Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Toll-like Receptor-8 Agonistic Activities in C2, C4, and C8 Modified Thiazolo[4,5-*c*]quinolines

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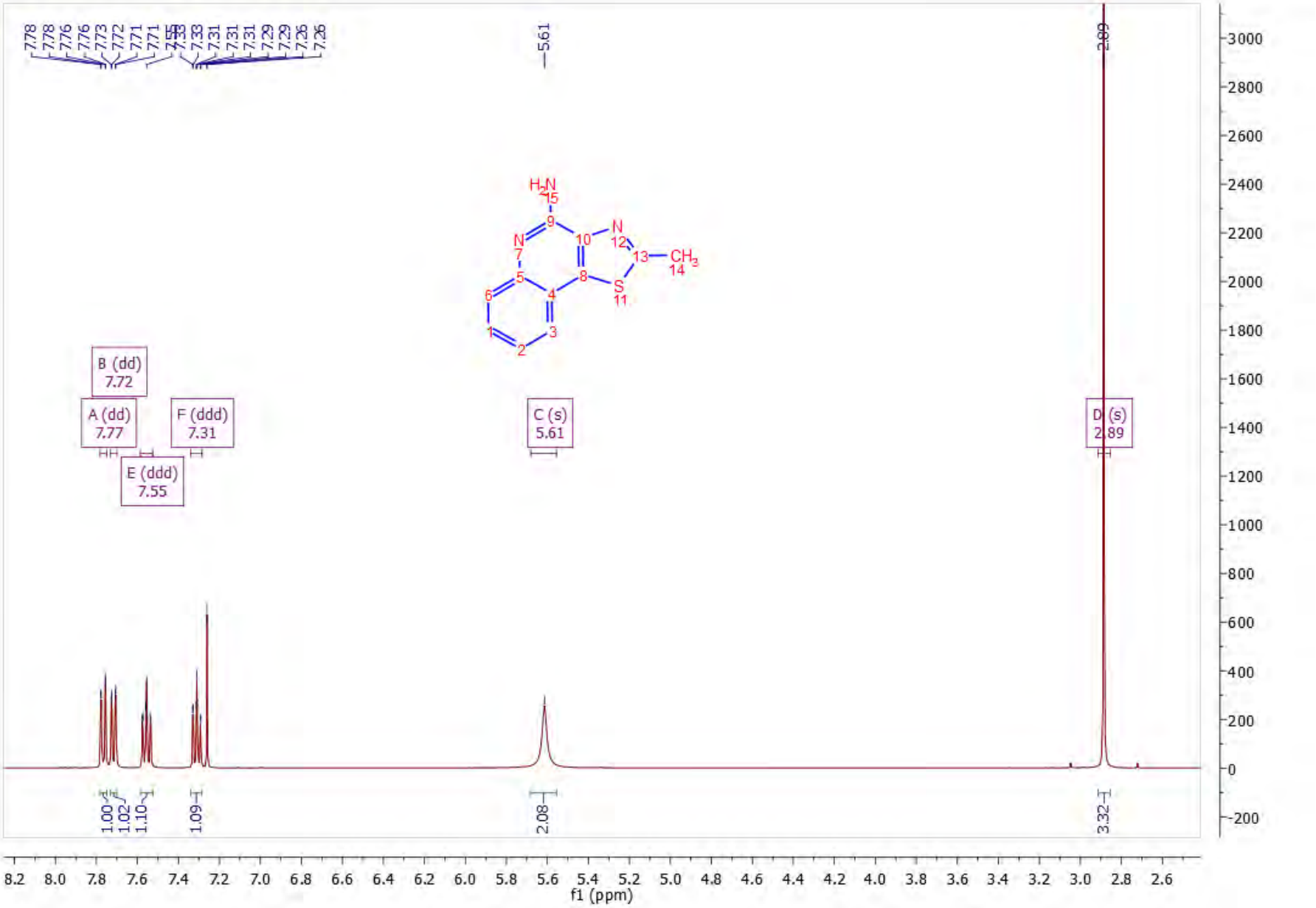
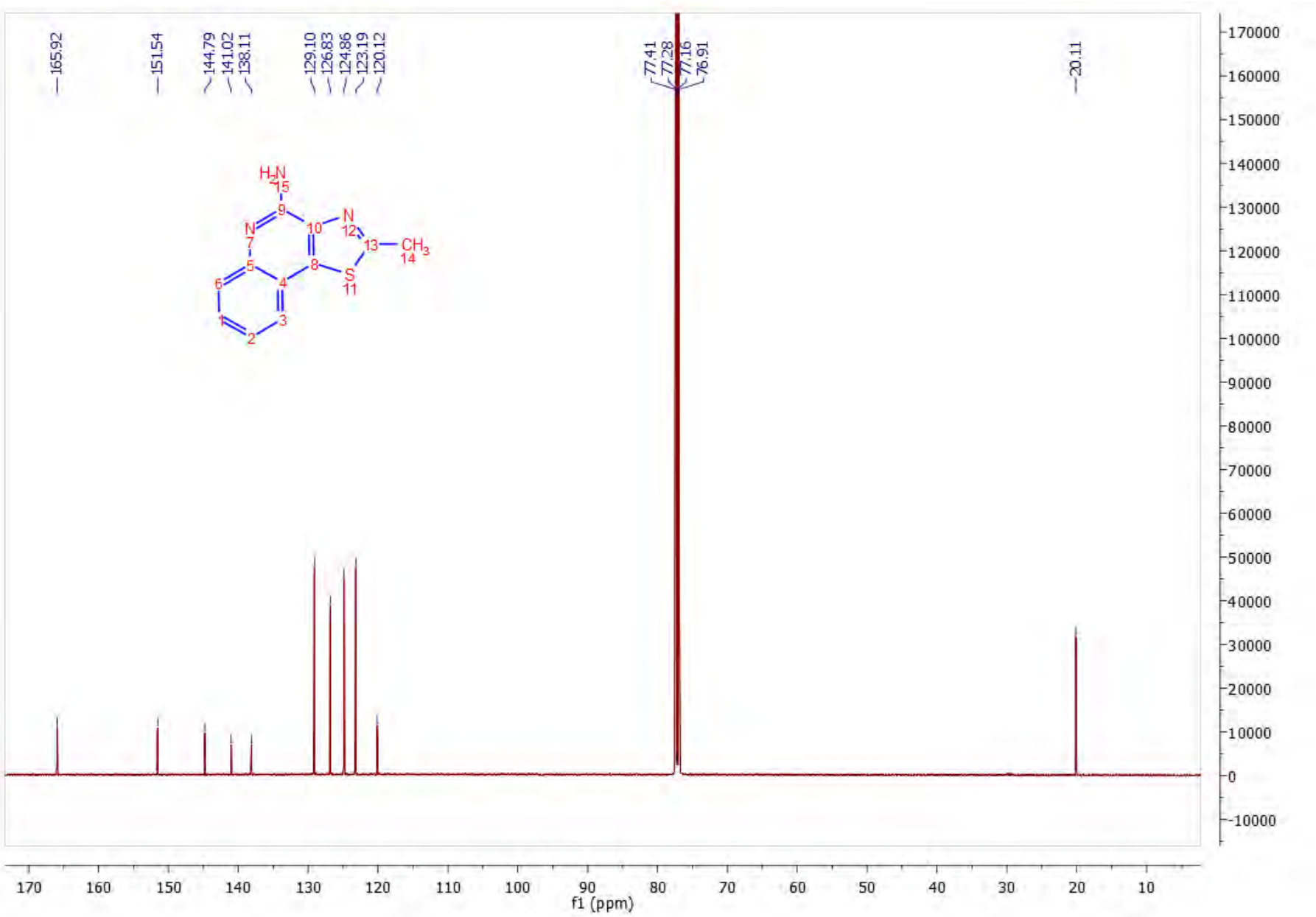
Department of Medicinal Chemistry
University of Kansas

8a ^{1}H NMR



8a ^{13}C NMR



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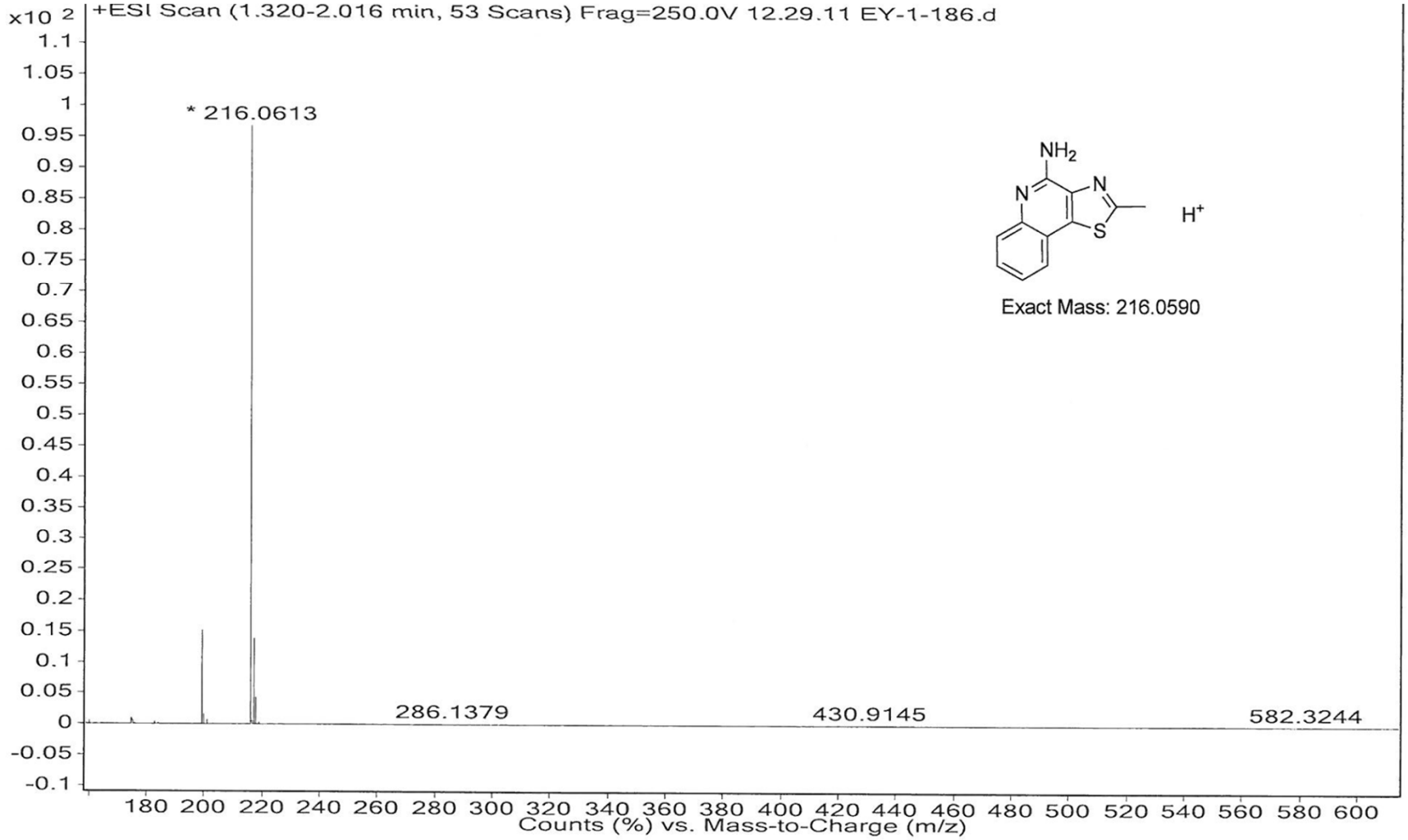

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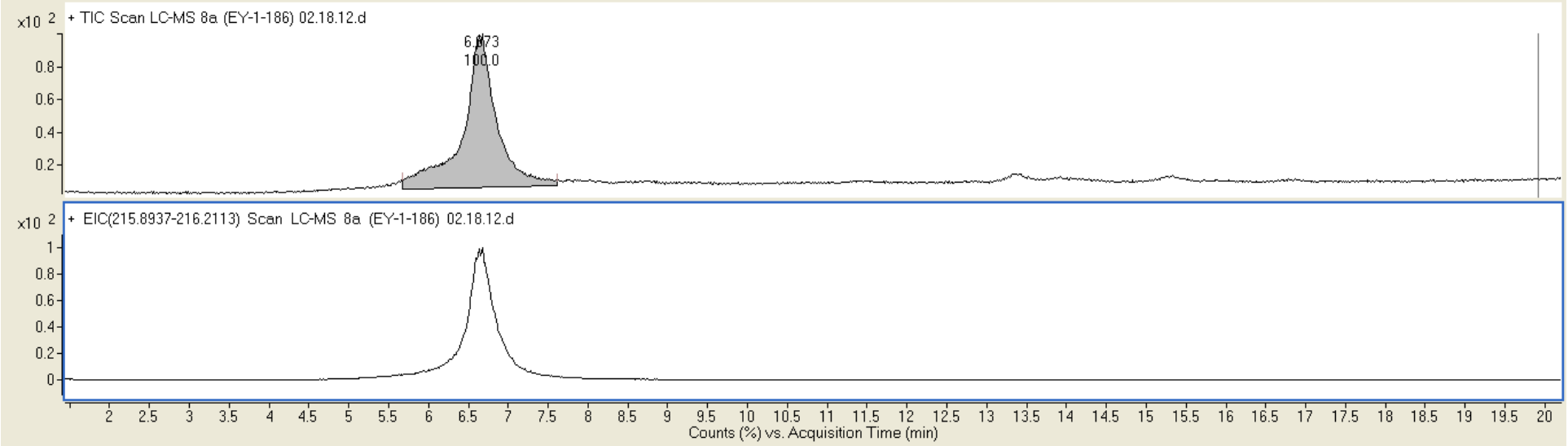

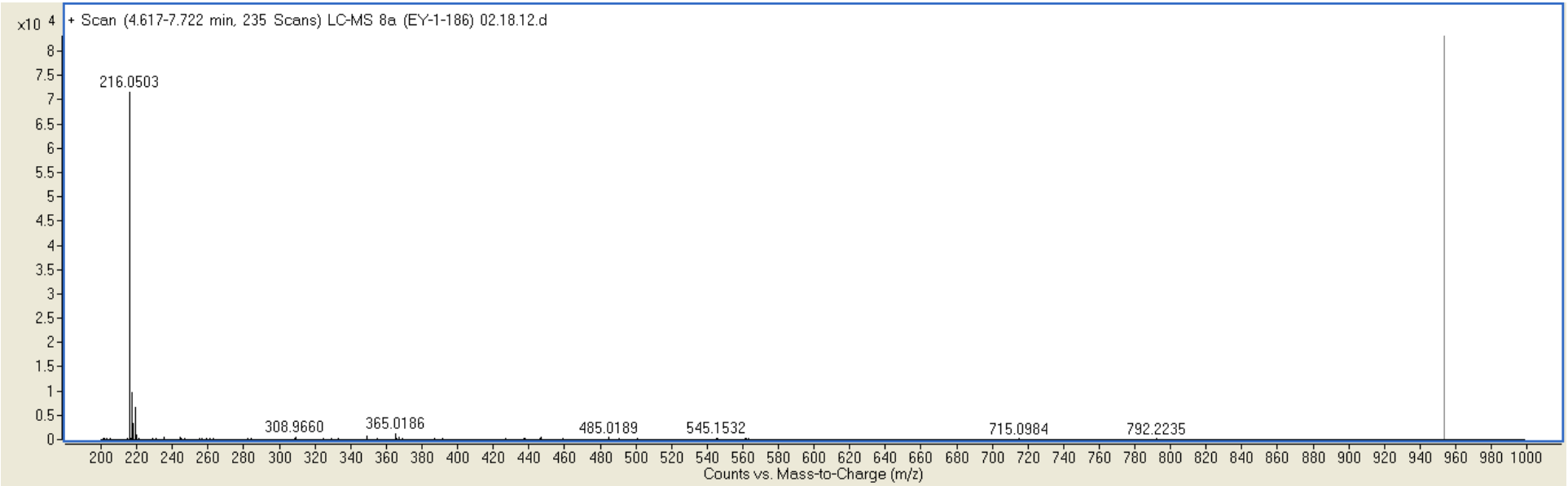

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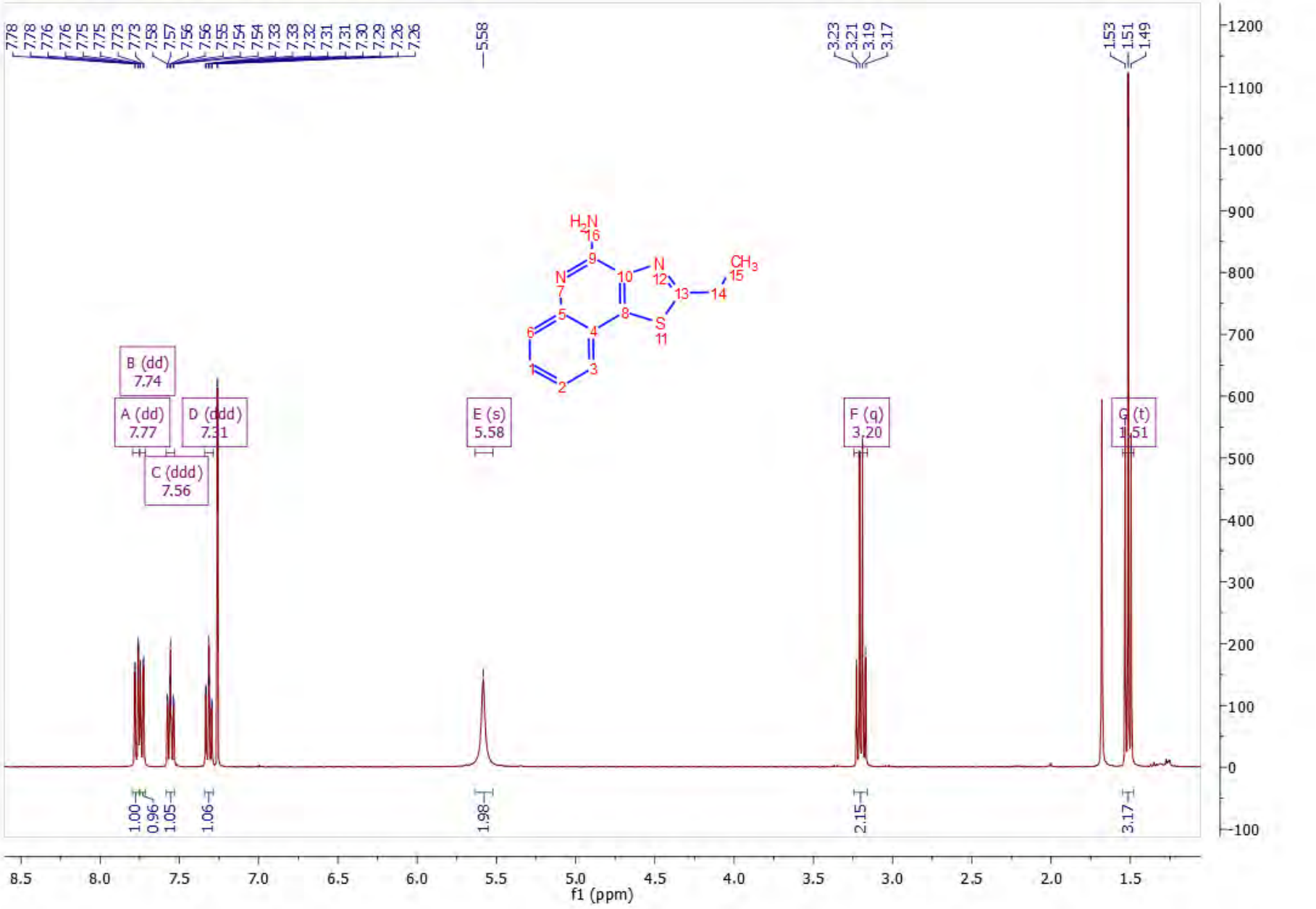

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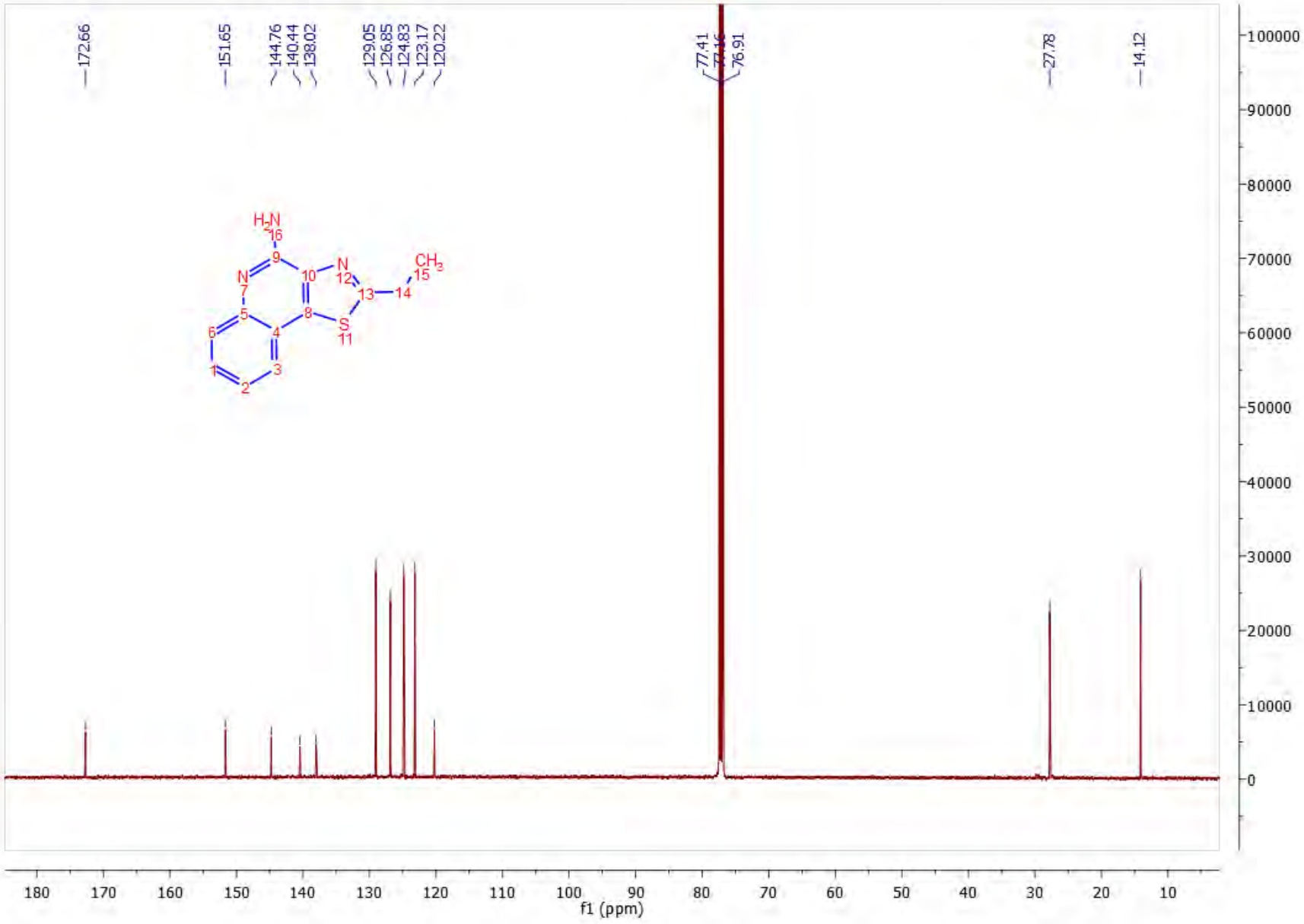

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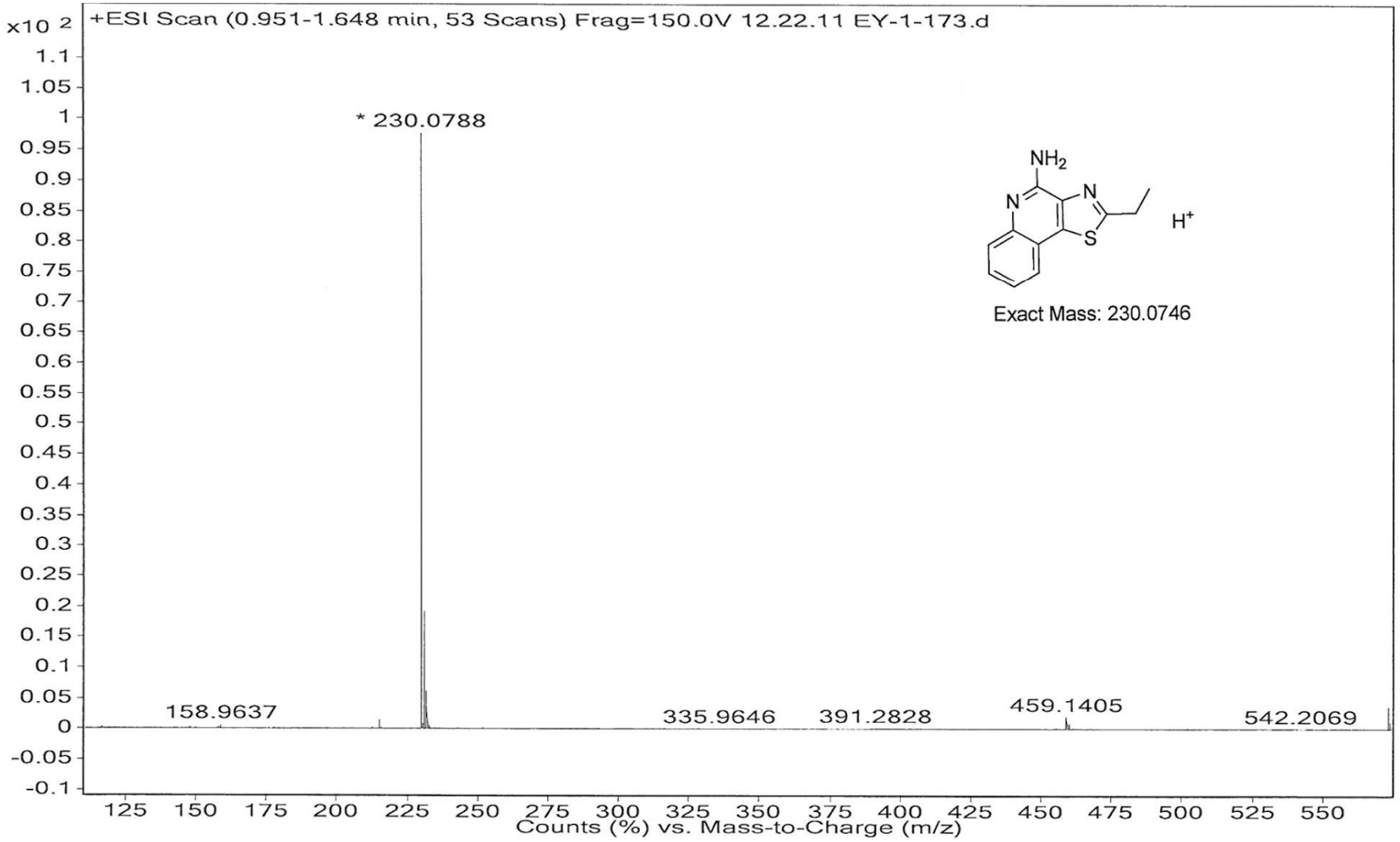

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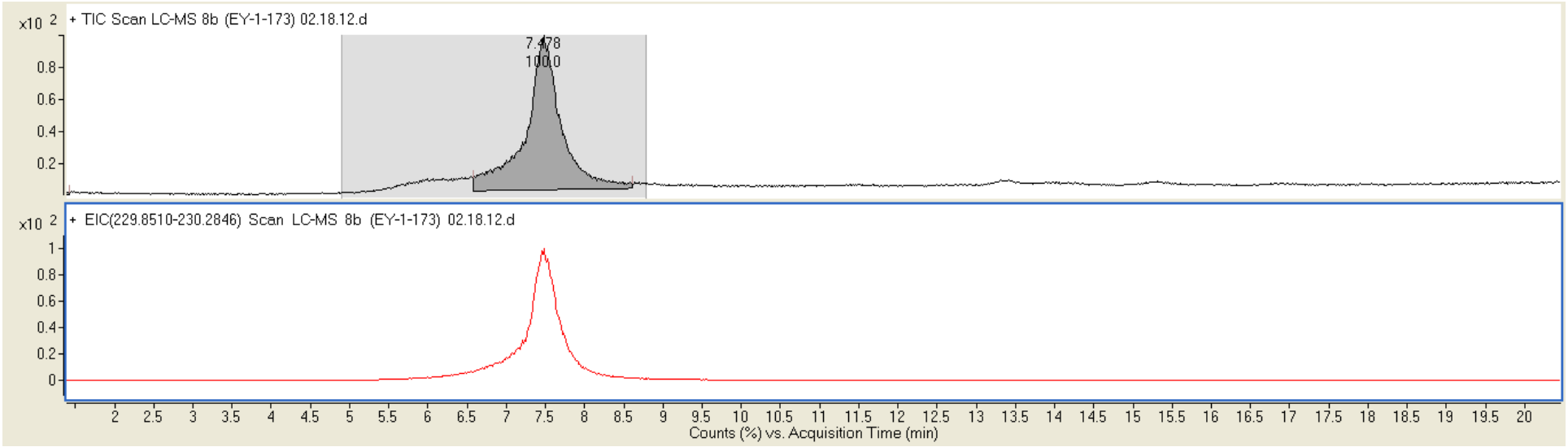

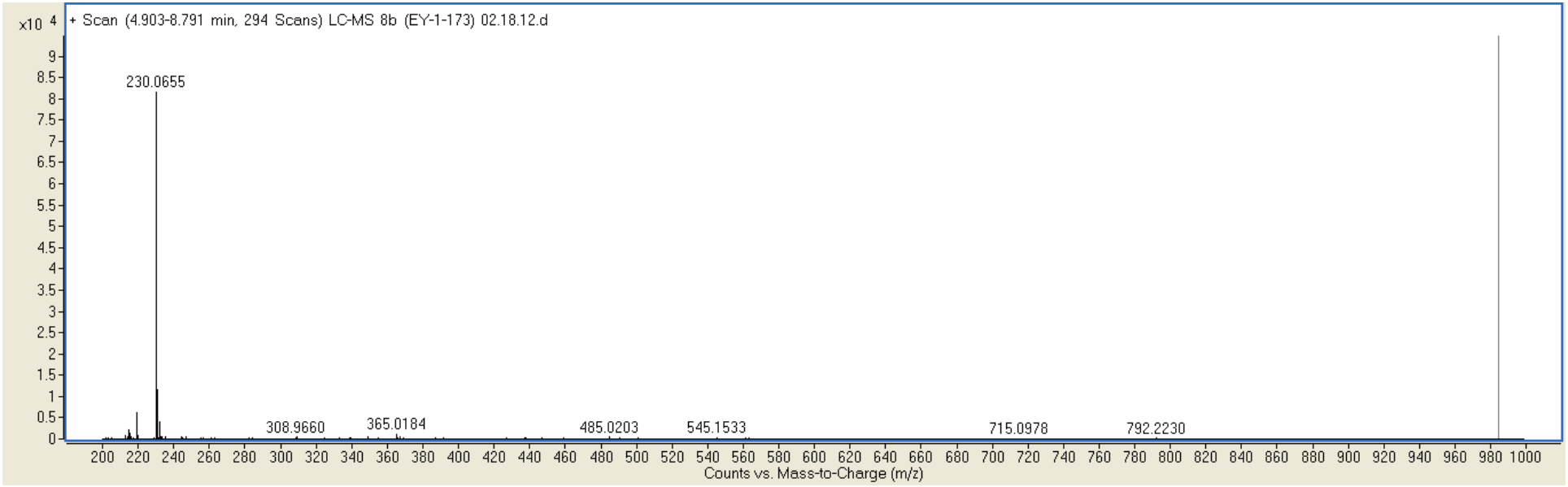

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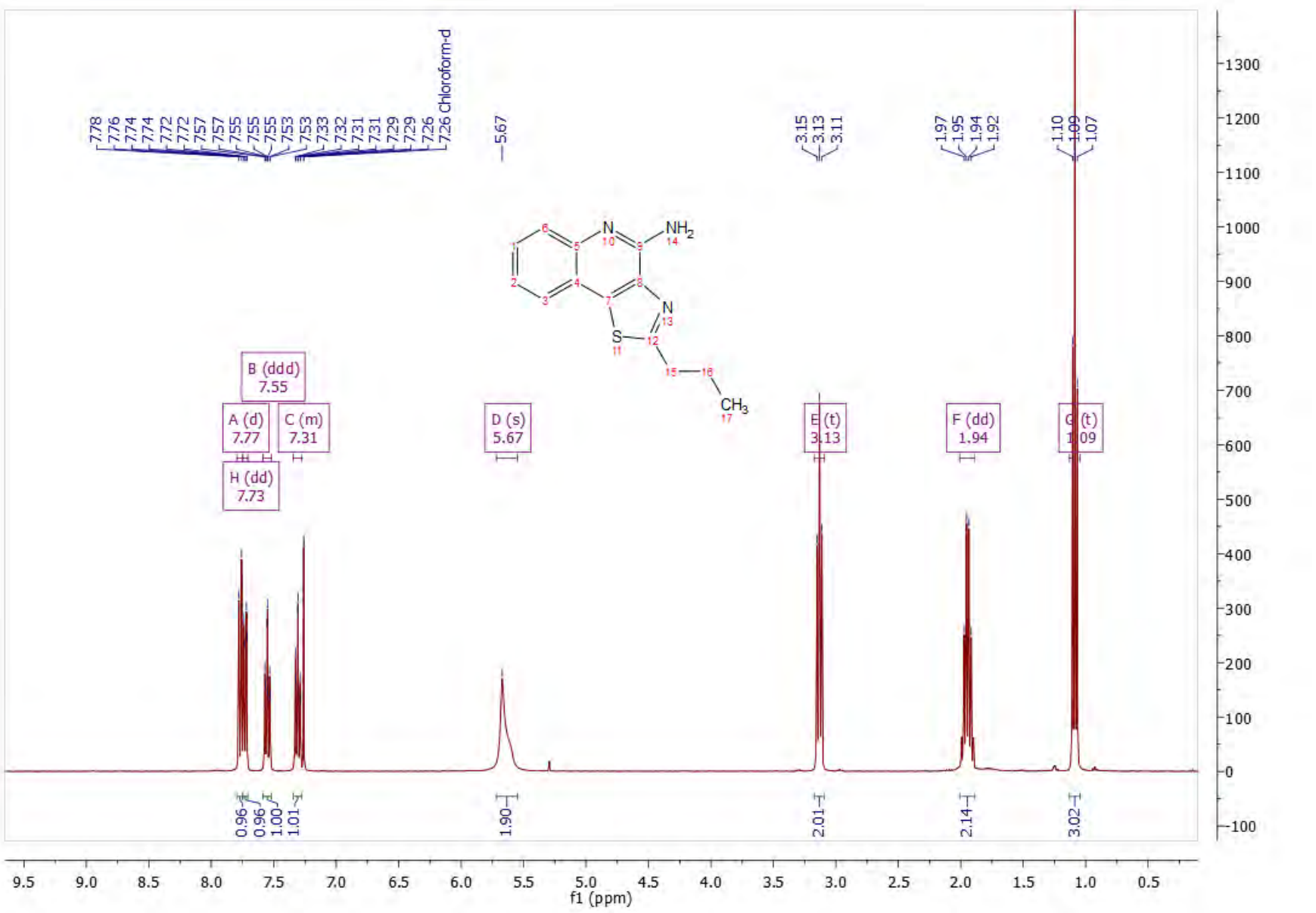

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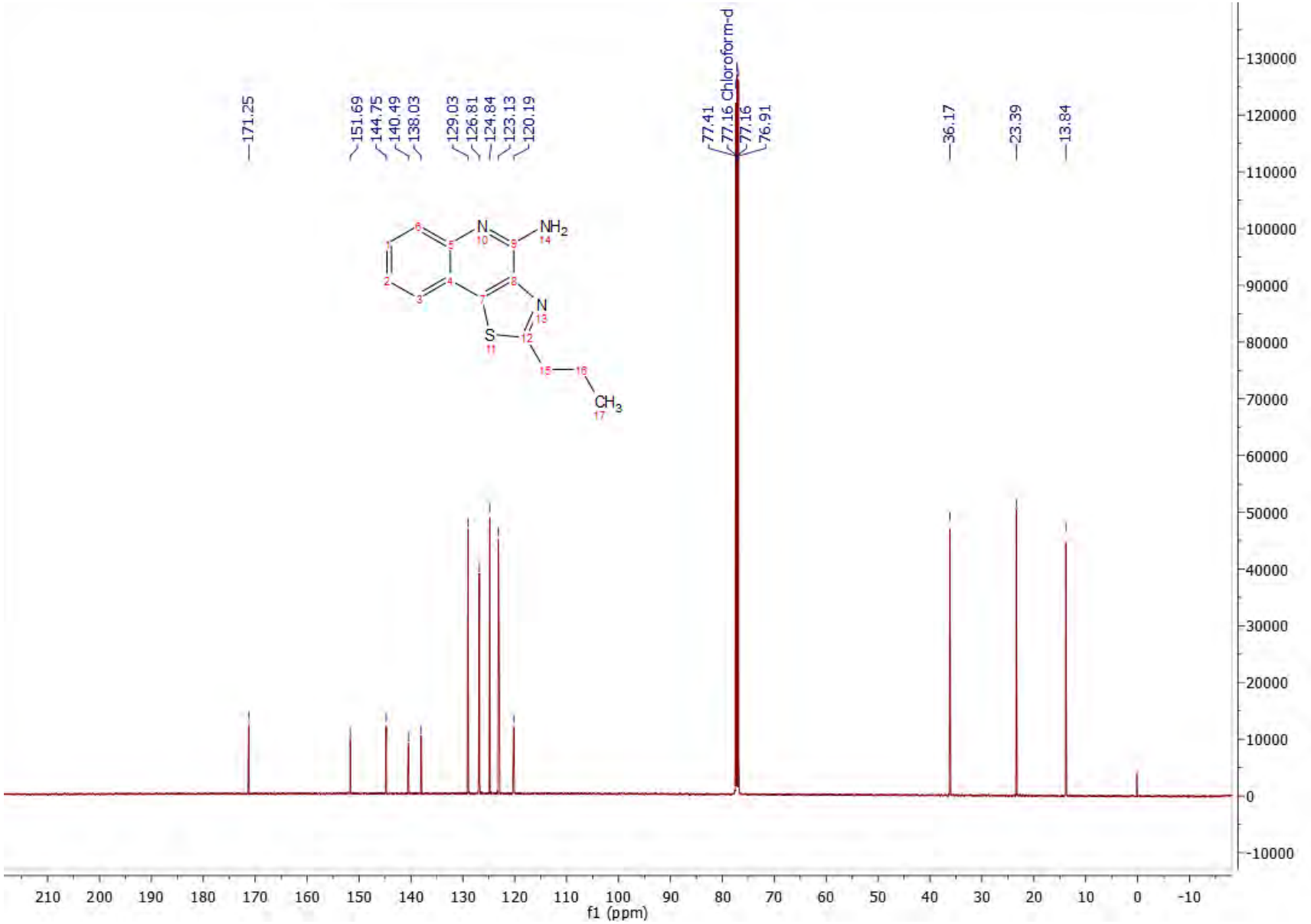

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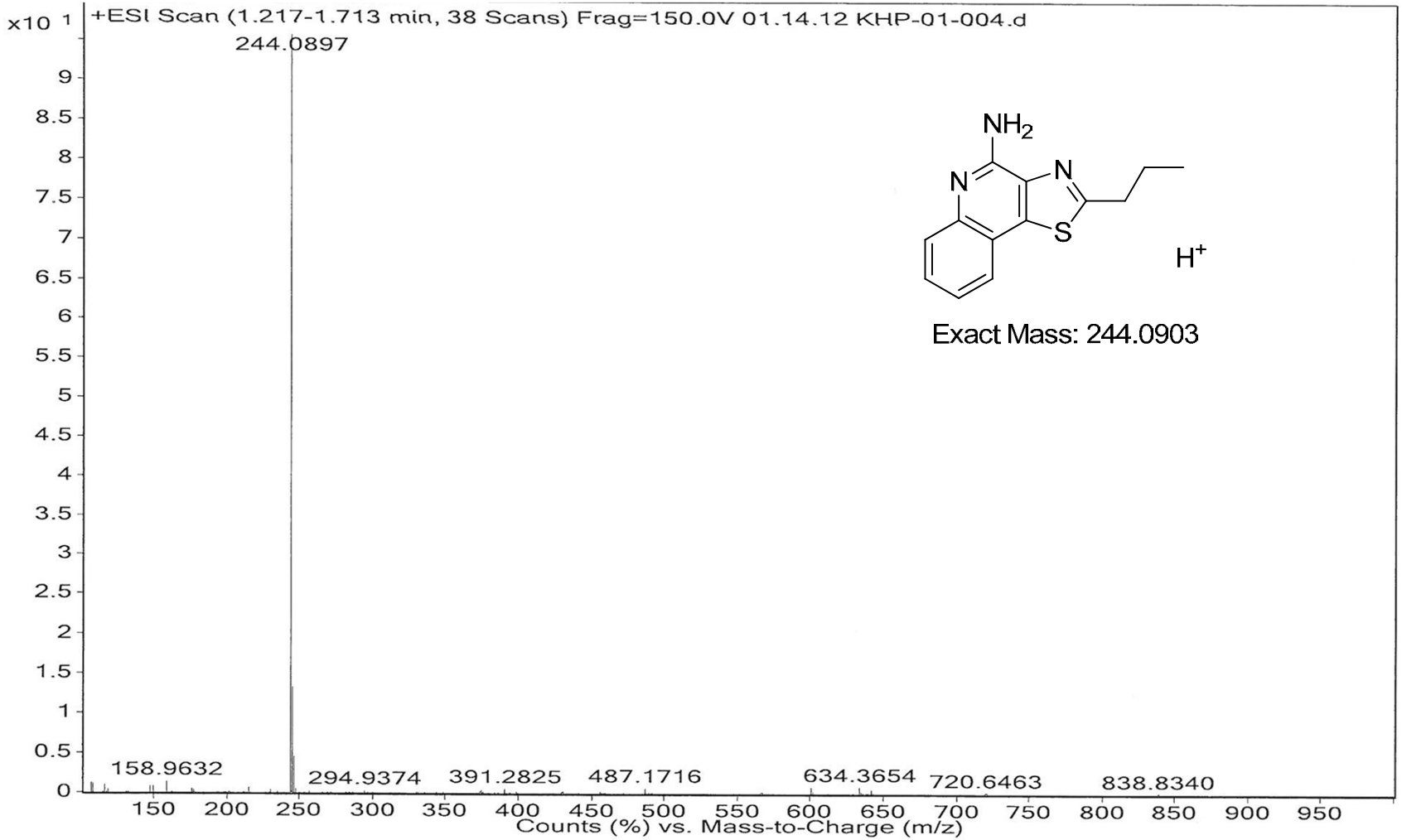

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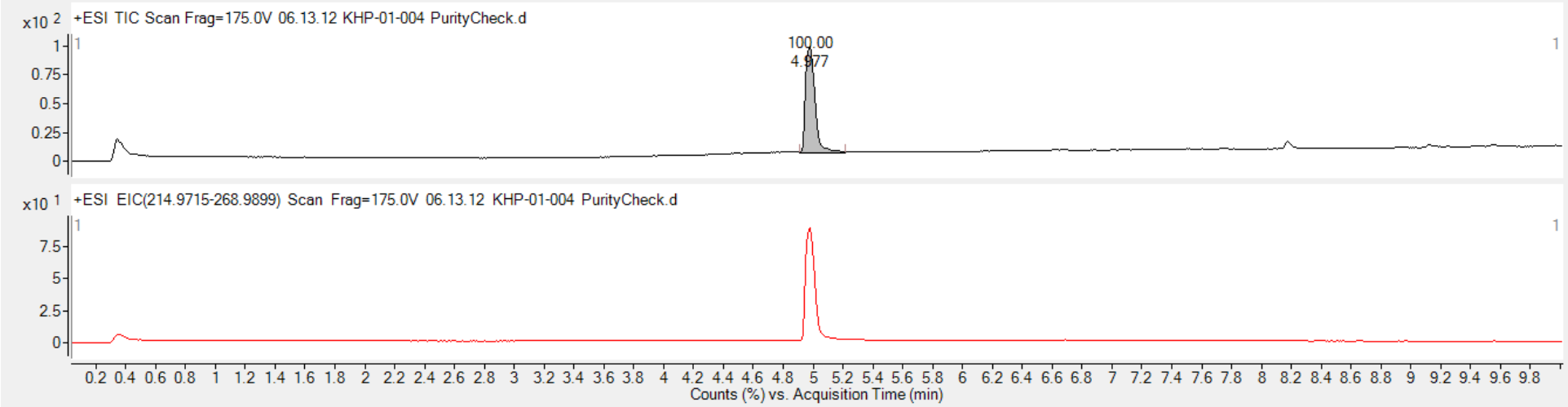

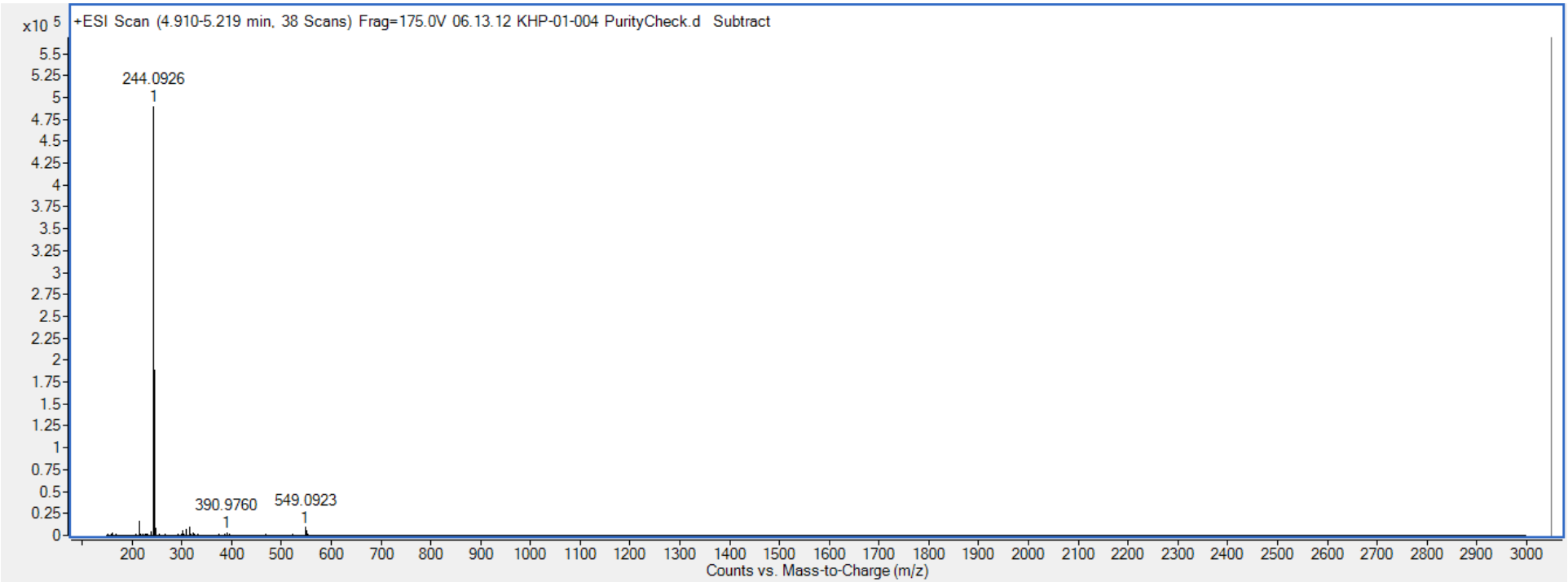

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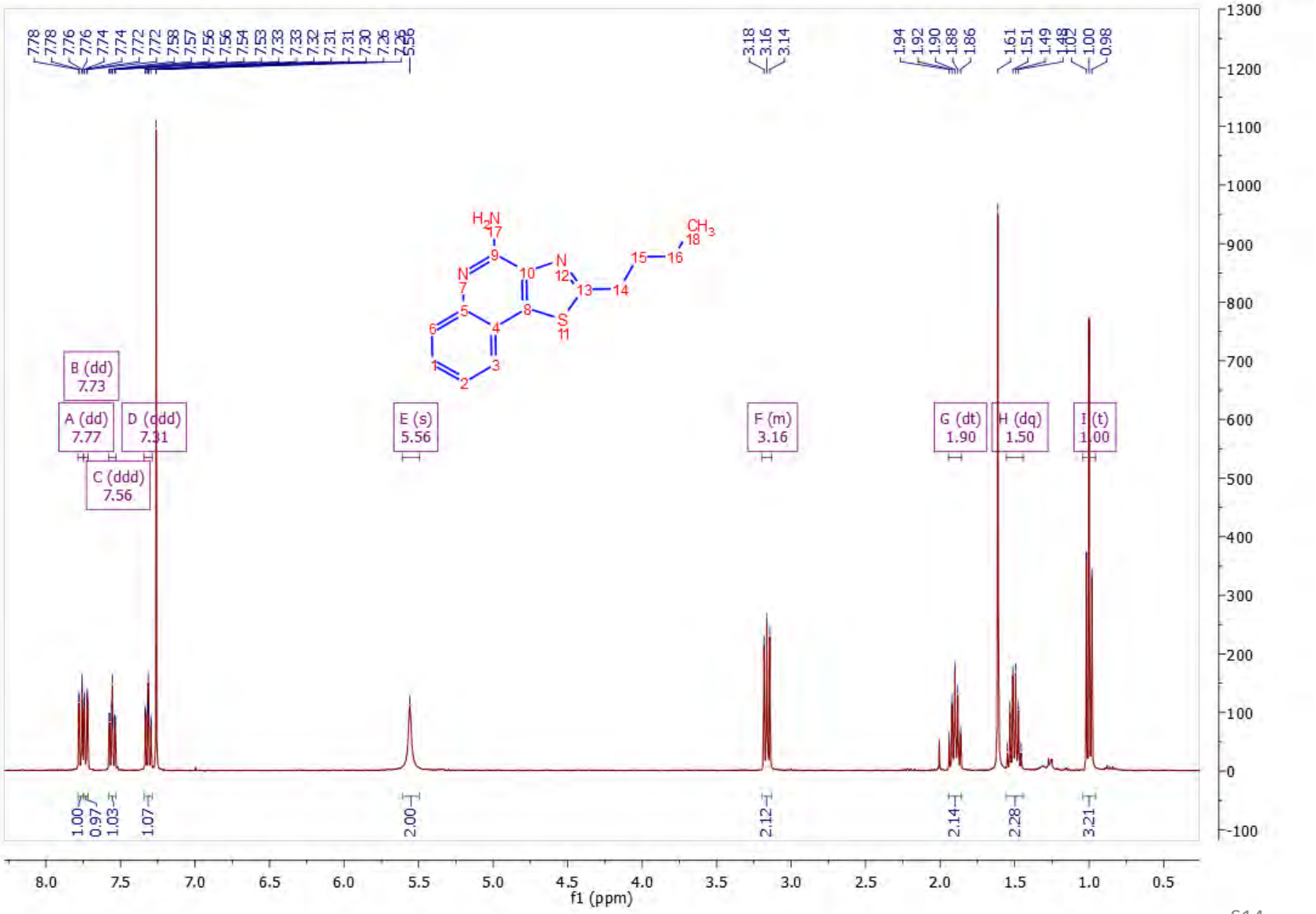

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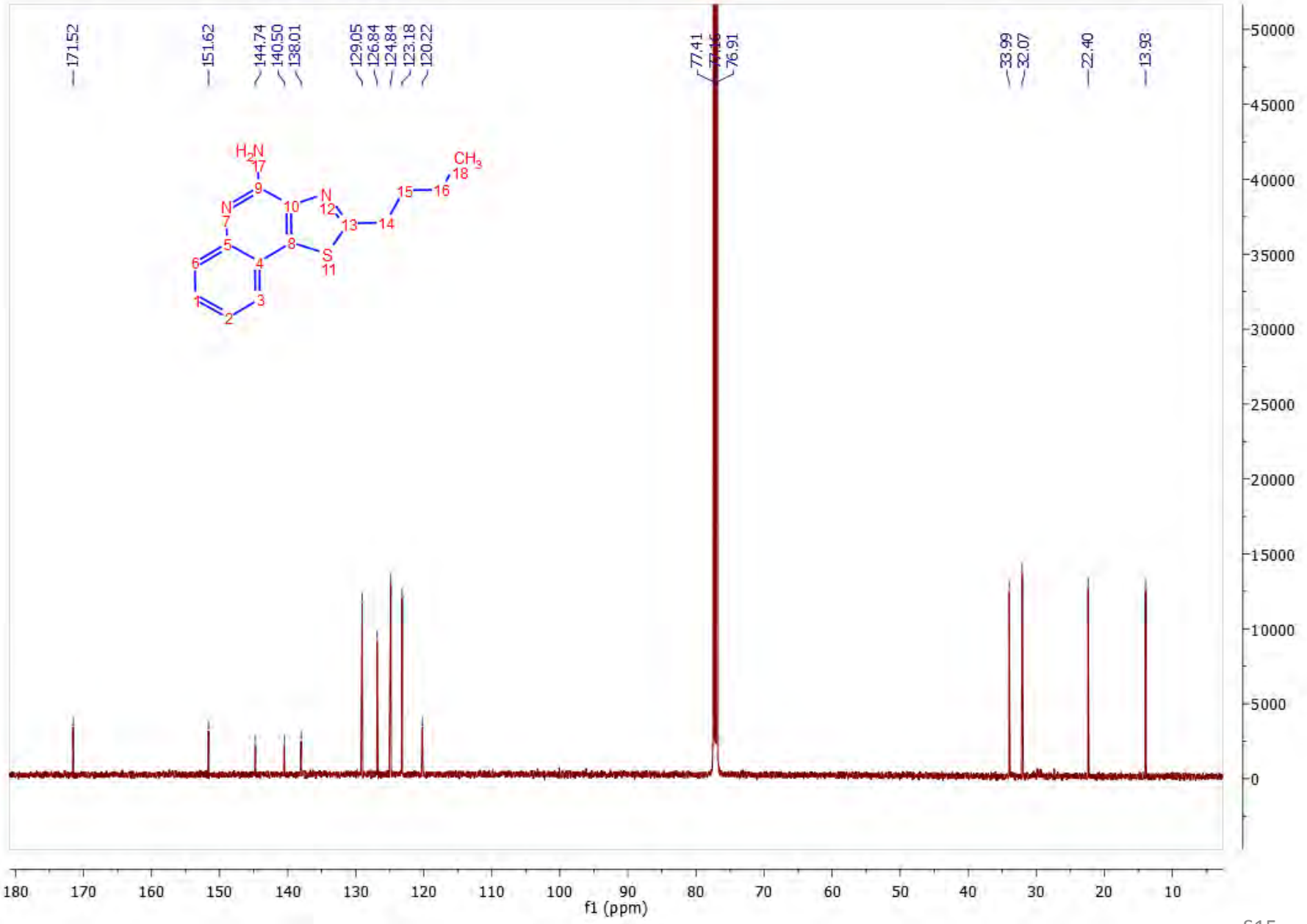

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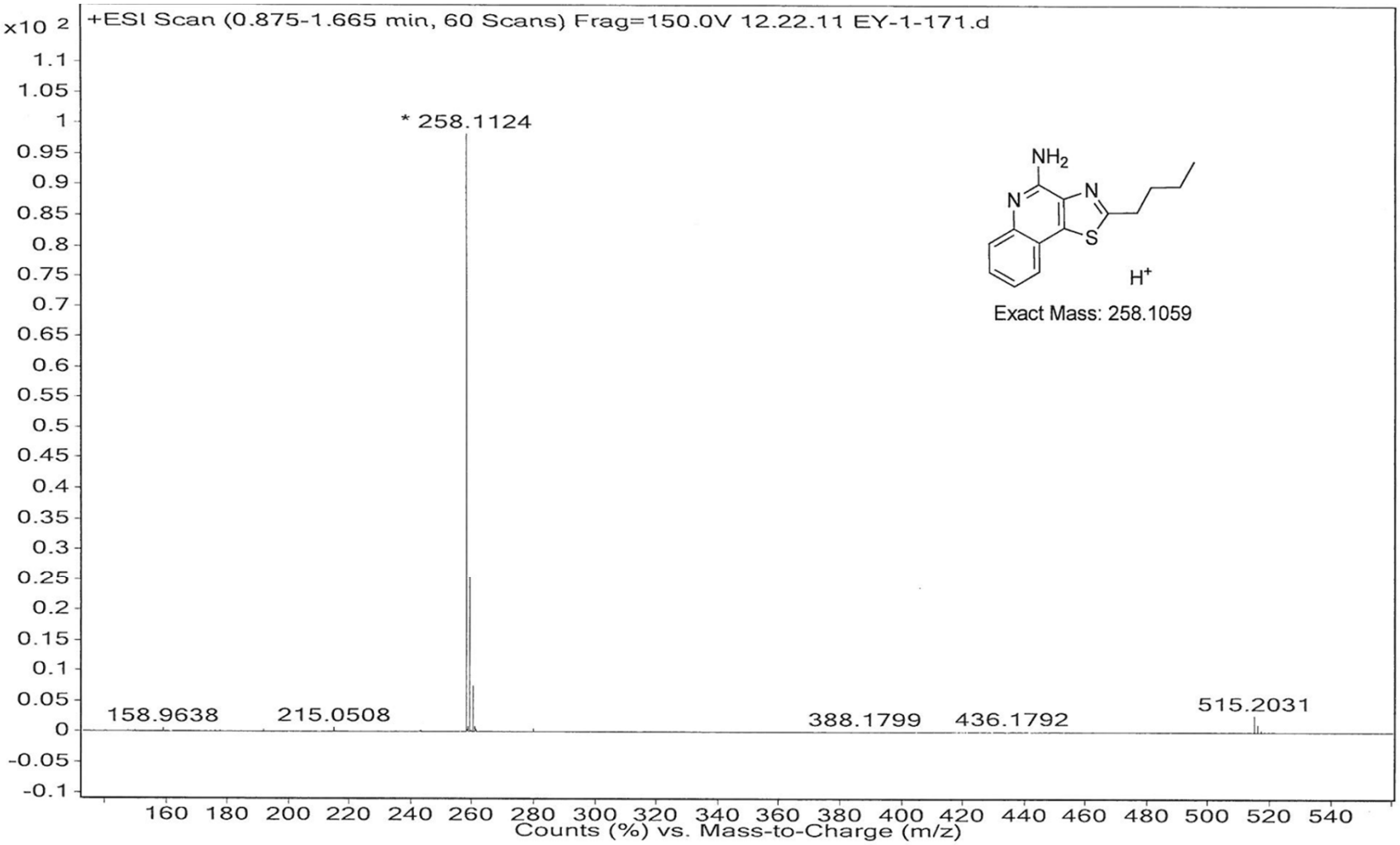

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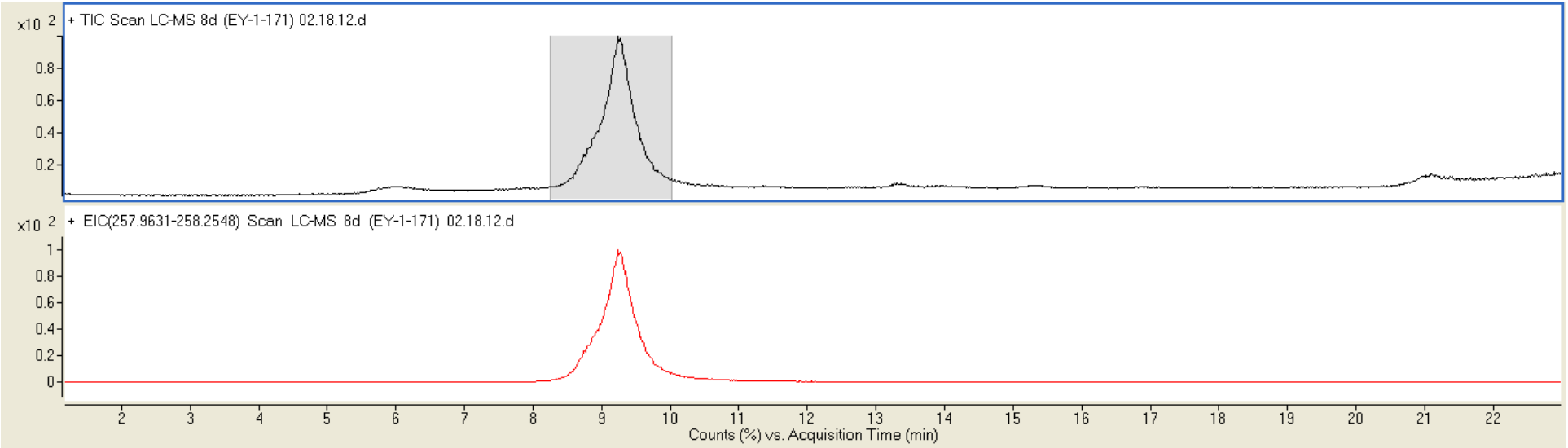

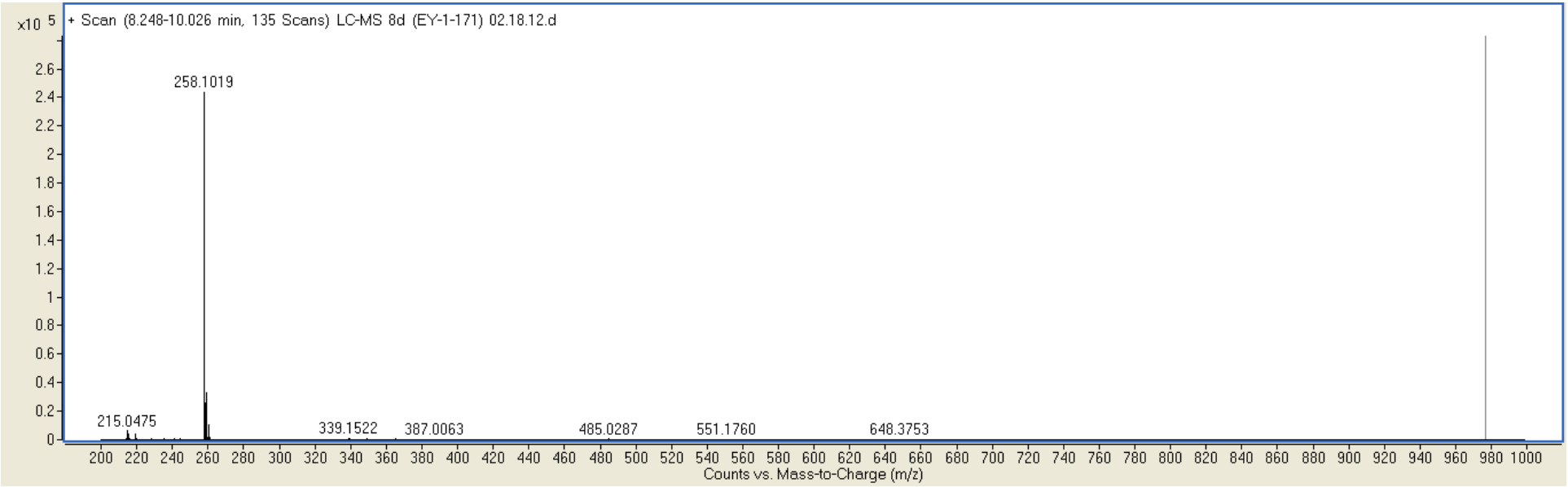

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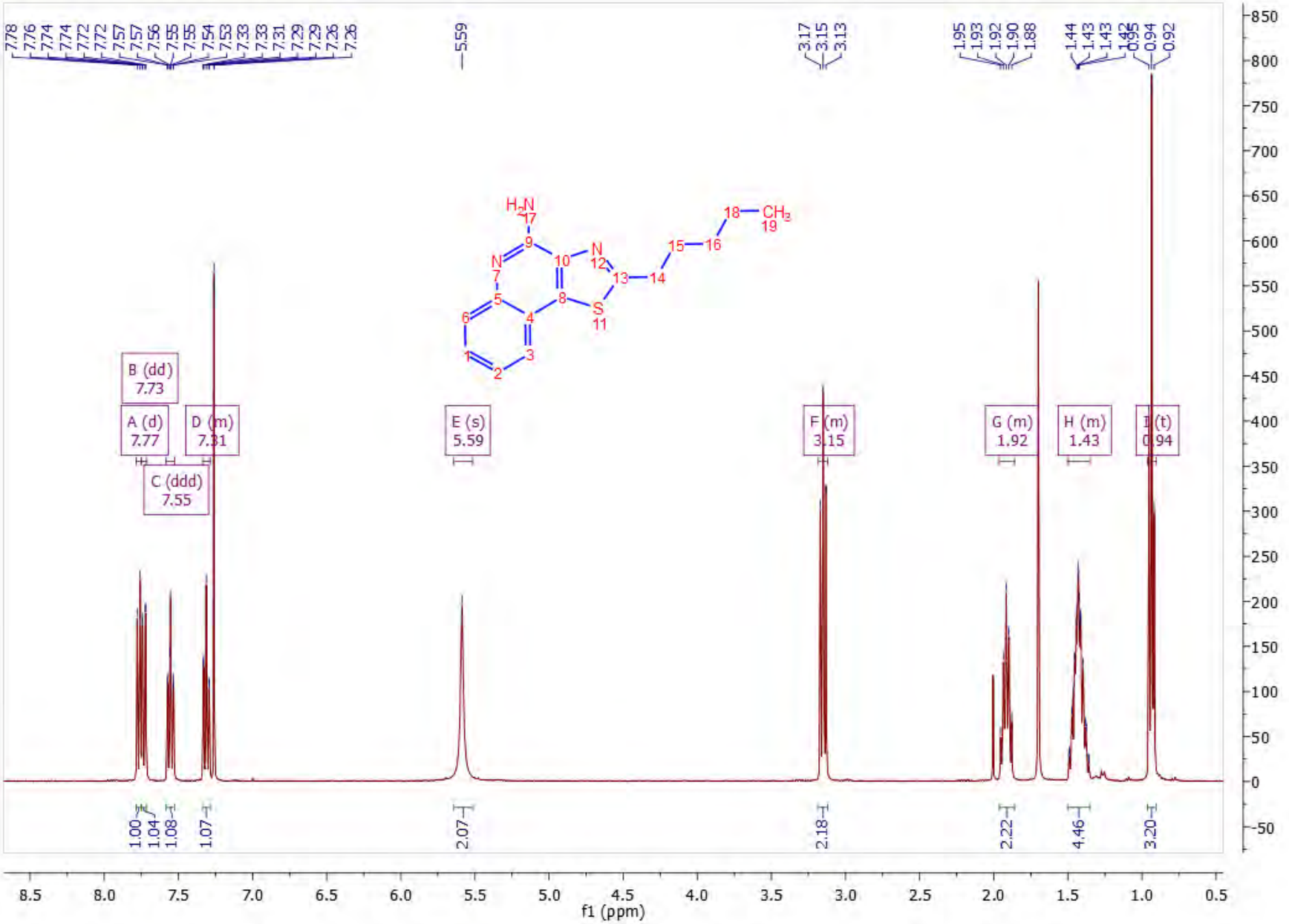

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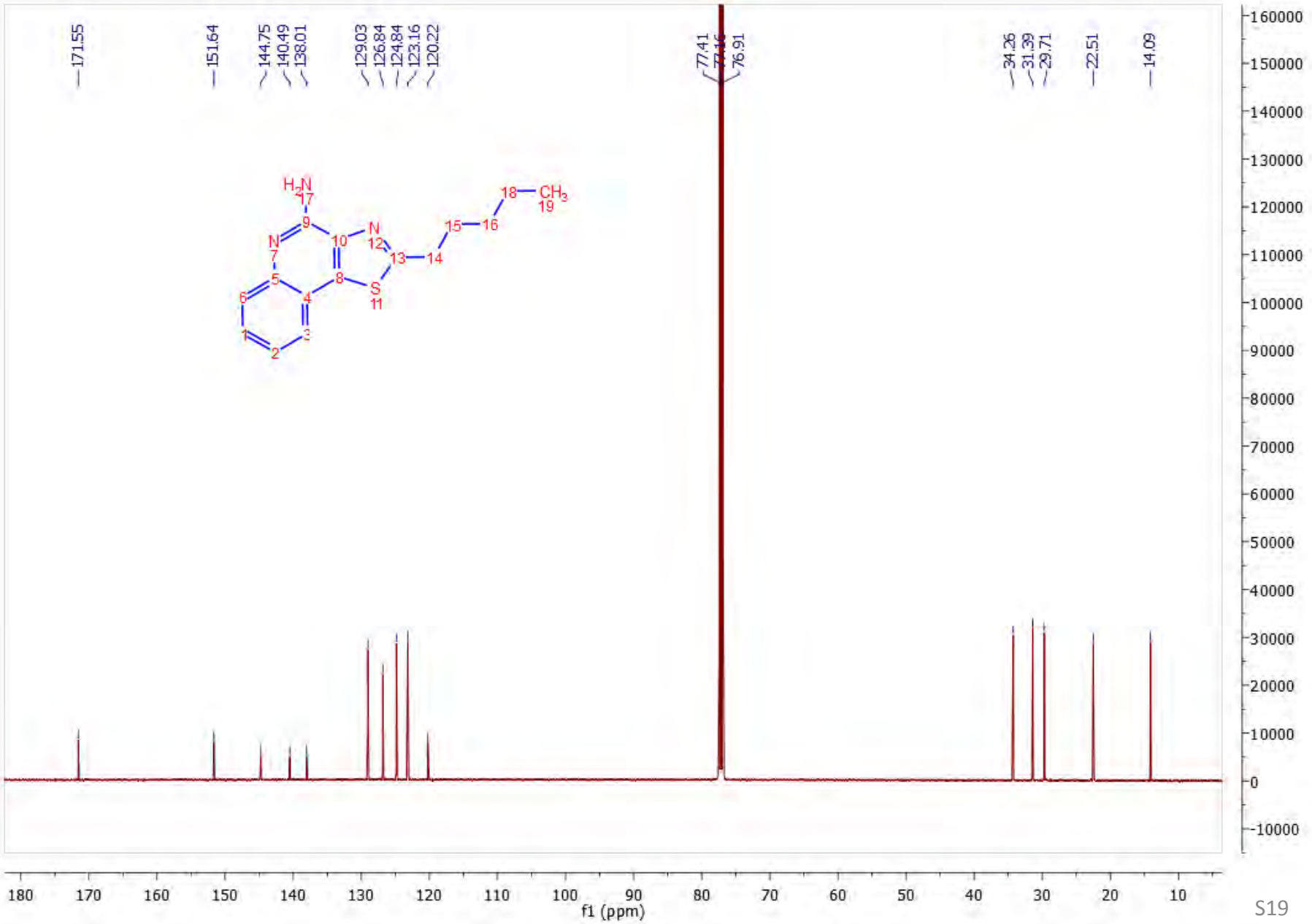

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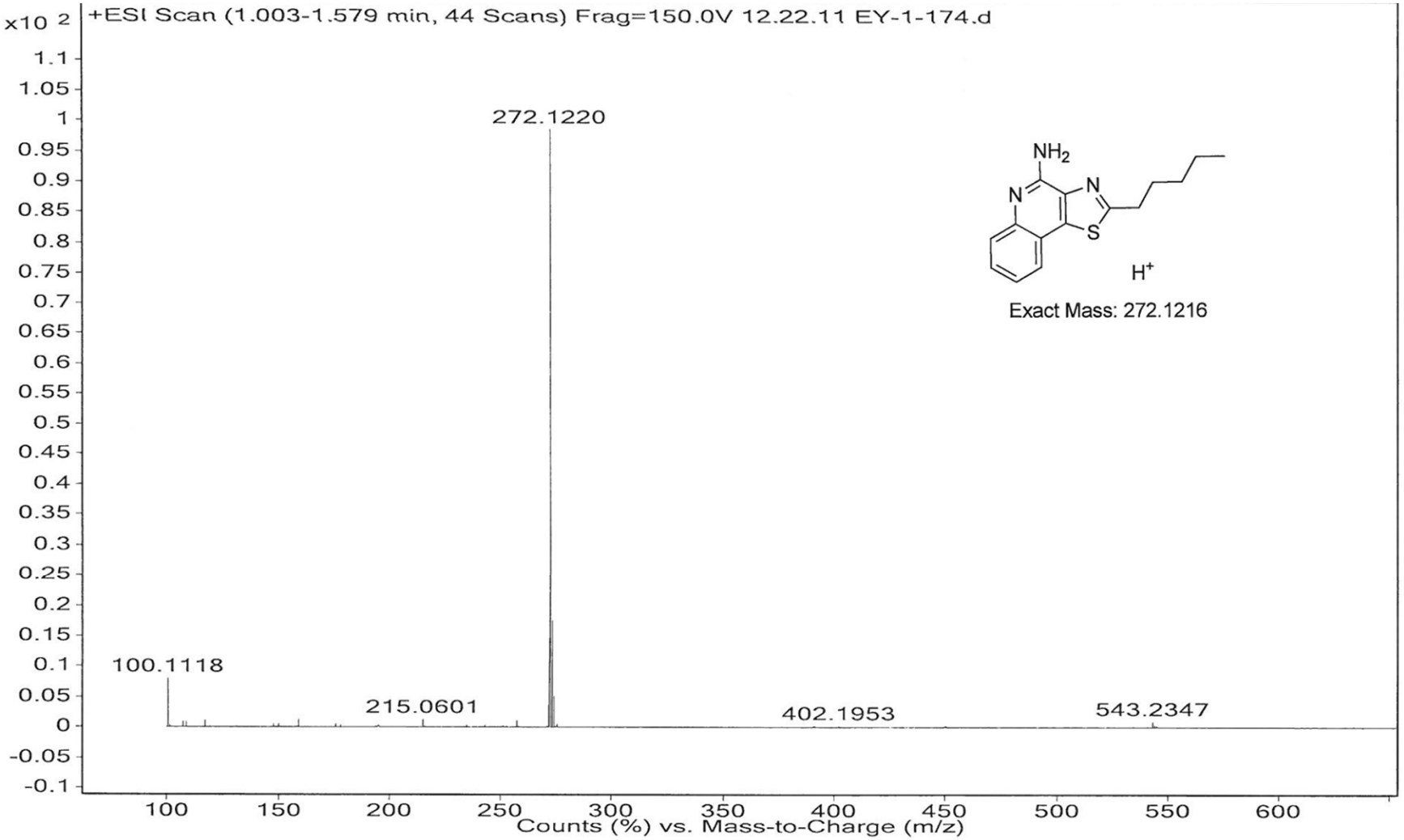

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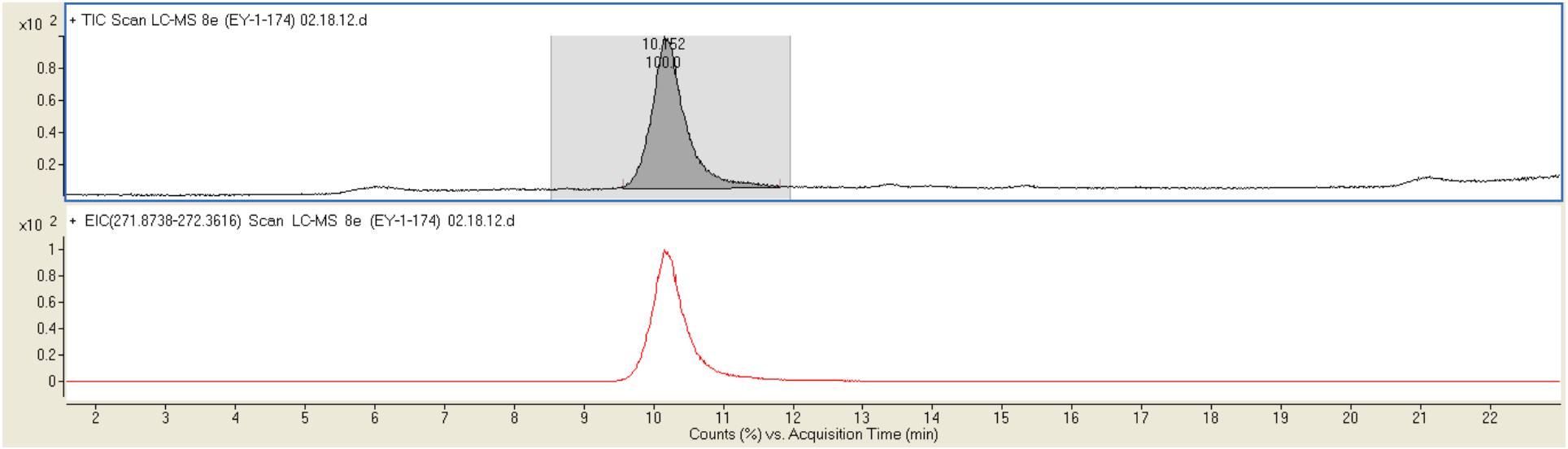

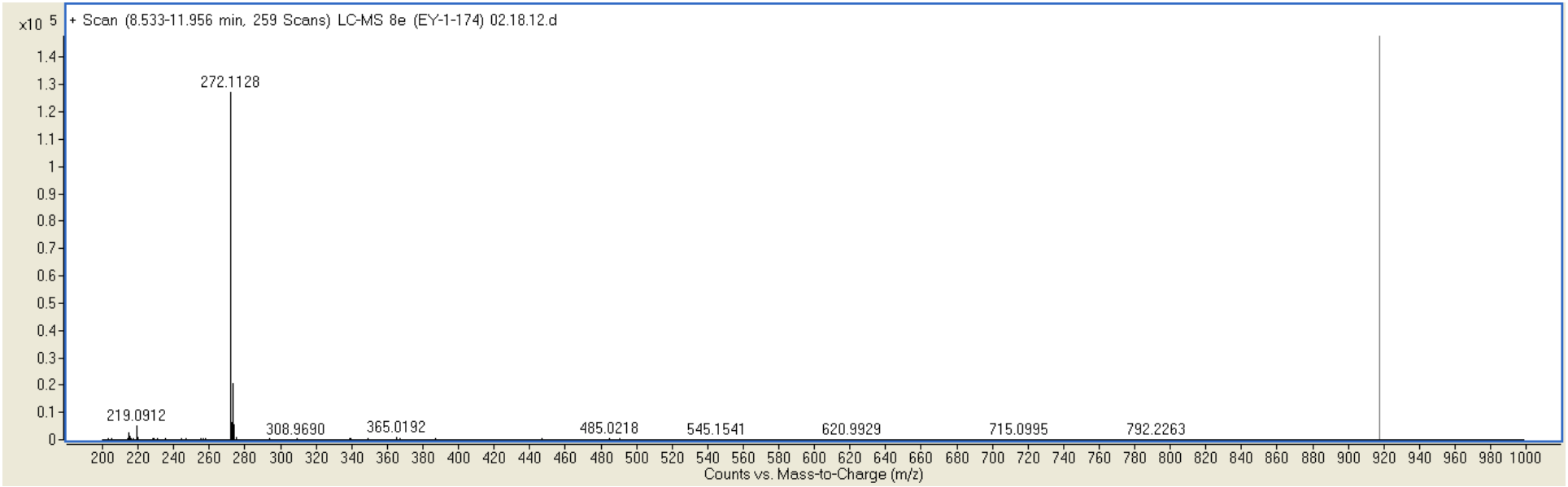

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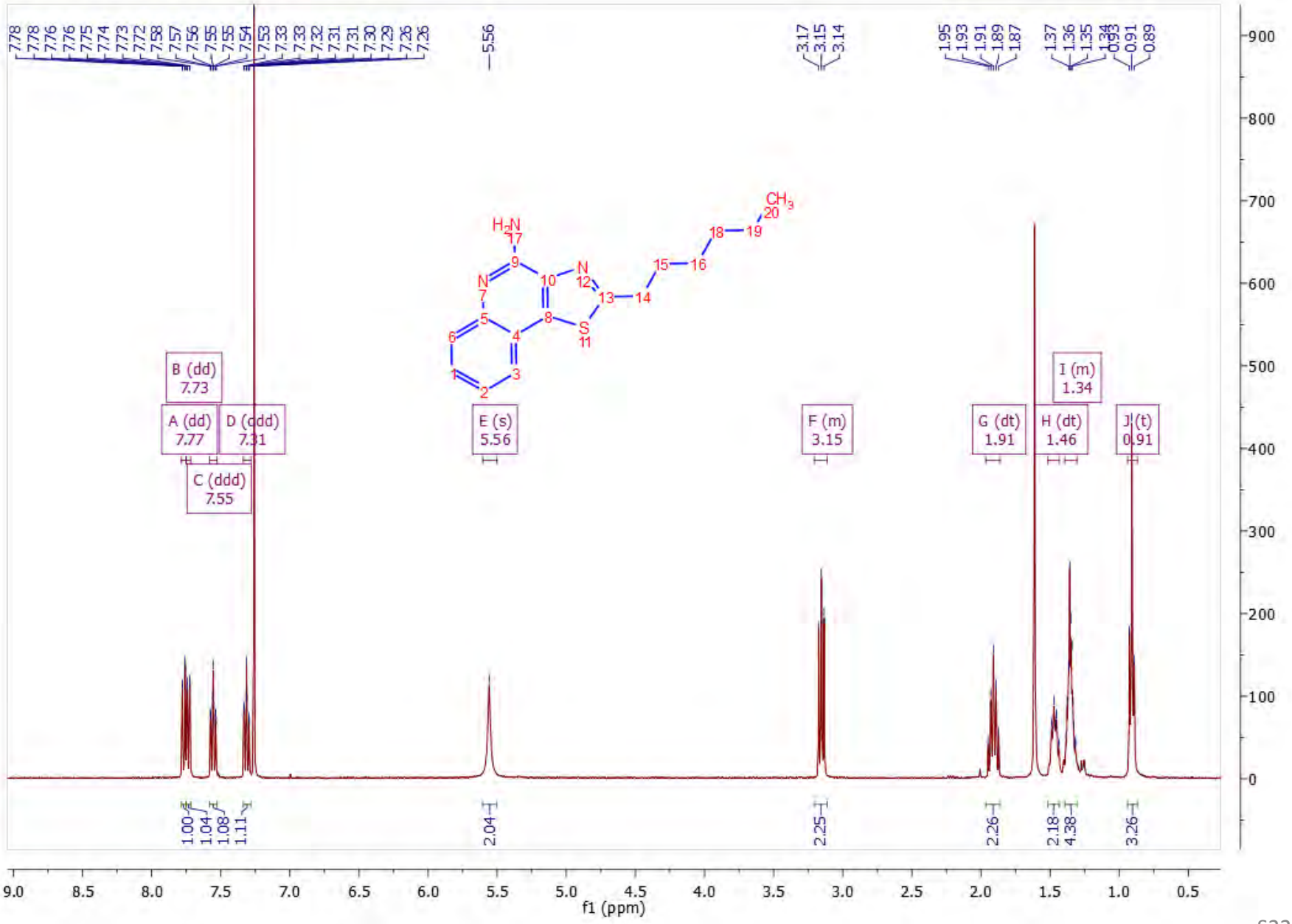

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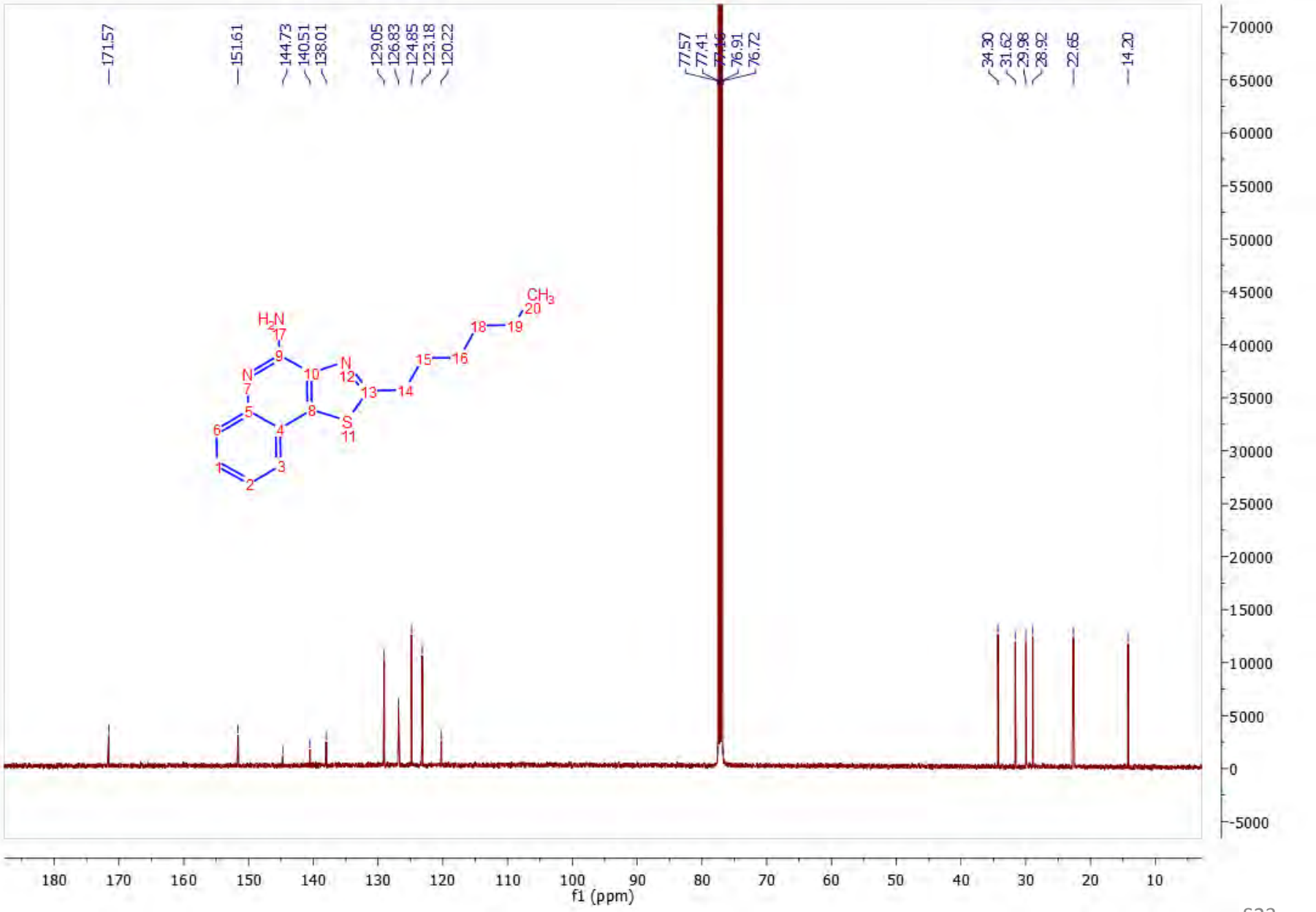

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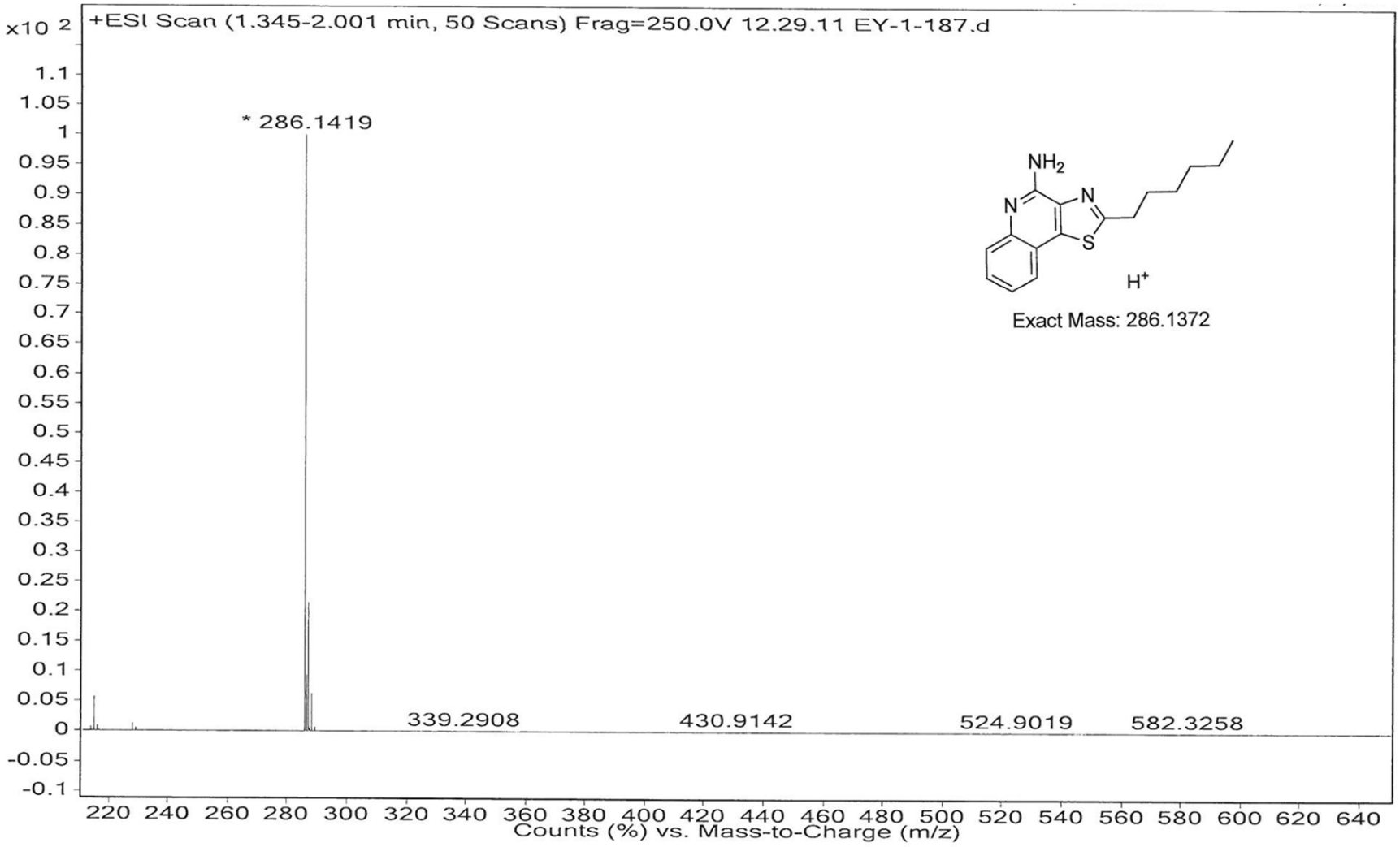

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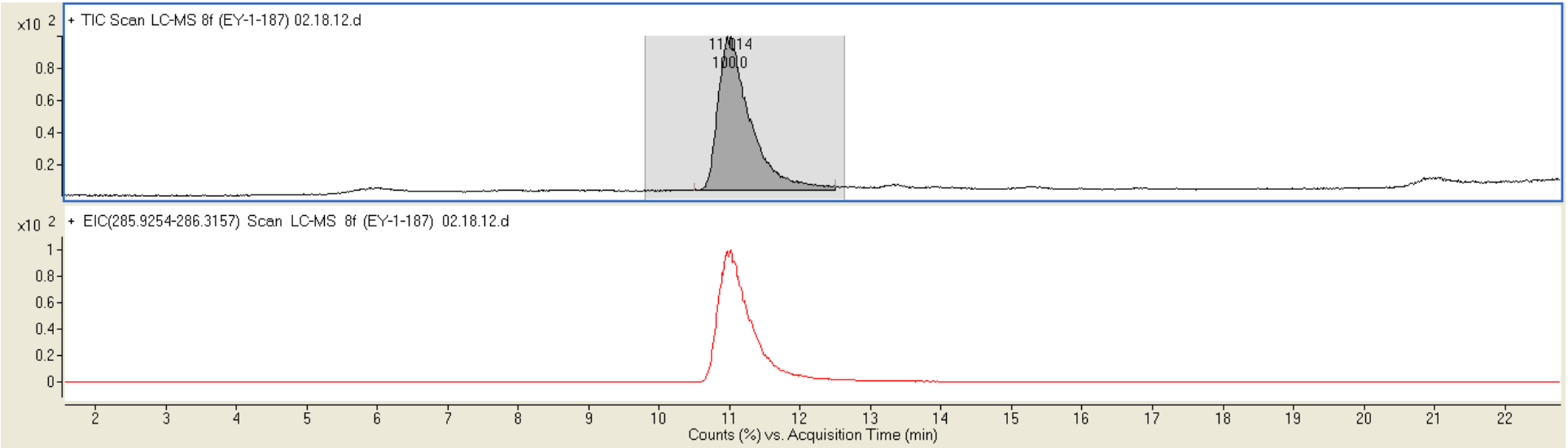

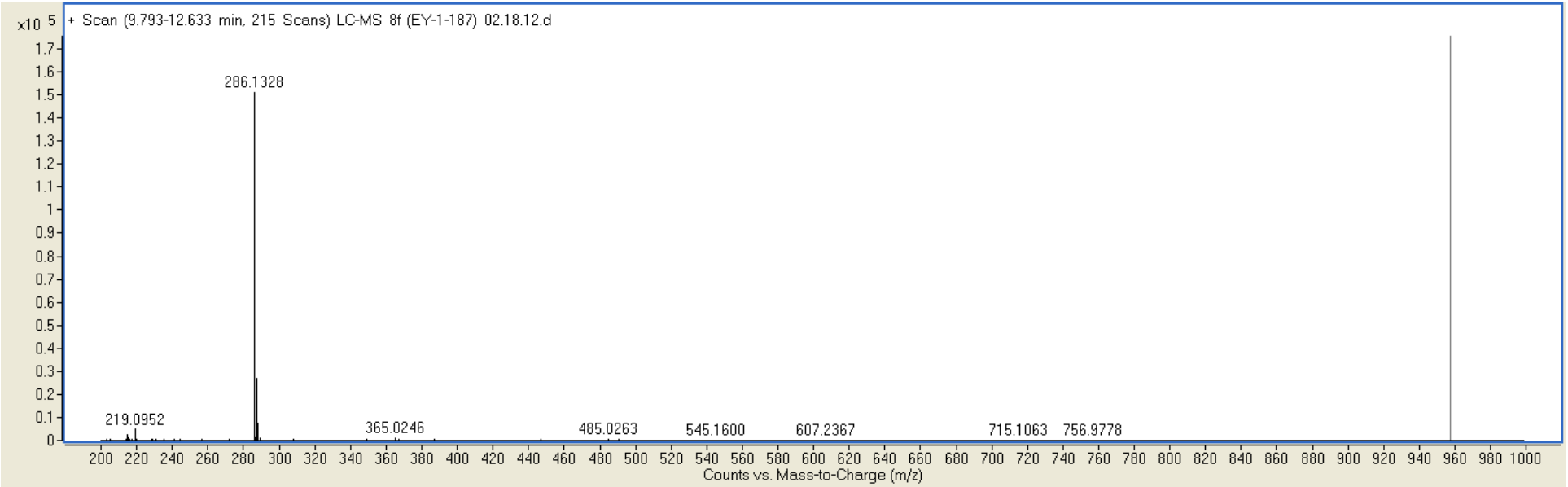

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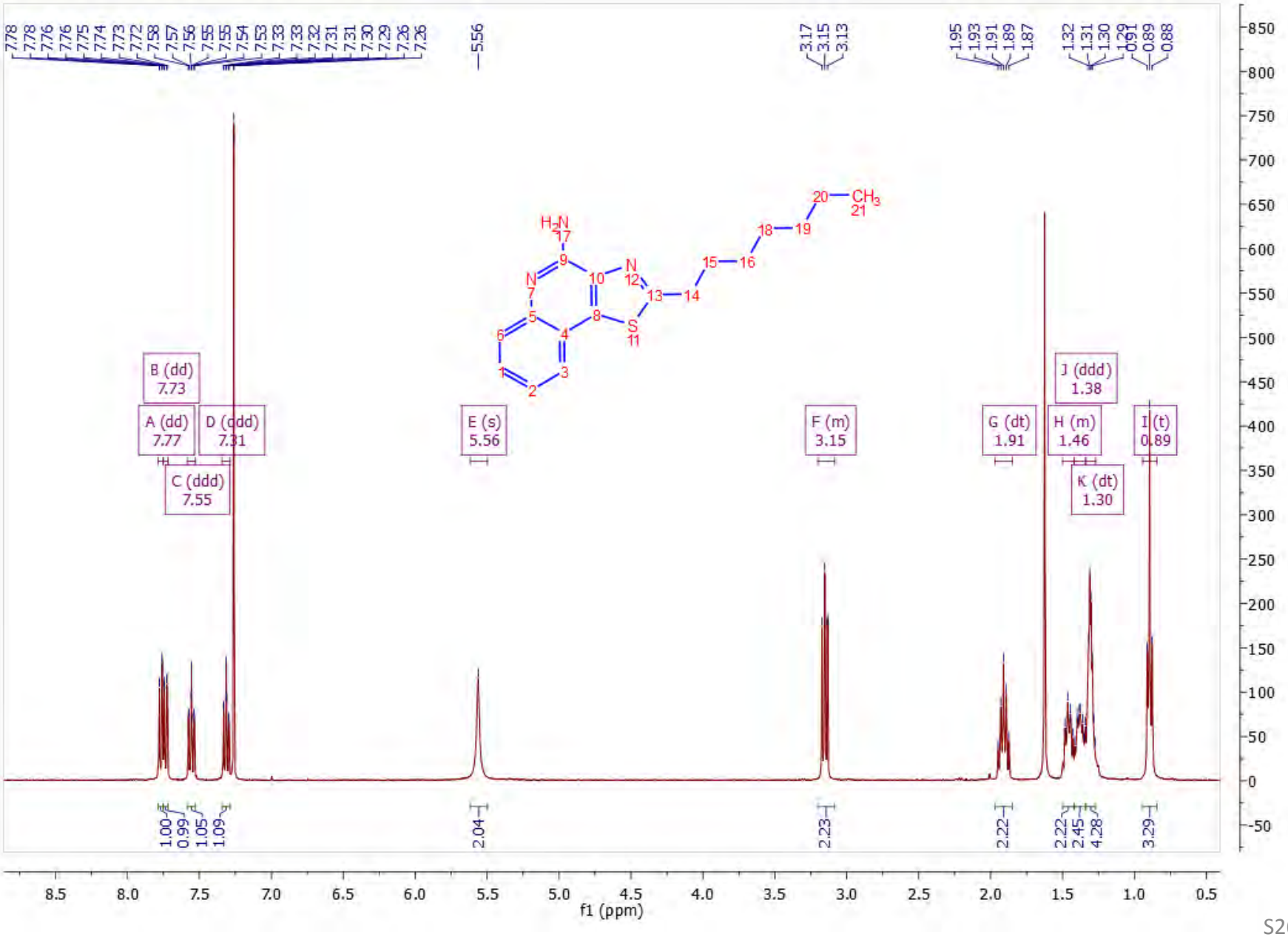

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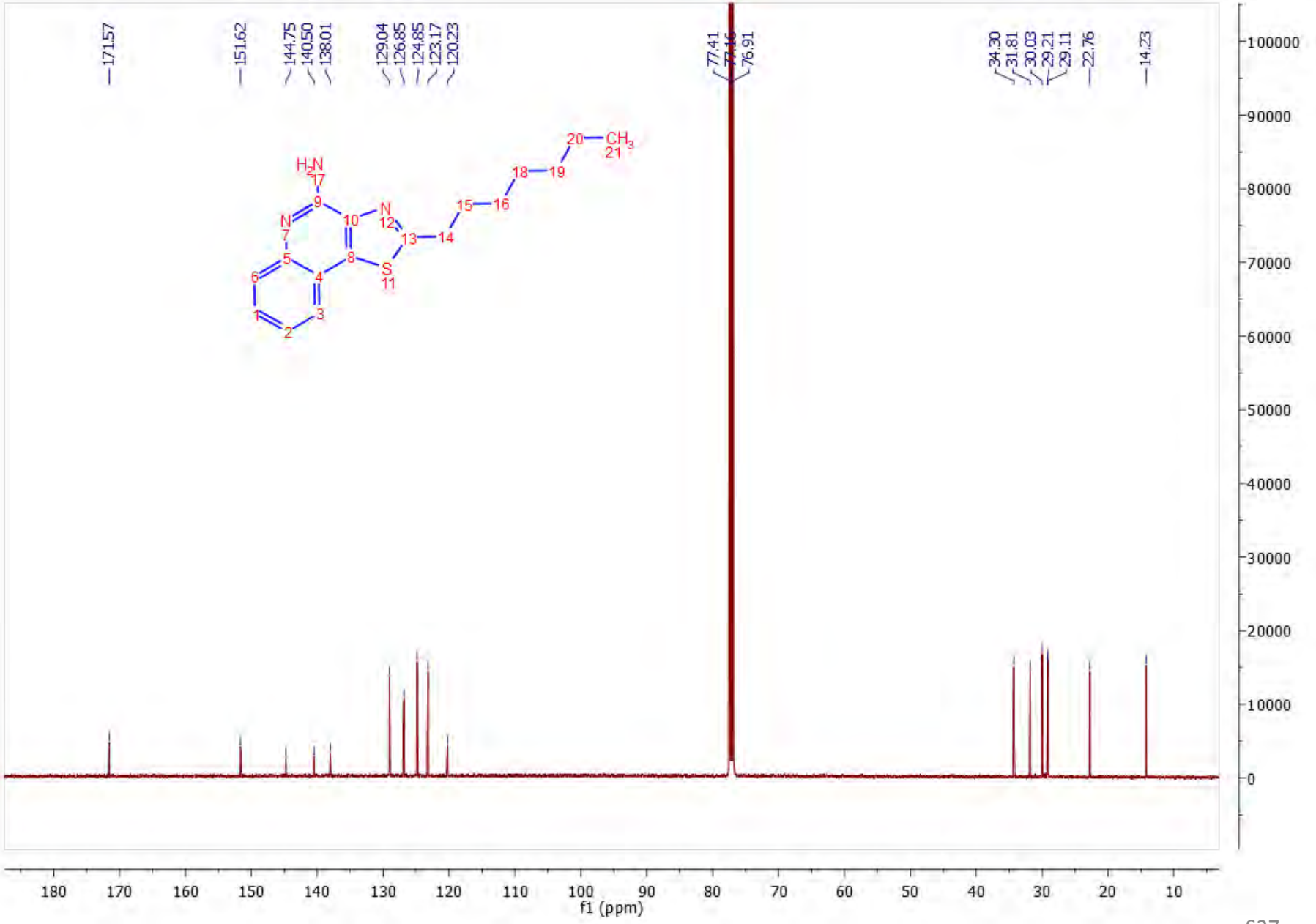

