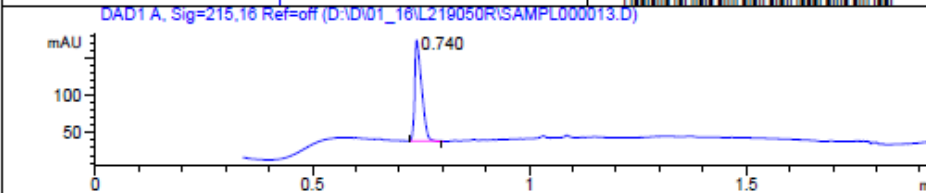
MaxPeak: 100.00%  
Ret\_Time: 0.740 min



Mol Wt 147.22  
Exact Mass 147.13

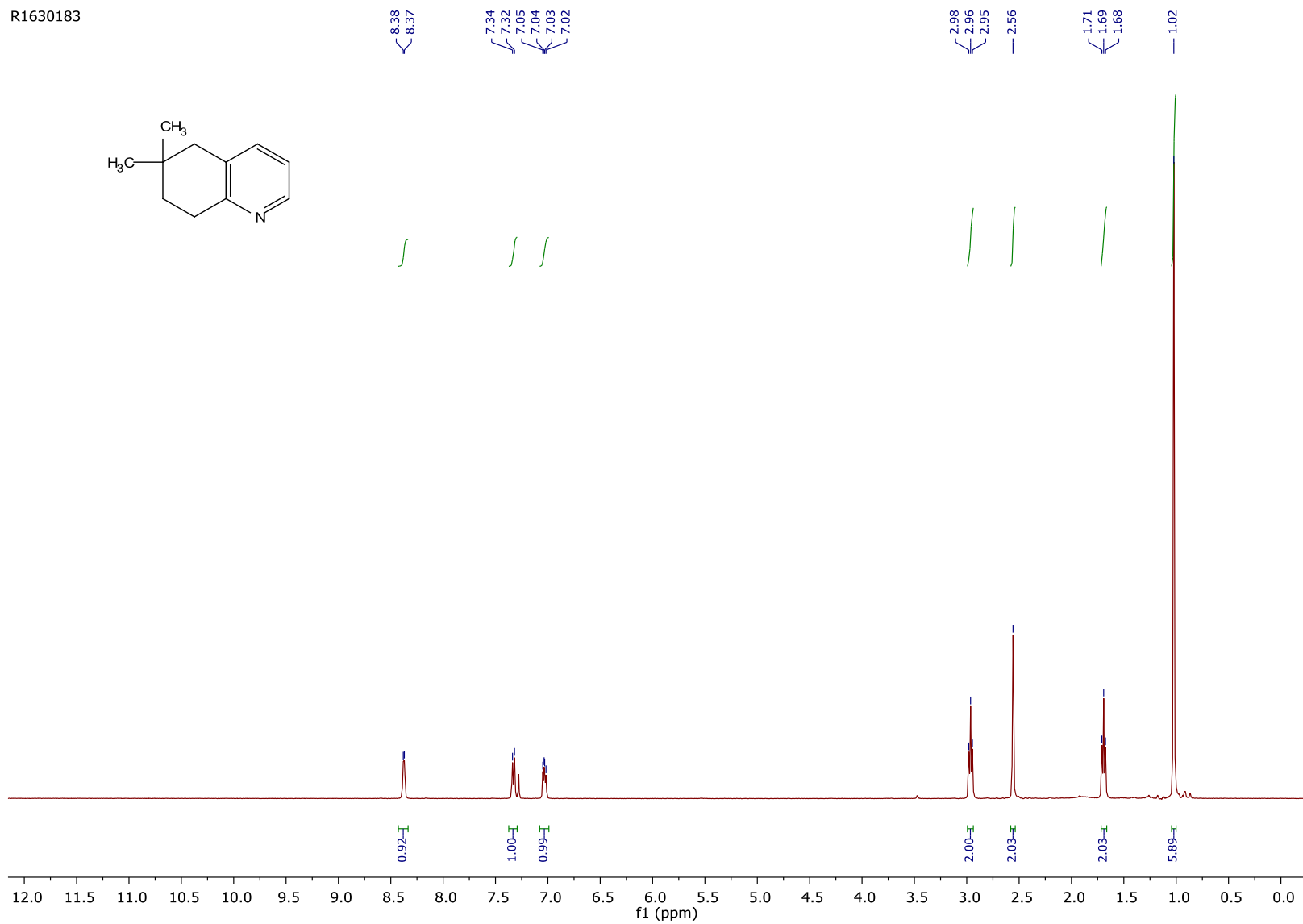
#	Time	Area%
1	0.740	100.00

R1644756

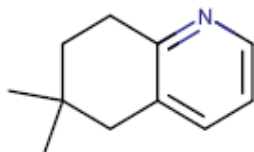


# <sup>1</sup>H and LCMS spectra of **3**

R1630183



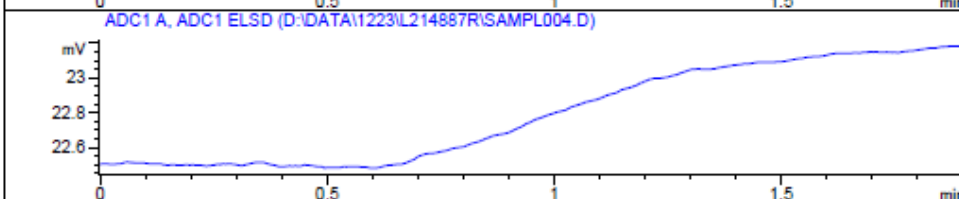
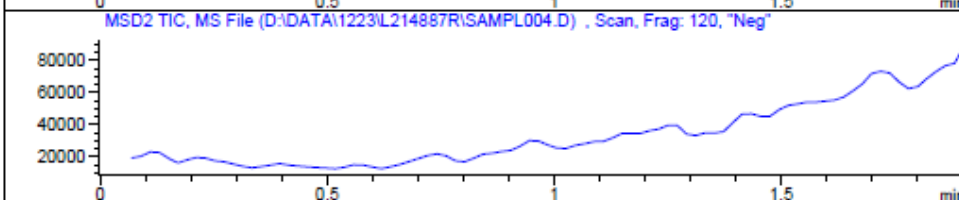
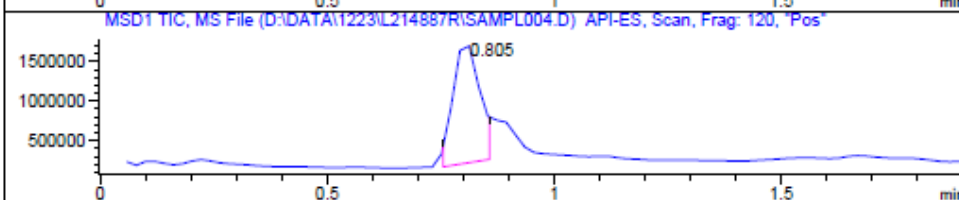
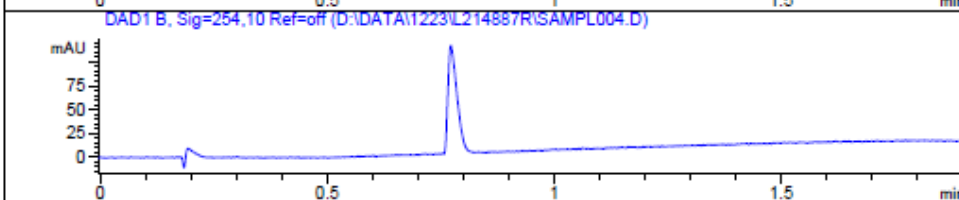
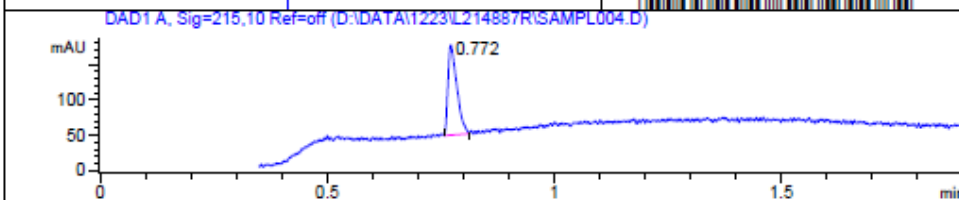
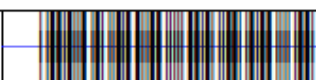
MaxPeak: 100.00%  
Ret\_Time: 0.772 min