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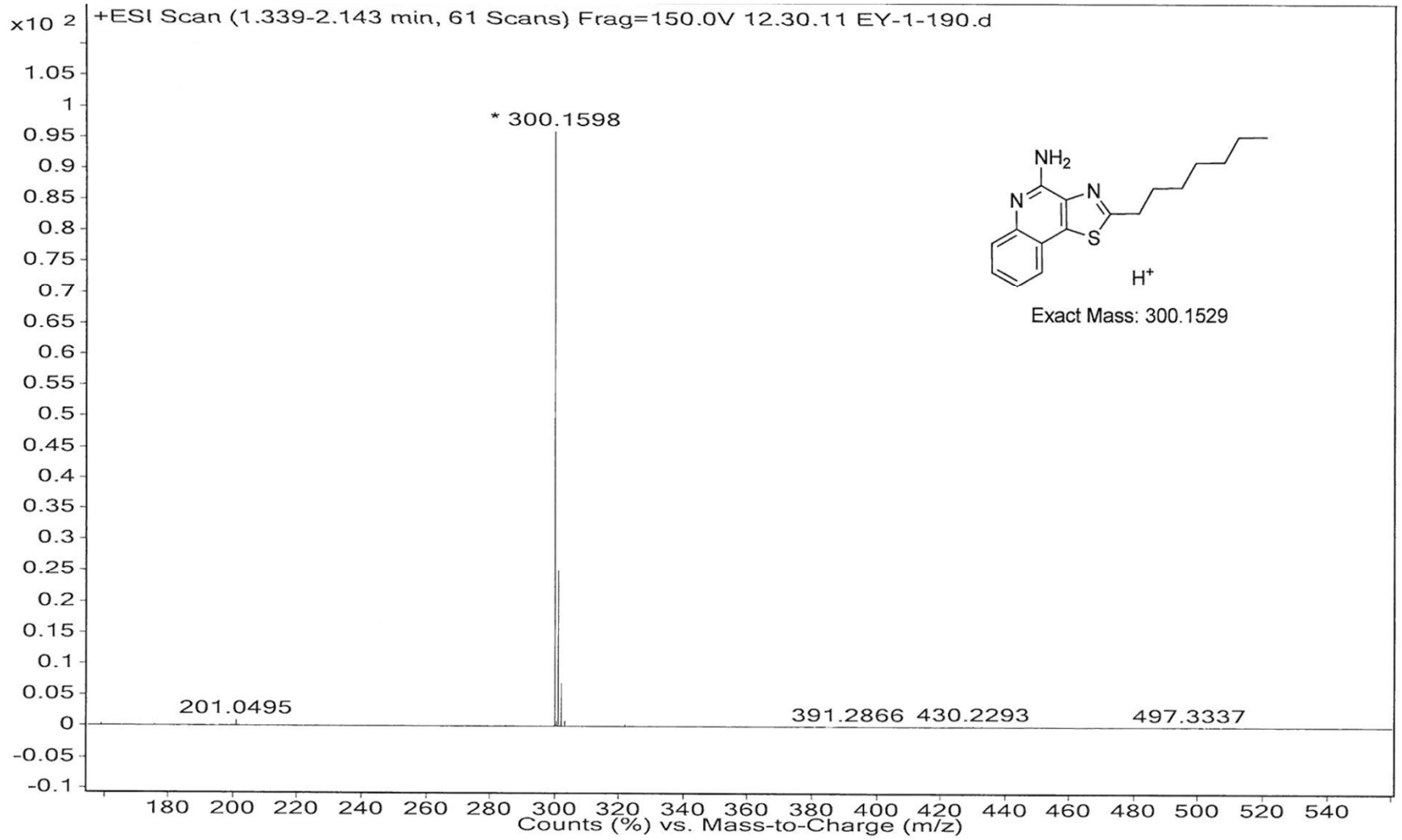

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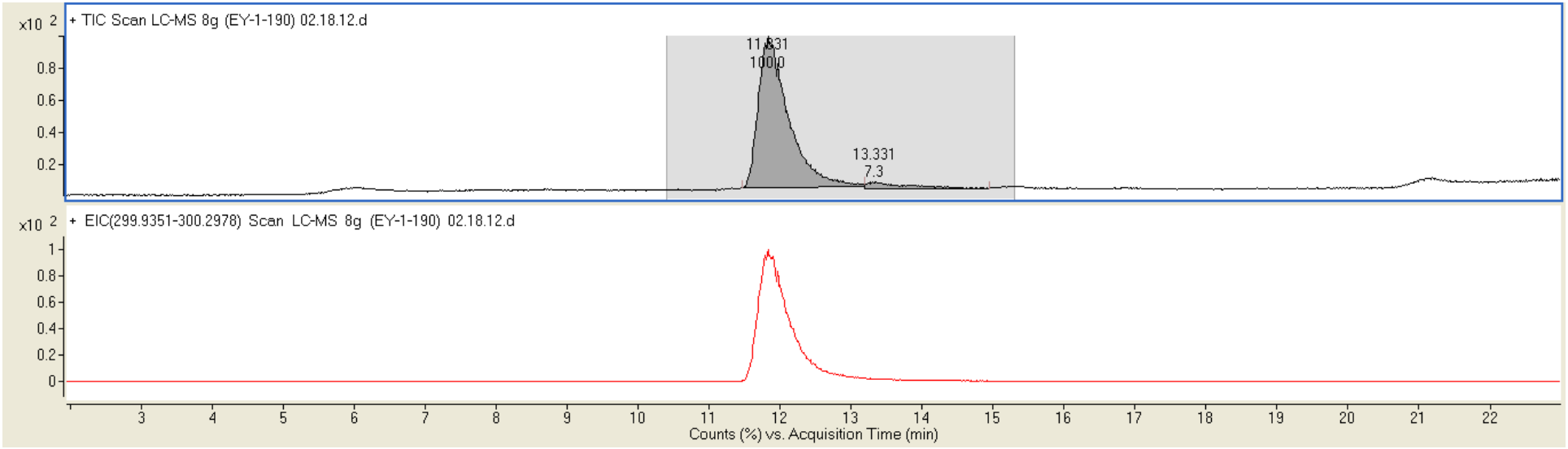

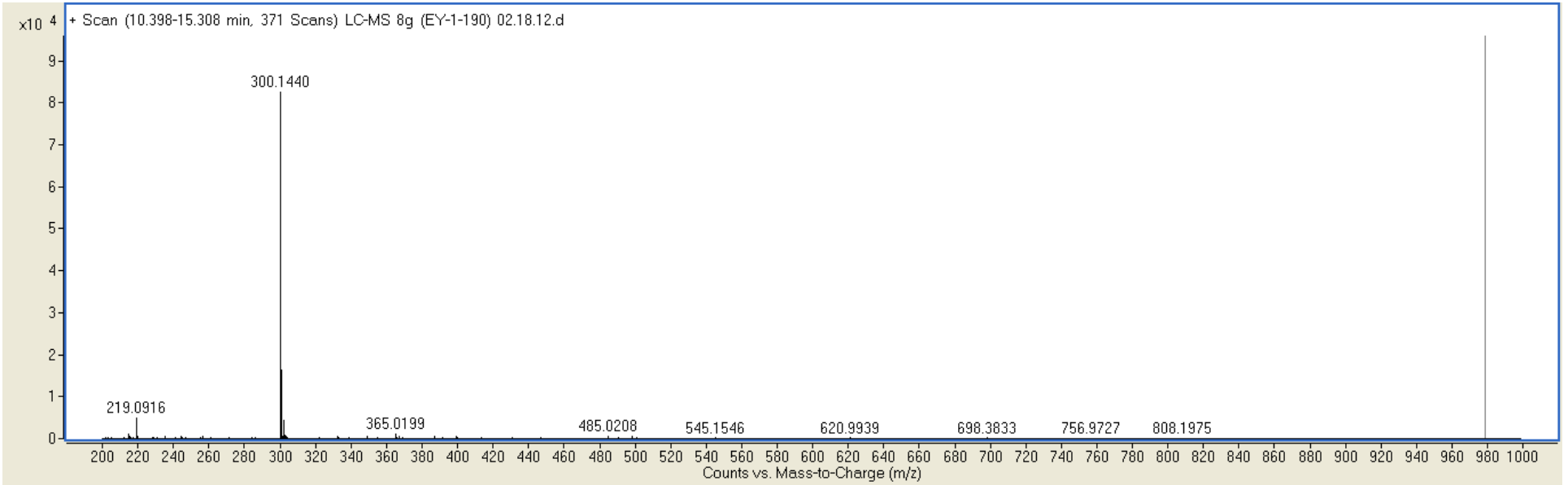

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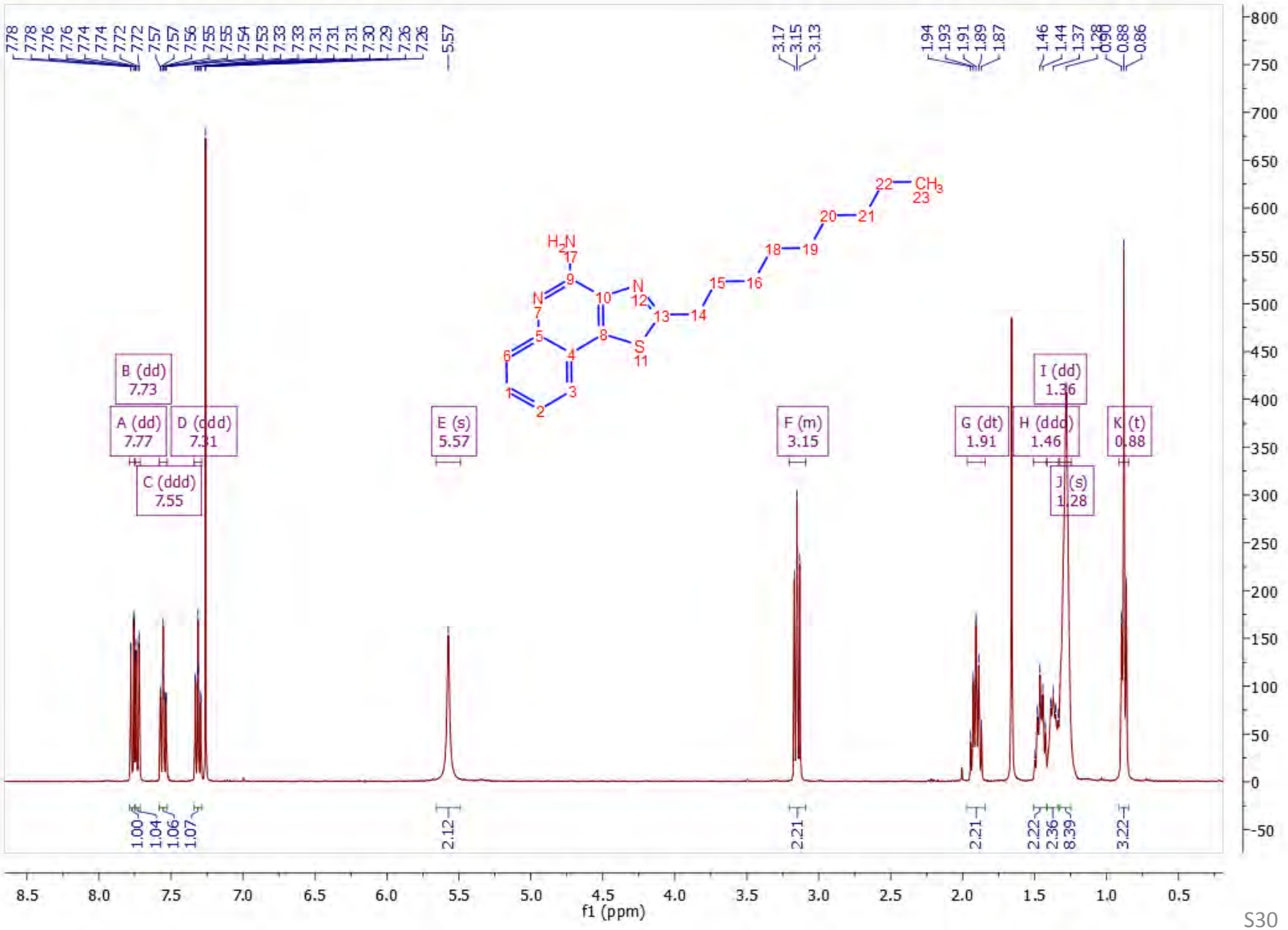

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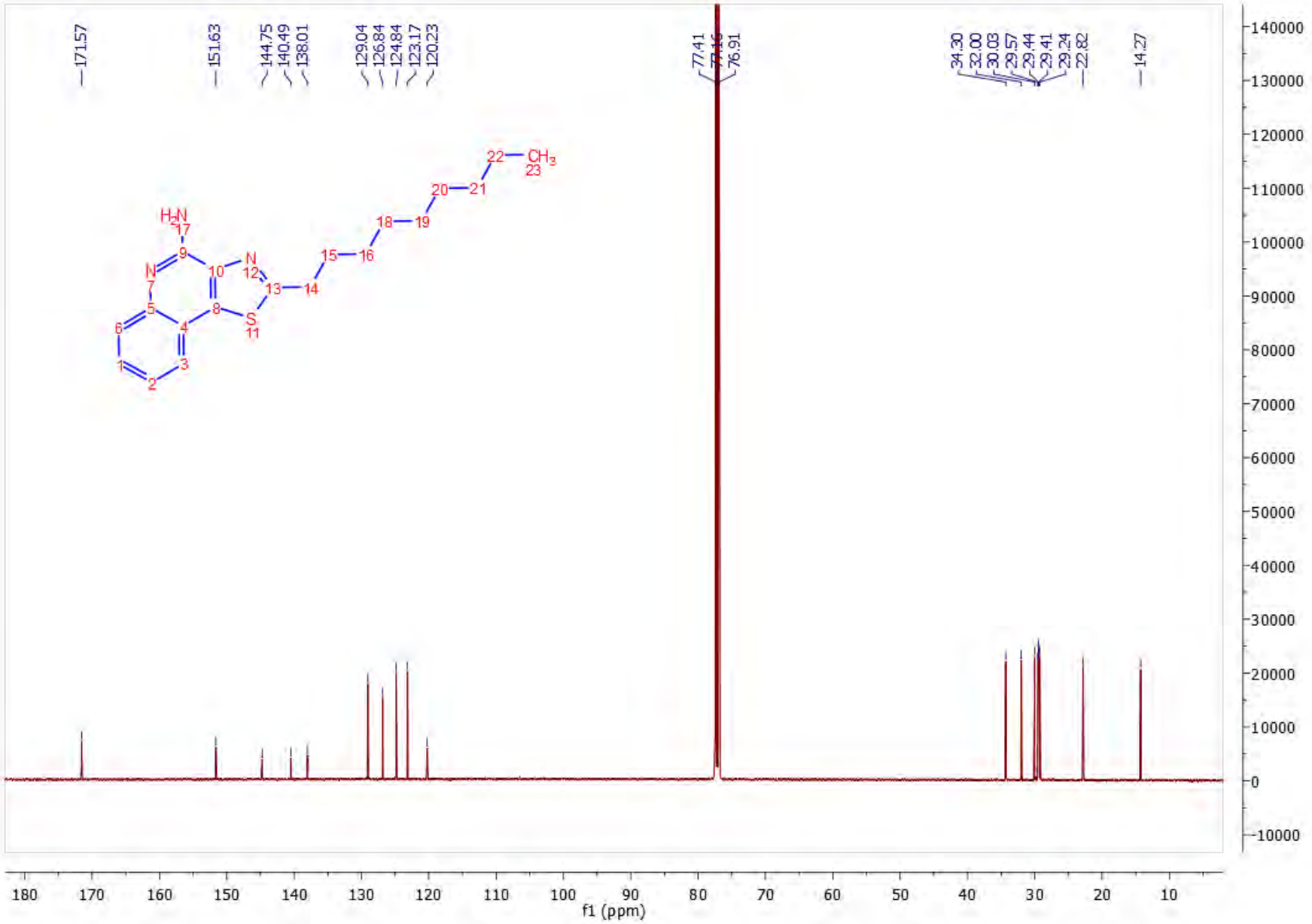

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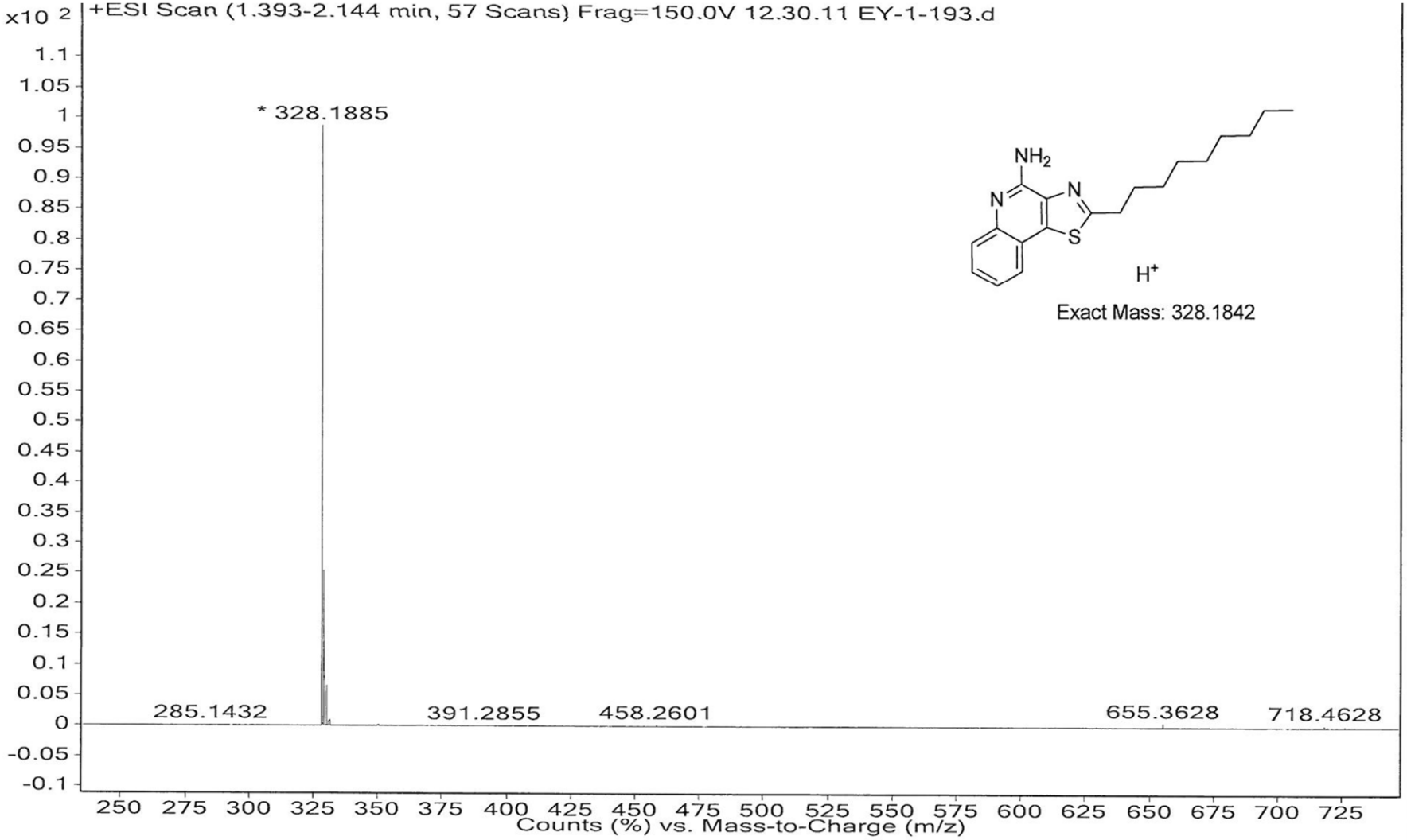

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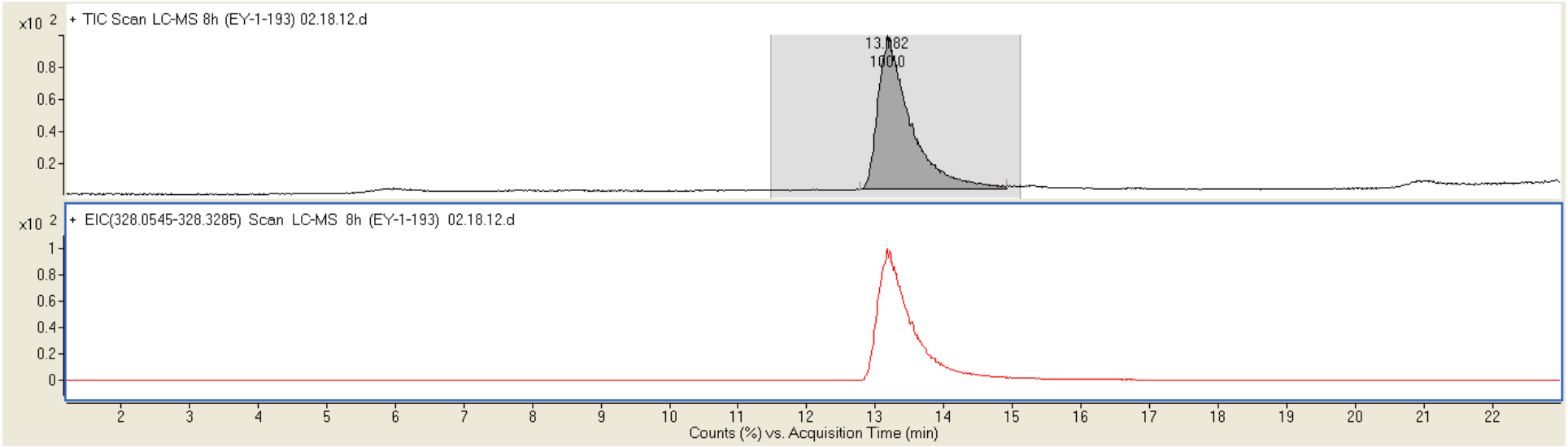

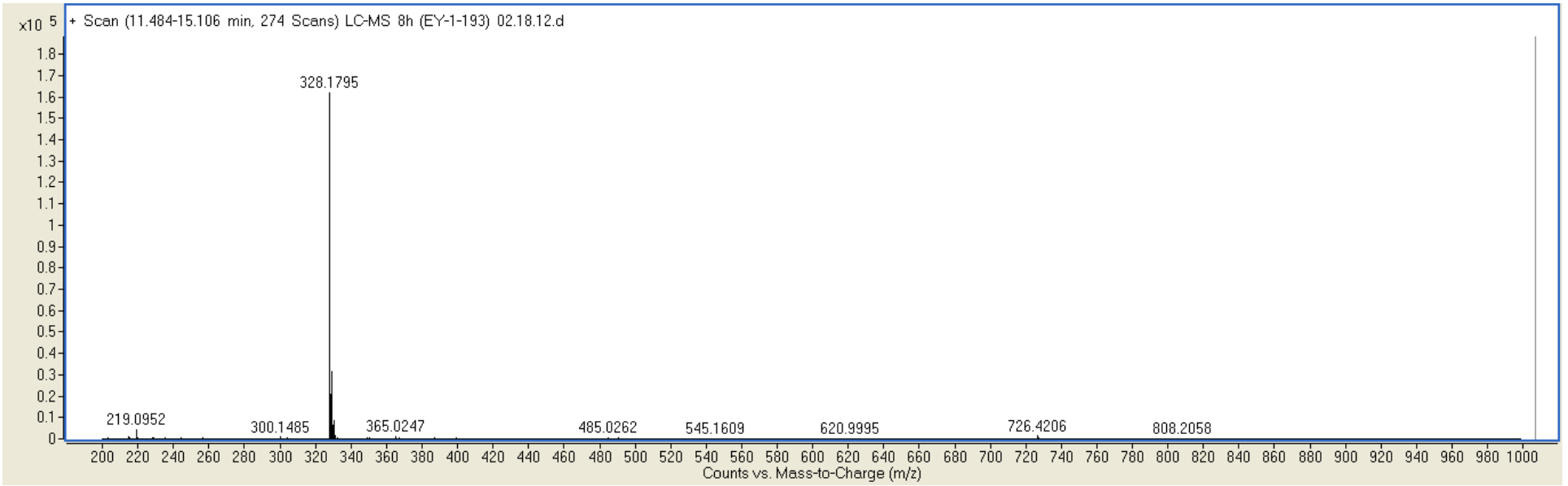

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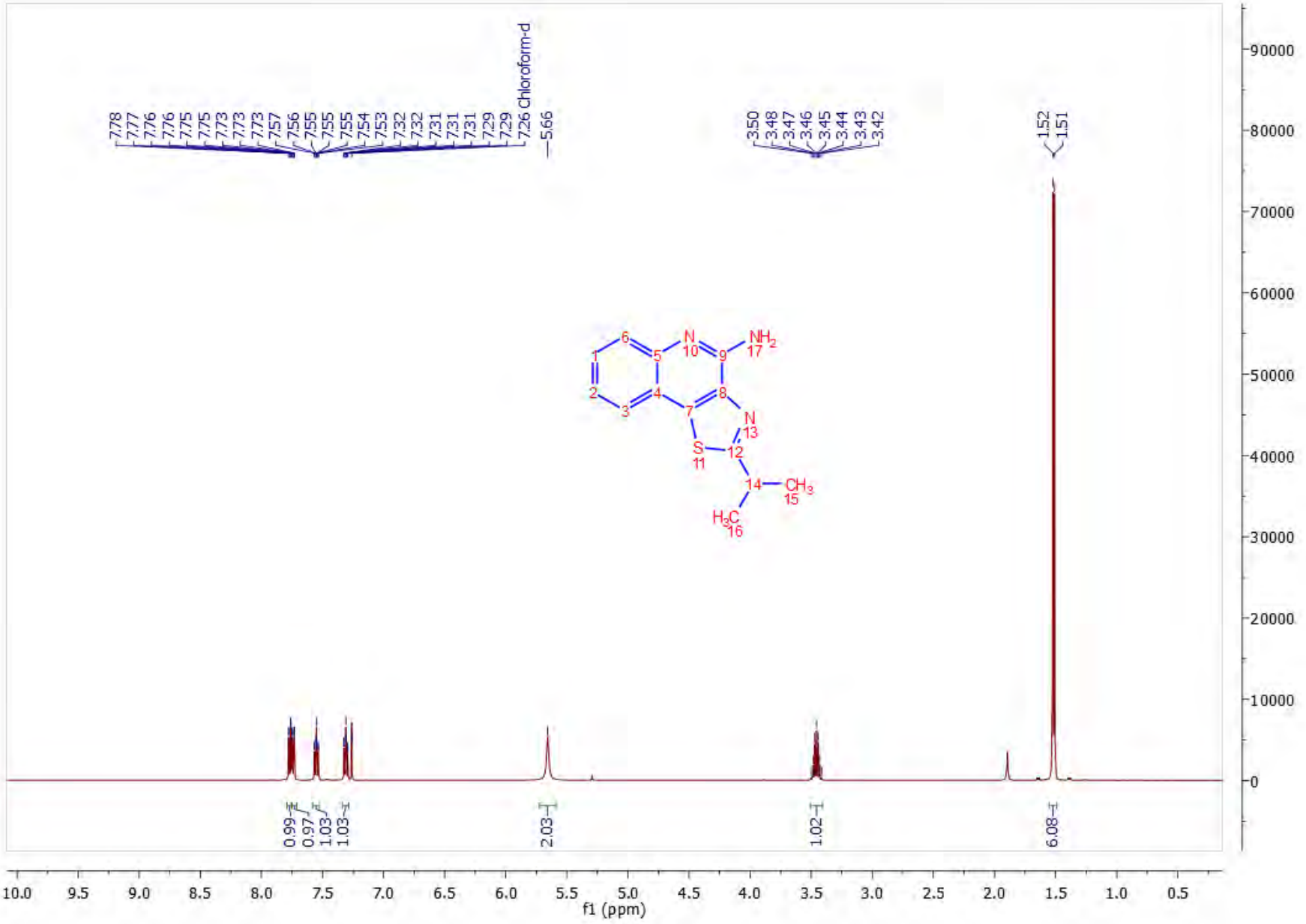

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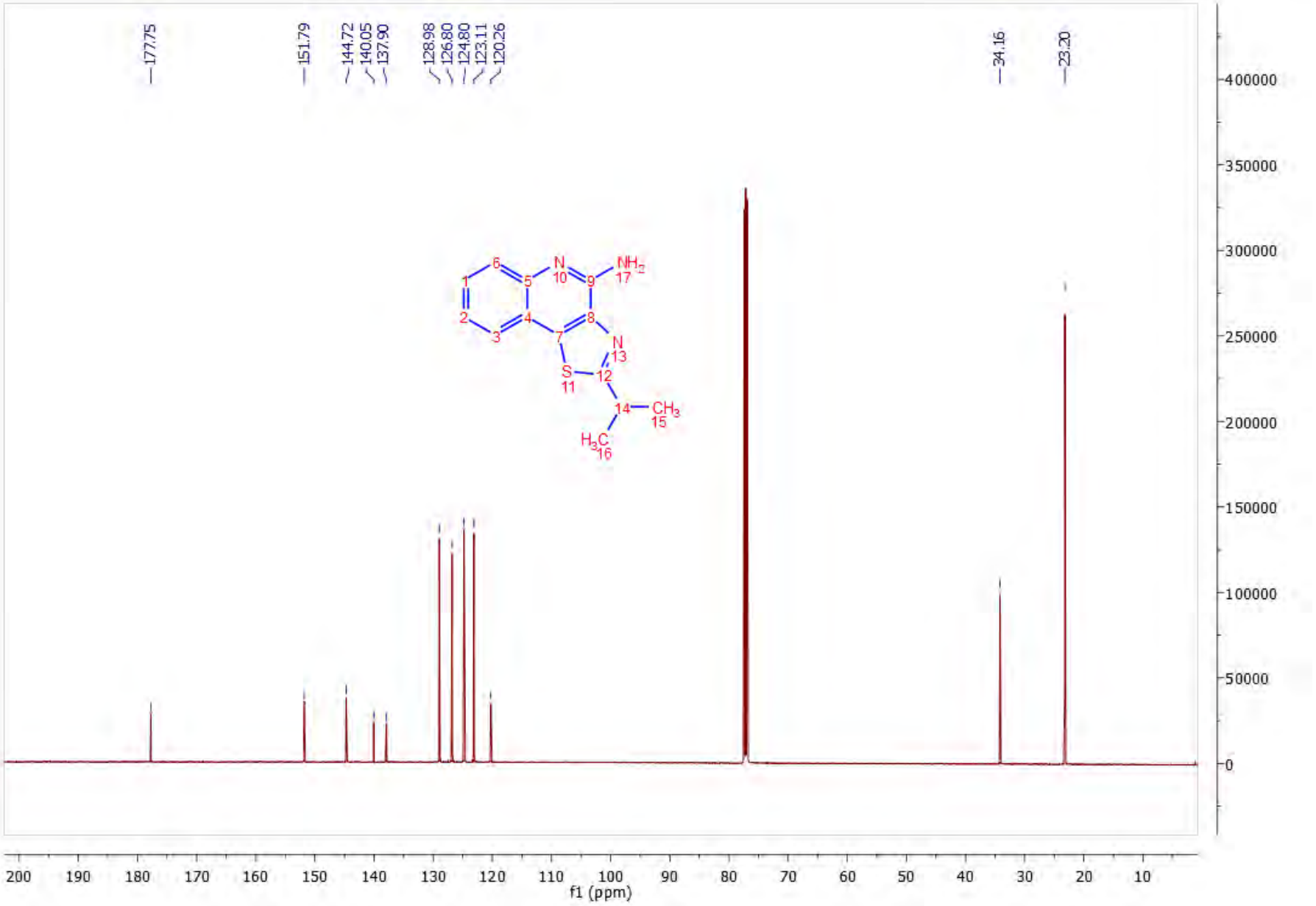

8i MS

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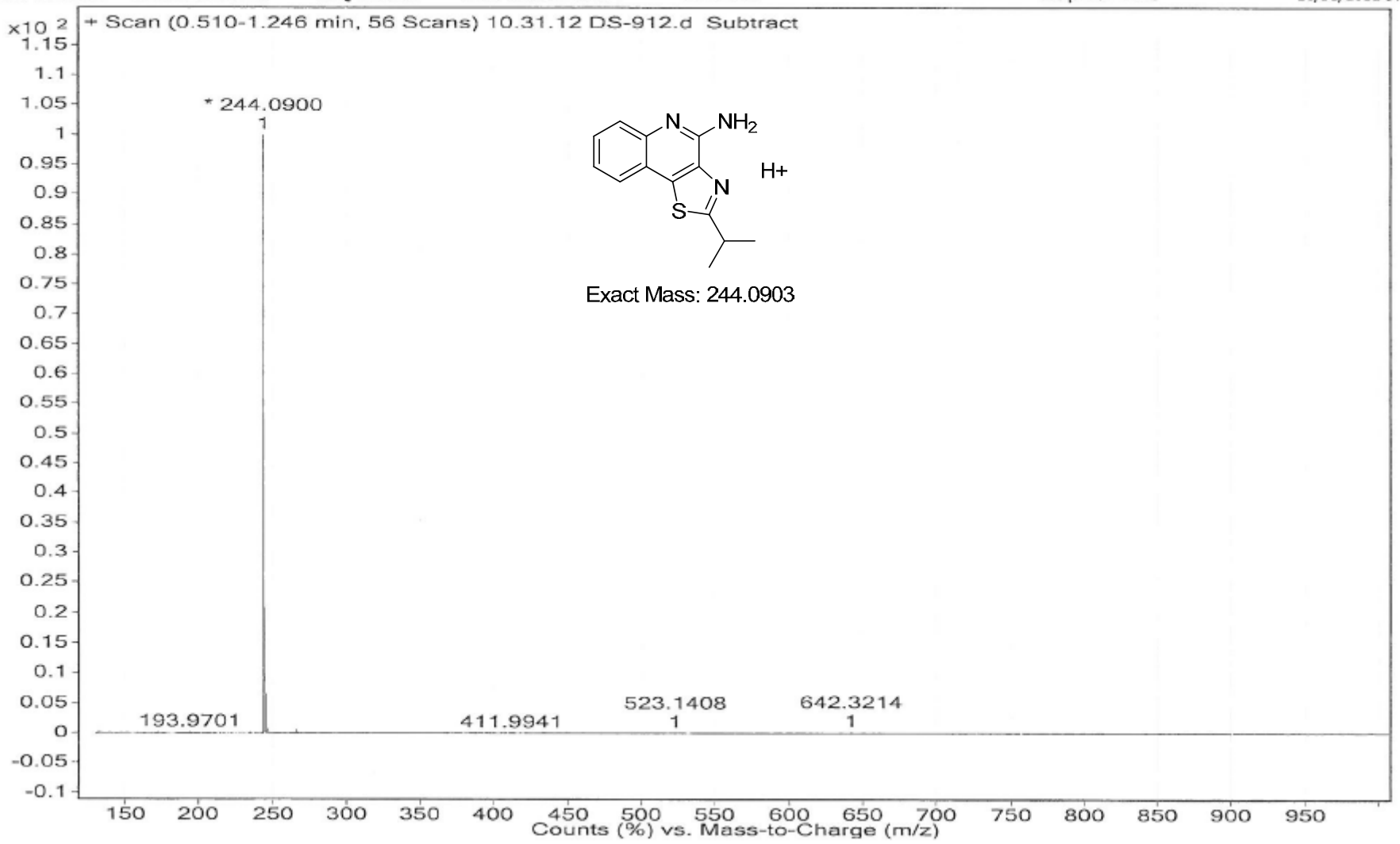

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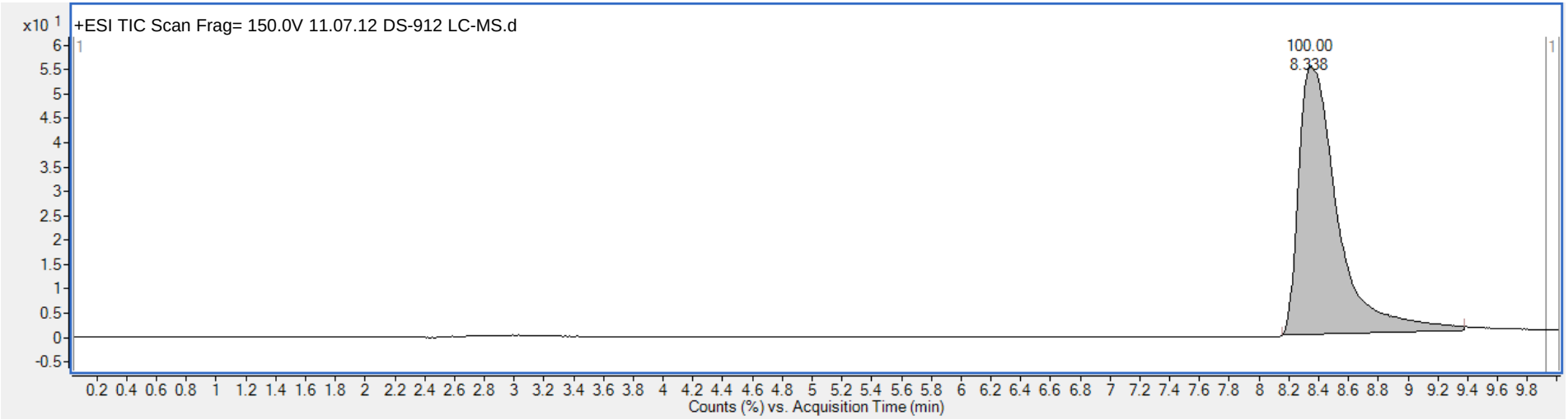

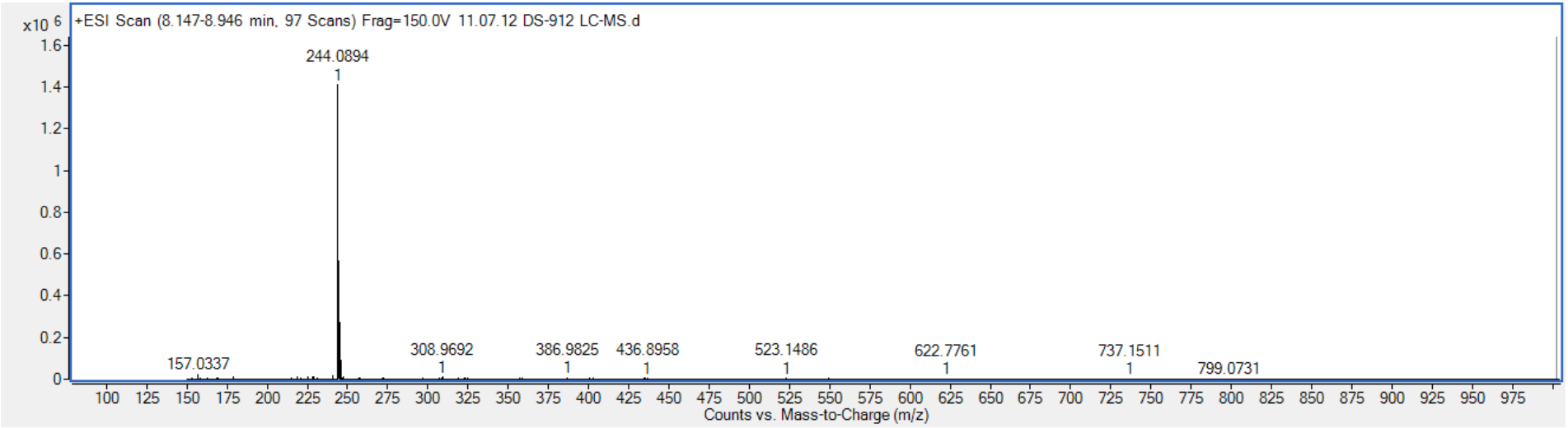

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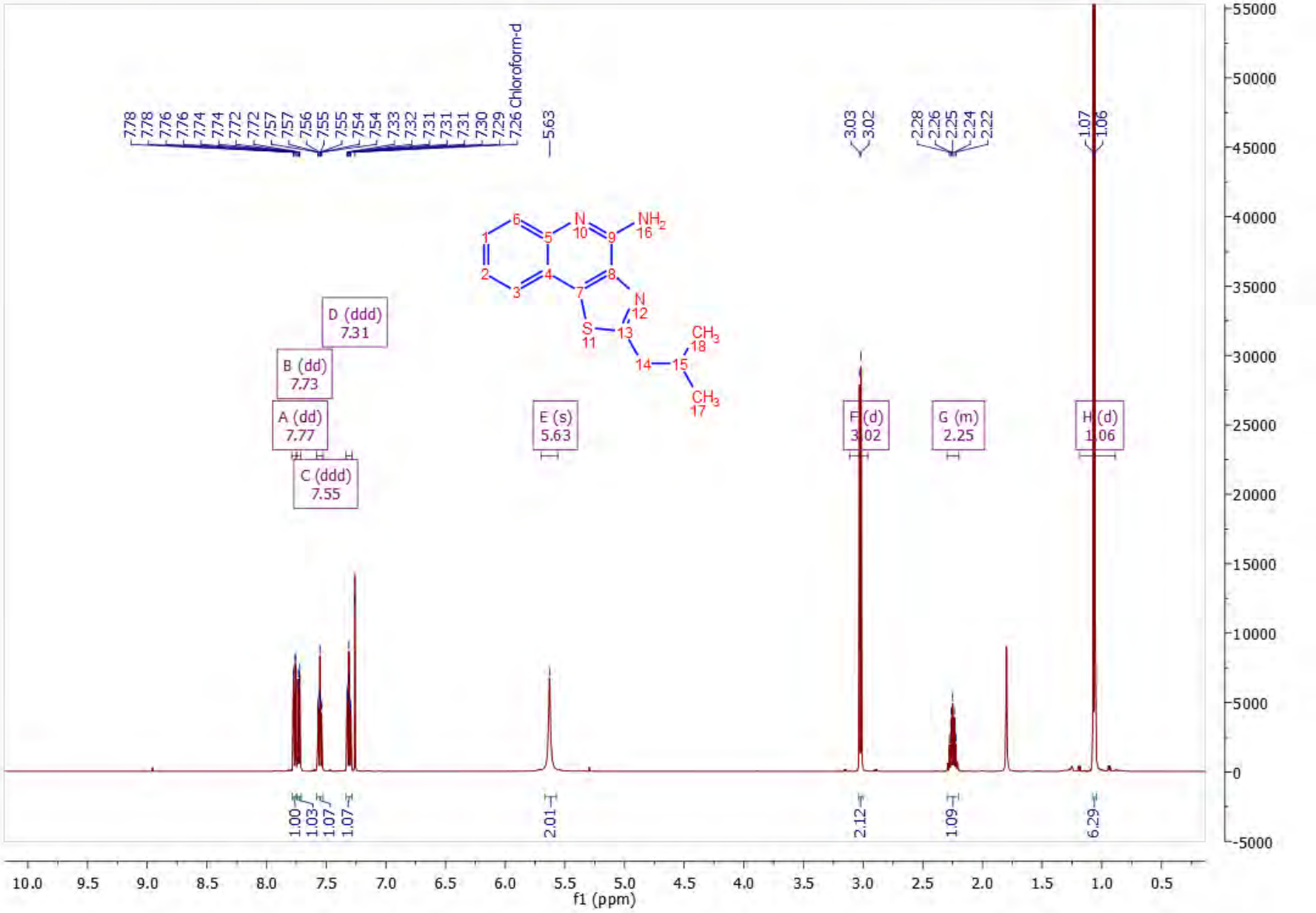
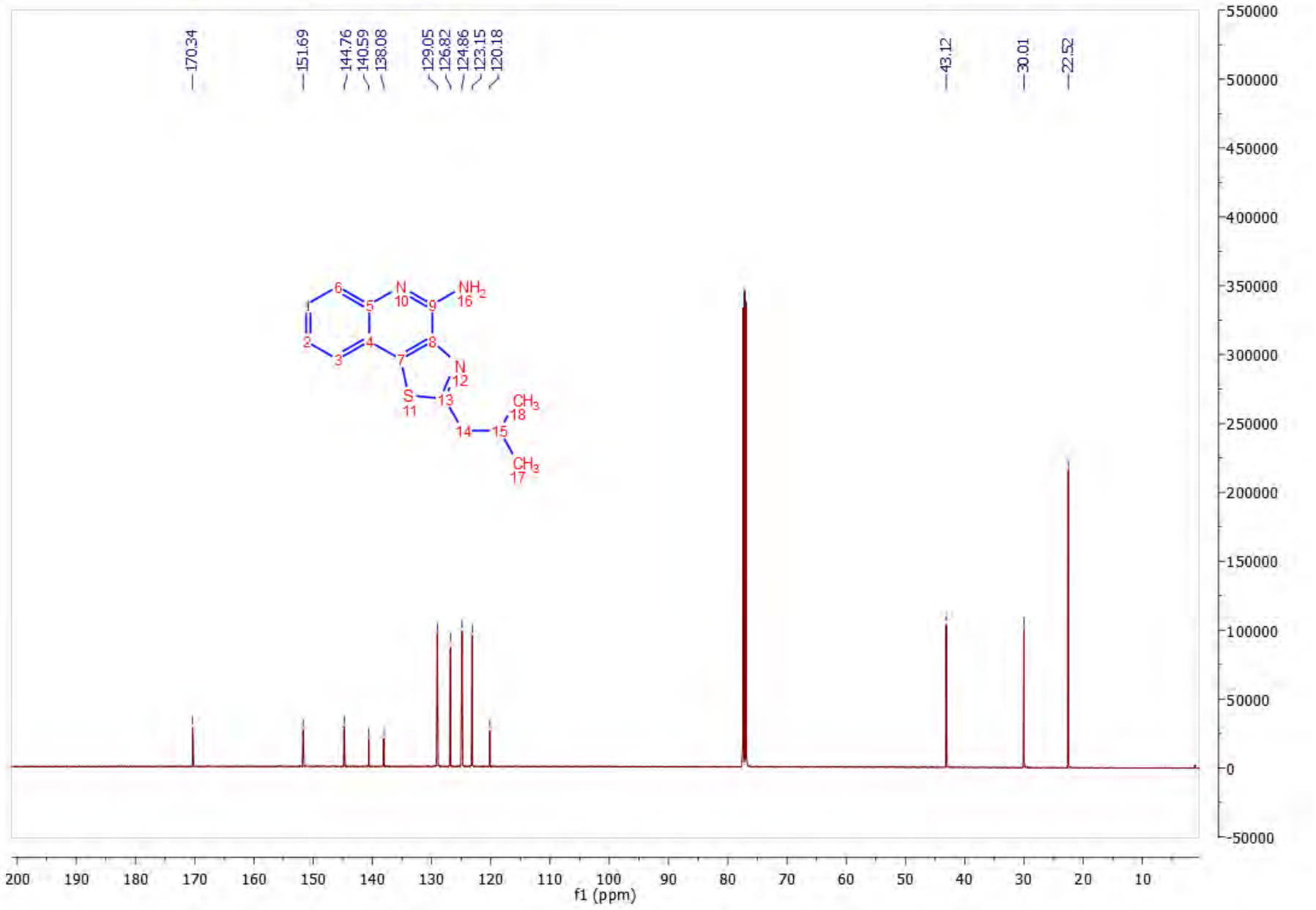


8j ^{13}C NMR



8j MS

Sample Name	10.17.12 DS-908 tube	Position	Vial 2	Instrument Name	Instrument 1	User Name	
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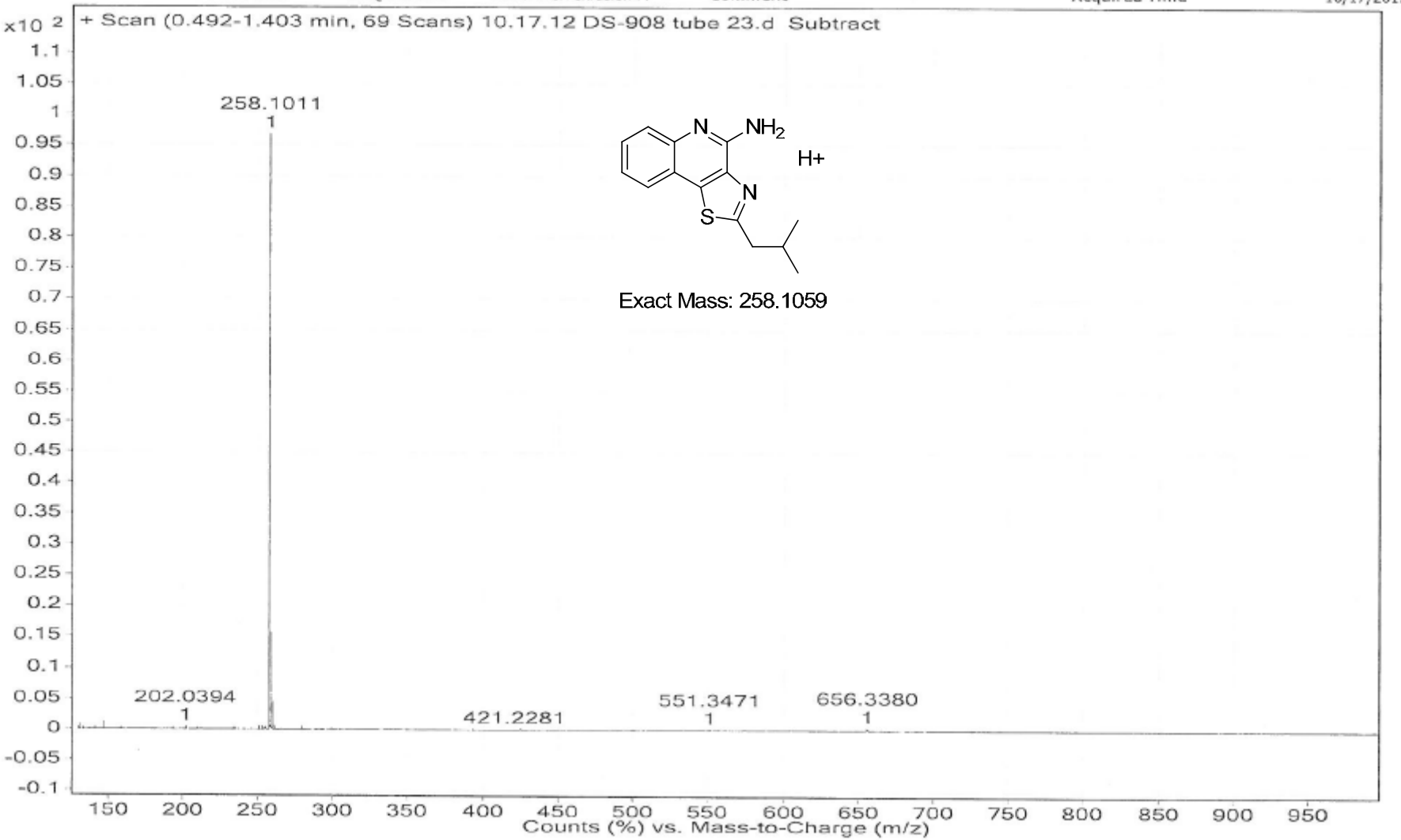
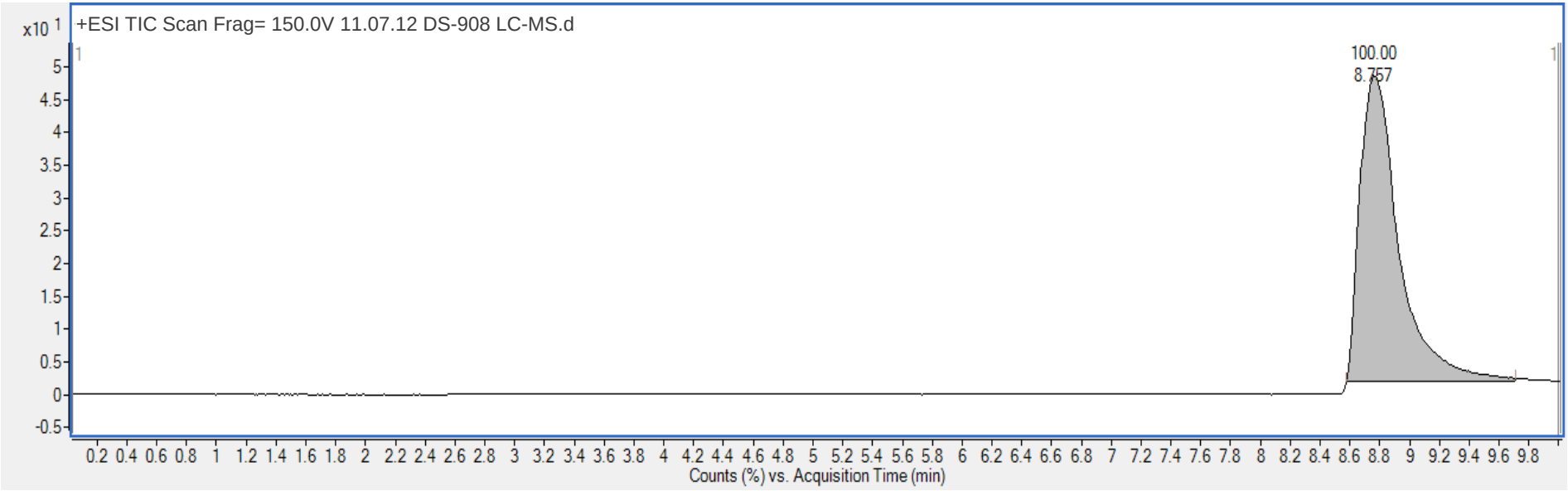
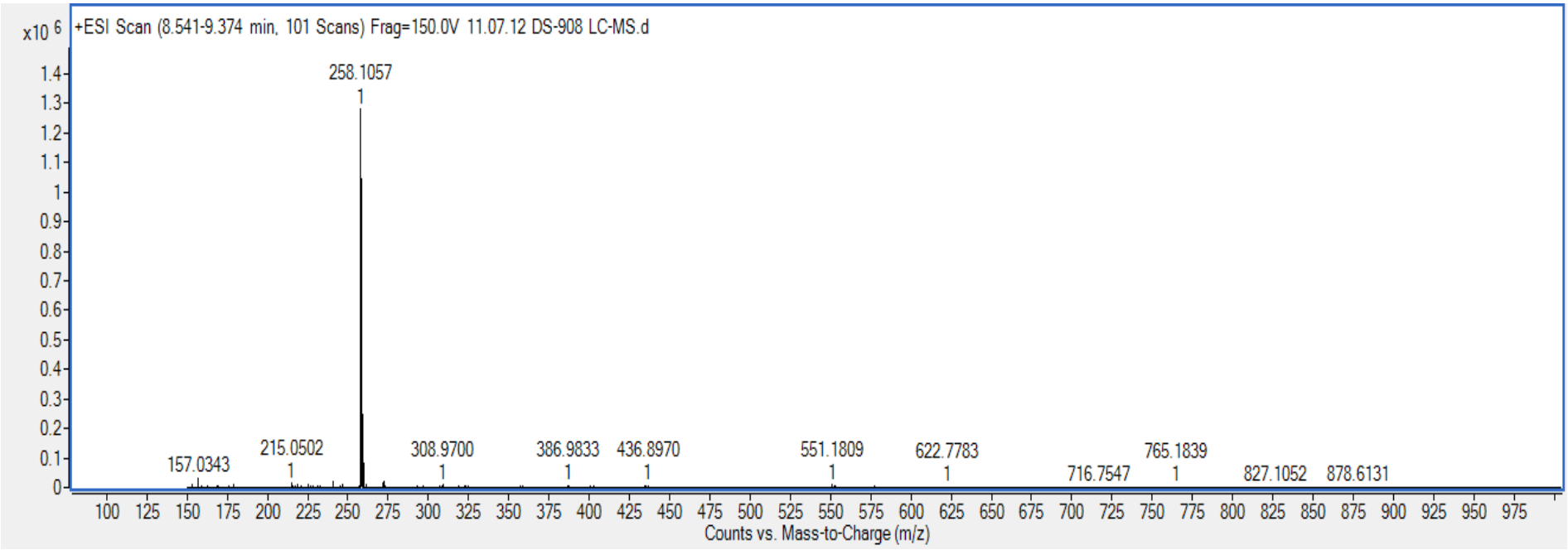
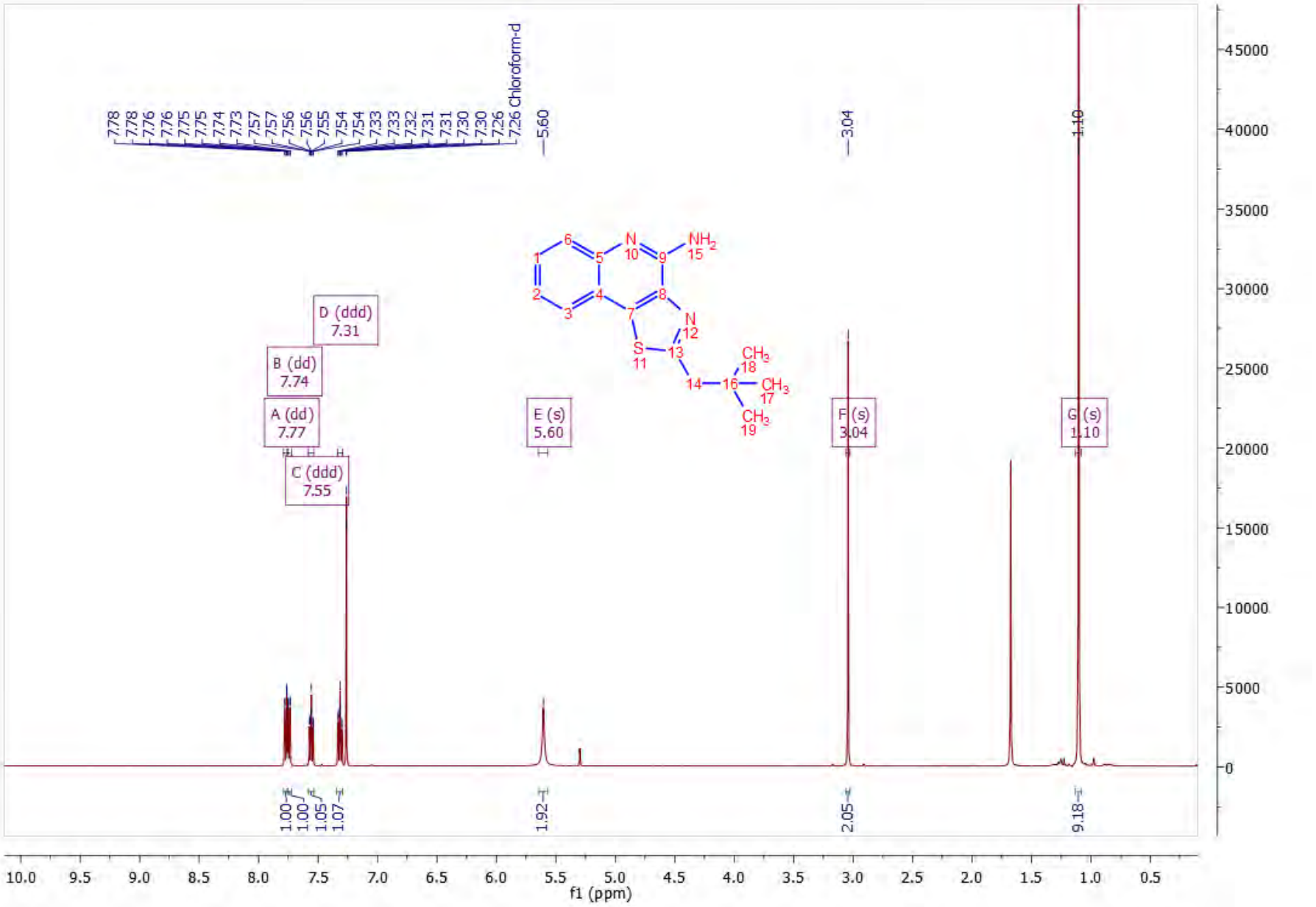


8j LC-MS





8k ^{1}H NMR



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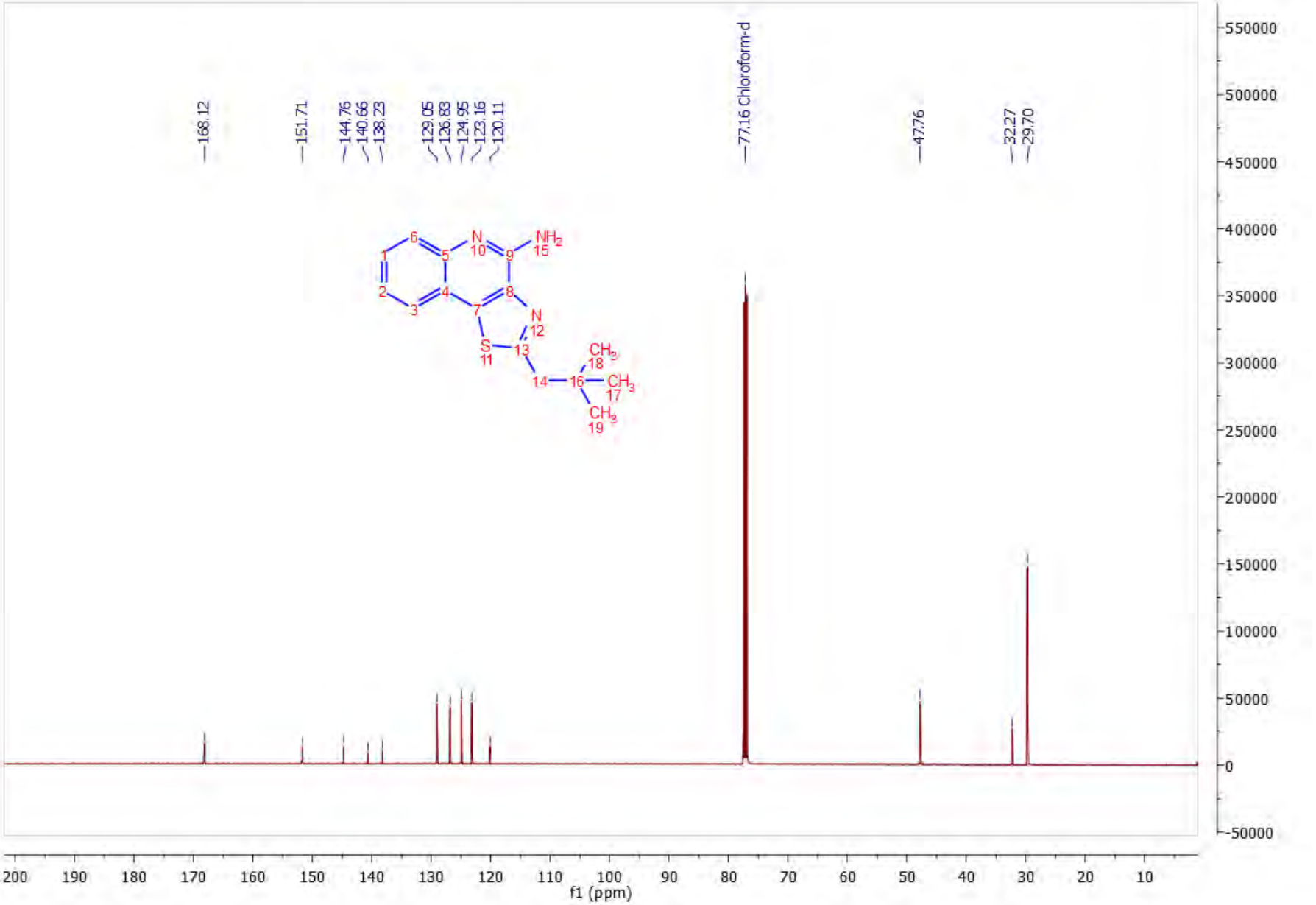

8k MS

Sample Name	10.17.12 ds909 tube	Position	Vial 2	Instrument Name	Instrument 1	User Name	
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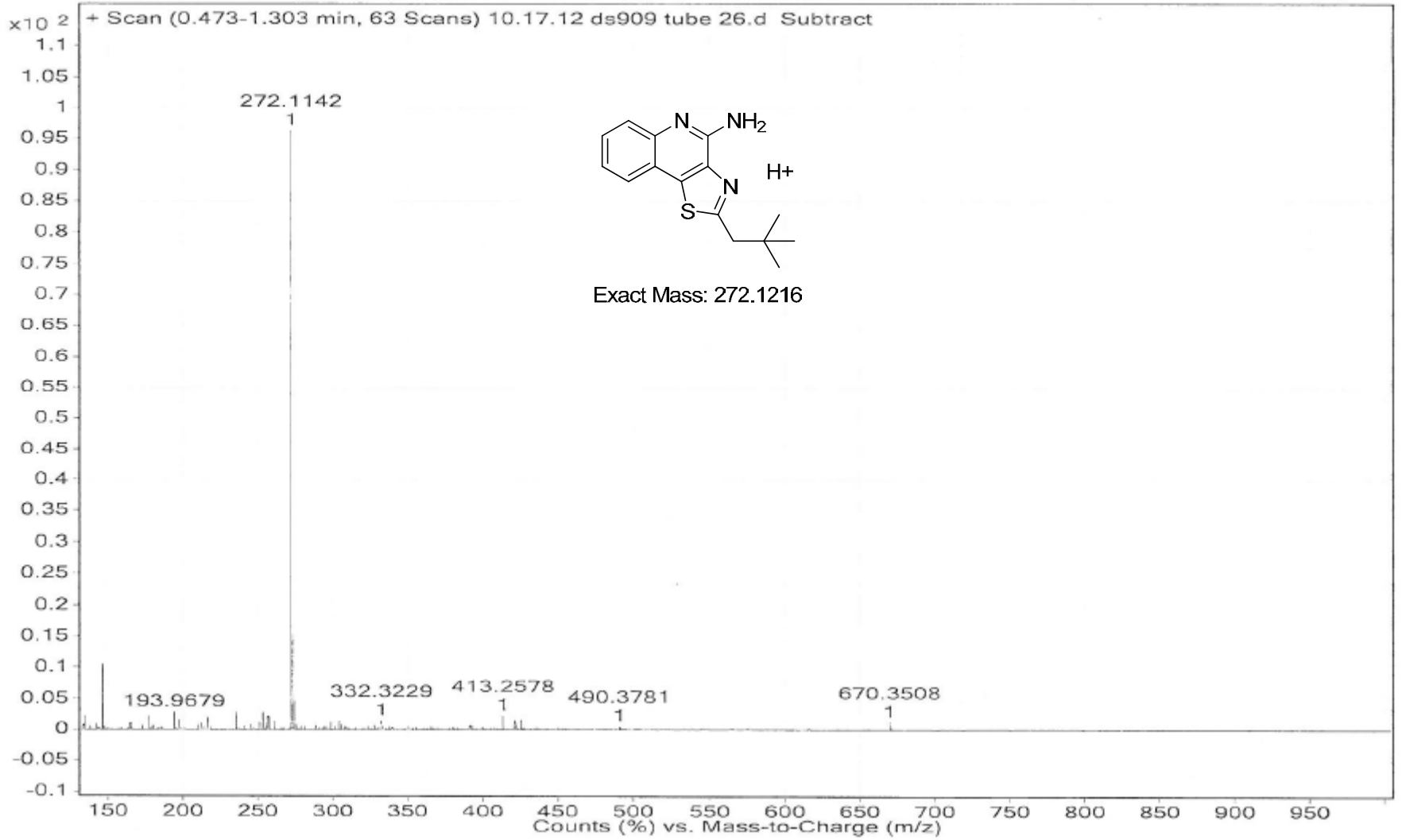
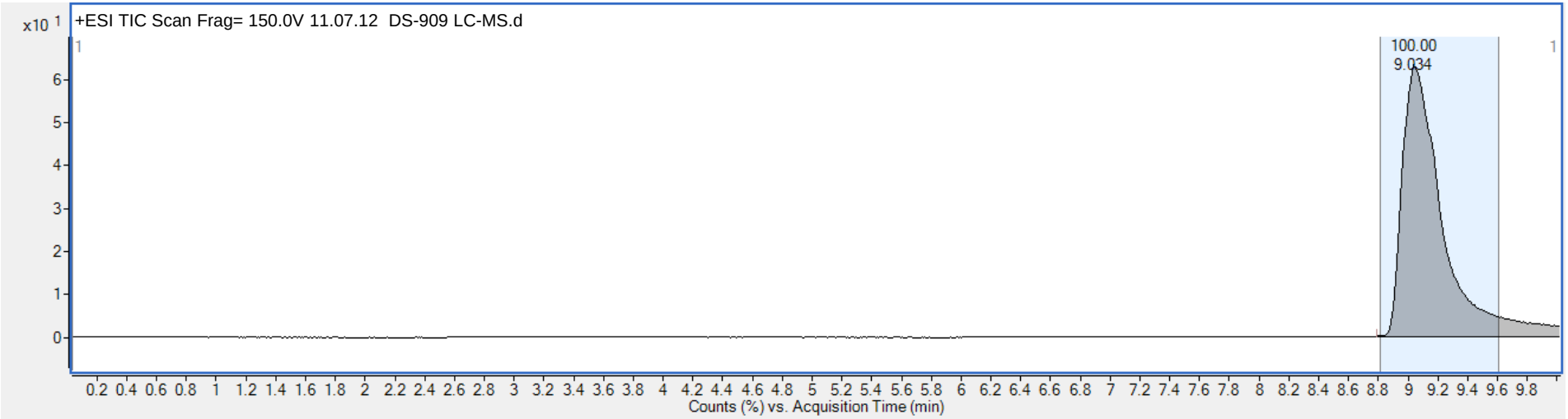
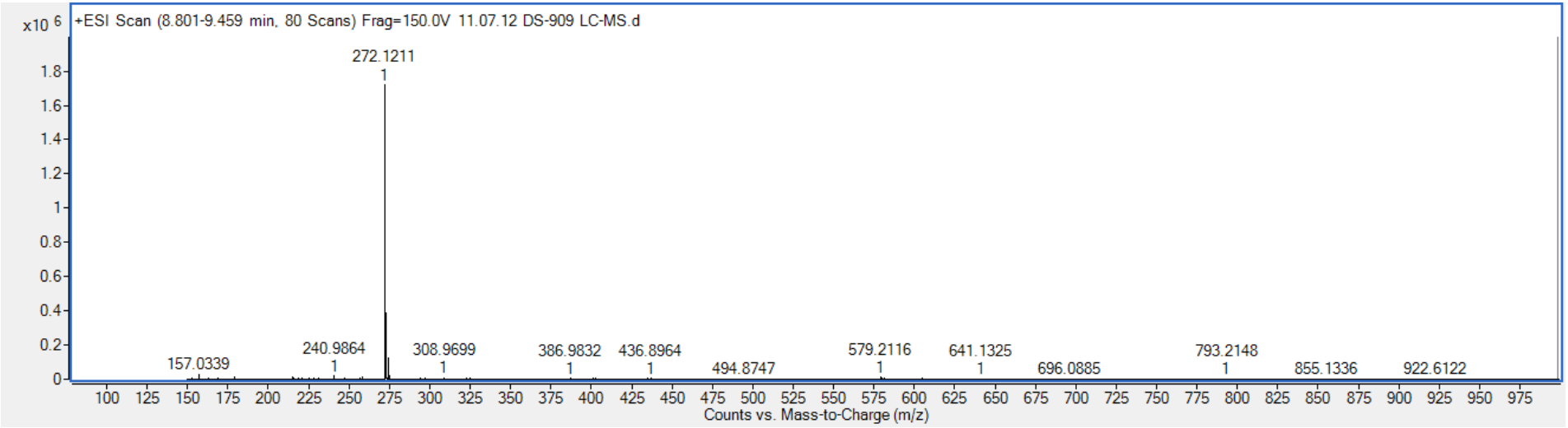
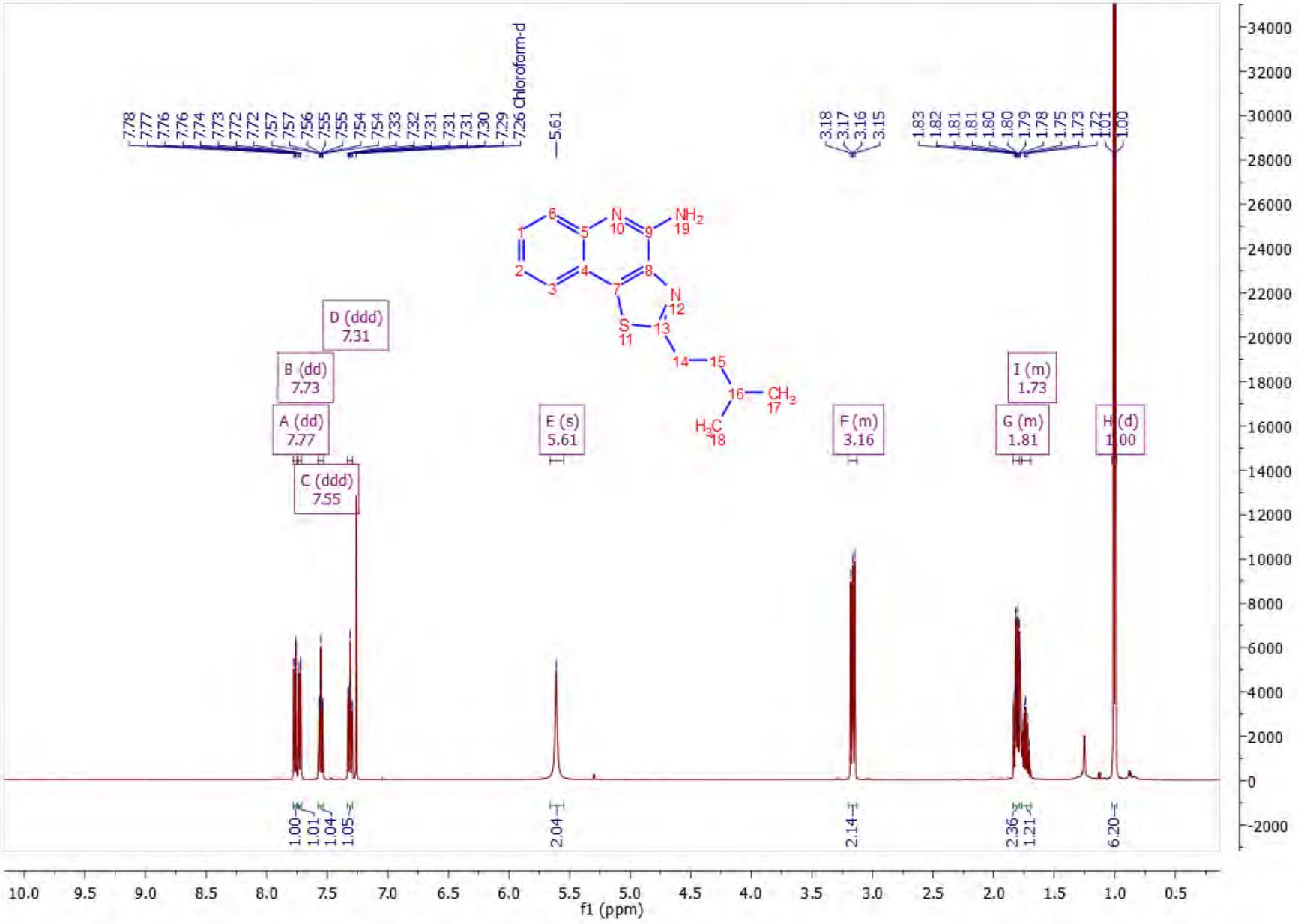


8k LC-MS

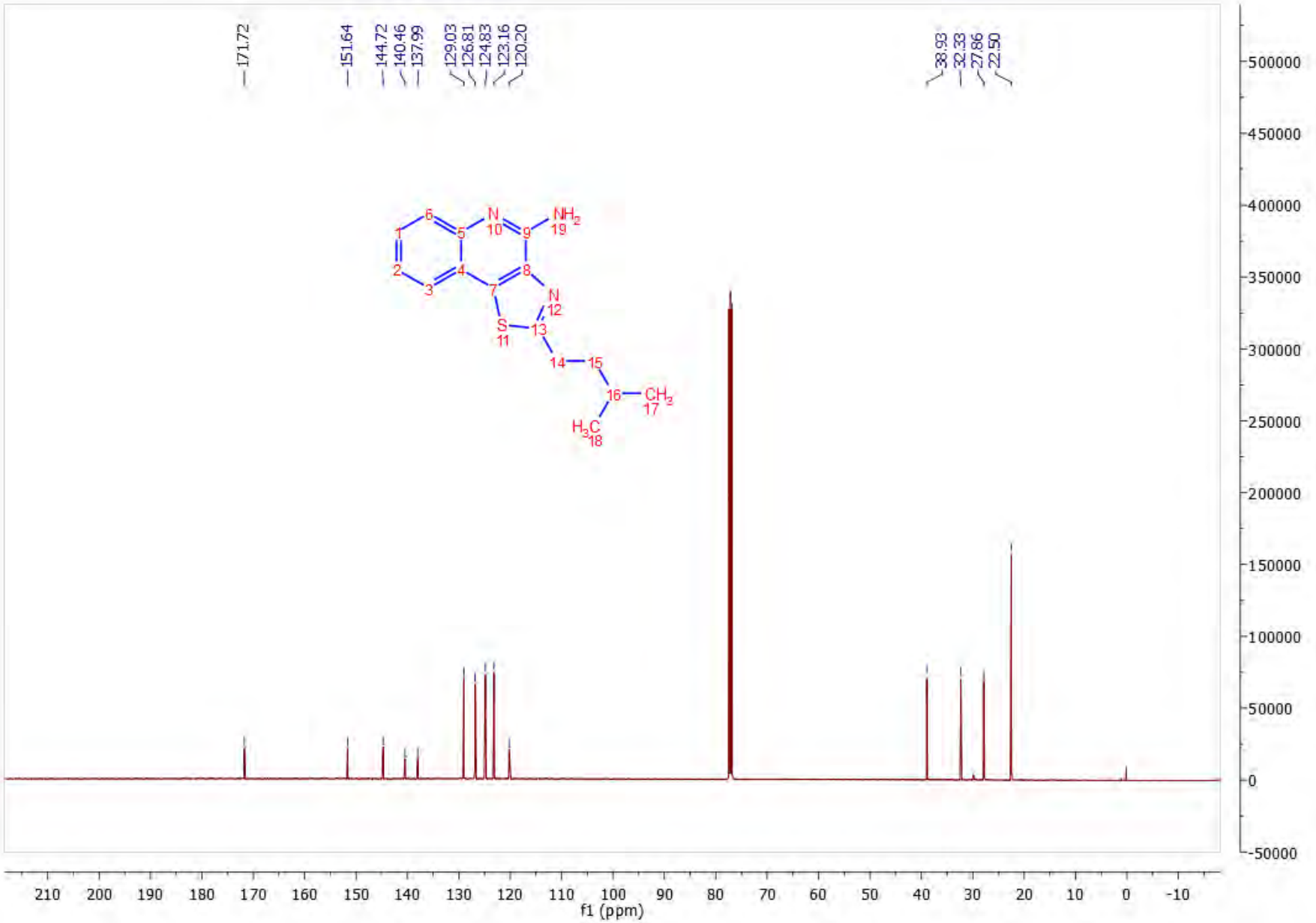




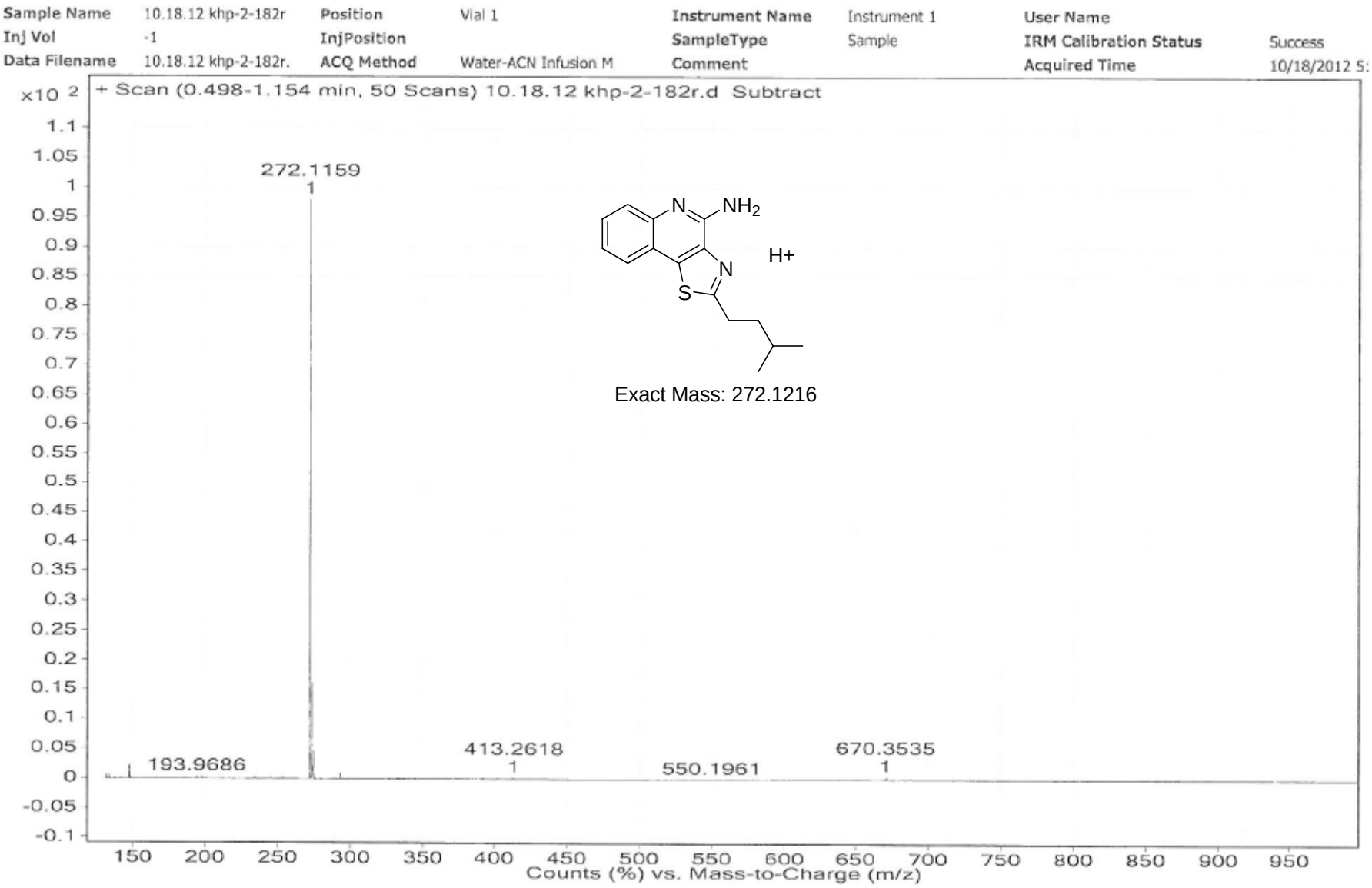
8l ^{1}H NMR



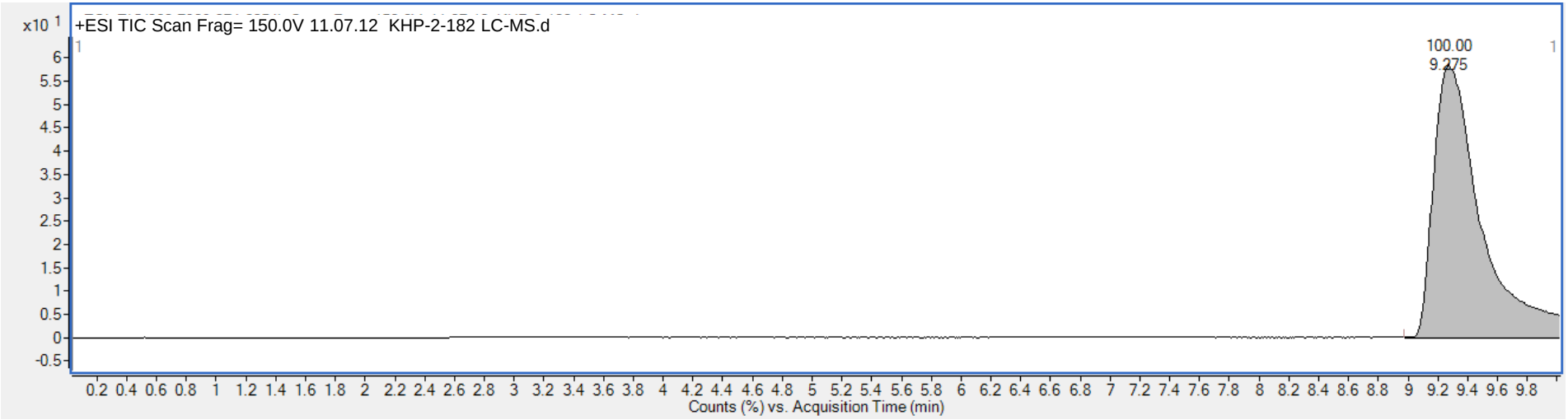
8l ^{13}C NMR

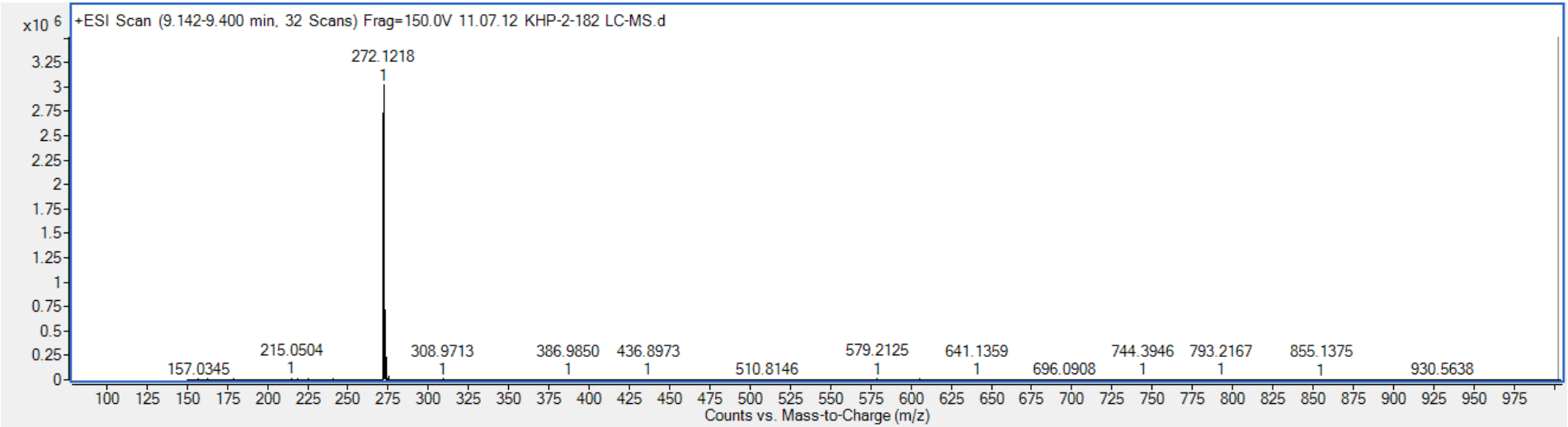


8l MS

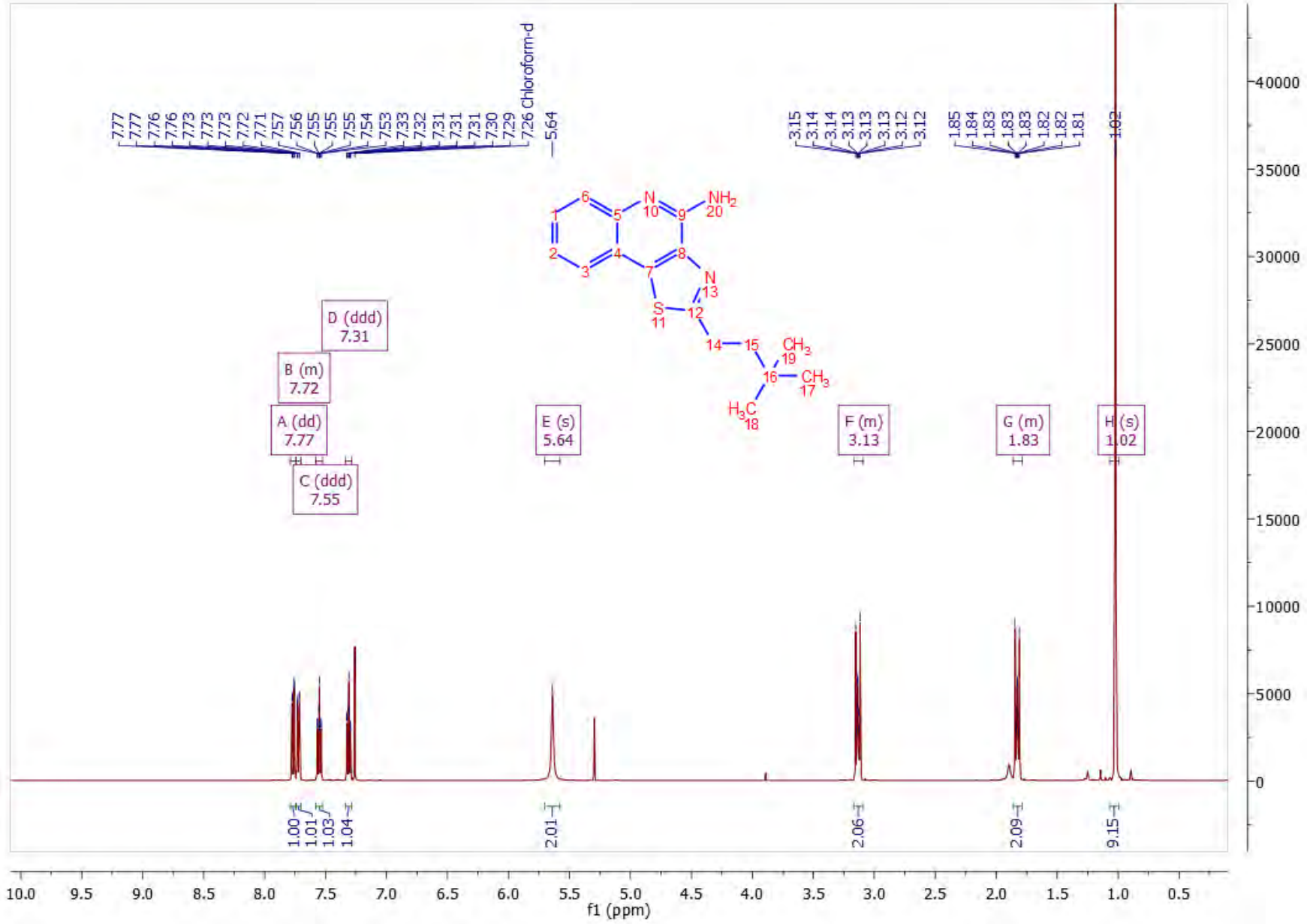


8l LC-MS

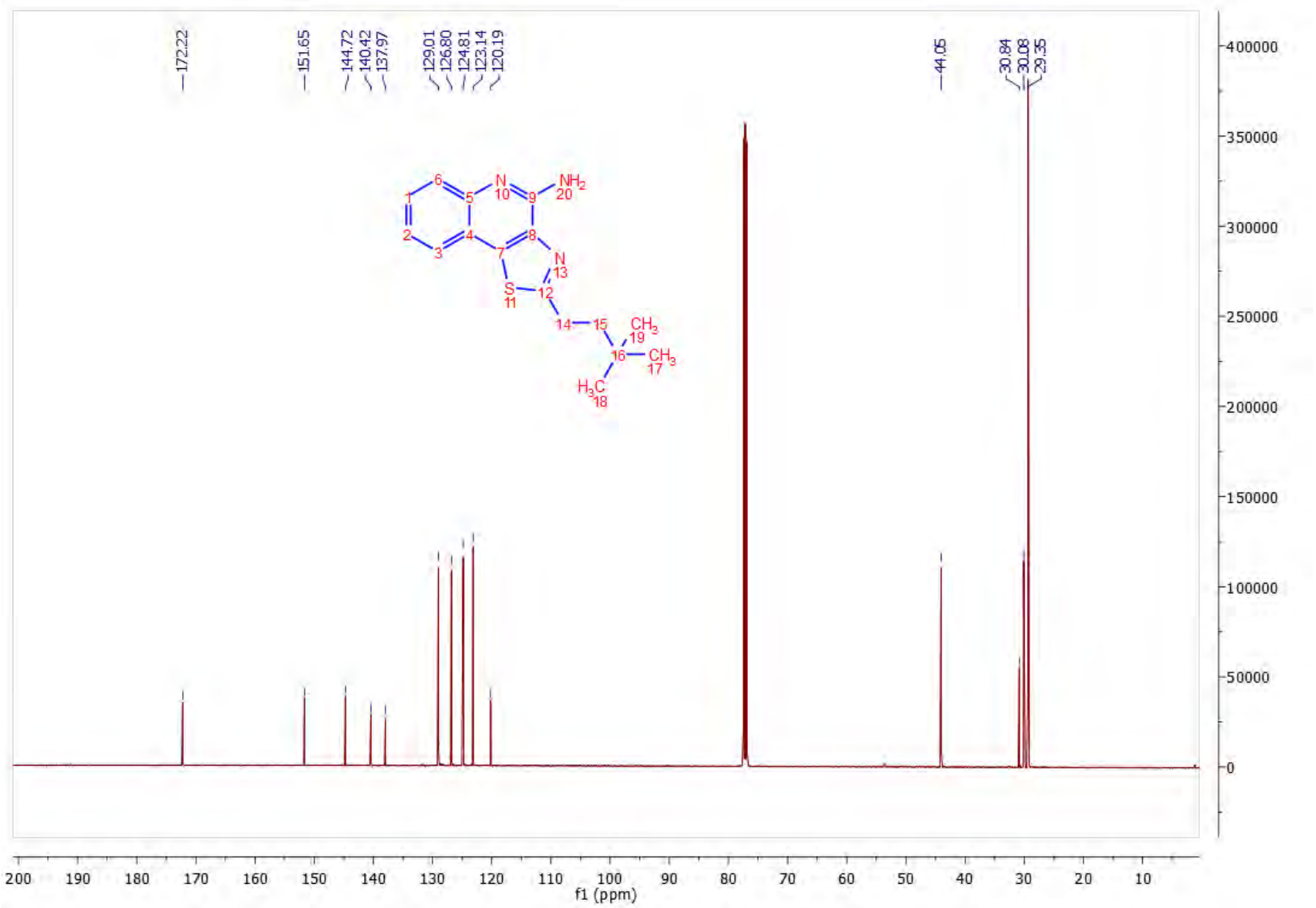




8m ^{1}H NMR

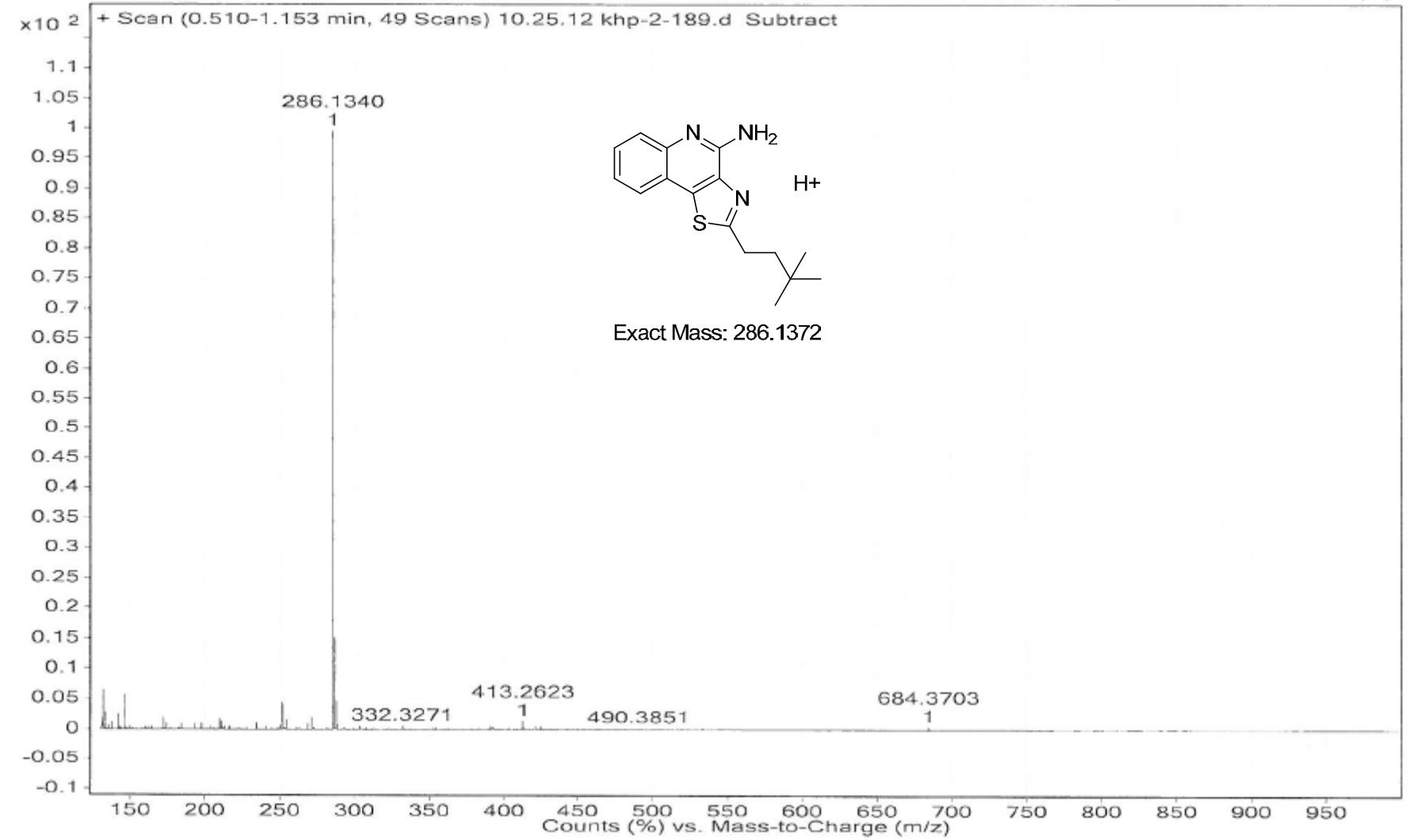


8m ^{13}C NMR

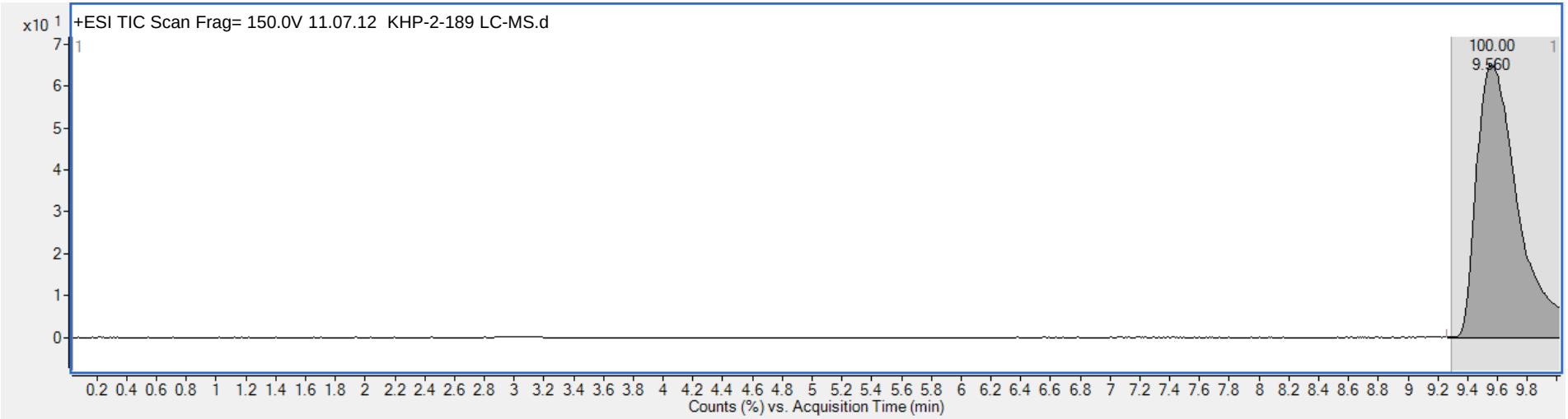


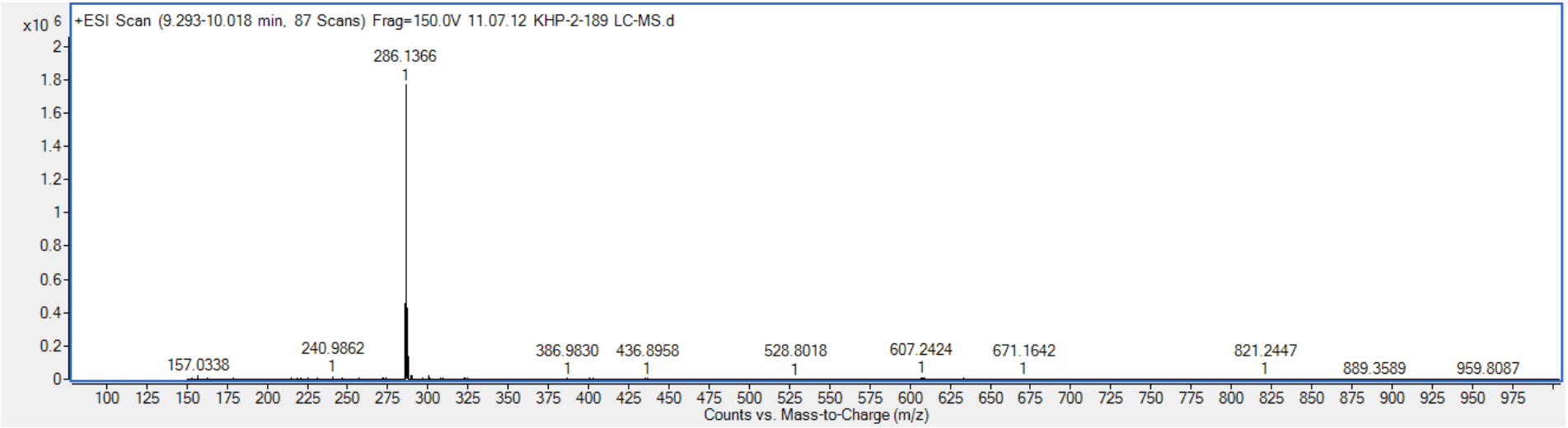
8m MS

Sample Name	10.25.12 khp-2-189	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	10.25.12 khp-2-189.d	ACQ Method	Water-ACN Infusion M	Comment		Acquired Time	10/25/2012