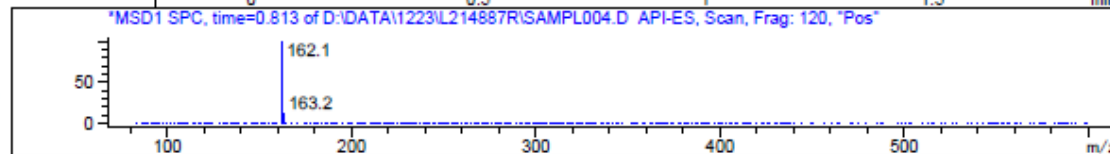
Mol Wt 161.24  
Exact Mass 161.15

#	Time	Area%
1	0.772	100.00

R1630183

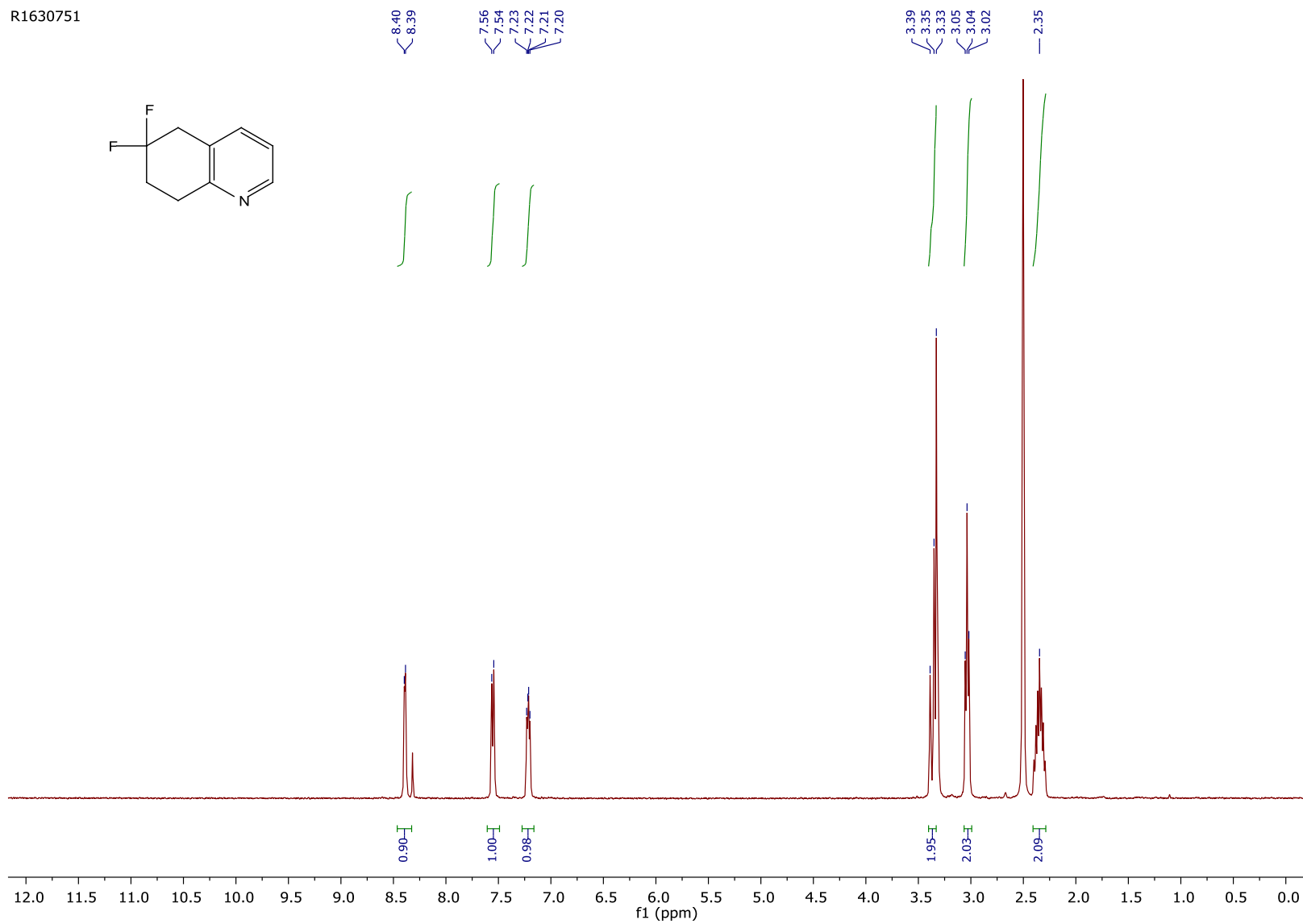


RT 0.805

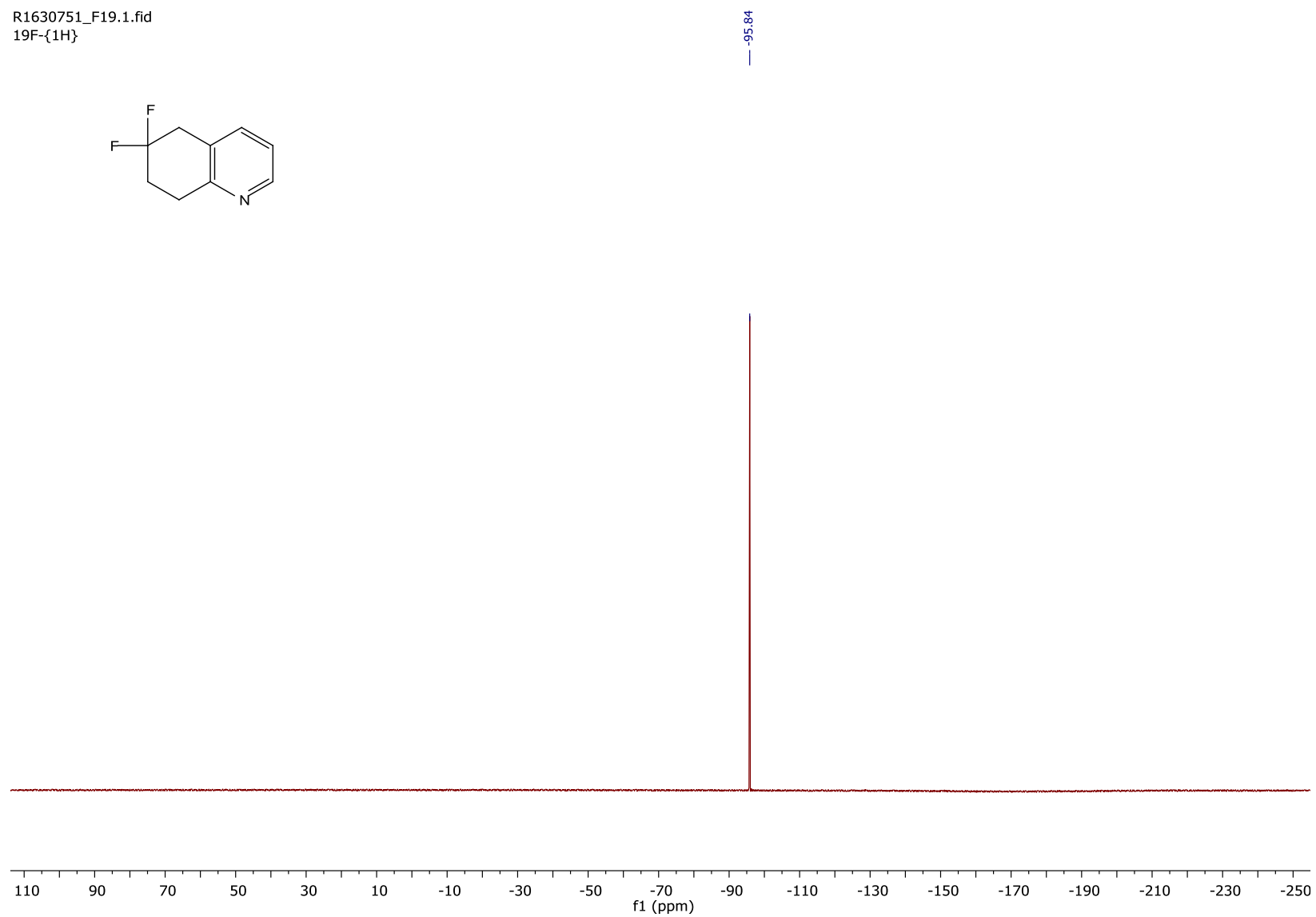
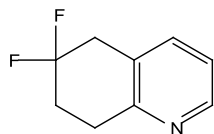


# $^1\text{H}$ , $^{19}\text{F}$ and LCMS spectra of **4**

R1630751

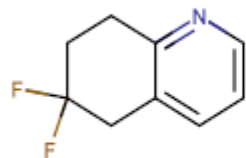


R1630751\_F19.1.fid  
19F-{1H}





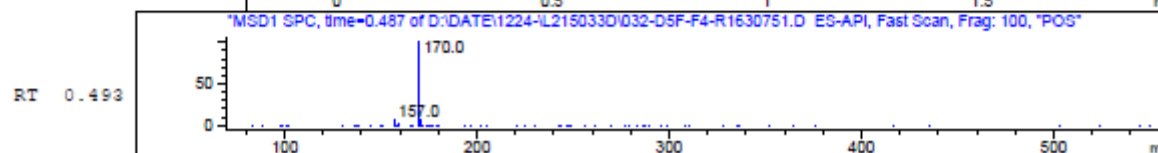
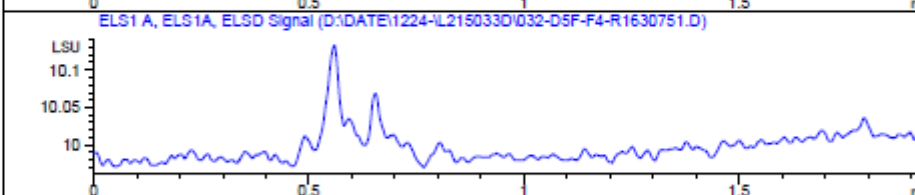
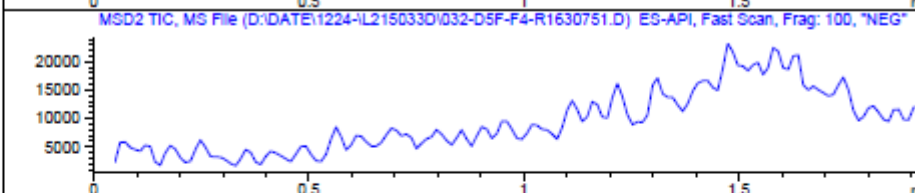
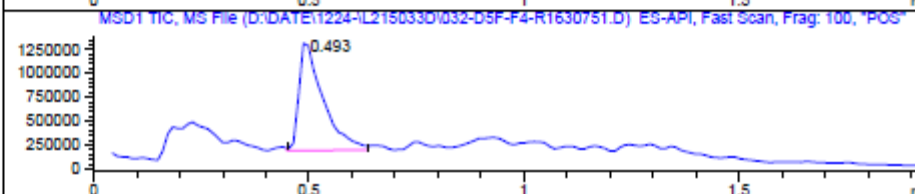
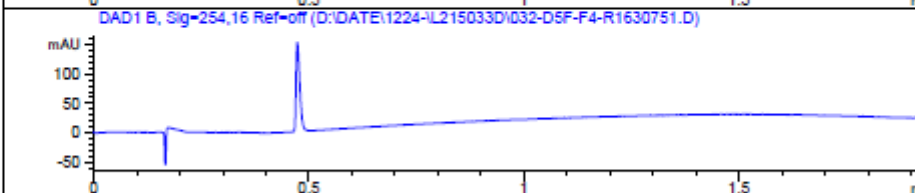
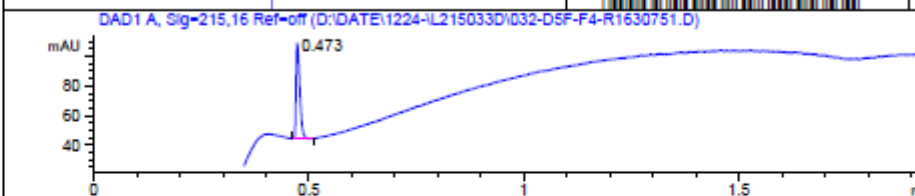
MaxPeak: 100.00%  
Ret\_Time: 0.473 min