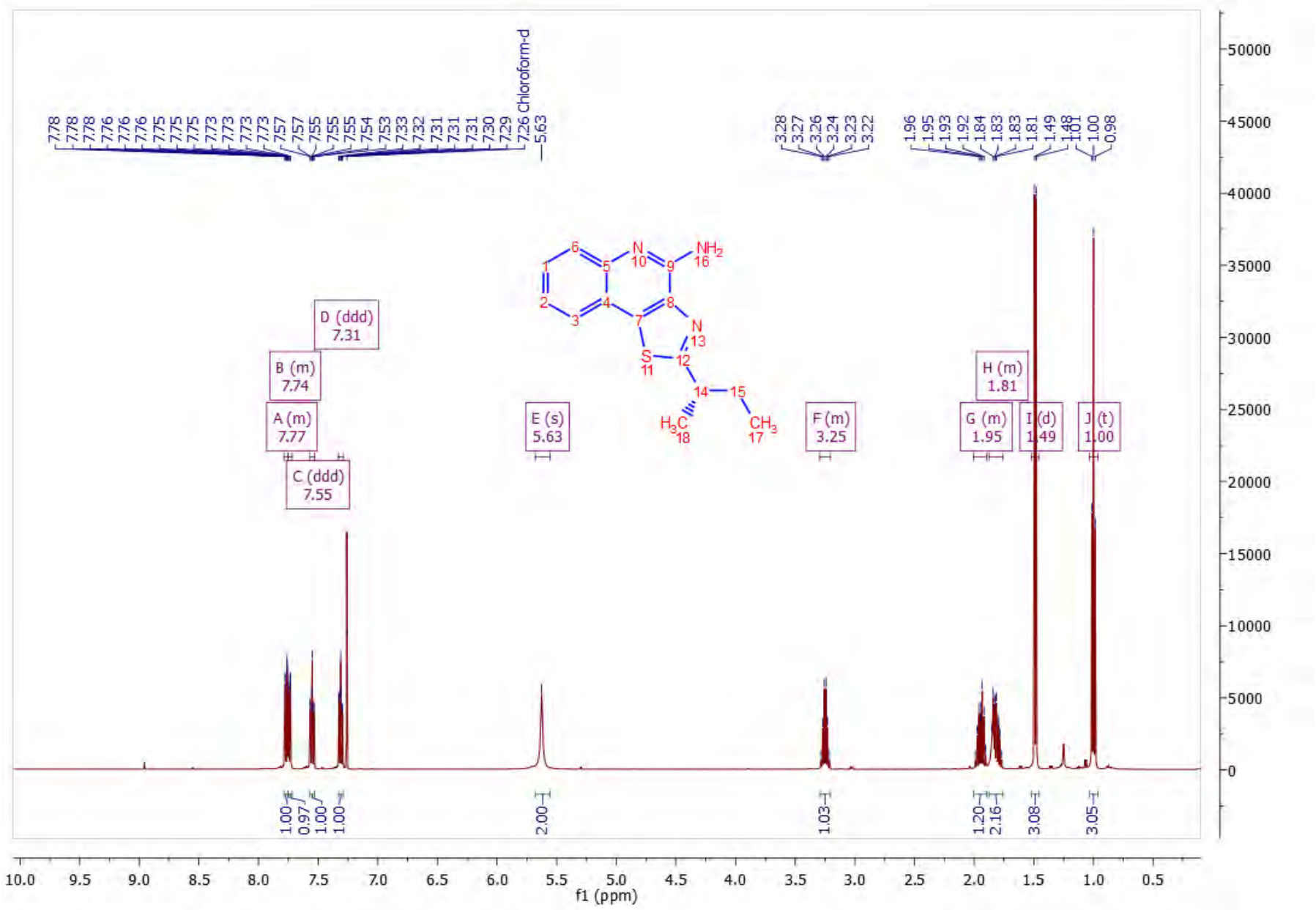


8m LC-MS

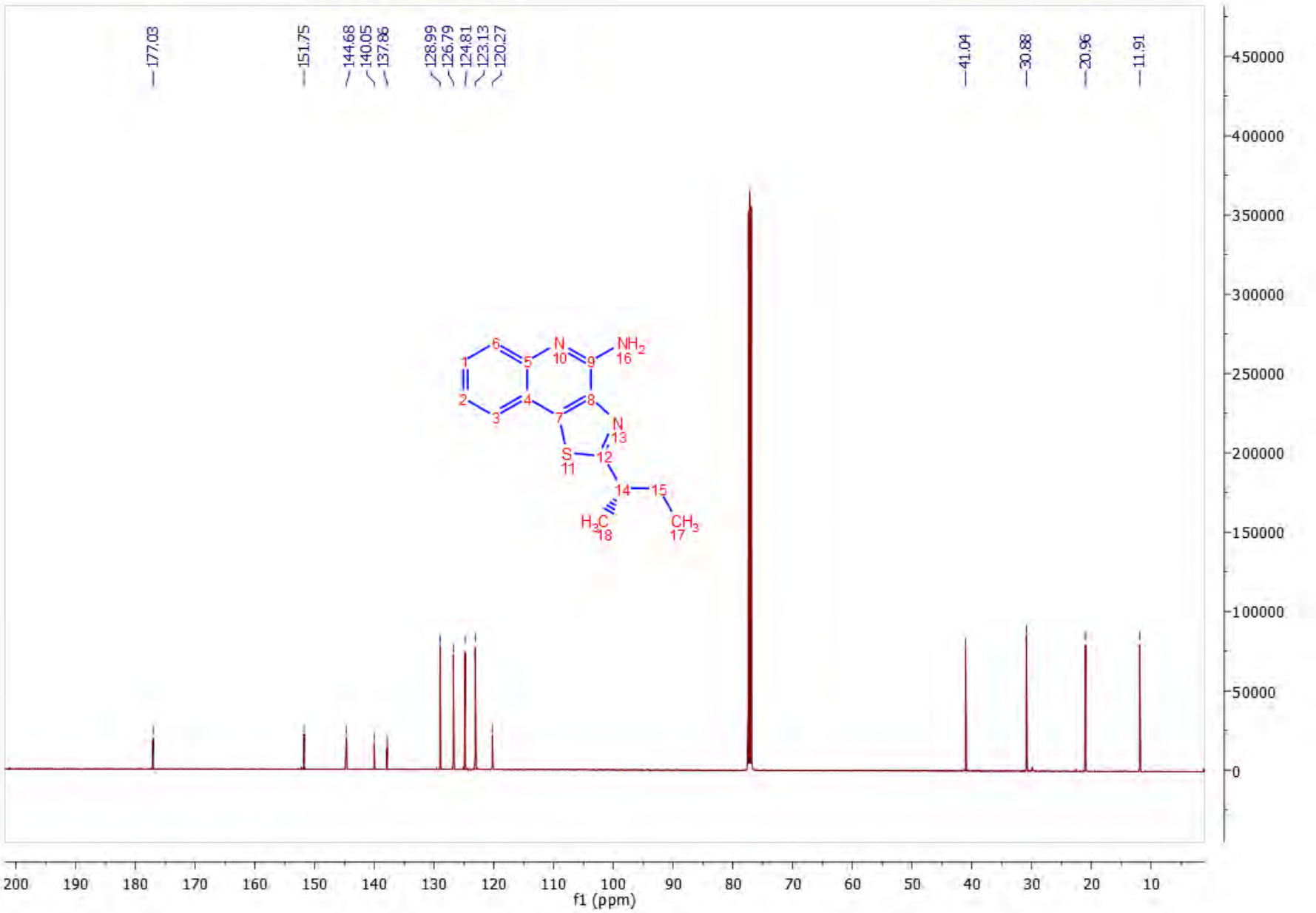




8n ^{1}H NMR

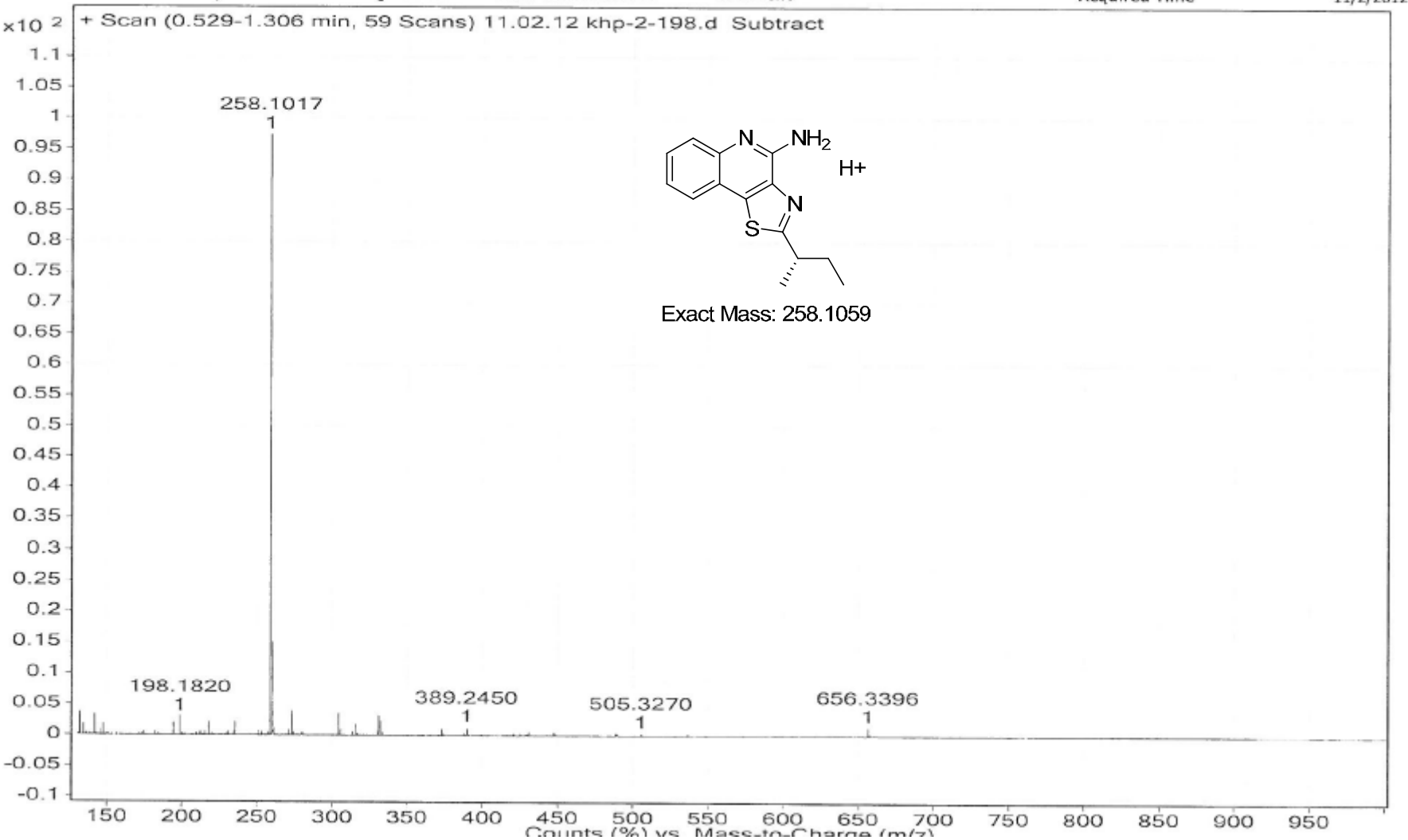


8n ^{13}C NMR

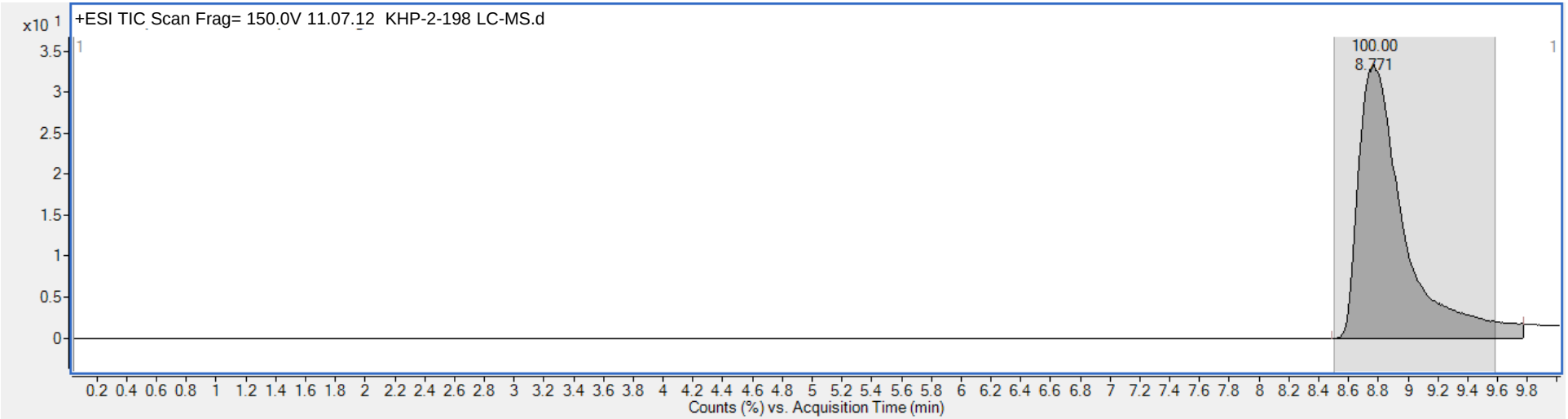


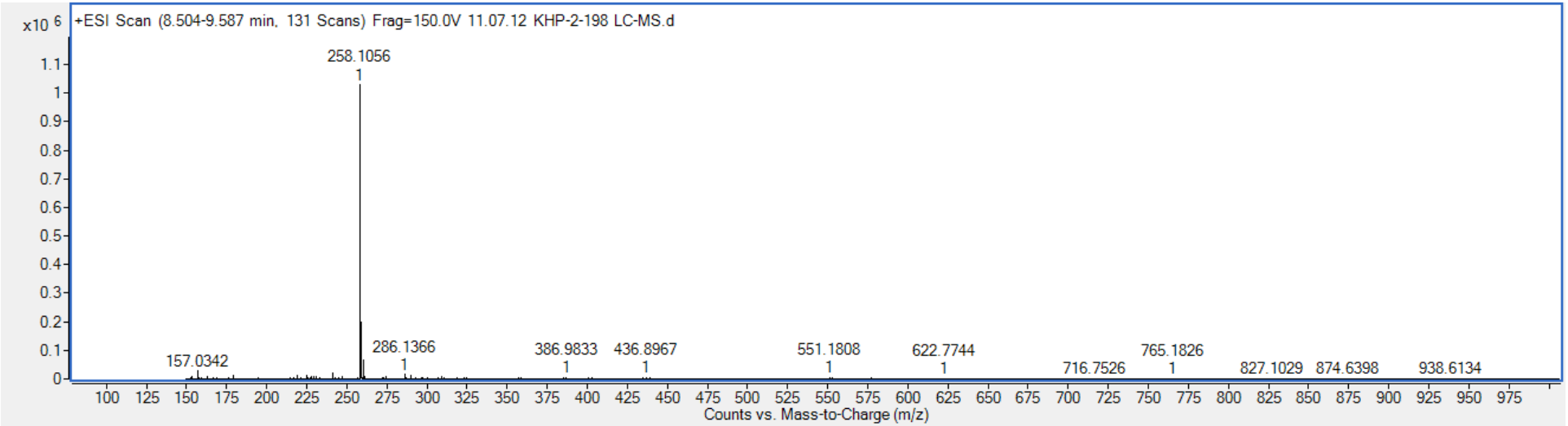
8n MS

Sample Name	11.02.12 khp-2-198	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	11.02.12 khp-2-198.d	ACQ Method	Water-ACN Infusion M	Comment		Acquired Time	11/2/2012

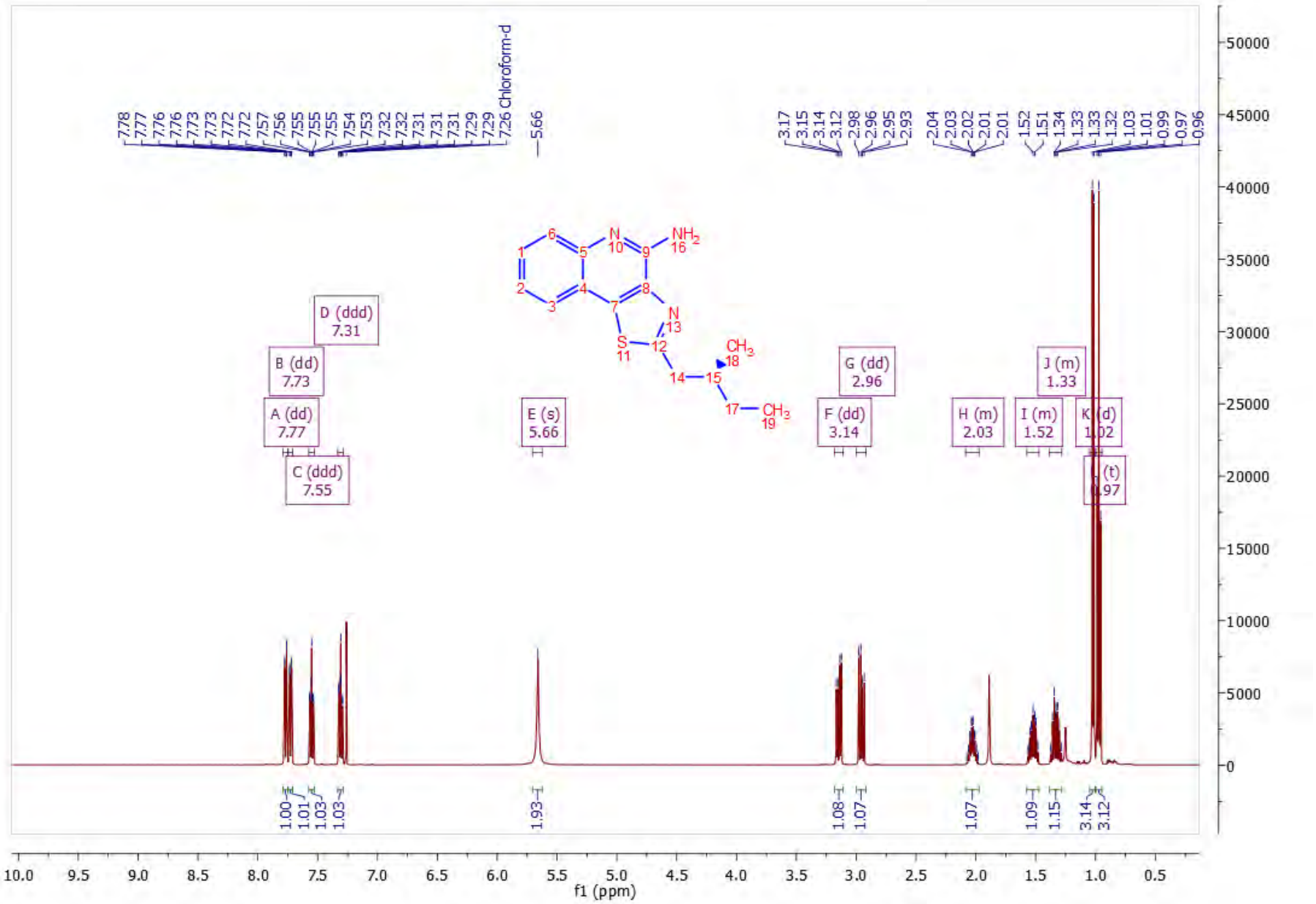


8n LC-MS

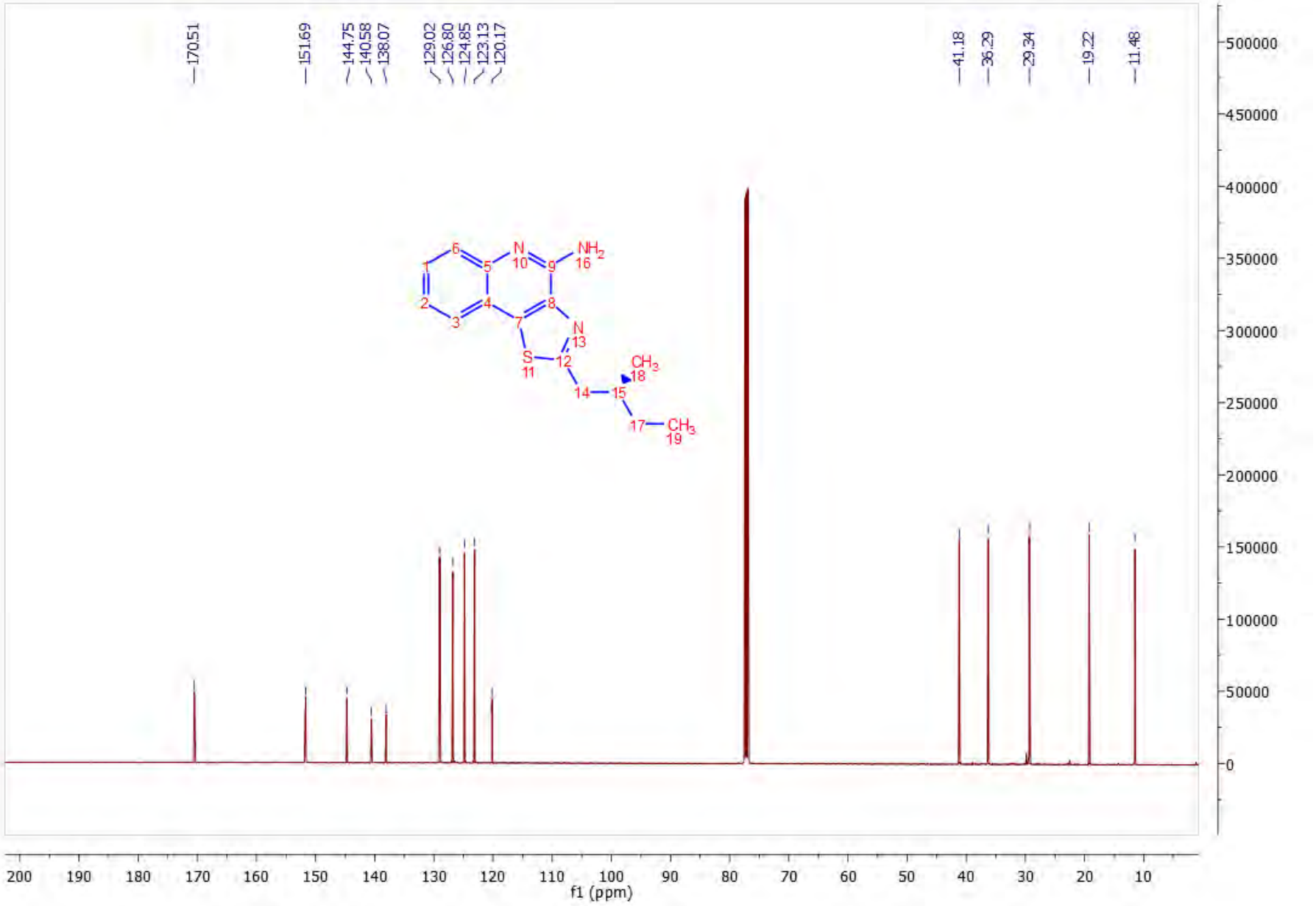




8o ^{1}H NMR

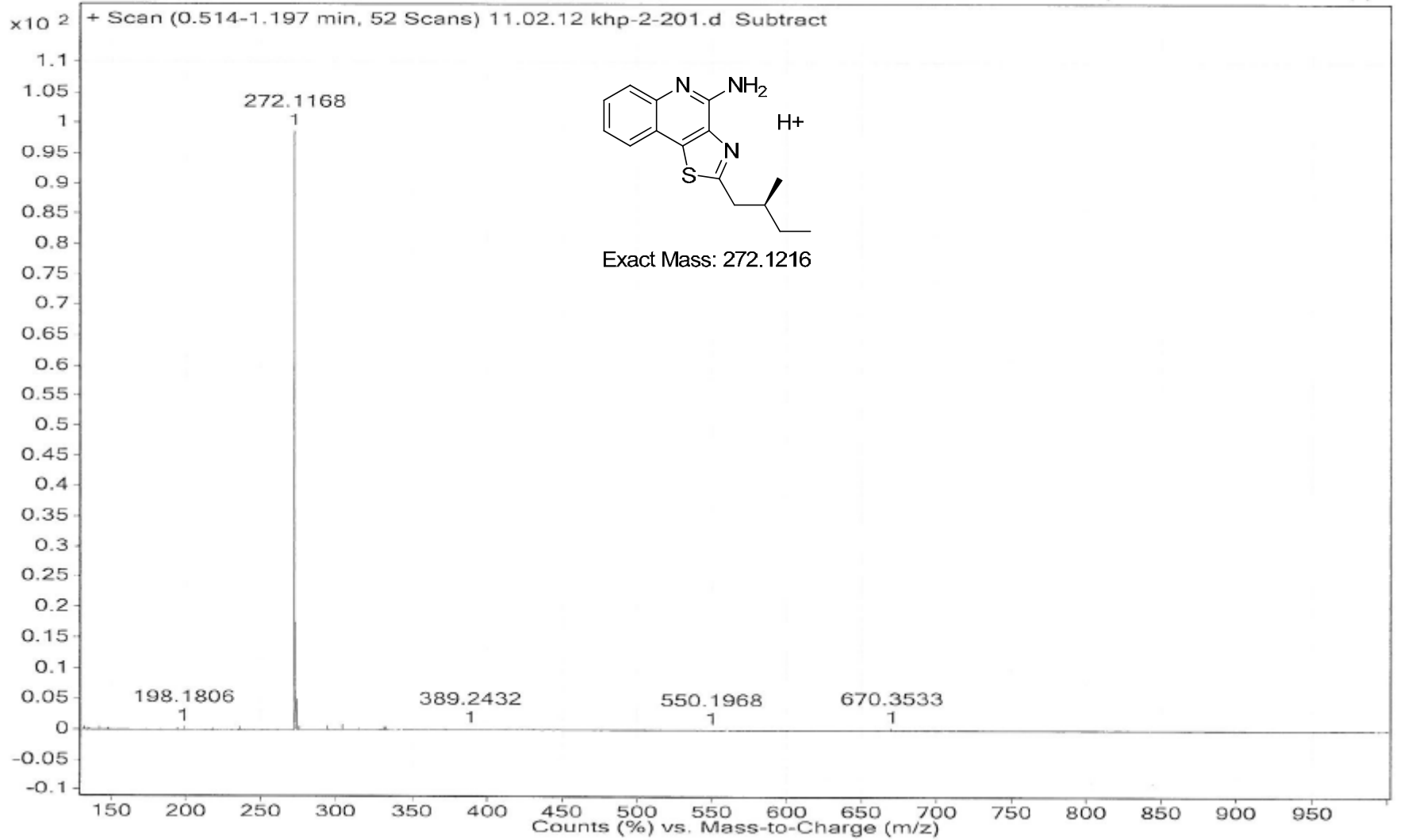


8o ^{13}C NMR

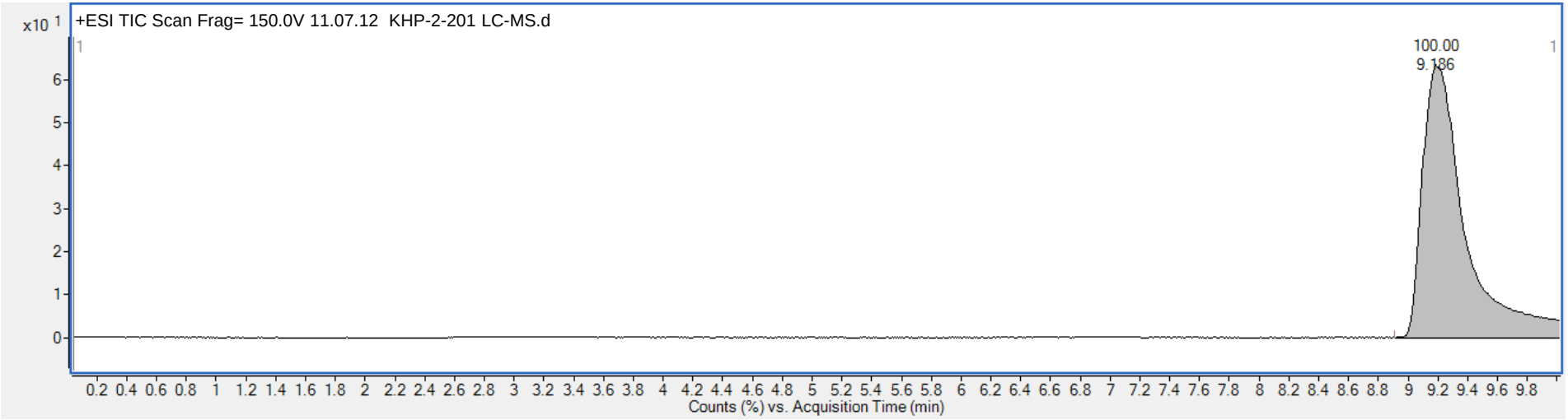


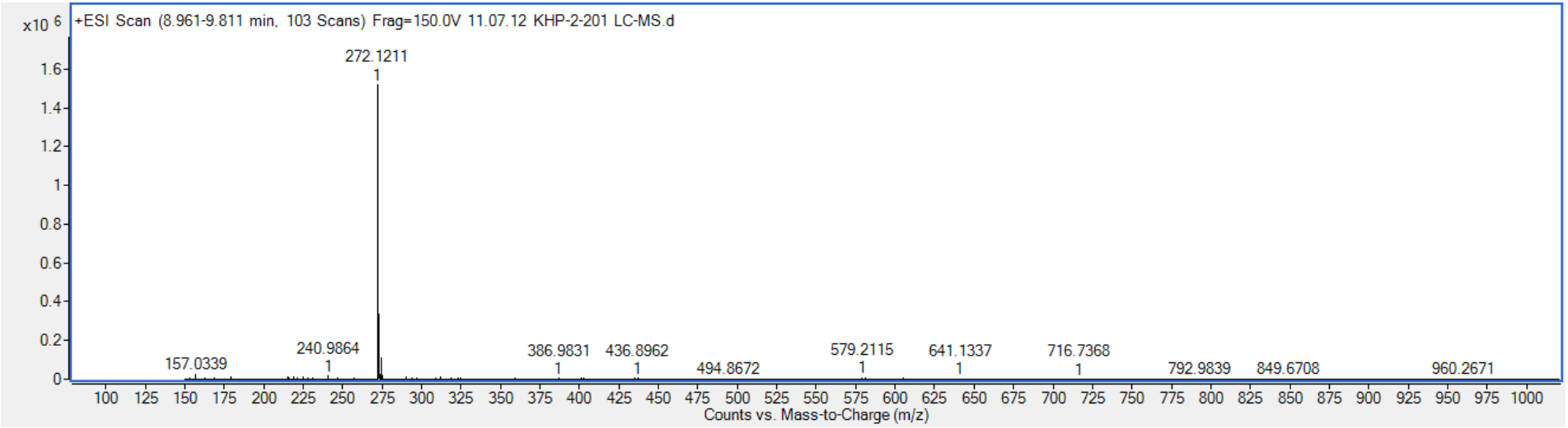
8o MS

Sample Name	11.02.12 khp-2-201	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	11.02.12 khp-2-201.d	ACQ Method	Water-ACN Infusion M	Comment		Acquired Time	11/2/2012

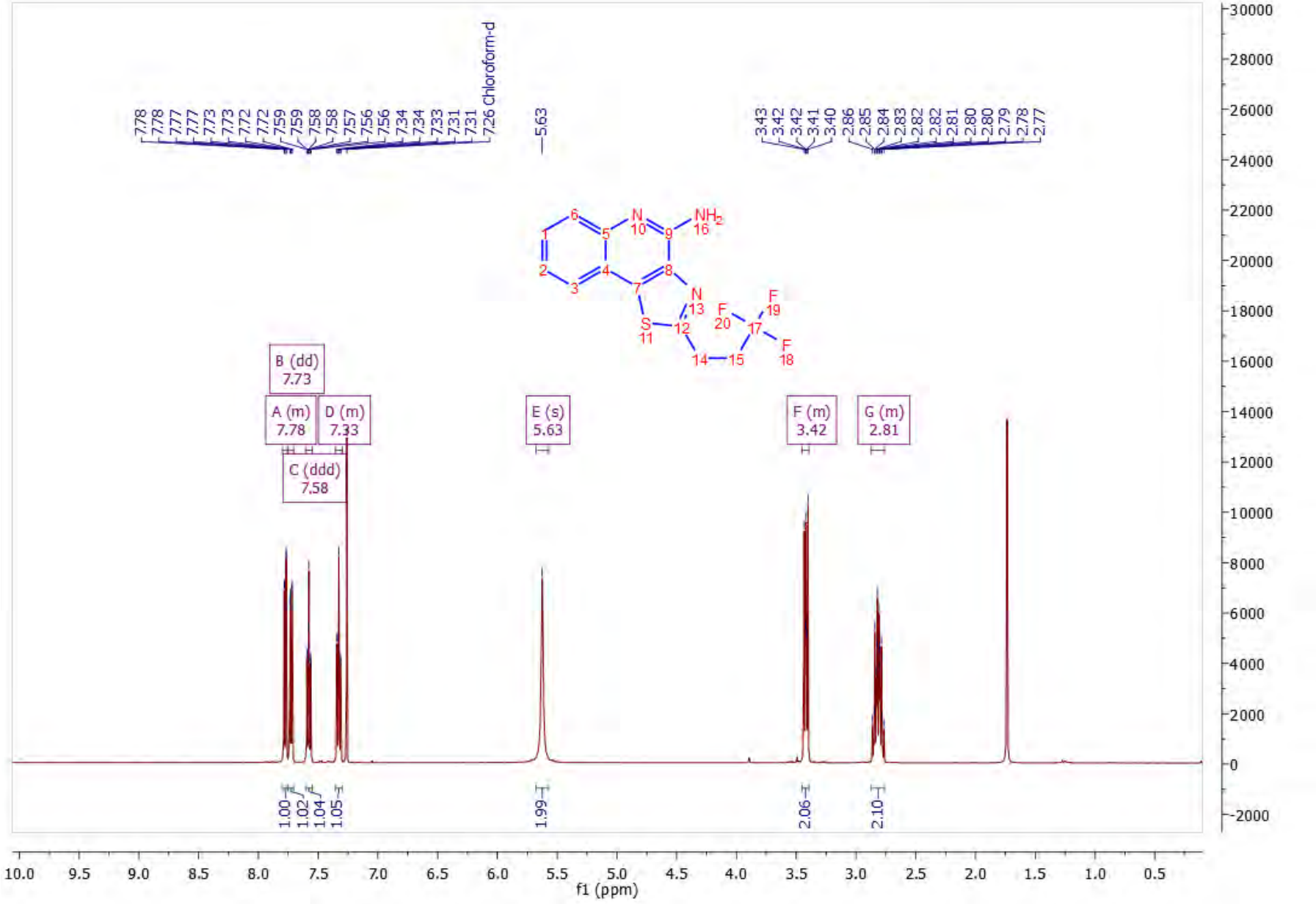


8o LC-MS

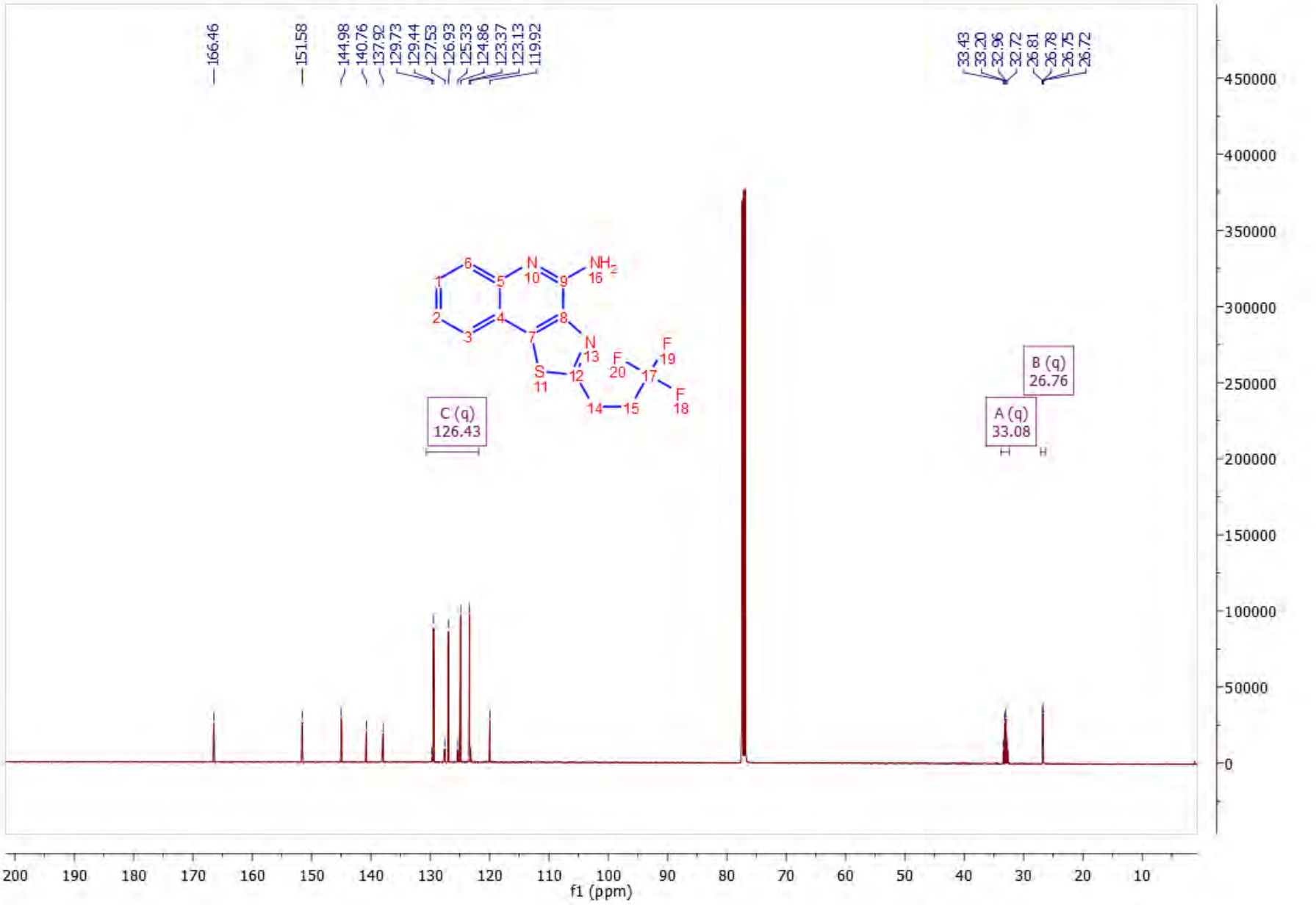




8p ^{1}H NMR

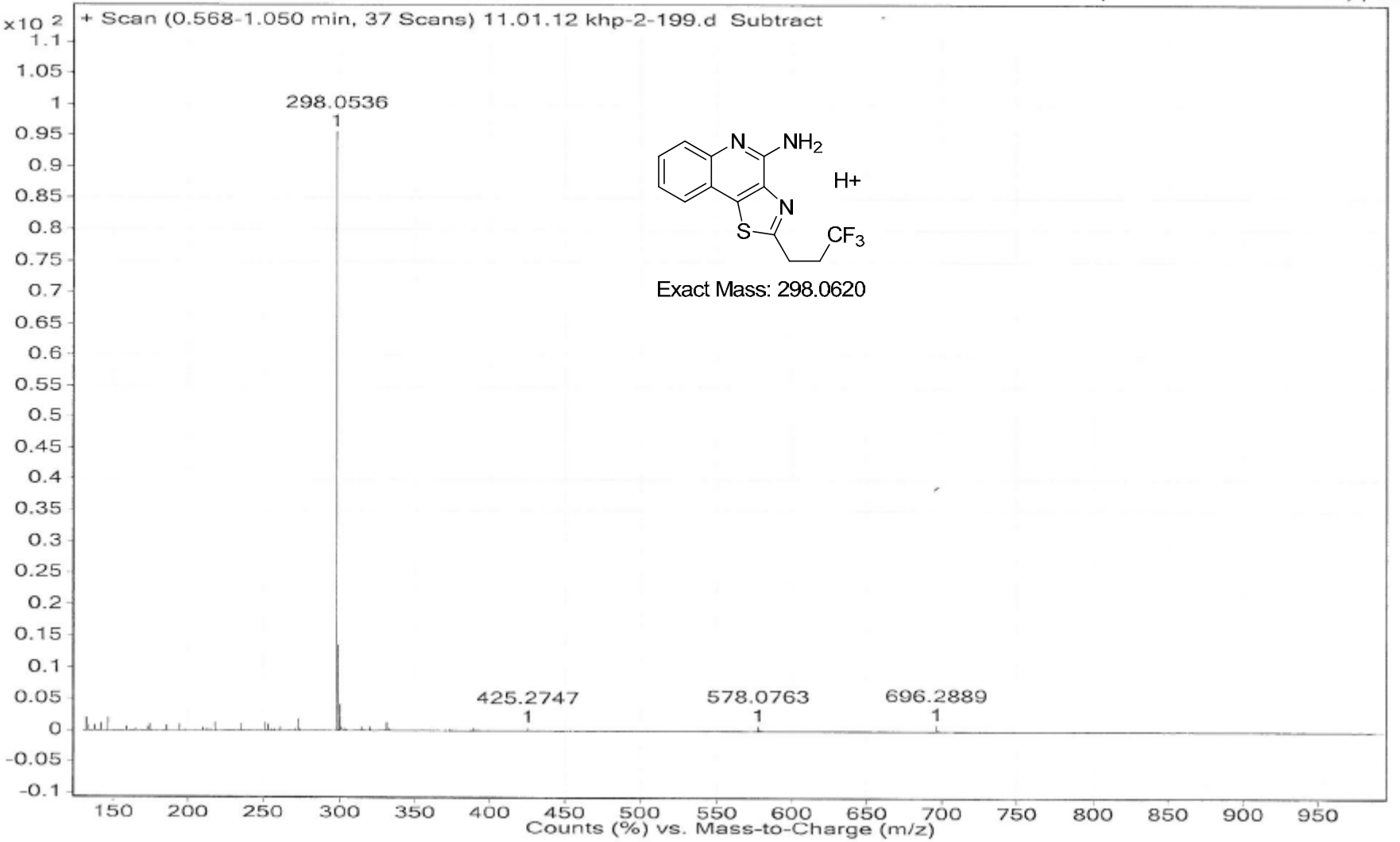


8p ^{13}C NMR

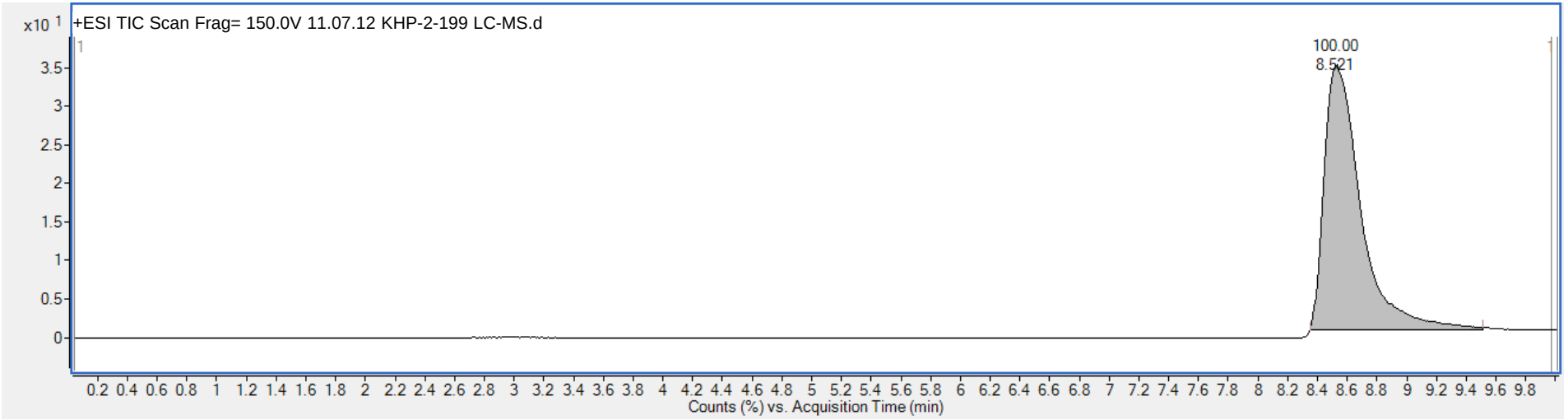


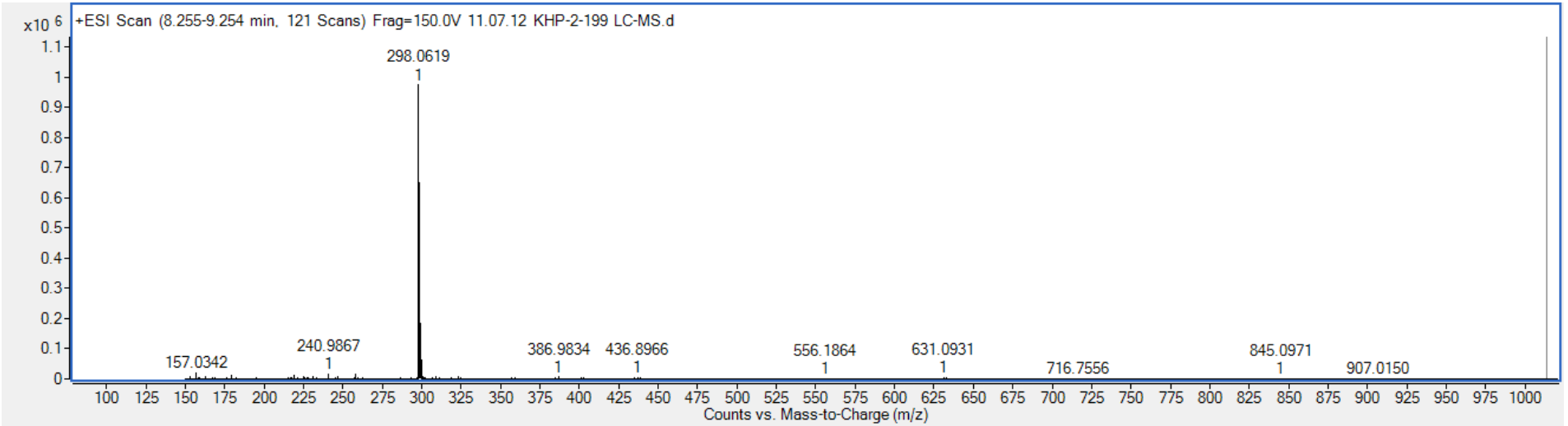
8p MS

Sample Name	11.01.12 khp-2-199	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	11.01.12 khp-2-199.d	ACQ Method	Water-ACN Infusion M	Comment		Acquired Time	11/1/2012

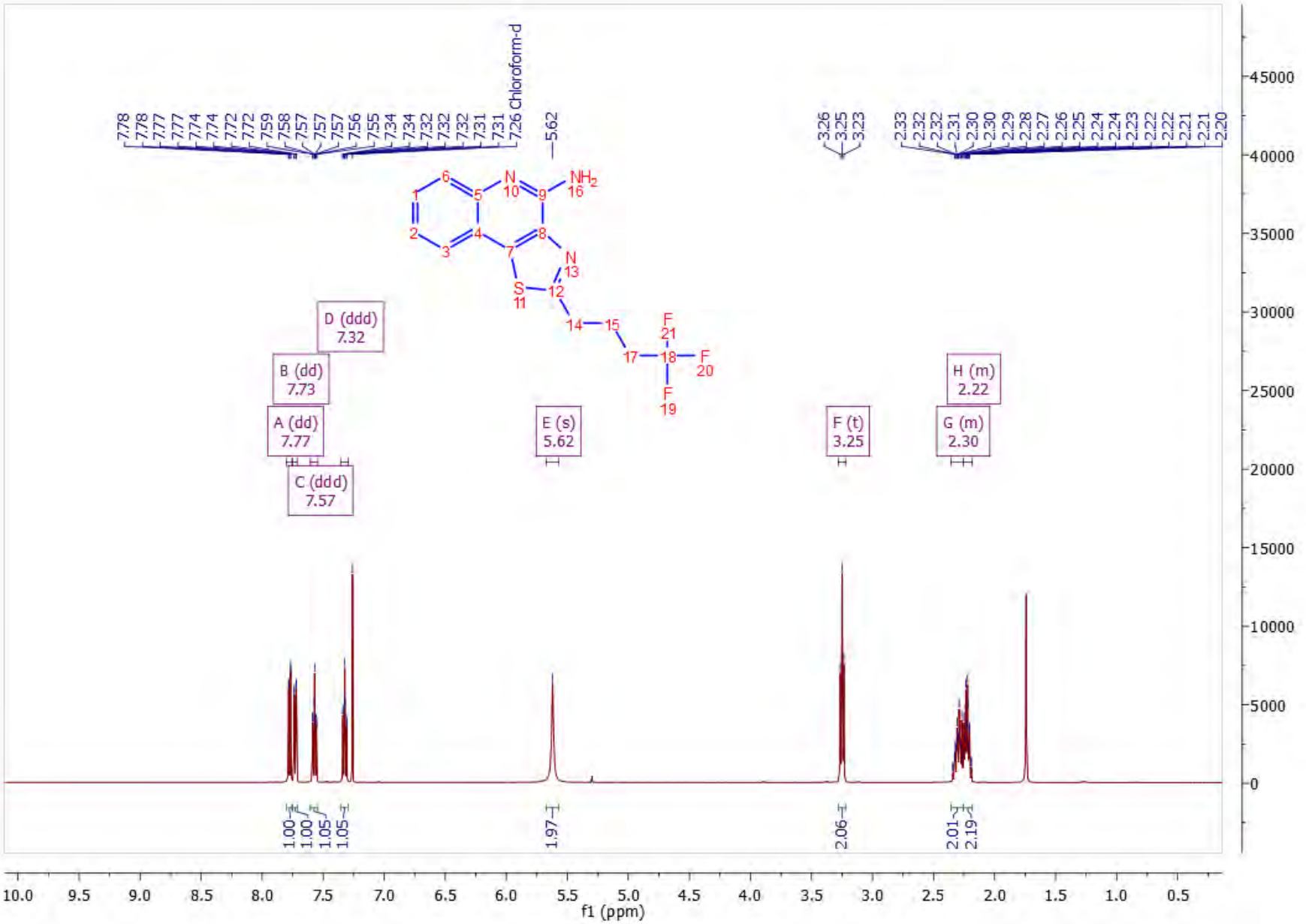


8p LC-MS

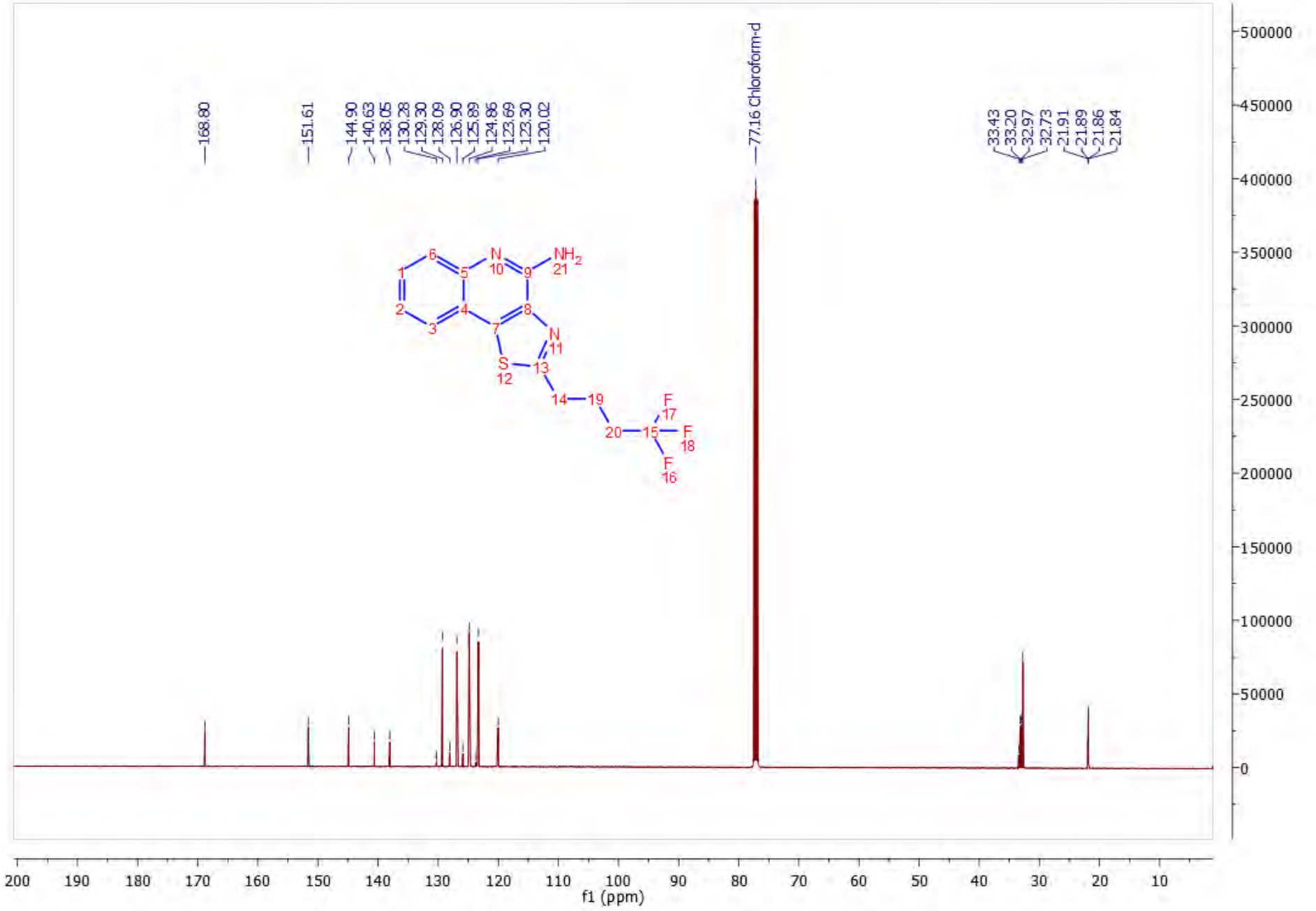




8q ^{1}H NMR

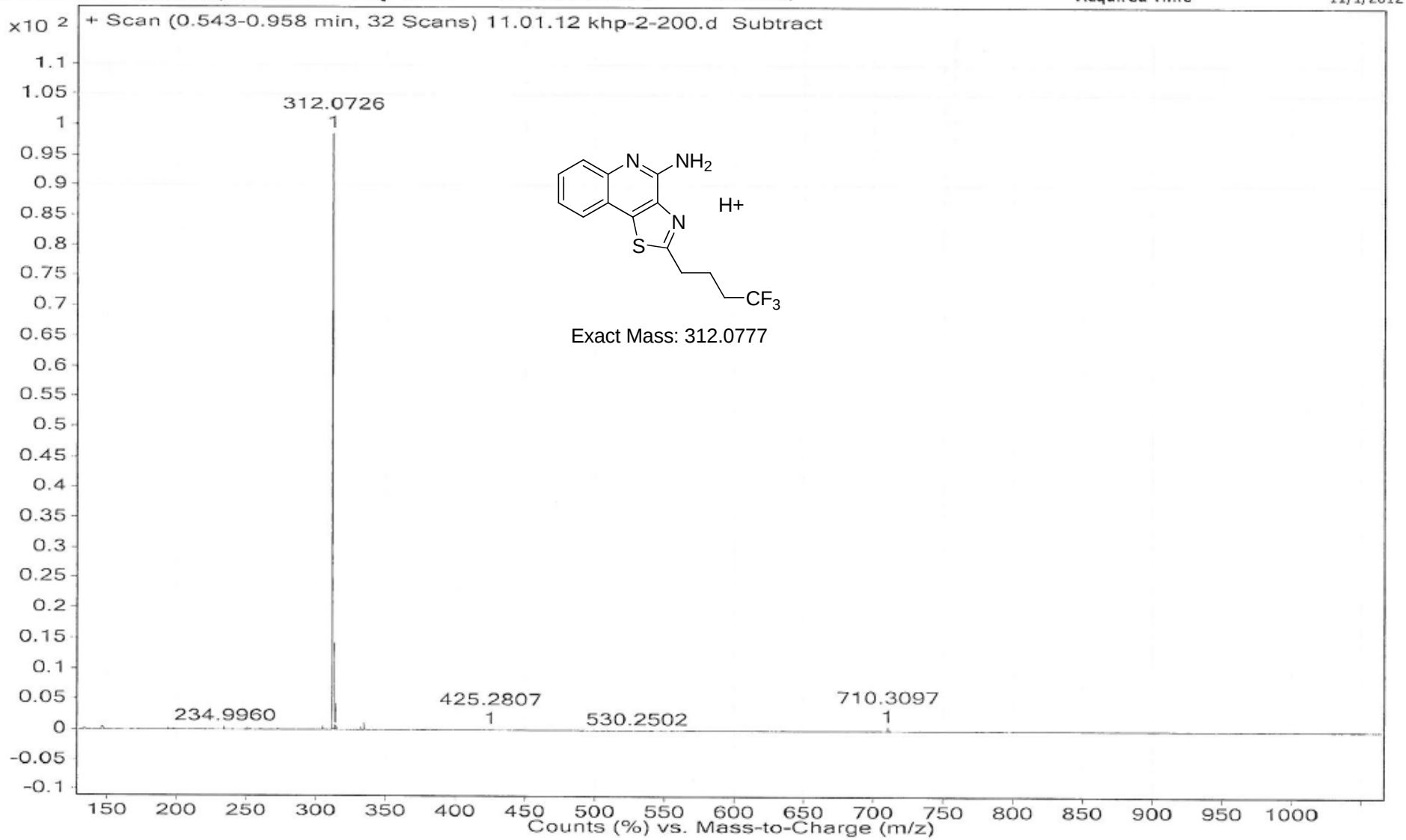


8q ^{13}C NMR



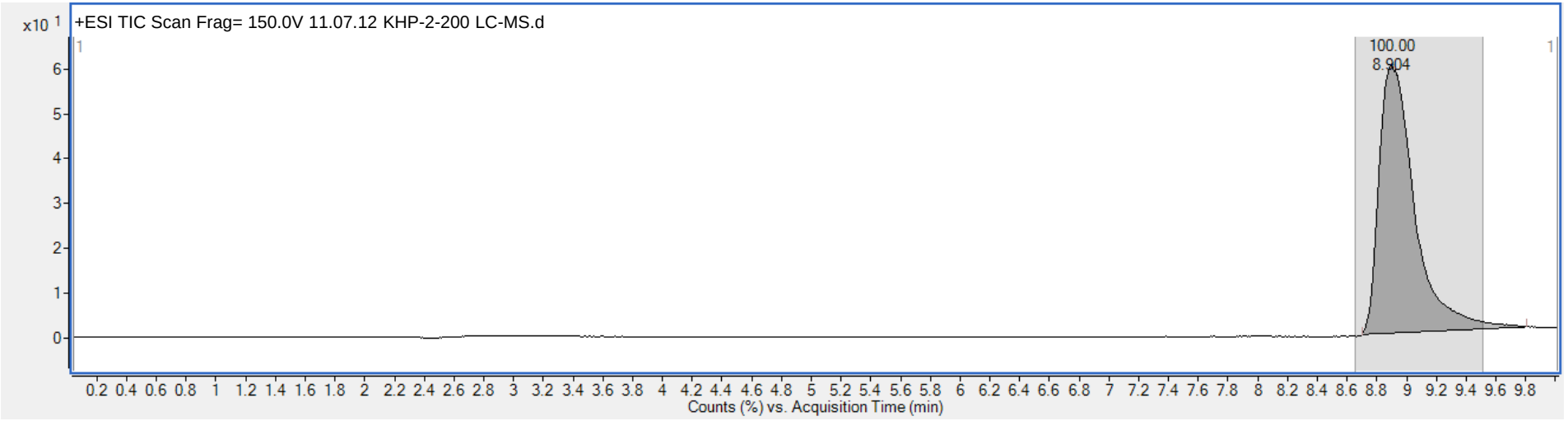
8q MS

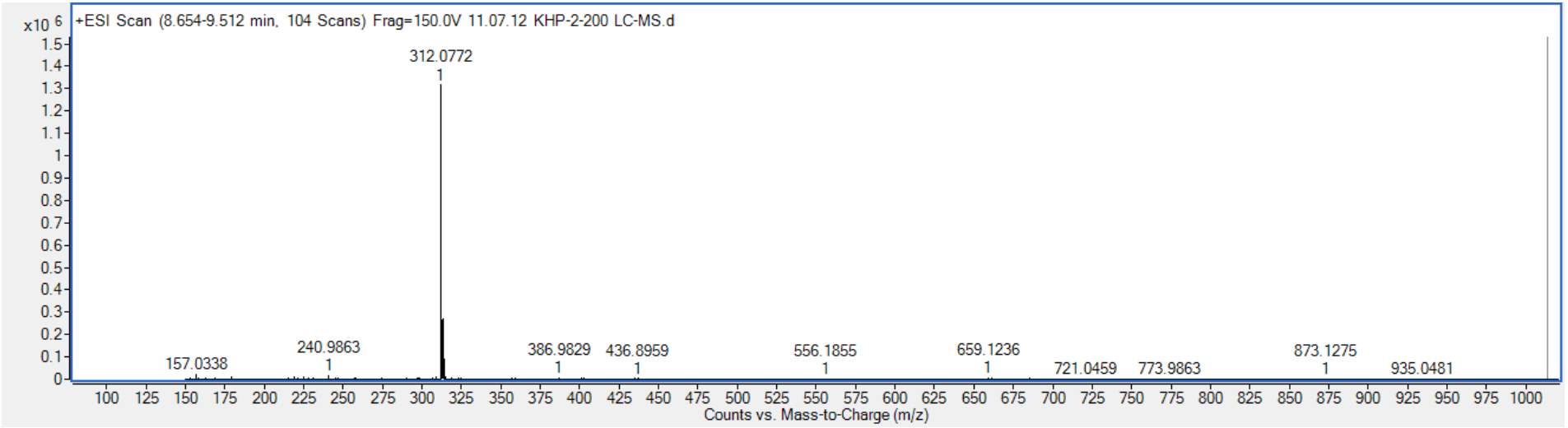
Sample Name	11.01.12 khp-2-200	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	11.01.12 khp-2-200.d	ACQ Method	Water-ACN Infusion M	Comment		Acquired Time	11/1/2012



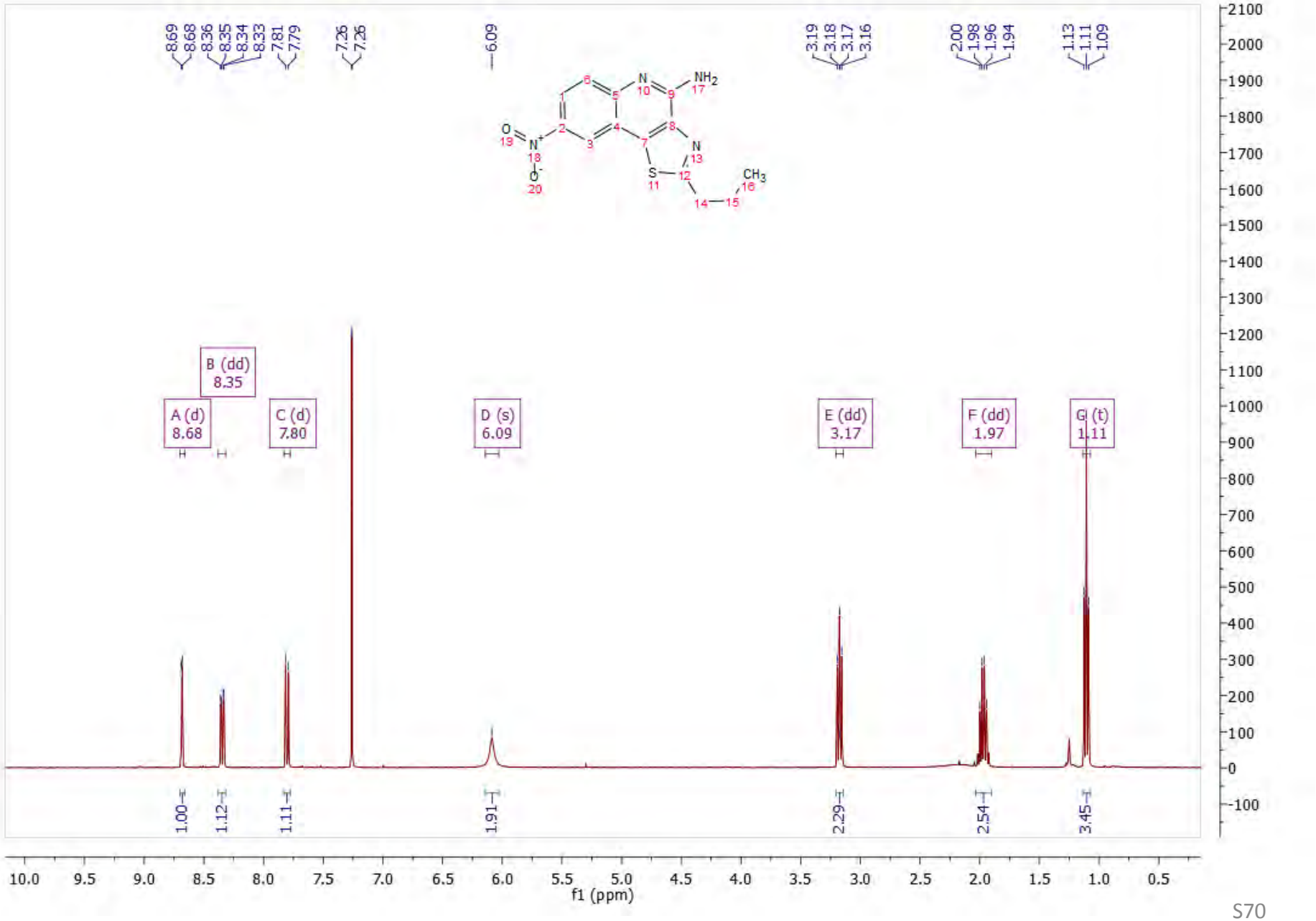
Exact Mass: 312.0777

8q LC-MS

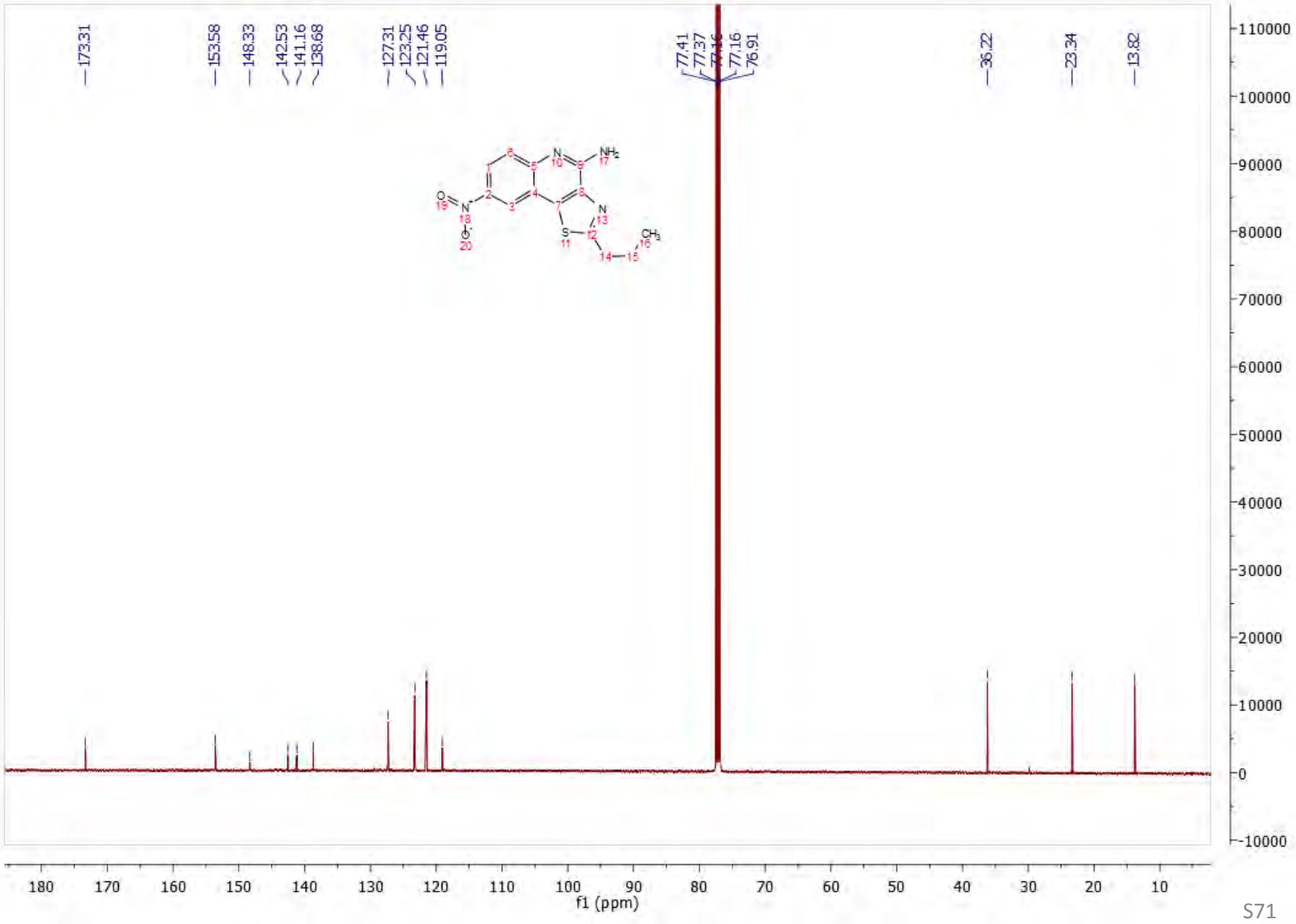




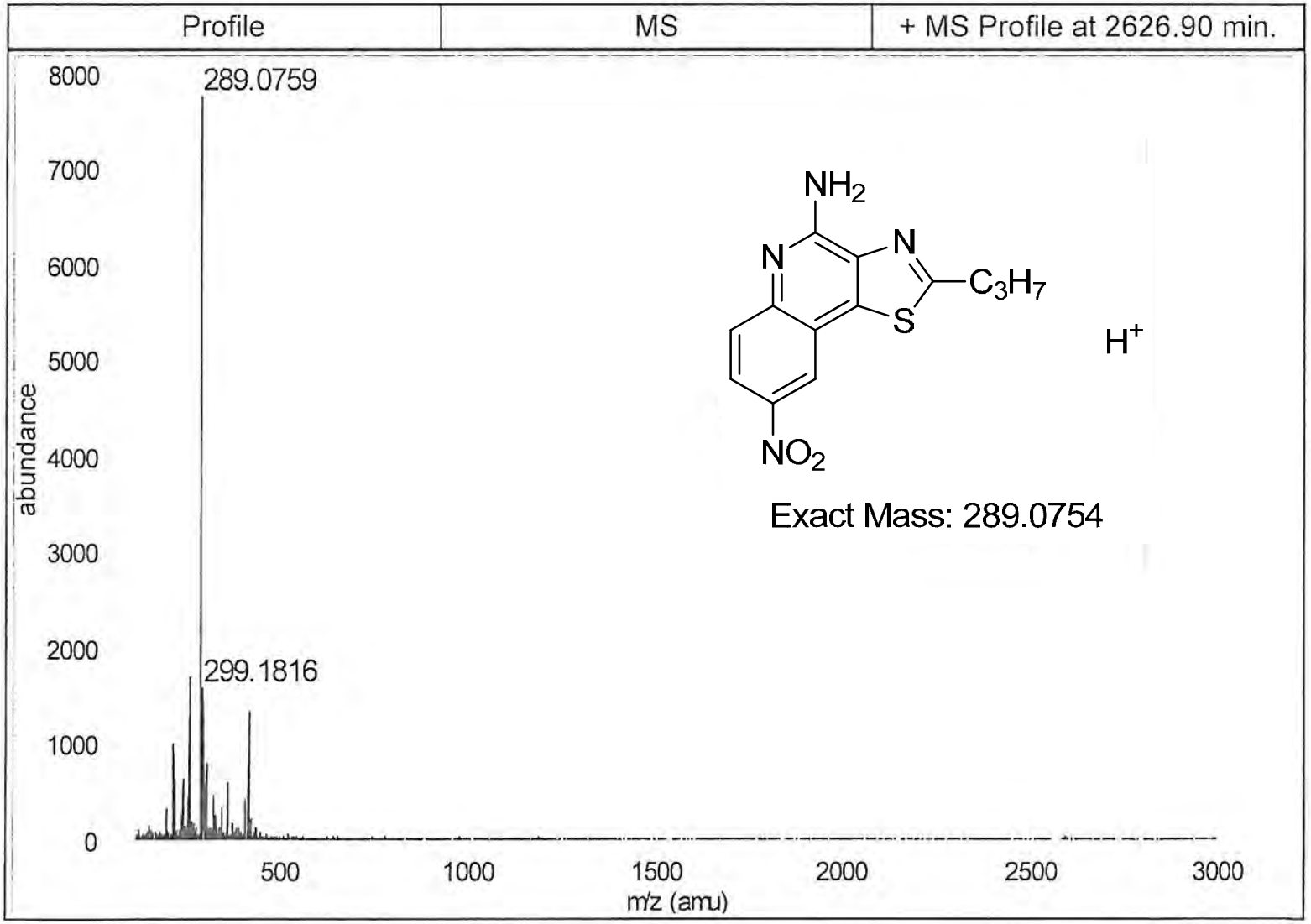
9 ^{1}H NMR



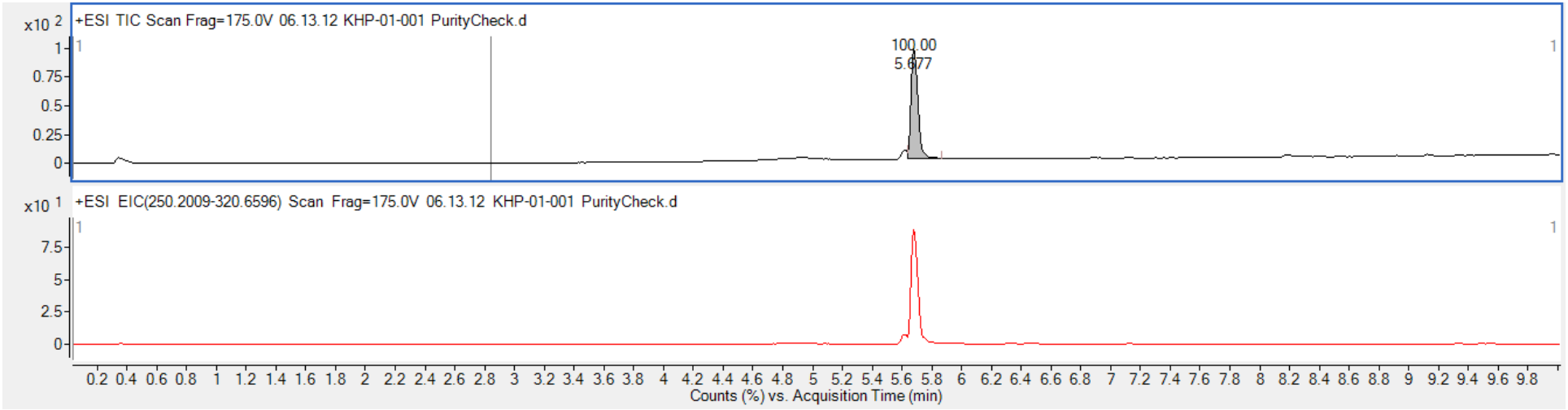
9 ^{13}C NMR

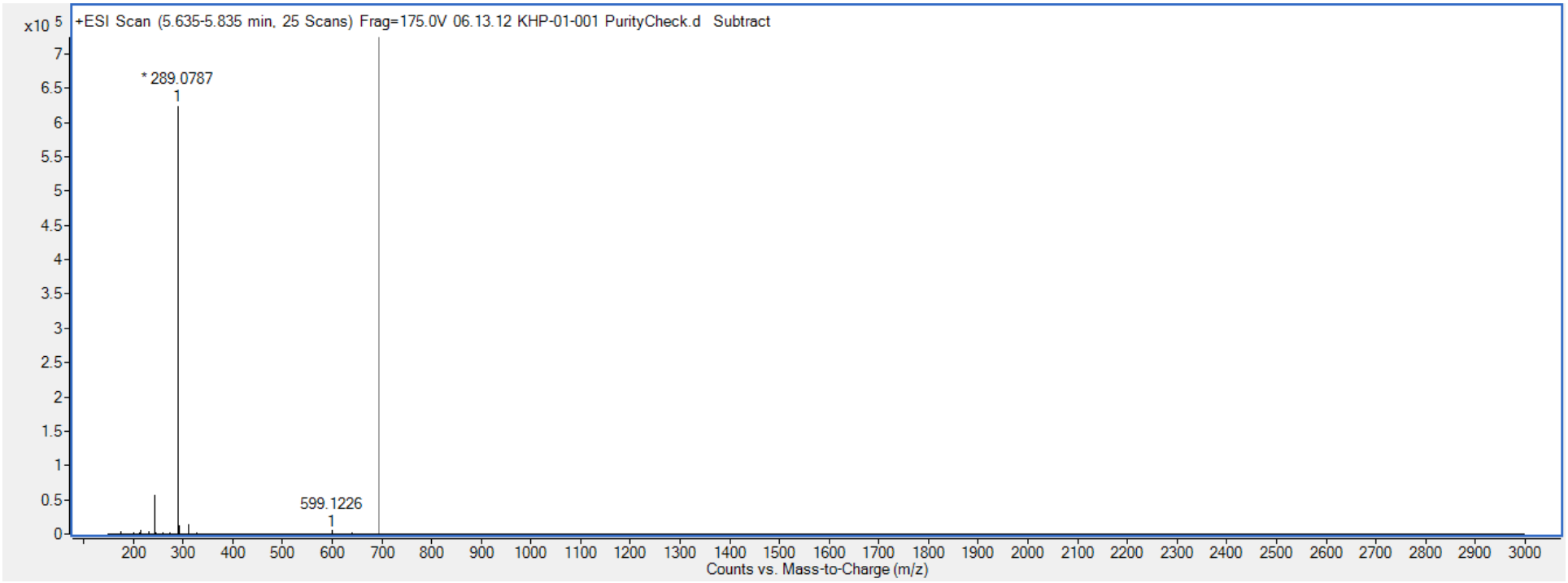


9 MS

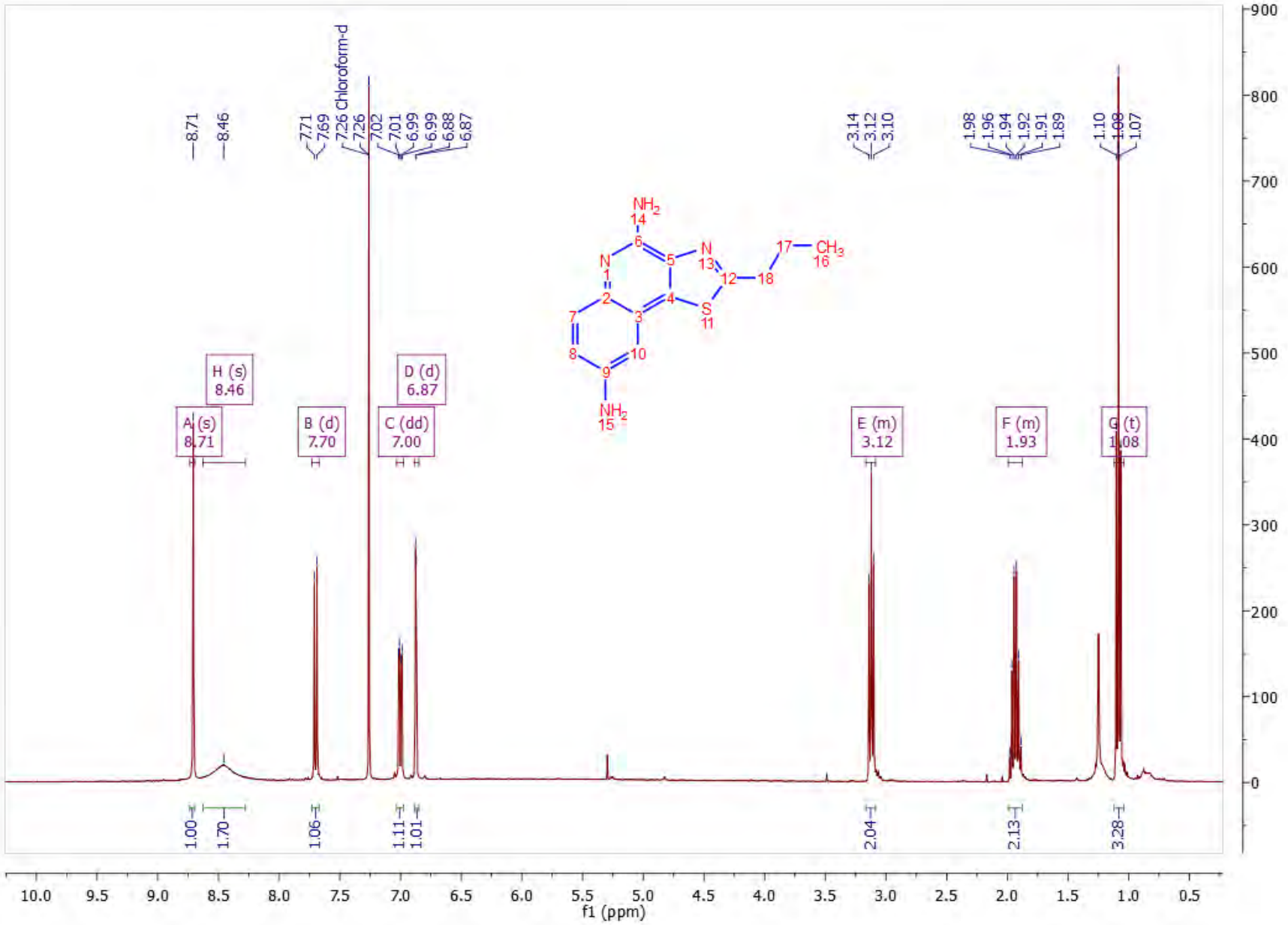


9 LC-MS

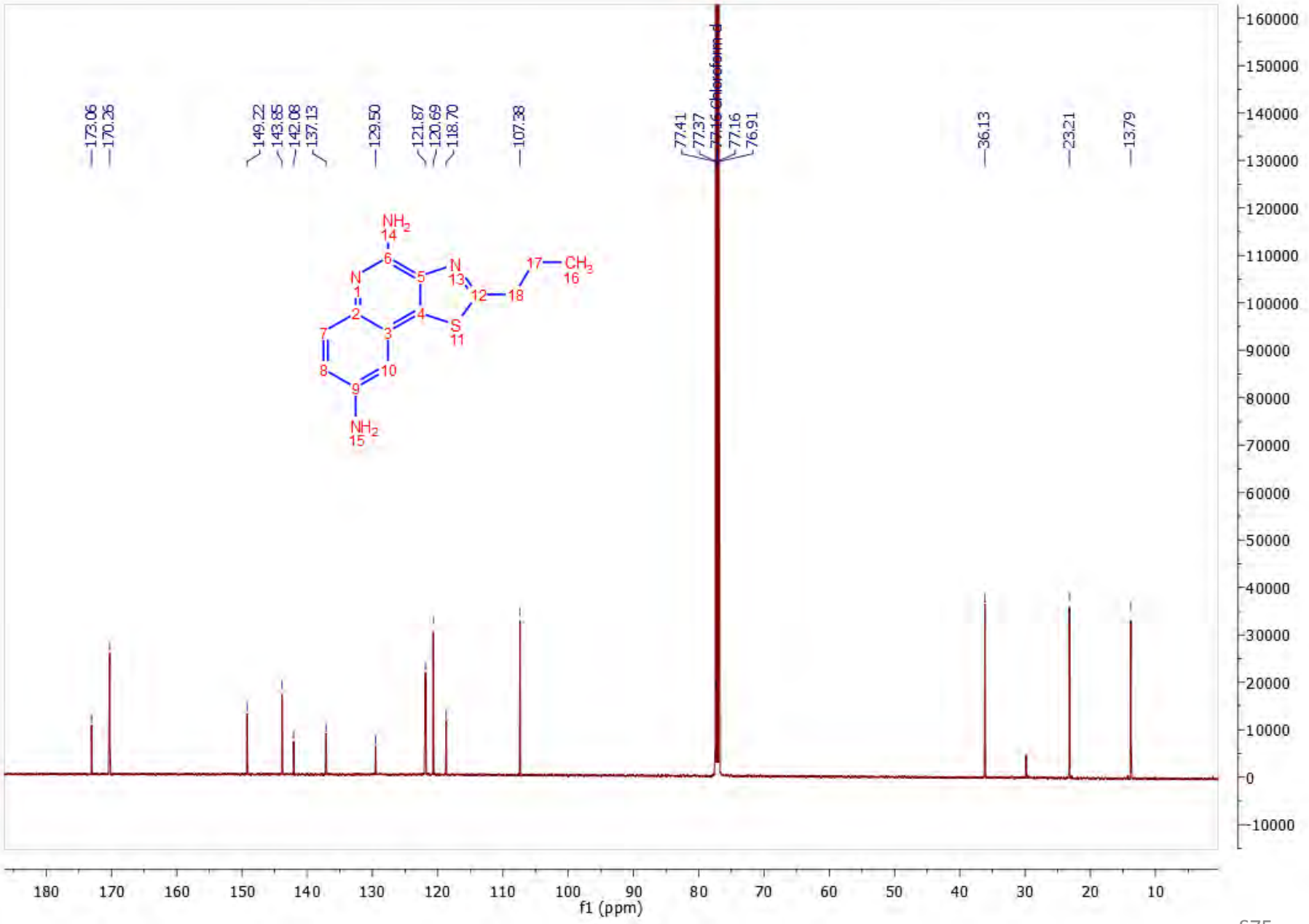




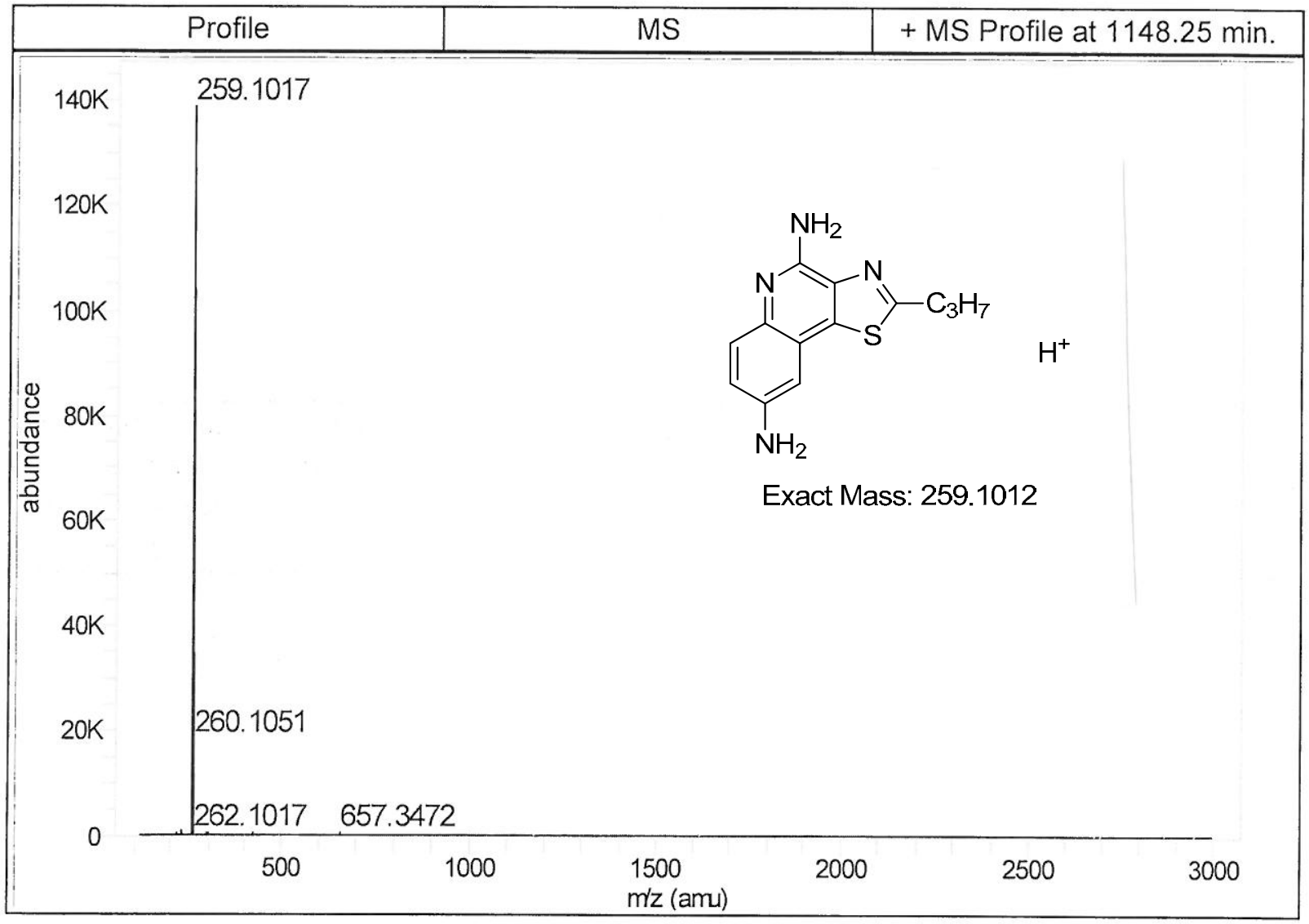
10 ^{1}H NMR


8.71
8.46
7.71
7.69
7.26 Chloroform-d
7.26
7.02
7.01
6.99
6.99
6.88
6.87
3.14
3.12
3.10
1.98
1.96
1.94
1.92
1.91
1.89
1.10
1.08
1.07
H (s) 8.46
A (s) 8.71
B (d) 7.70
D (d) 6.87
C (dd) 7.00
E (m) 3.12
F (m) 1.93
G (t) 1.08
1.00
1.70
1.06
1.11
1.01
2.04
2.13
3.28
f1 (ppm)

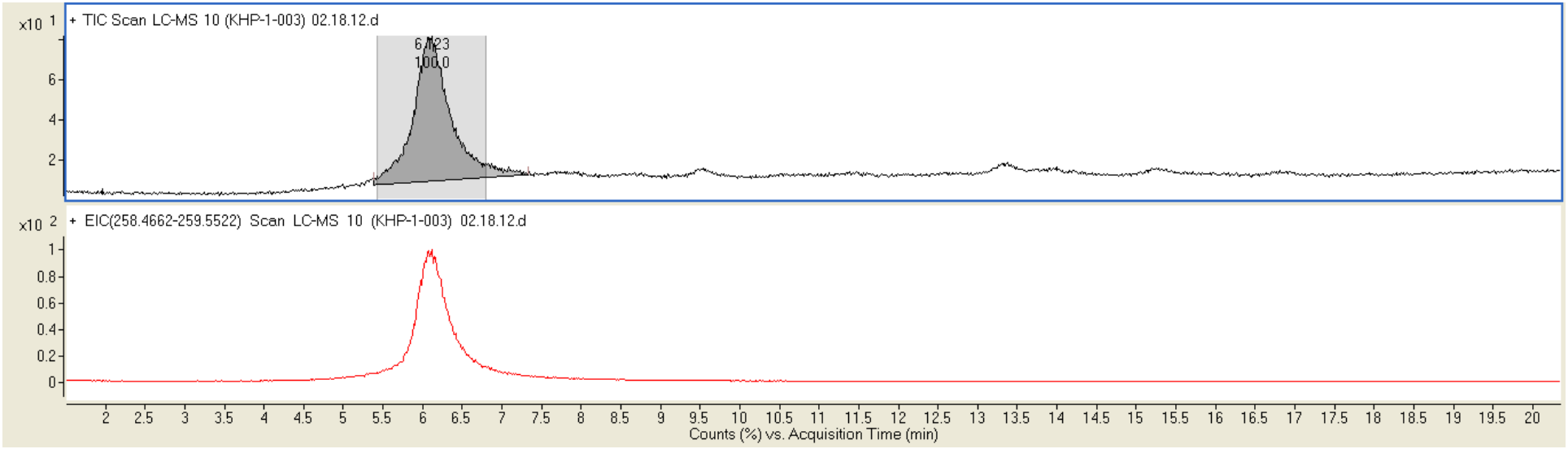
10 ^{13}C NMR

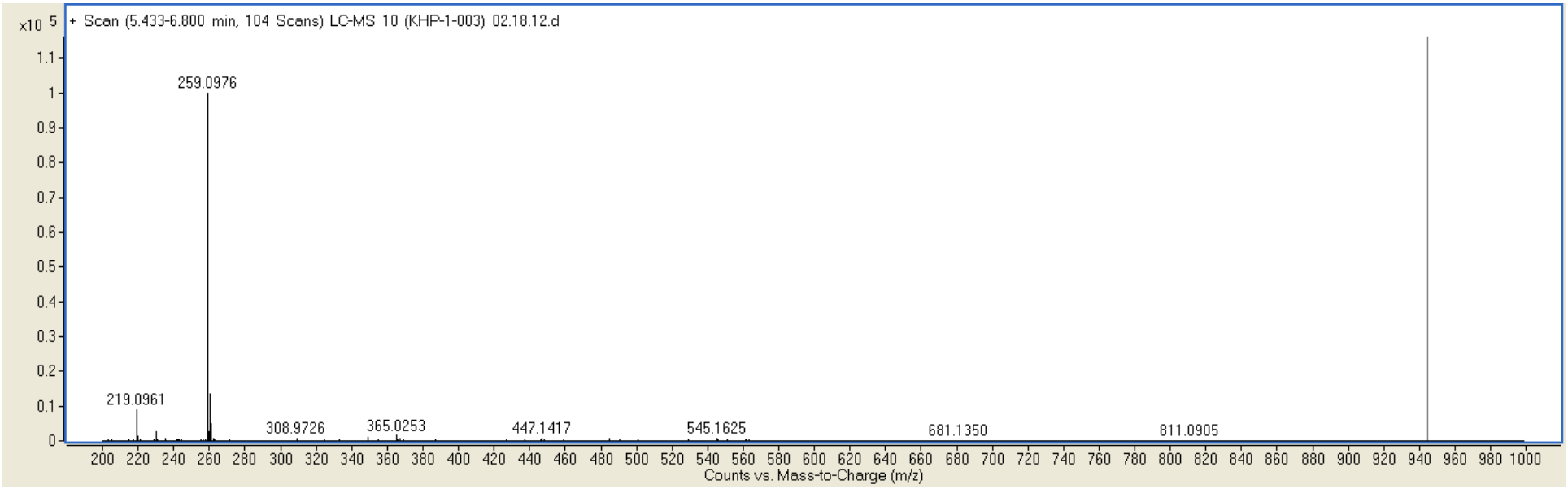


10 MS

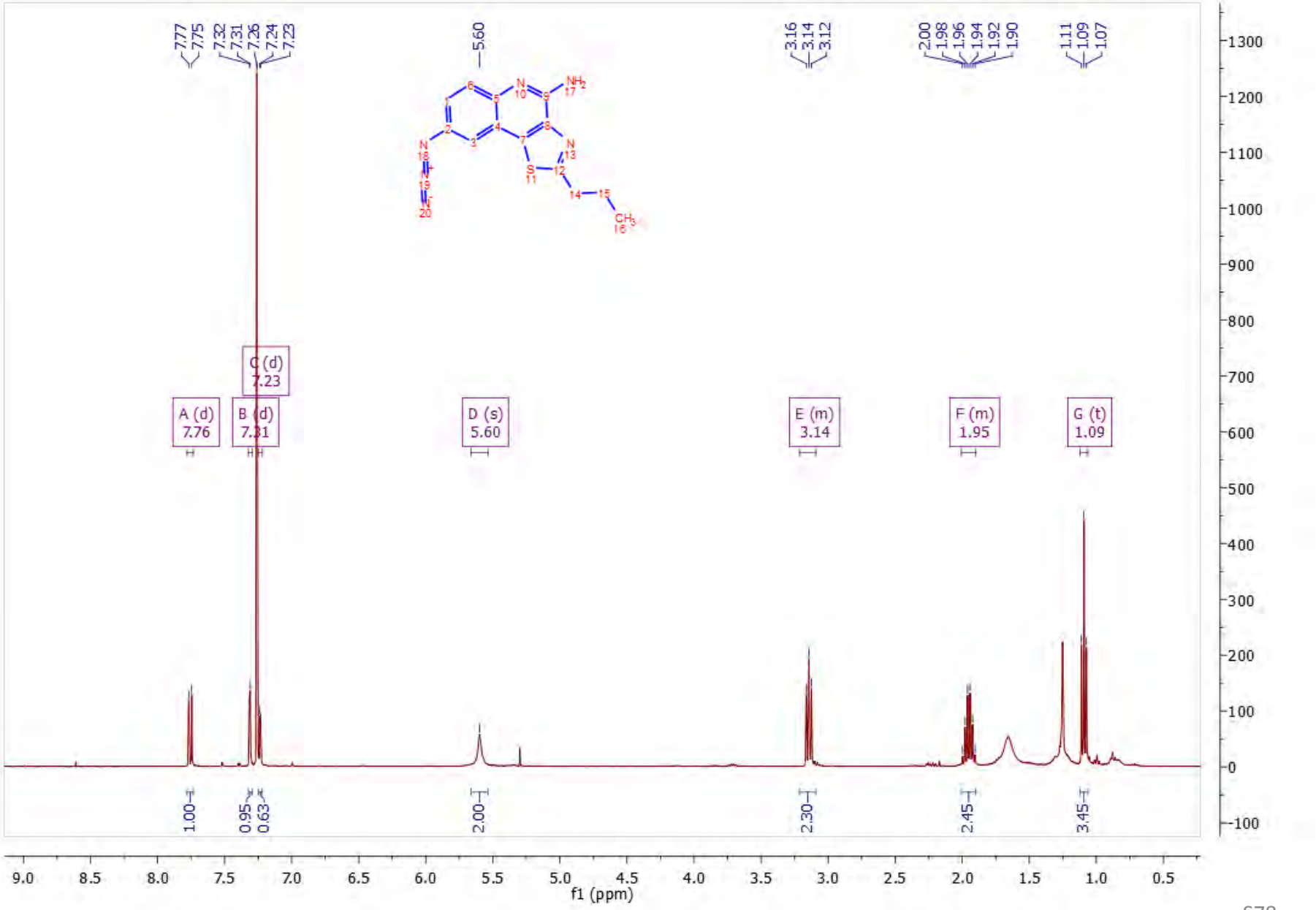


10 LC-MS

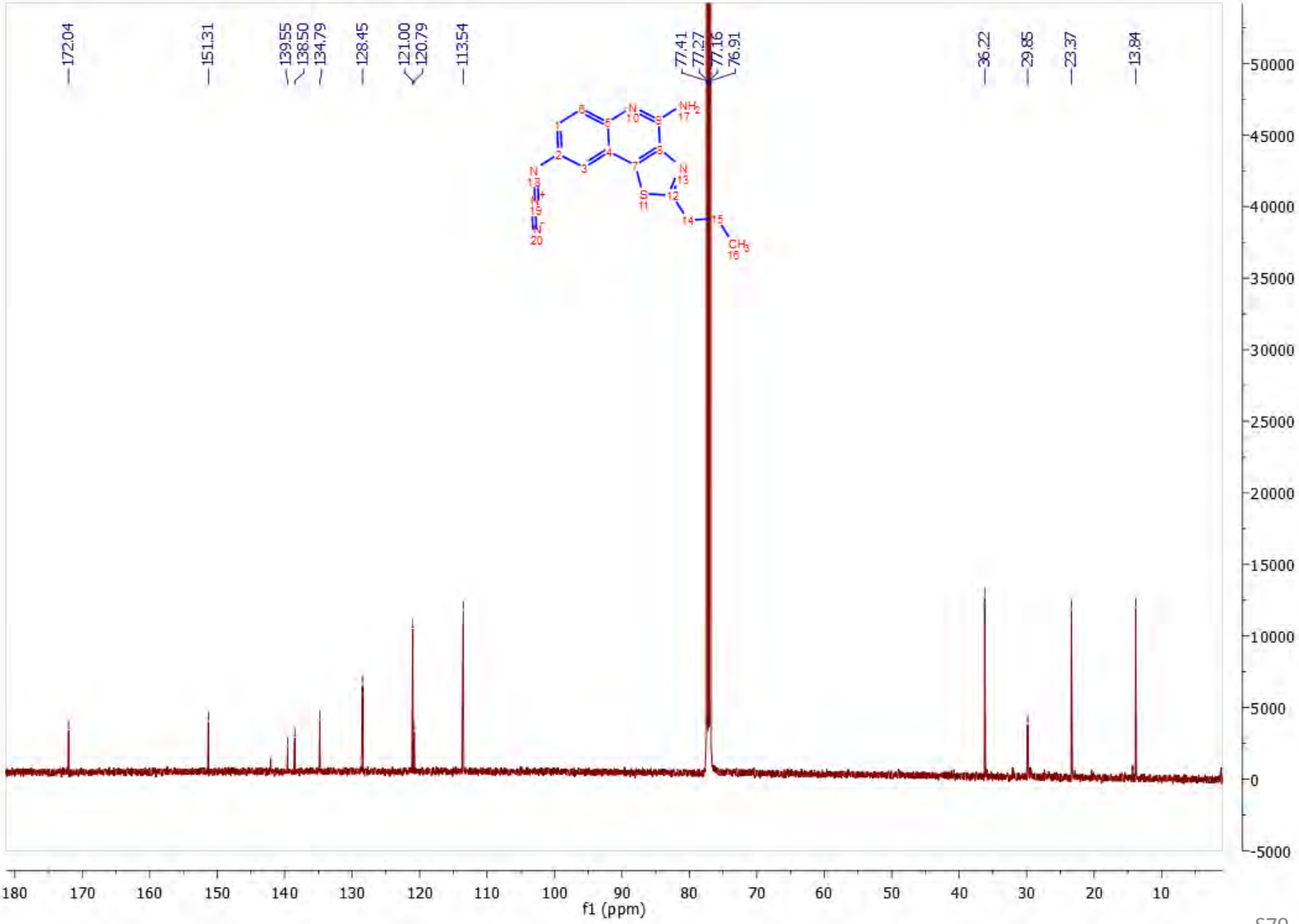




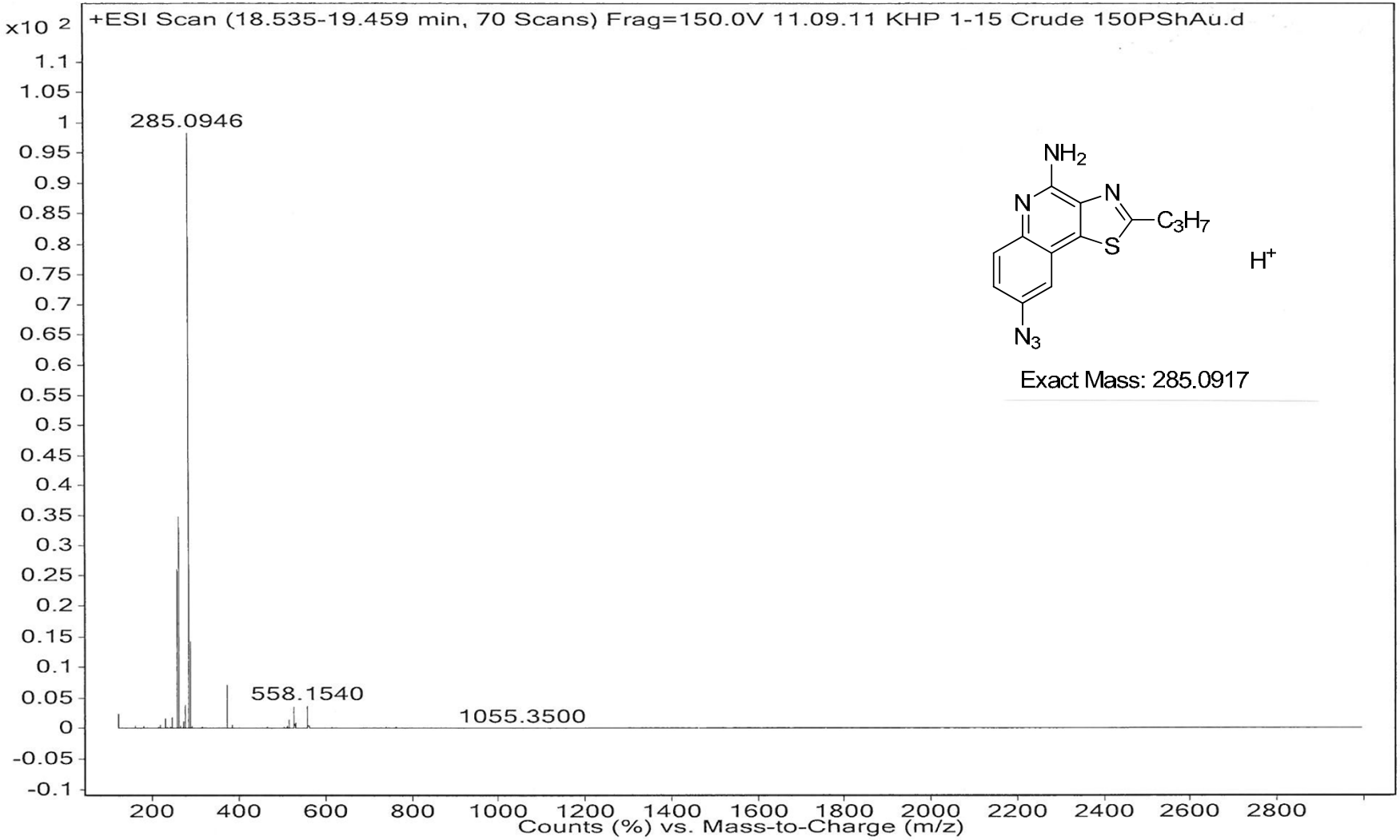
11 ^{1}H NMR



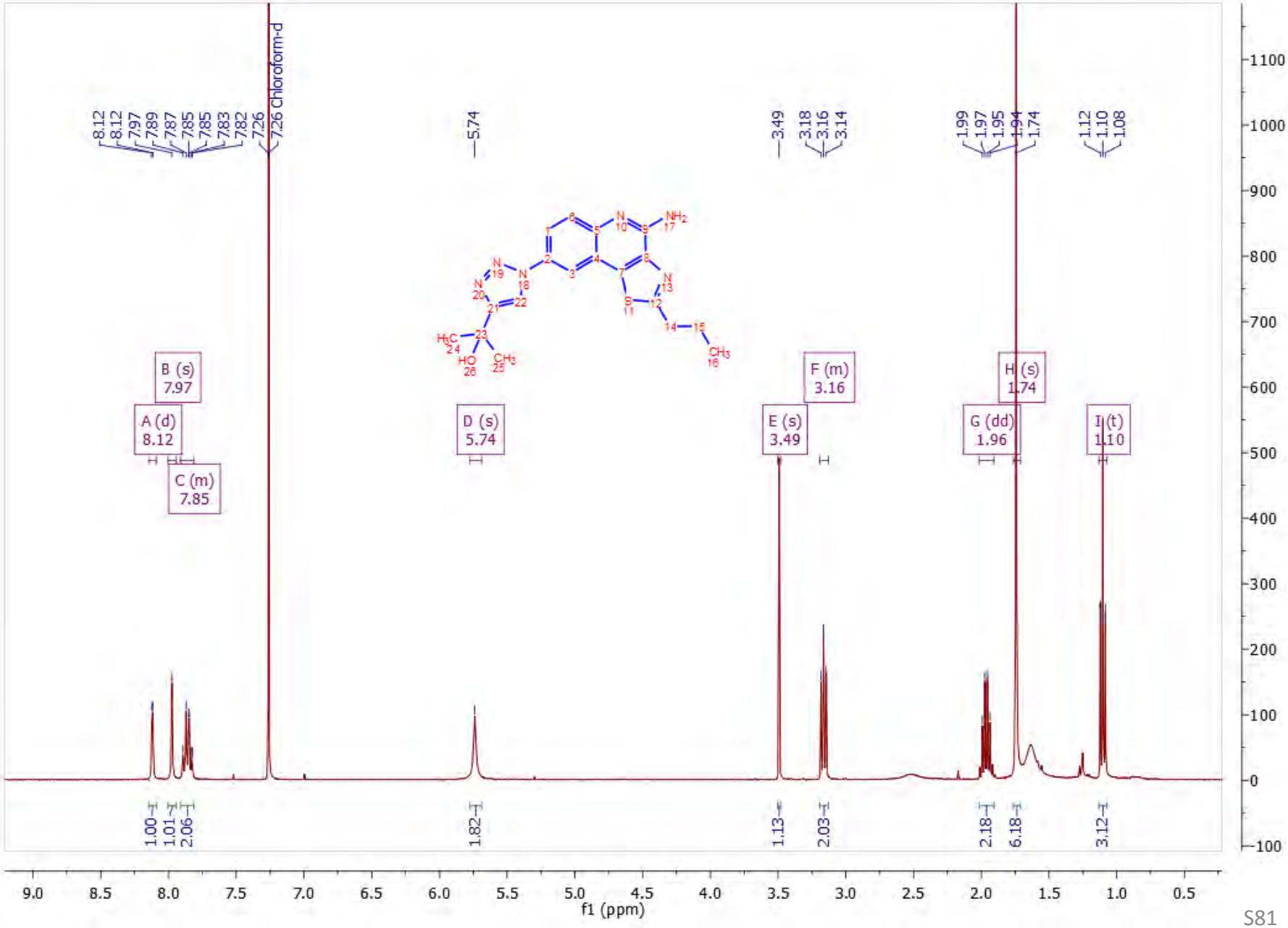
11 ^{13}C NMR



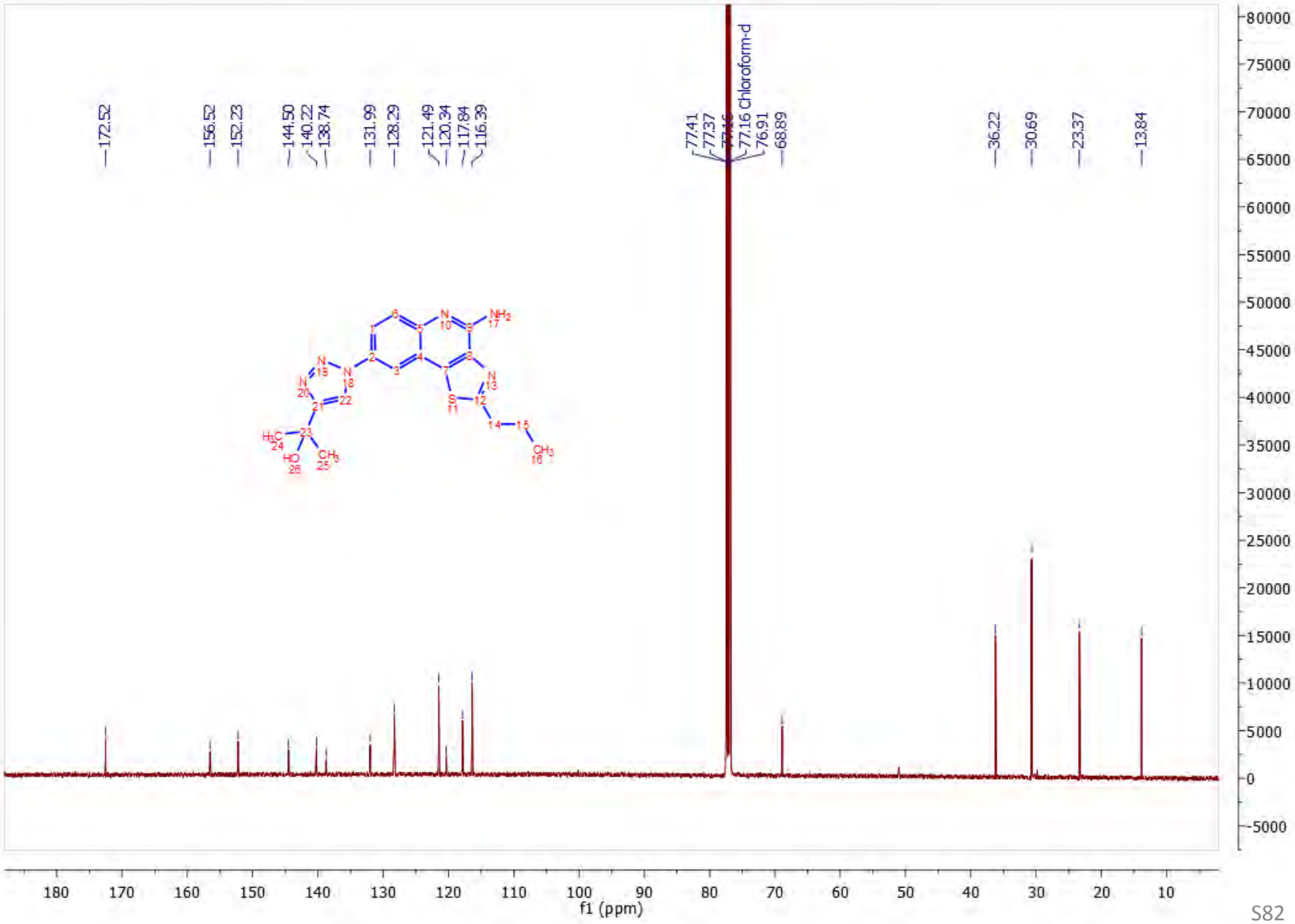
11 MS



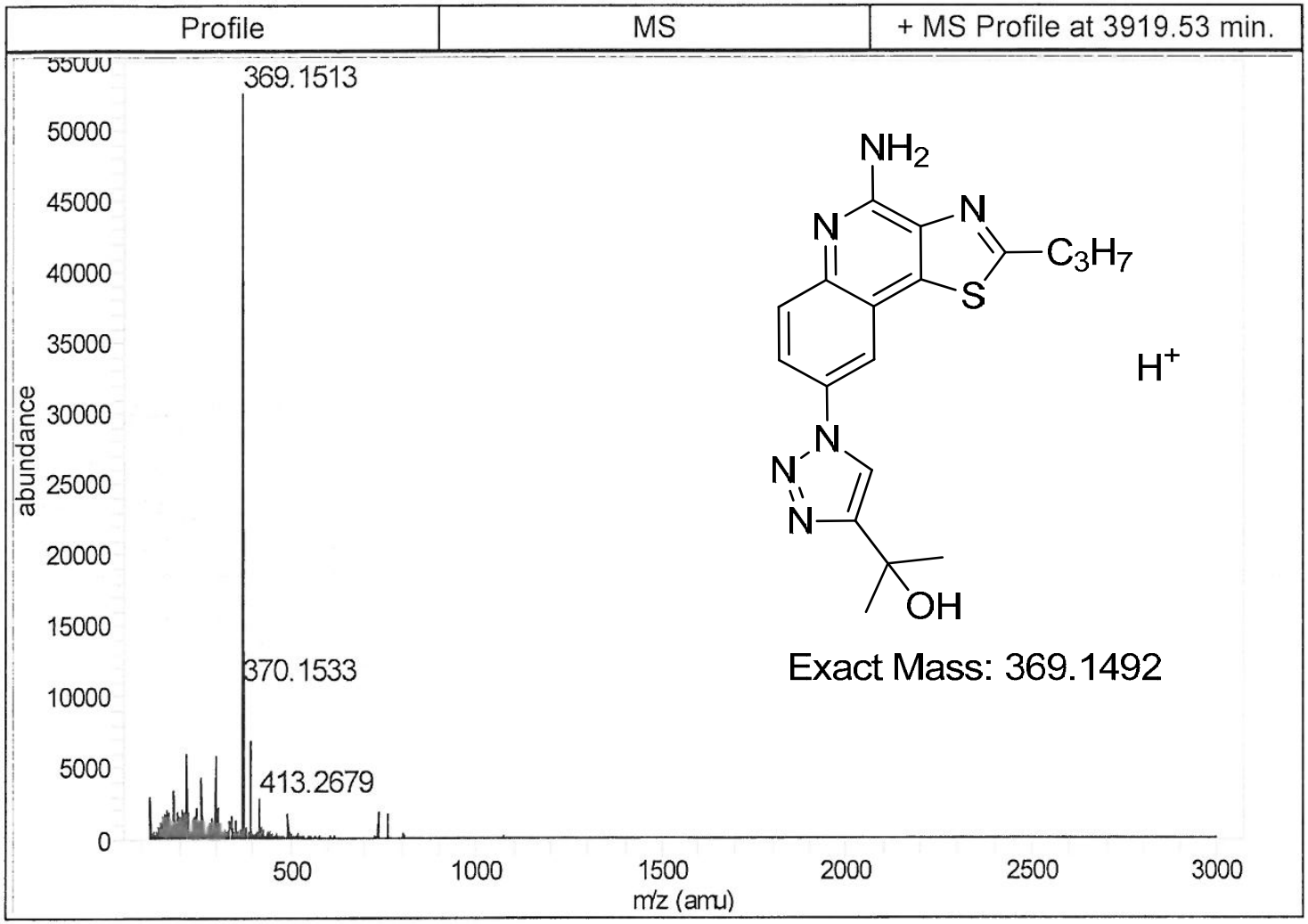
12a ^{1}H NMR



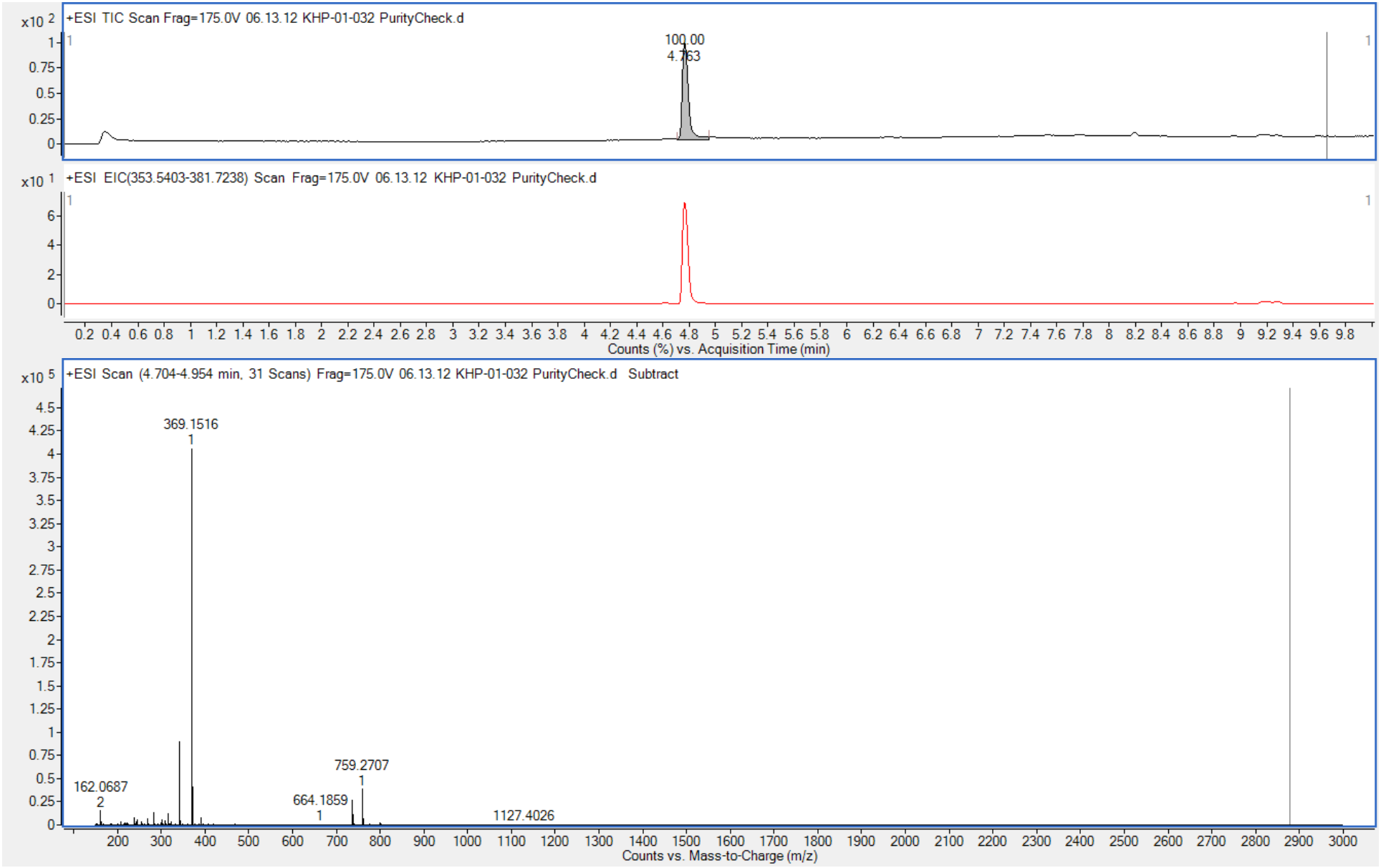
12a ^{13}C NMR



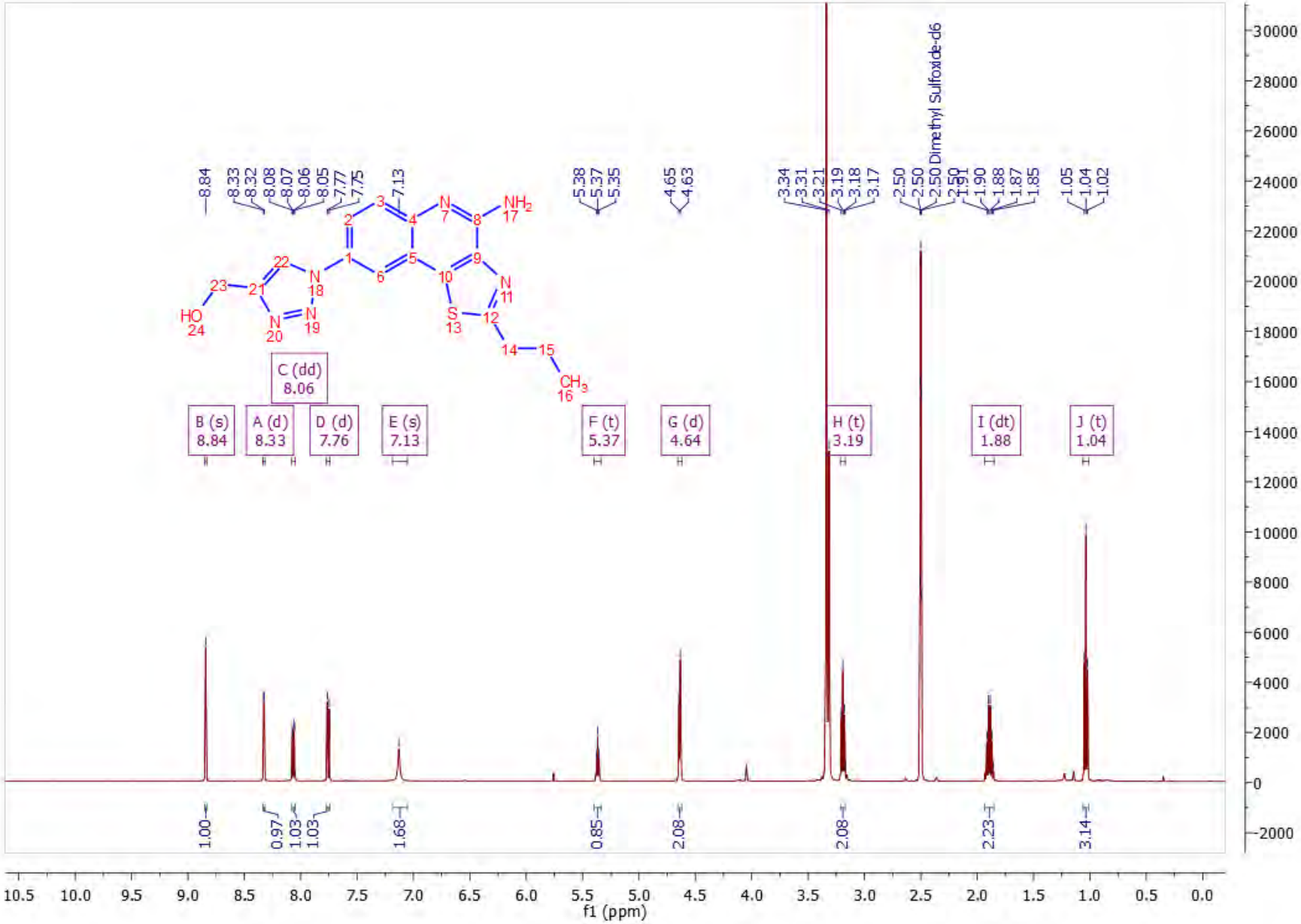
12a MS



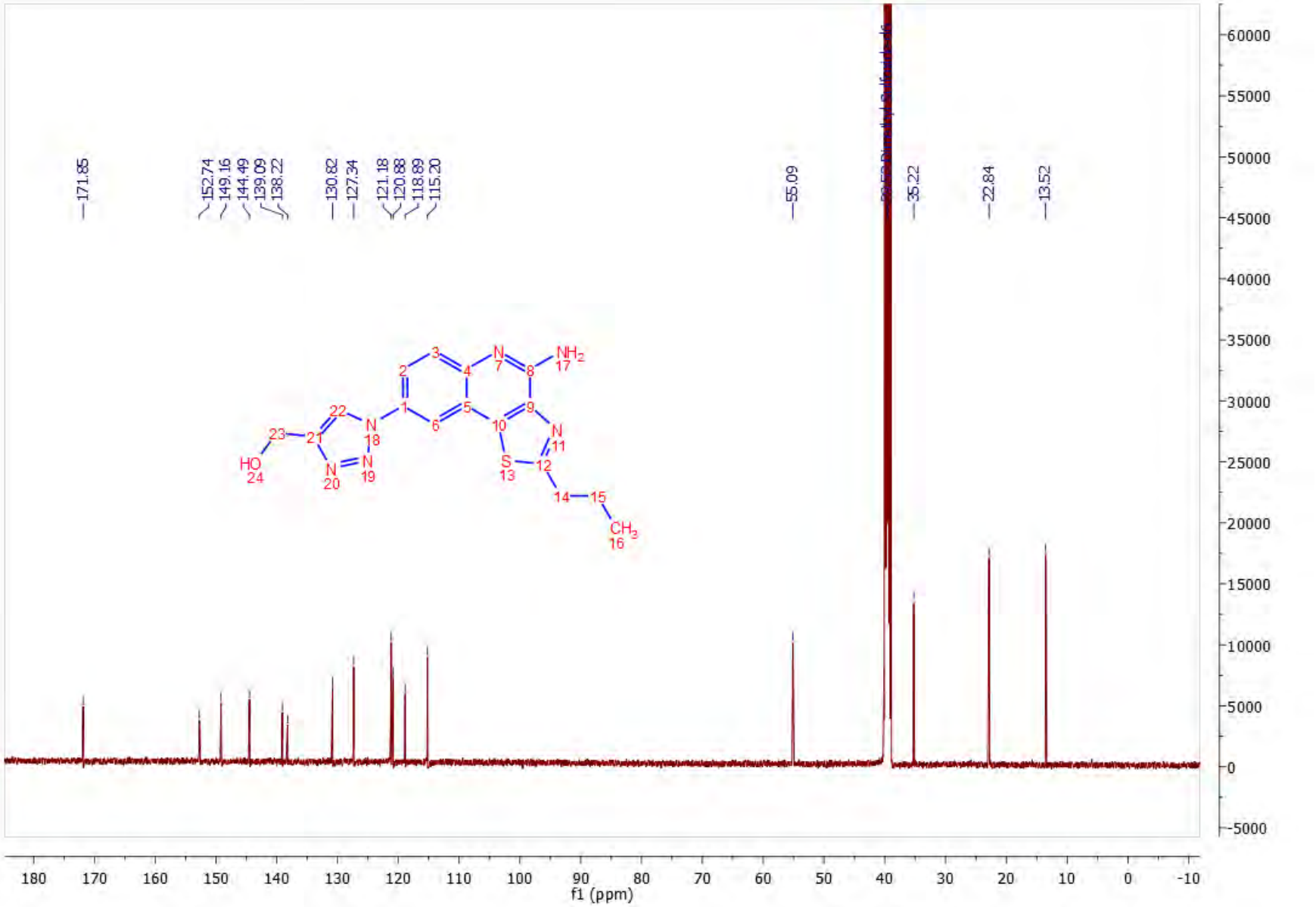
12a LC-MS



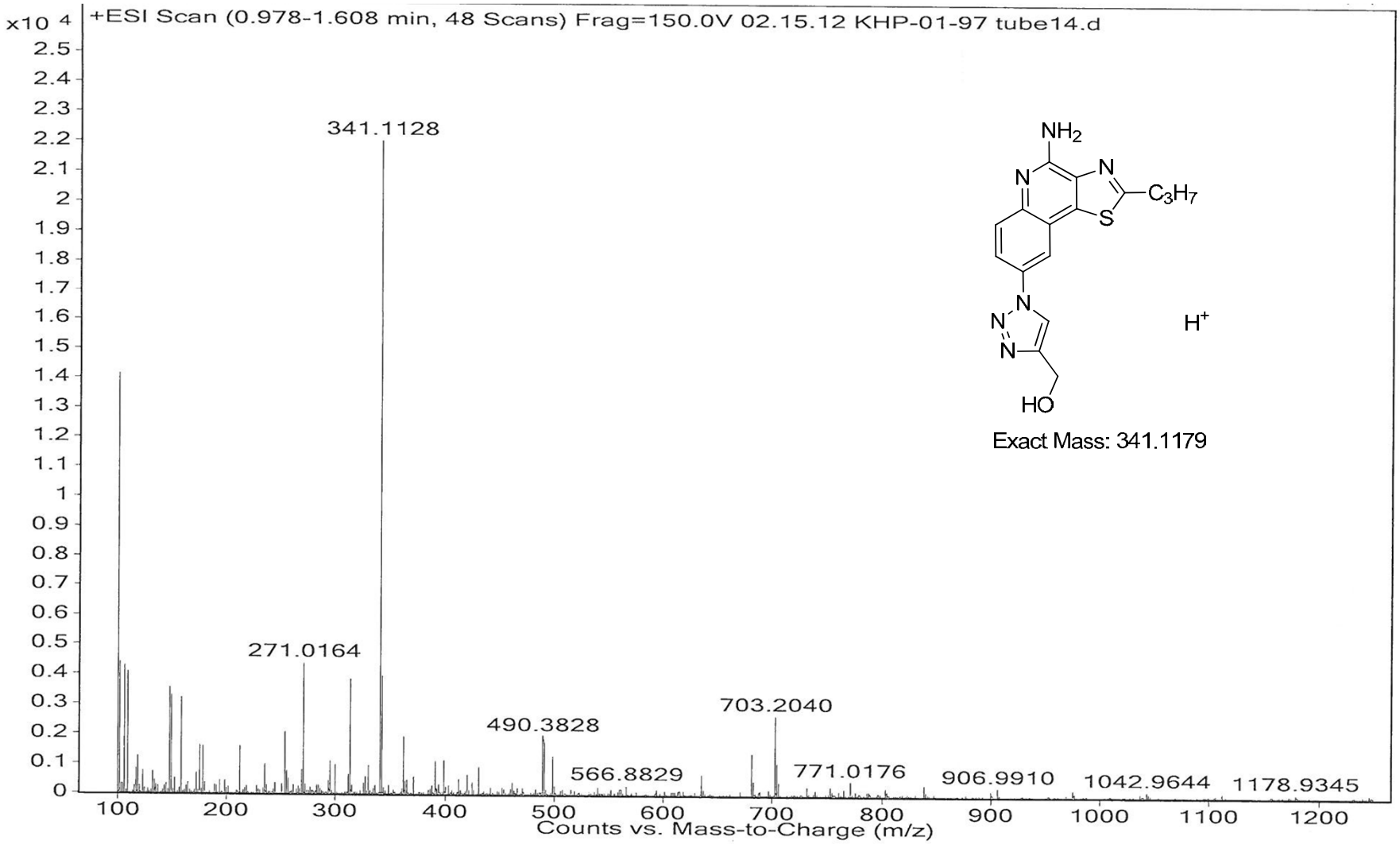
12b ^{1}H NMR


8.84
8.33
8.32
8.08
8.07
8.06
8.05
7.77
7.75
7.13
5.38
5.37
5.35
4.65
4.63
3.34
3.31
3.21
3.19
3.18
3.17
2.50
2.50
2.50 Dimethyl Sulfoxide-d6
2.50
1.91
1.90
1.88
1.87
1.85
1.05
1.04
1.02
NH2
17
HO
24
CH3
16
B (s) 8.84
A (d) 8.33
C (dd) 8.06
D (d) 7.76
E (s) 7.13
F (t) 5.37
G (d) 4.64
H (t) 3.19
I (dt) 1.88
J (t) 1.04
1.00
0.97
1.03
1.03
1.68
0.85
2.08
2.08
2.23
3.14
f1 (ppm)

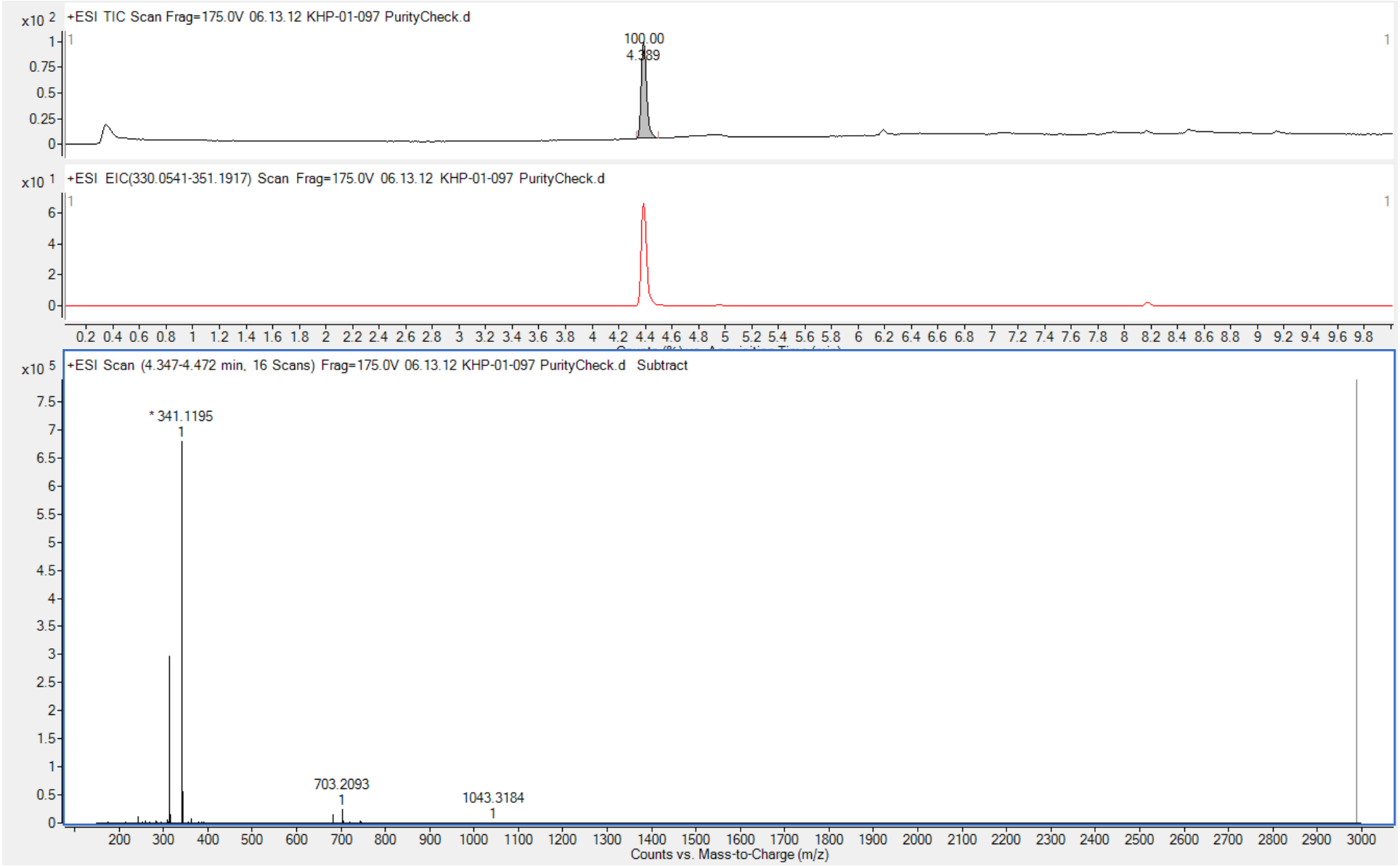
12b ^{13}C NMR



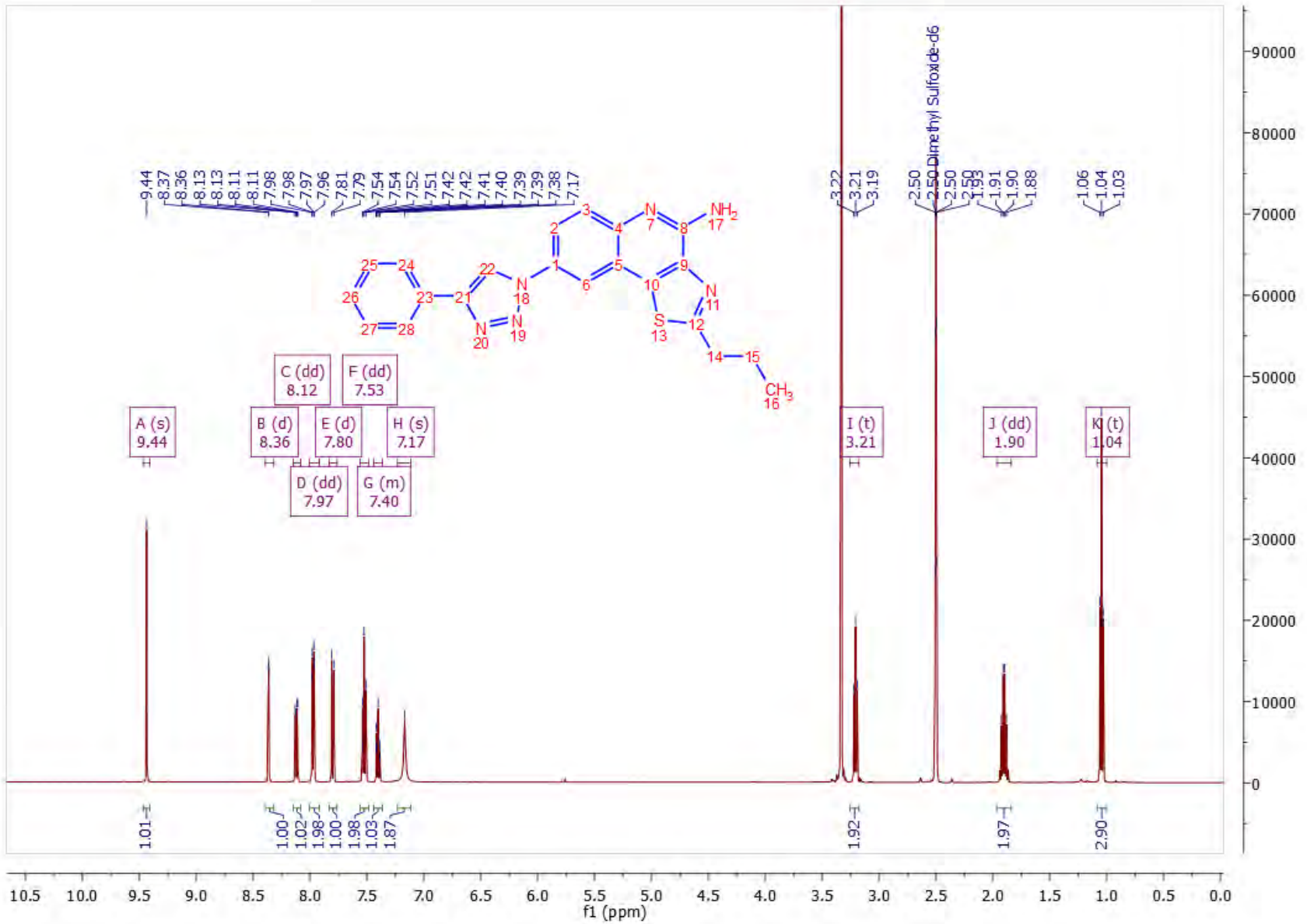
12b MS



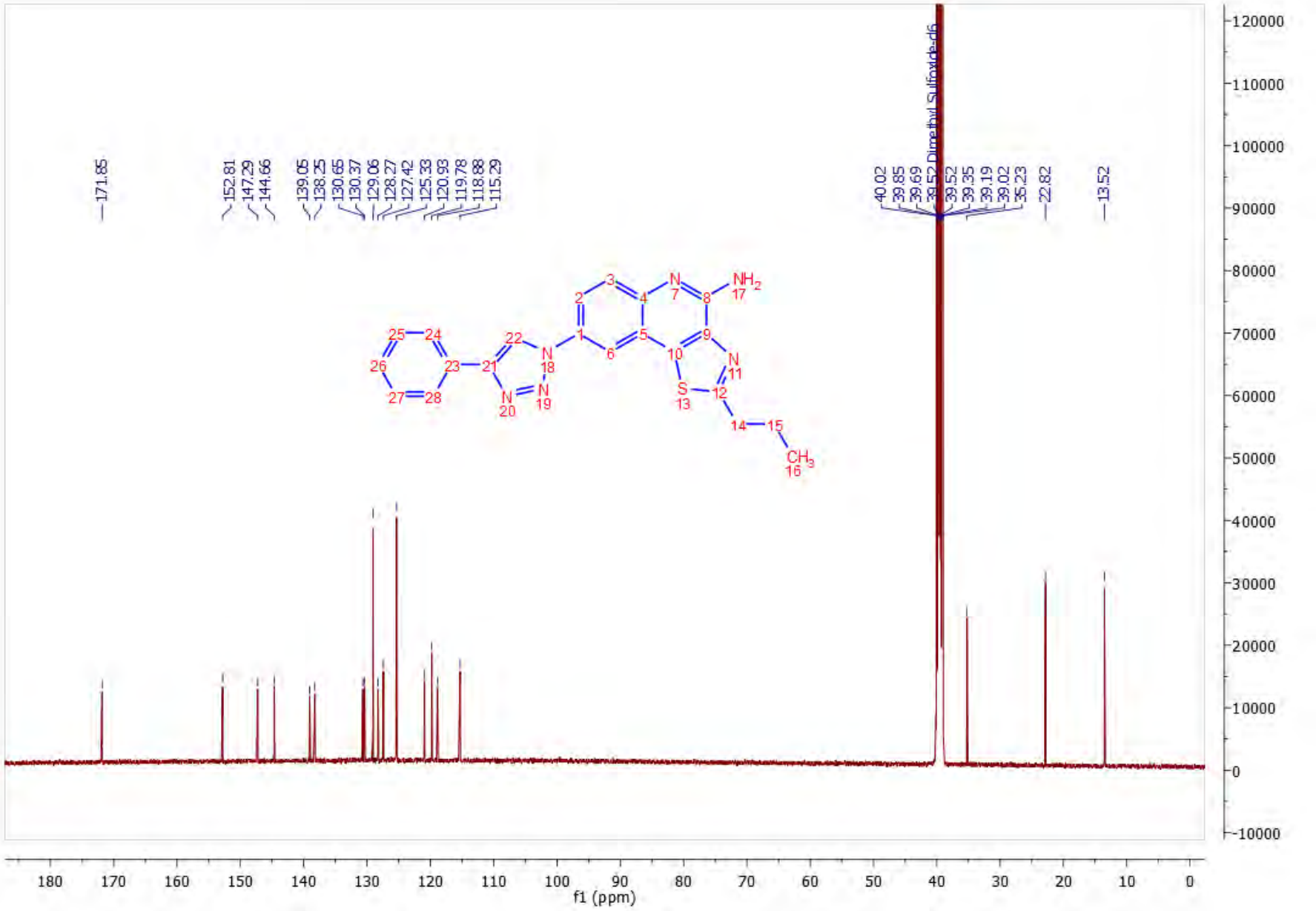
12b LC-MS



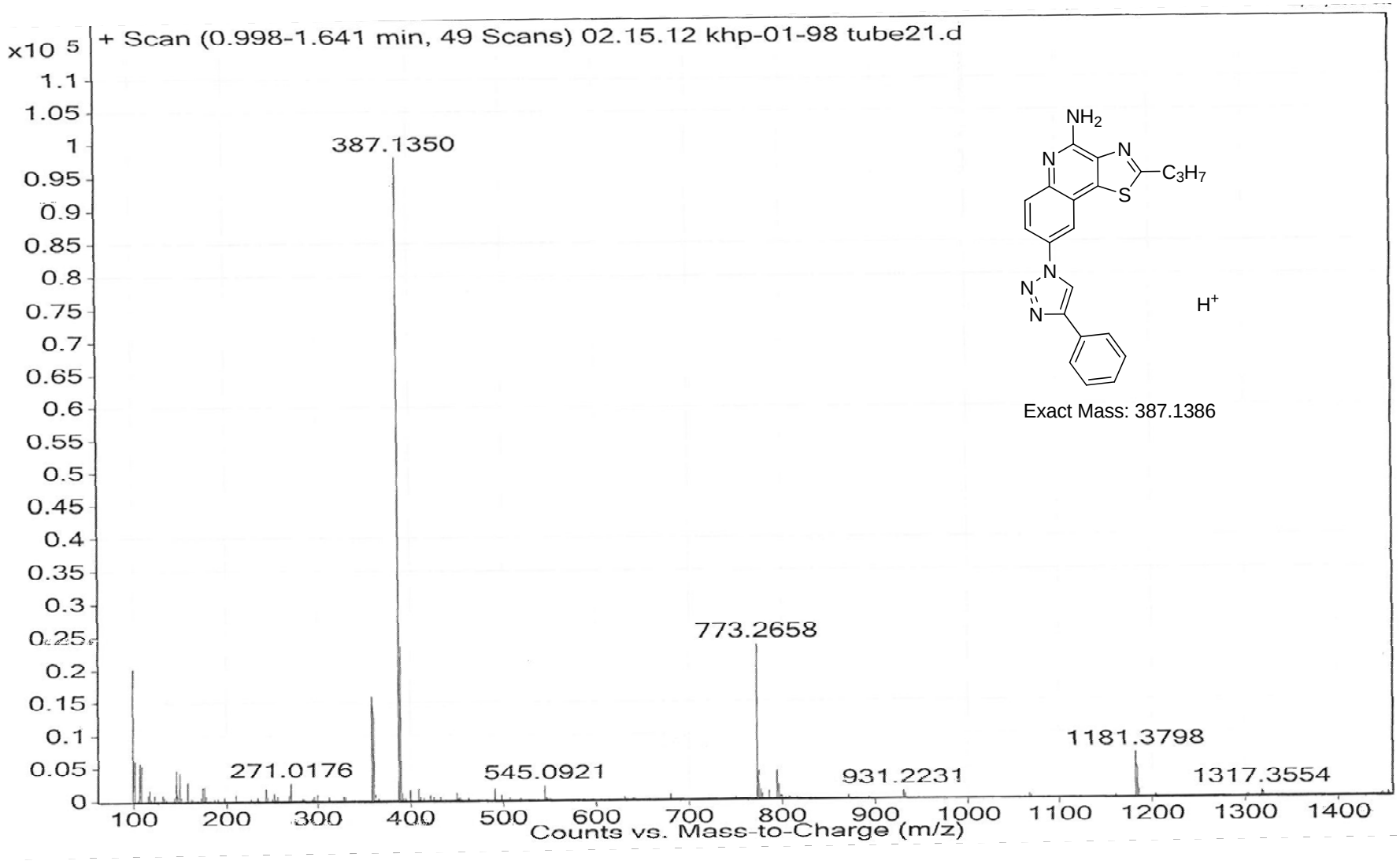
12c ^{1}H NMR



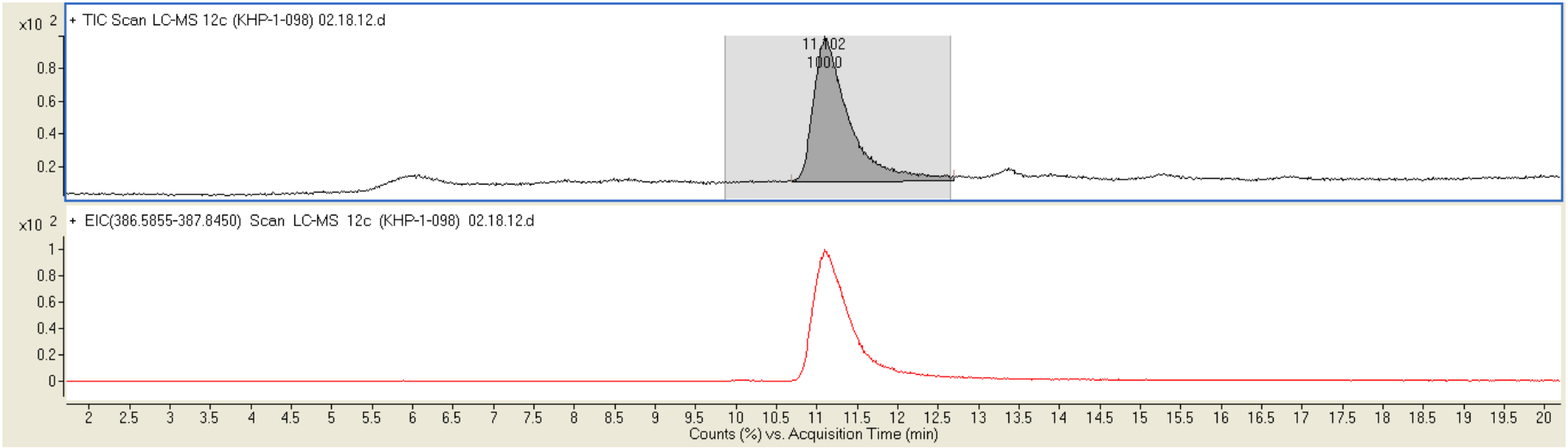
12c ^{13}C NMR

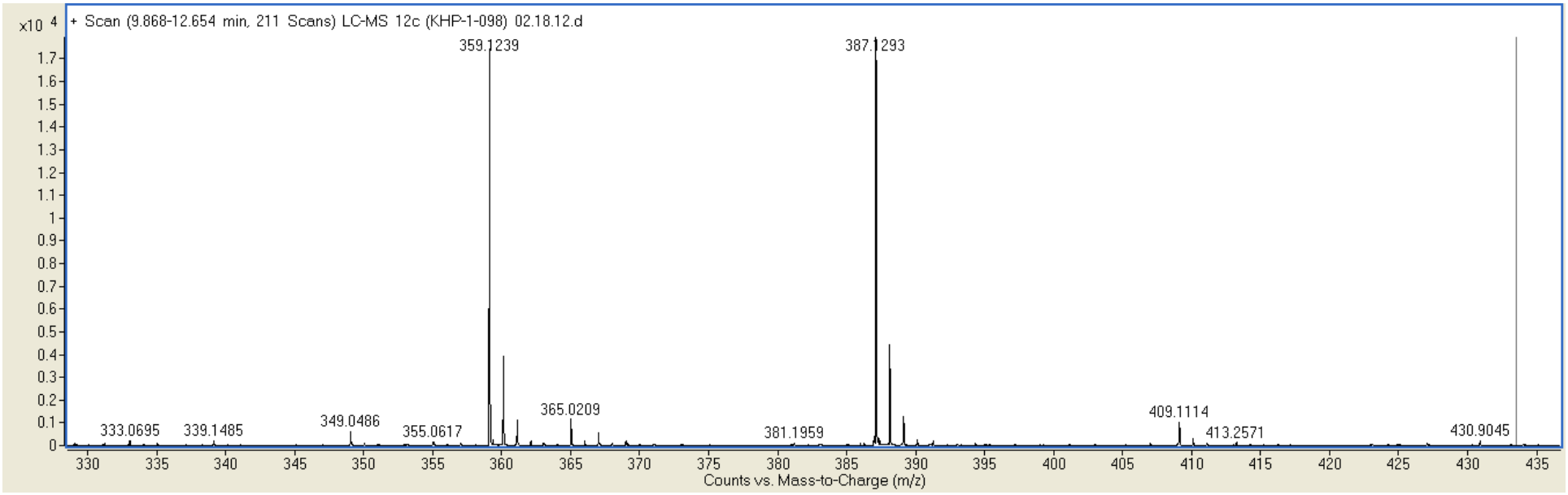


12c MS

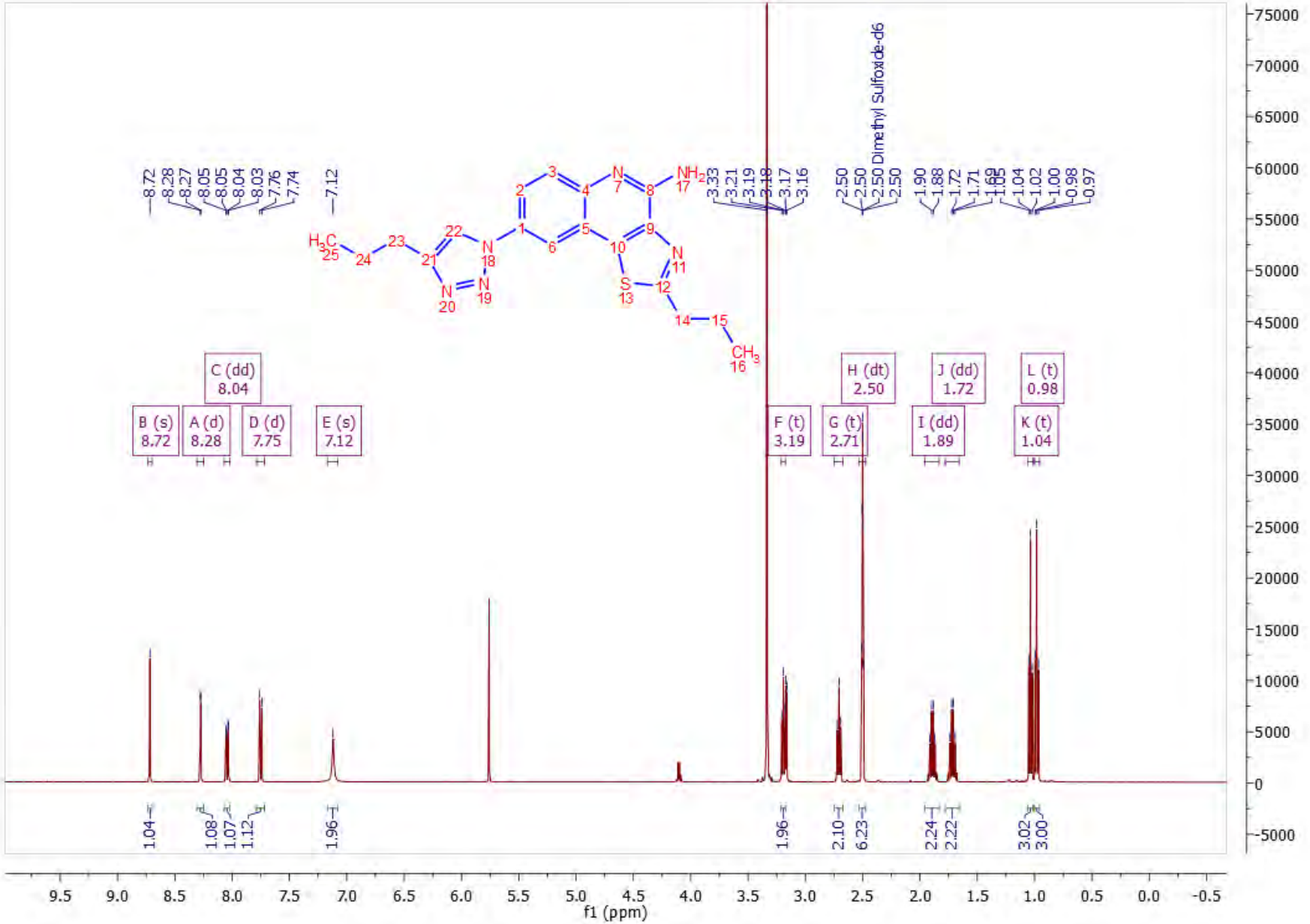


12c LC-MS

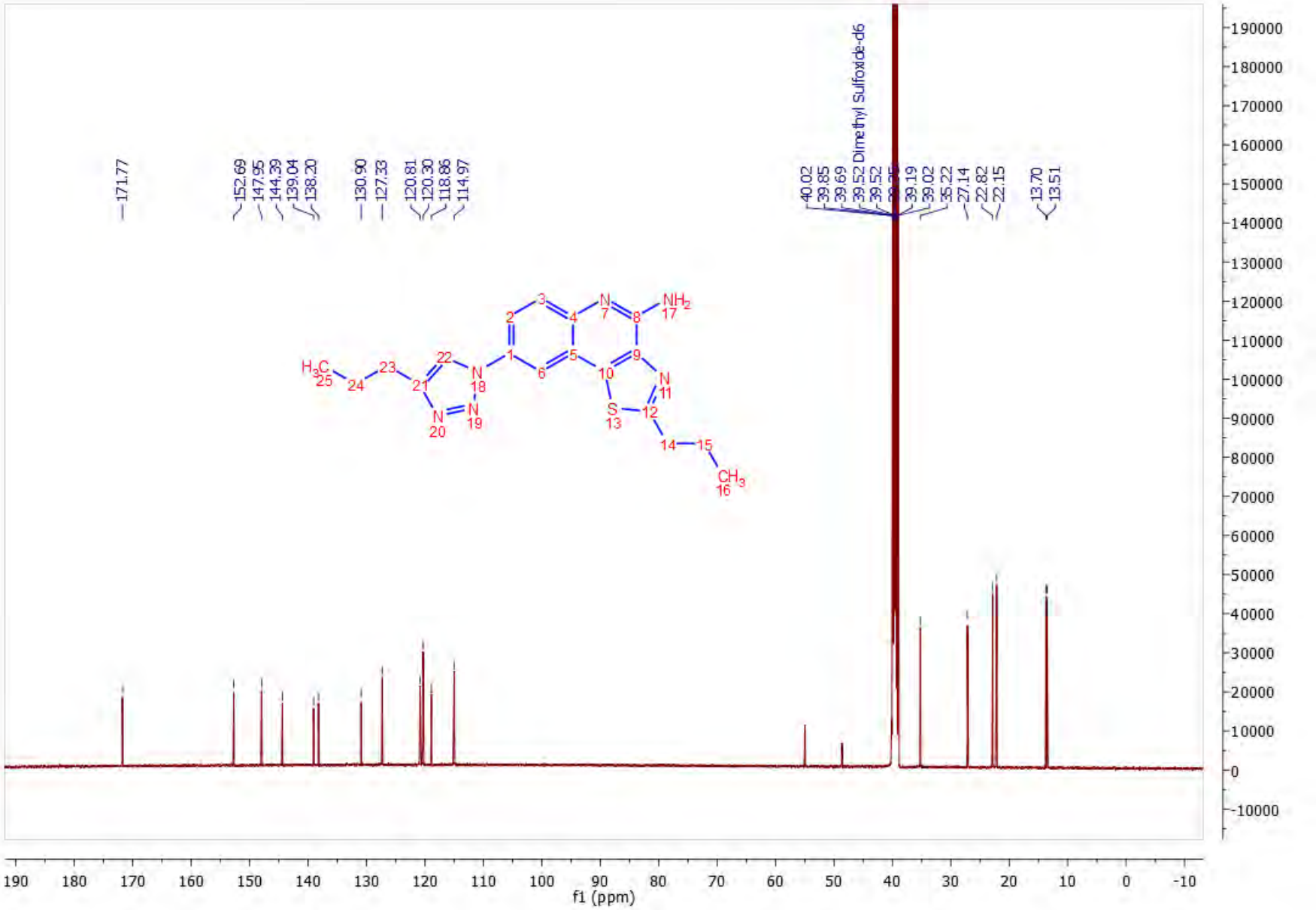




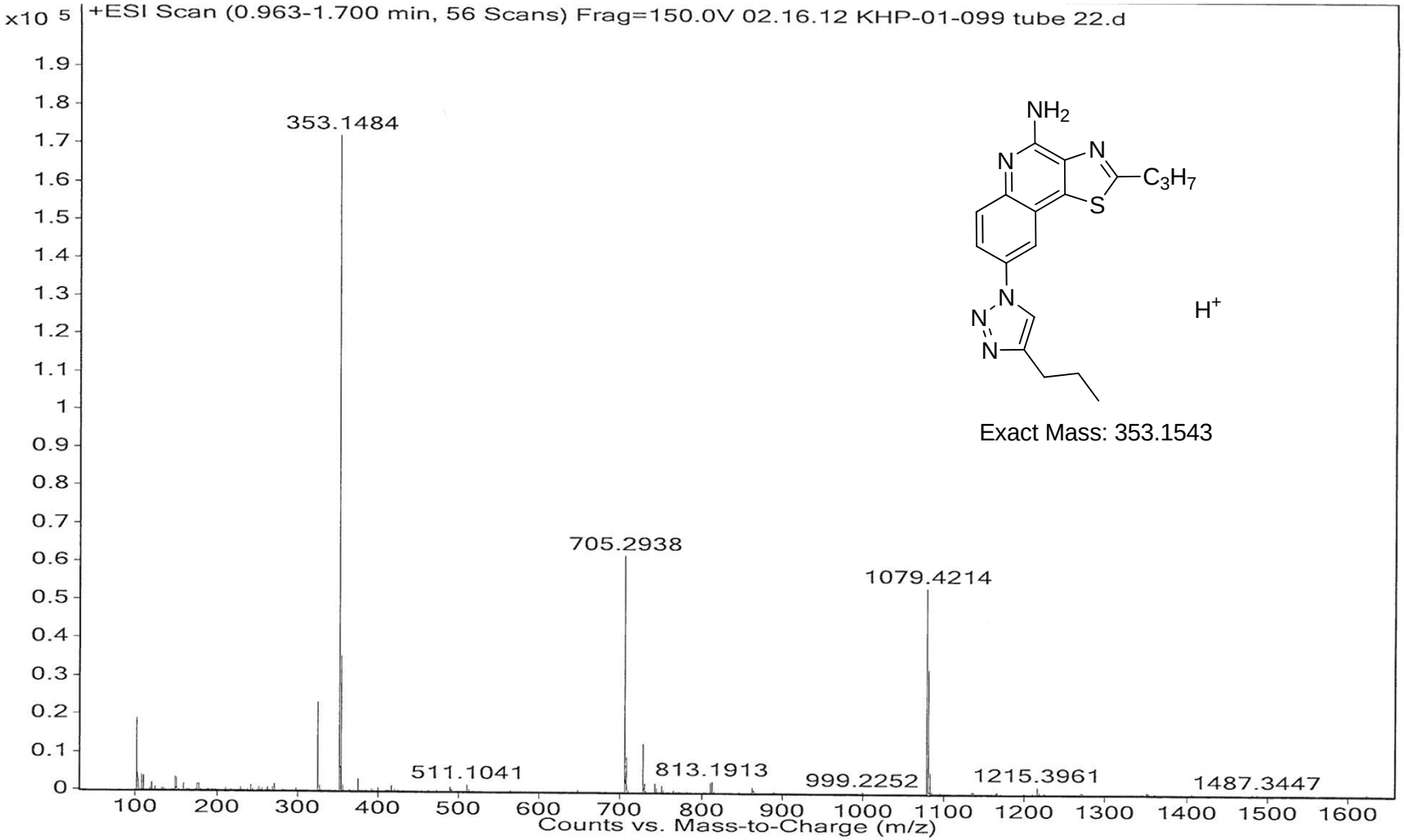
12d ^{1}H NMR



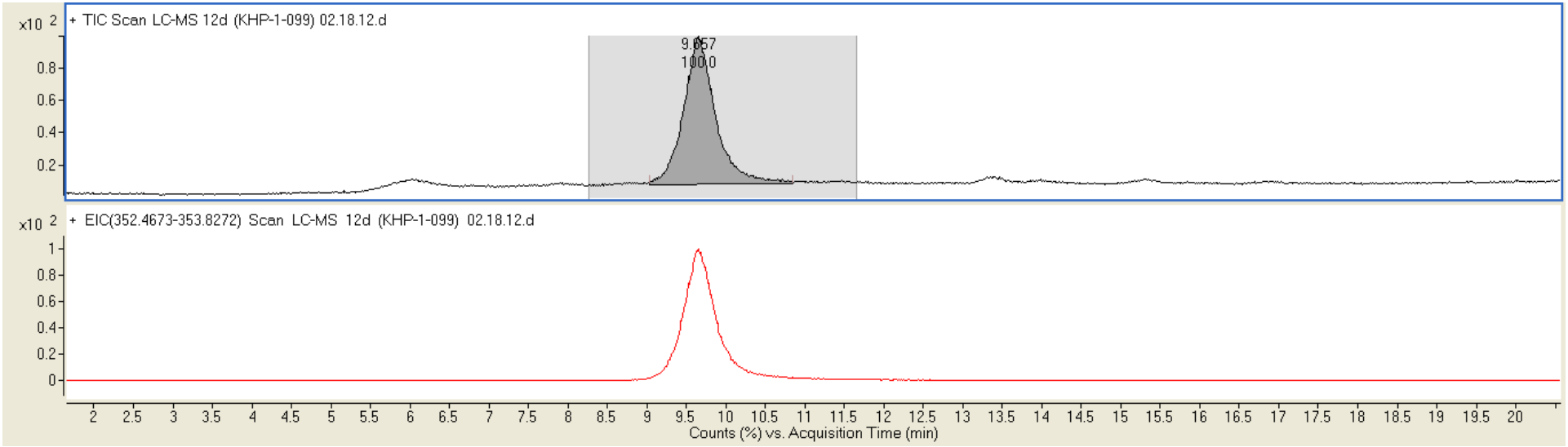
12d ^{13}C NMR

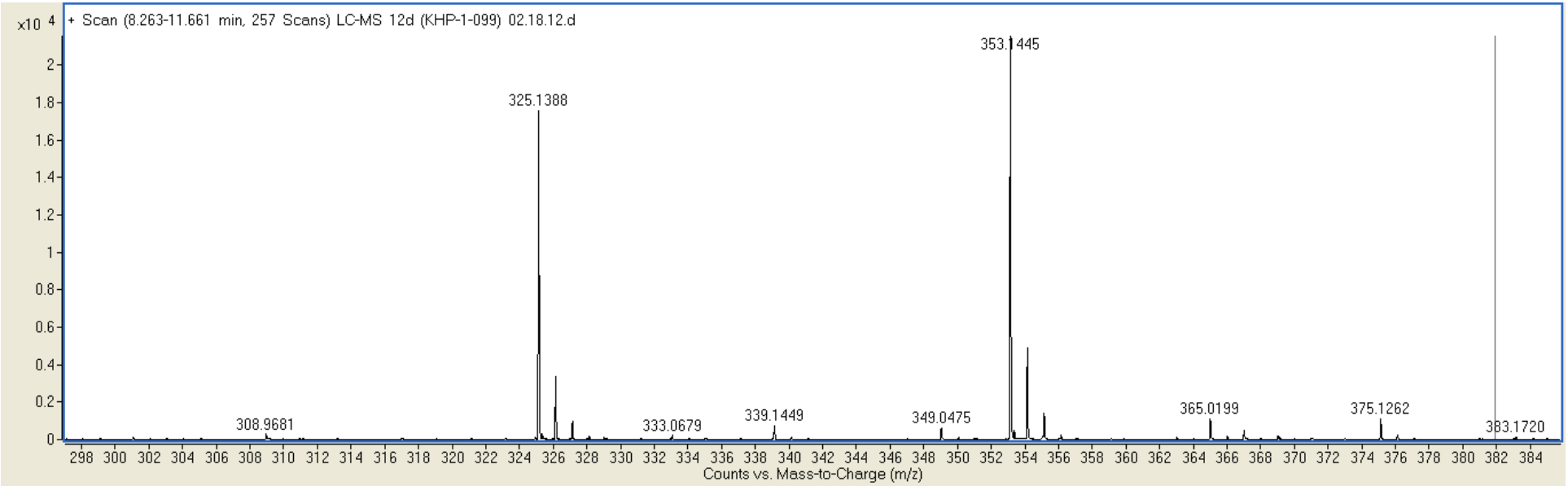


12d MS

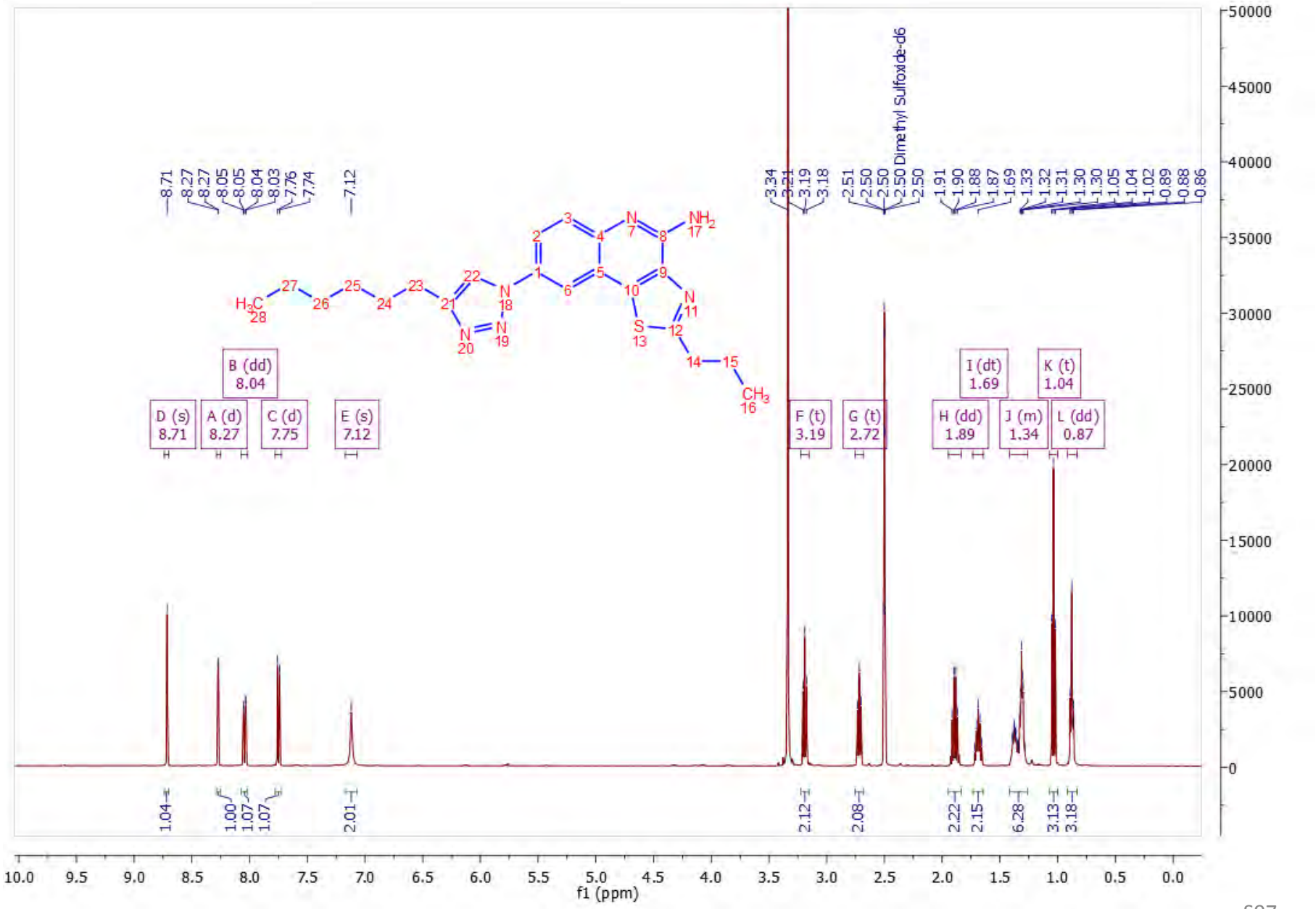


12d LC-MS

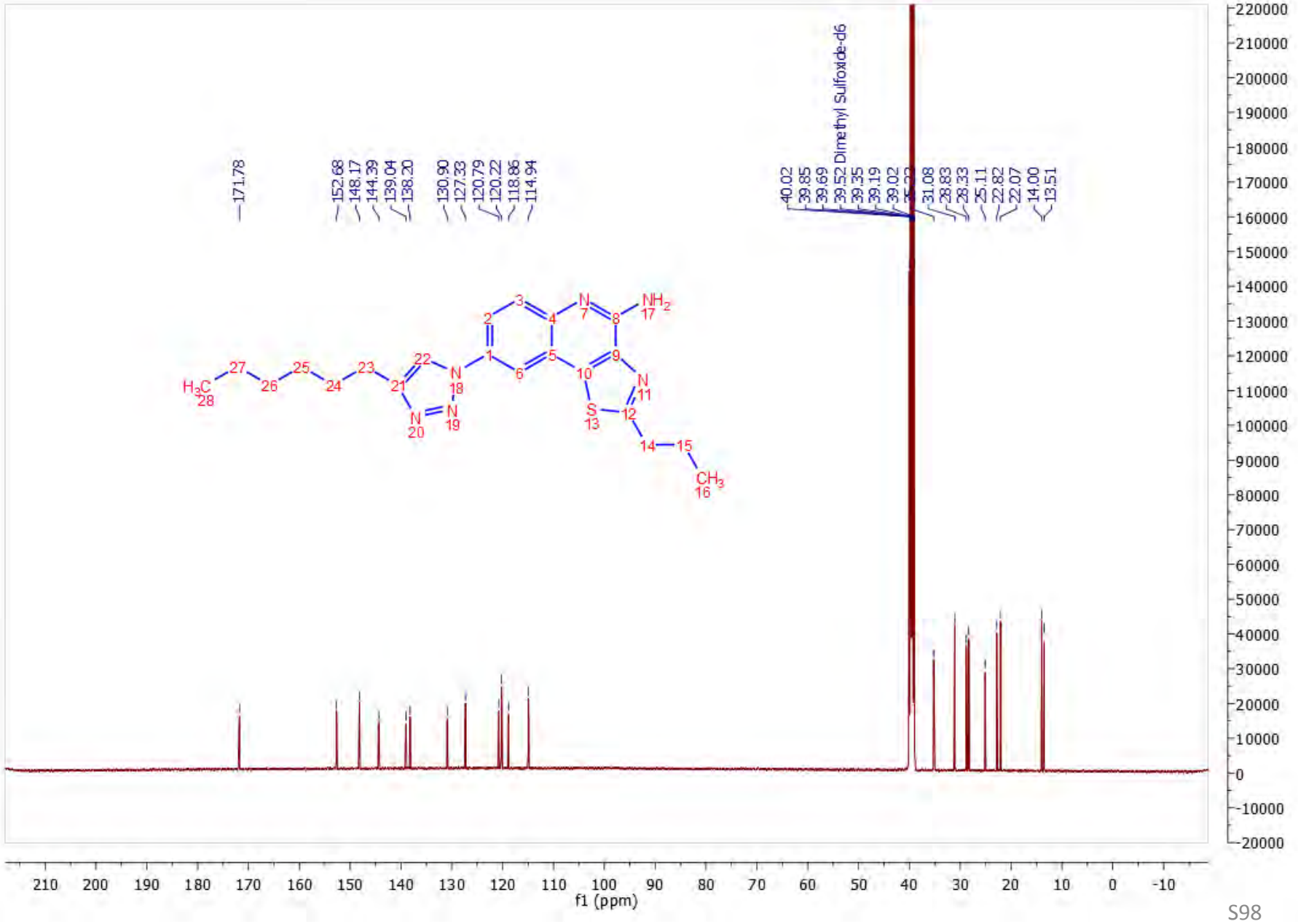




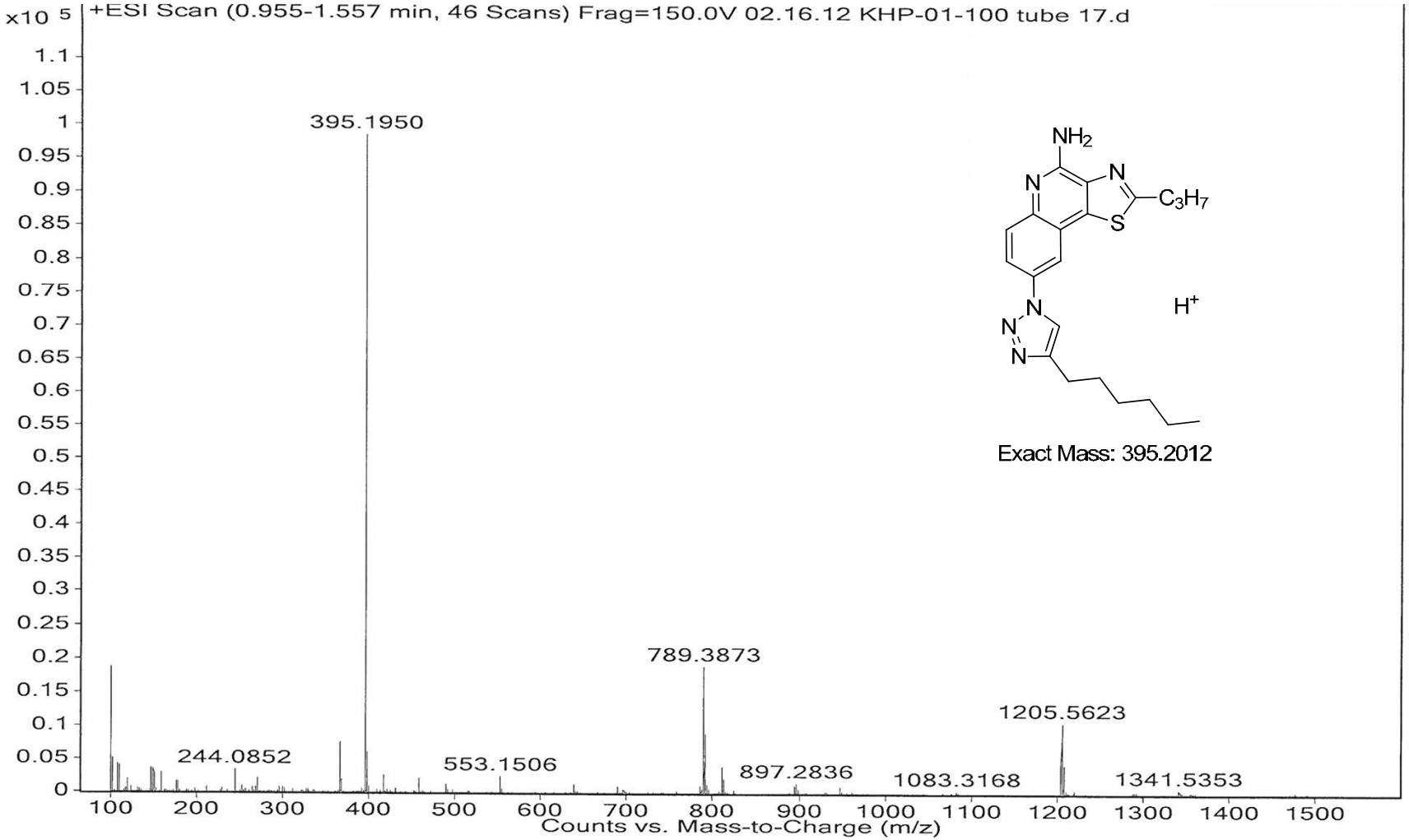
12e ^{1}H NMR


8.71
8.27
8.27
8.05
8.05
8.04
8.03
7.76
7.74
7.12
3.34
3.21
3.19
3.18
2.51
2.50
2.50
2.50 Dimethyl Sulfoxide-d6
2.50
1.91
1.90
1.88
1.87
1.69
1.33
1.32
1.31
1.30
1.30
1.05
1.04
1.02
0.89
0.88
0.86
B (dd) 8.04
D (s) 8.71
A (d) 8.27
C (d) 7.75
E (s) 7.12
F (t) 3.19
G (t) 2.72
I (dt) 1.69
K (t) 1.04
H (dd) 1.89
J (m) 1.34
L (dd) 0.87
1.04
1.00
1.07
1.07
2.01
2.12
2.08
2.22
2.15
6.28
3.13
3.18
f1 (ppm)

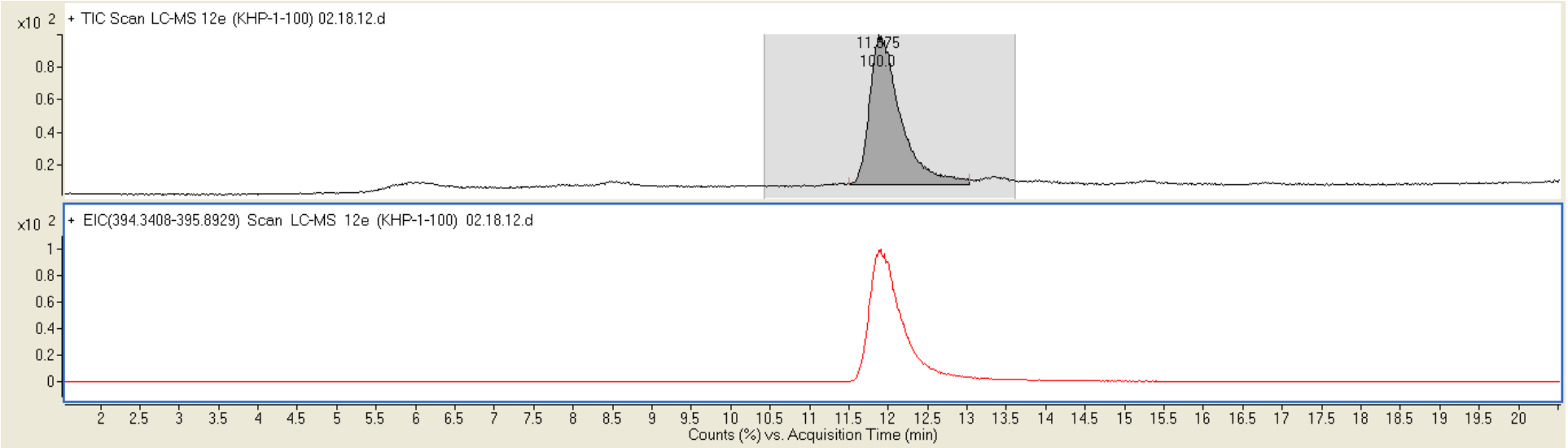
12e ^{13}C NMR

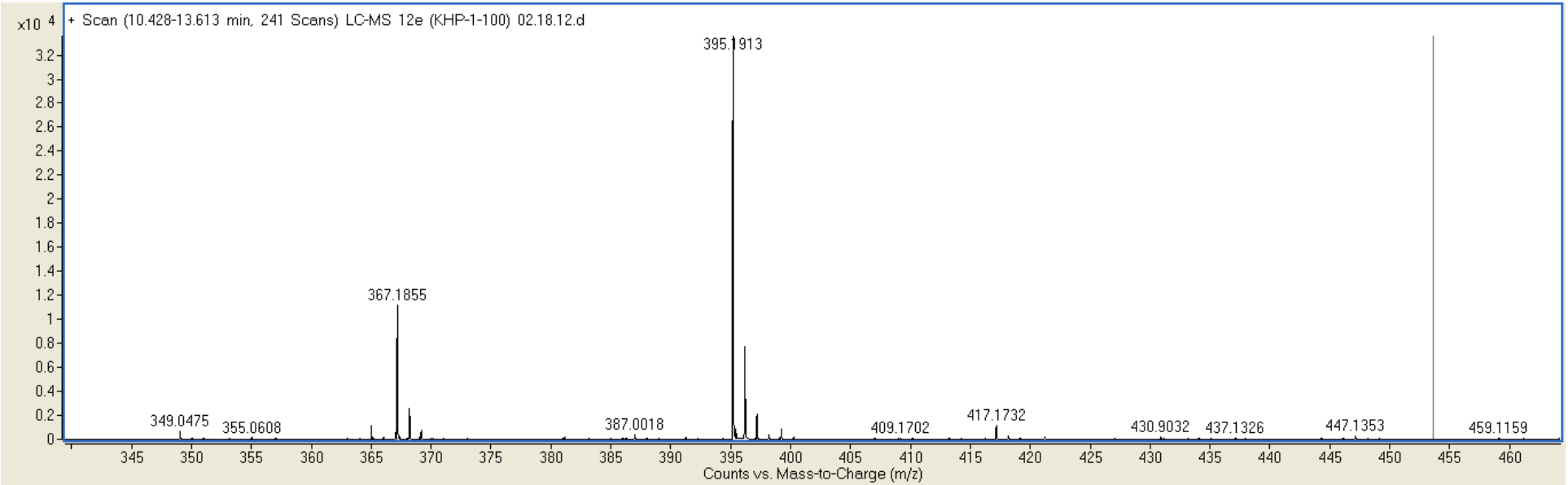


12e MS

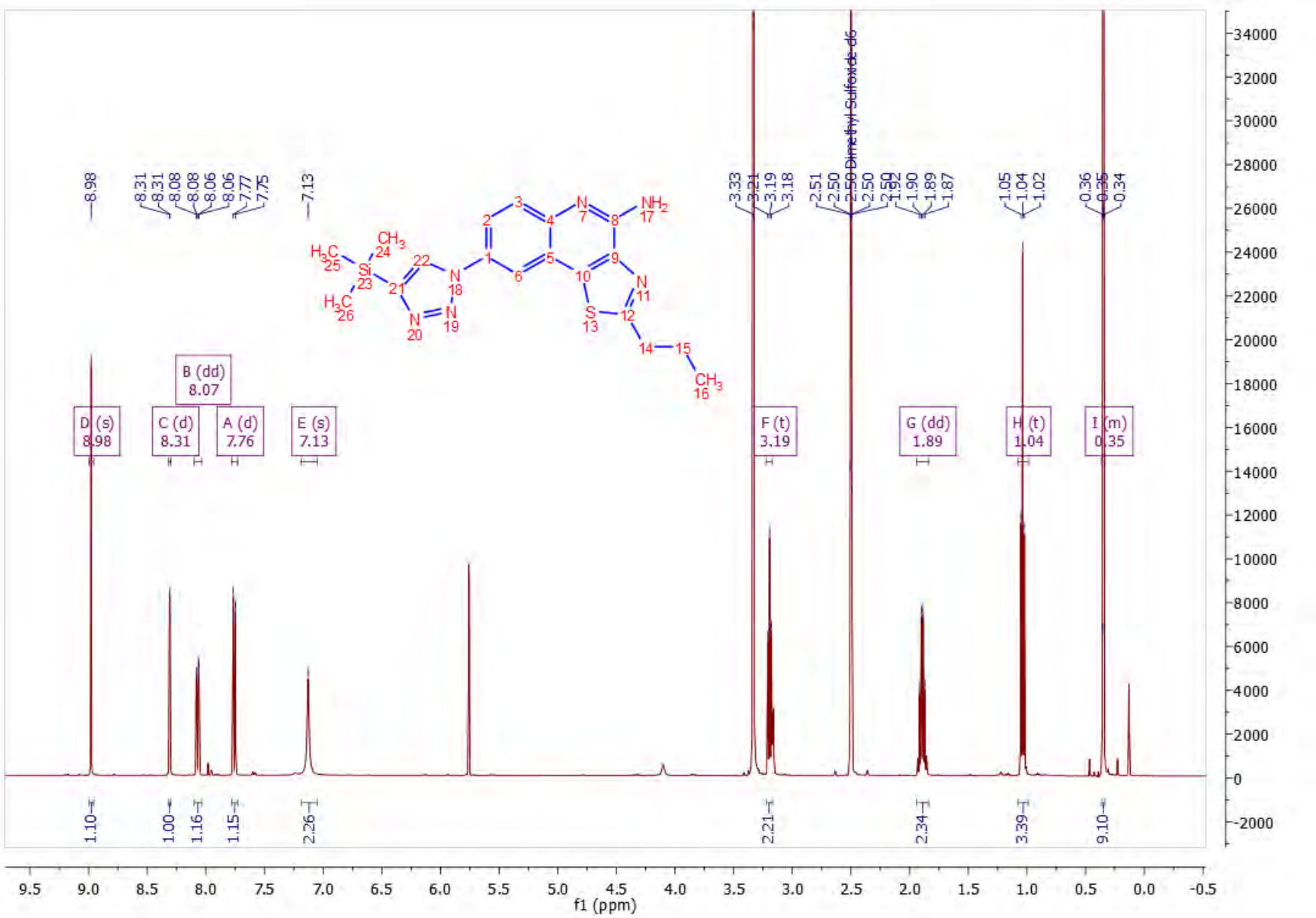


12e LC-MS

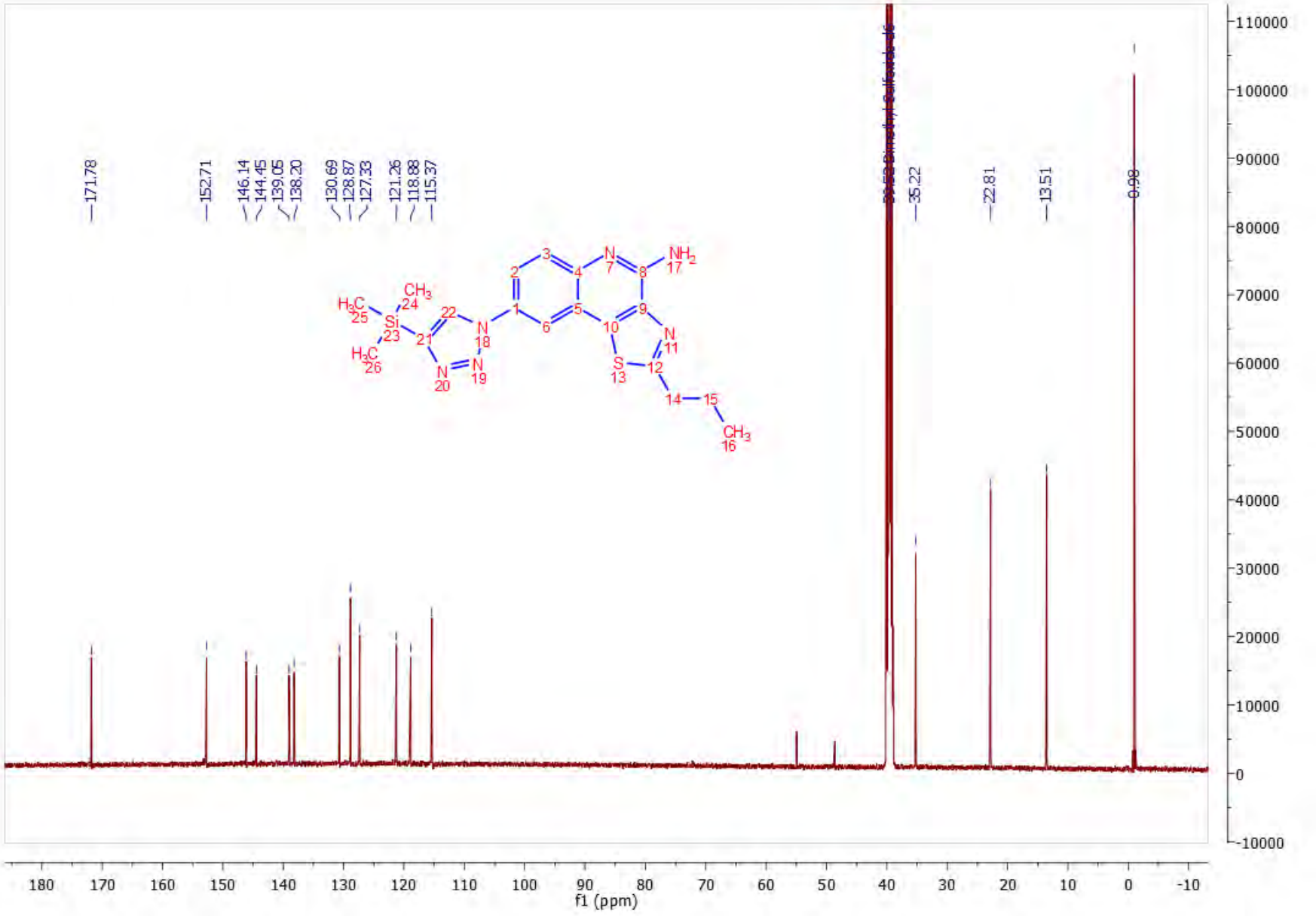




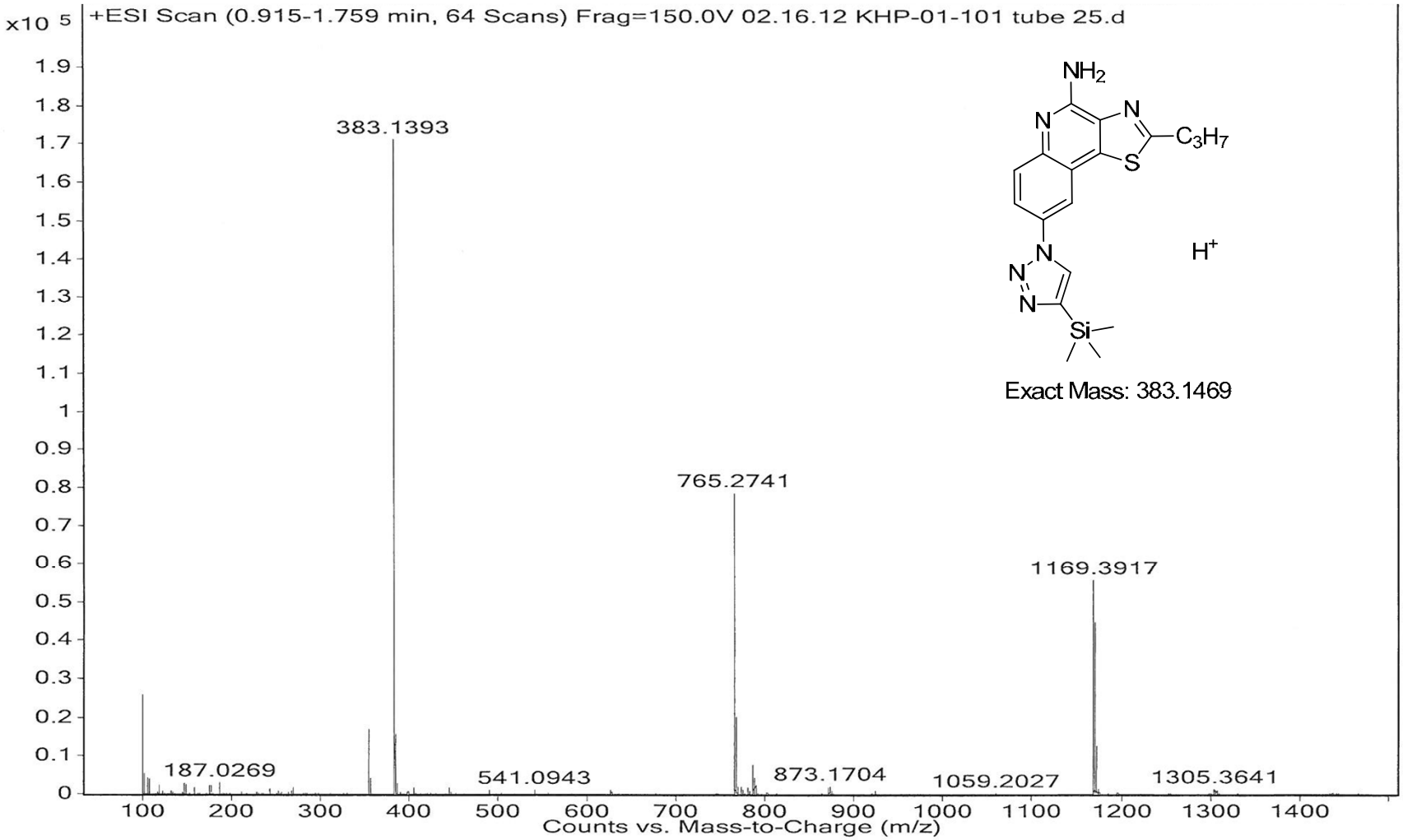
12f ^{1}H NMR



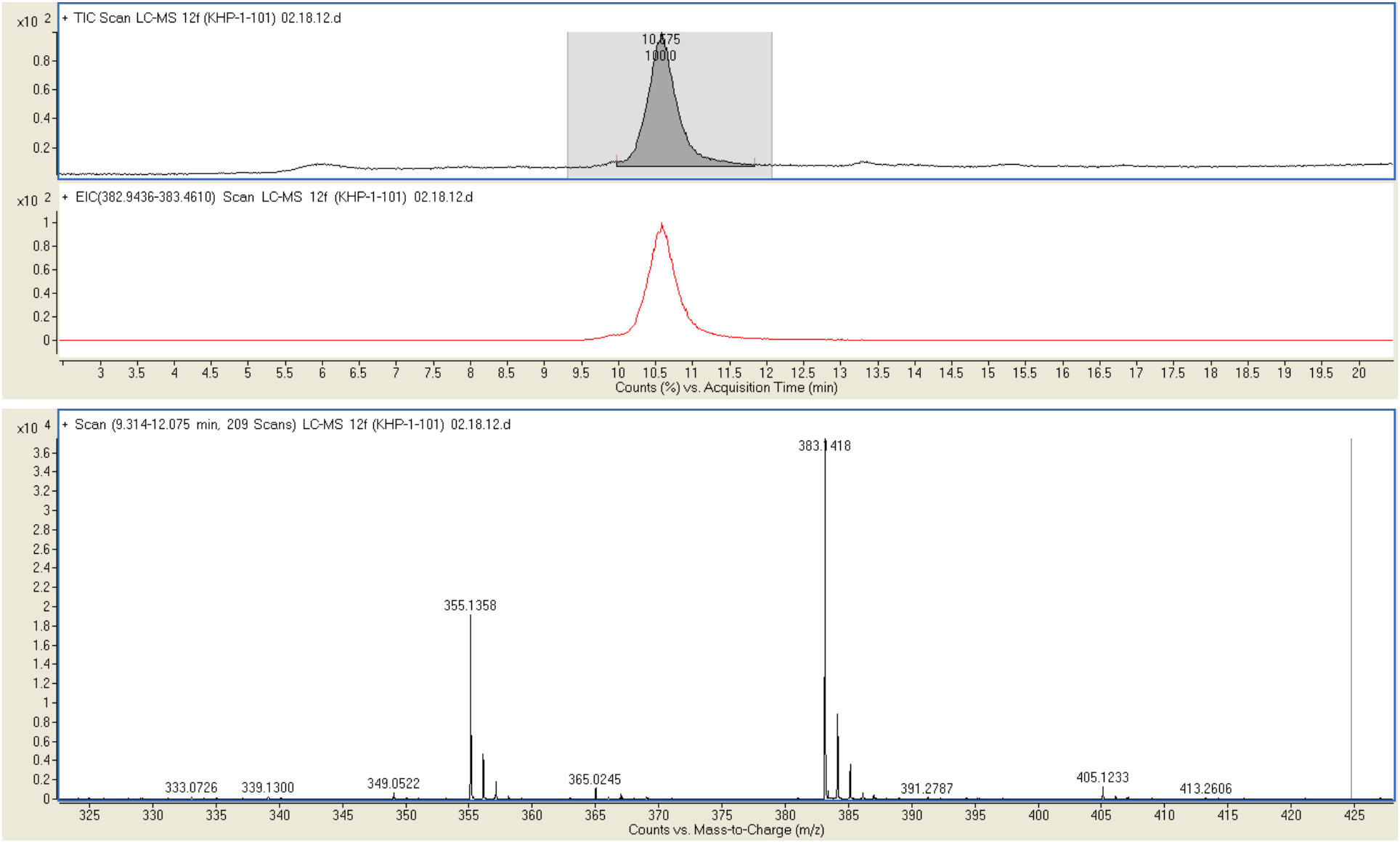
12f ^{13}C NMR



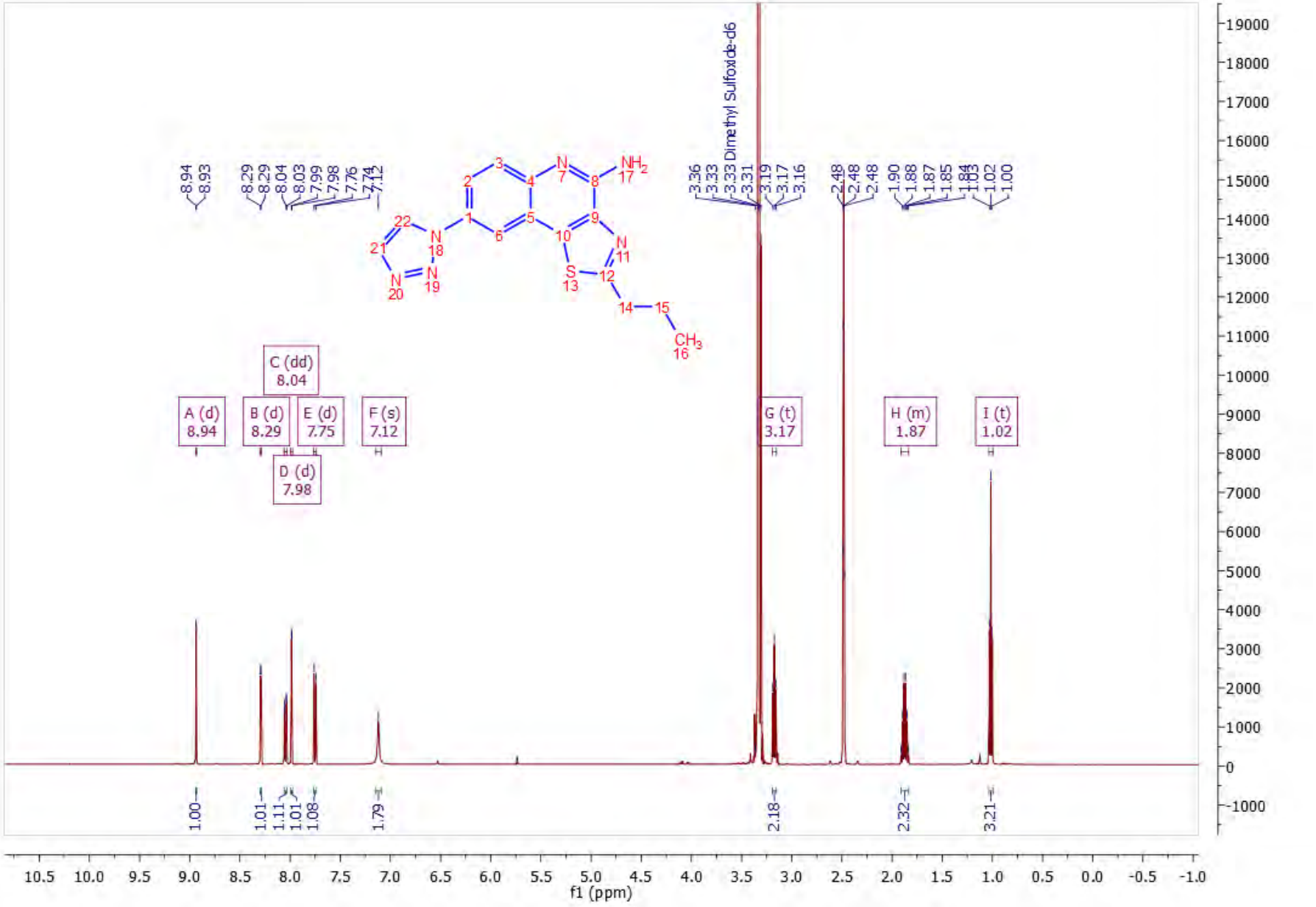
12f MS



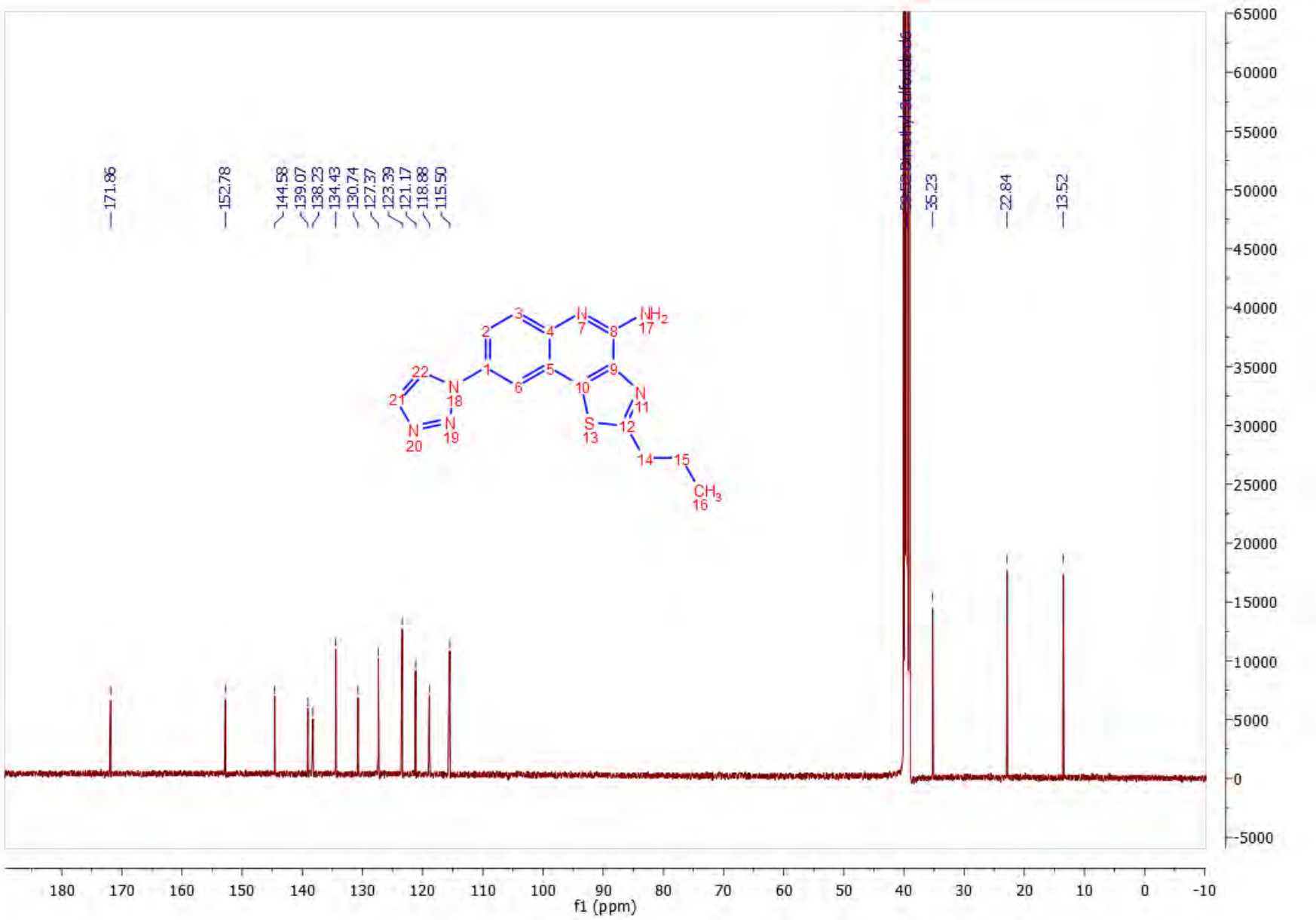
12f LC-MS



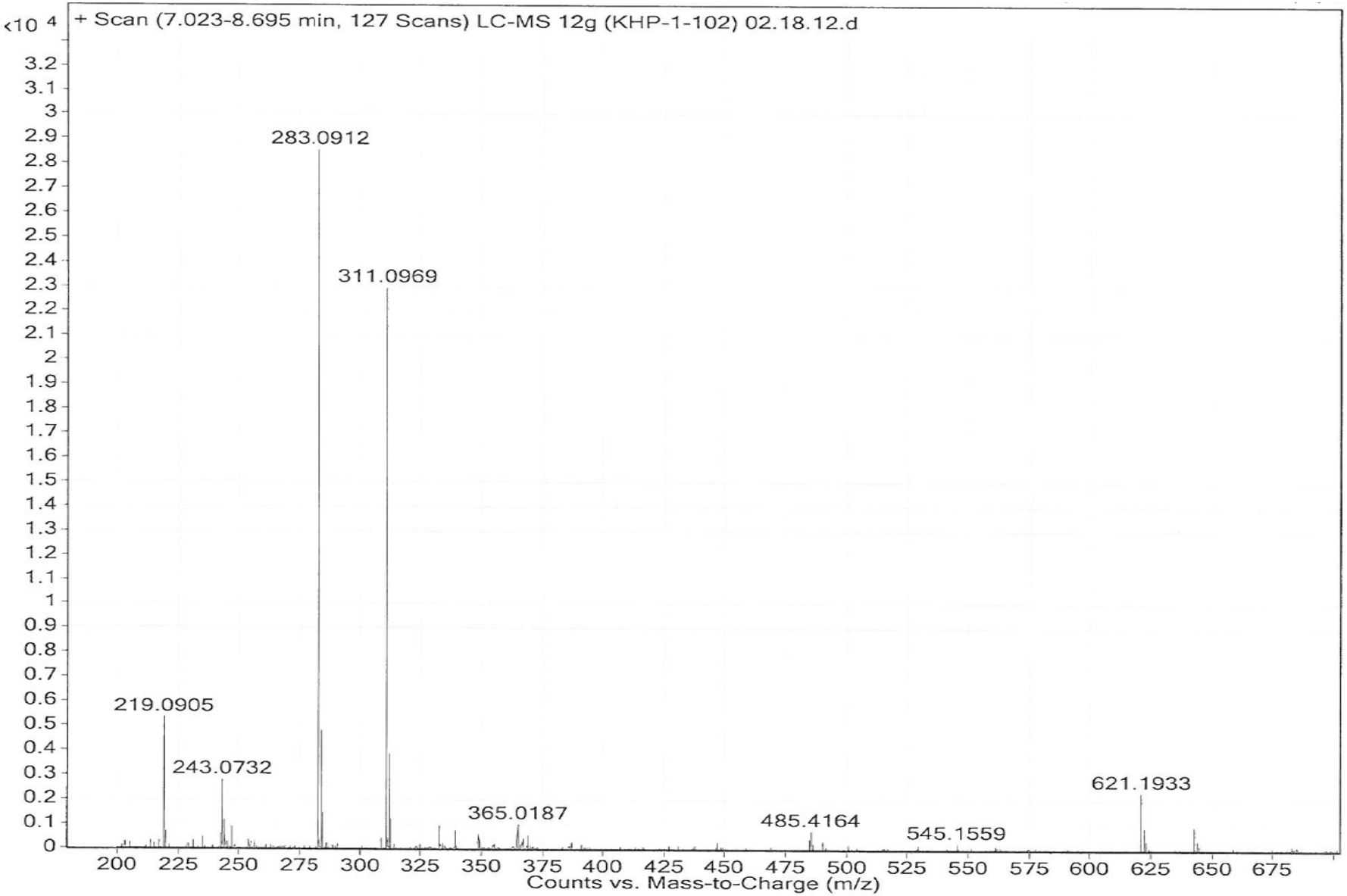
12g ^{1}H NMR


Dimethyl Sulfoxide-d6
A (d) 8.94
B (d) 8.29
C (dd) 8.04
D (d) 7.98
E (d) 7.75
F (s) 7.12
G (t) 3.17
H (m) 1.87
I (t) 1.02
f1 (ppm)