Mol Wt 169.17  
Exact Mass 169.09

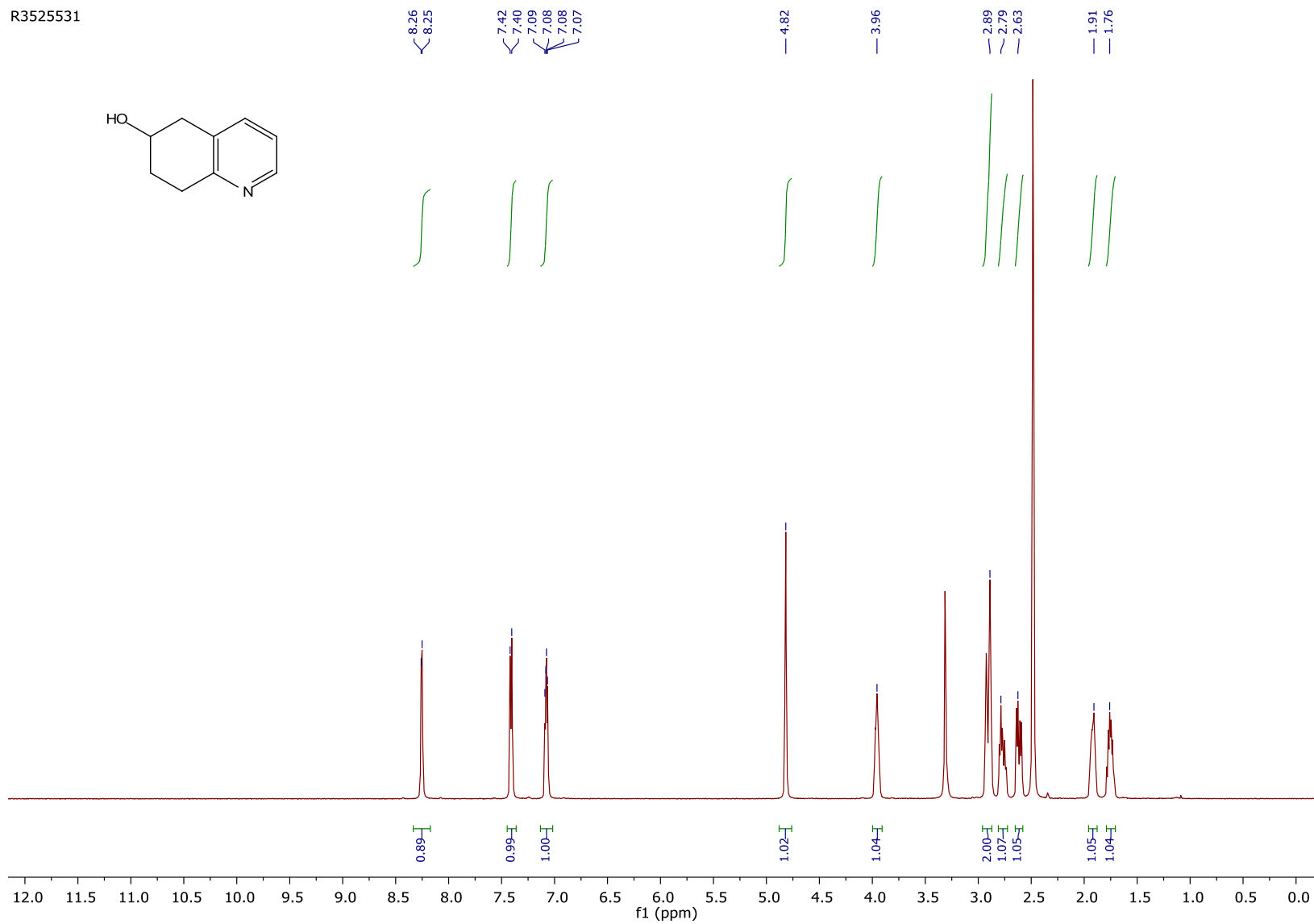
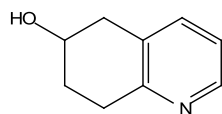
#	Time	Area%
1	0.473	100.00

R1630751

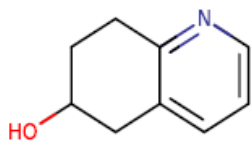


# <sup>1</sup>H and LCMS spectra of **5**

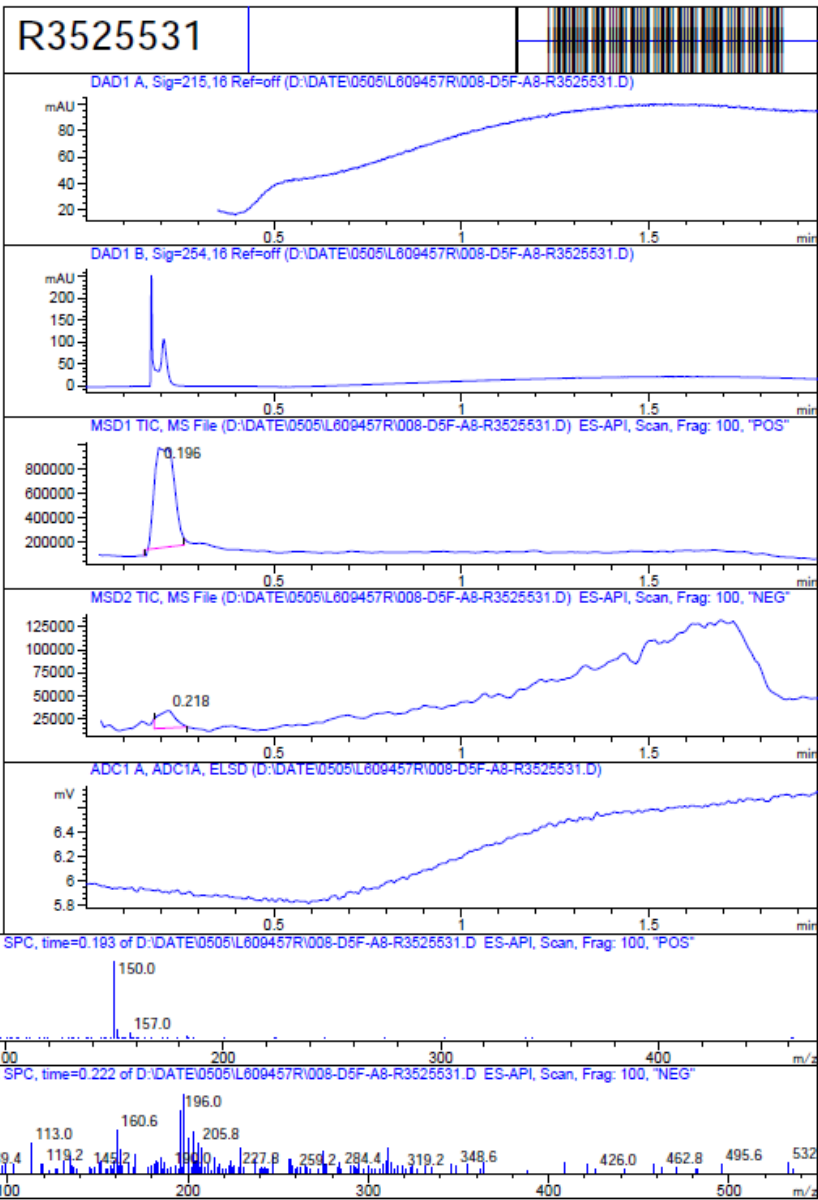
R3525531



Error: Peaks not found!

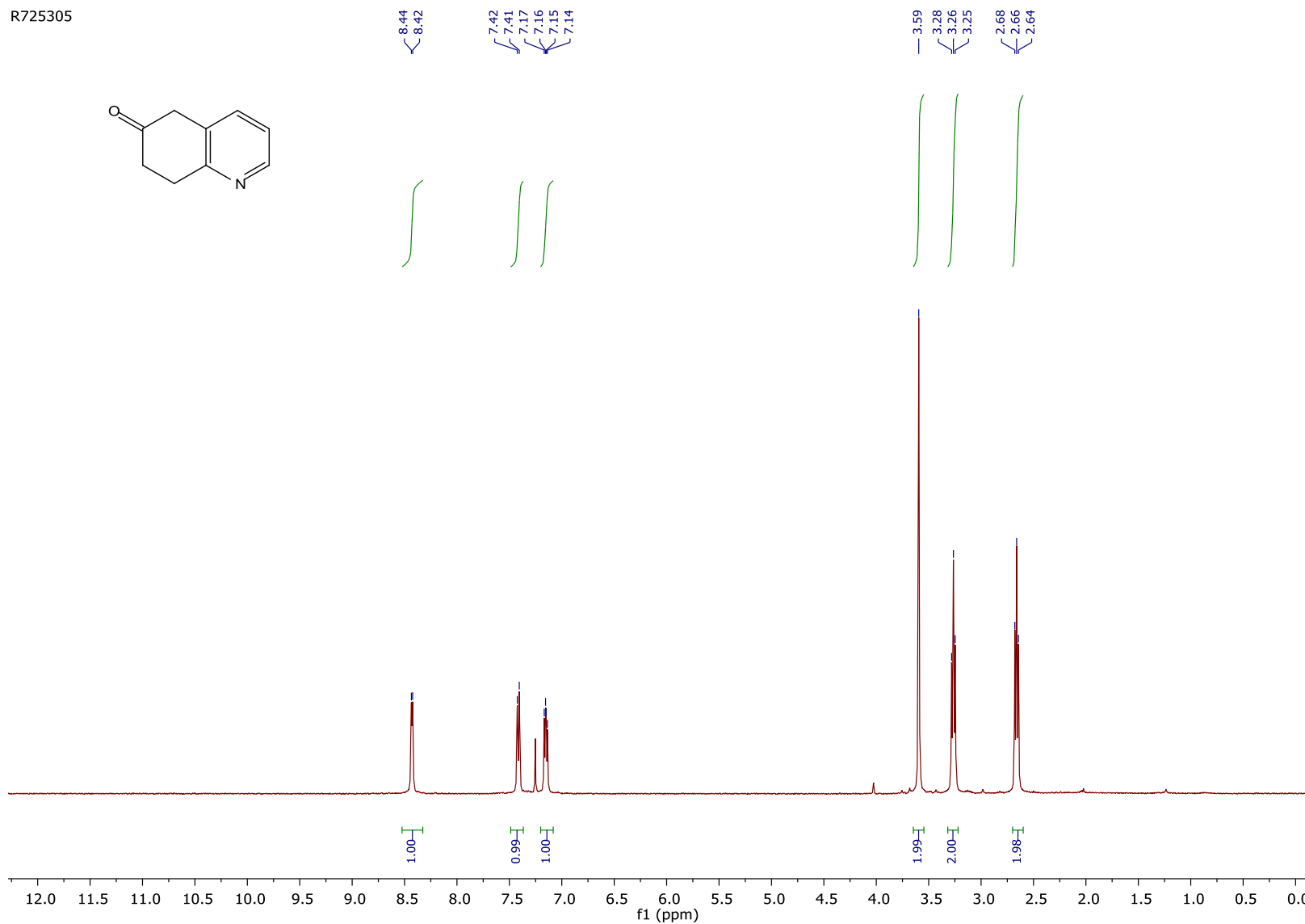


Mol Wt 149.19  
Exact Mass 149.1  
Error: Peaks not found!

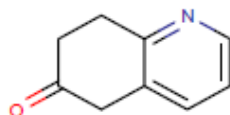


# <sup>1</sup>H and LCMS spectra of **6b**

R725305



Error: Peaks not found!