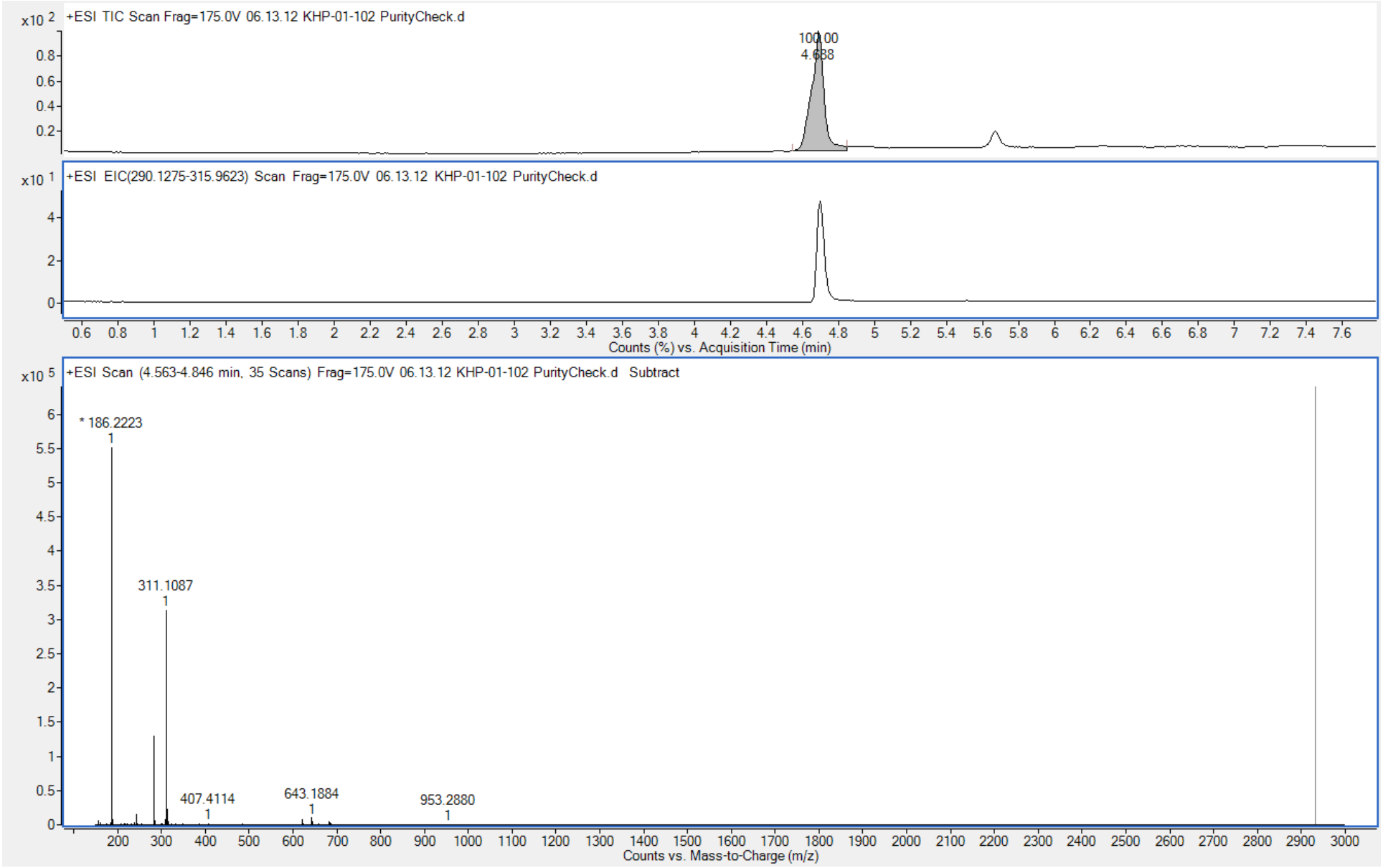
12g ^{13}C NMR



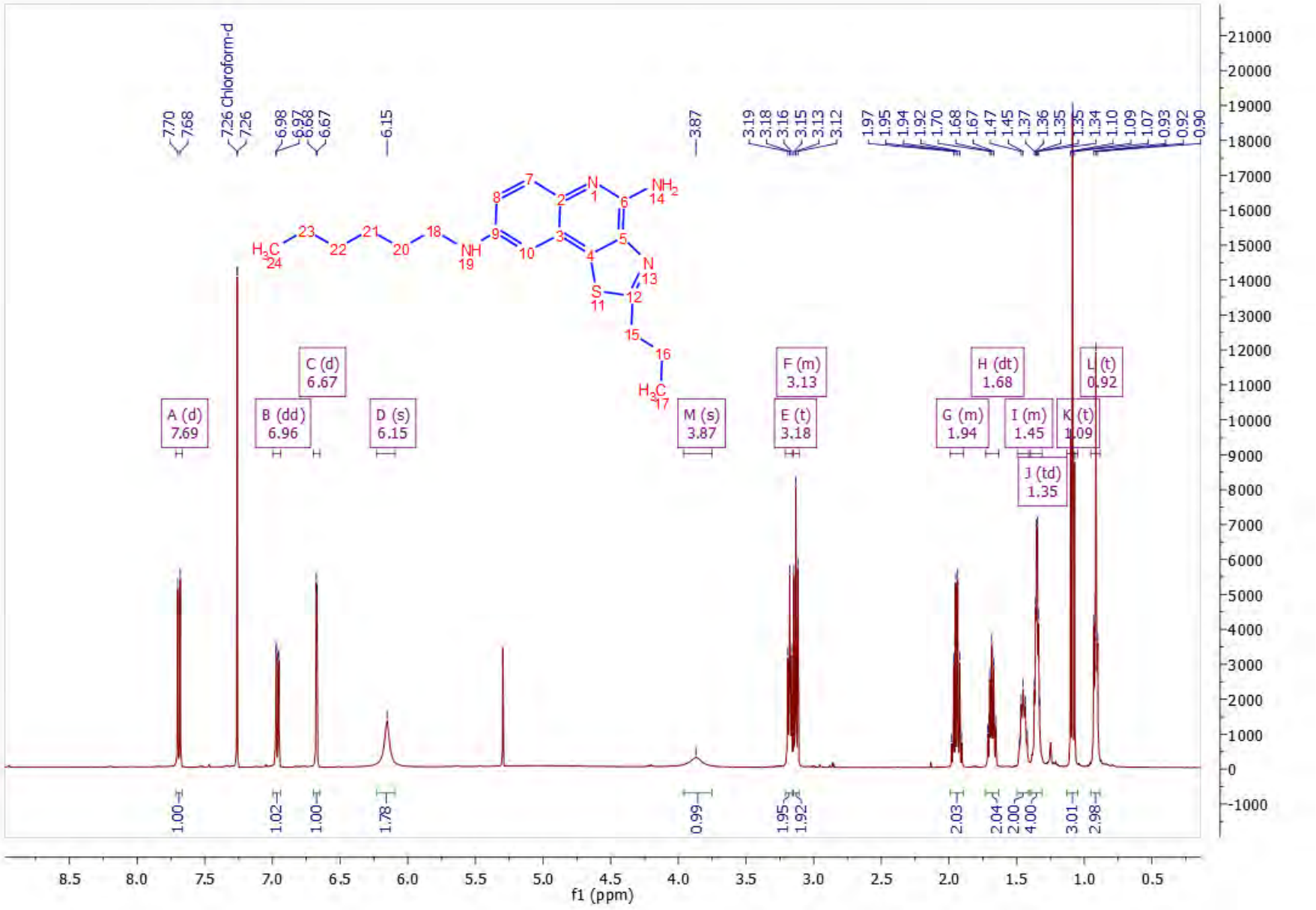
12g MS



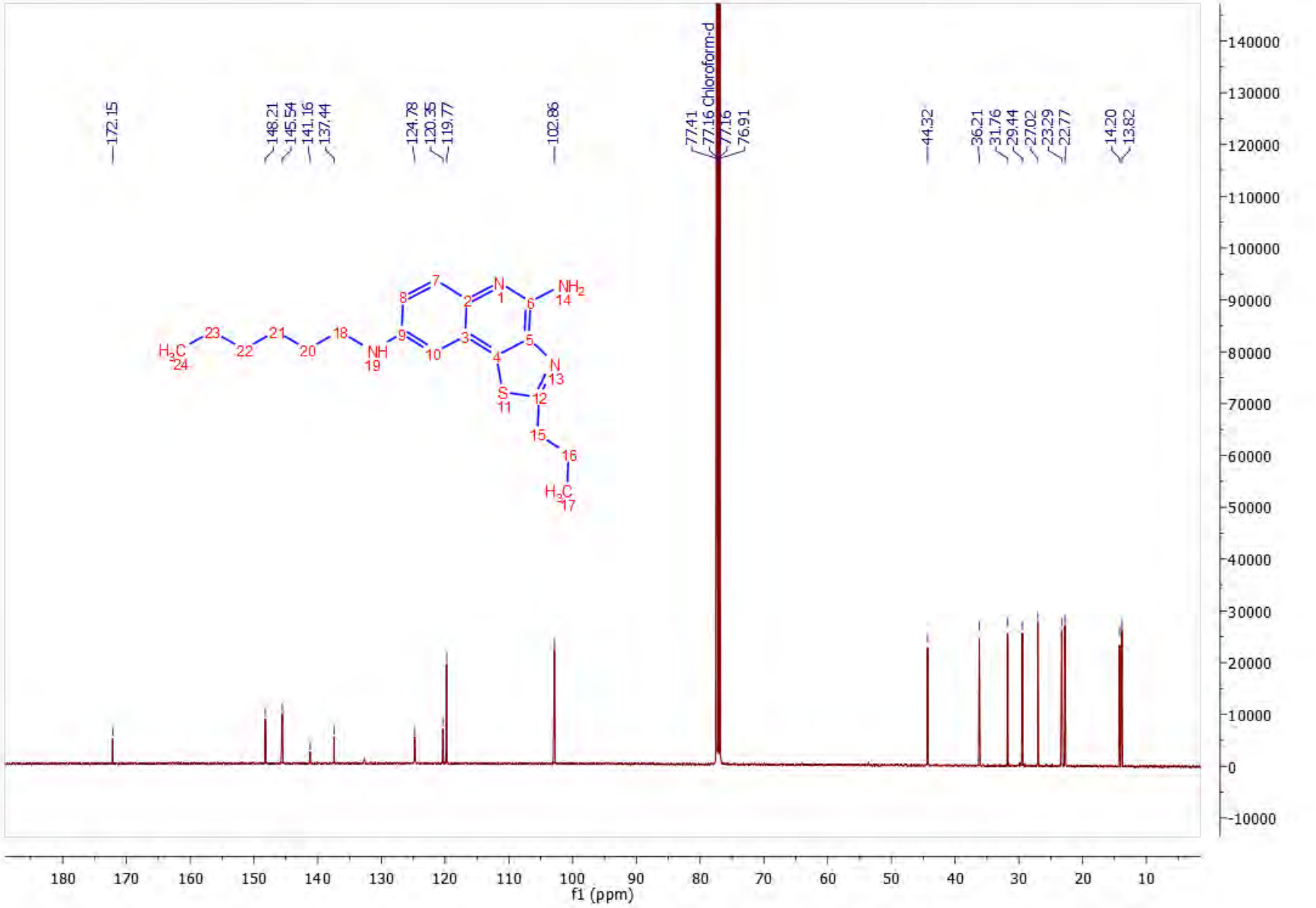
12g LC-MS



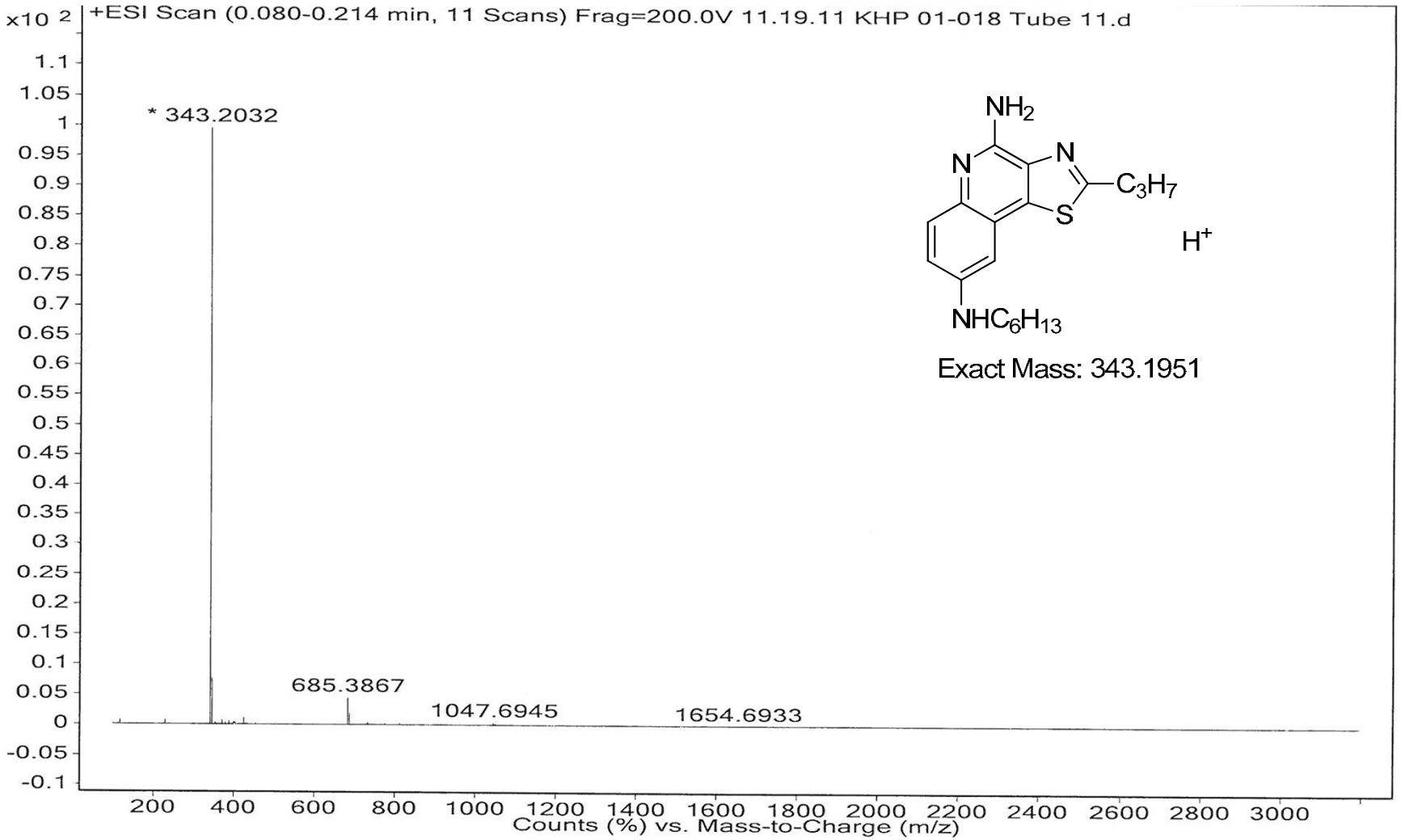
13a ^{1}H NMR



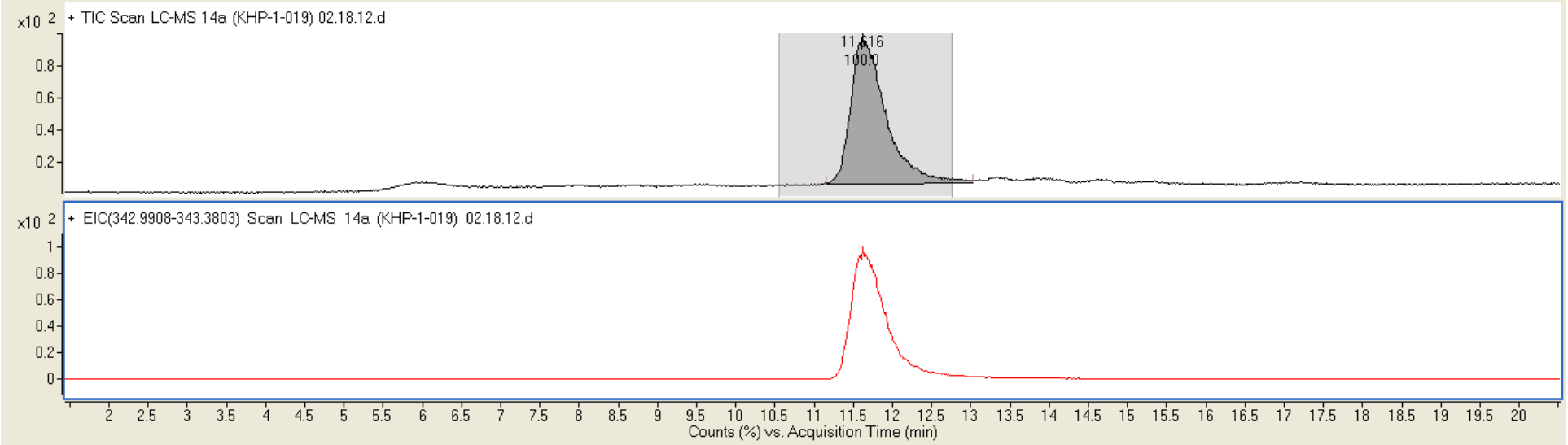
13a ^{13}C NMR

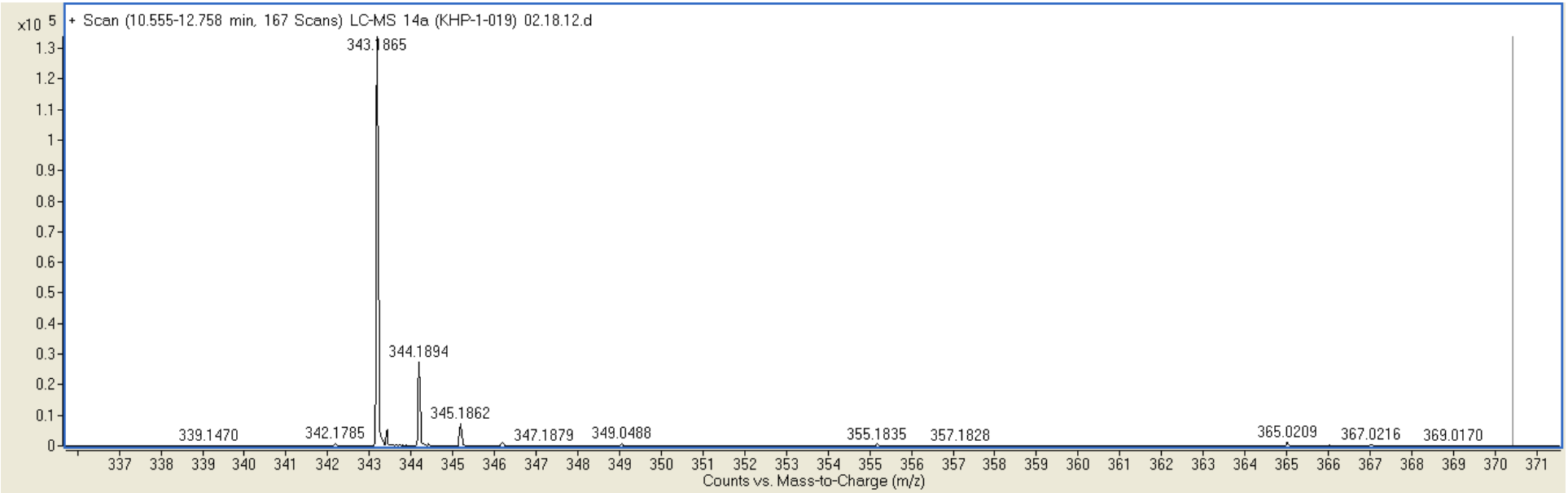


13a MS

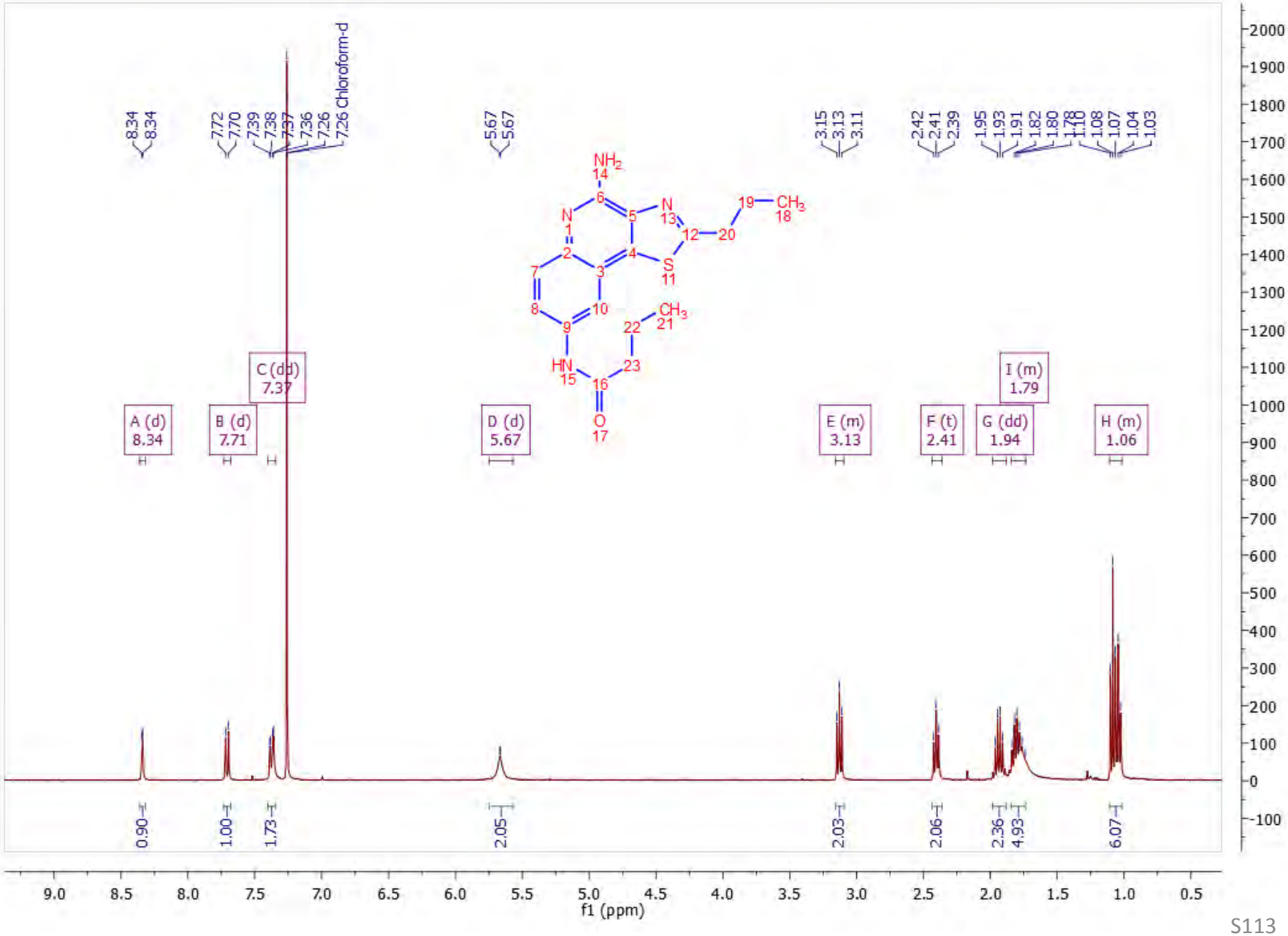


13a LC-MS

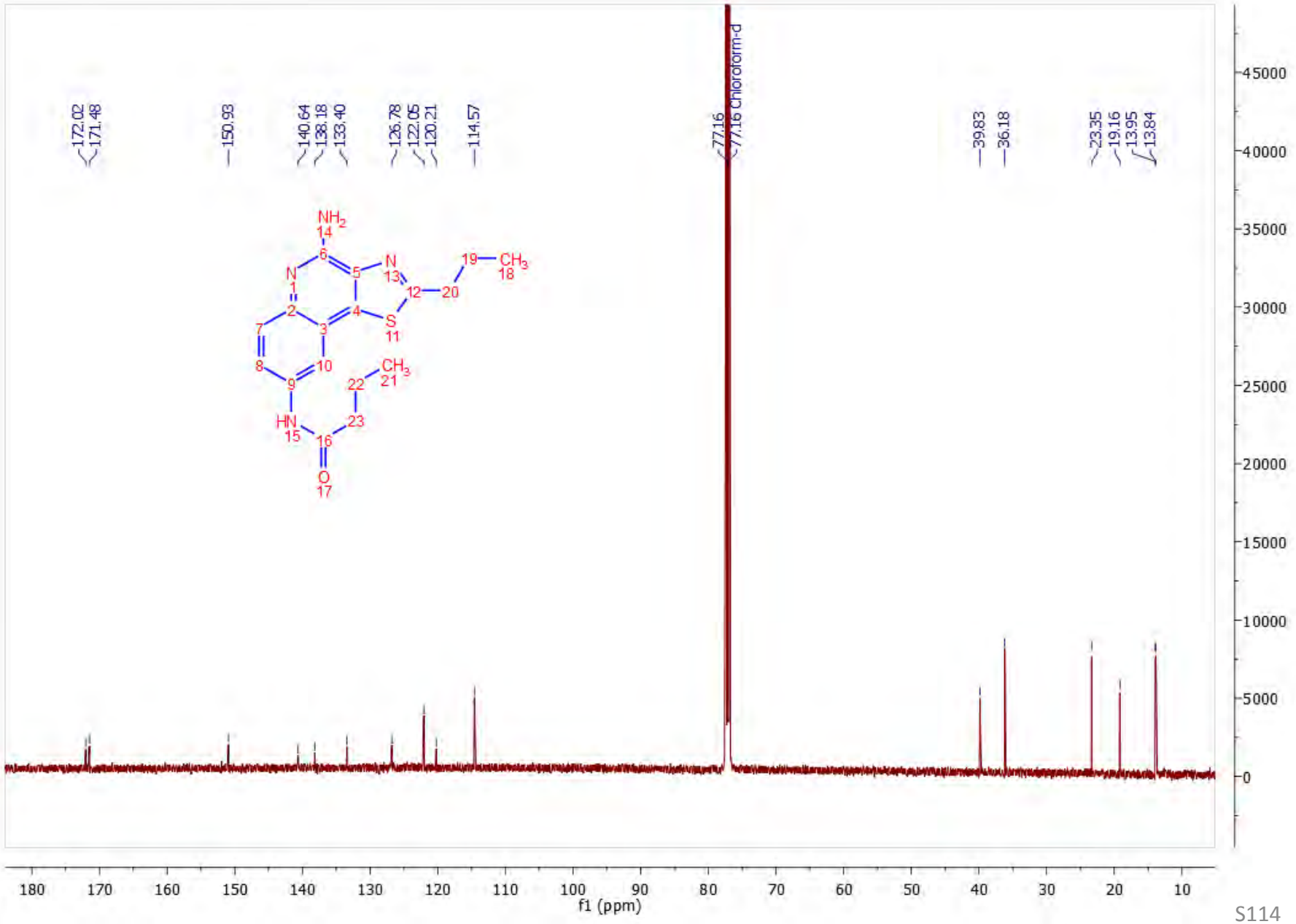




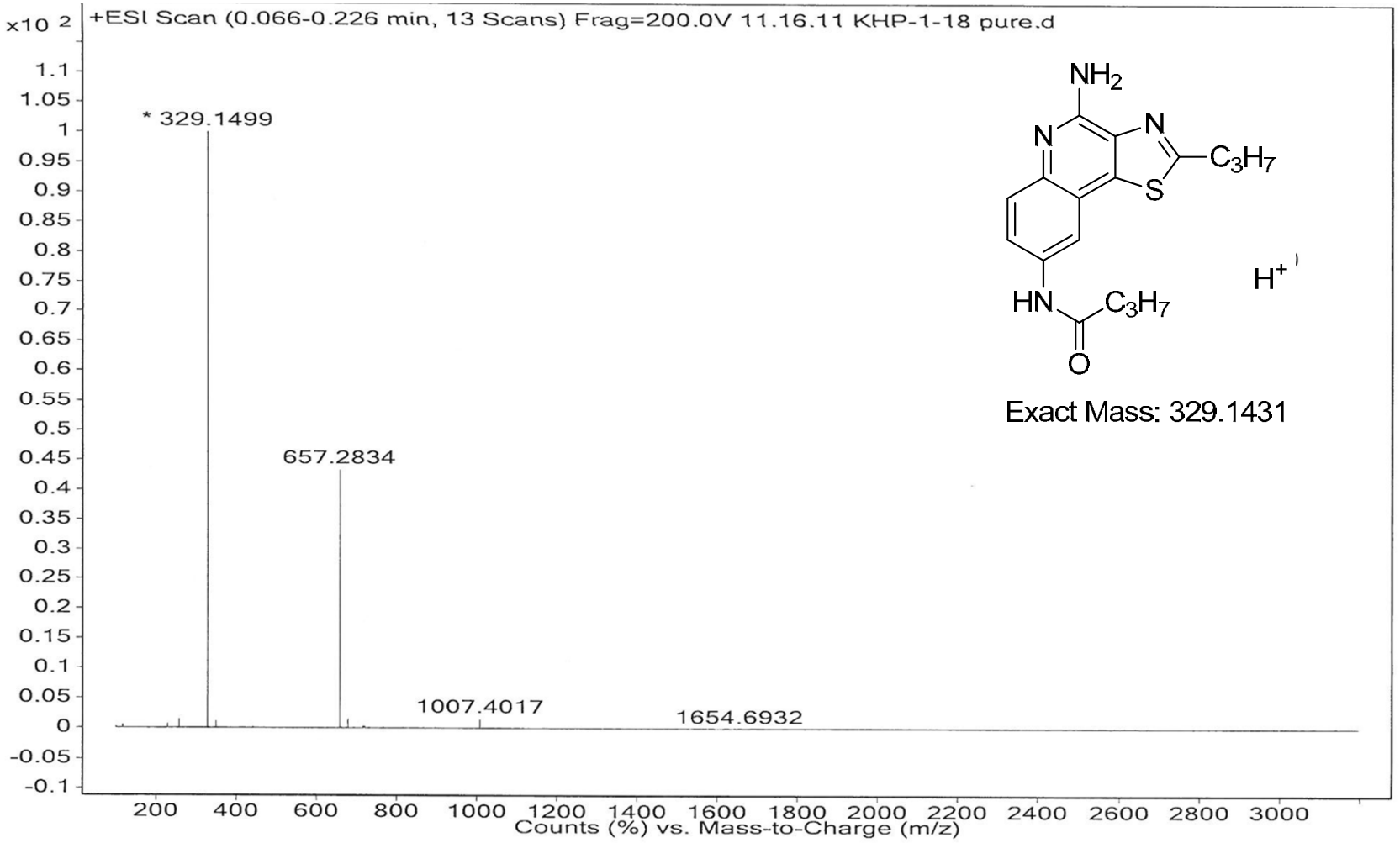
13b ^{1}H NMR



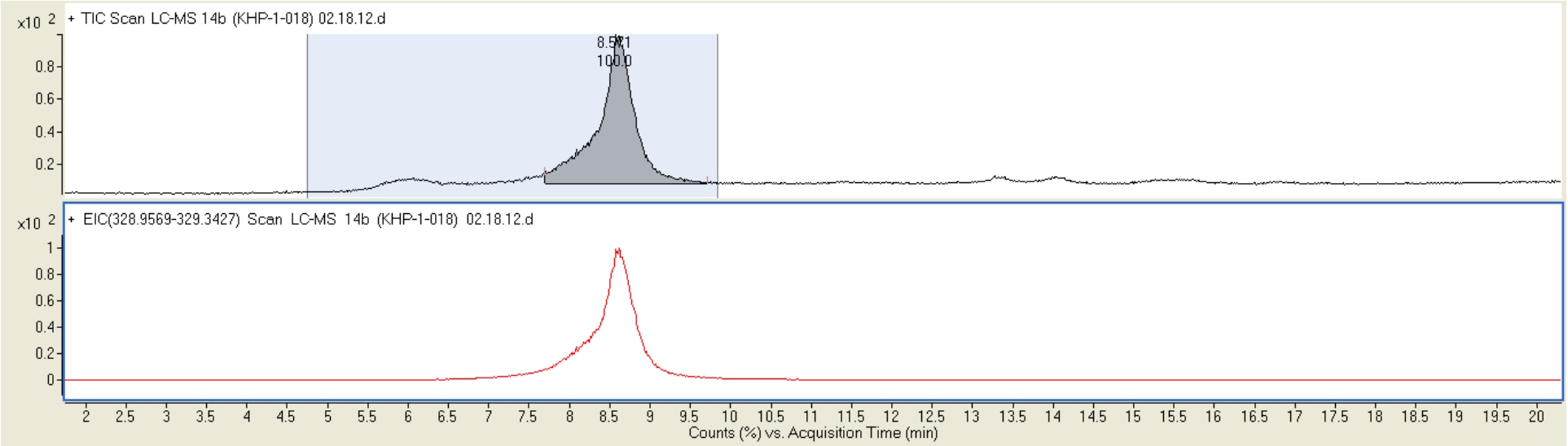
13b ^{13}C NMR

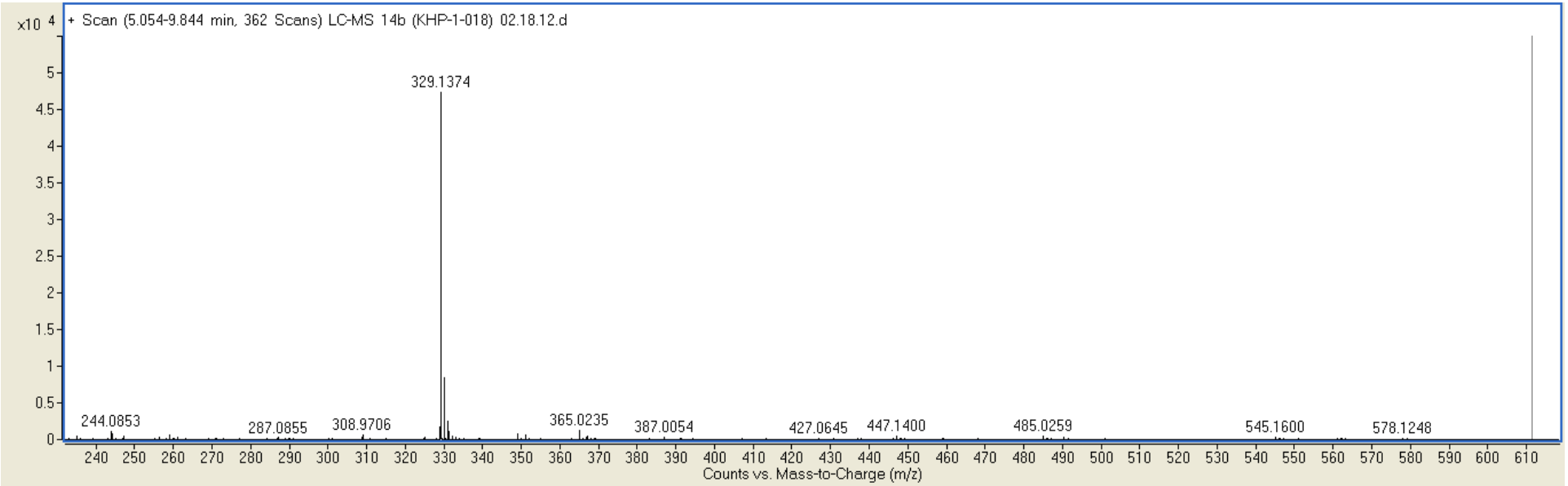


13b MS

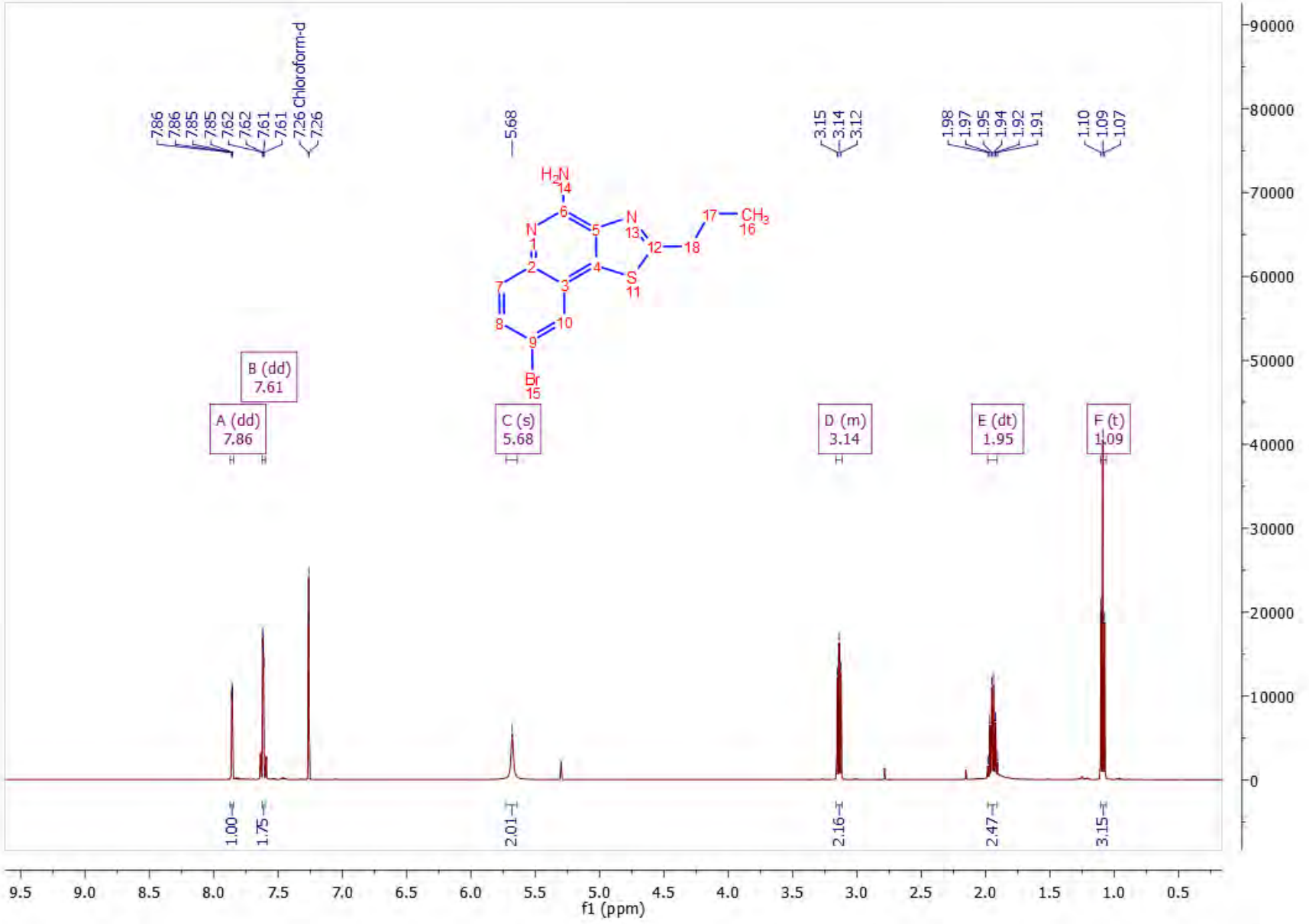


13b LC-MS

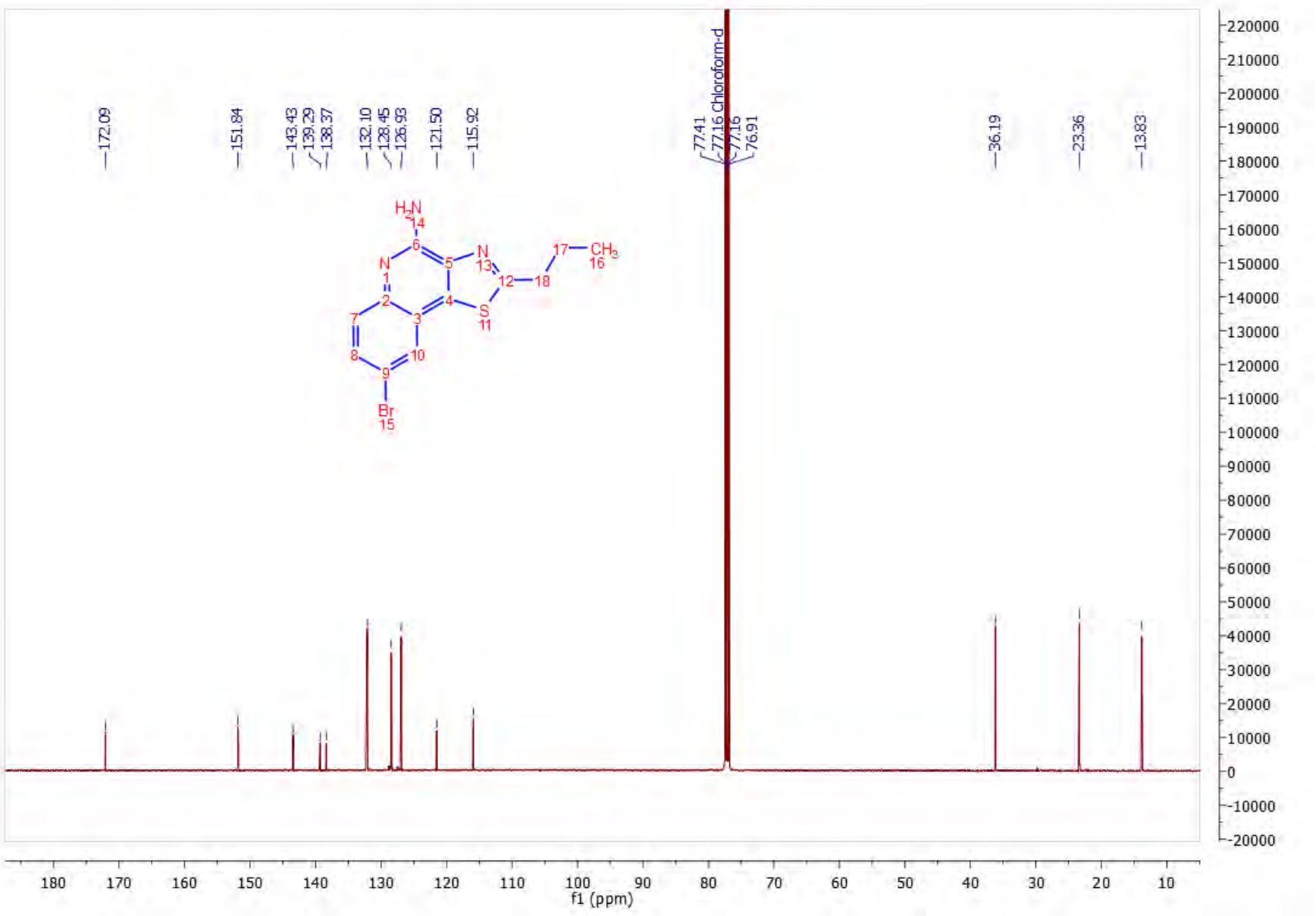




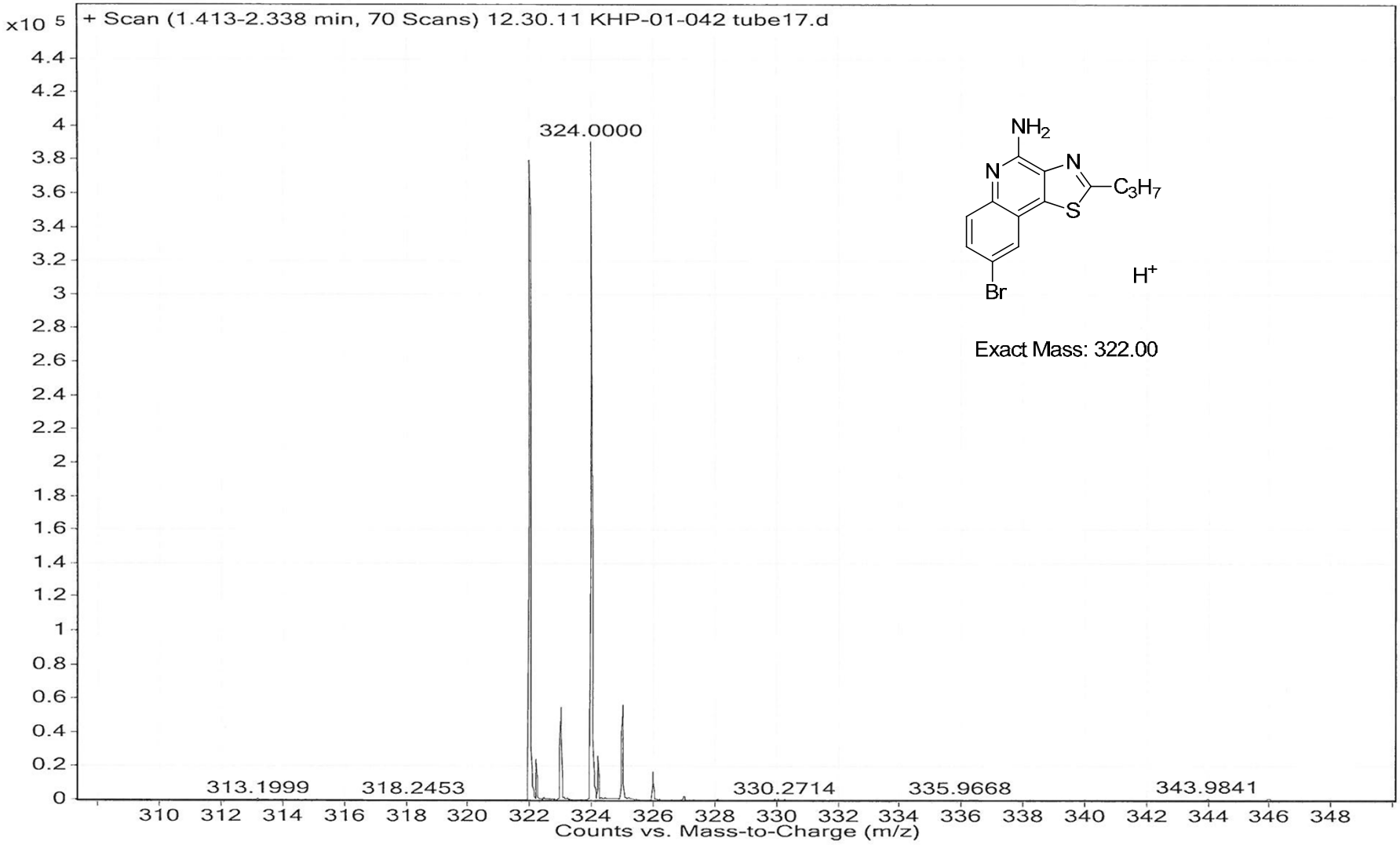
14 ^{1}H NMR



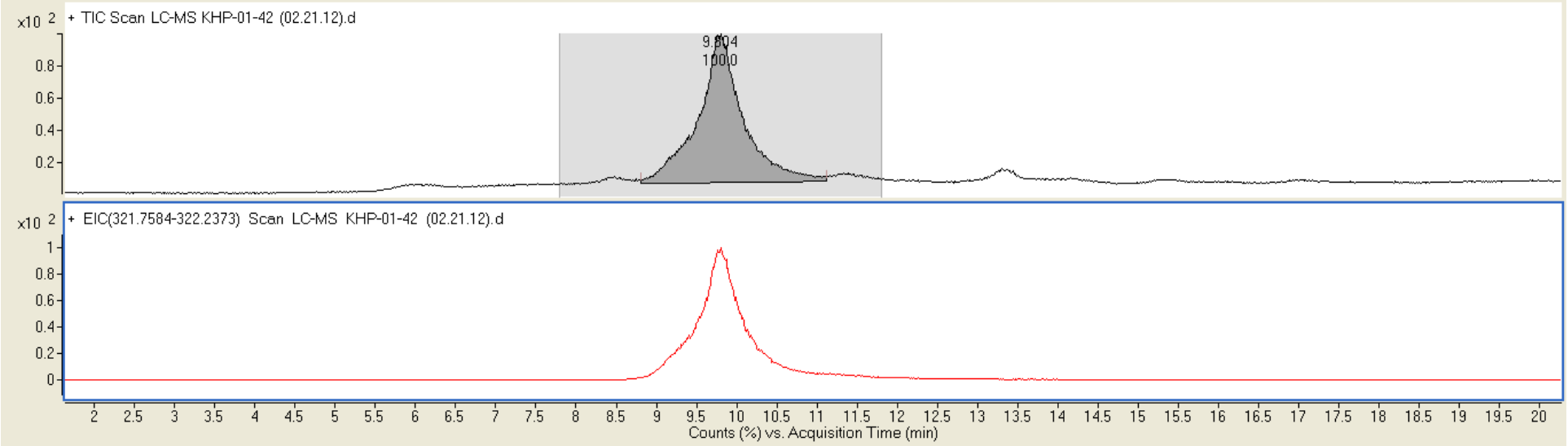
14 ^{13}C NMR

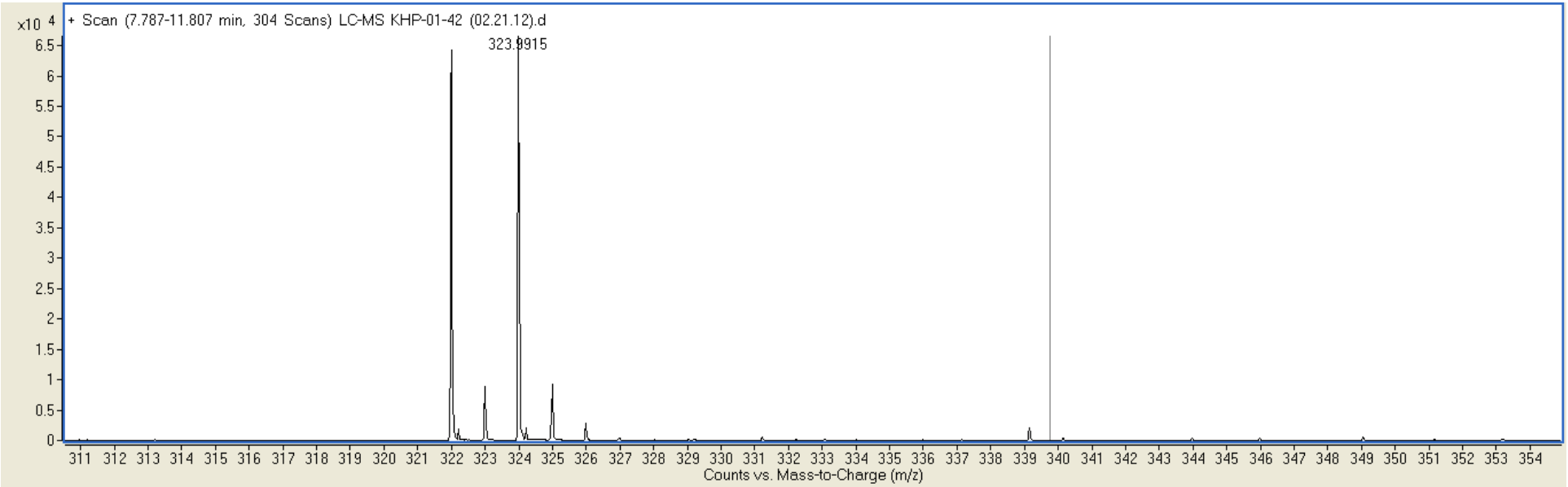


14 MS

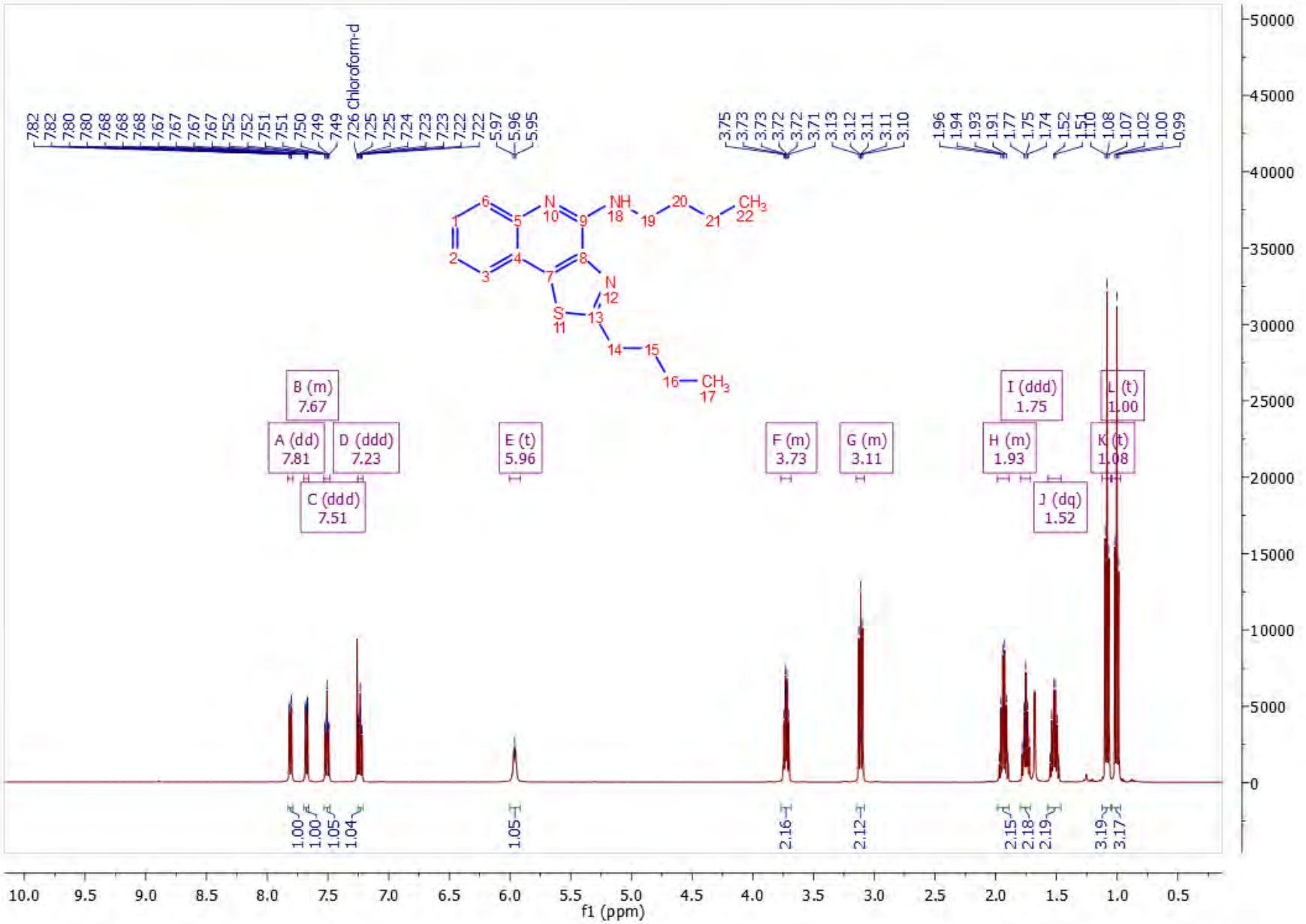


14 LC-MS

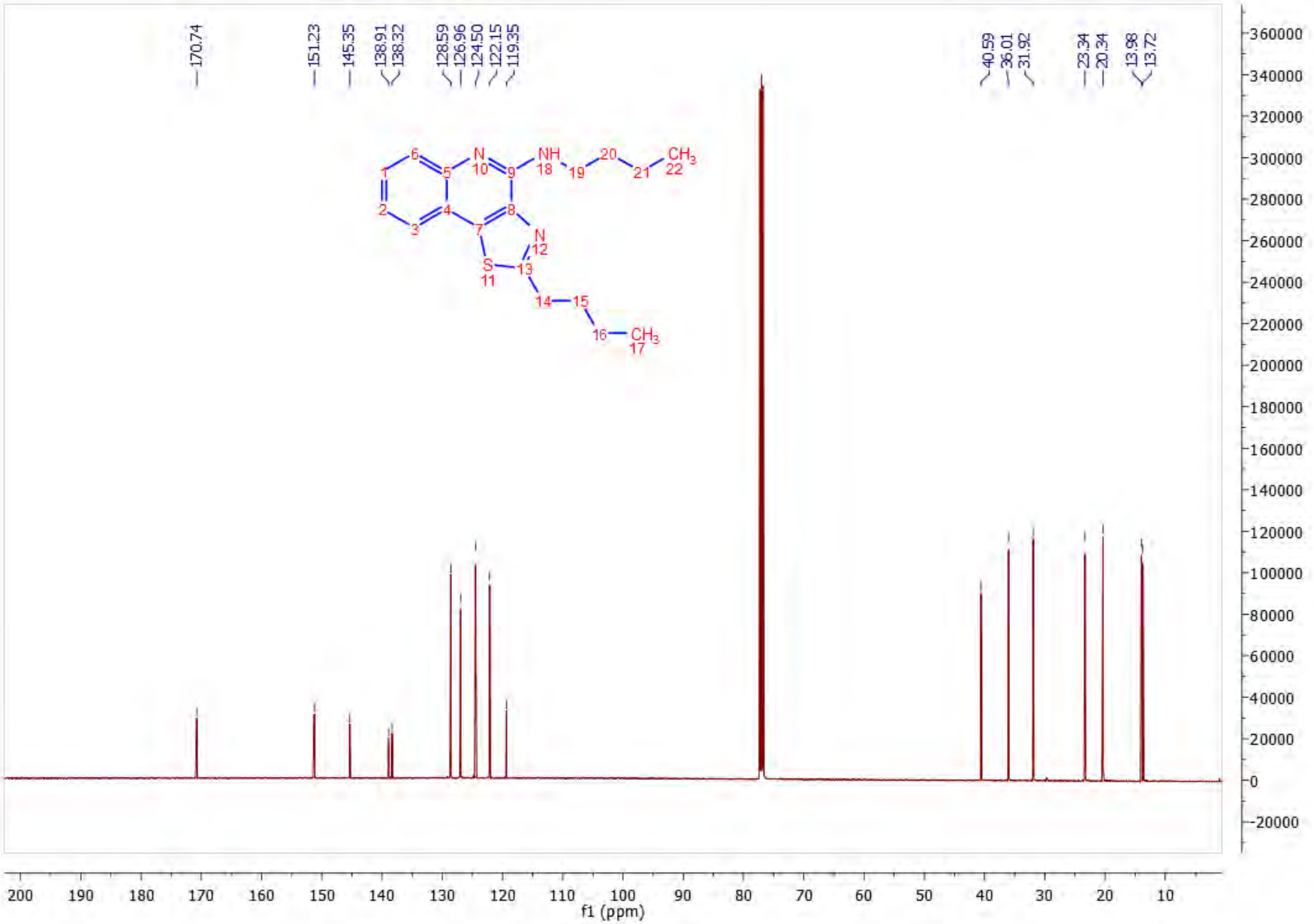




15a ^{1}H NMR

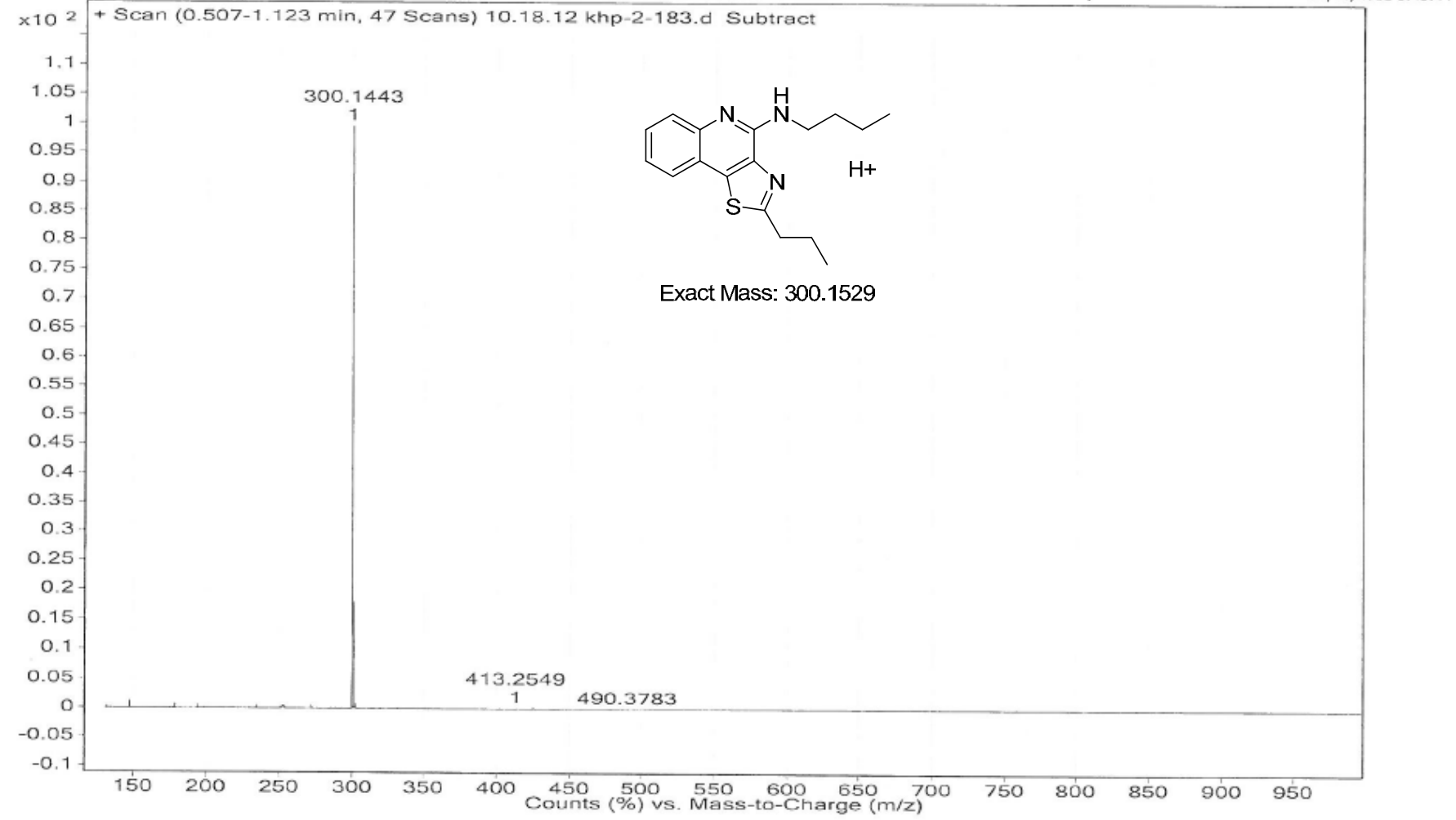


15a ^{13}C NMR



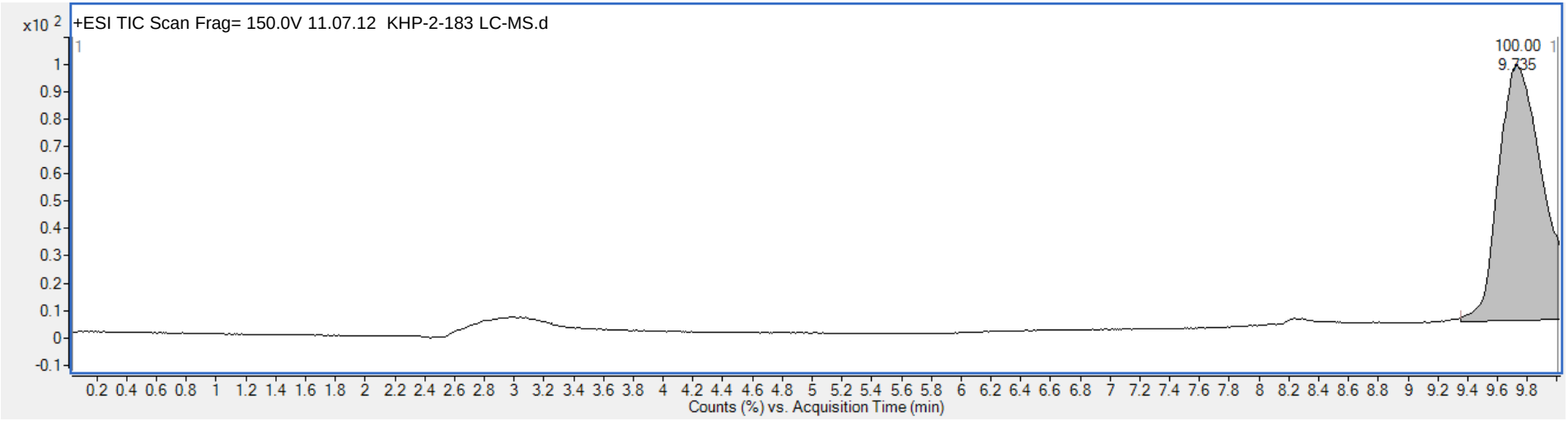
15a MS

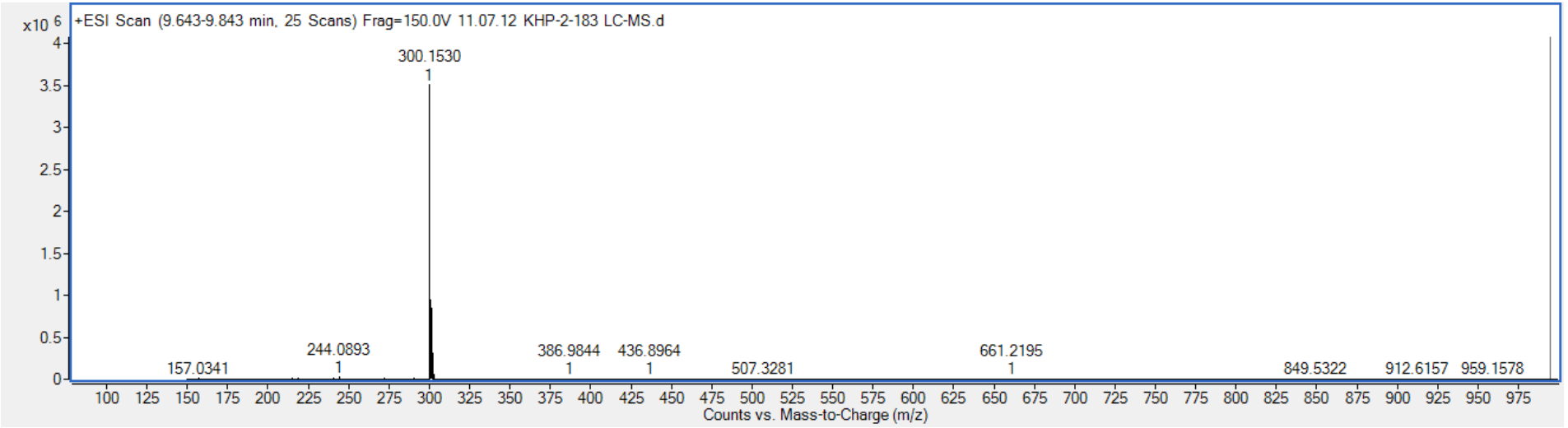
Sample Name	10.18.12 khp-2-183	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	10.18.12 khp-2-183.d	ACQ Method	Water-ACN Infusion M	Comment		Acquired Time	10/18/2012 1:41:44



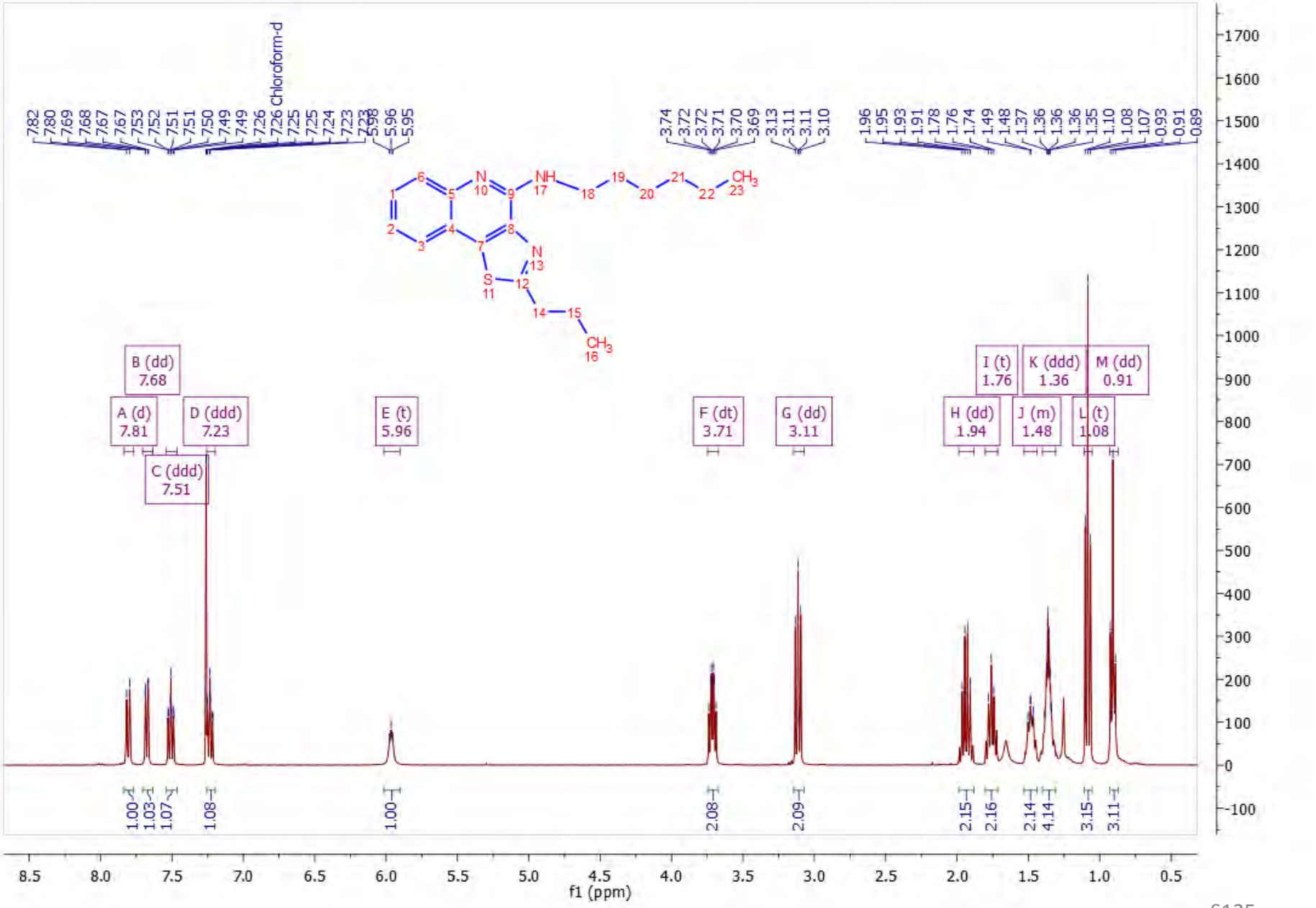
Exact Mass: 300.1529

15a LC-MS

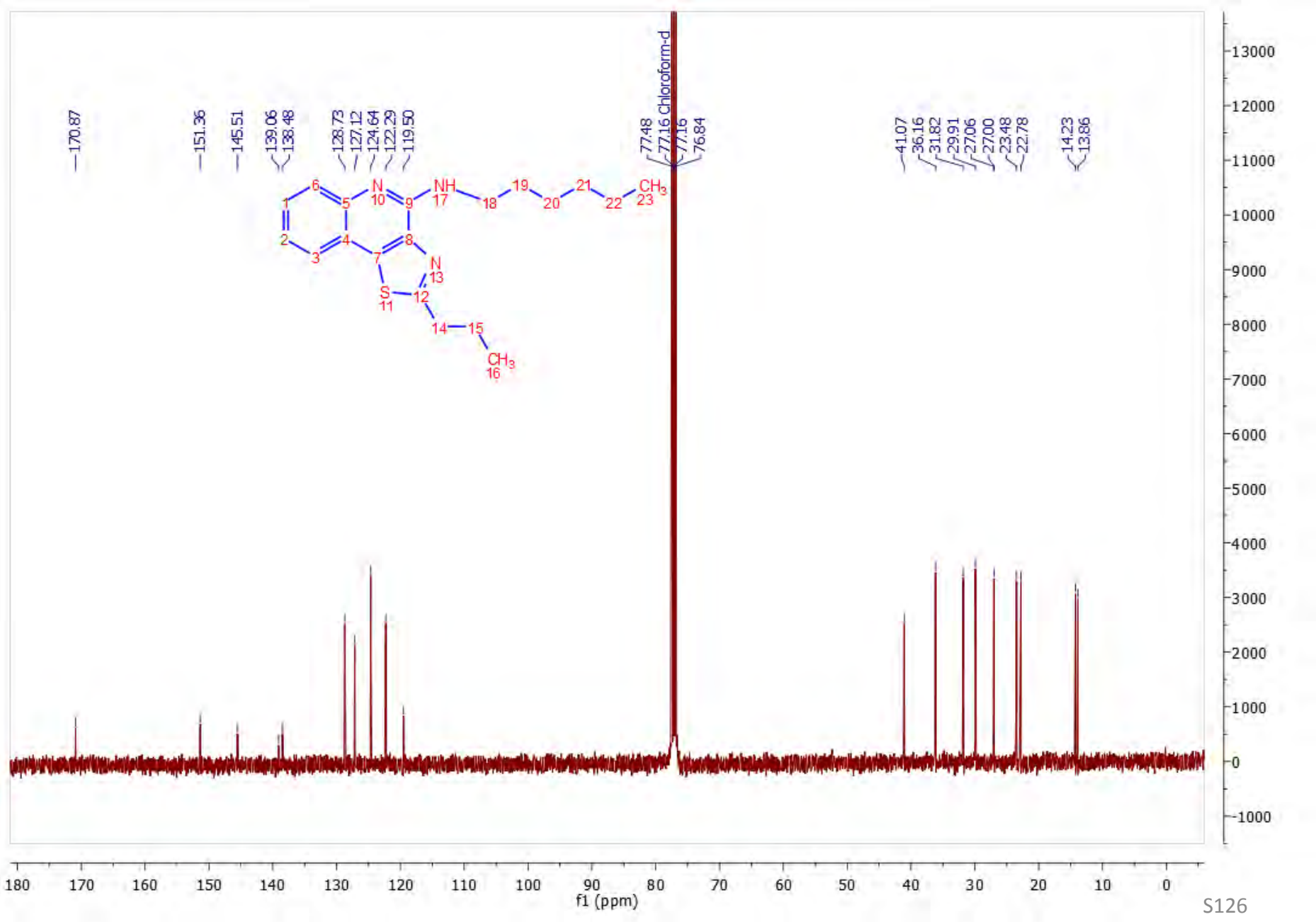




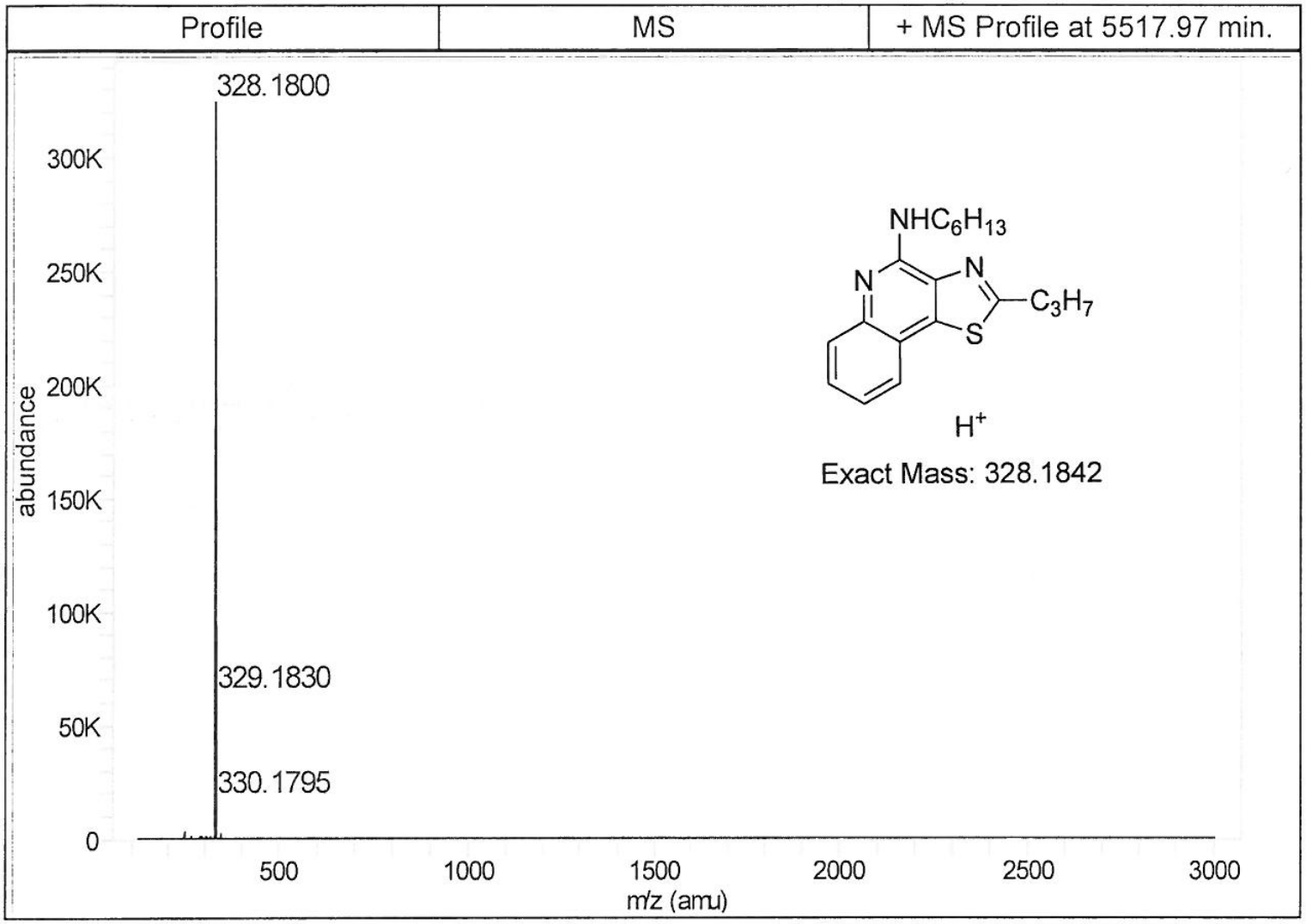
15b ^{1}H NMR



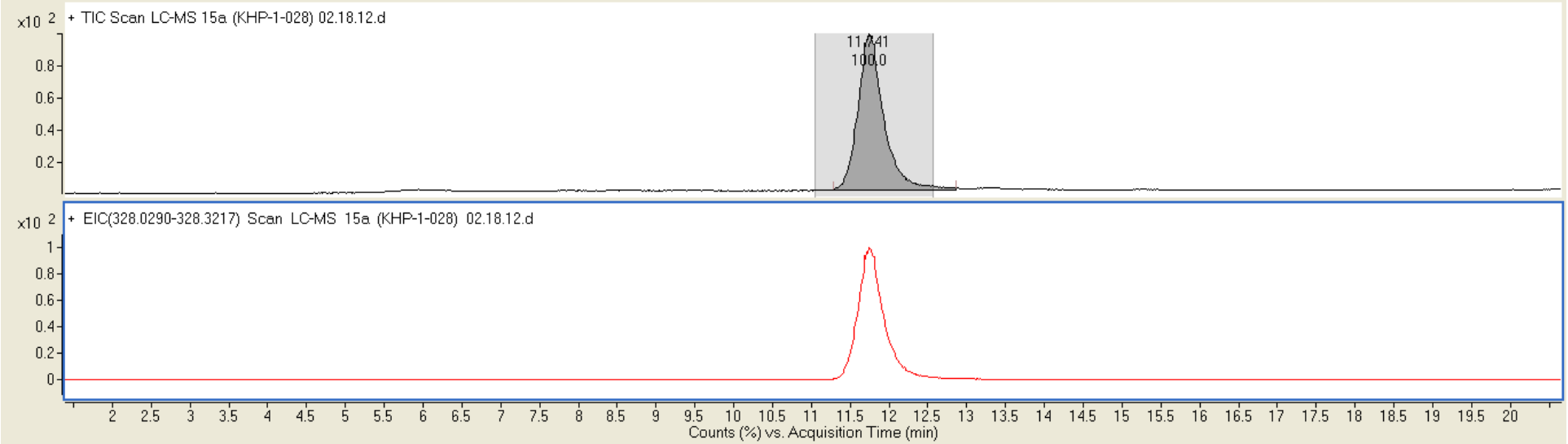
15b ^{13}C NMR

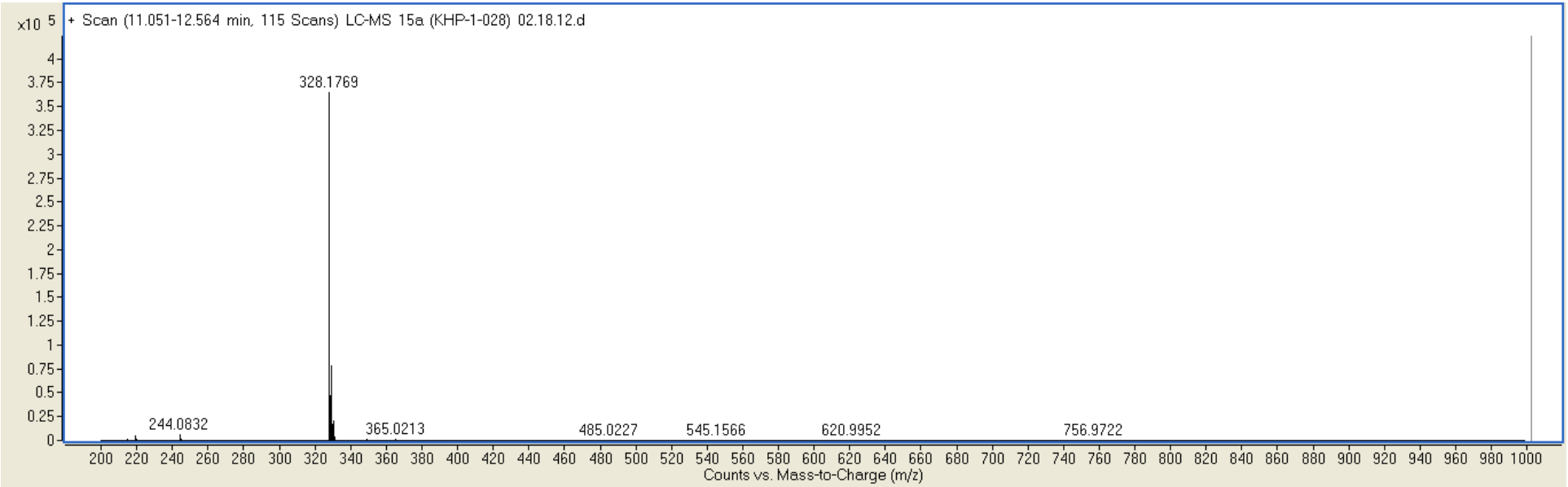


15b MS

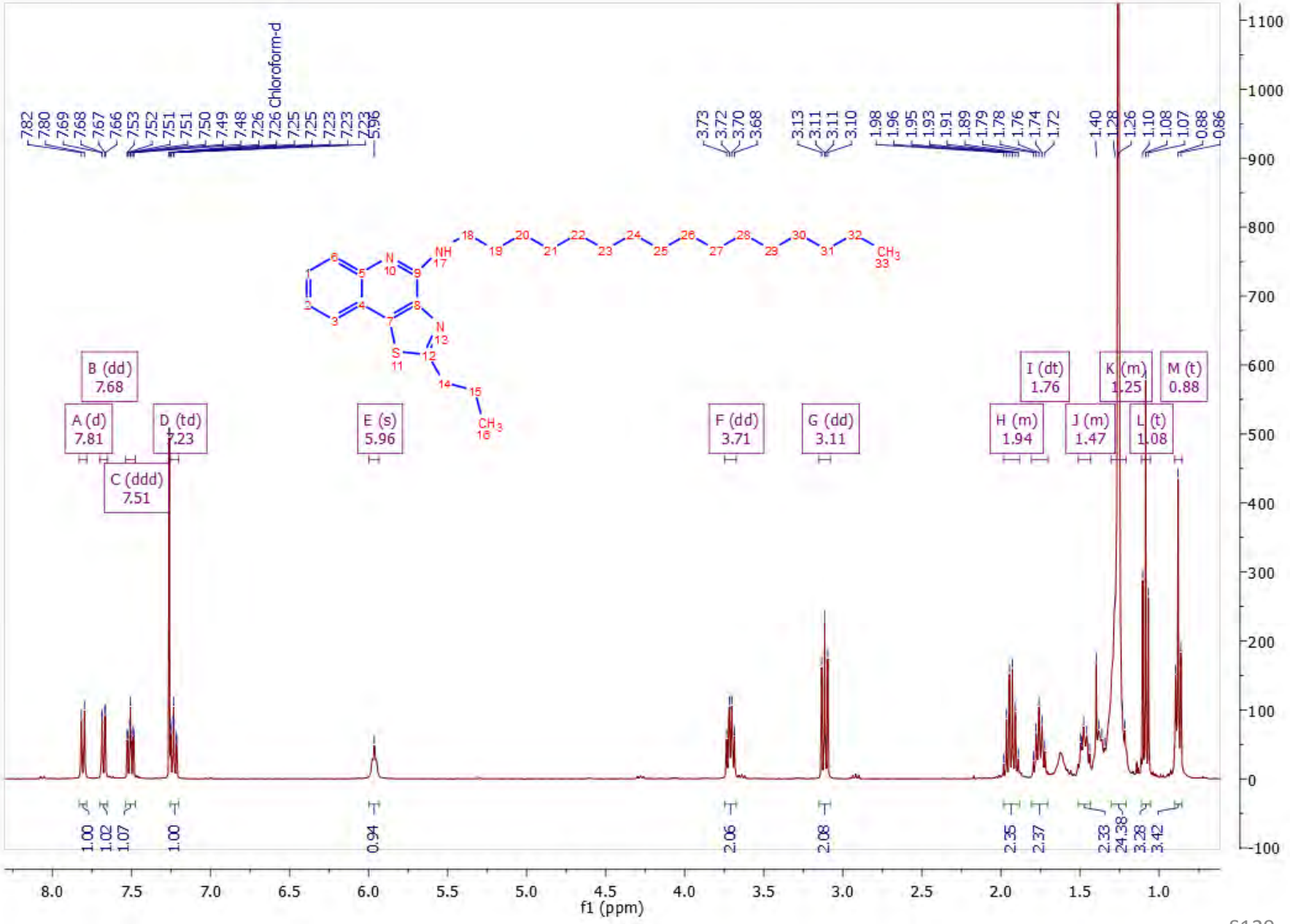


15b LC-MS

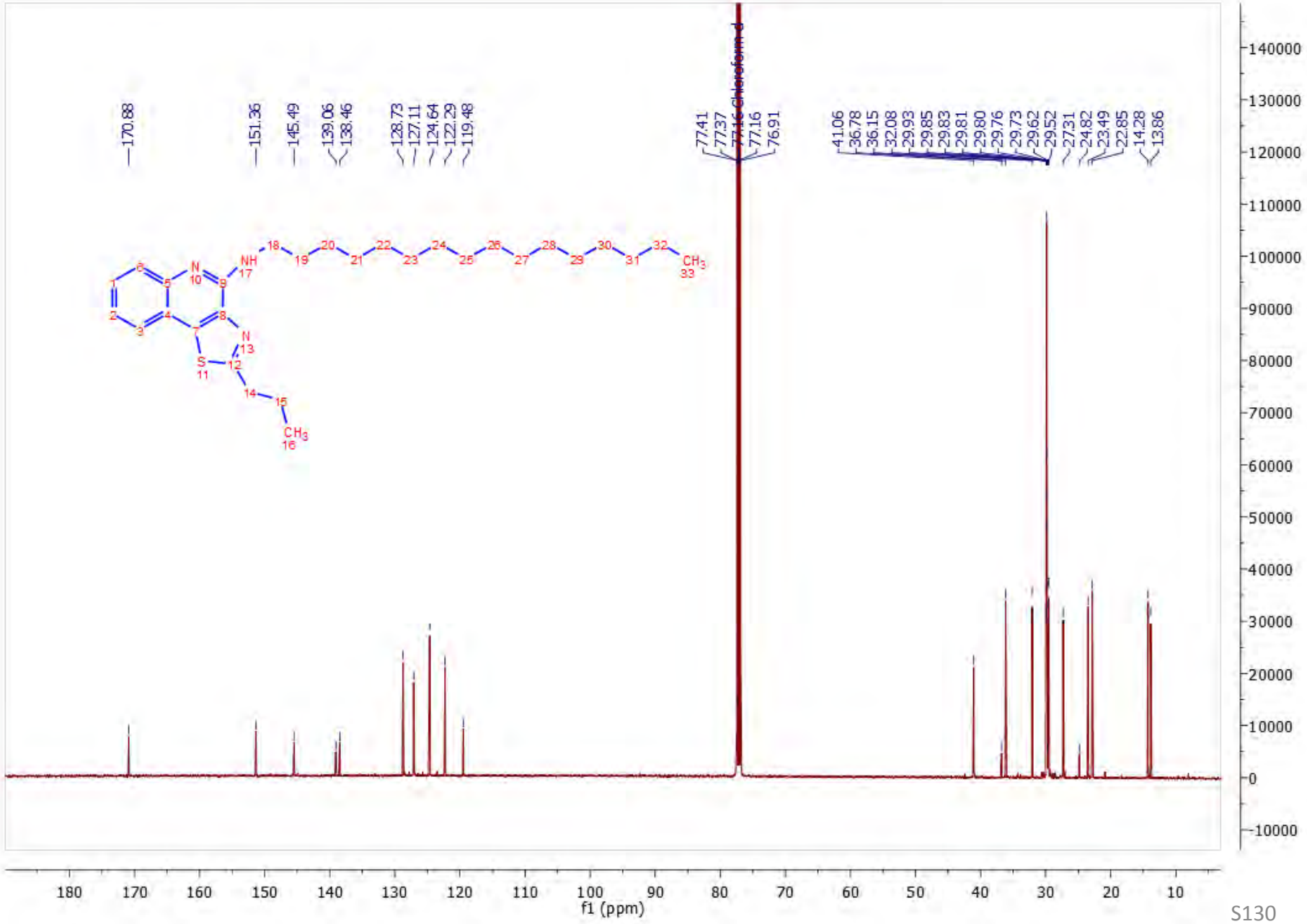




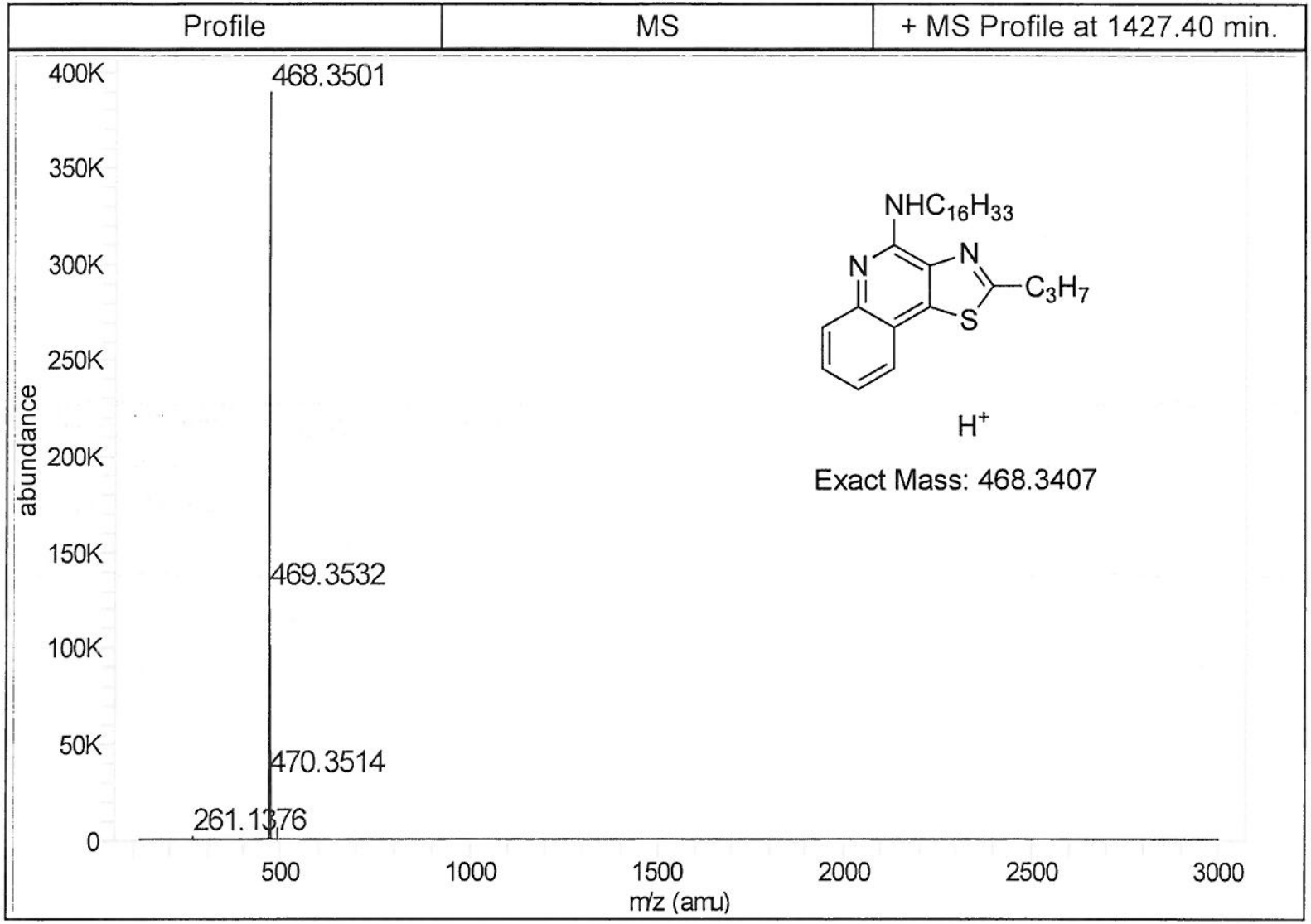
15c ^{1}H NMR



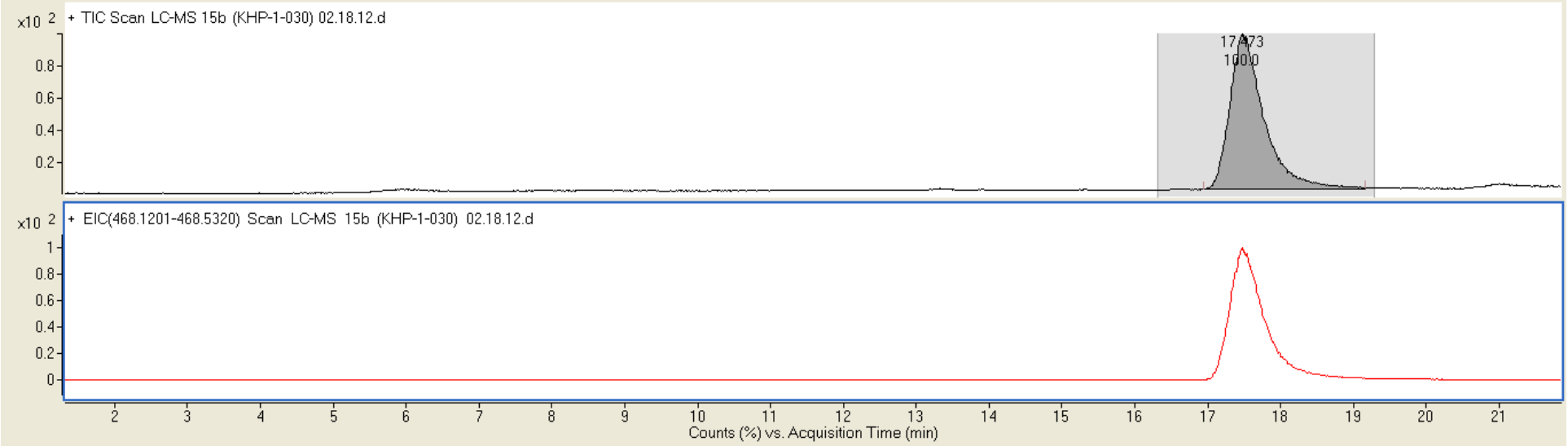
15c ^{13}C NMR

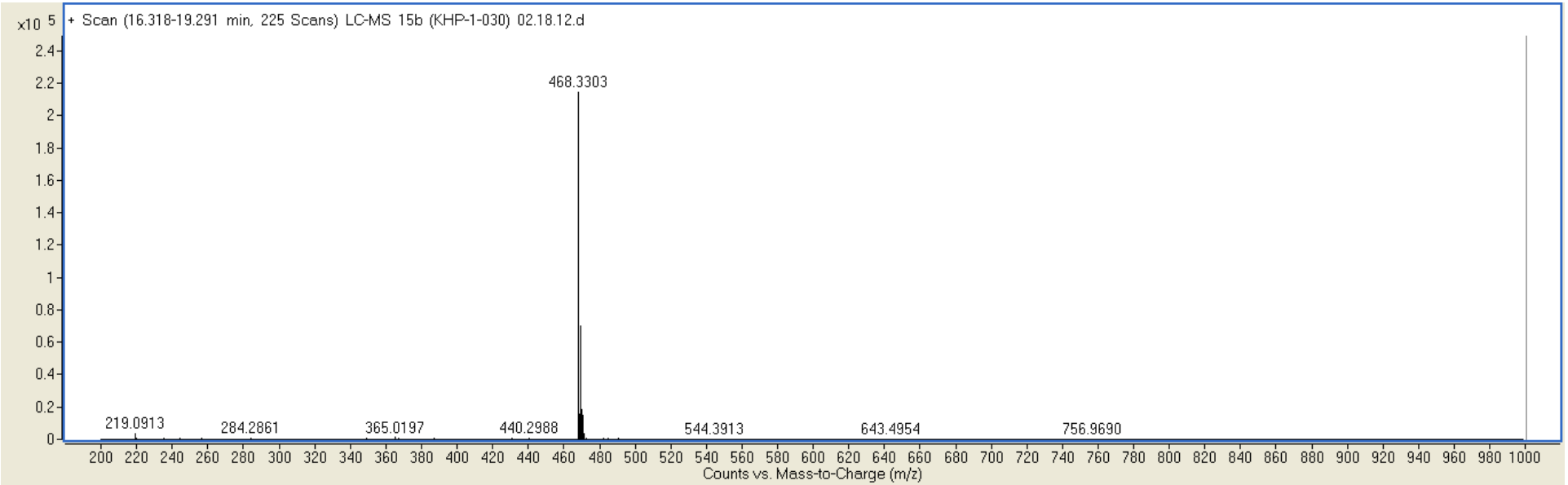


15c MS

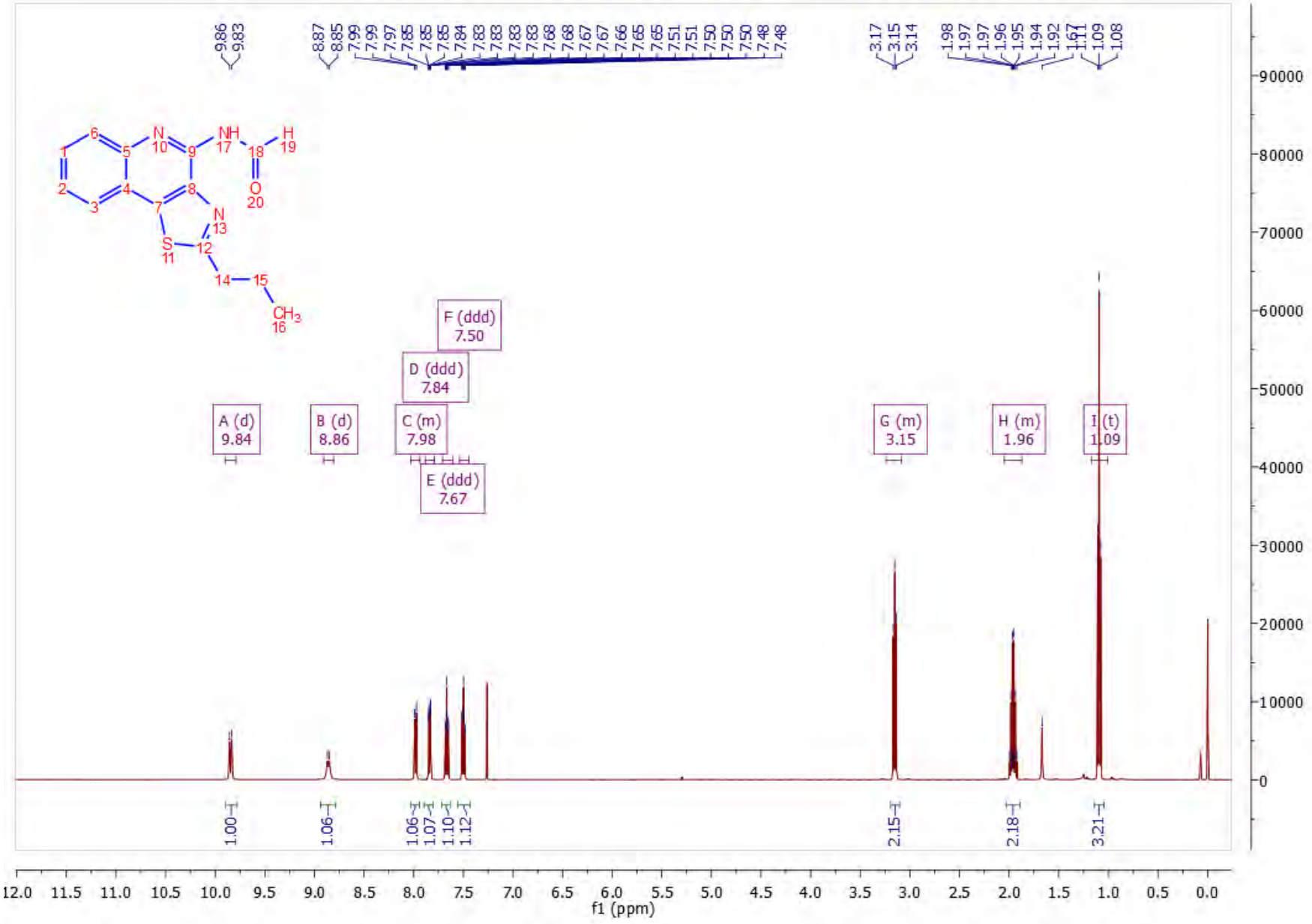


15c LC-MS

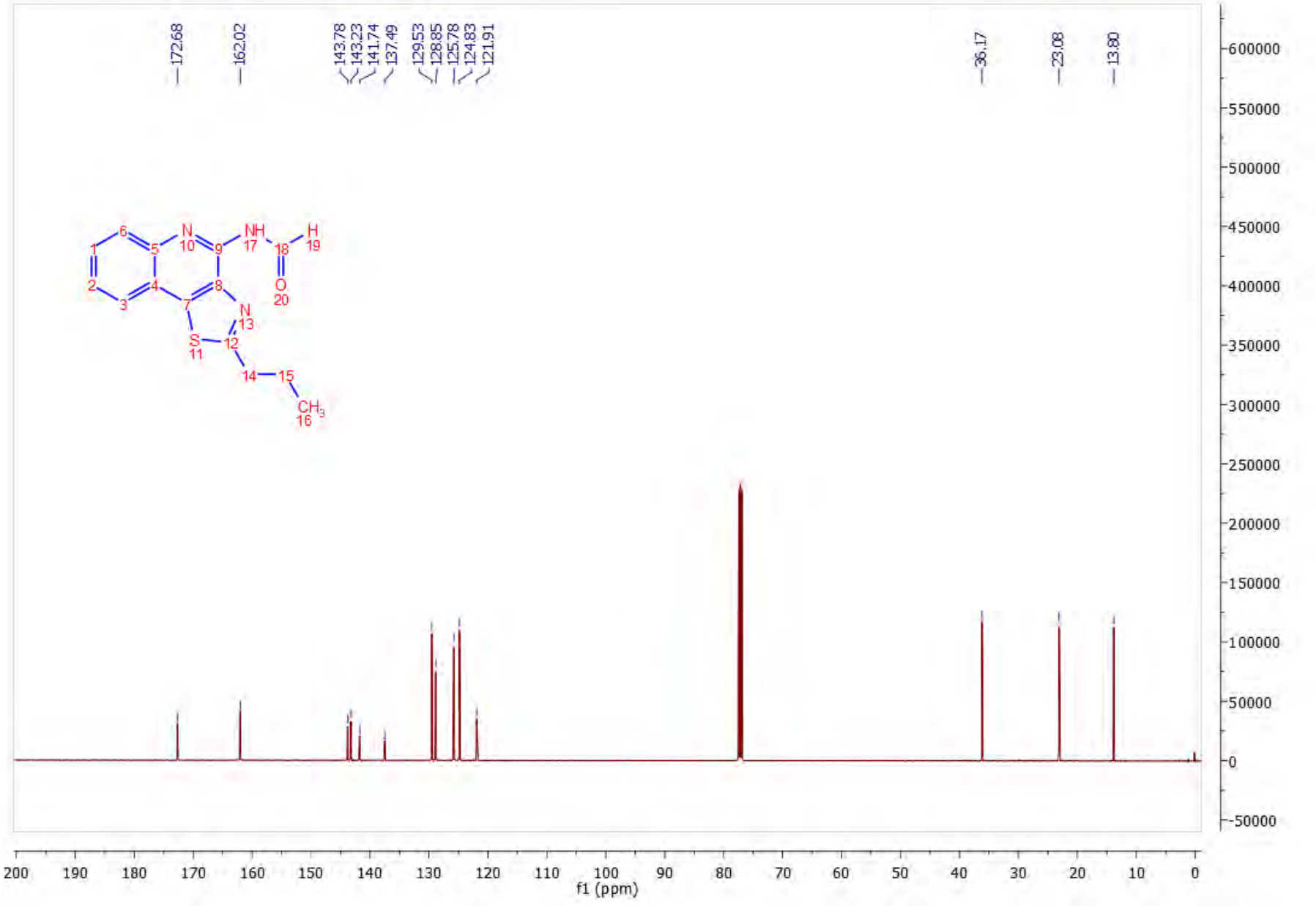




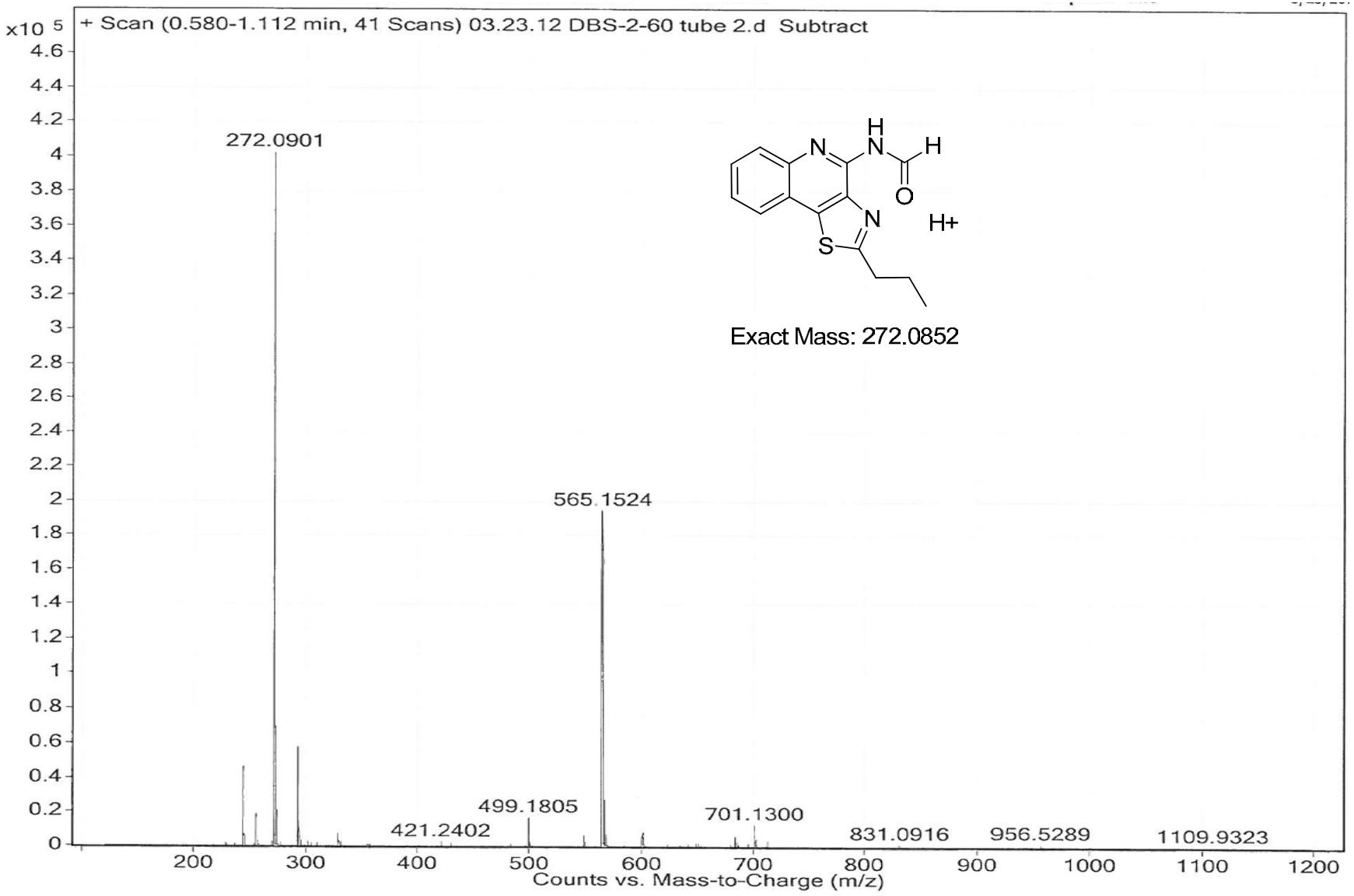
15d ^{1}H NMR



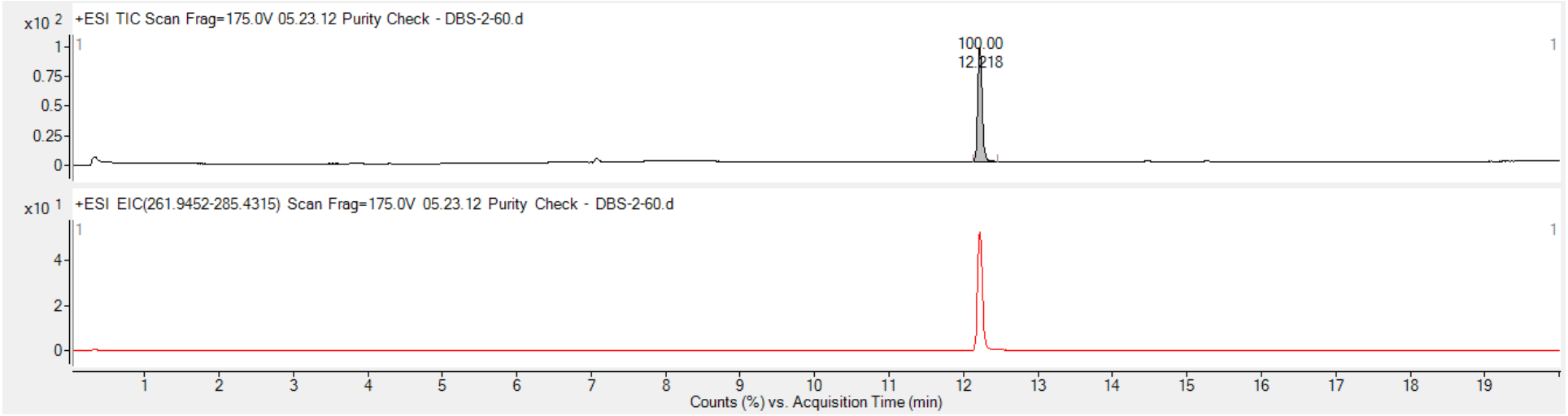
15d ^{13}C NMR

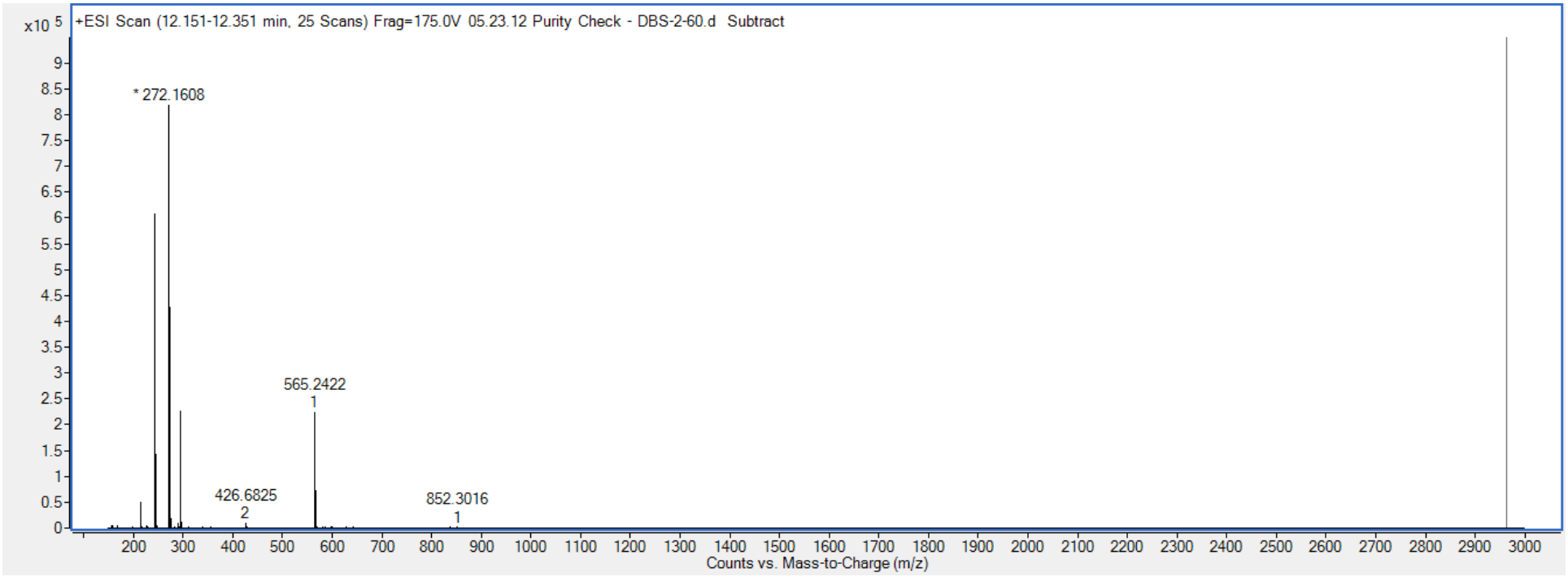


15d MS

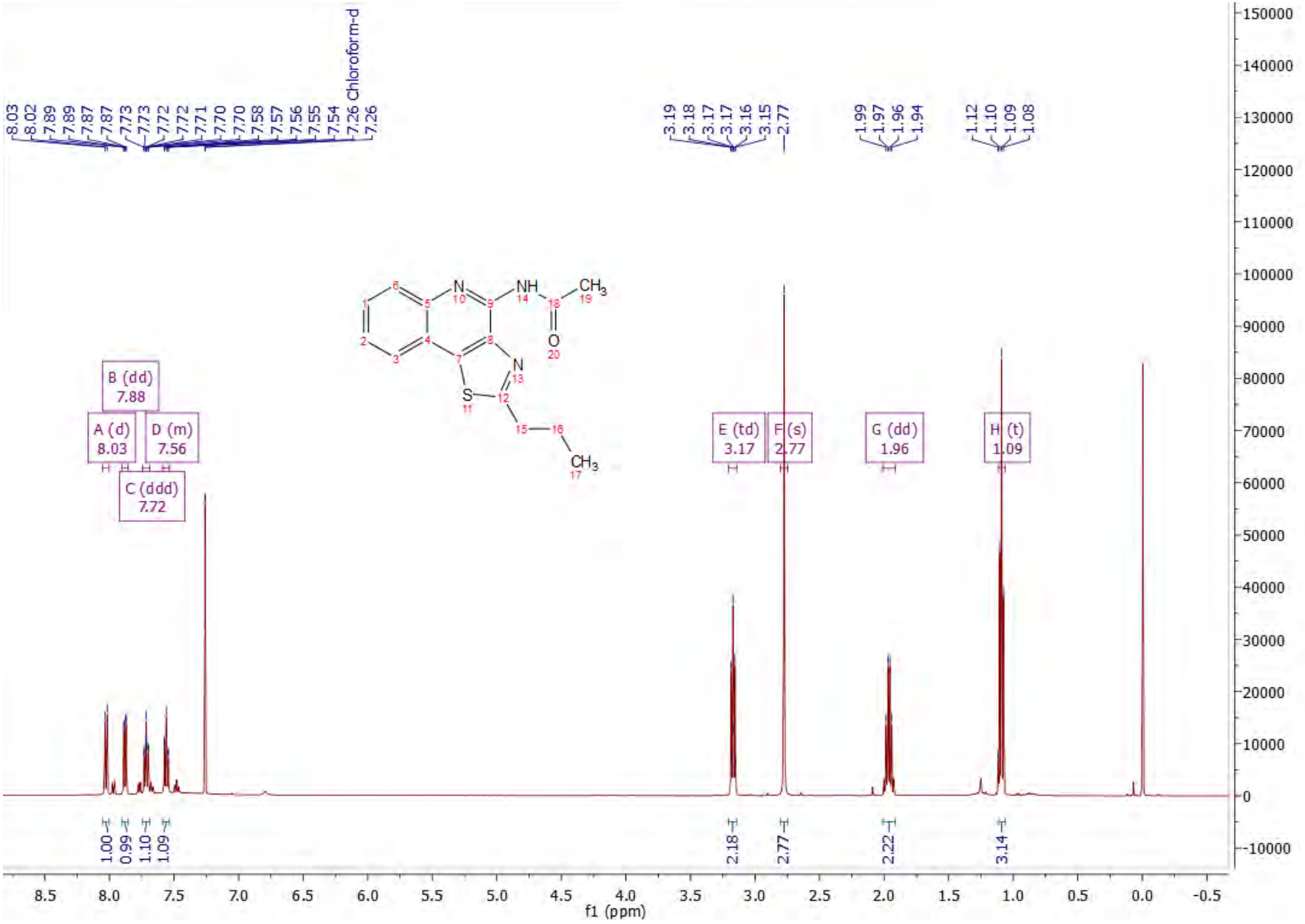


15d LC-MS





15e ^{1}H NMR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7.89
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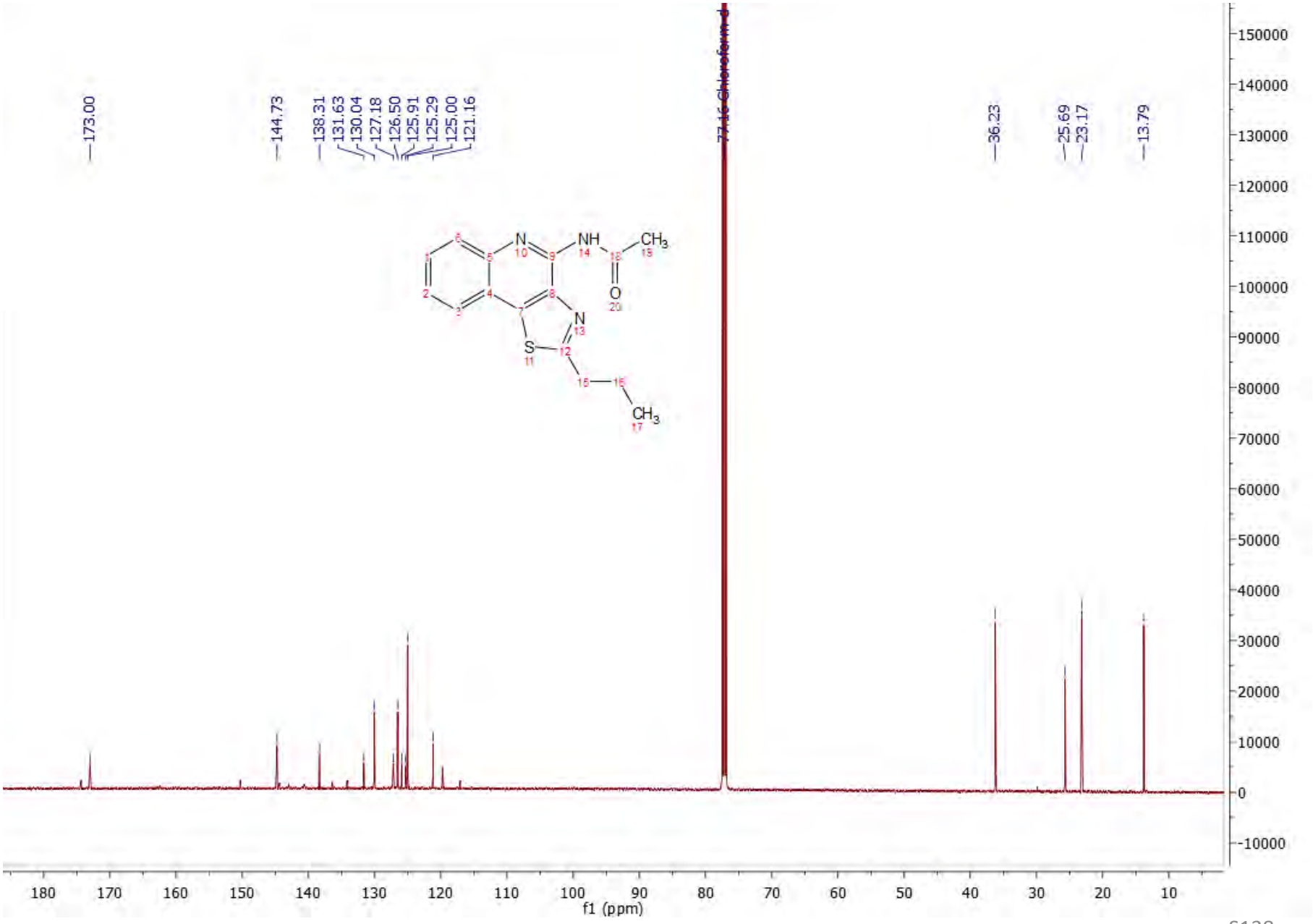
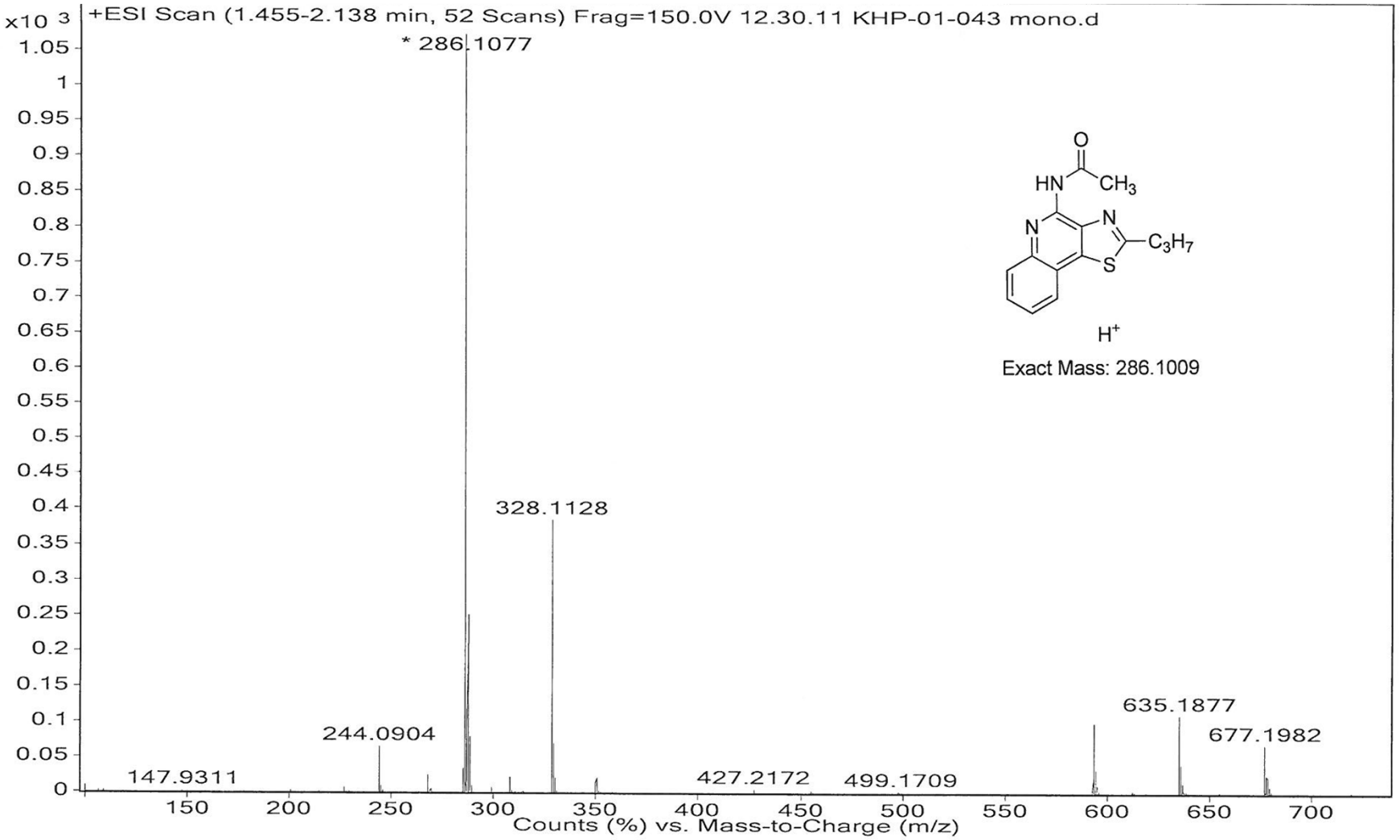
7.73
7.73
7.72
7.72
7.71
7.70
7.70
7.58
7.57
7.56
7.55
7.54
7.26 Chloroform-d
7.26
3.19
3.18
3.17
3.17
3.16
3.15
2.77
1.99
1.97
1.96
1.94
1.12
1.10
1.09
1.08
B (dd)
7.88
A (d)
8.03
D (m)
7.56
C (ddd)
7.72
E (td)
3.17
F (s)
2.77
G (dd)
1.96
H (t)
1.09
1.00
0.99
1.10
1.09
2.18
2.77
2.22
3.14
f1 (ppm)

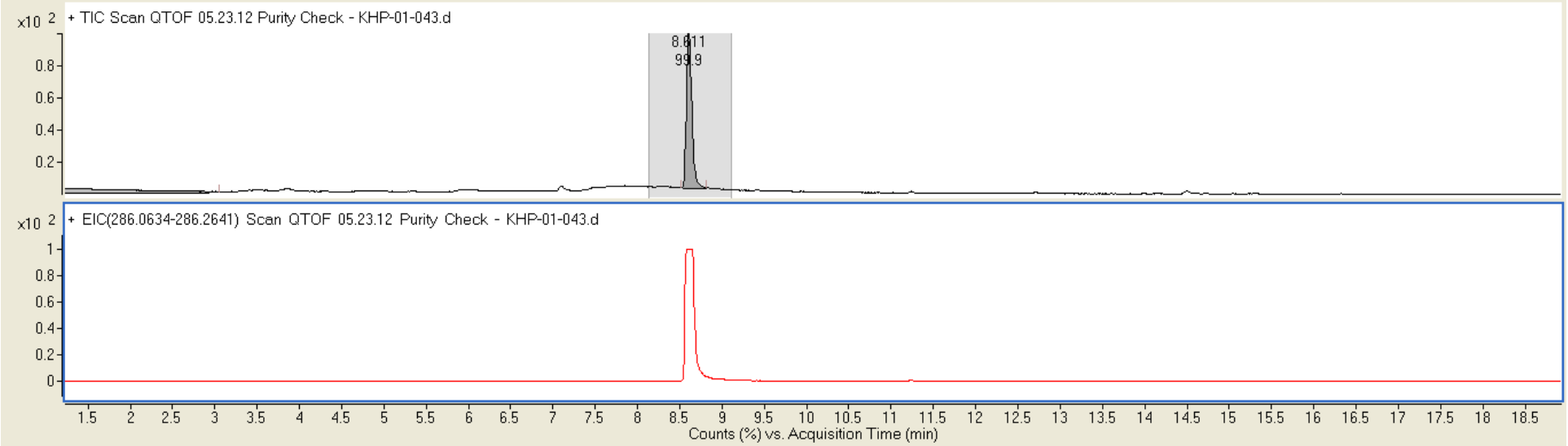
15e ^{13}C NMR

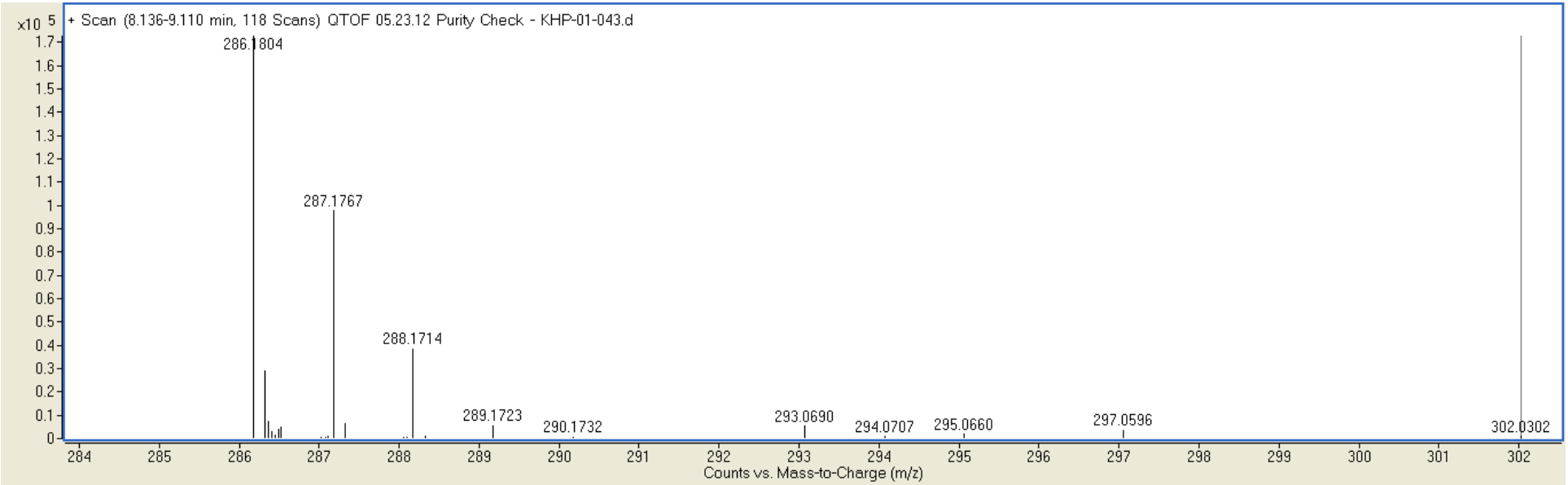


15e MS

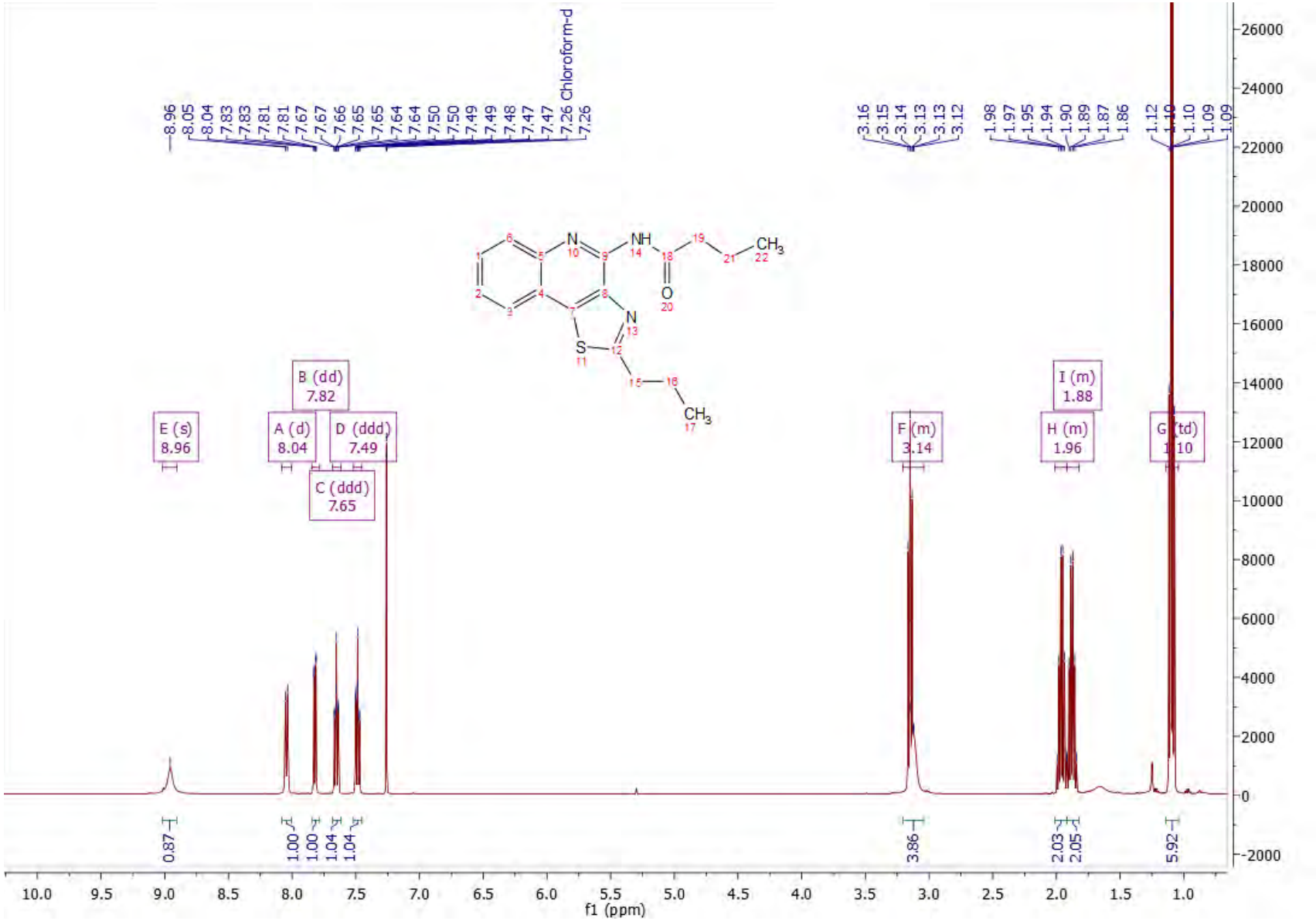


15e LC-MS

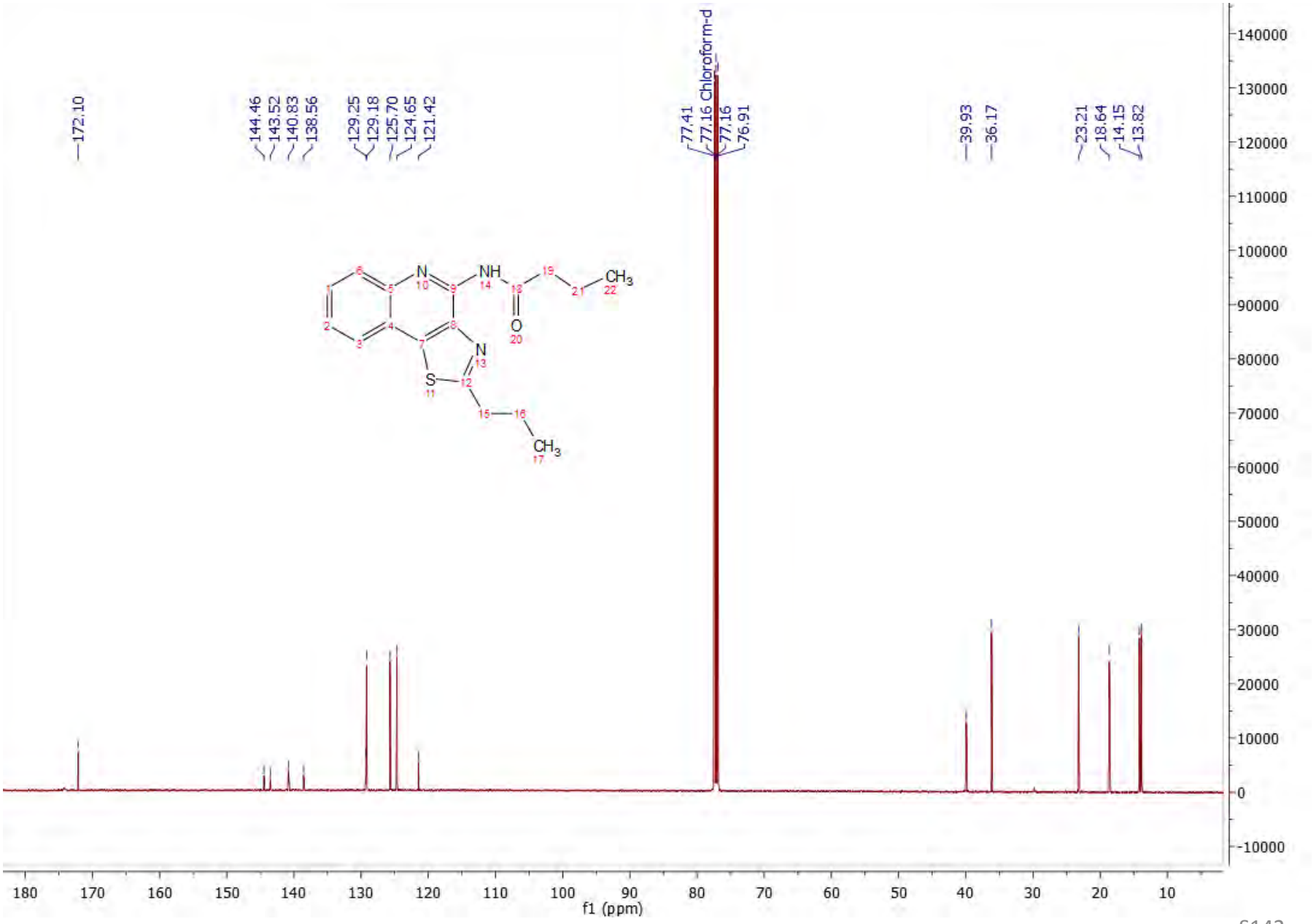




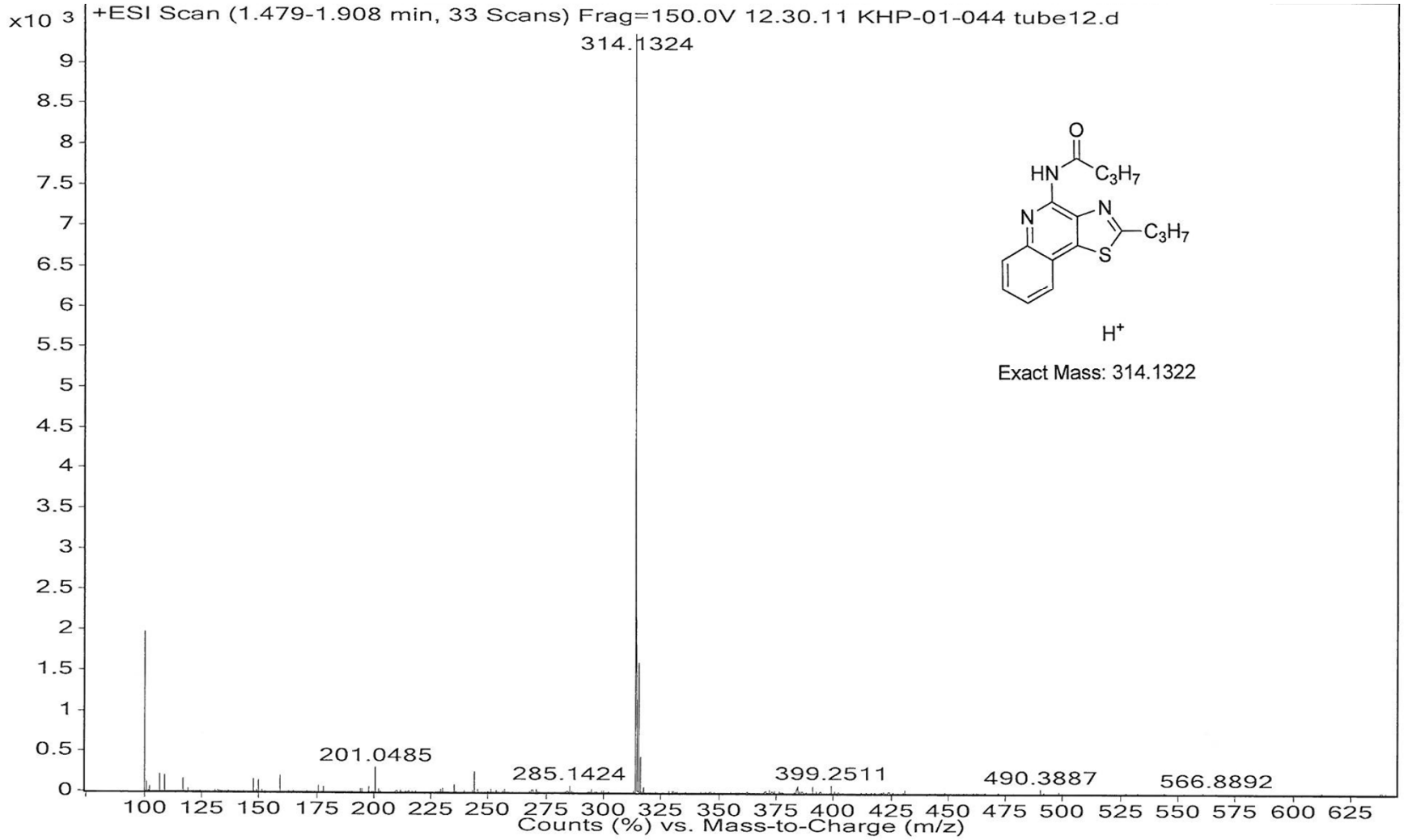
15f ^{1}H NMR



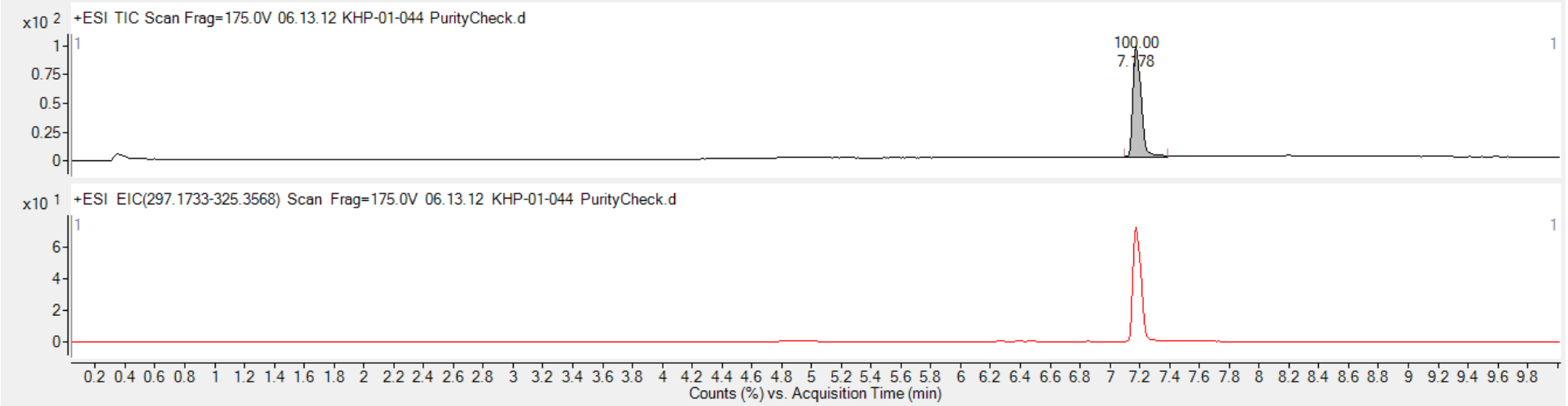
15f ^{13}C NMR

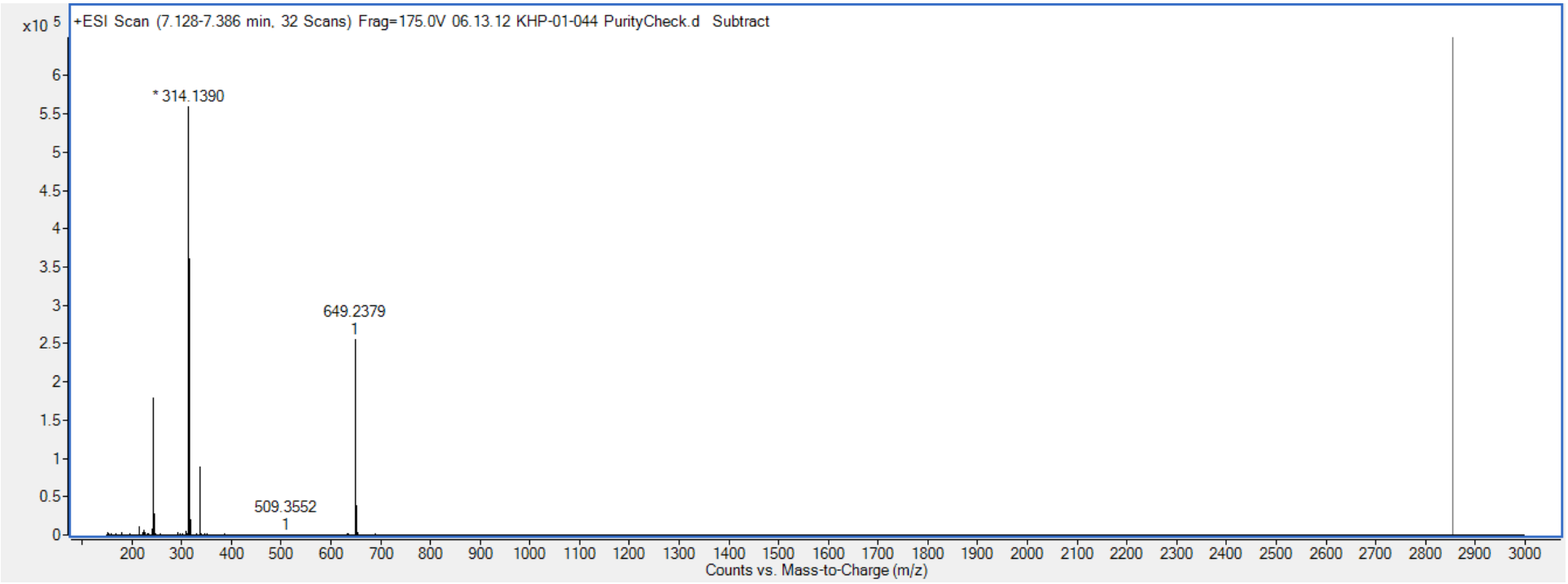


15f MS

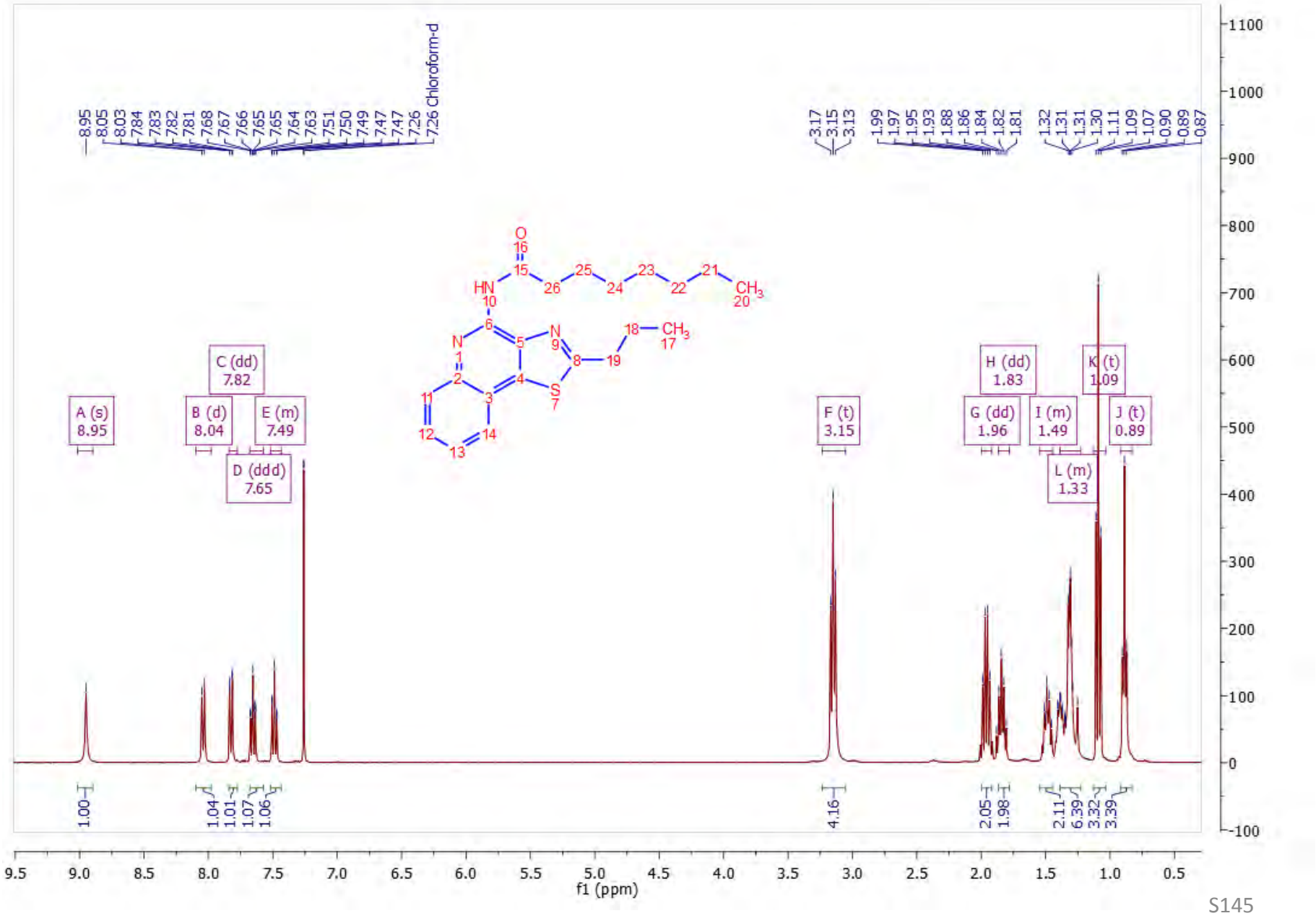


15f LC-MS

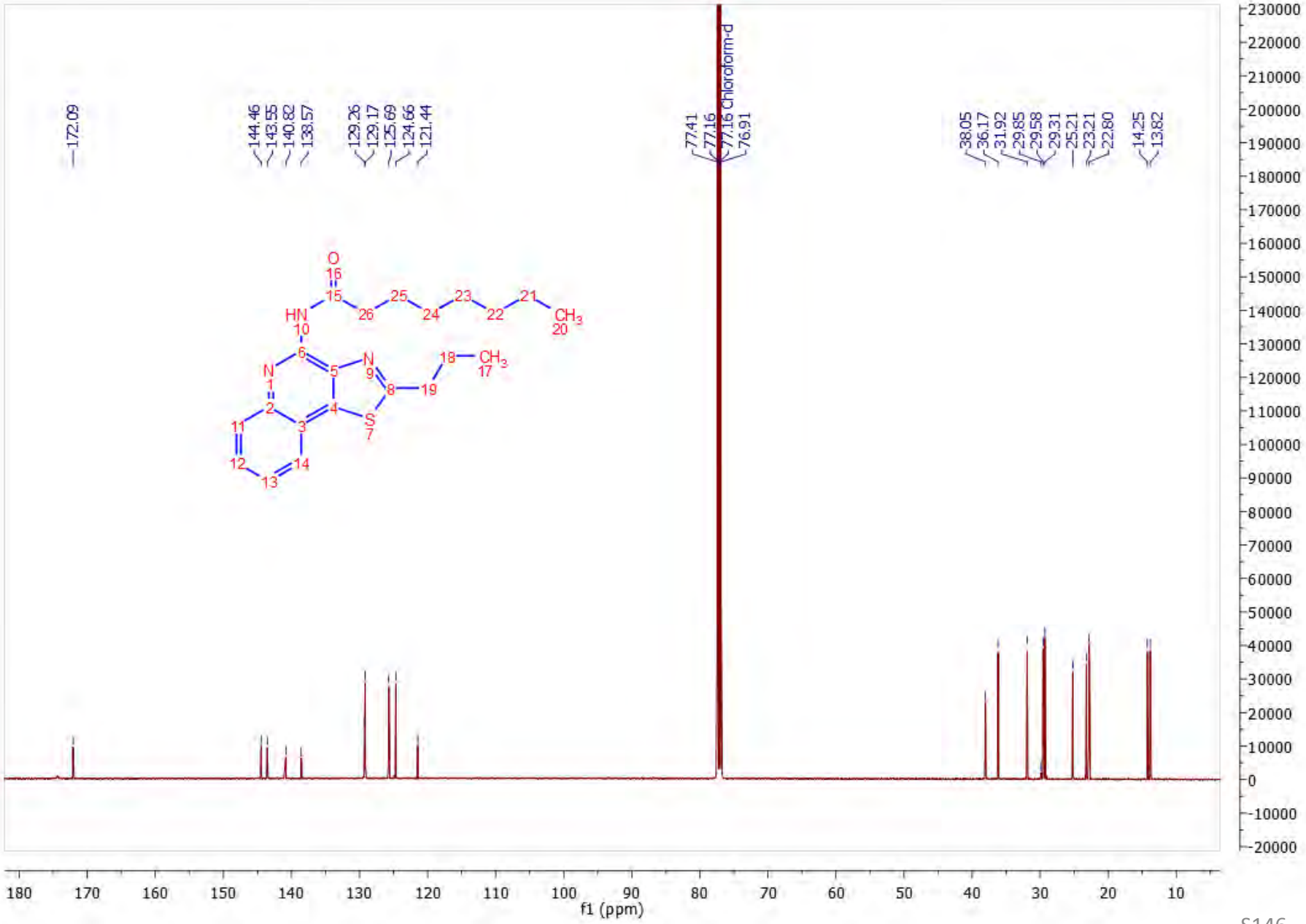




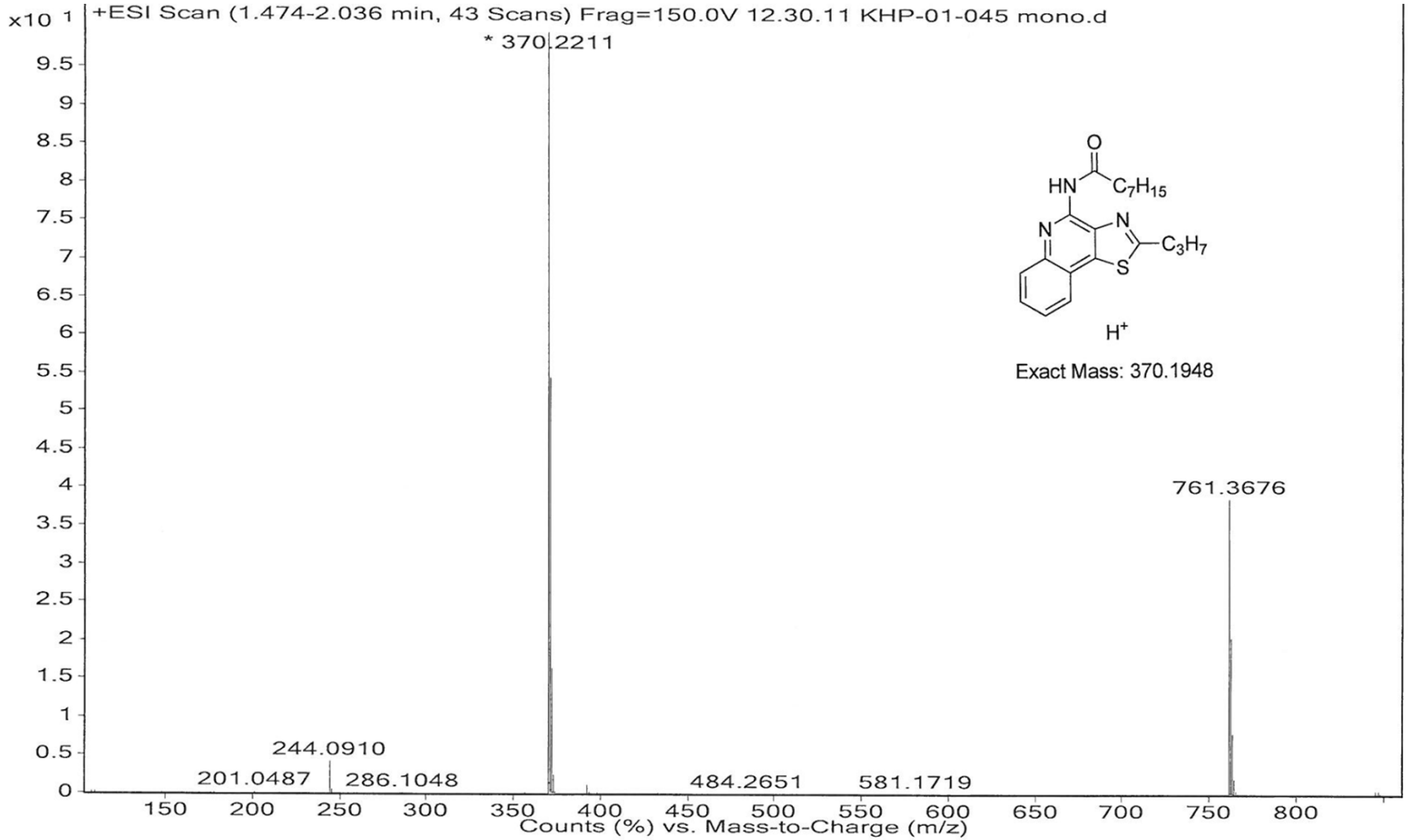
15h ^{1}H NMR



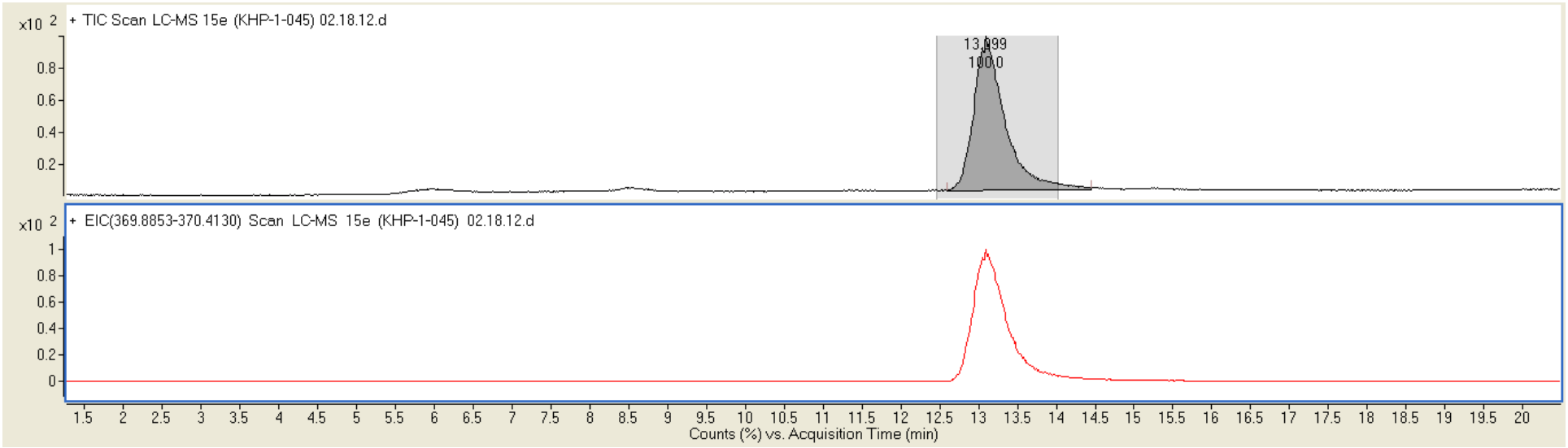
15g ^{13}C NMR

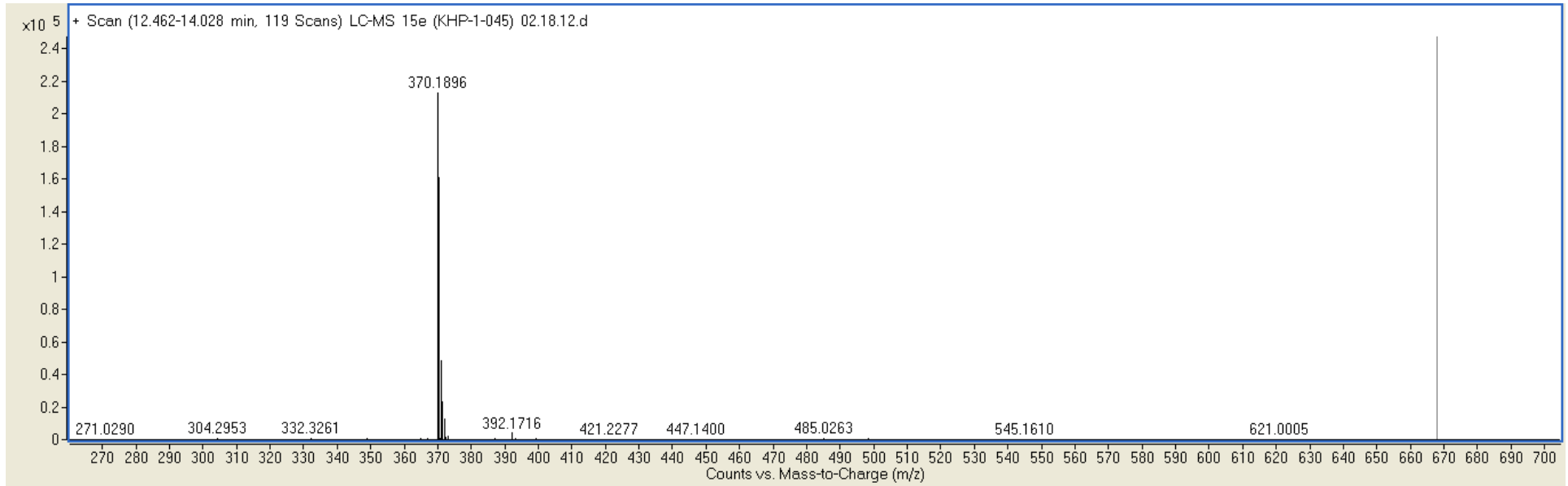


15g MS

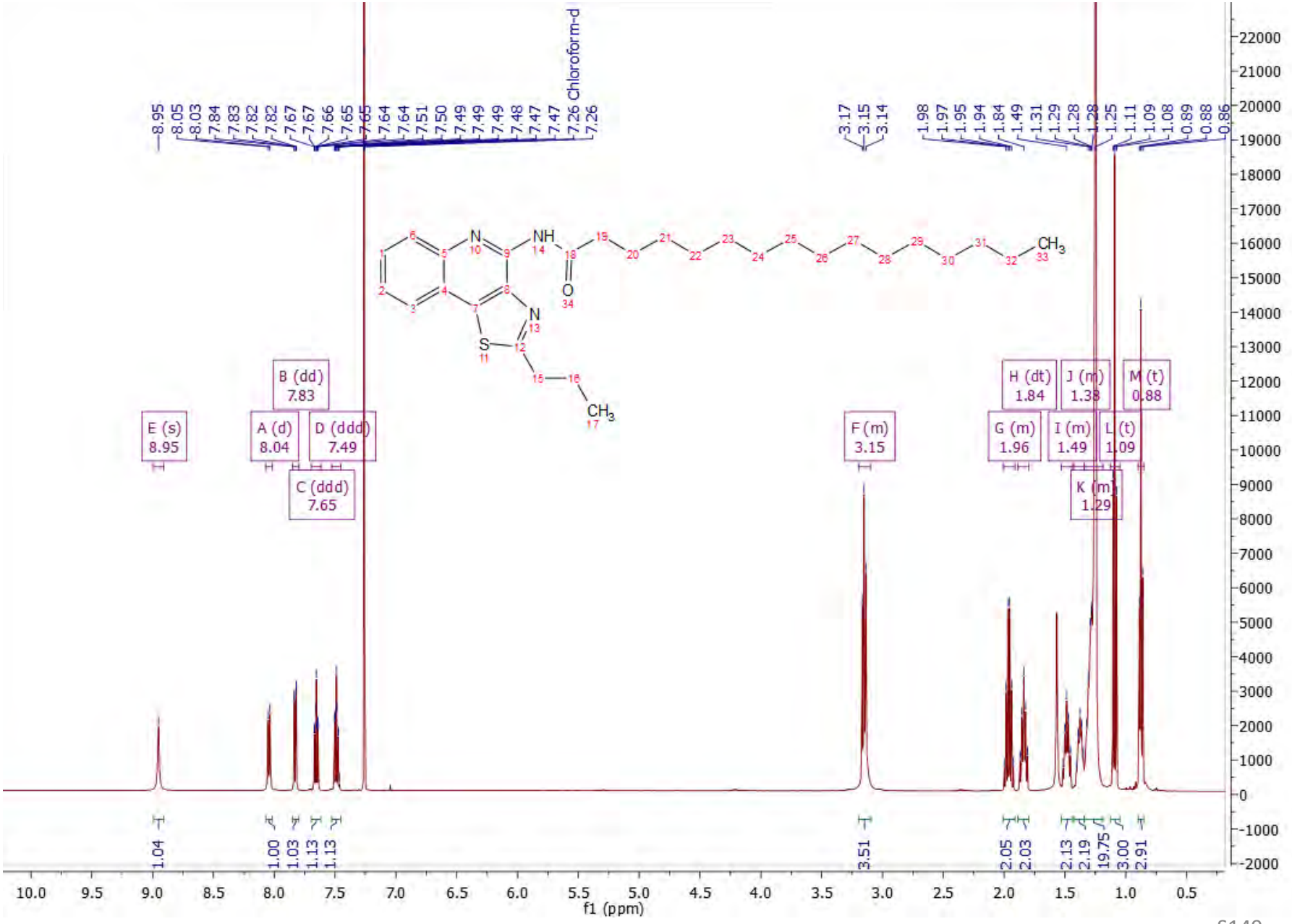


15g LC-MS

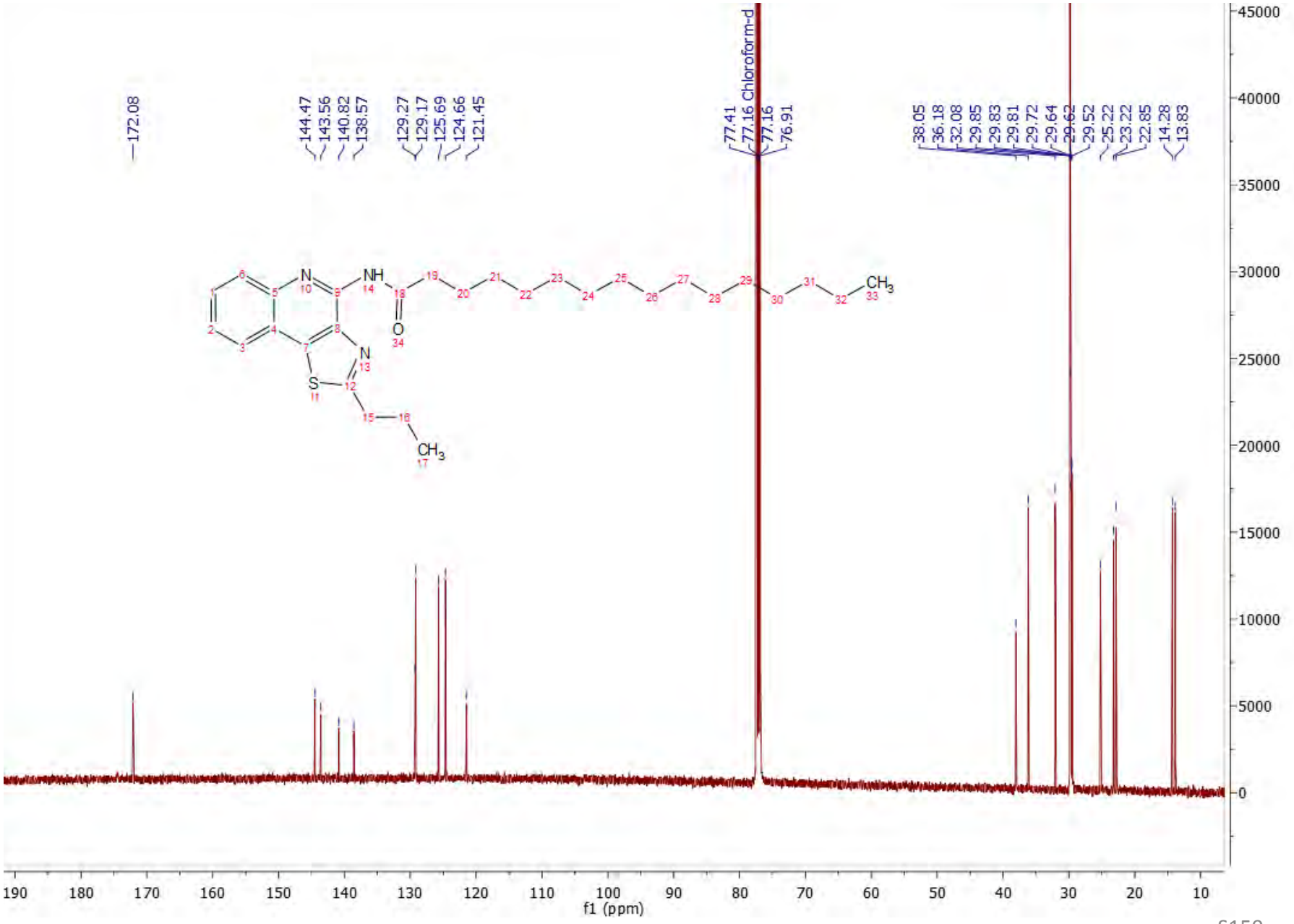




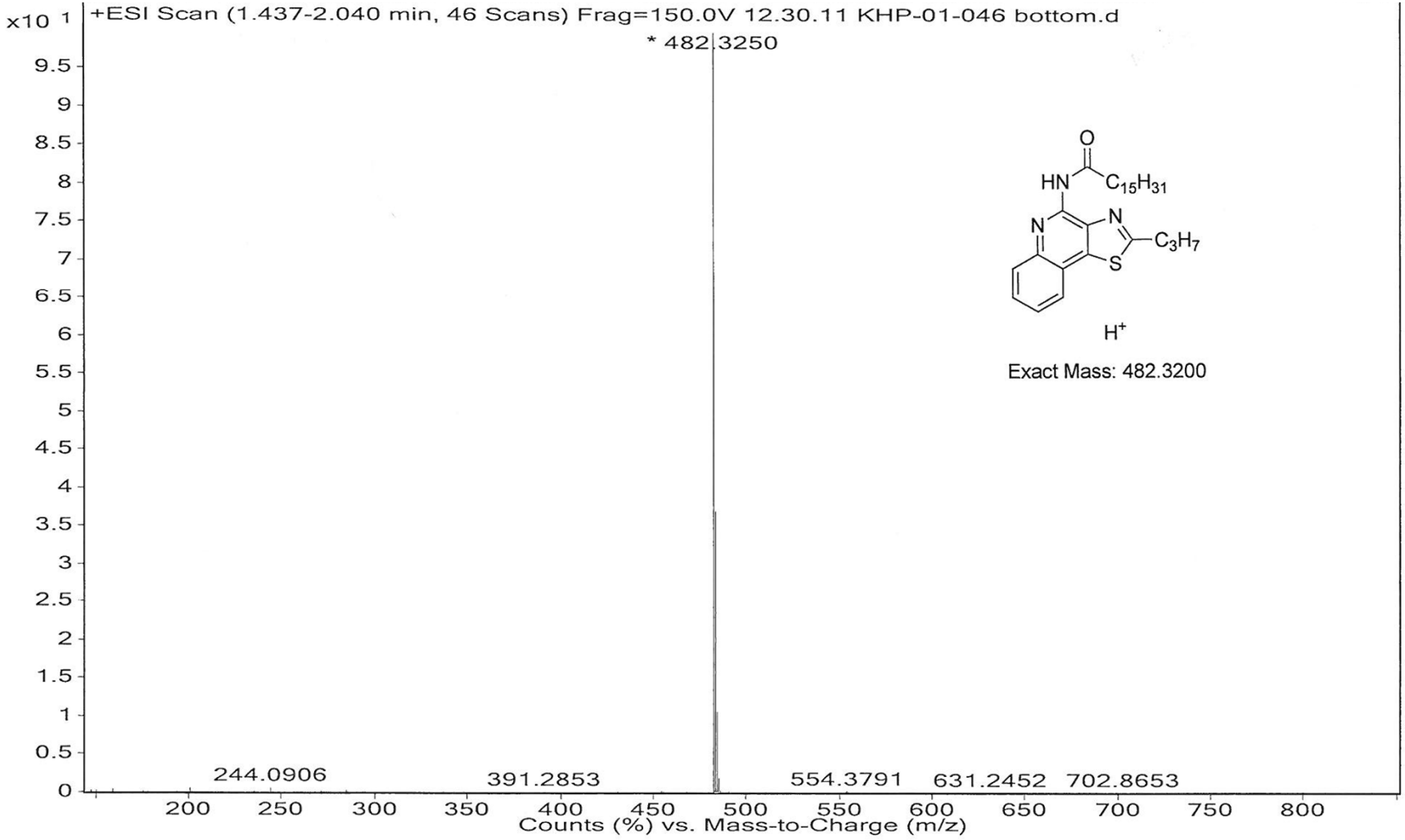
15h ^{1}H NMR



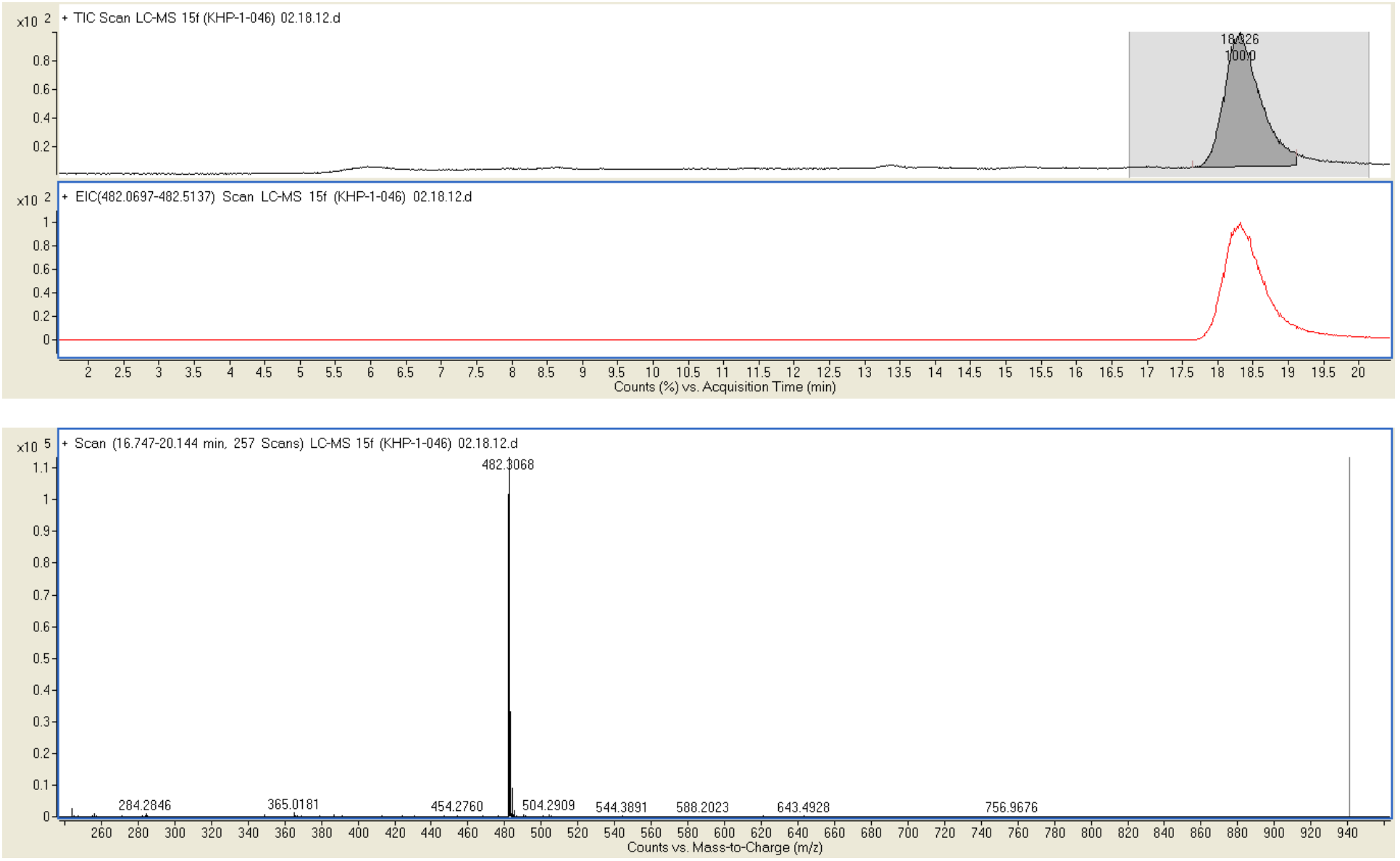
15h ^{13}C NMR



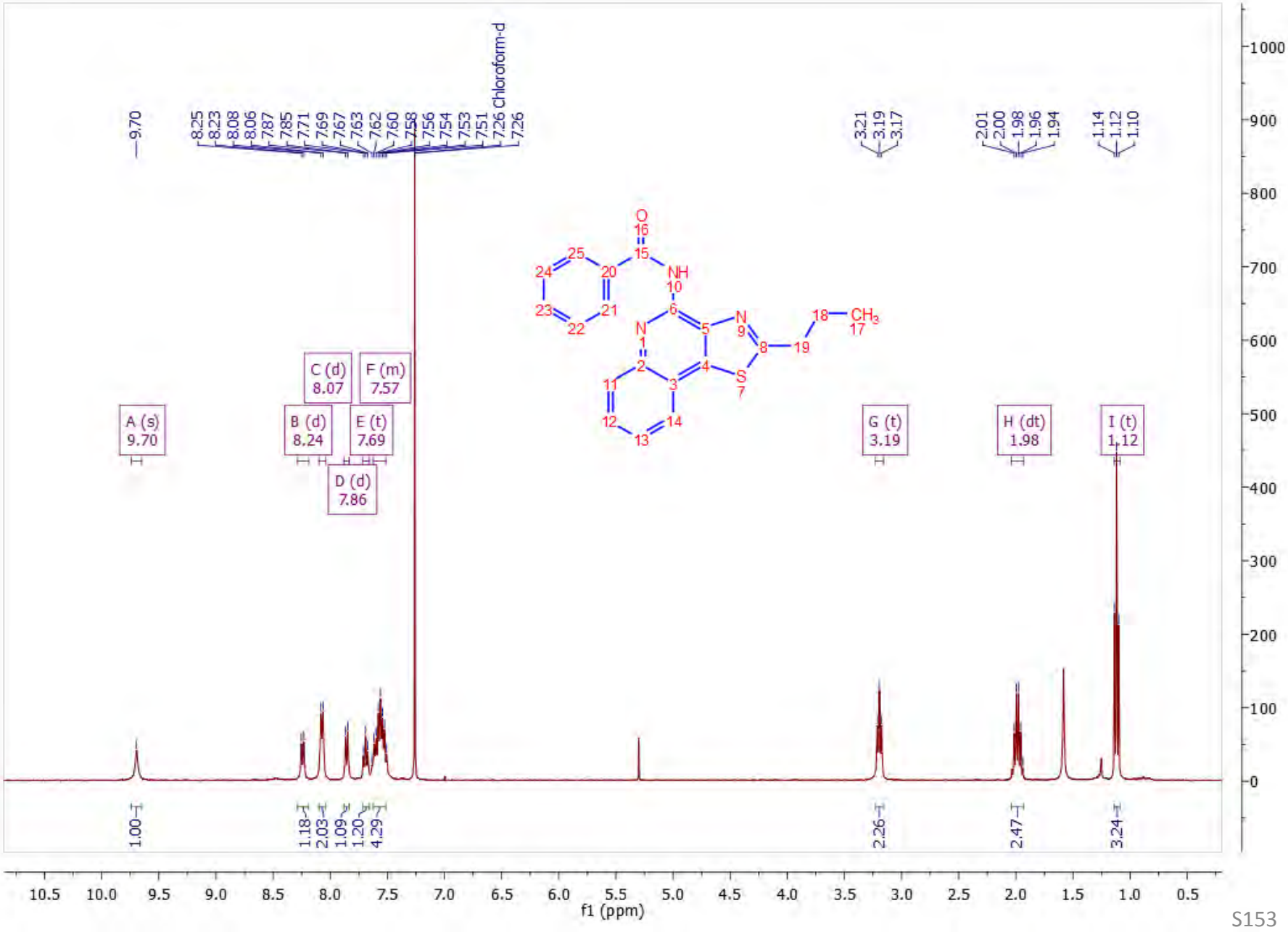
15h MS



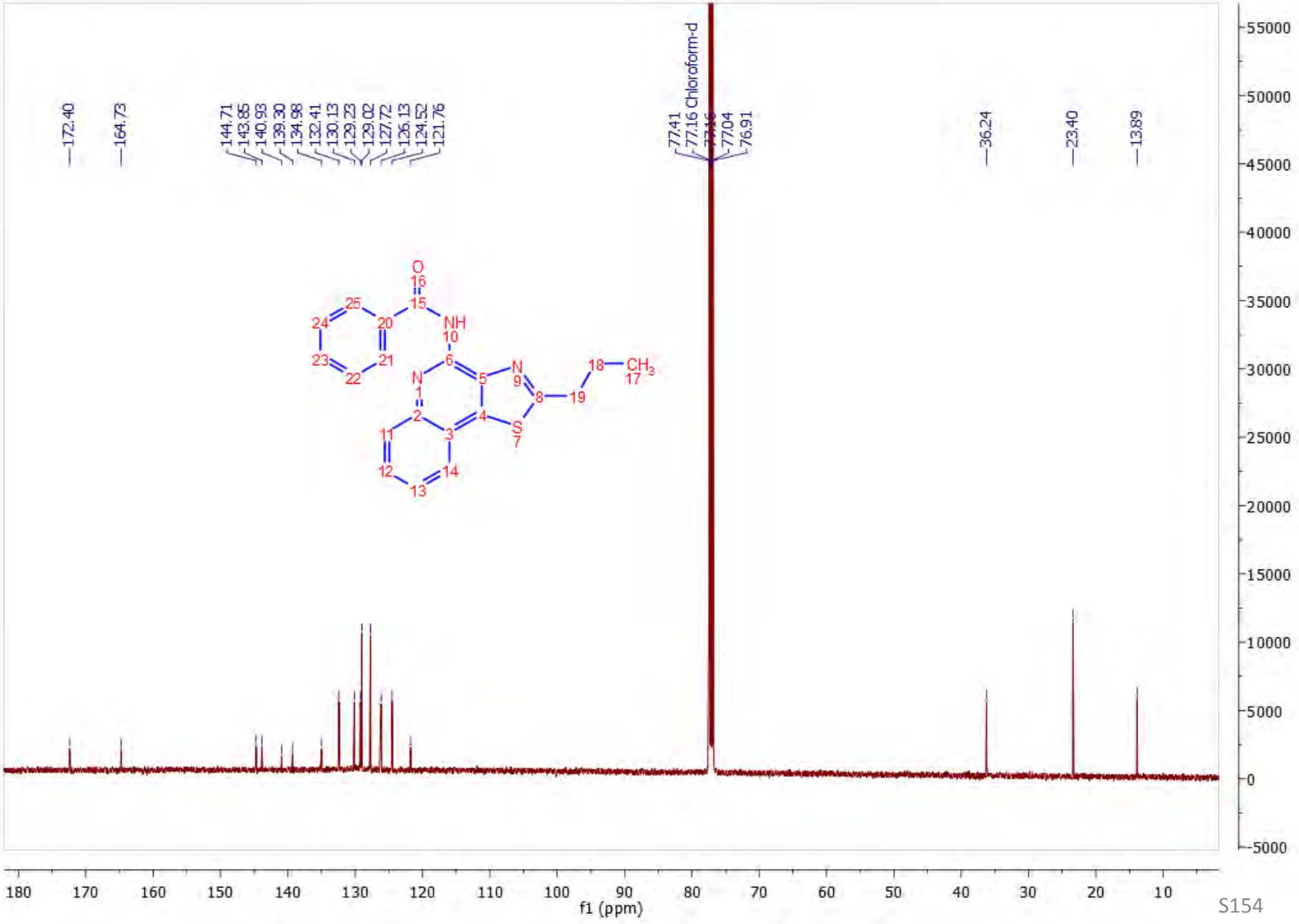
15h LC-MS



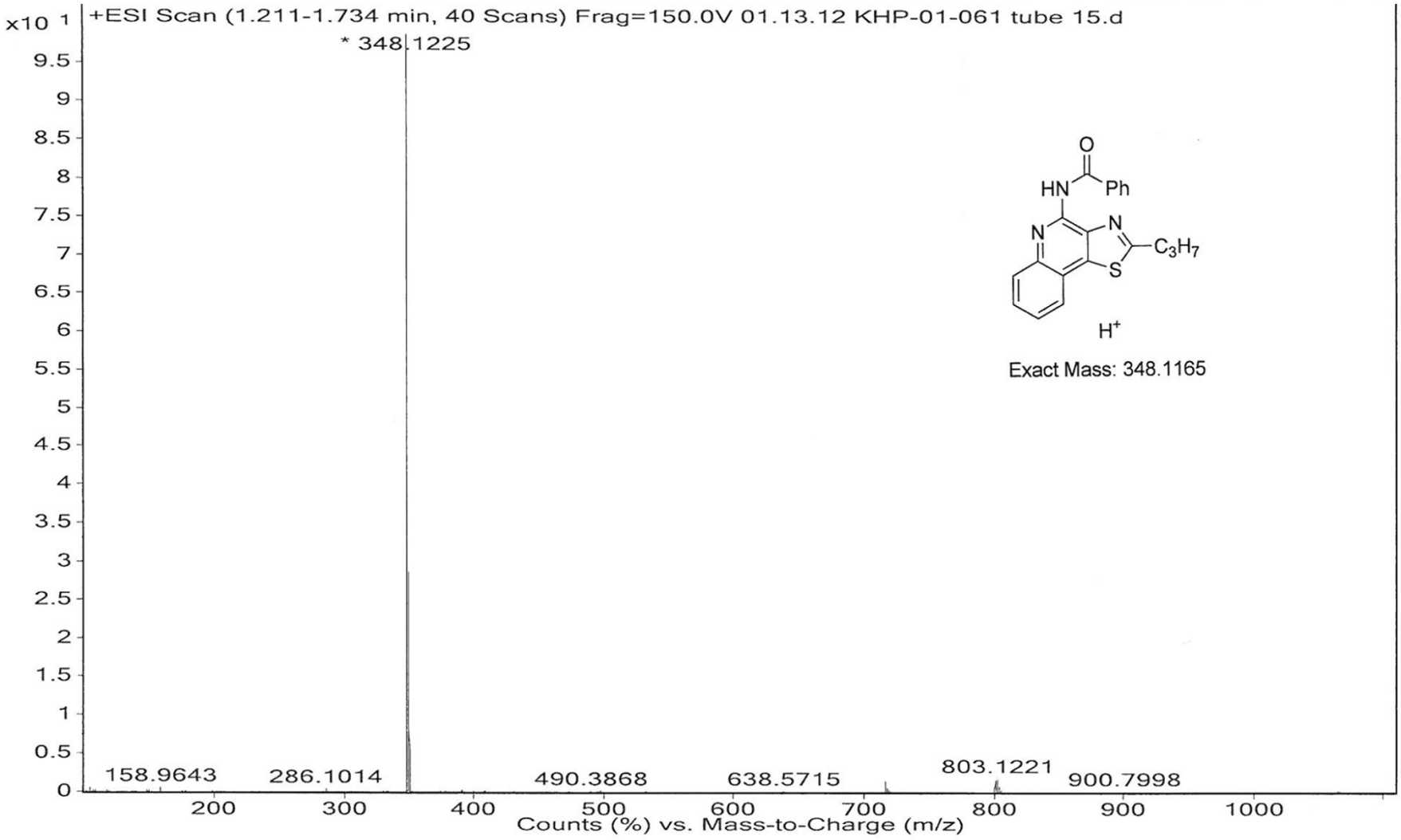
15i ^{1}H NMR



15i ^{13}C NMR



15i MS



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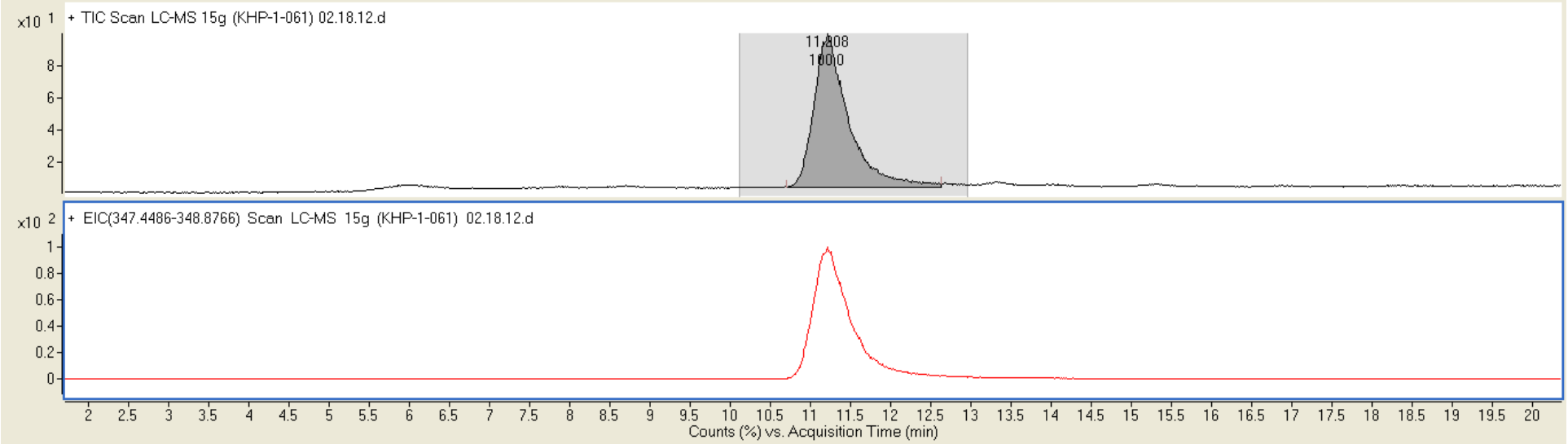
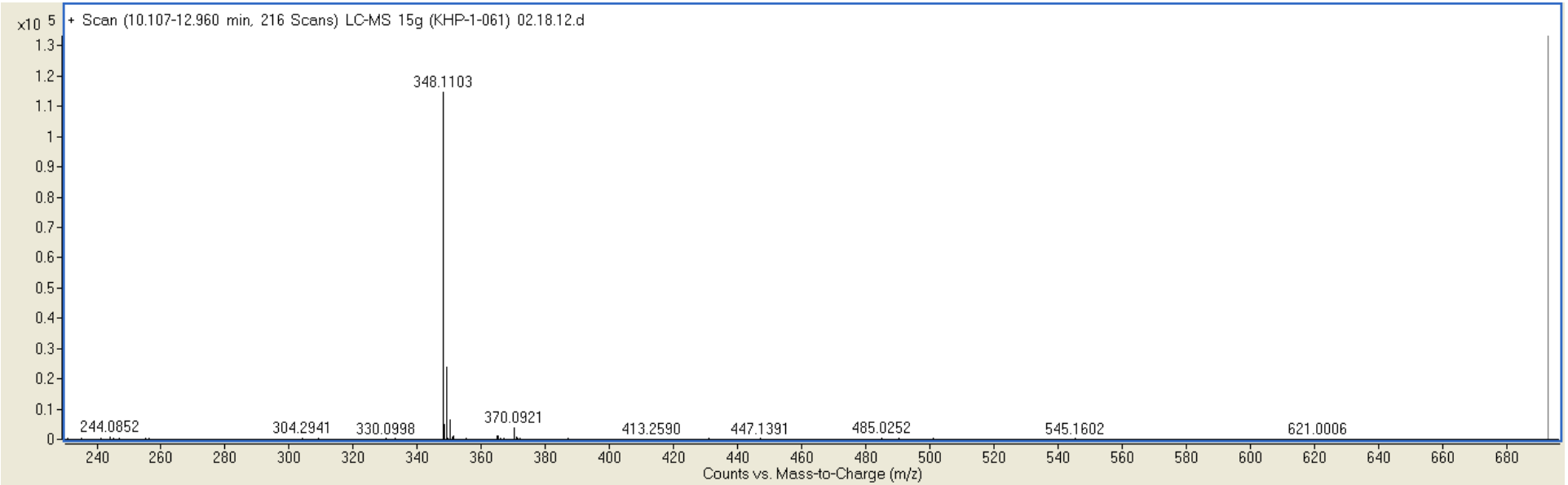
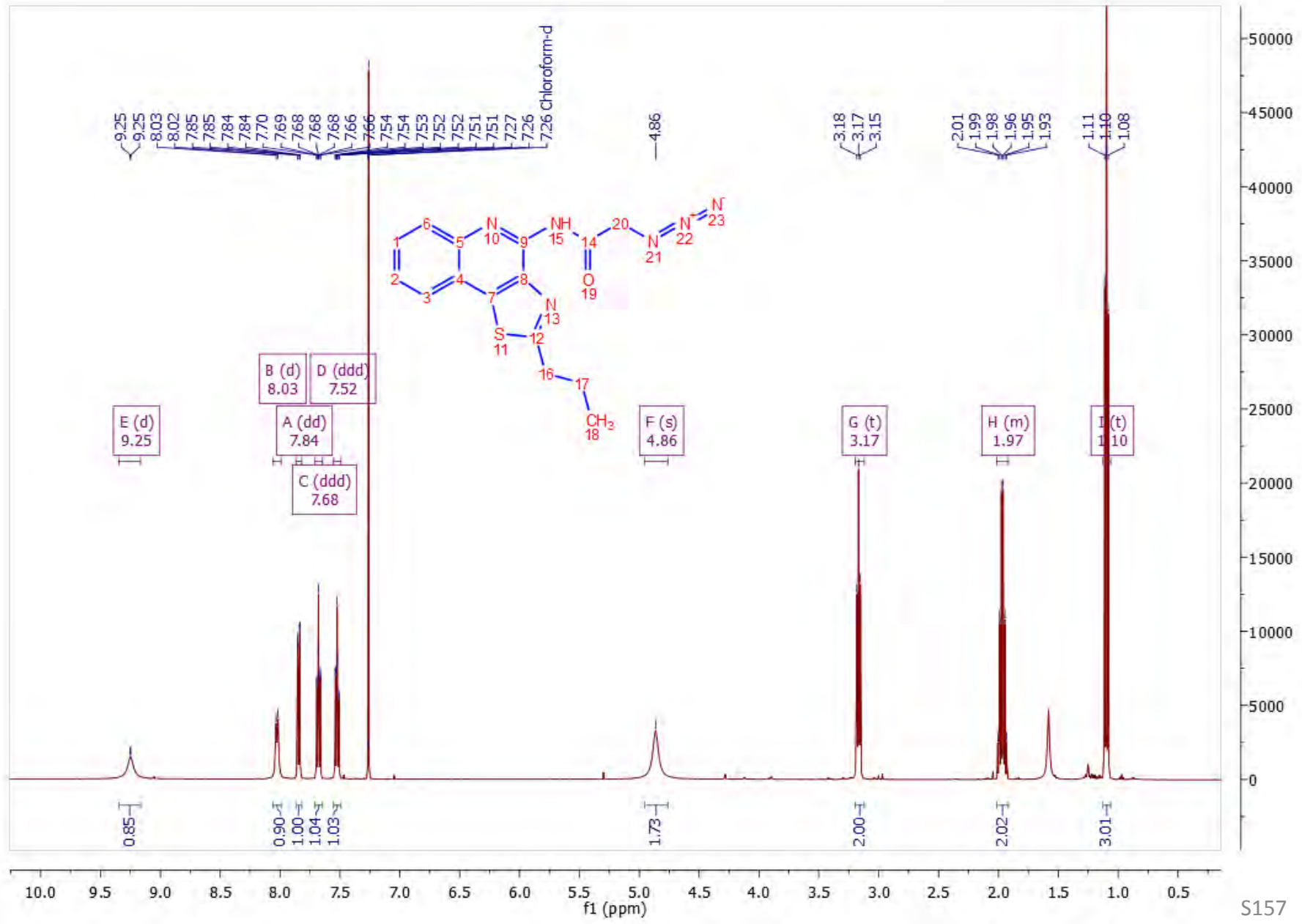




15j ^{1}H NMR



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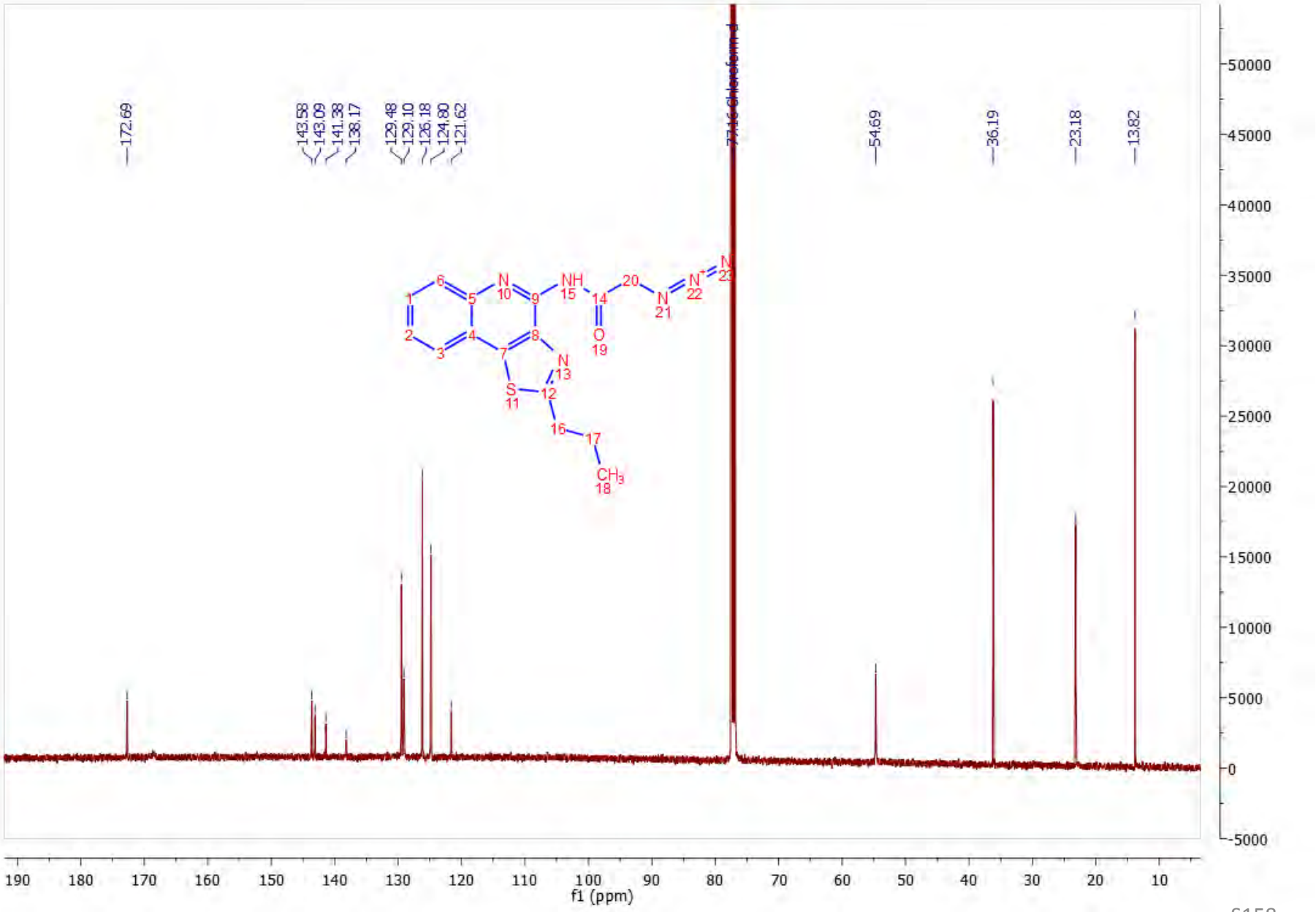