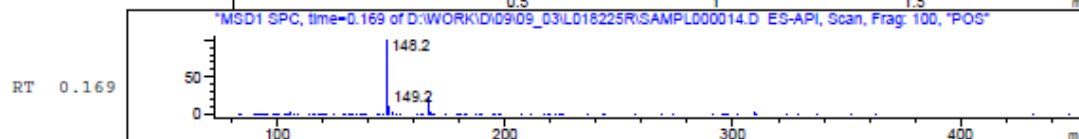
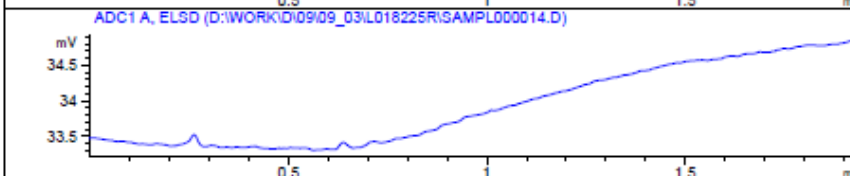
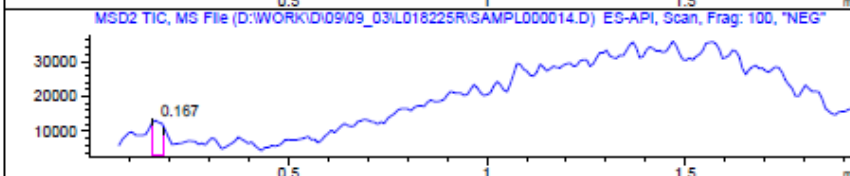
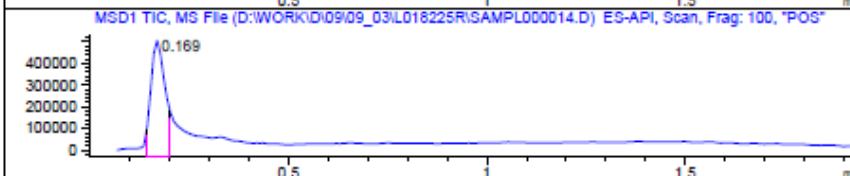
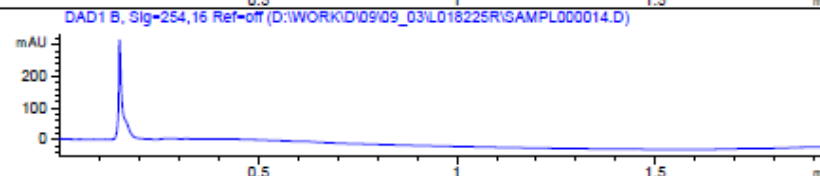
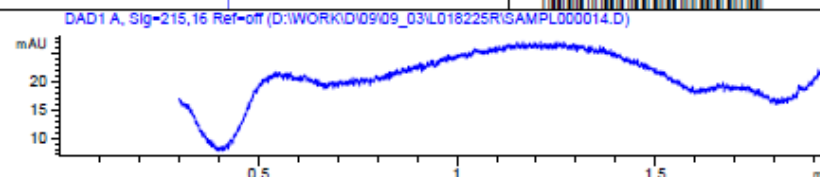


Mol Wt 147.17

Exact Mass 147.08

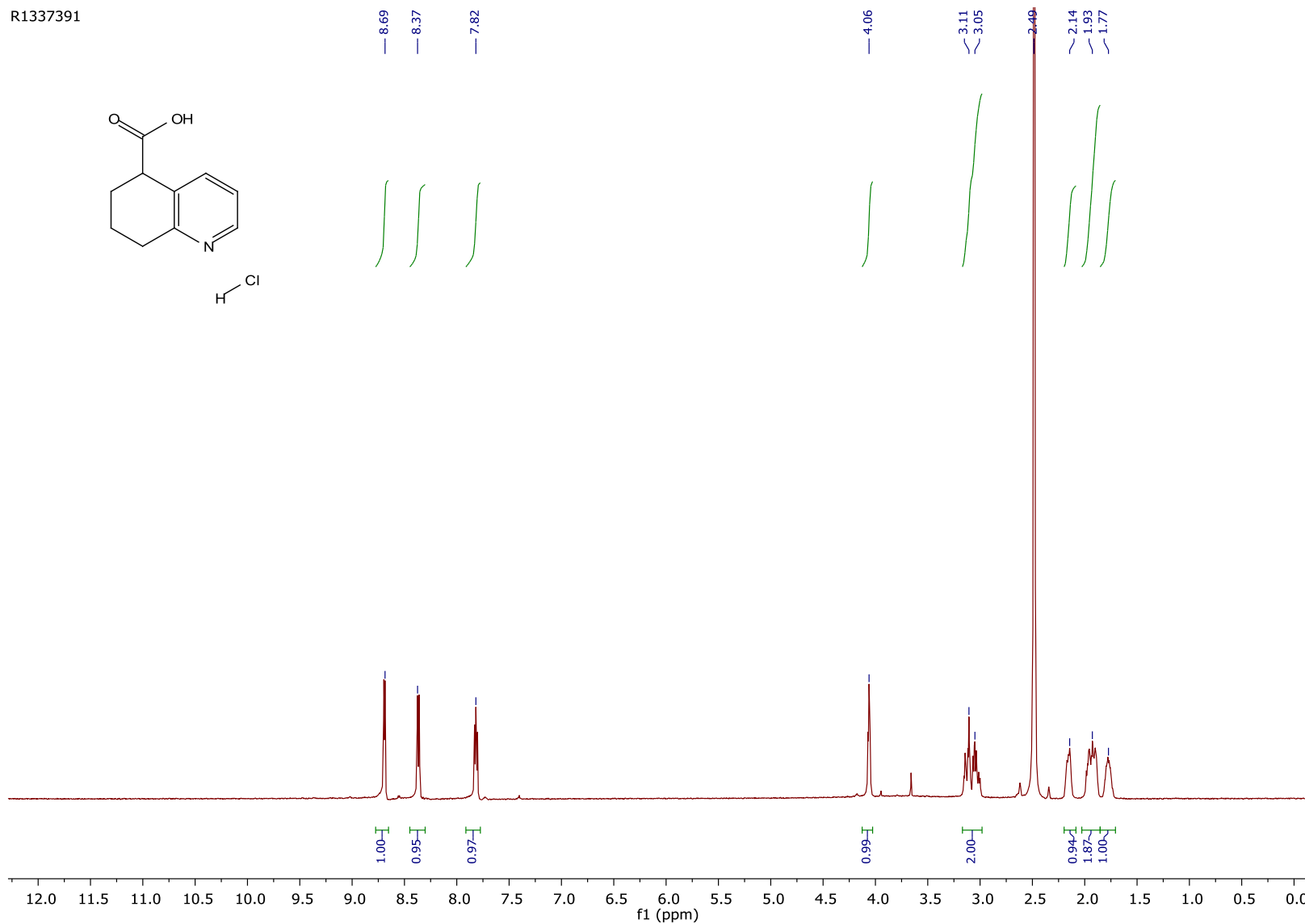
Error: Peaks not found!

R725305



# $^1\text{H}$ and LCMS spectra of **7a**·HCl

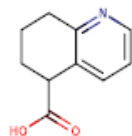
R1337391



R1337391



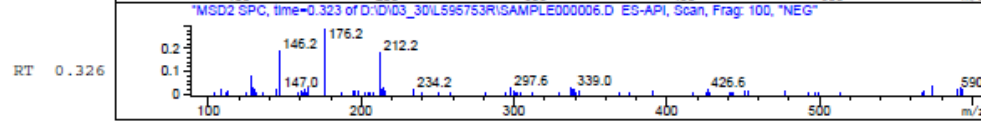
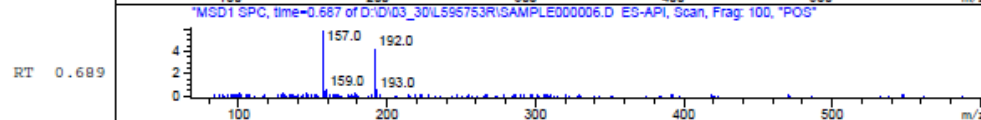
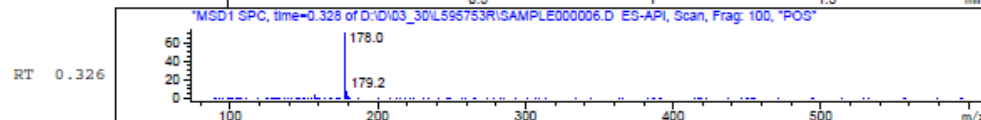
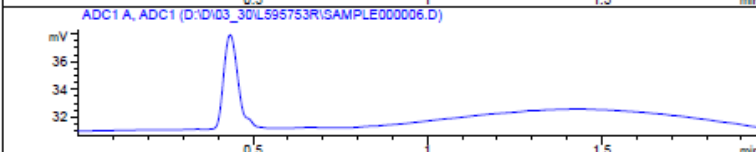
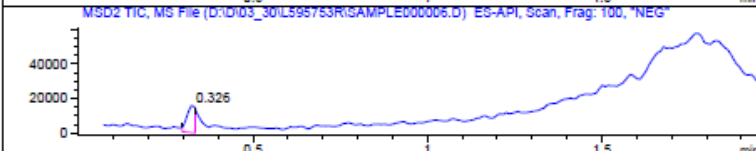
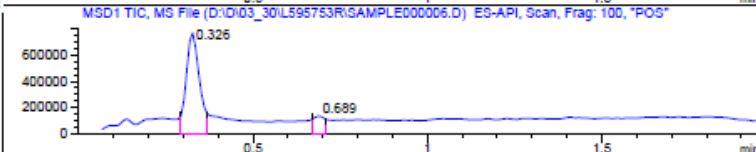
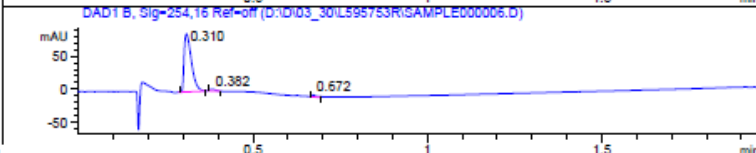
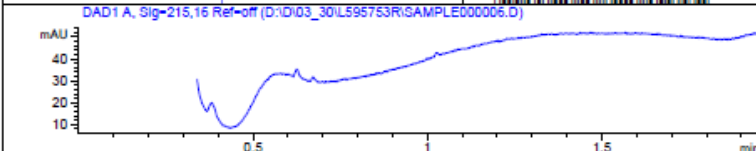
HCl



Mol Wt 213.66  
Exact Mass 177.09

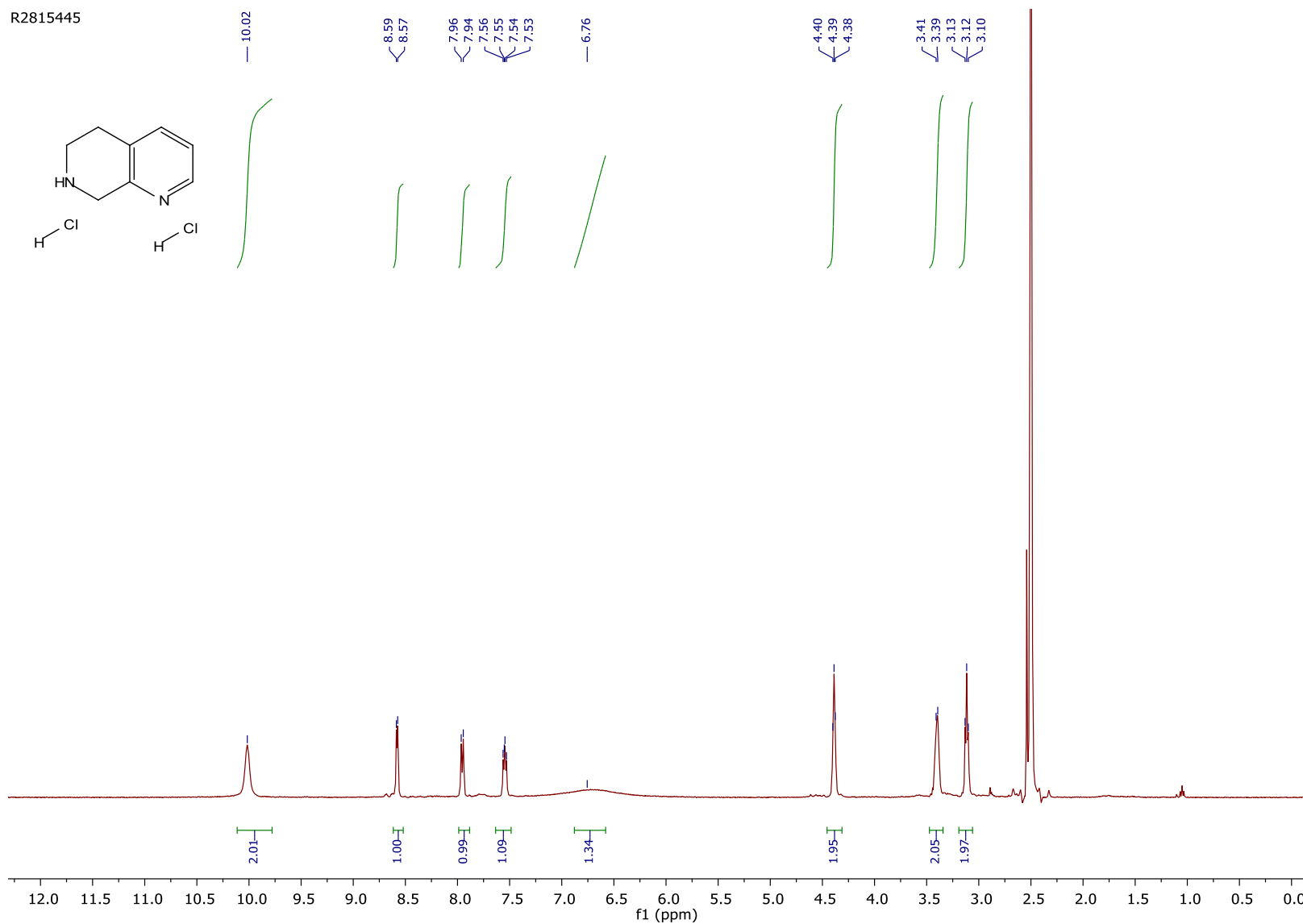
Error: Peaks not found!

#	Time	Area%
---	DAD1 B	---
1	0.310	95.68
2	0.382	2.16
3	0.672	2.16



# $^1\text{H}$ and LCMS spectra of **9c**·2HCl

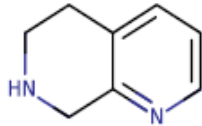
R2815445



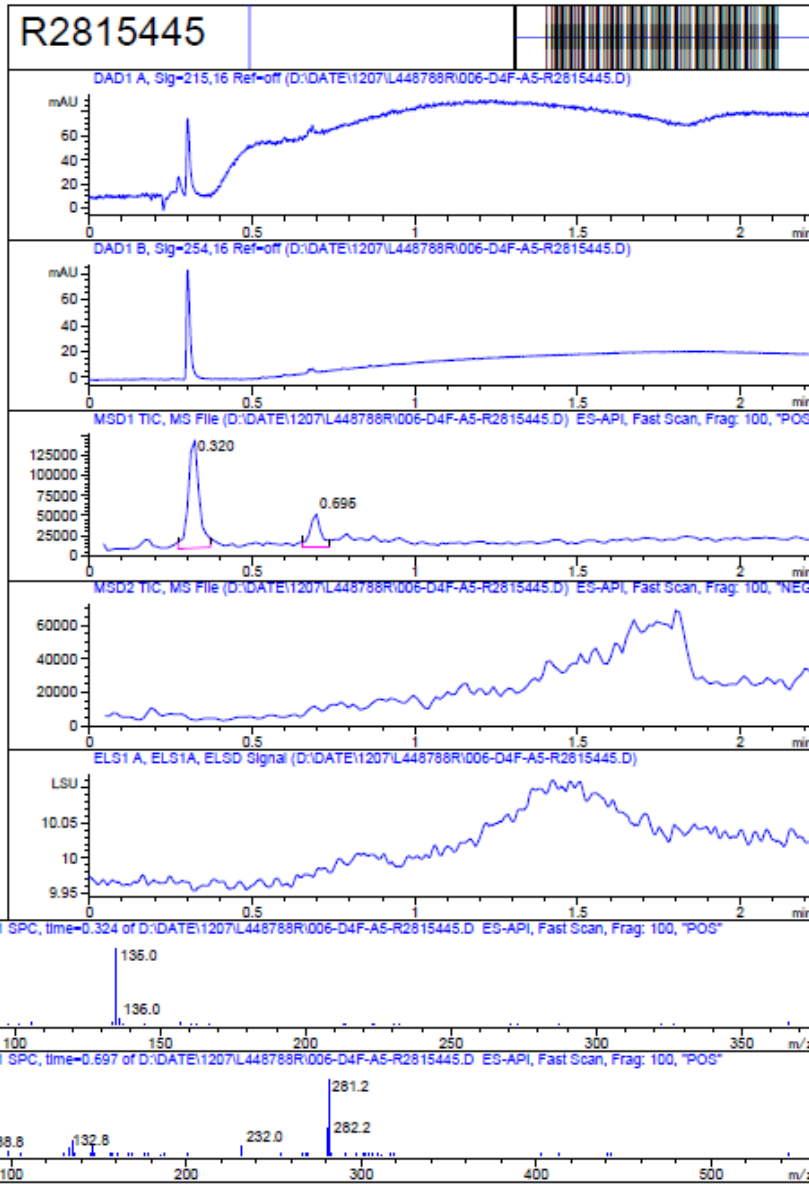


Error: Peaks not found!

HCl HCl

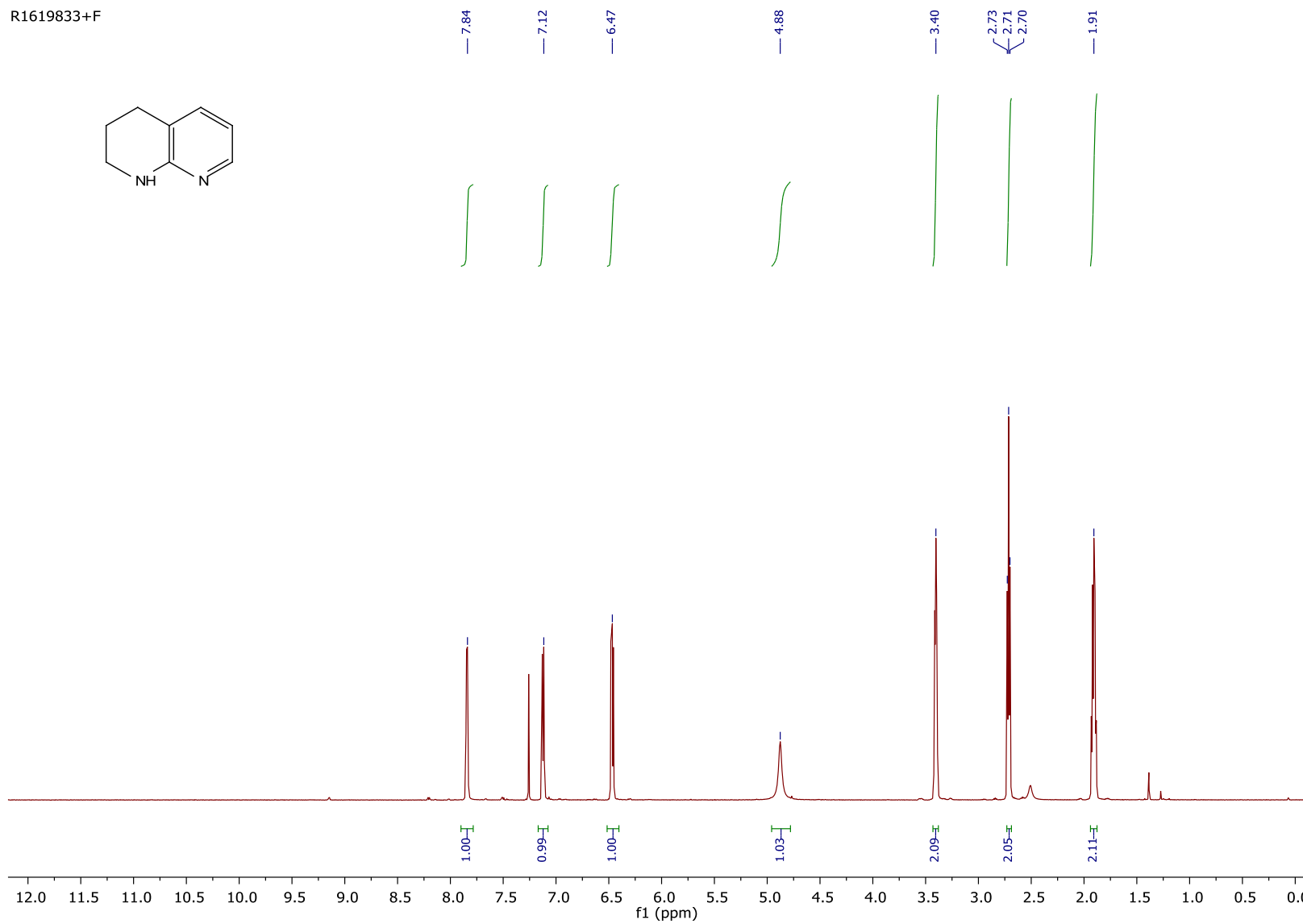
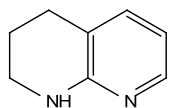


Mol Wt 207.1  
Exact Mass 134.1  
Error: Peaks not found!

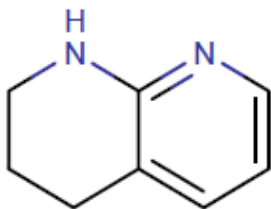


# <sup>1</sup>H and LCMS spectra of **9d**

R1619833+F



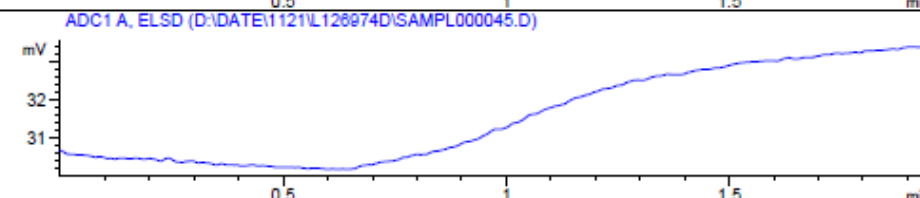
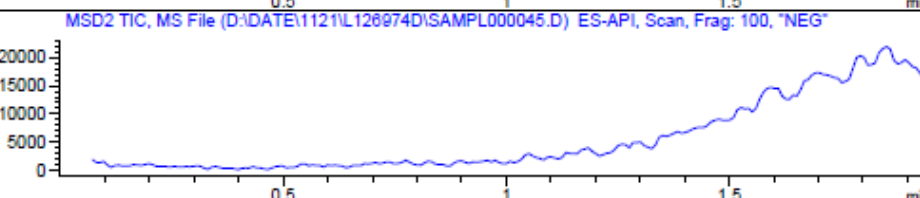
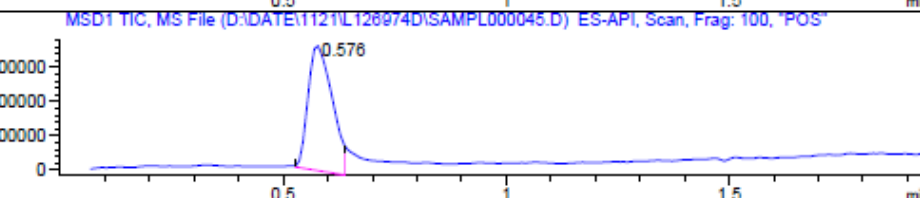
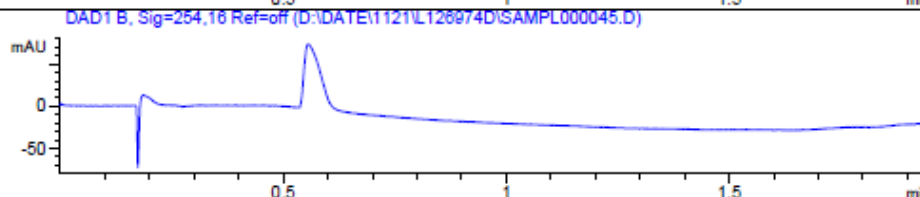
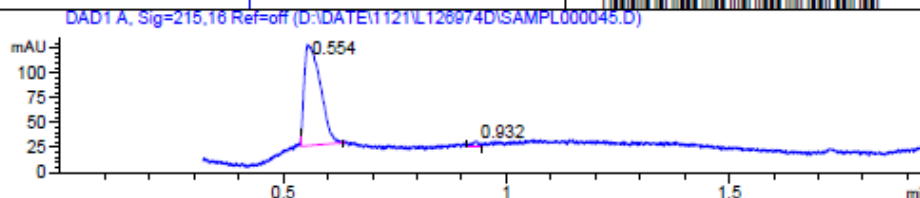
MaxPeak: 98.59%  
Ret\_Time: 0.554 min