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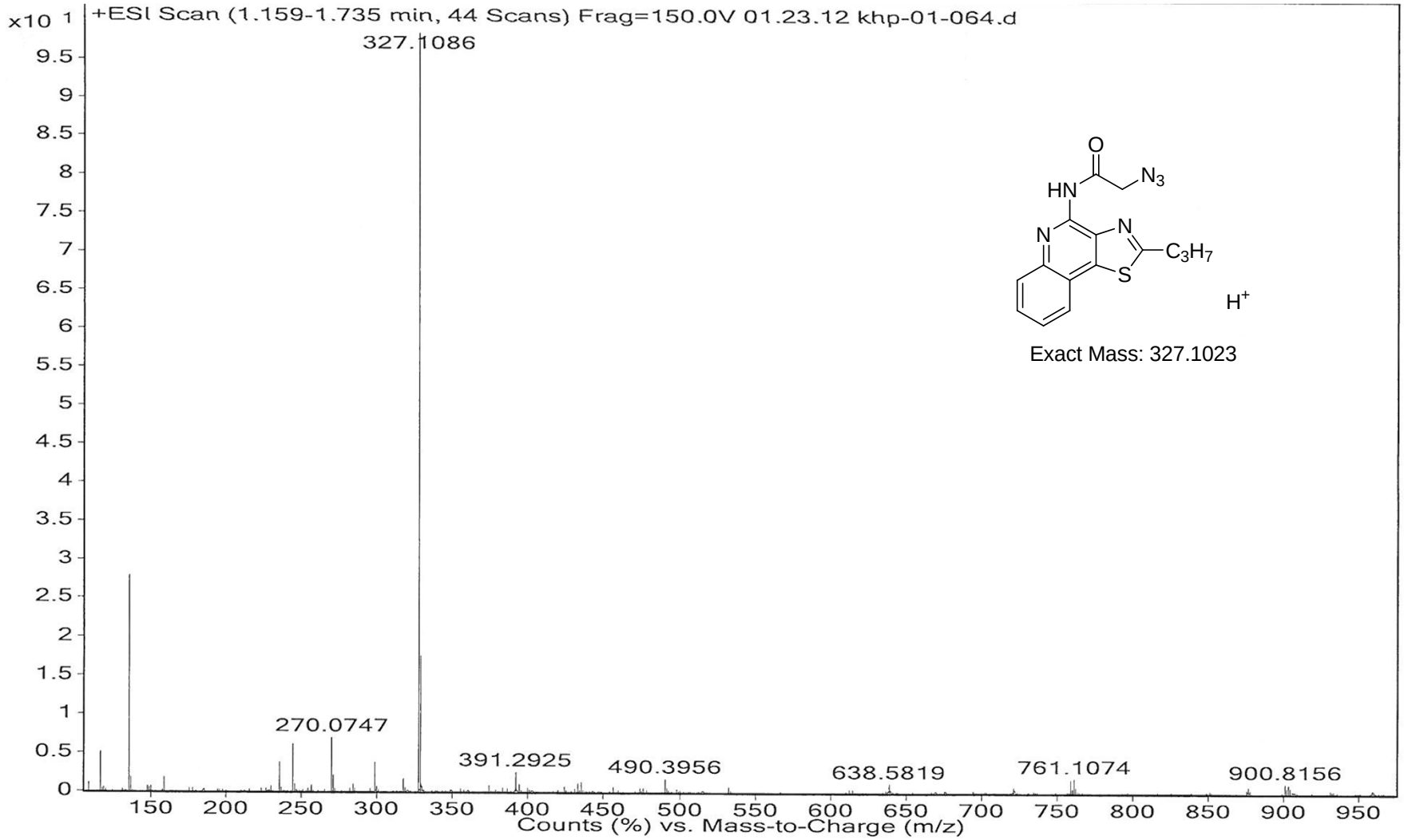

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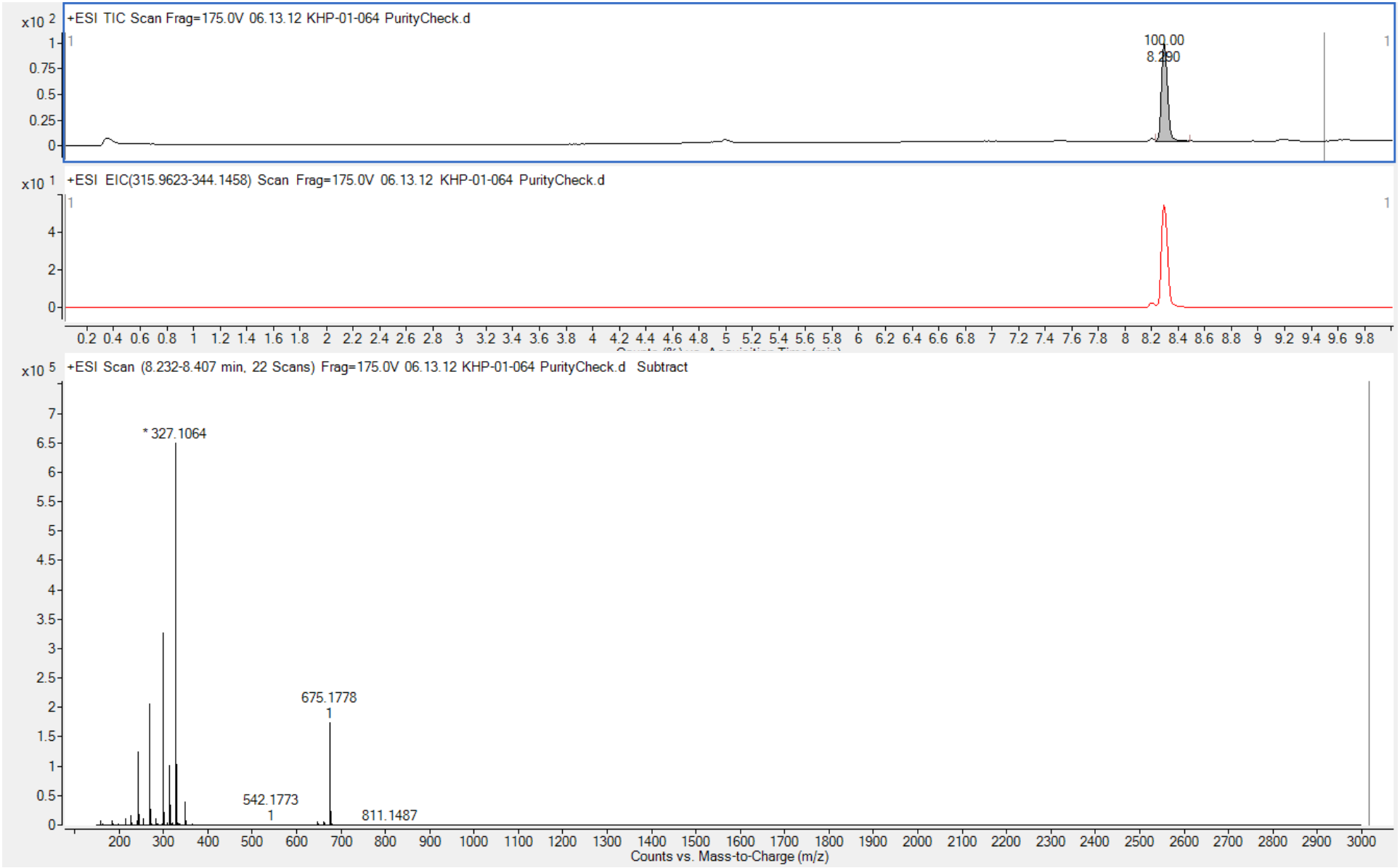
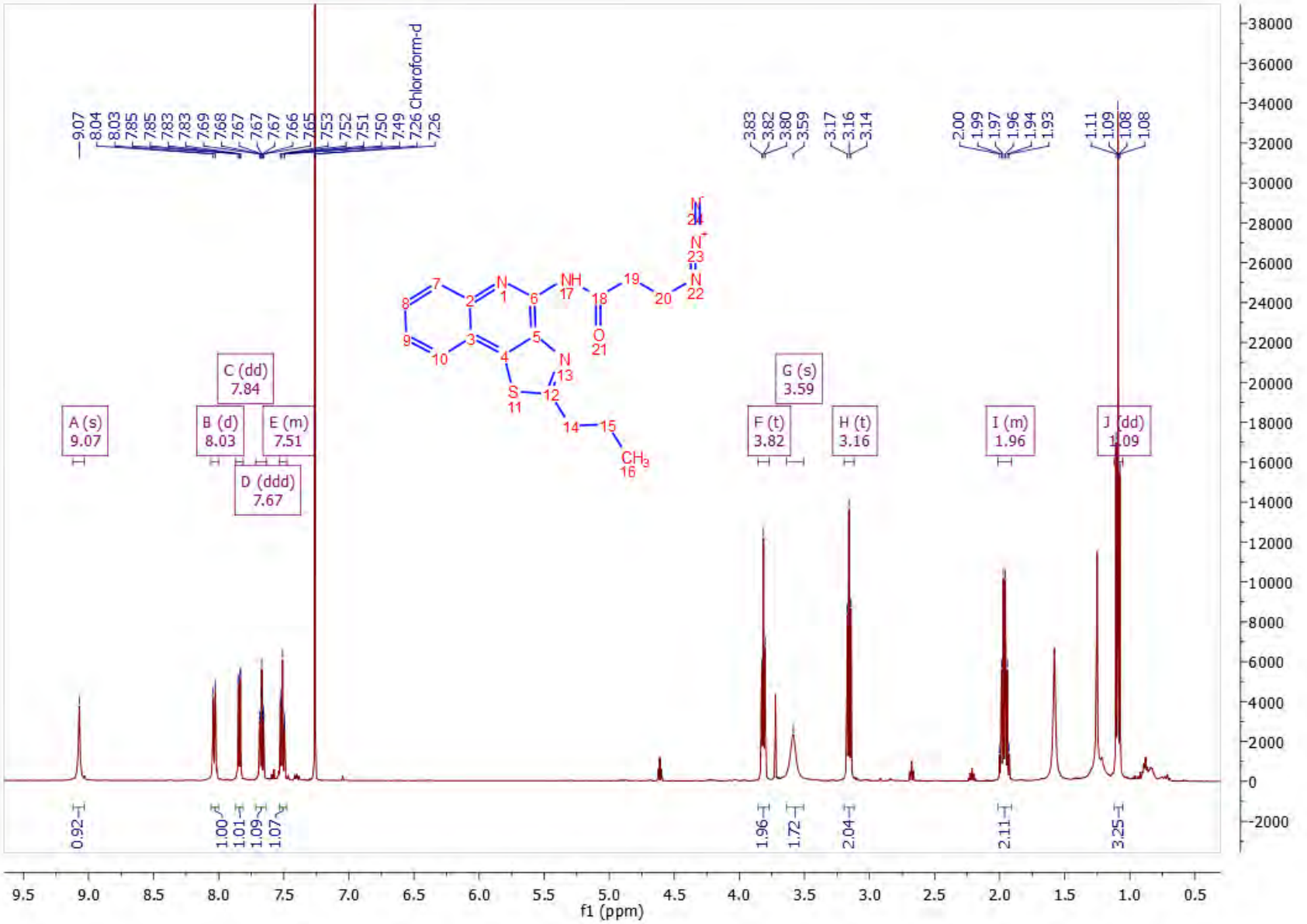
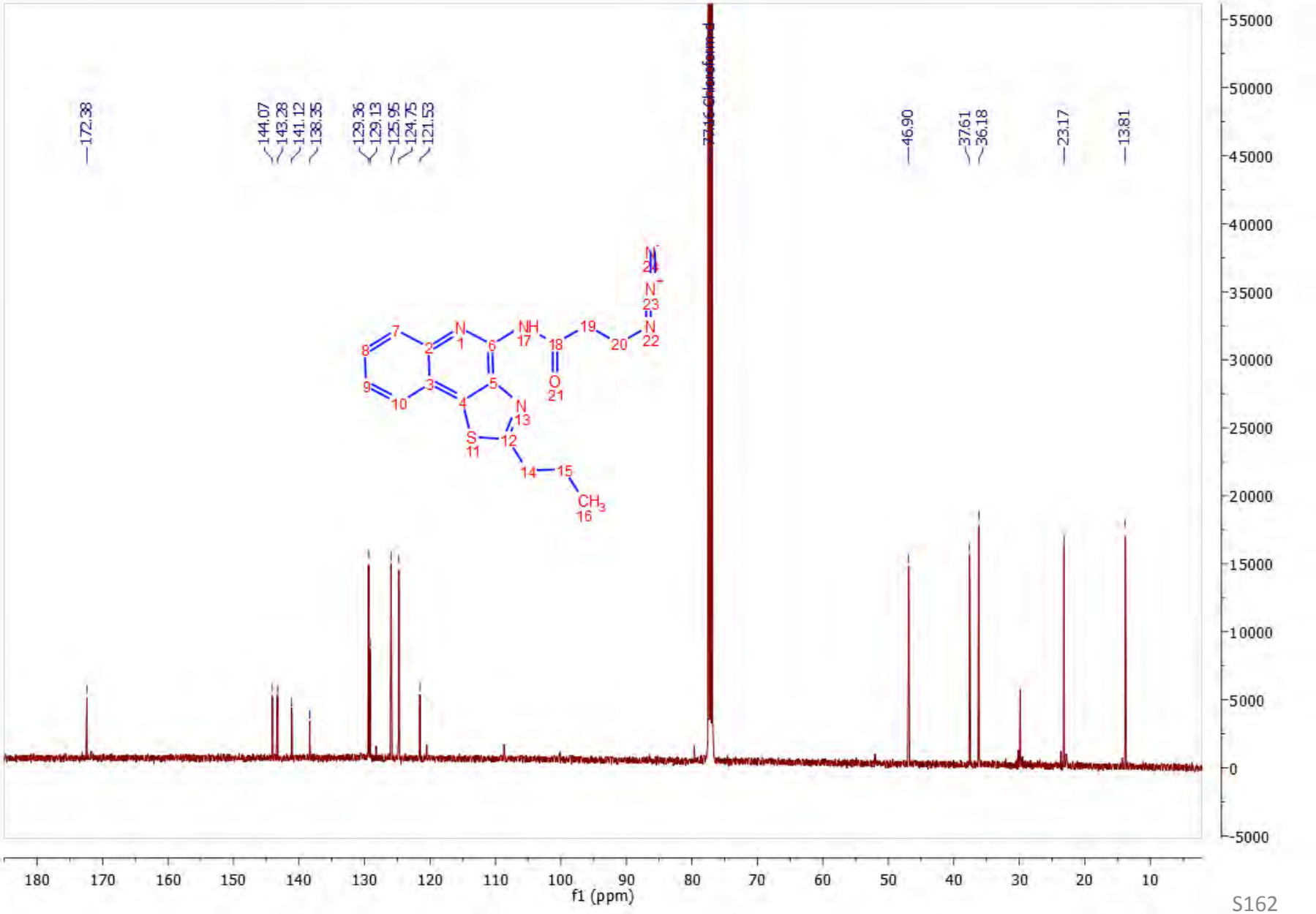


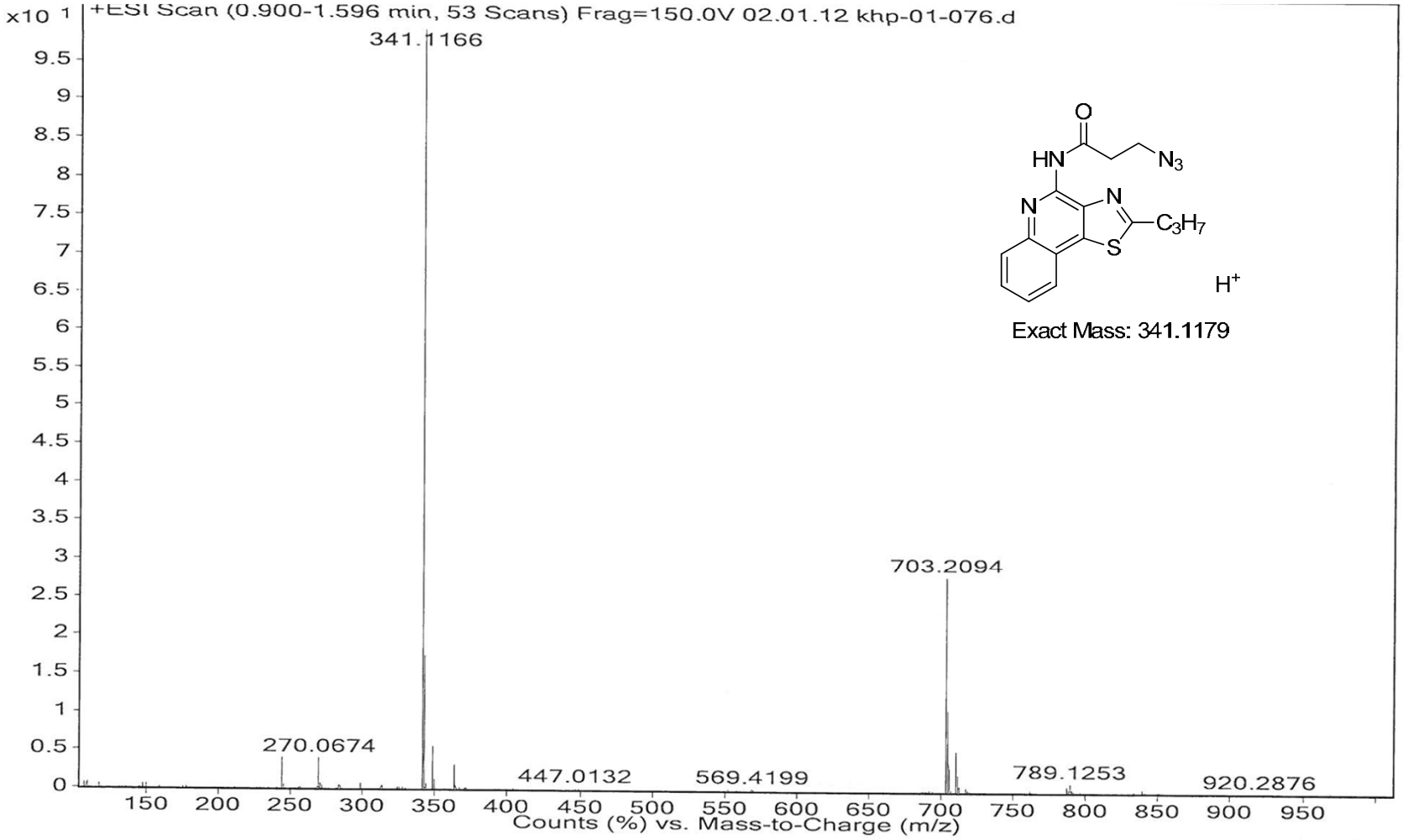
15k ^{1}H NMR



15k ^{13}C NMR



15k MS



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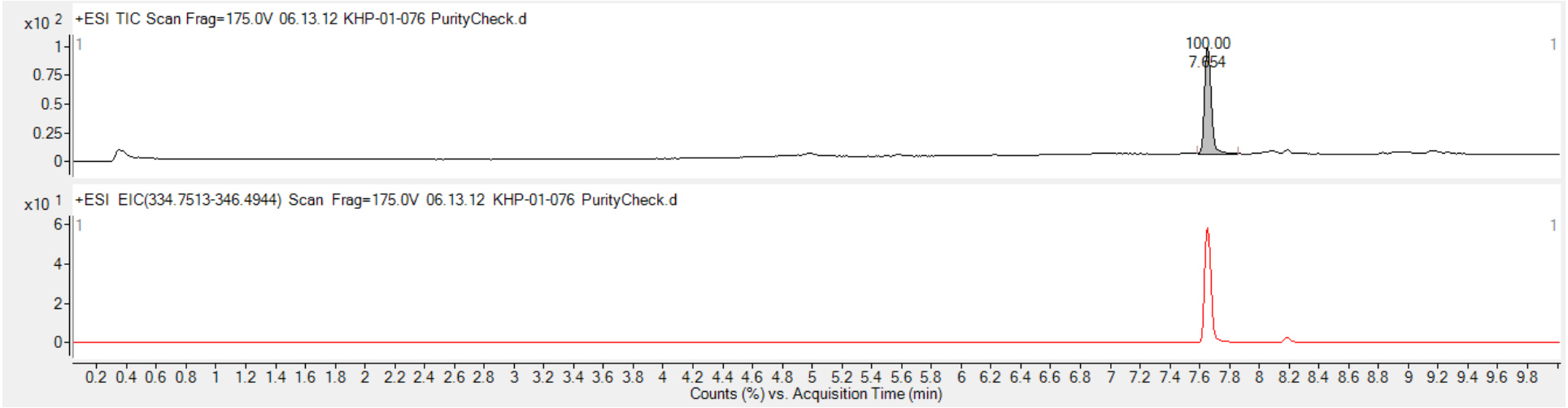
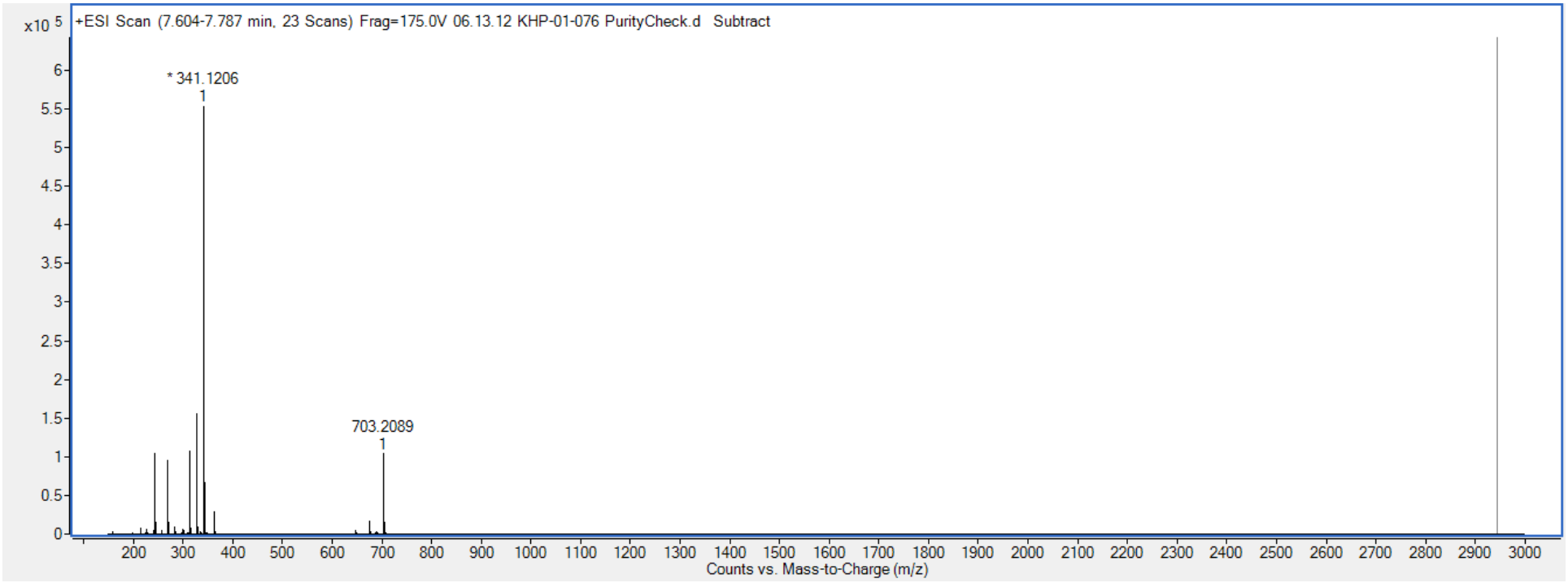
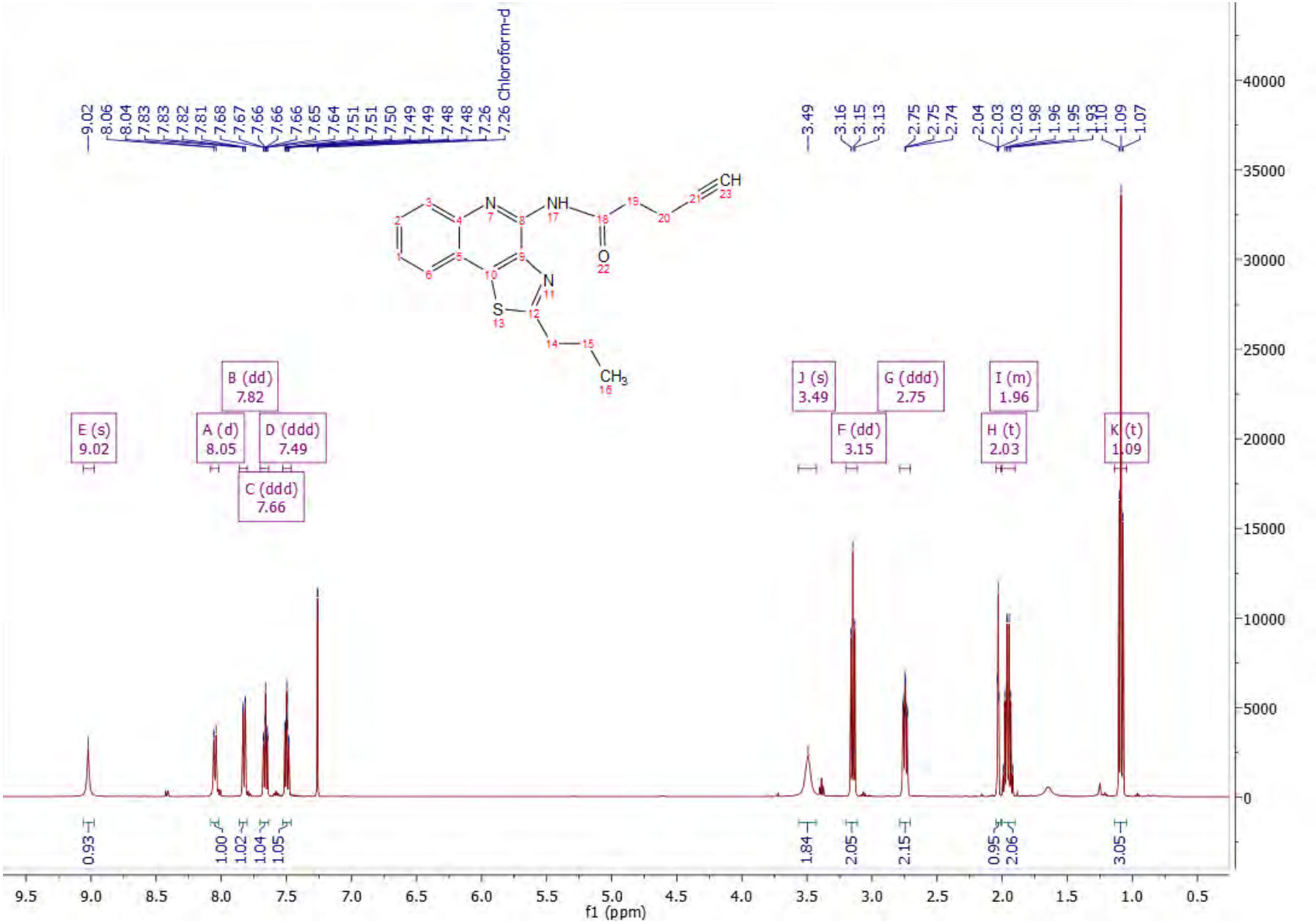
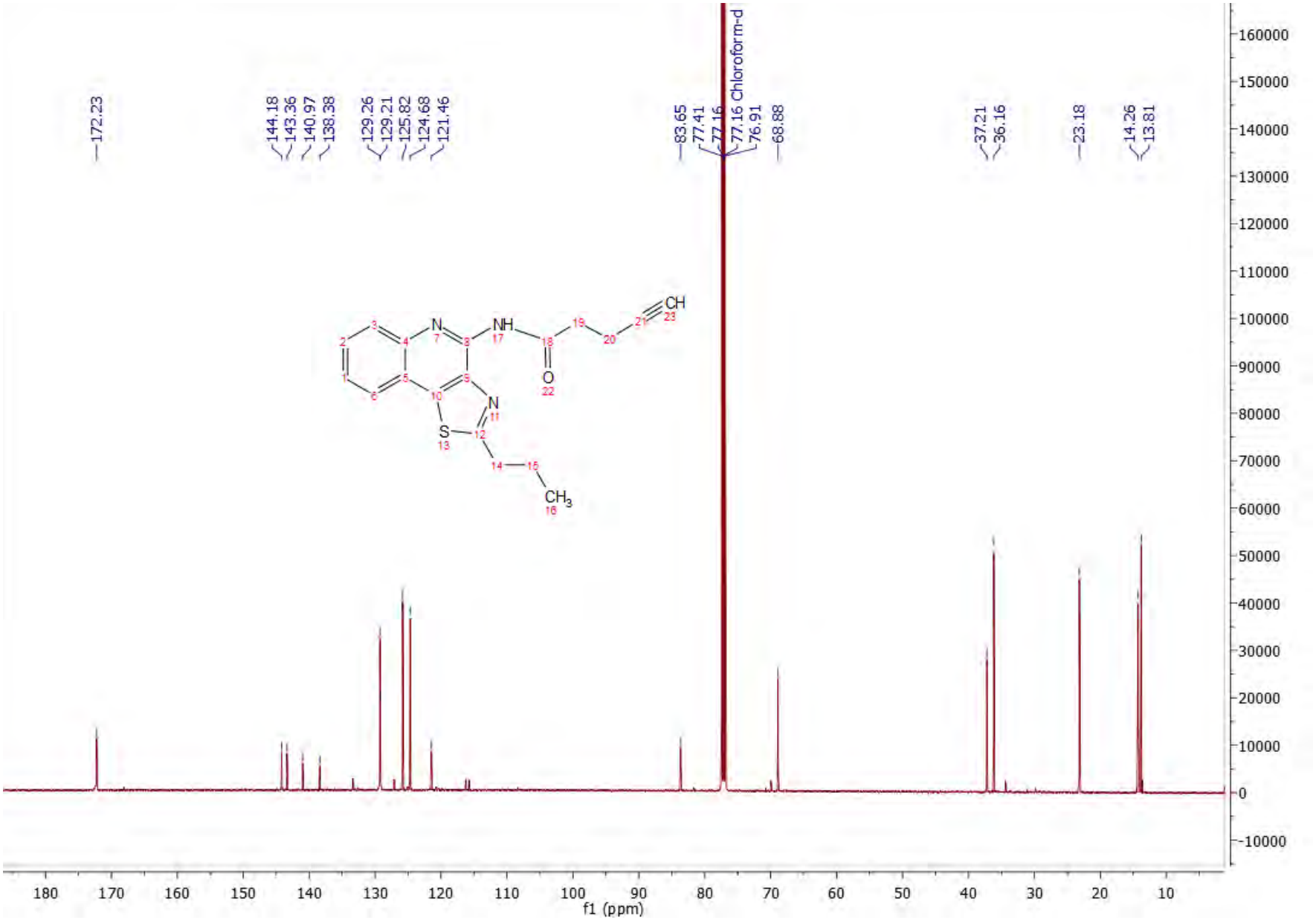




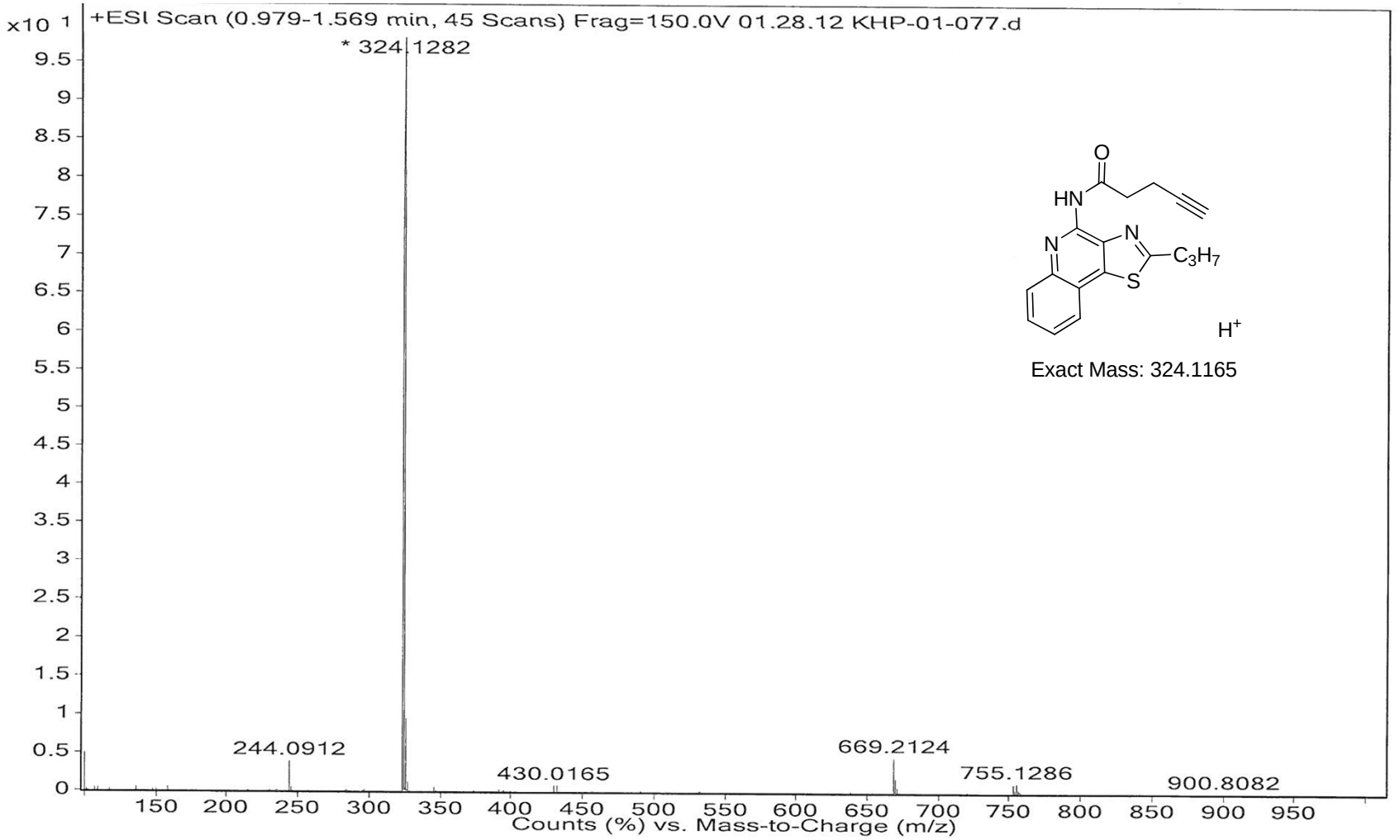
15l ^{1}H NMR



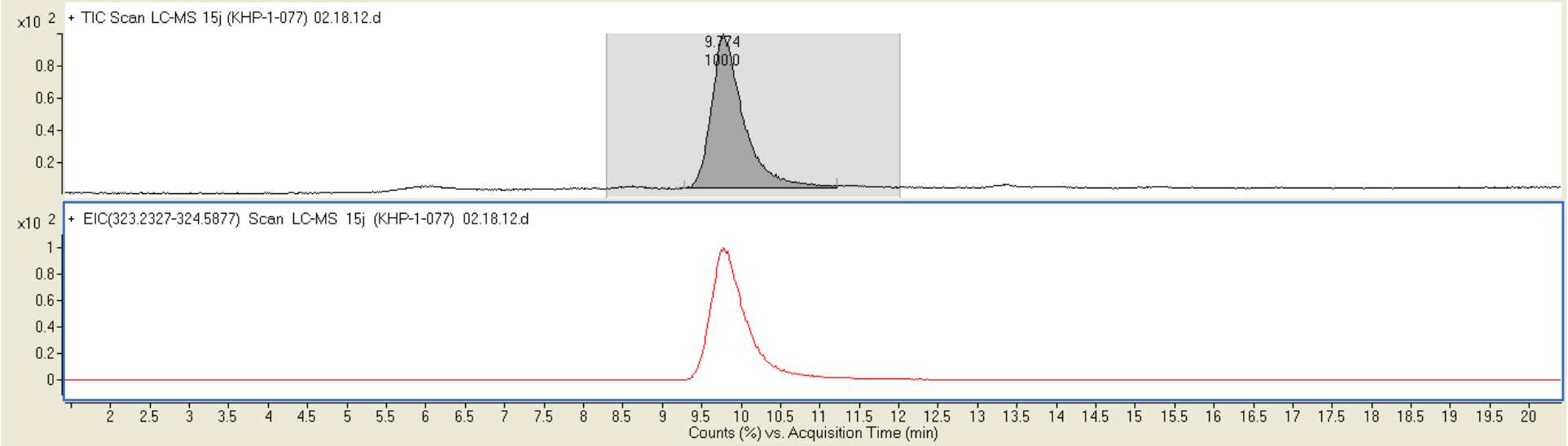
15l ^{13}C NMR

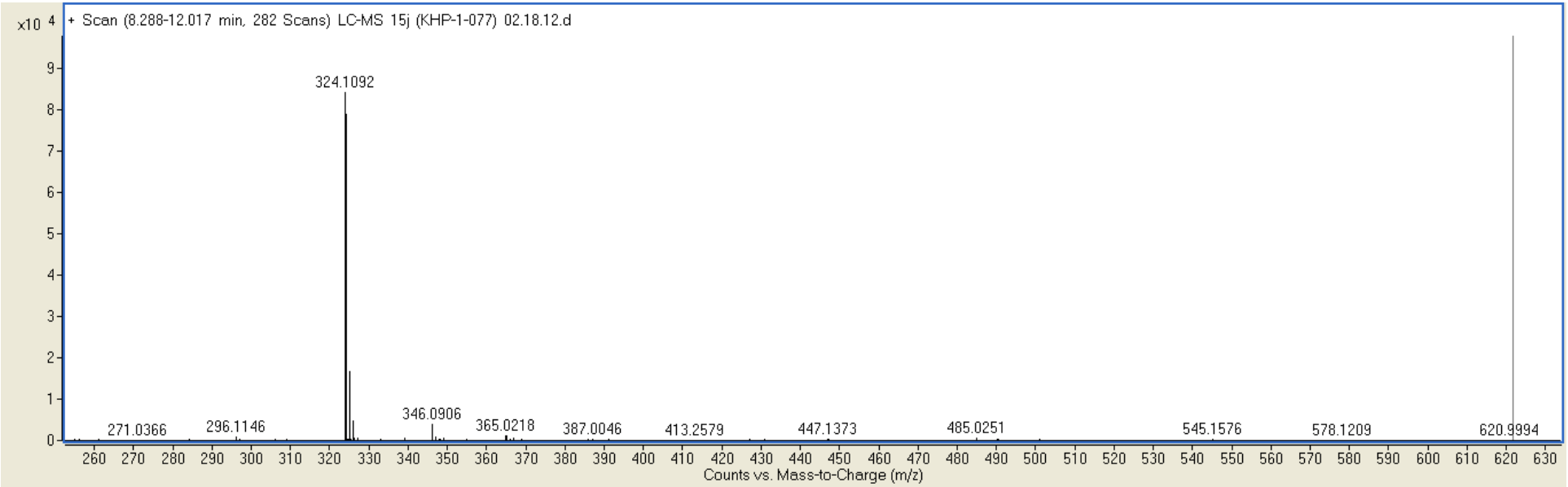


15l MS

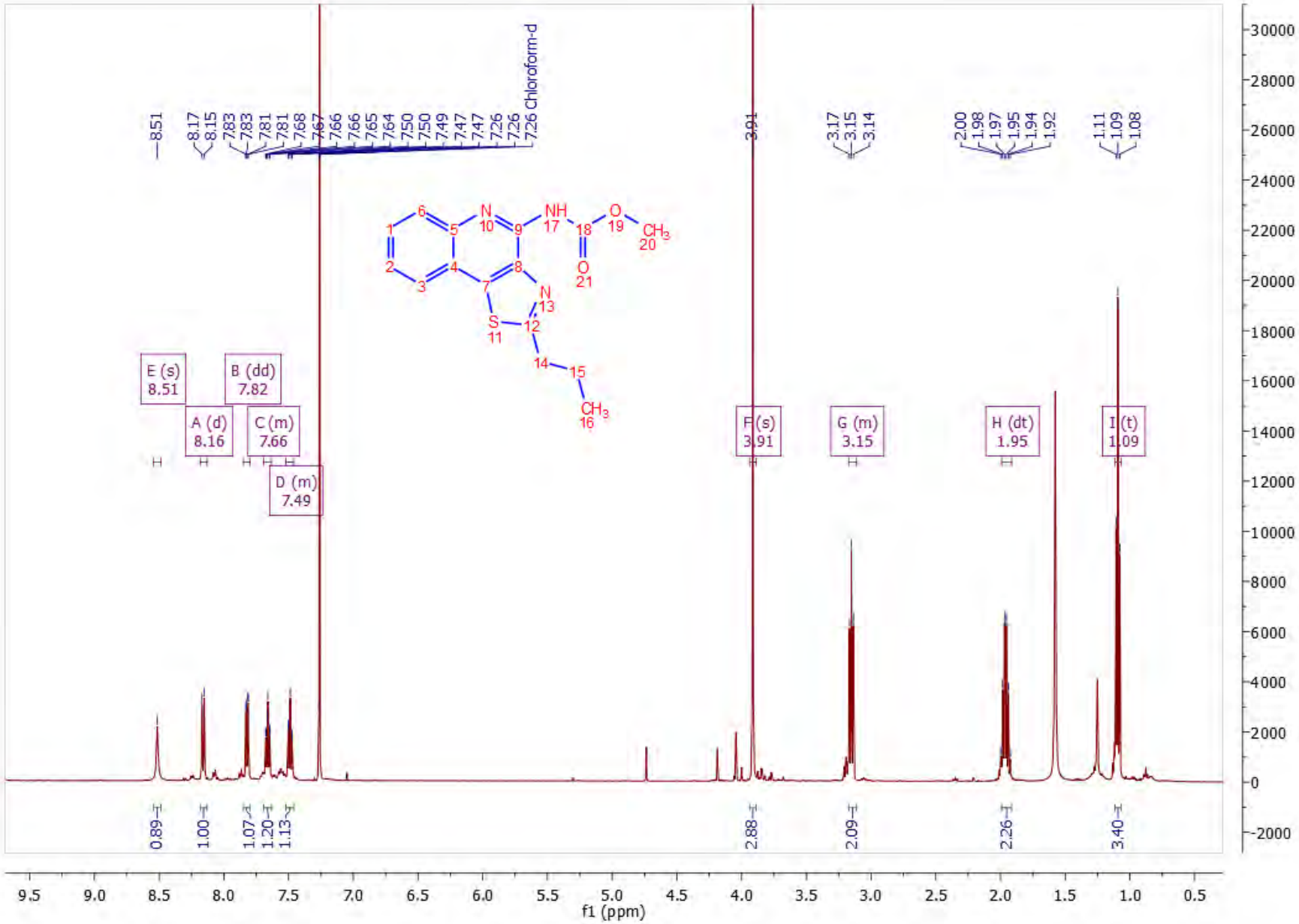


15l LC-MS

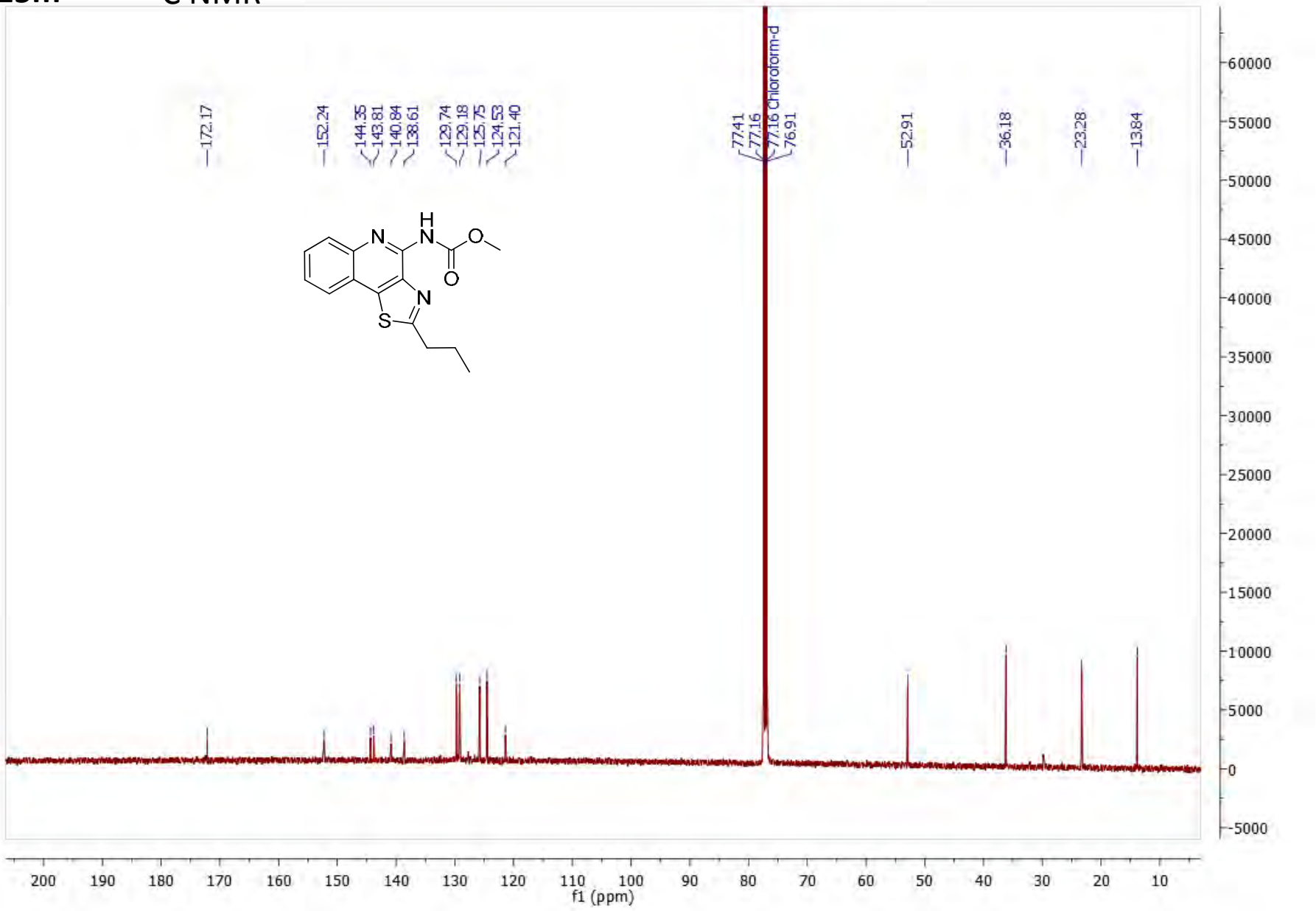




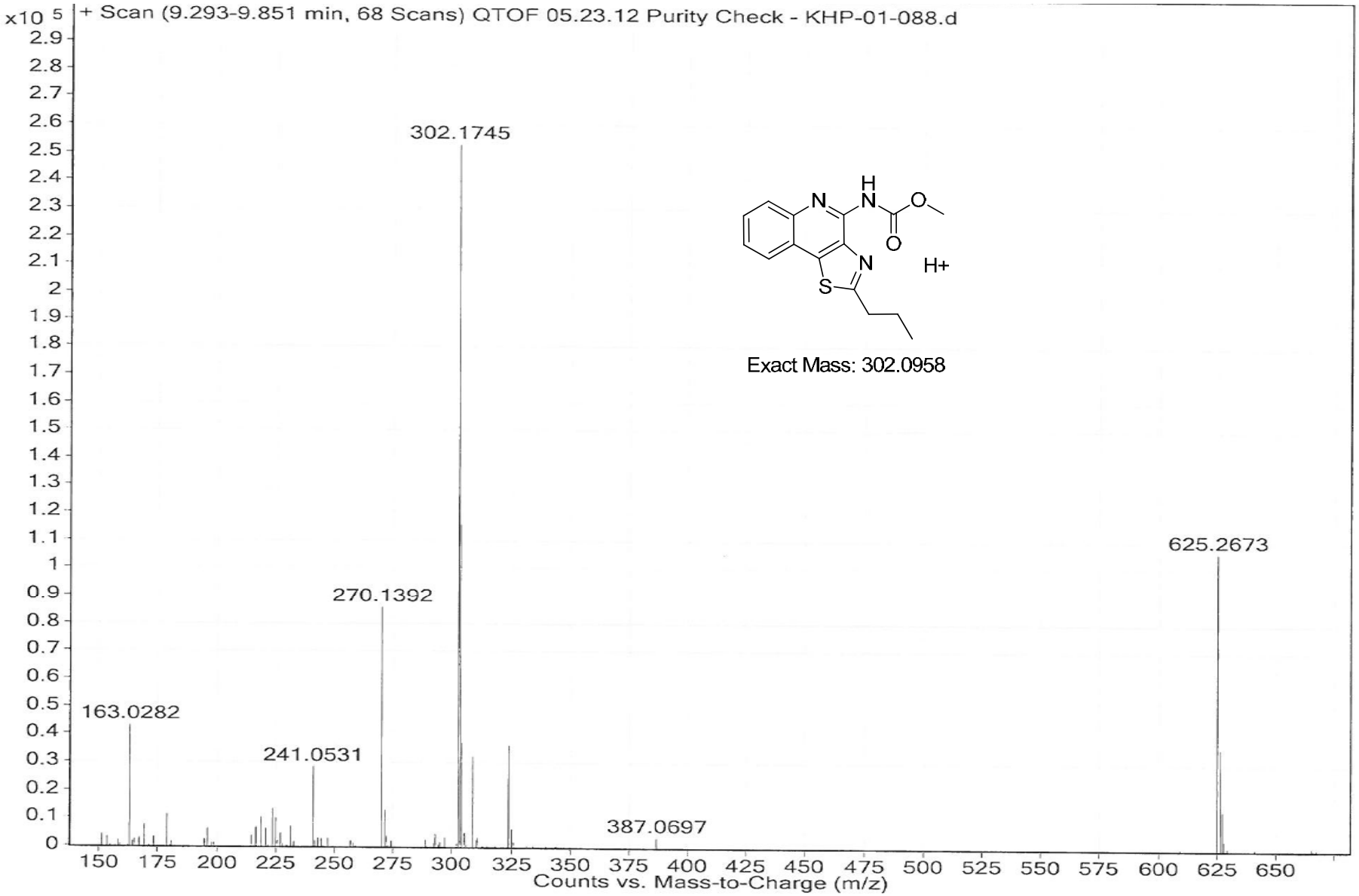
15m ^{1}H NMR



15m ^{13}C NMR



15m MS



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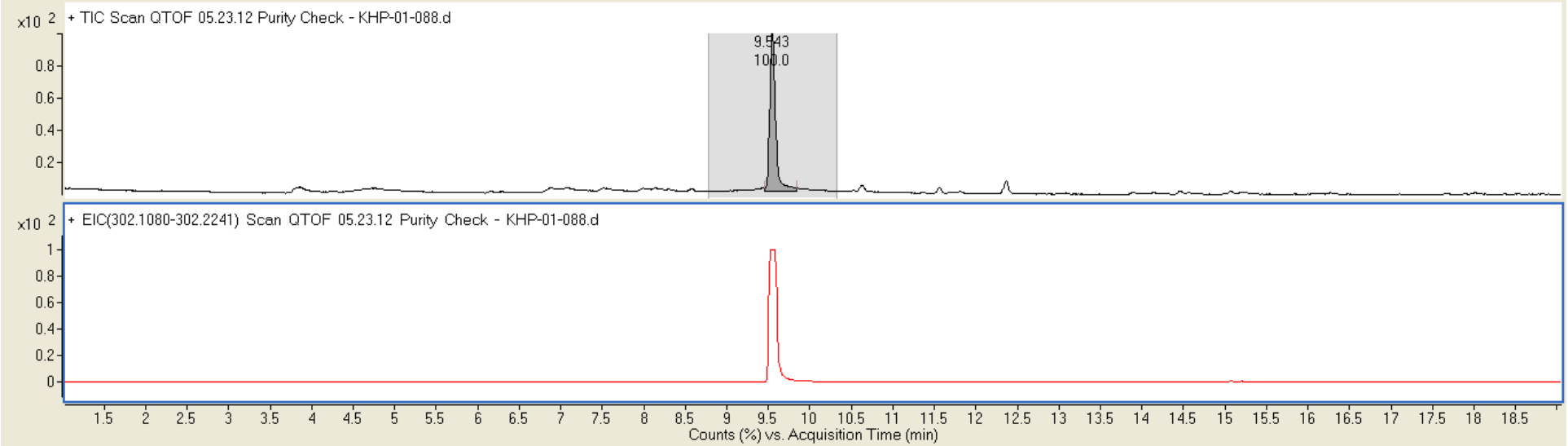
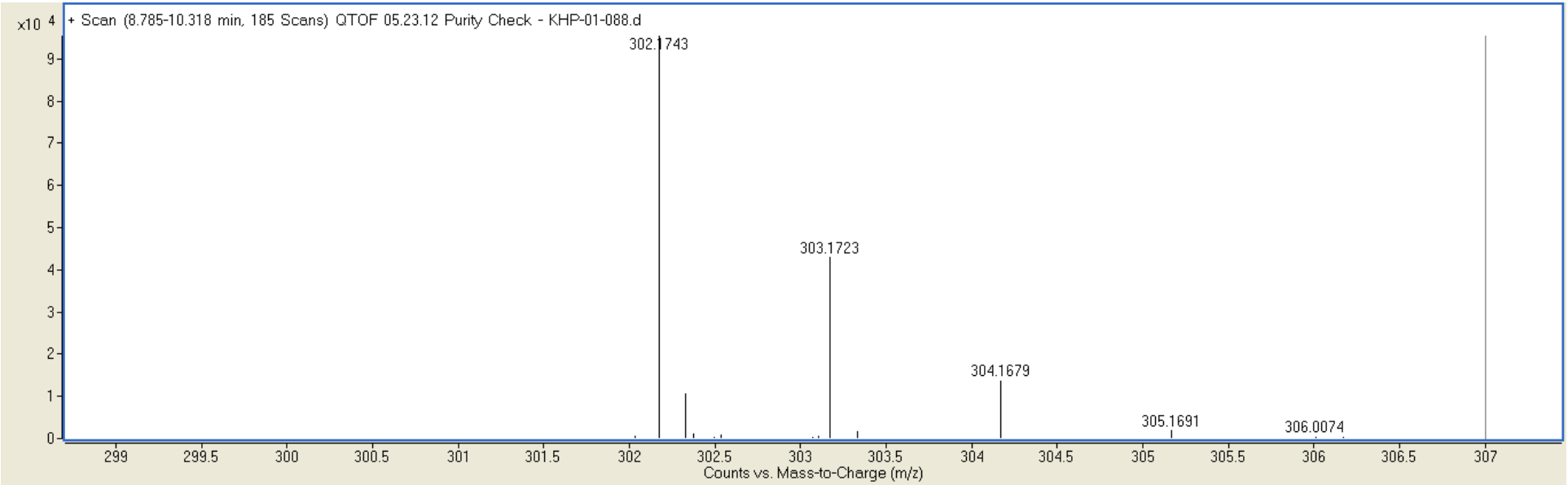
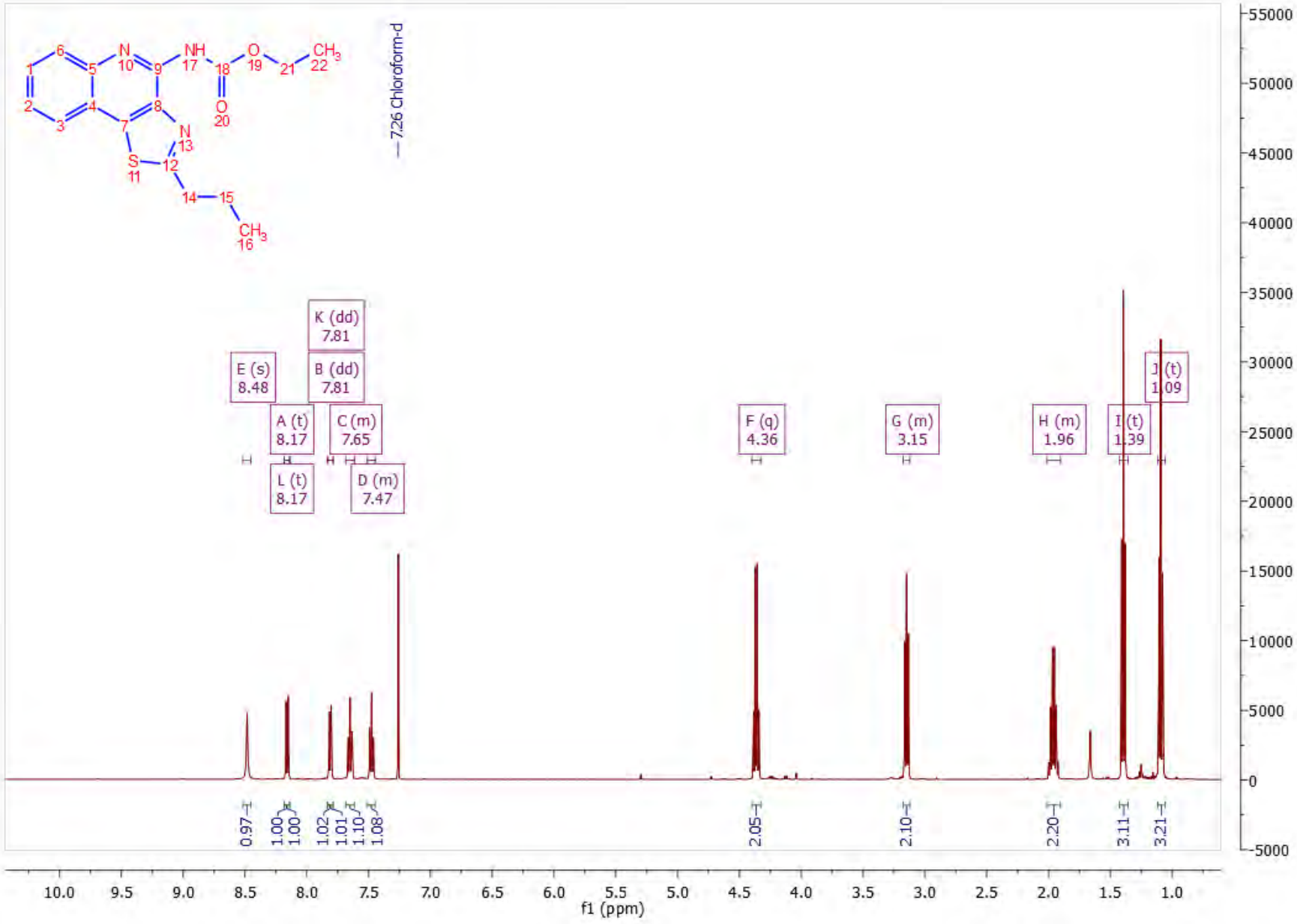
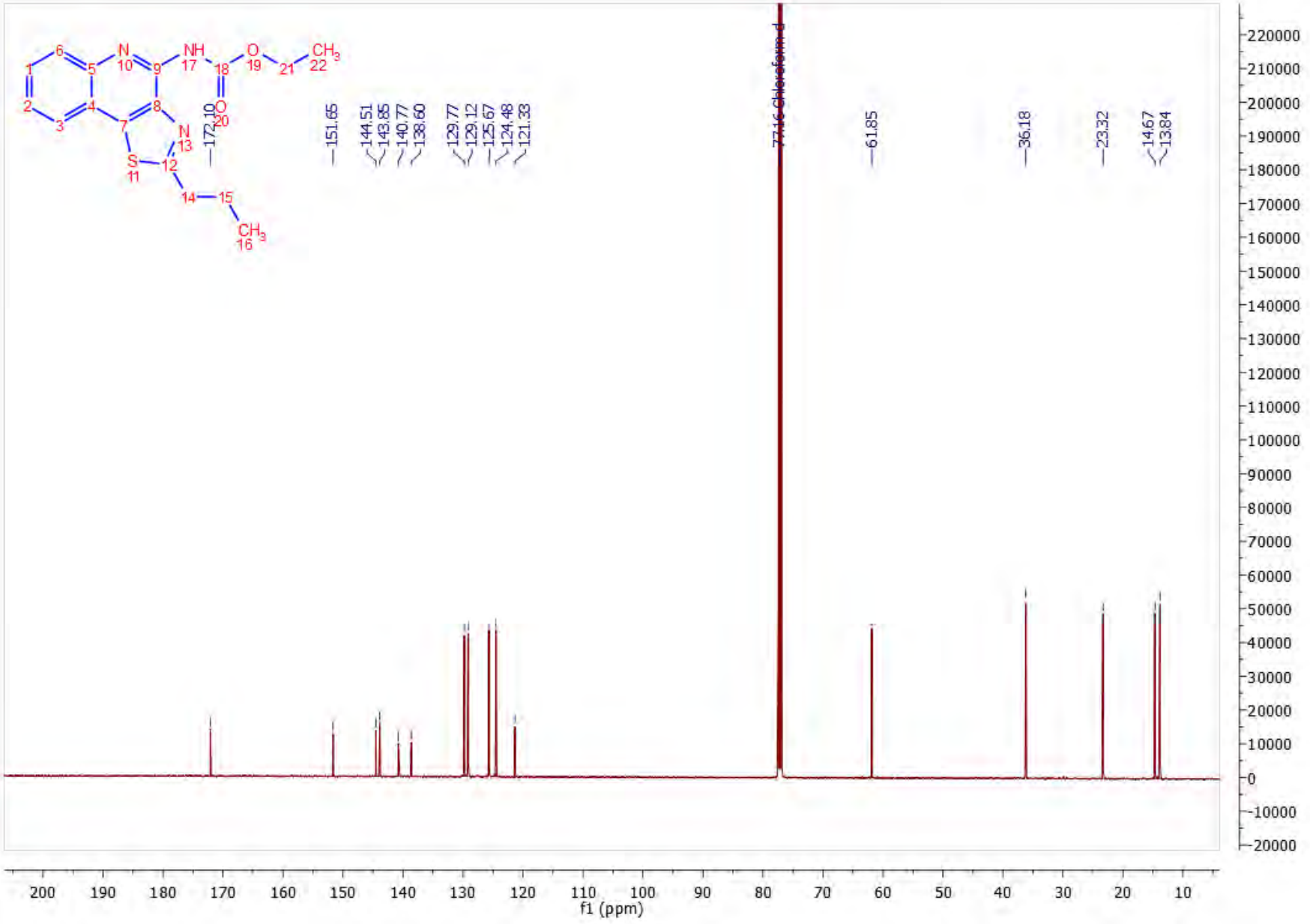