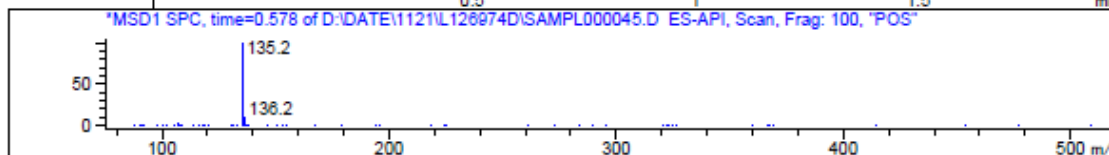
Mol Wt 134.18  
Exact Mass 134.1

#	Time	Area%
1	0.554	98.59
2	0.932	1.41

R1331370

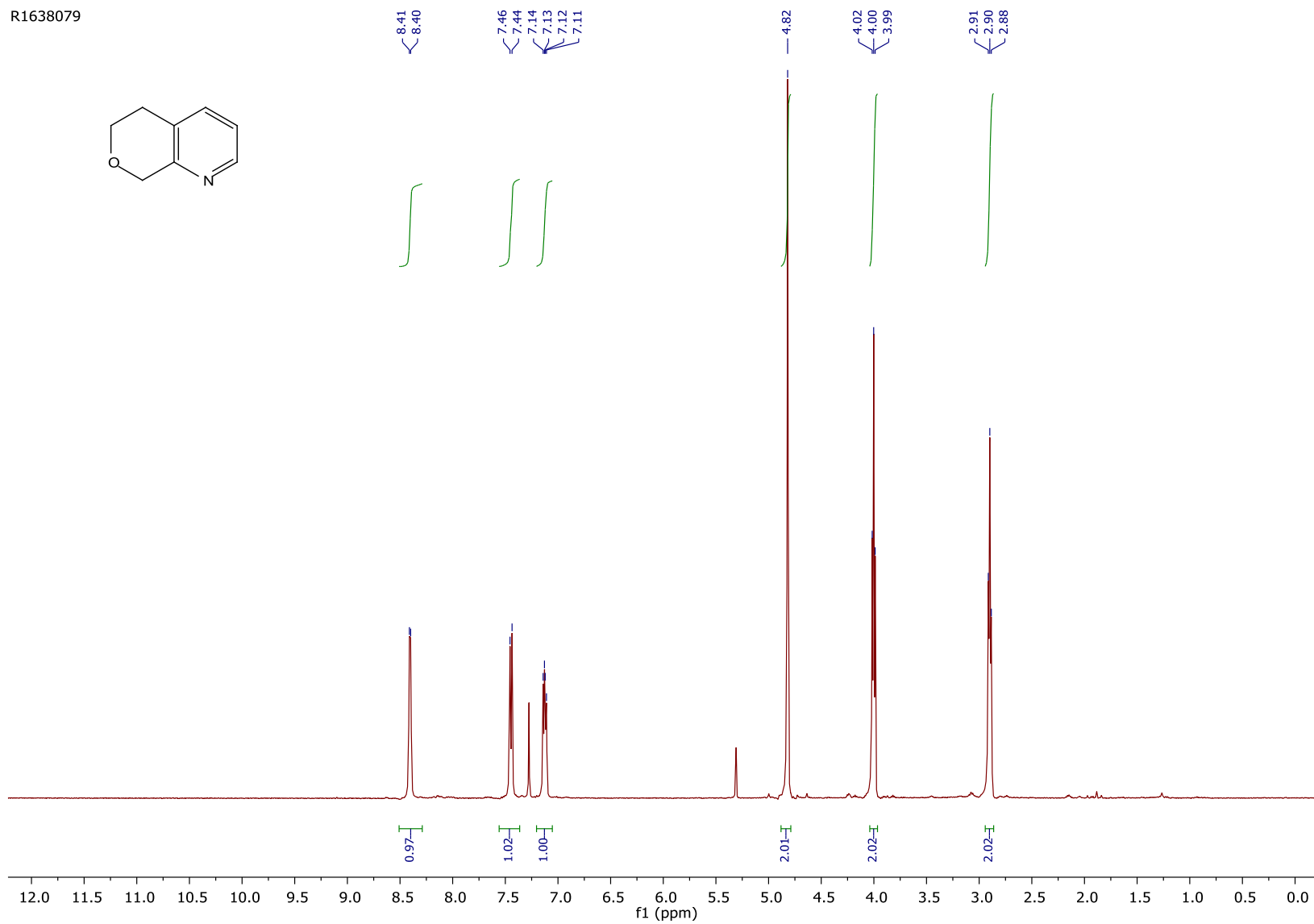


RT 0.576

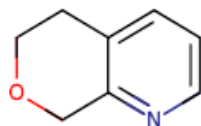


# <sup>1</sup>H and LCMS spectra of **10c**

R1638079

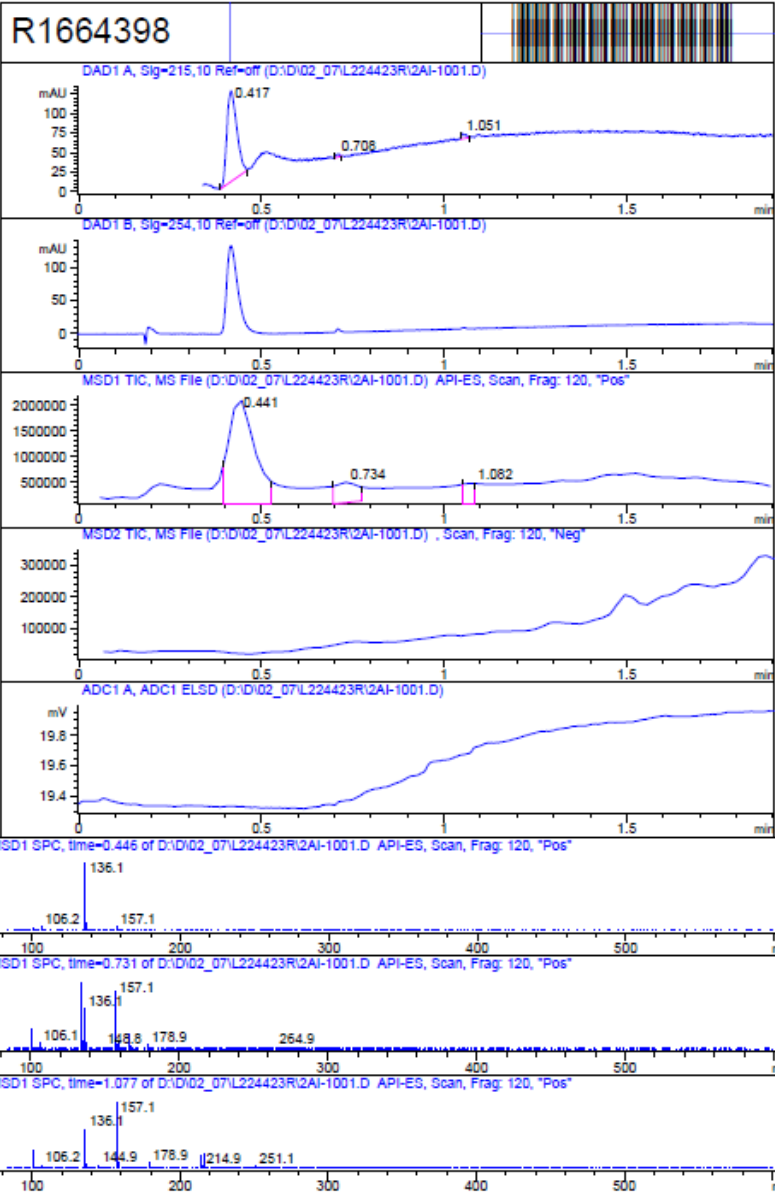


MaxPeak: 96.60%  
Ret\_Time: 0.417 min



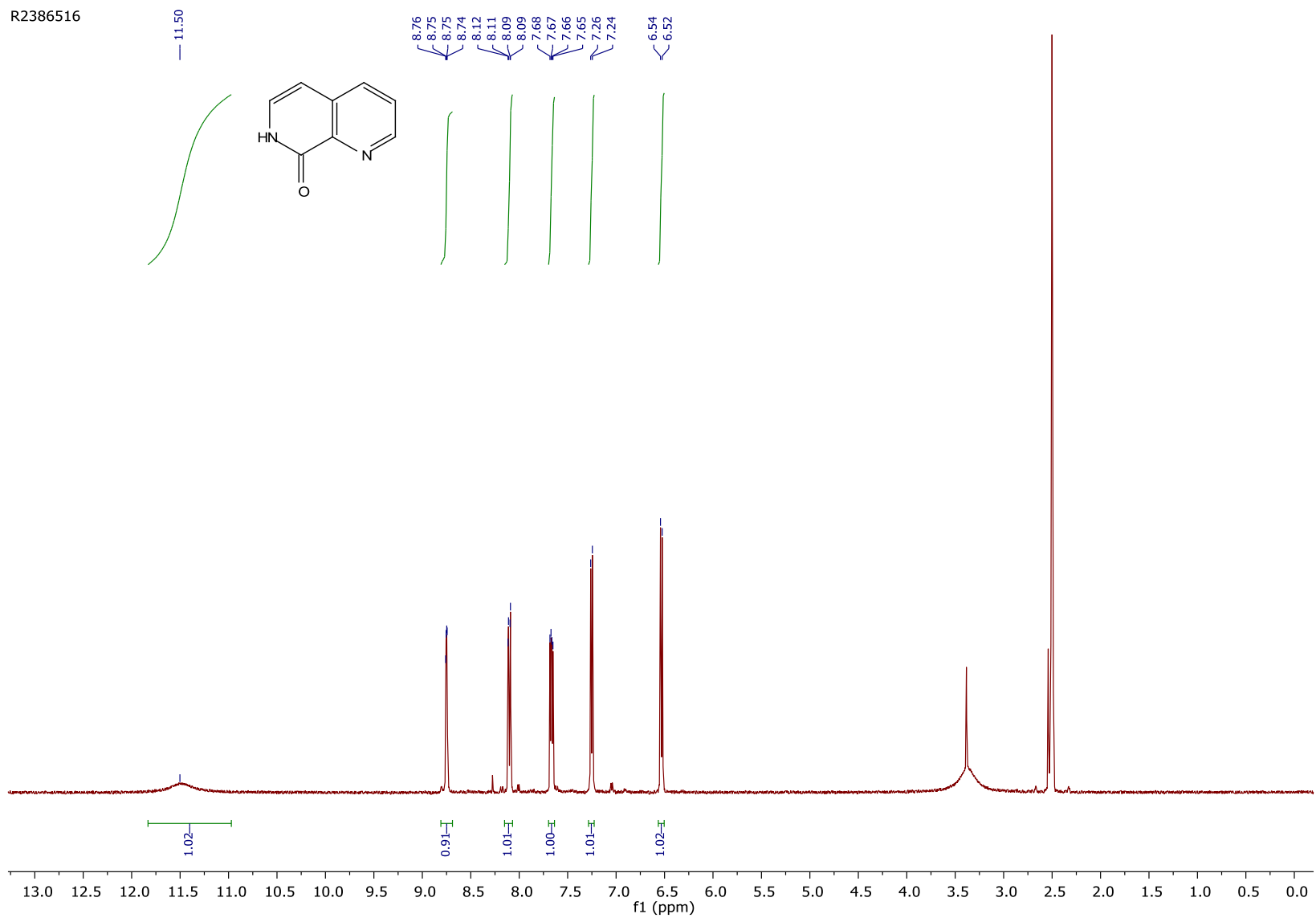
Mol Wt 135.16  
Exact Mass 135.08

#	Time	Area%
1	0.417	96.60
2	0.708	1.18
3	1.051	2.21

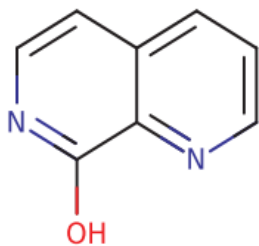


# <sup>1</sup>H and LCMS spectra of **21**

R2386516



MaxPeak: 100.00%  
Ret\_Time: 0.511 min



Mol Wt 146.15

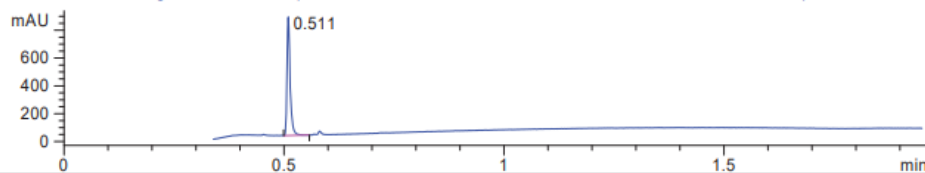
Exact Mass 146.05

#	Time	Area%
1	0.511	100.00

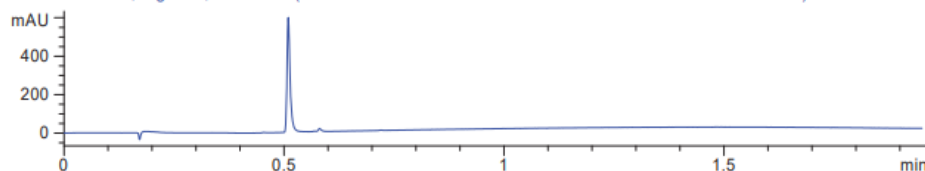
R2386516



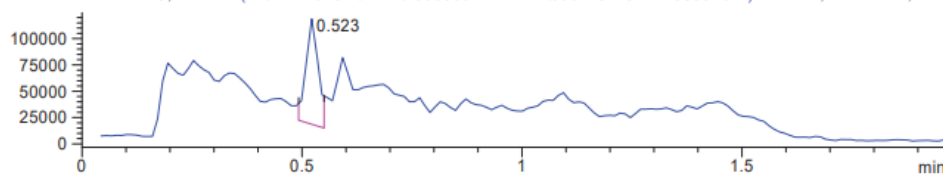
DAD1 A, Sig=215,16 Ref-off (D:\DATE\NOV\11\11\305569R-PART1\009-D5F-C2-R2386516.D)



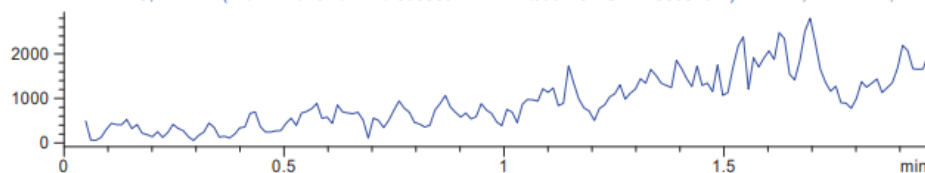
DAD1 B, Sig=254,16 Ref-off (D:\DATE\NOV\11\11\305569R-PART1\009-D5F-C2-R2386516.D)



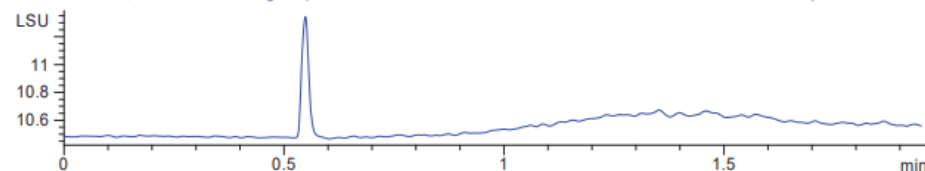
MSD1 TIC, MS File (D:\DATE\NOV\11\11\305569R-PART1\009-D5F-C2-R2386516.D) ES-API, Fast Scan, Frag



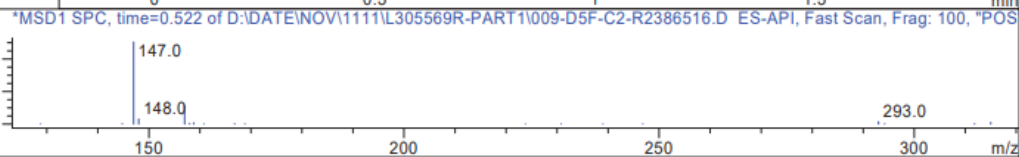
MSD2 TIC, MS File (D:\DATE\NOV\11\11\305569R-PART1\009-D5F-C2-R2386516.D) ES-API, Fast Scan, Frag



ELS1 A, ELS1A, ELS1A Signal (D:\DATE\NOV\11\11\305569R-PART1\009-D5F-C2-R2386516.D)

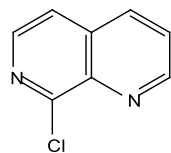


RT 0.523

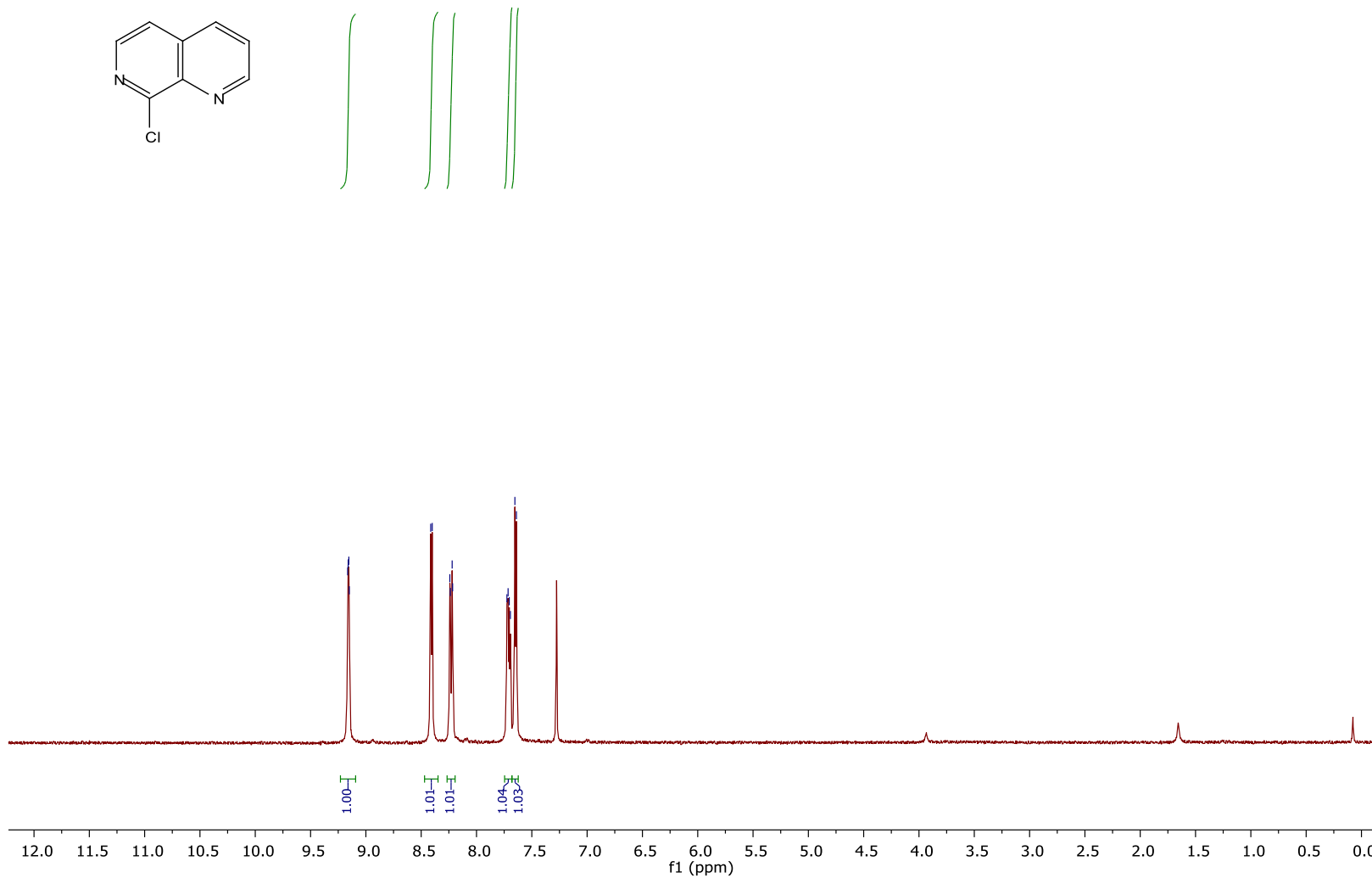


# <sup>1</sup>H and LCMS spectra of **22**

R1725775

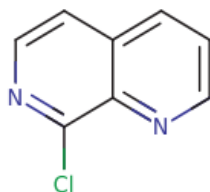


9.16  
9.16  
9.15  
9.15  
8.41  
8.40  
8.24  
8.24  
8.22  
8.22  
7.72  
7.71  
7.70  
7.69  
7.65  
7.64





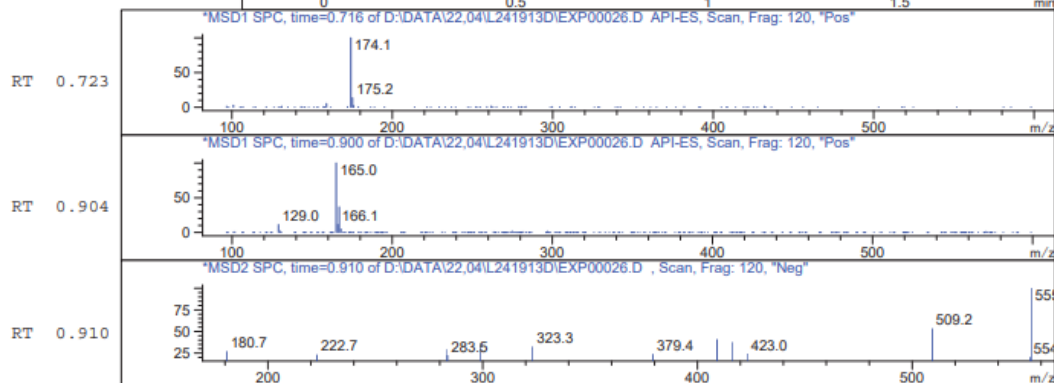
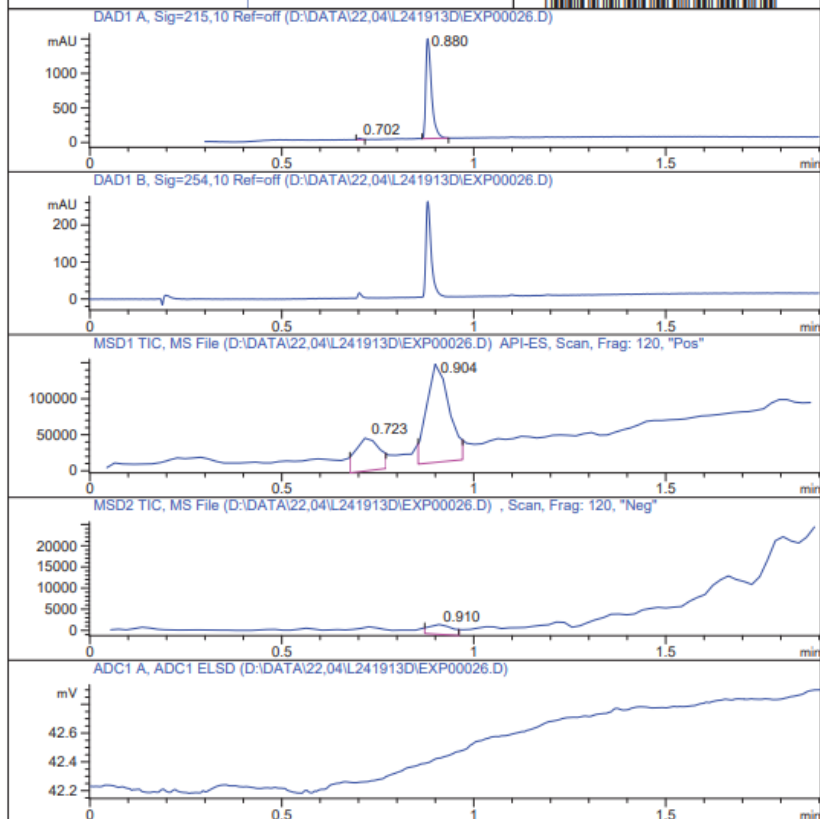
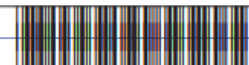
MaxPeak: 98.98%  
Ret\_Time: 0.880 min



Mol Wt 164.59  
Exact Mass 164.02

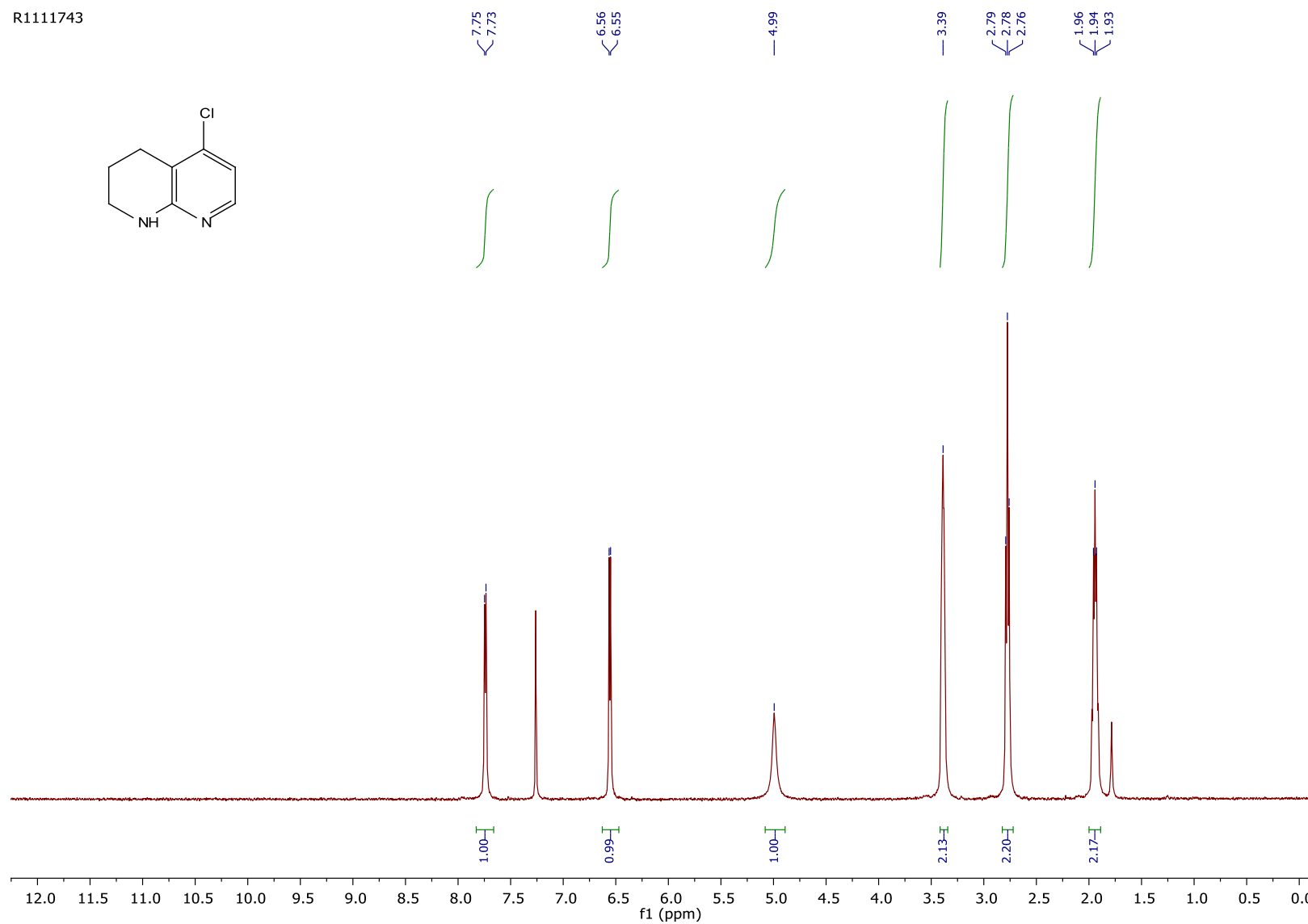
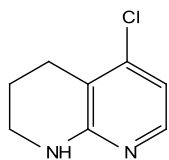
#	Time	Area%
1	0.702	1.02
2	0.880	98.98

R1725775



# <sup>1</sup>H and LCMS spectra of **24**

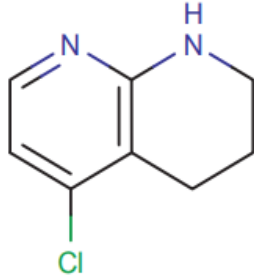
R1111743



# R1111743



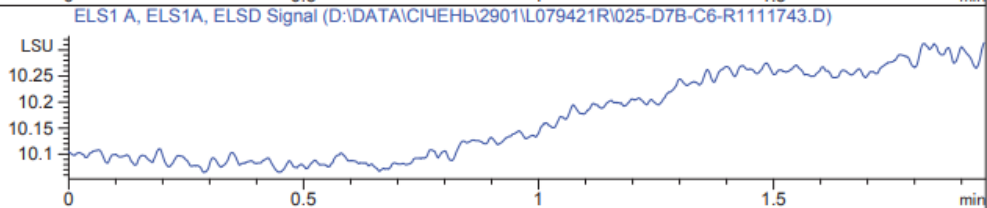
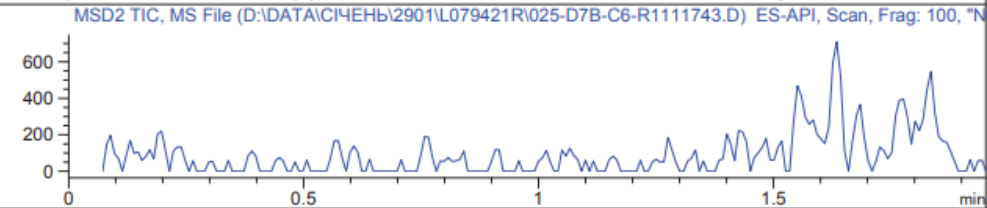
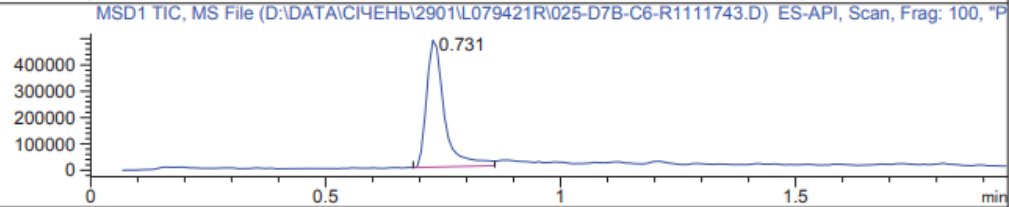
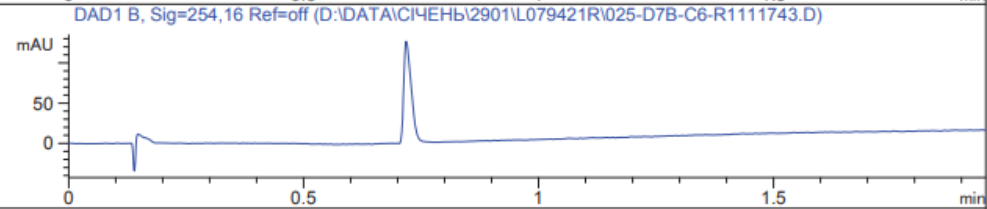
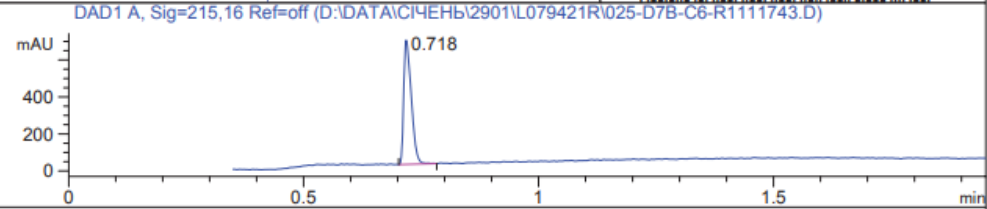
MaxPeak: 100.00%  
Ret\_Time: 0.718 min



Mol Wt 168.62

Exact Mass 168.06

#	Time	Area%
1	0.718	100.00



RT 0.731