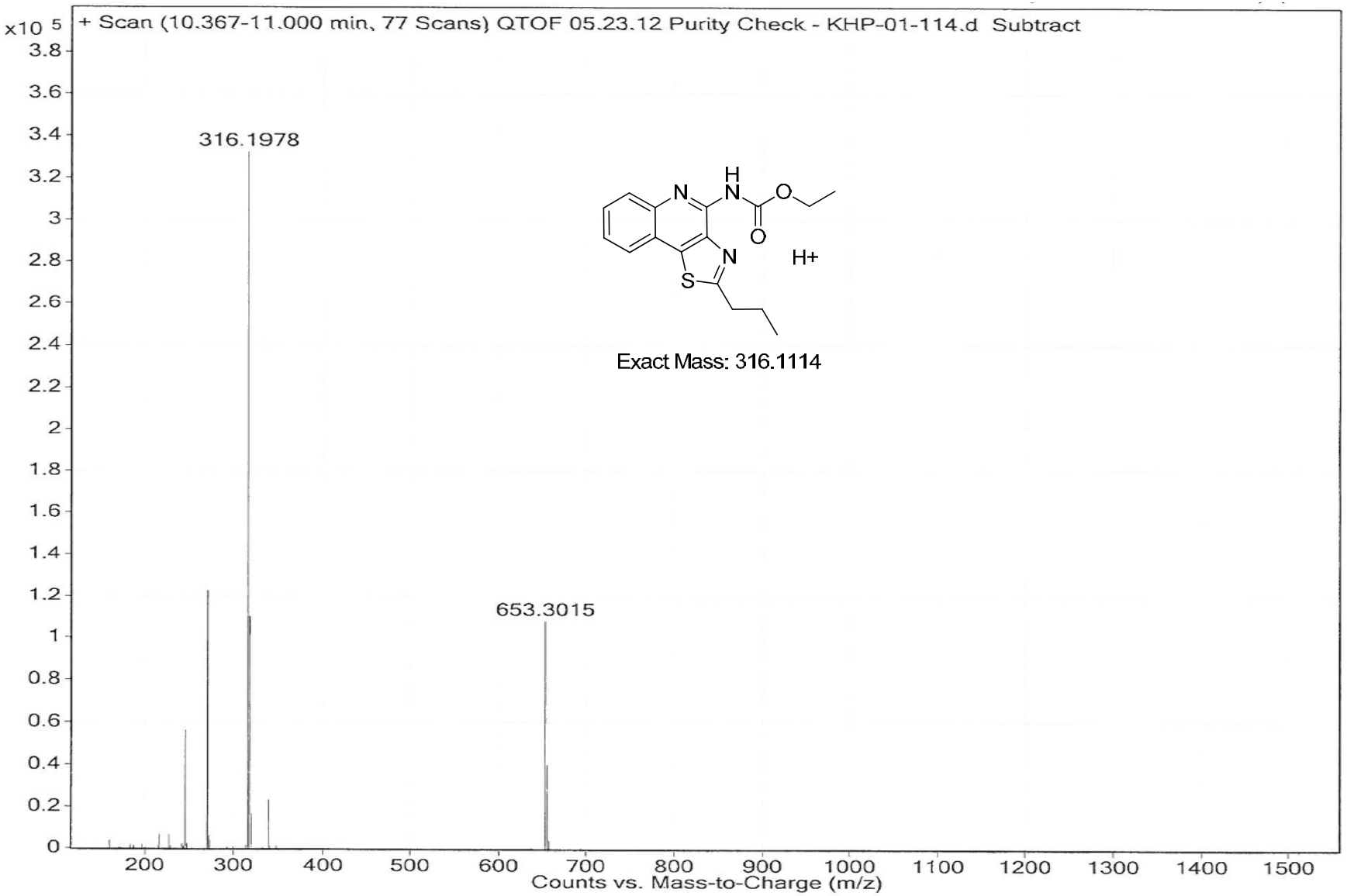
15n ^{1}H NMR



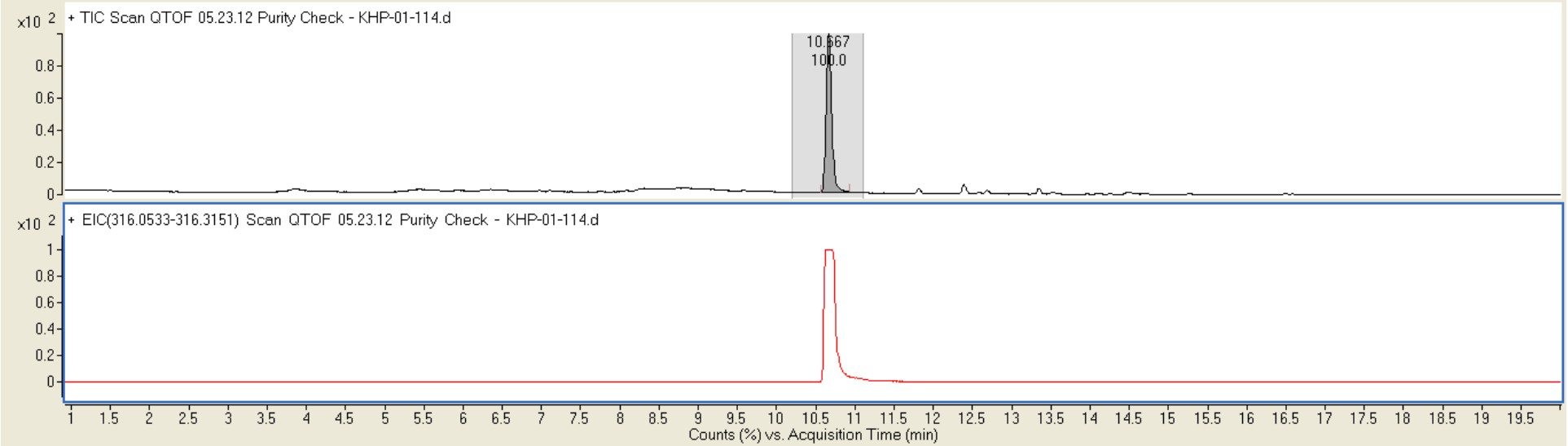
15n ^{13}C NMR

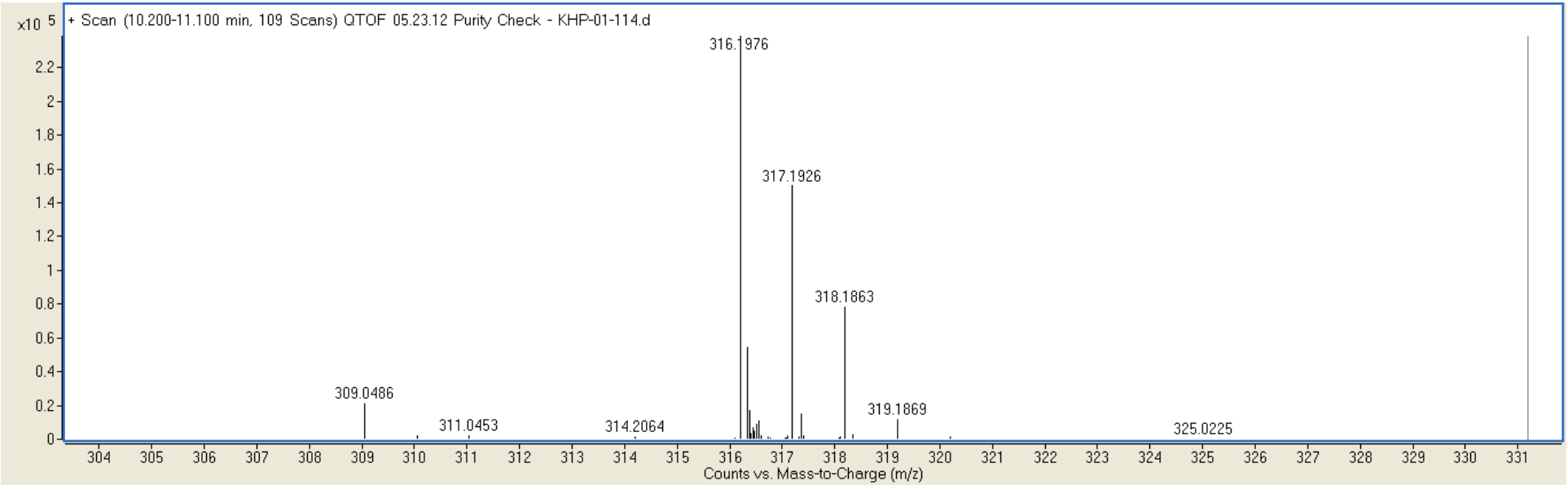


15n MS

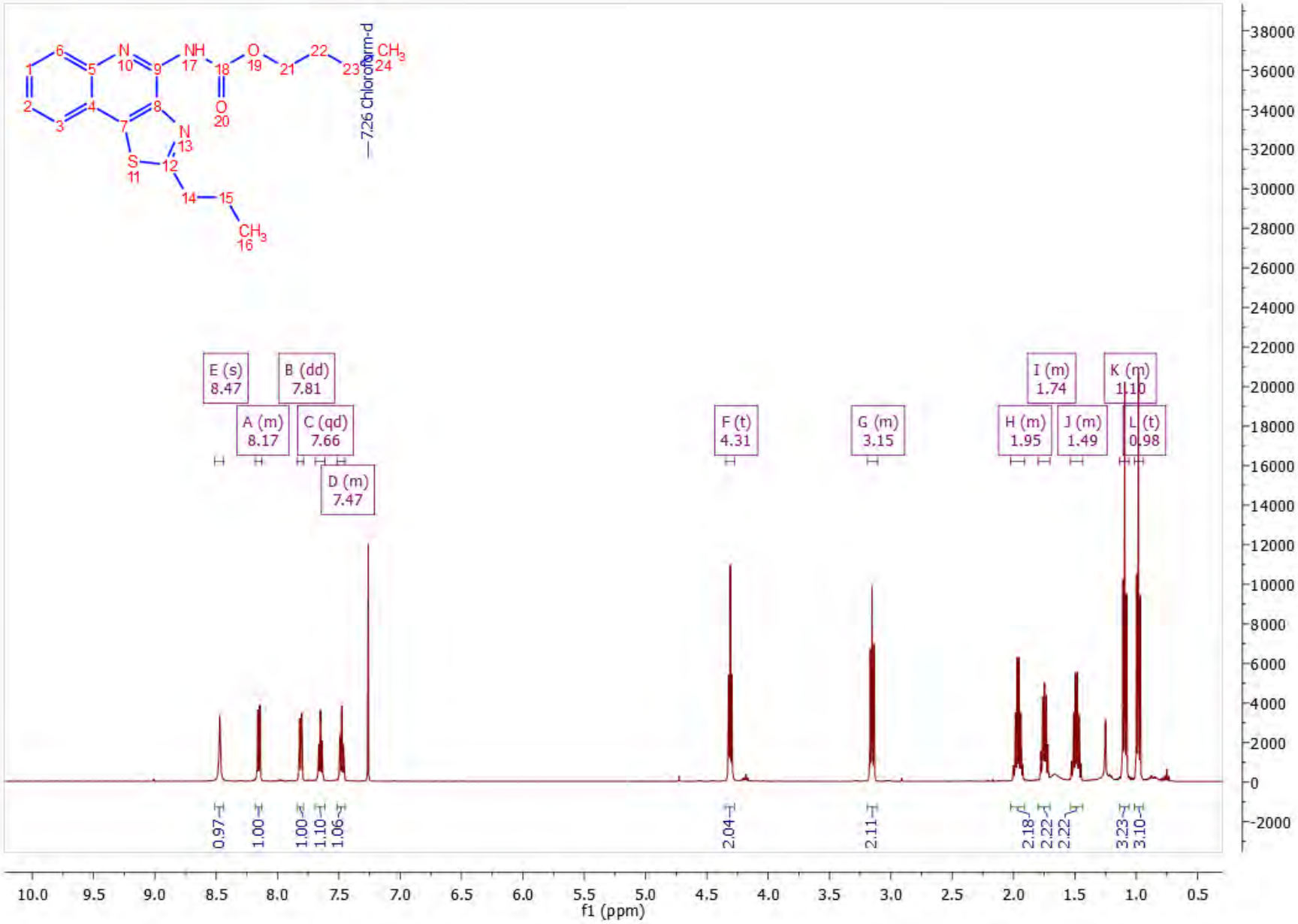


15n LC-MS

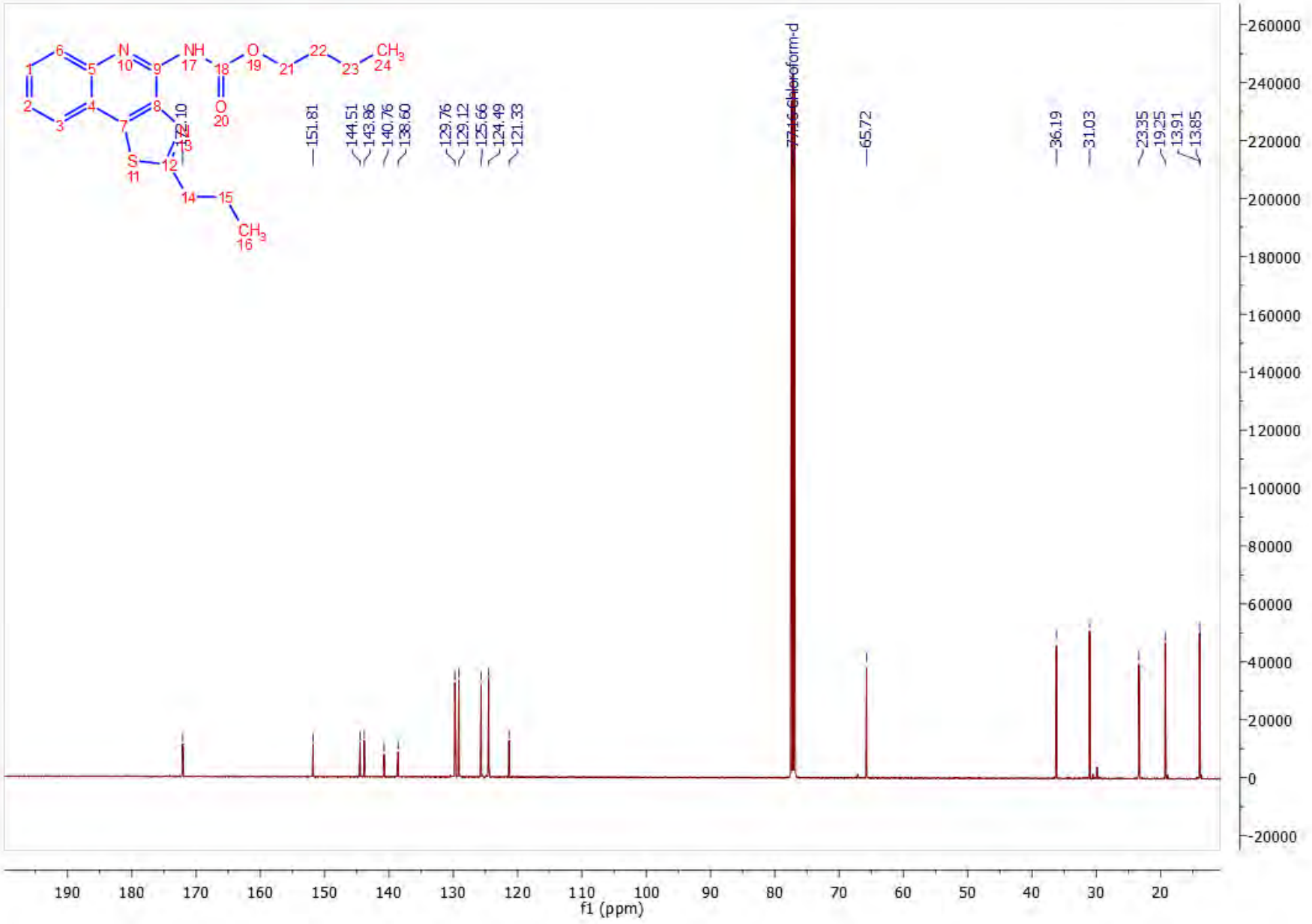




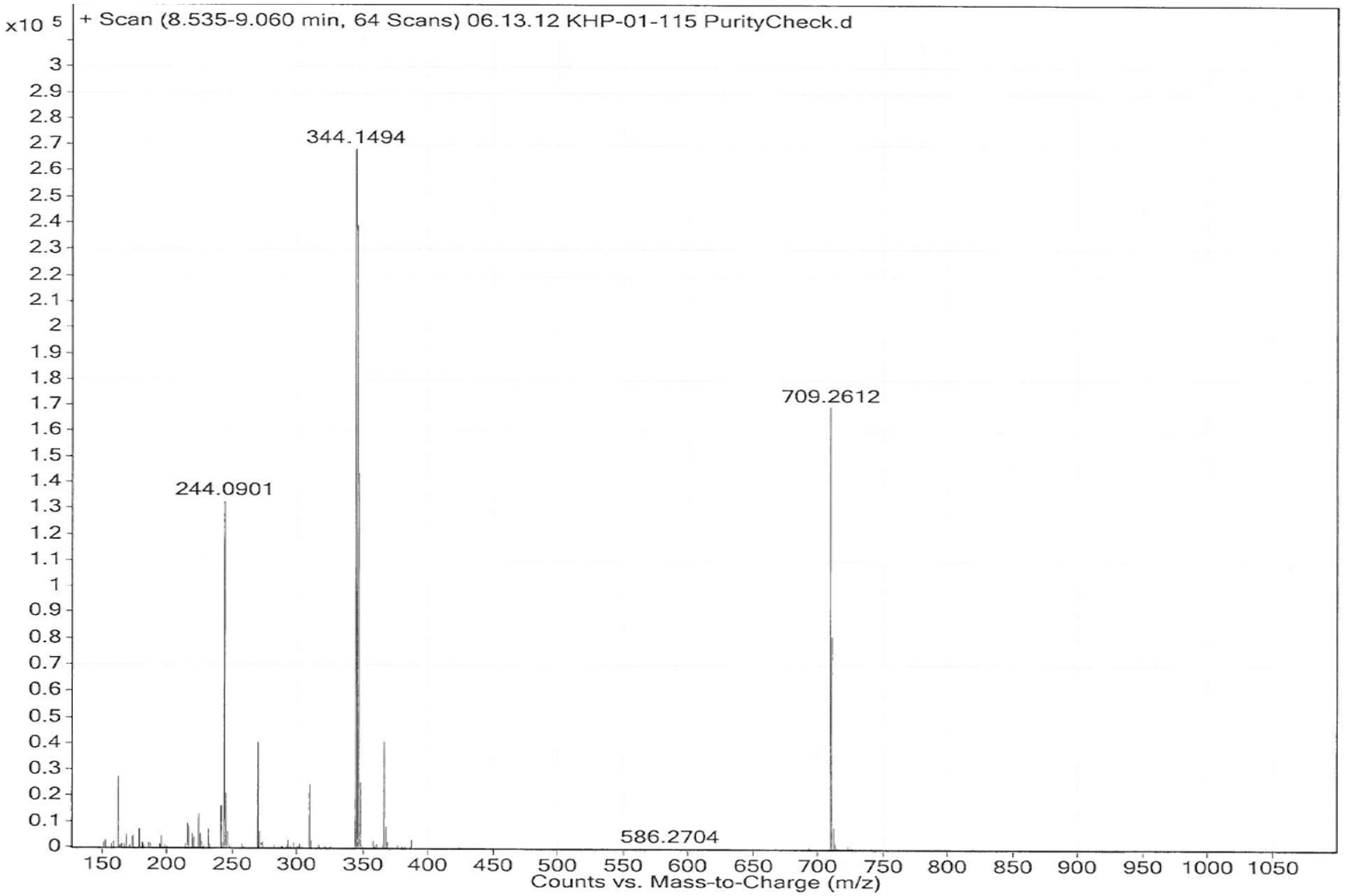
15o ^{1}H NMR



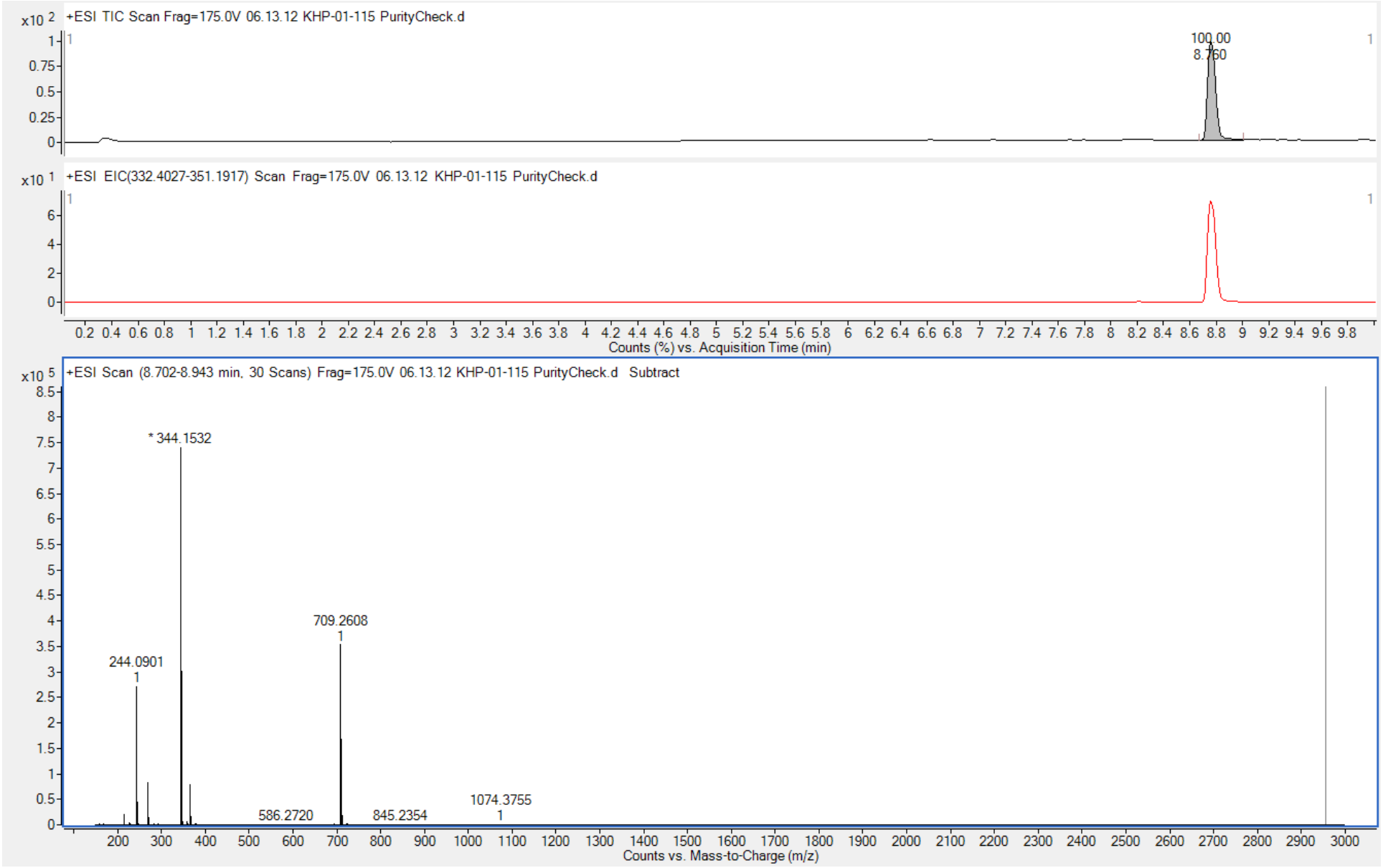
15o ^{13}C NMR



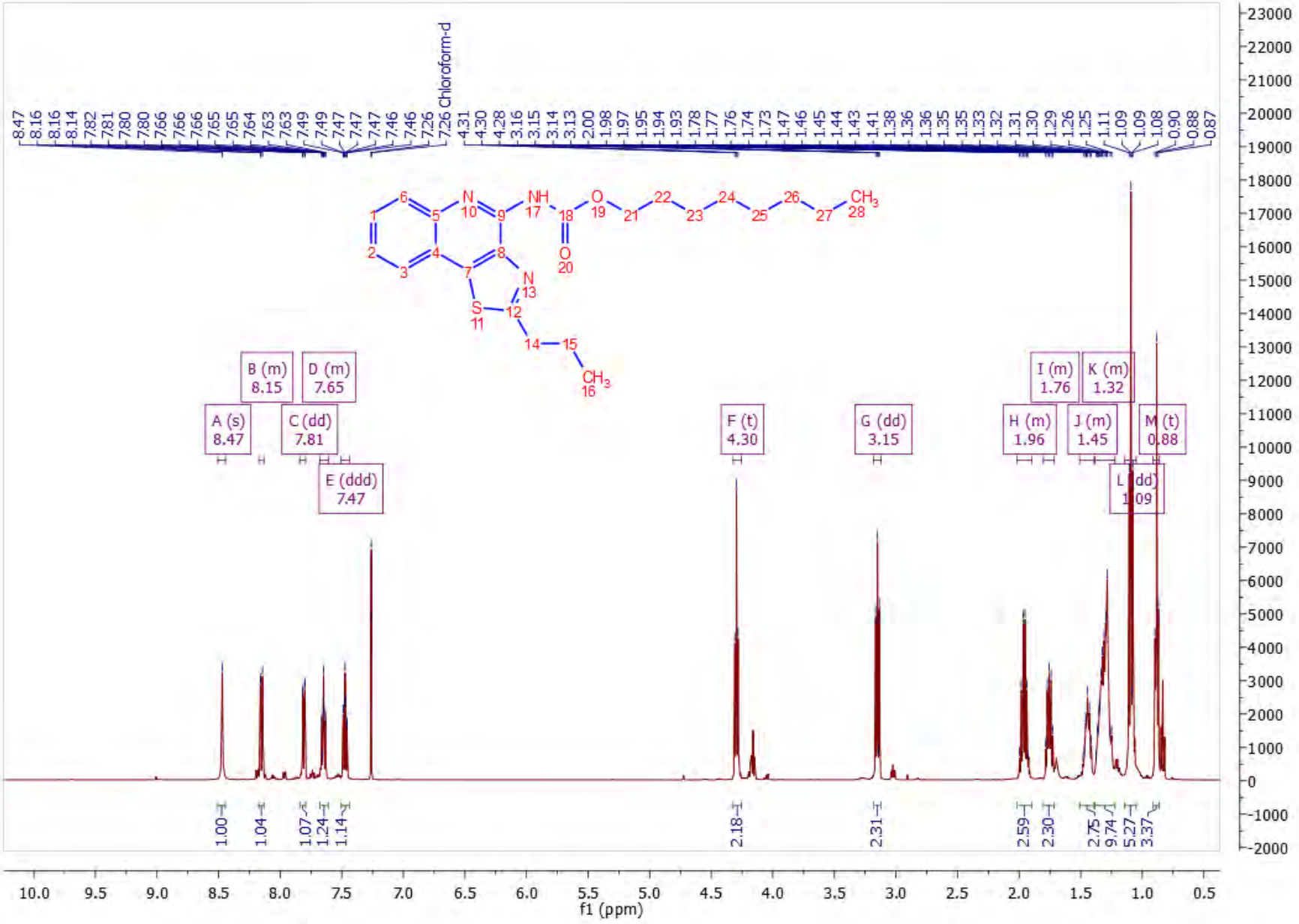
15o MS



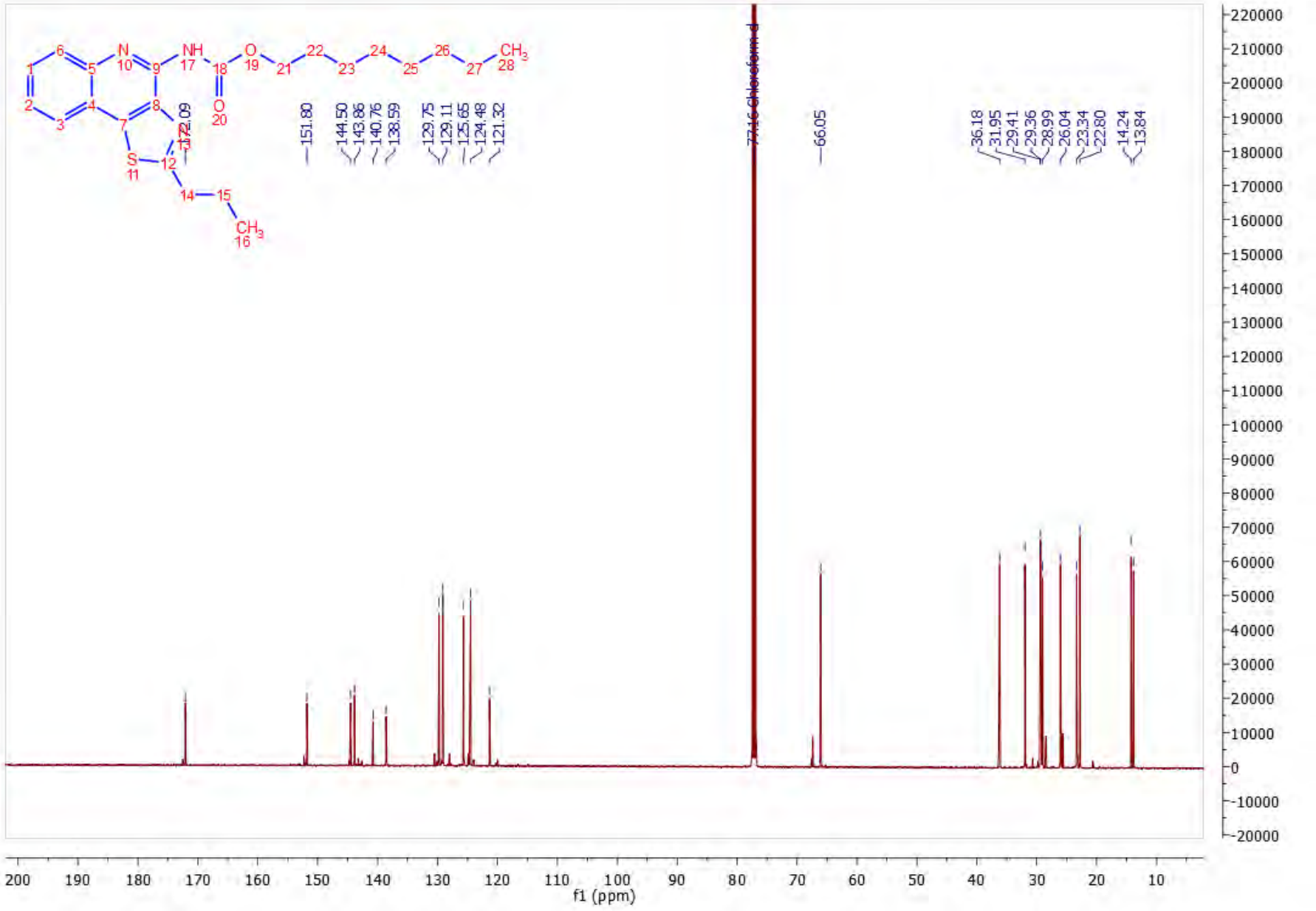
15o LC-MS



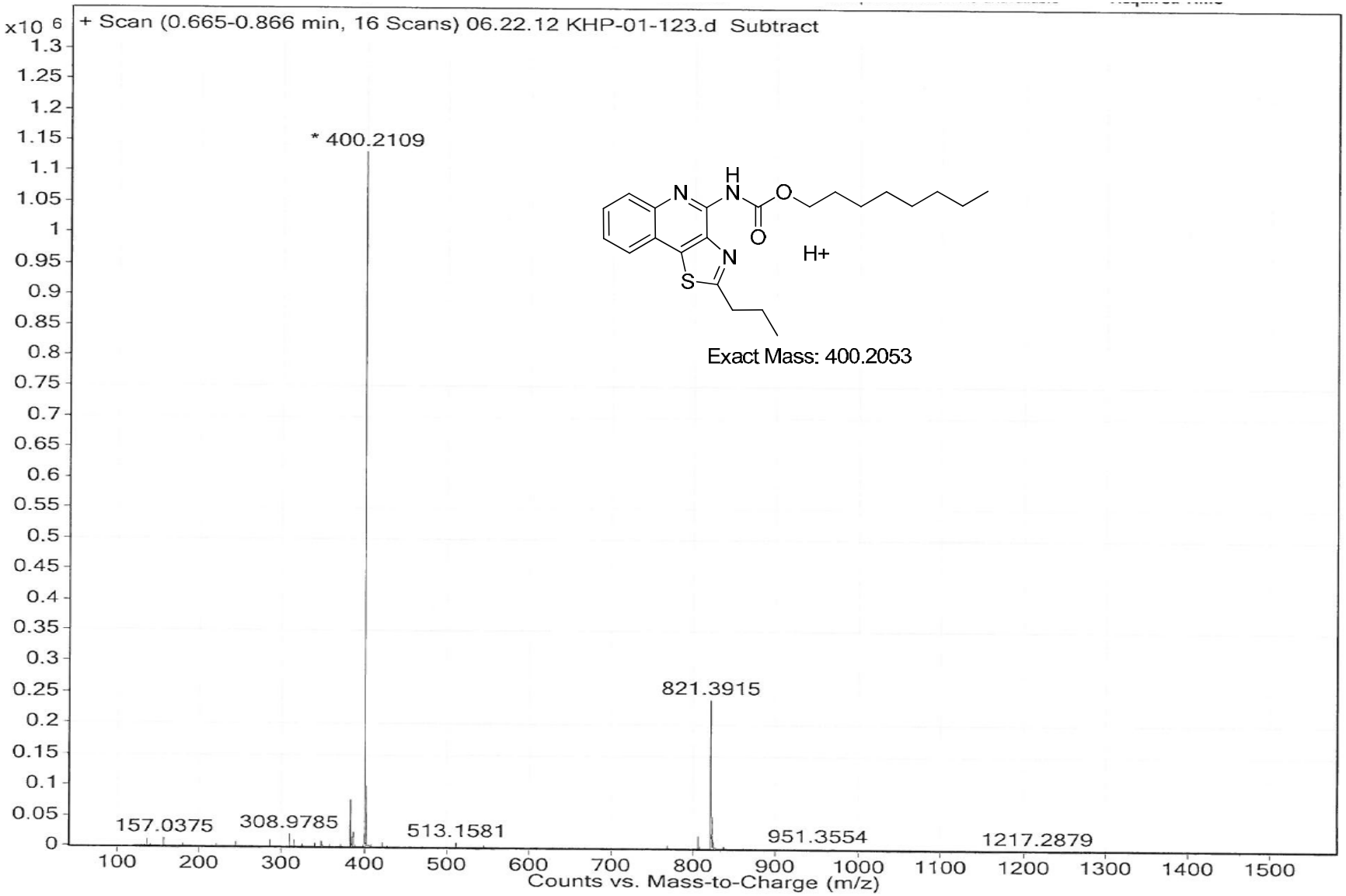
15p ^{1}H NMR



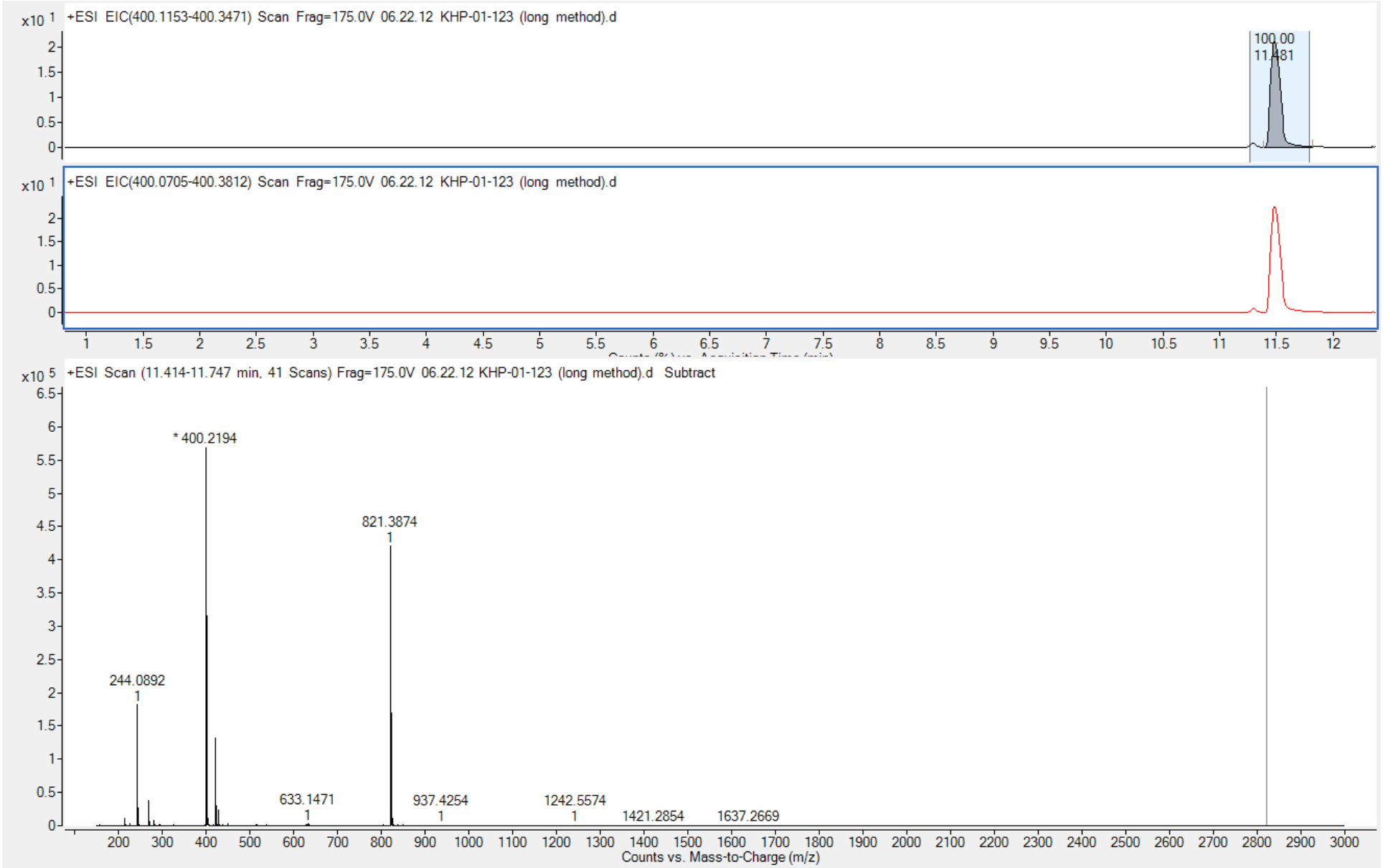
15p ^{13}C NMR



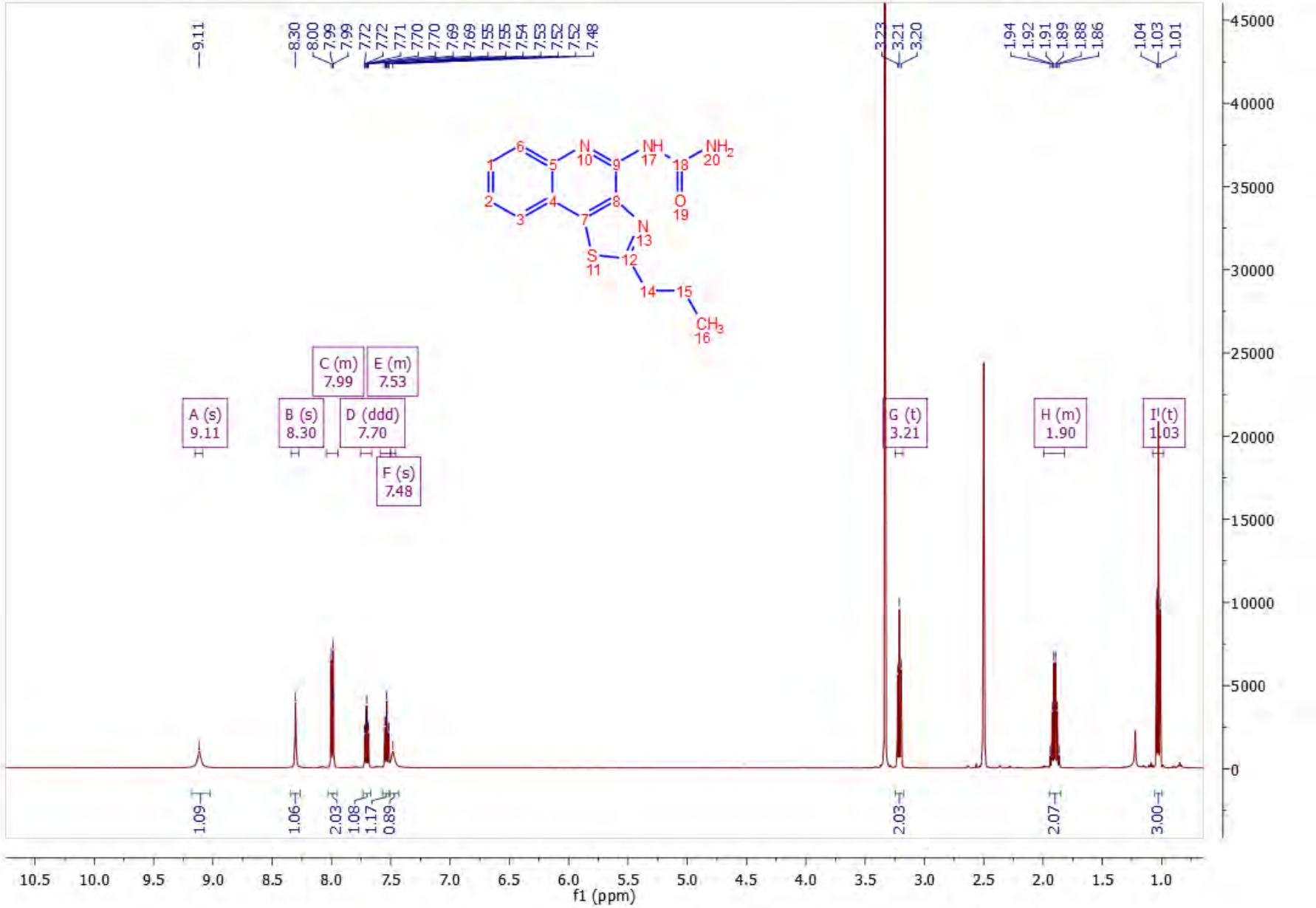
15p MS



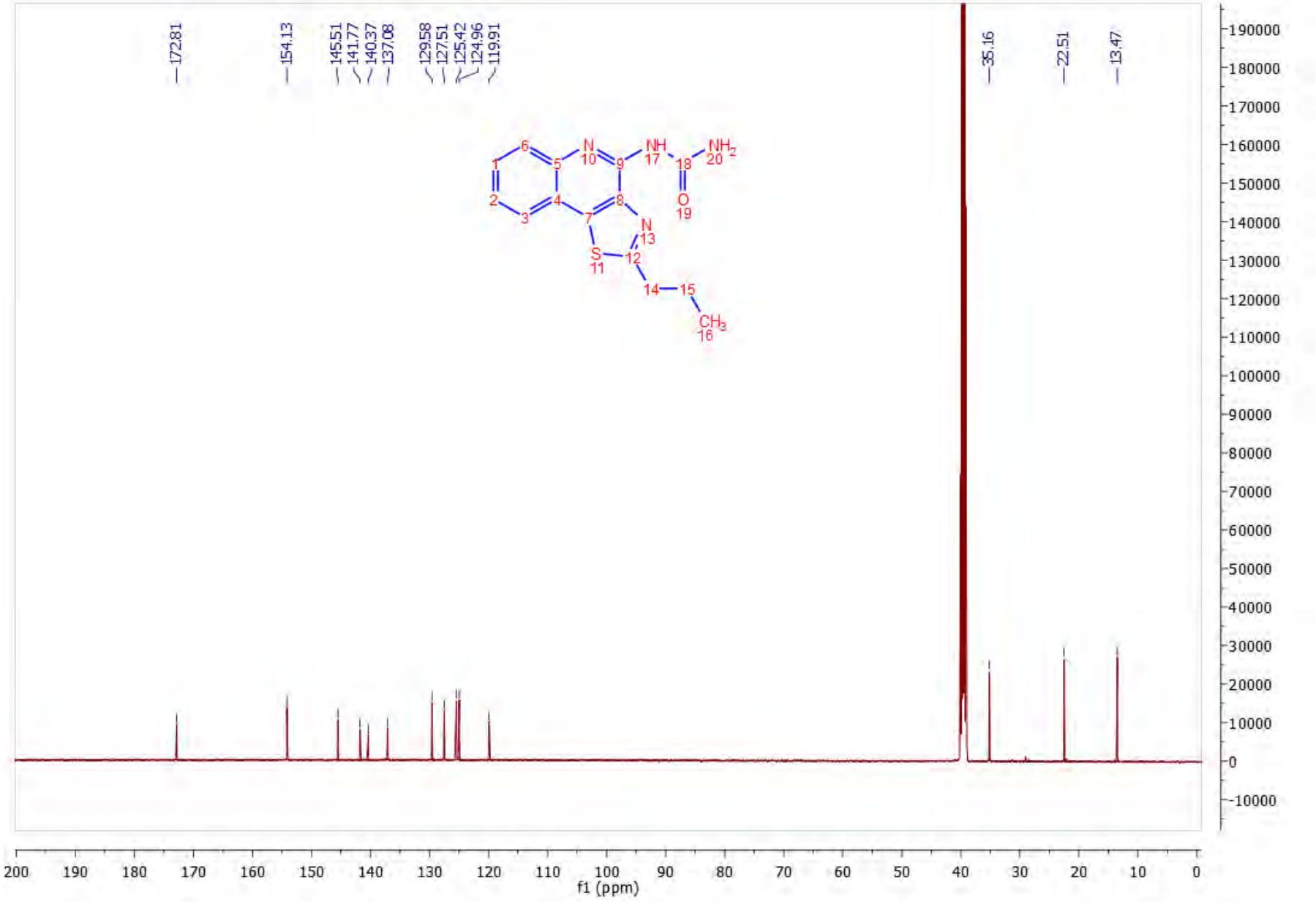
15p LC-MS



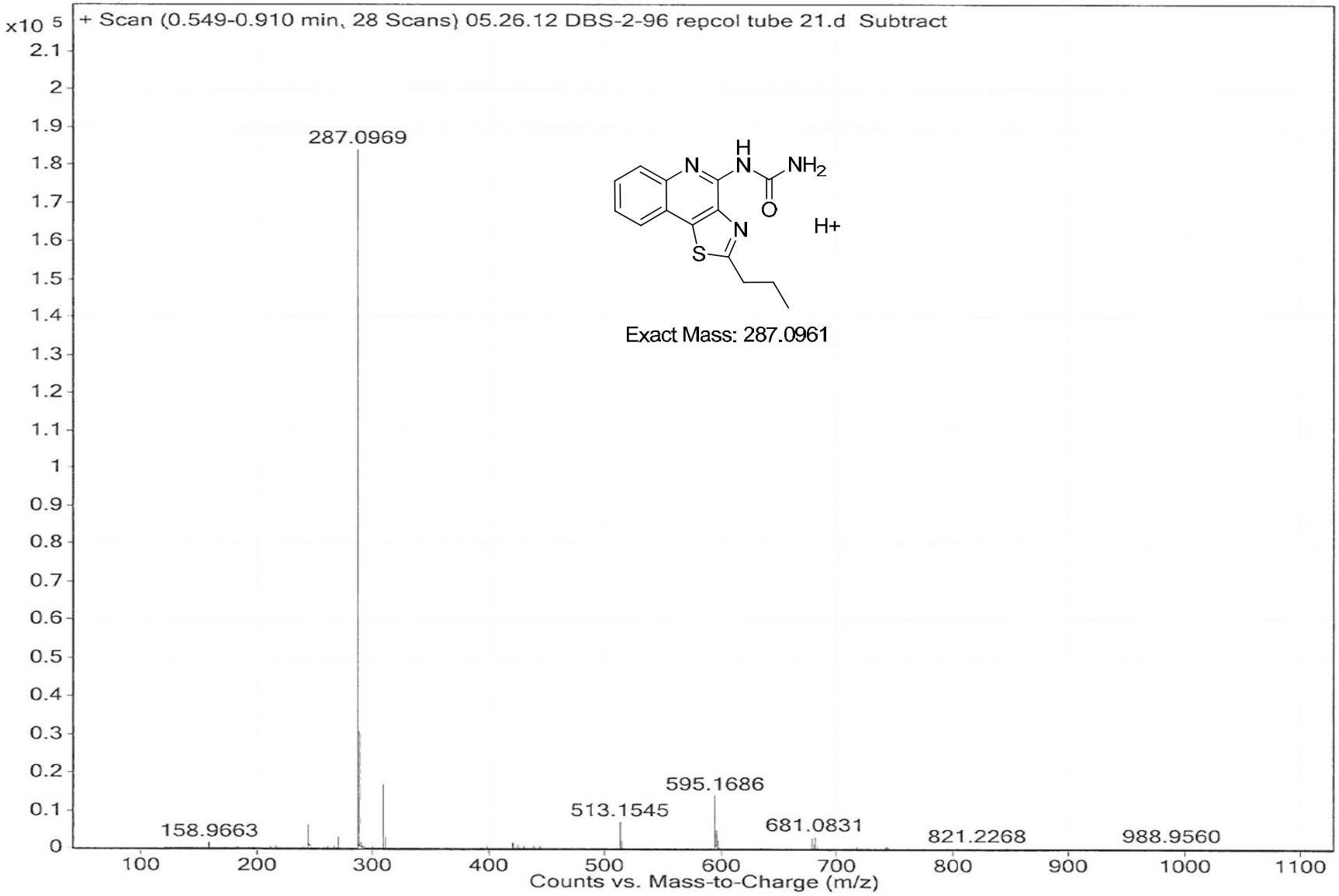
15q ^{1}H NMR



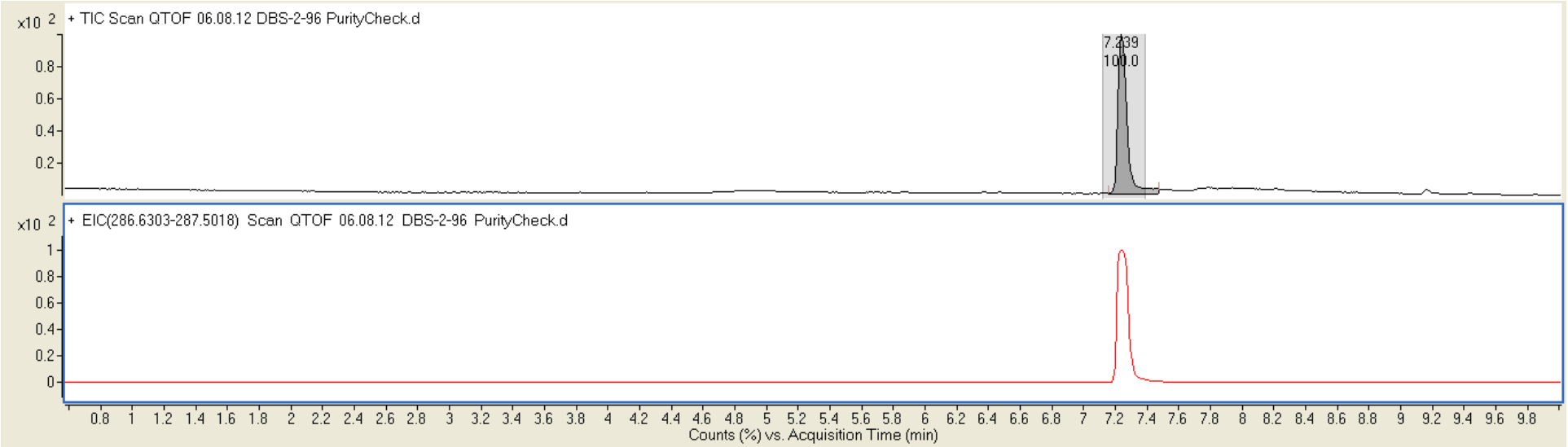
15q ^{13}C NMR

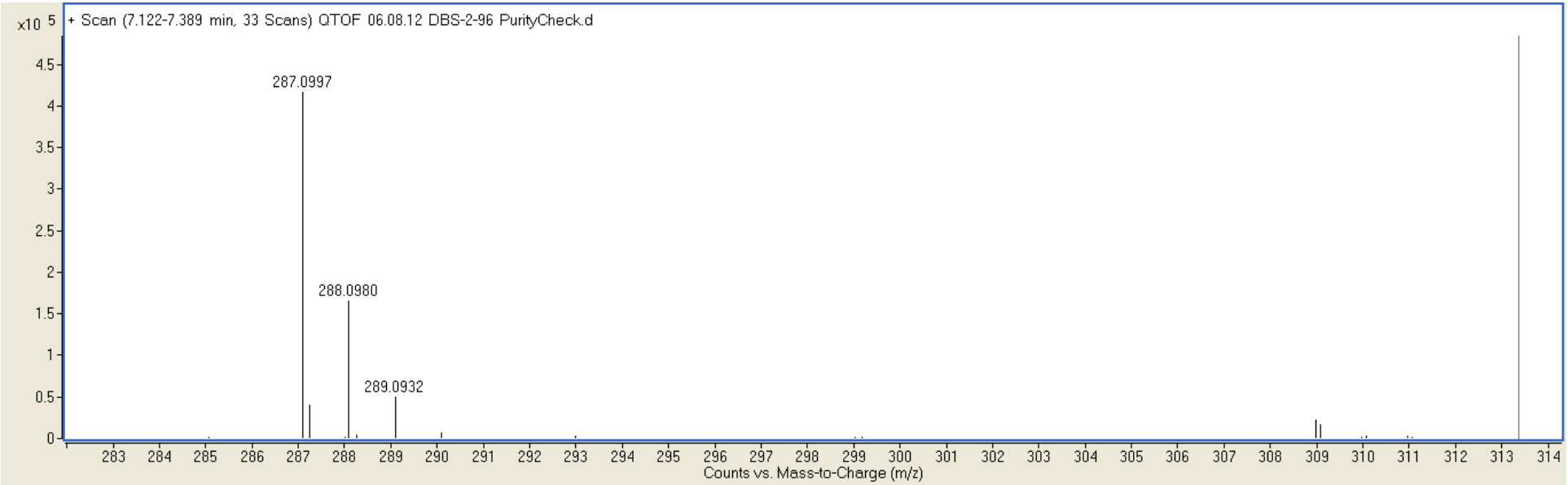


15q MS

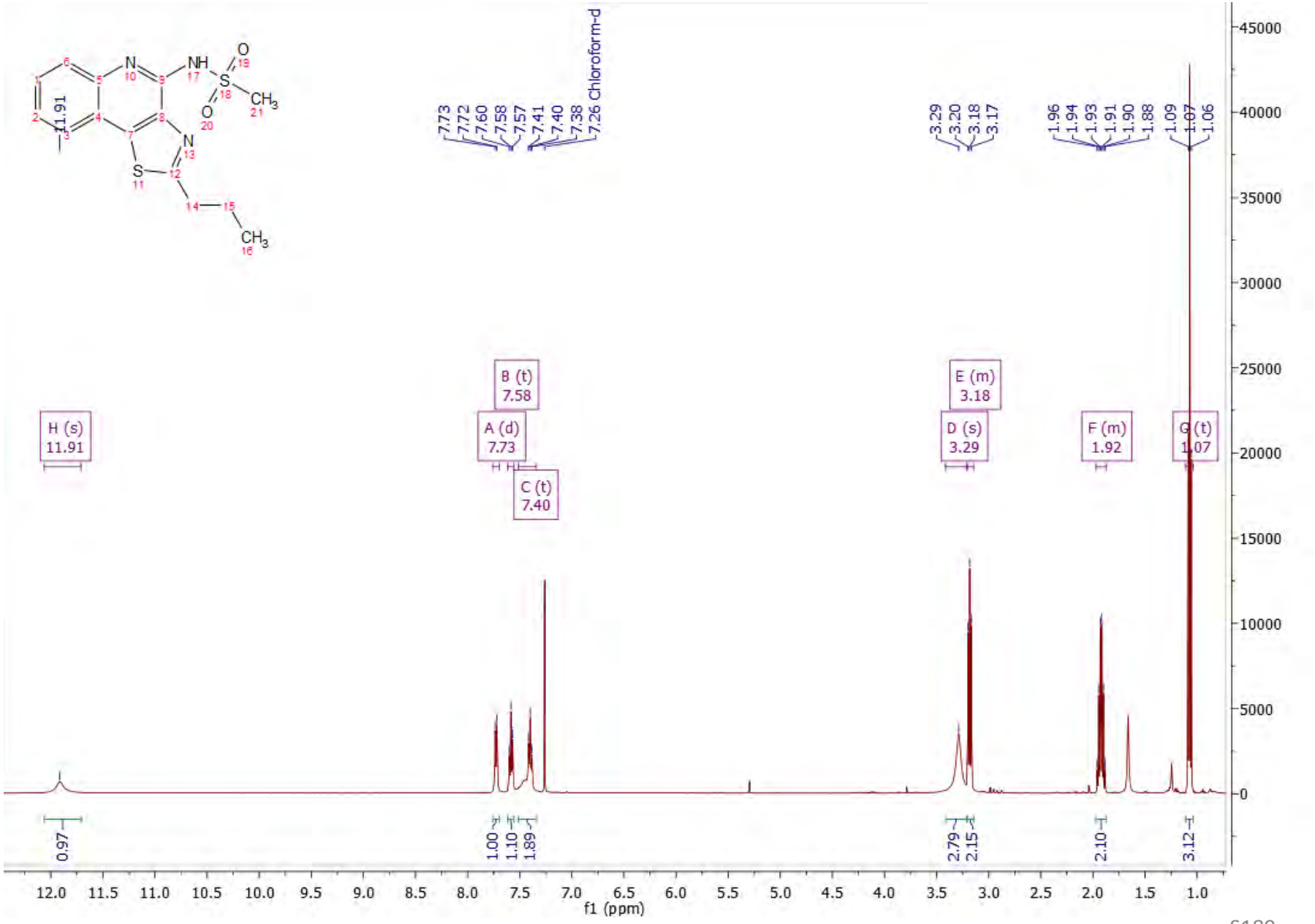


15q LC-MS

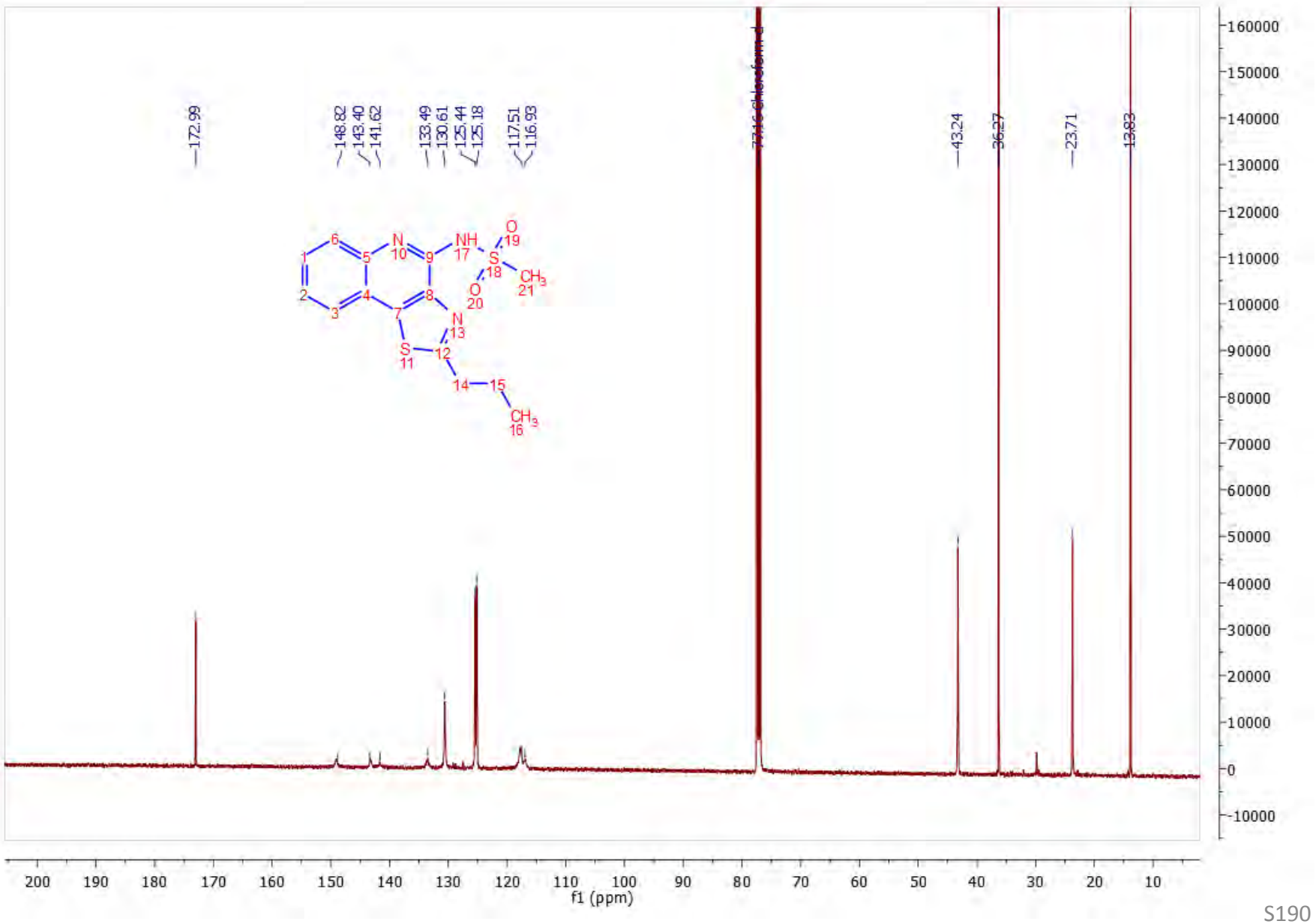




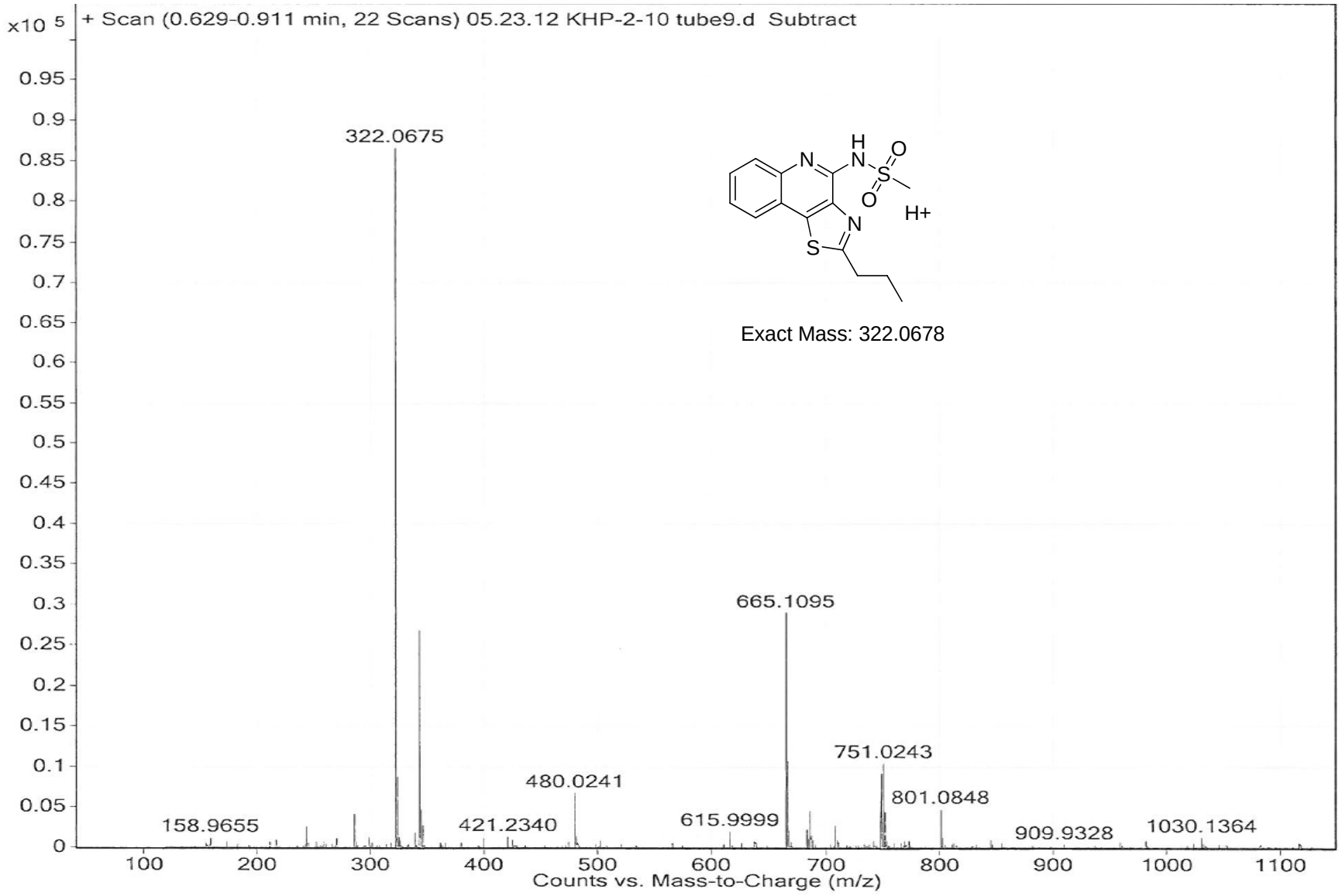
15r ^{1}H NMR



15r ^{13}C NMR



15r MS



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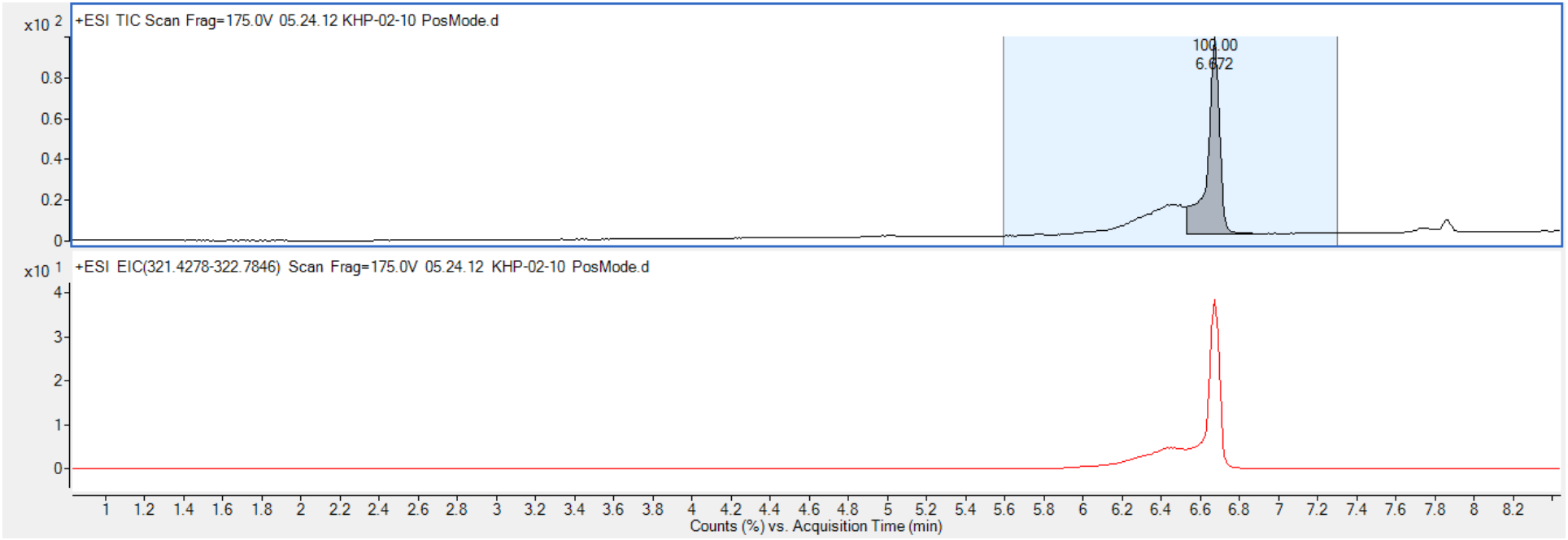
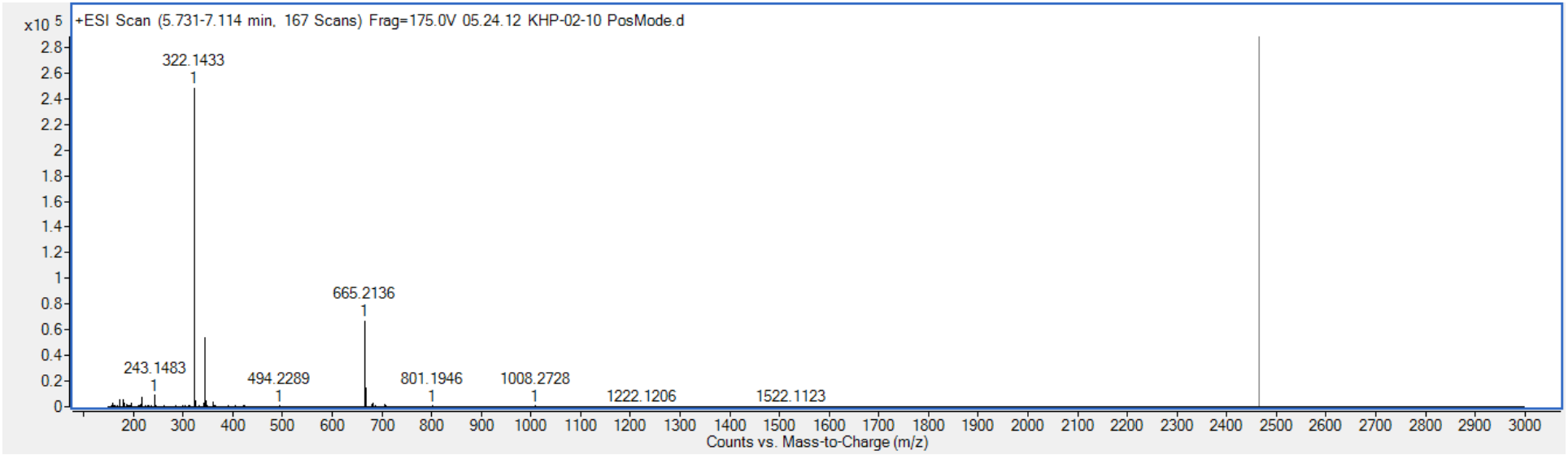
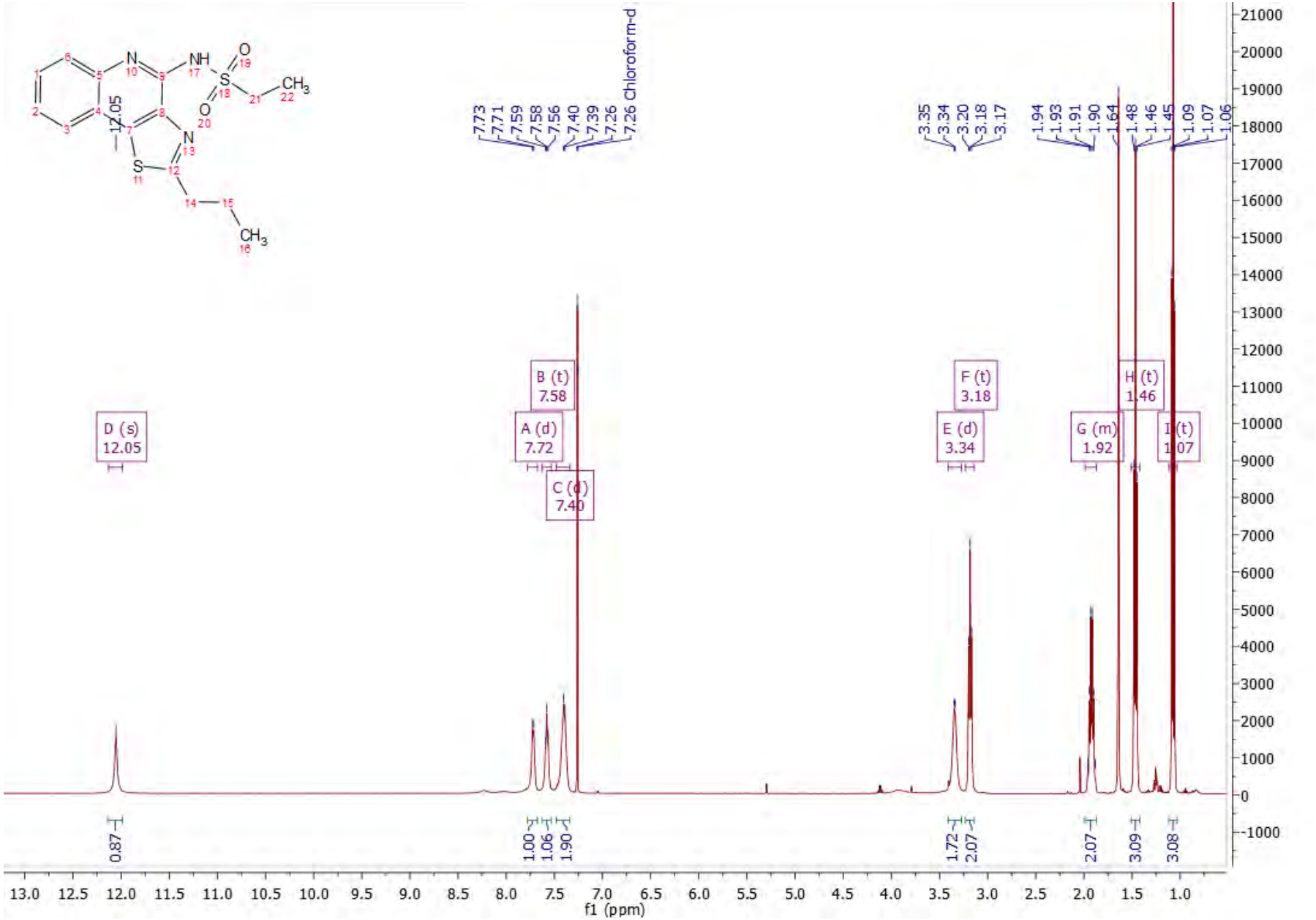
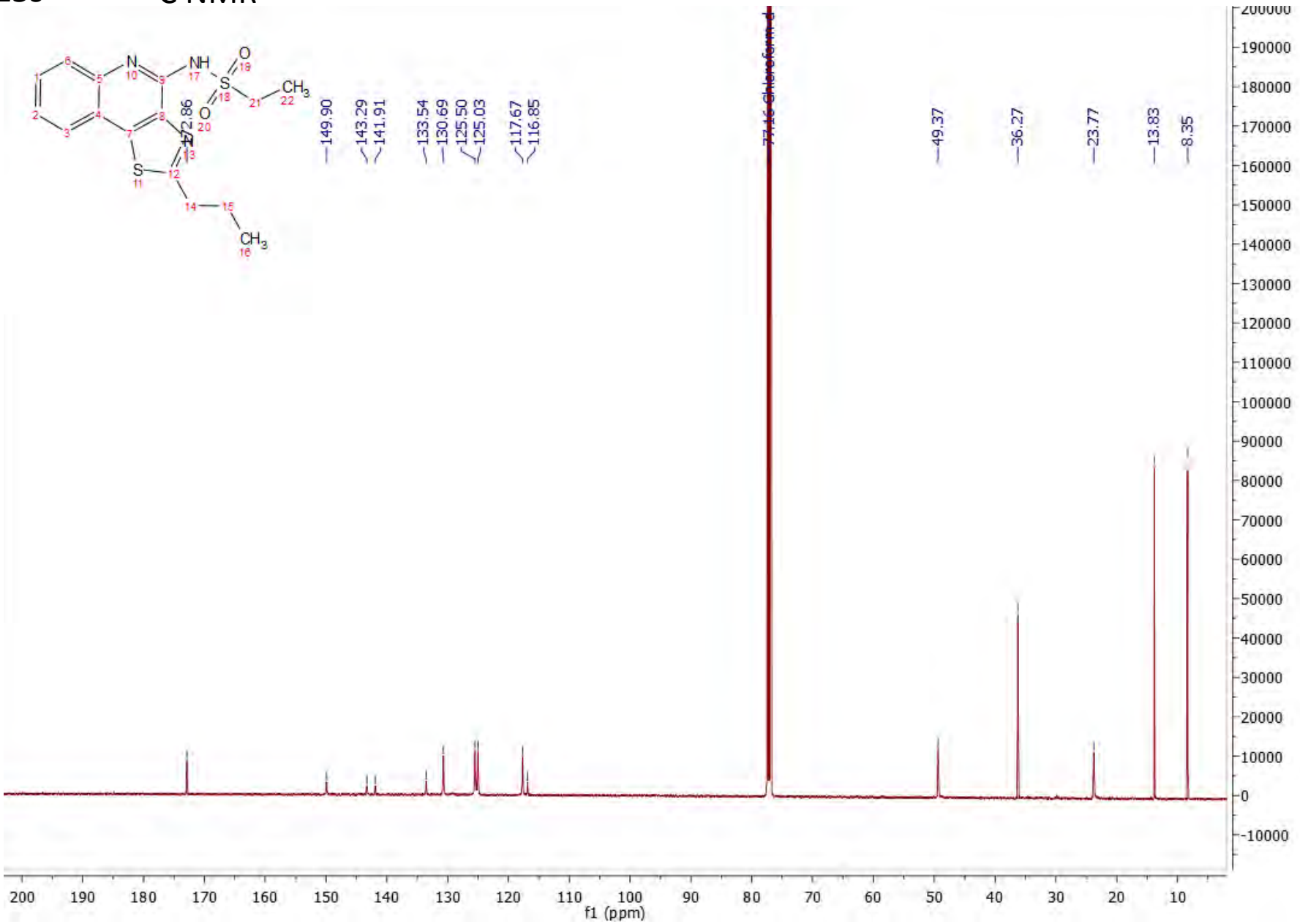




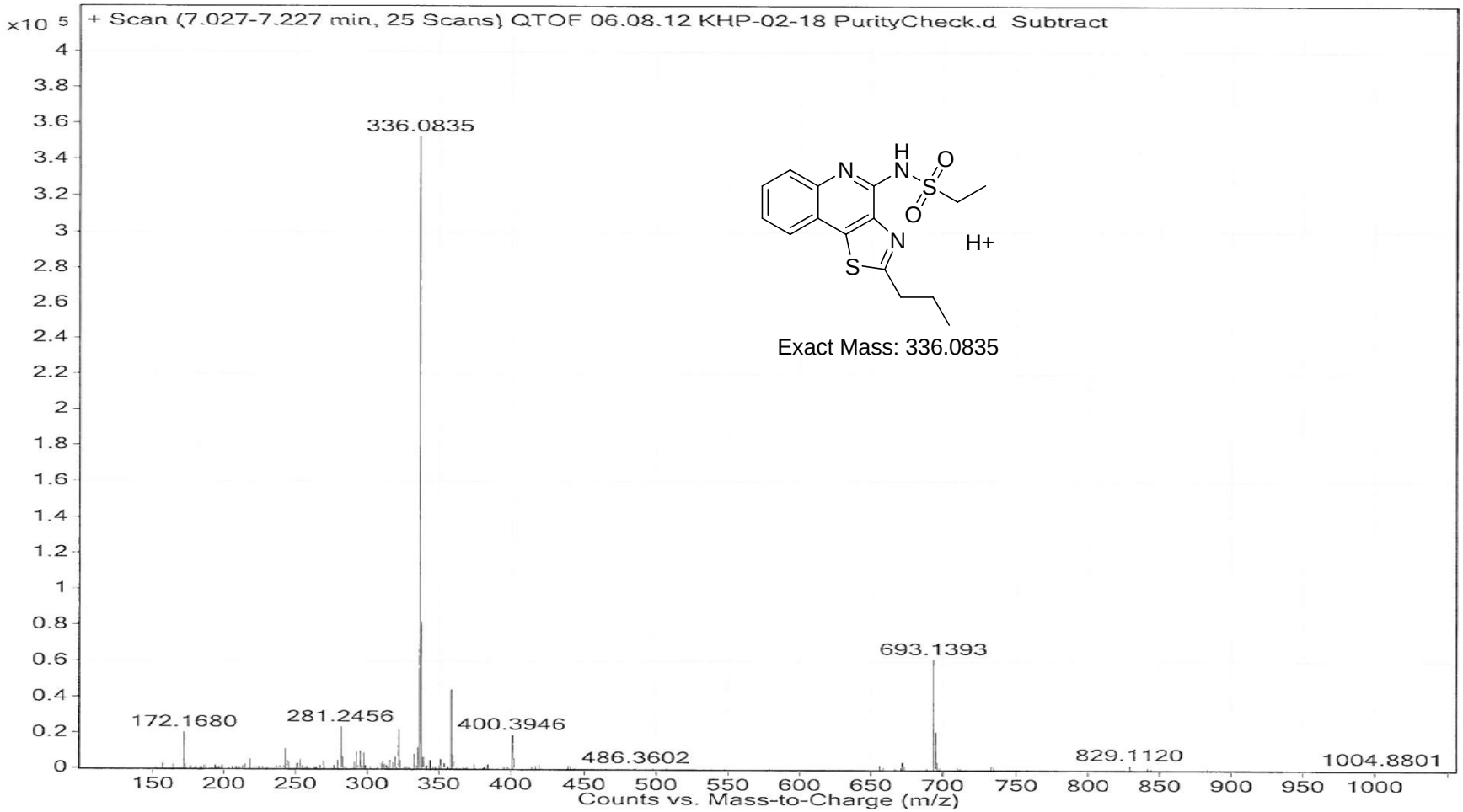
15s ^{1}H NMR



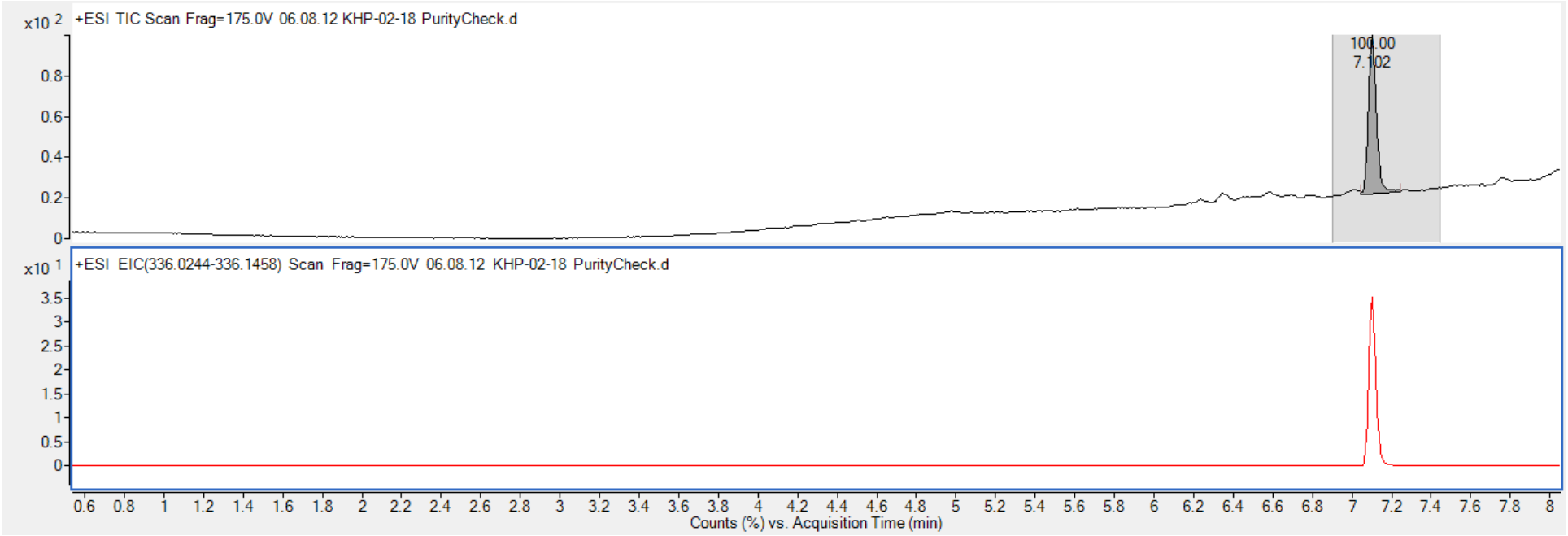
15s ^{13}C NMR

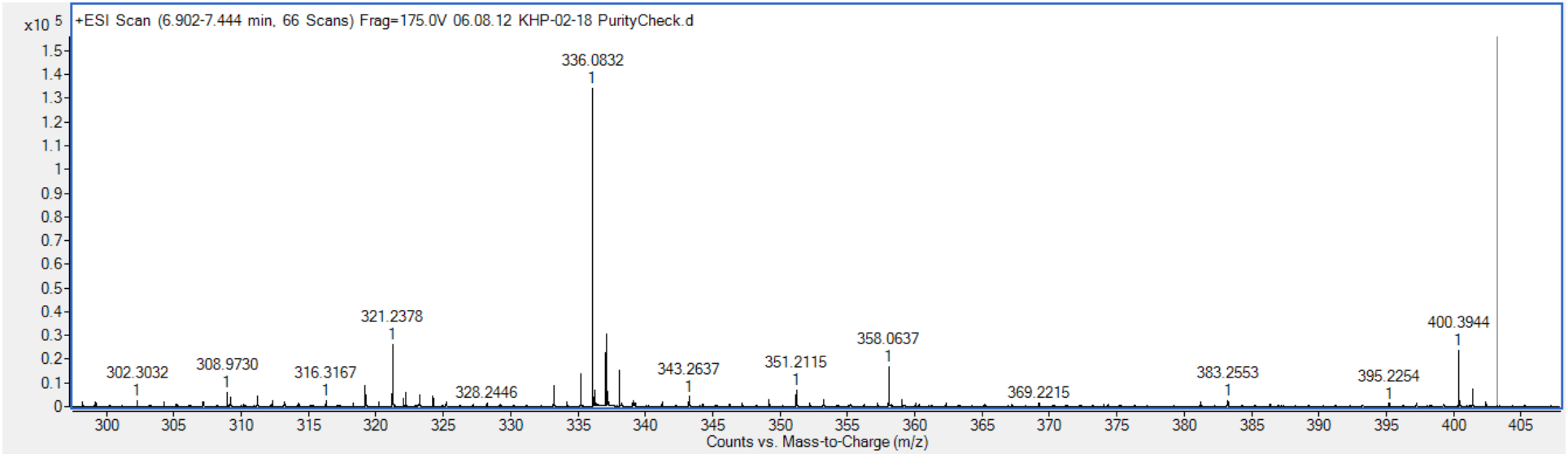


15s MS

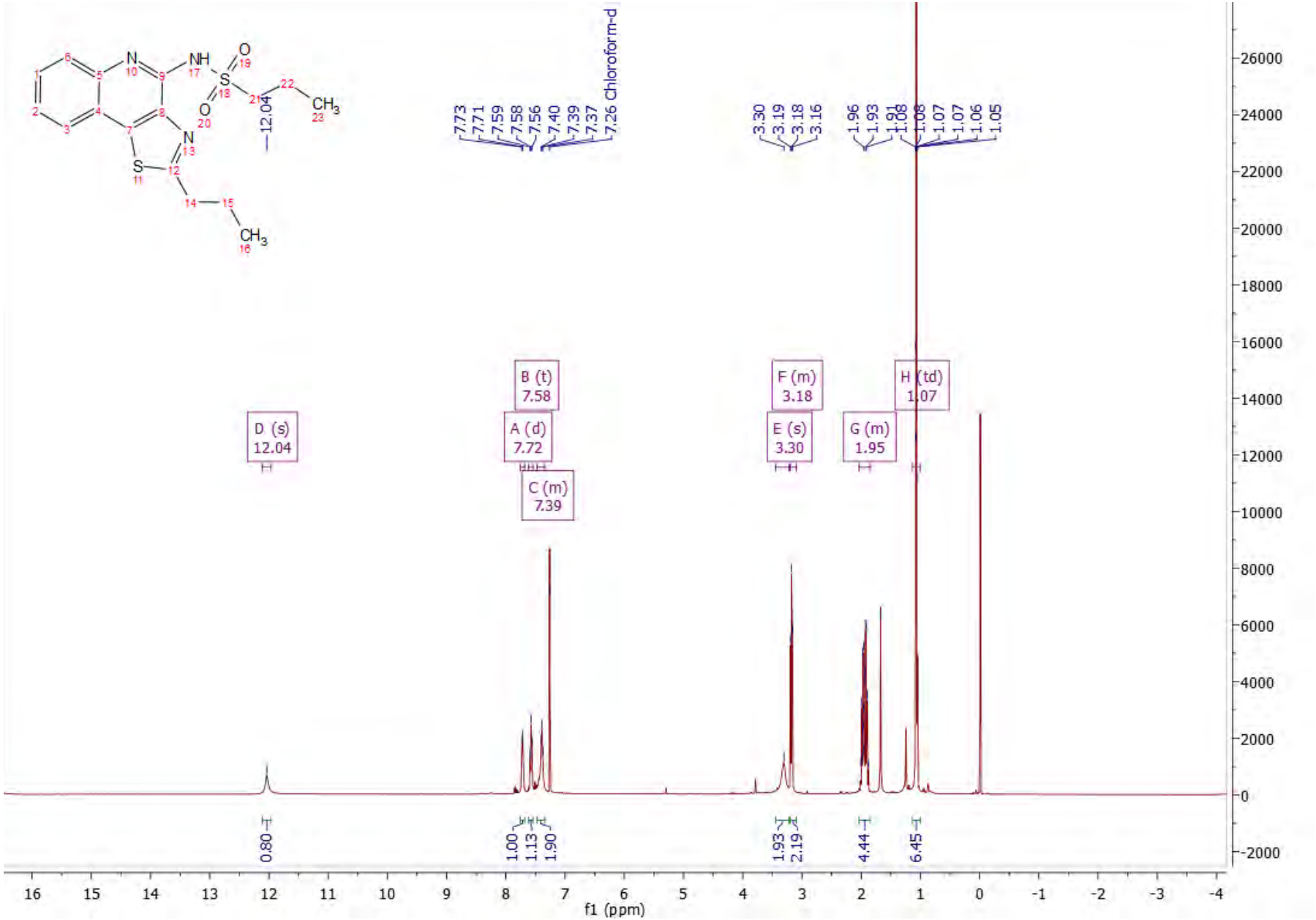


15s LC-MS

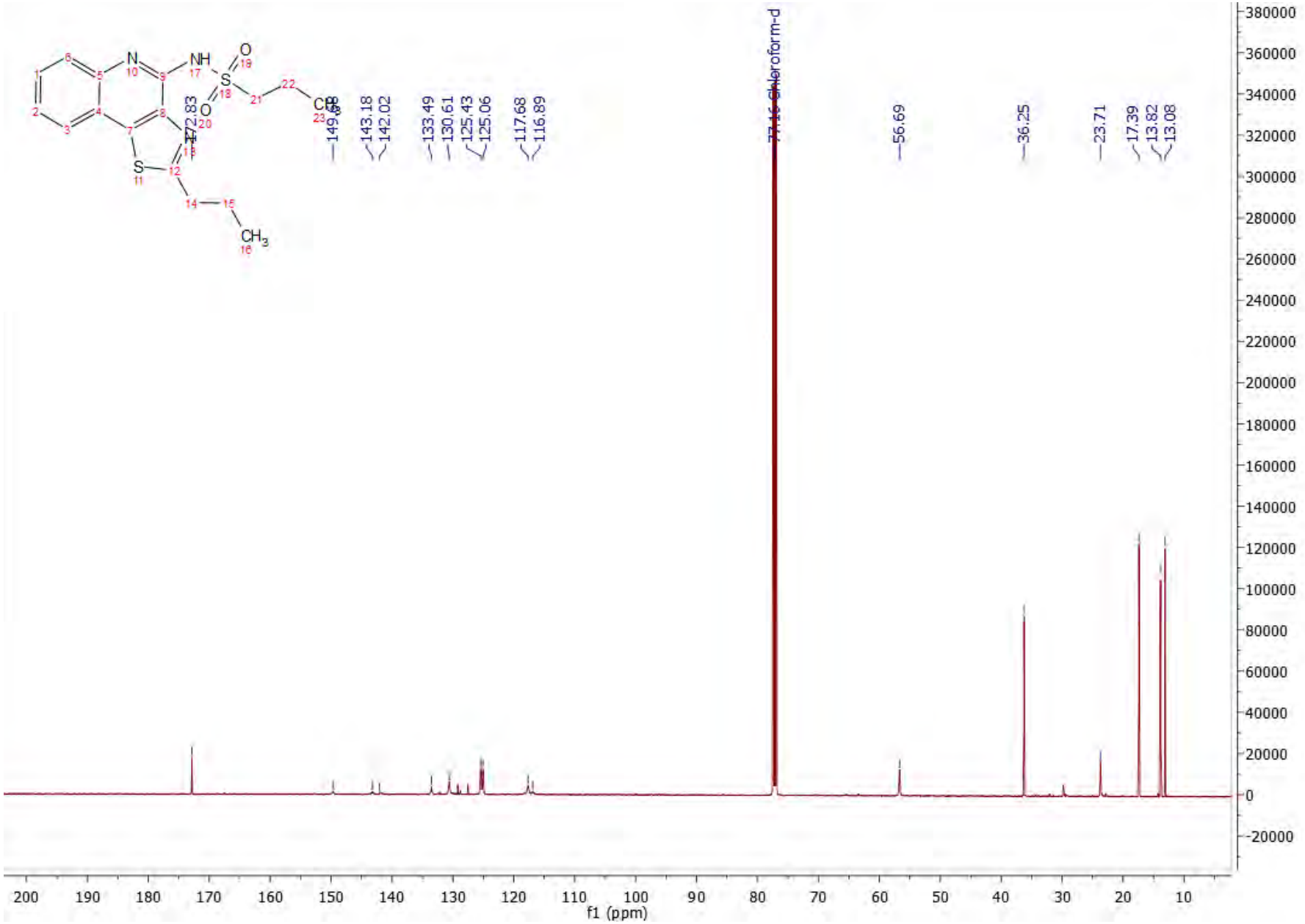




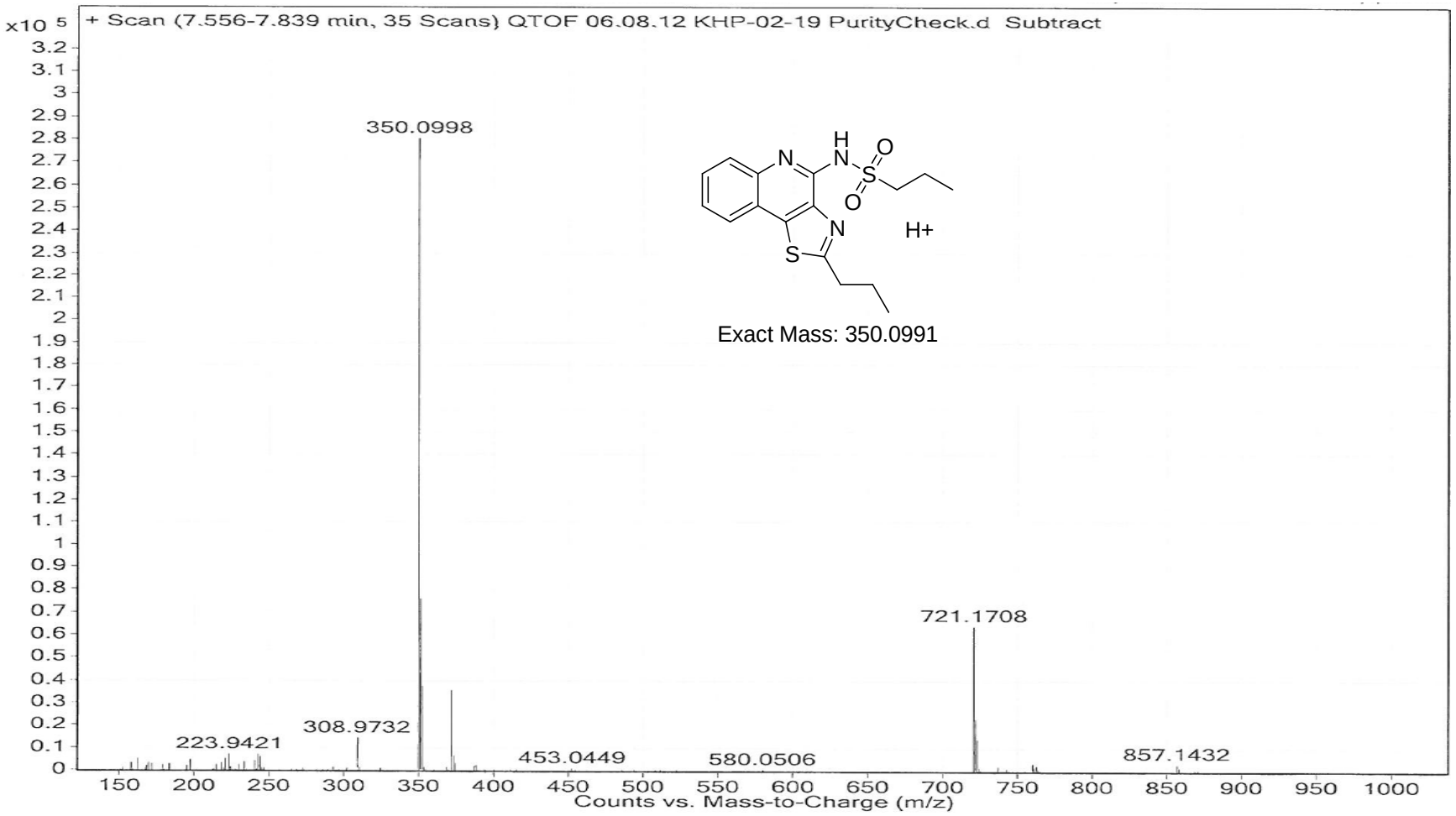
15t ^{1}H NMR



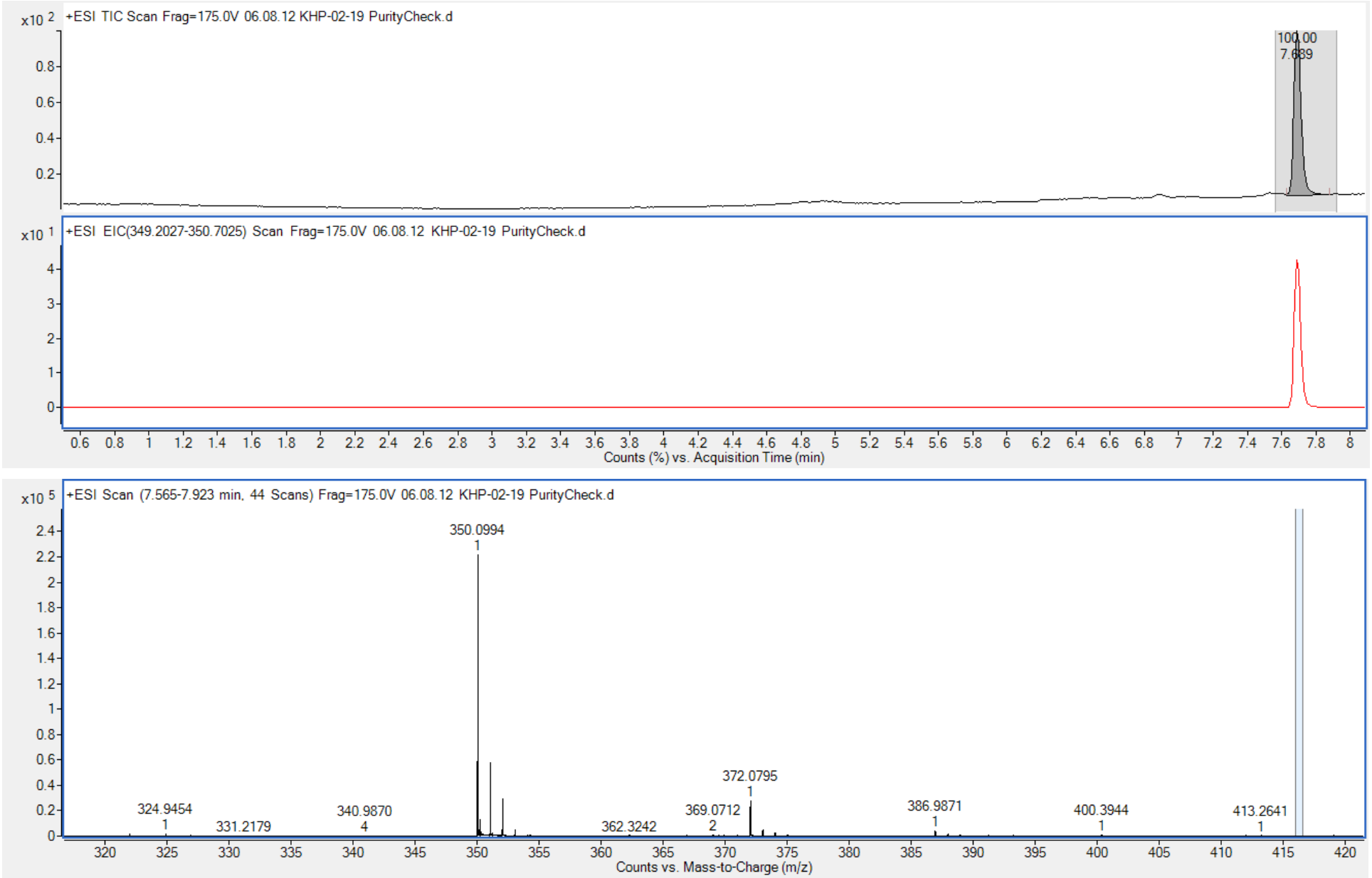
15t ^{13}C NMR



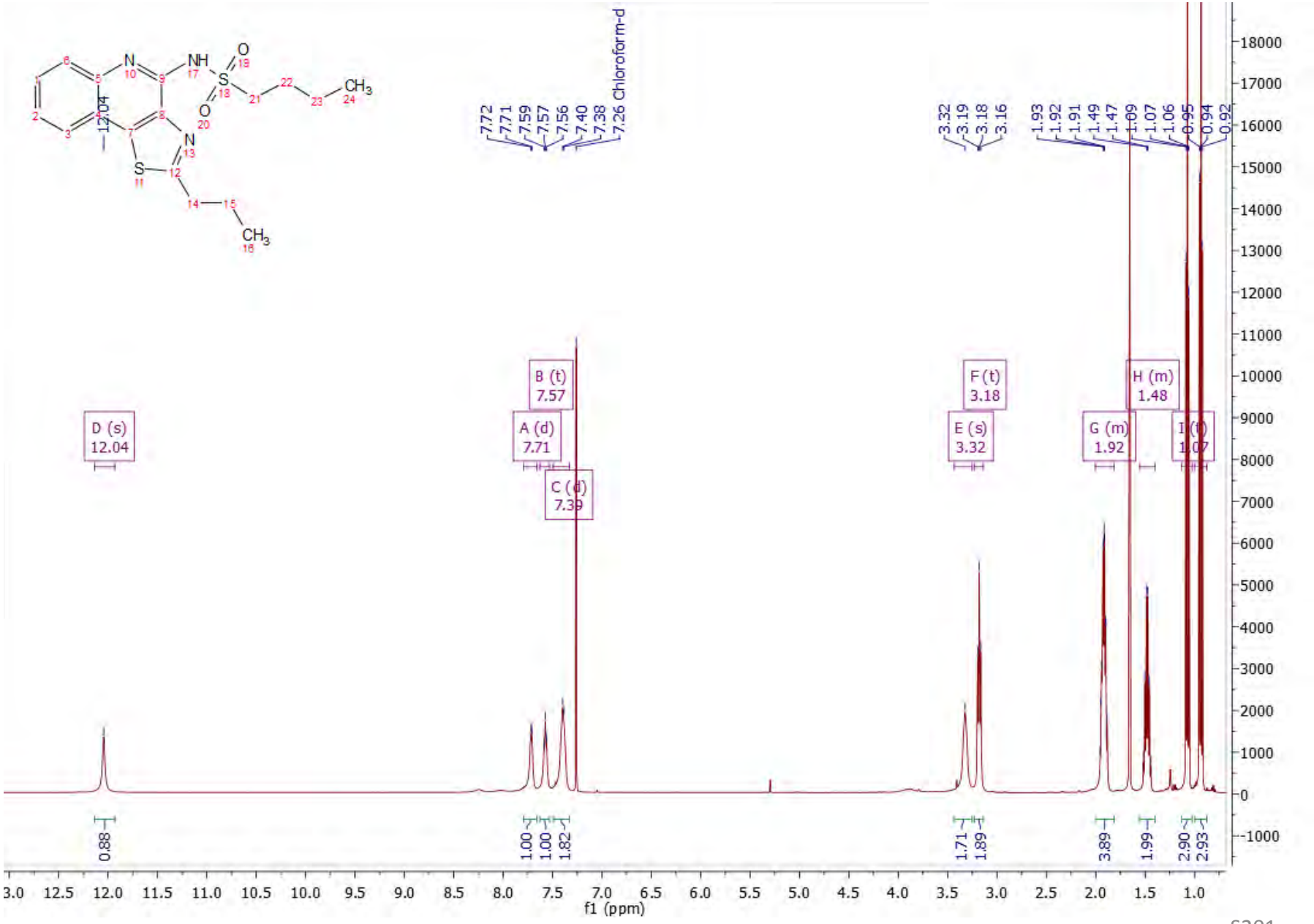
15t MS



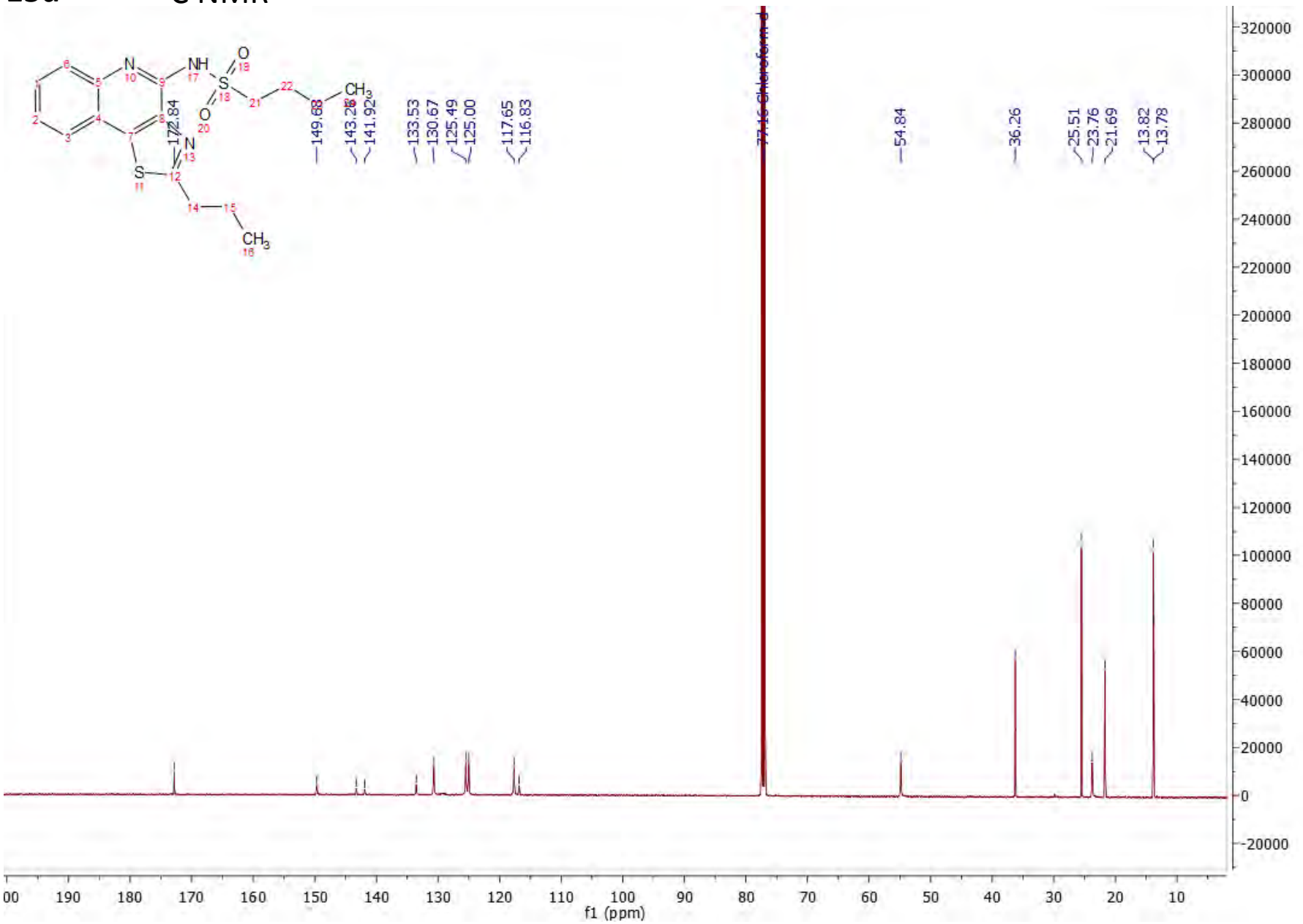
15t LC-MS



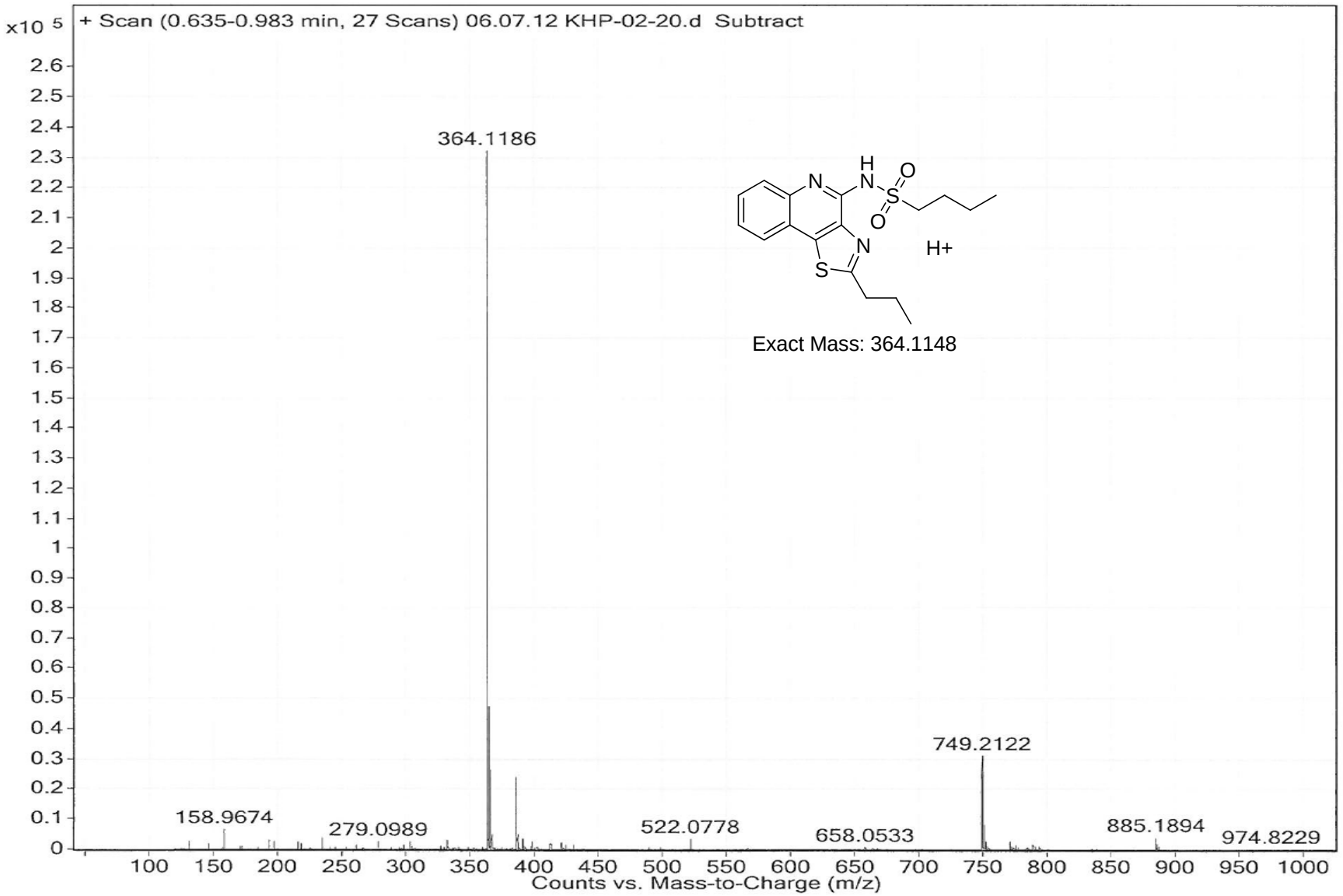
15u ^{1}H NMR



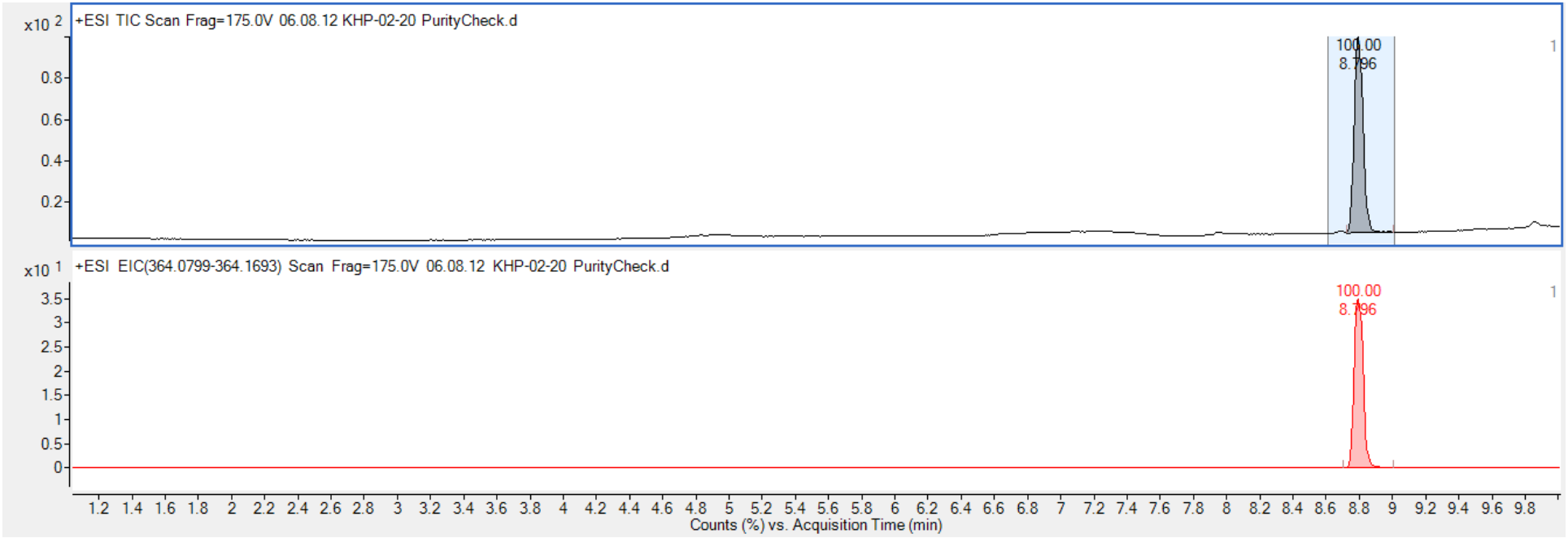
15u ^{13}C NMR

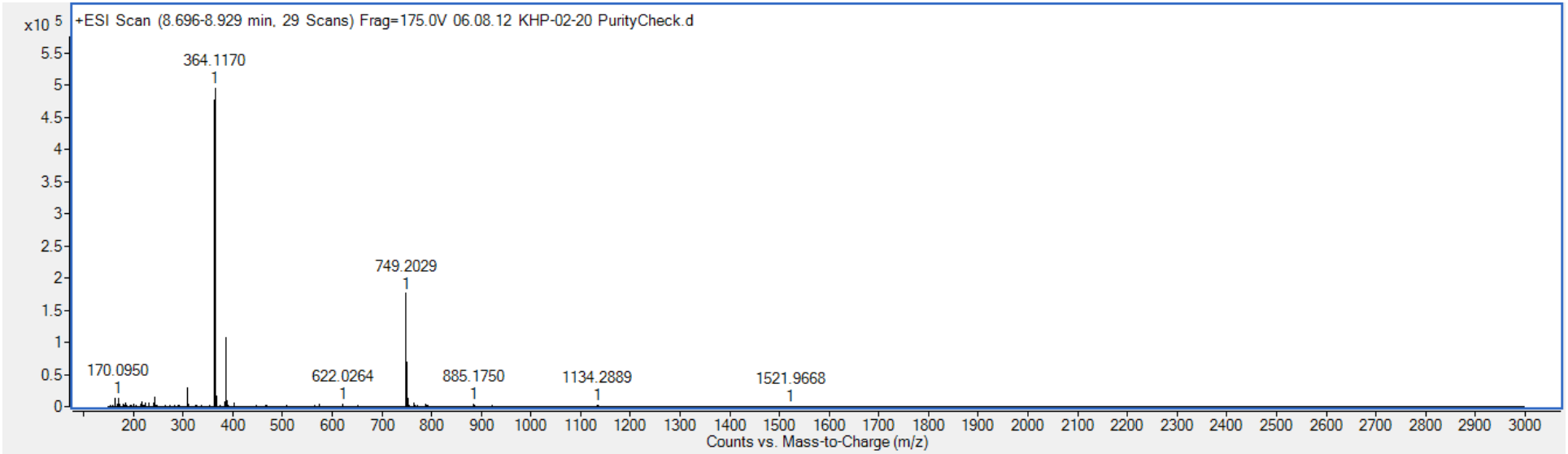


15u MS

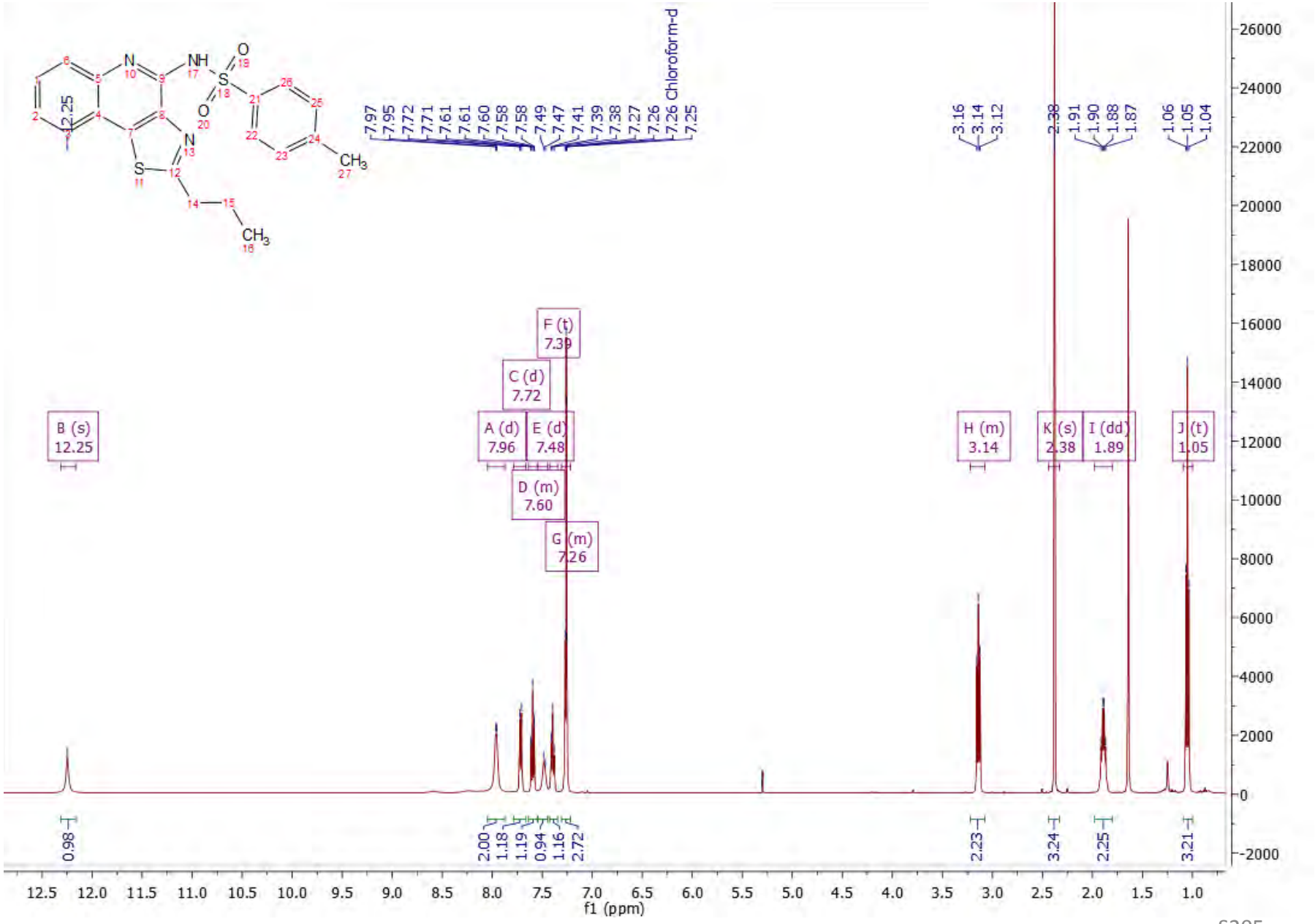


15u LC-MS

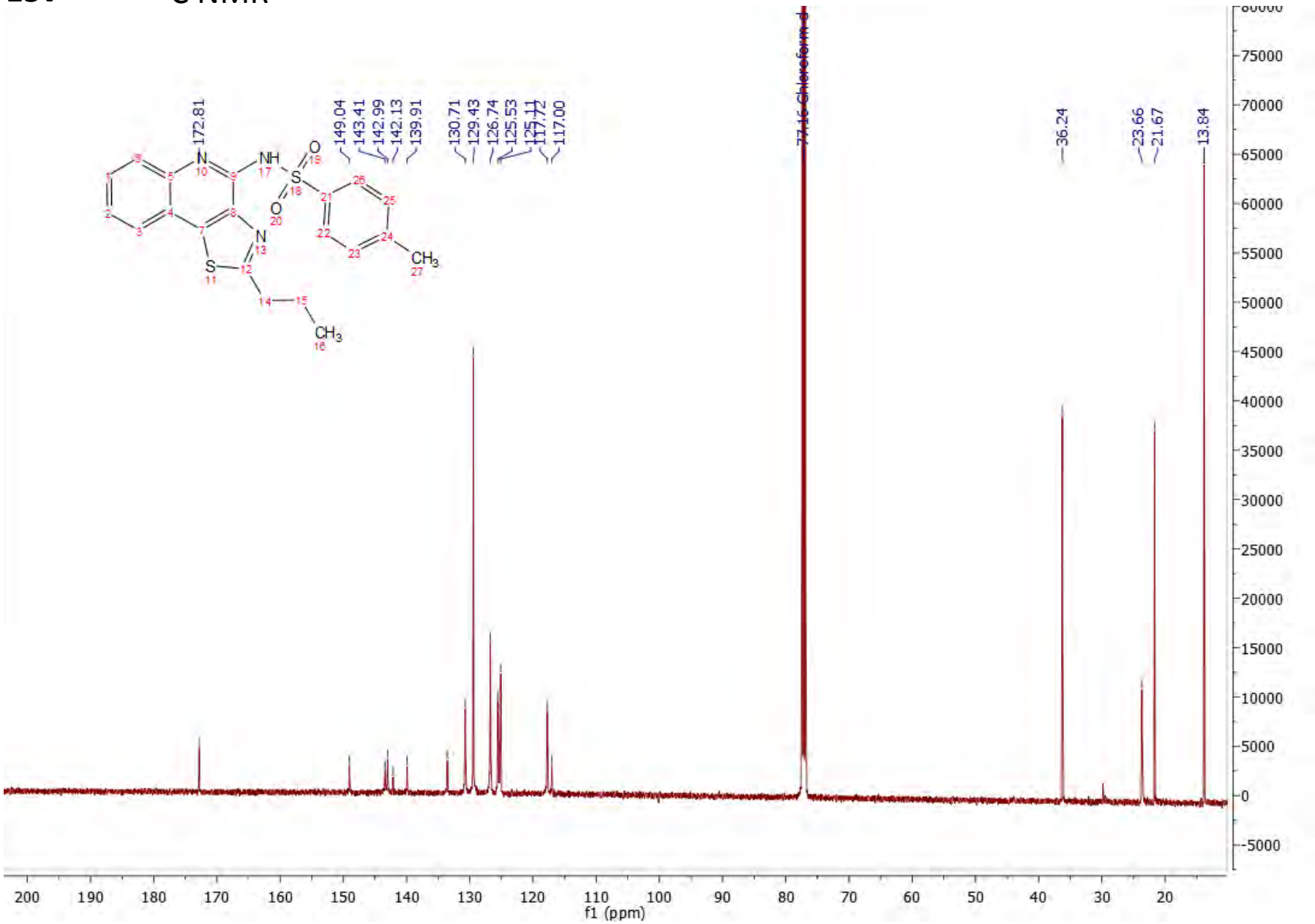




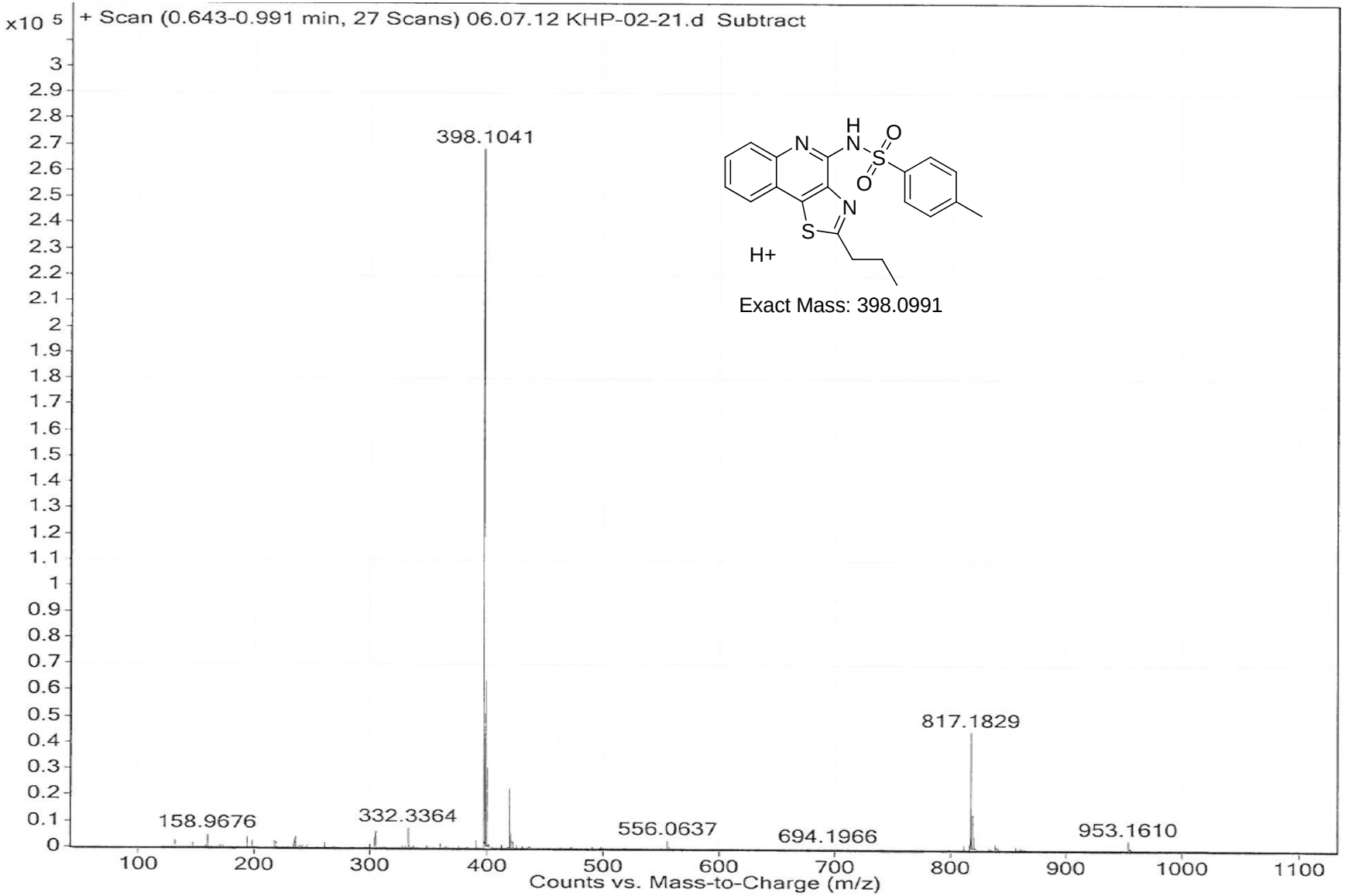
15v ^{1}H NMR


B (s) 12.25
A (d) 7.96
E (d) 7.48
F (t) 7.39
C (d) 7.72
D (m) 7.60
G (m) 7.26
H (m) 3.14
K (s) 2.38
I (dd) 1.89
J (t) 1.05
Chloroform-d
f1 (ppm)

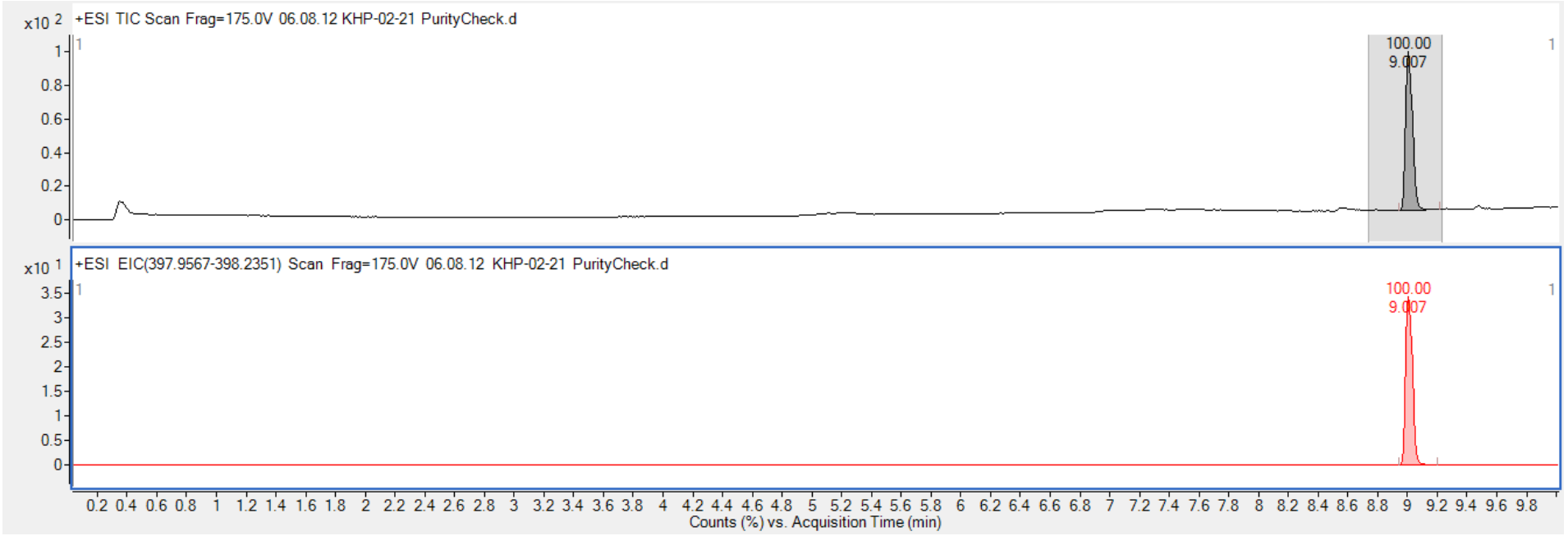
15v ^{13}C NMR

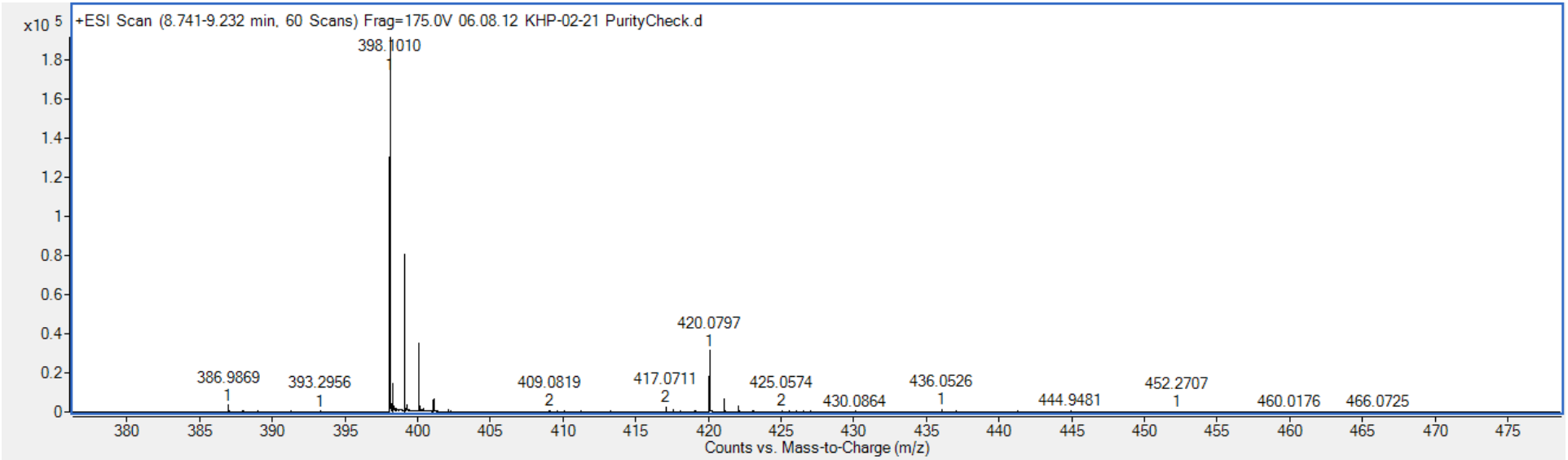


15v MS

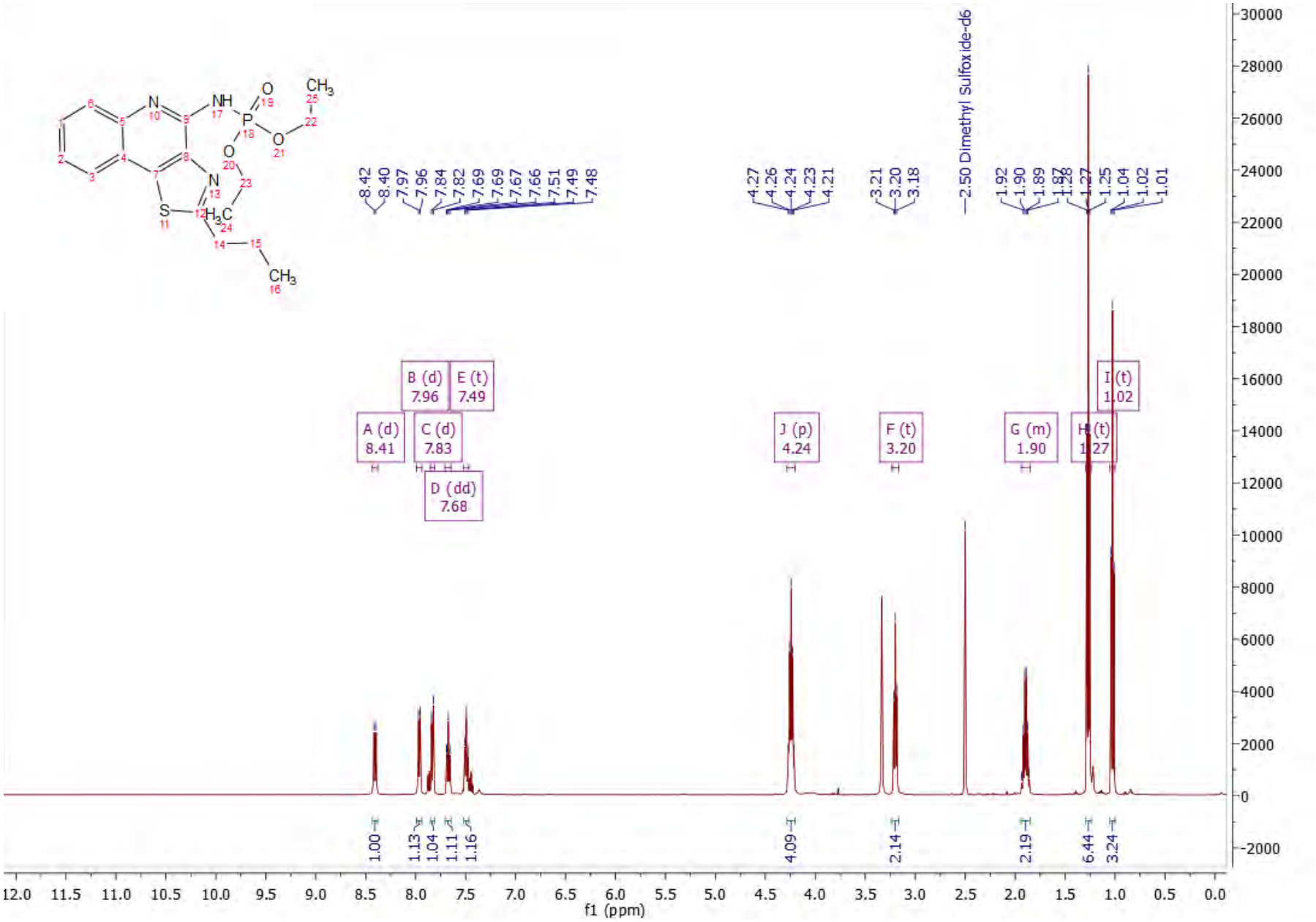


15v LC-MS

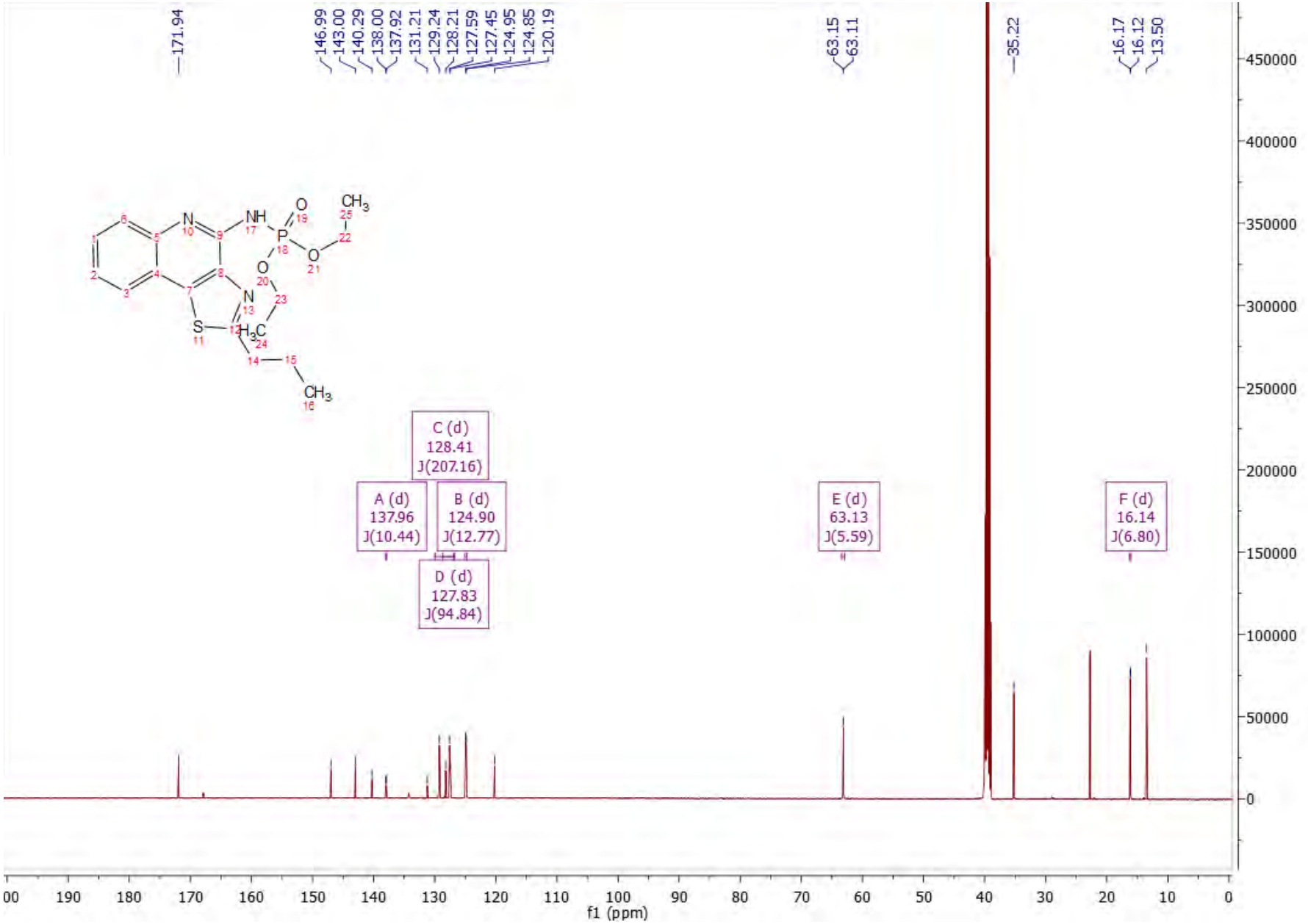




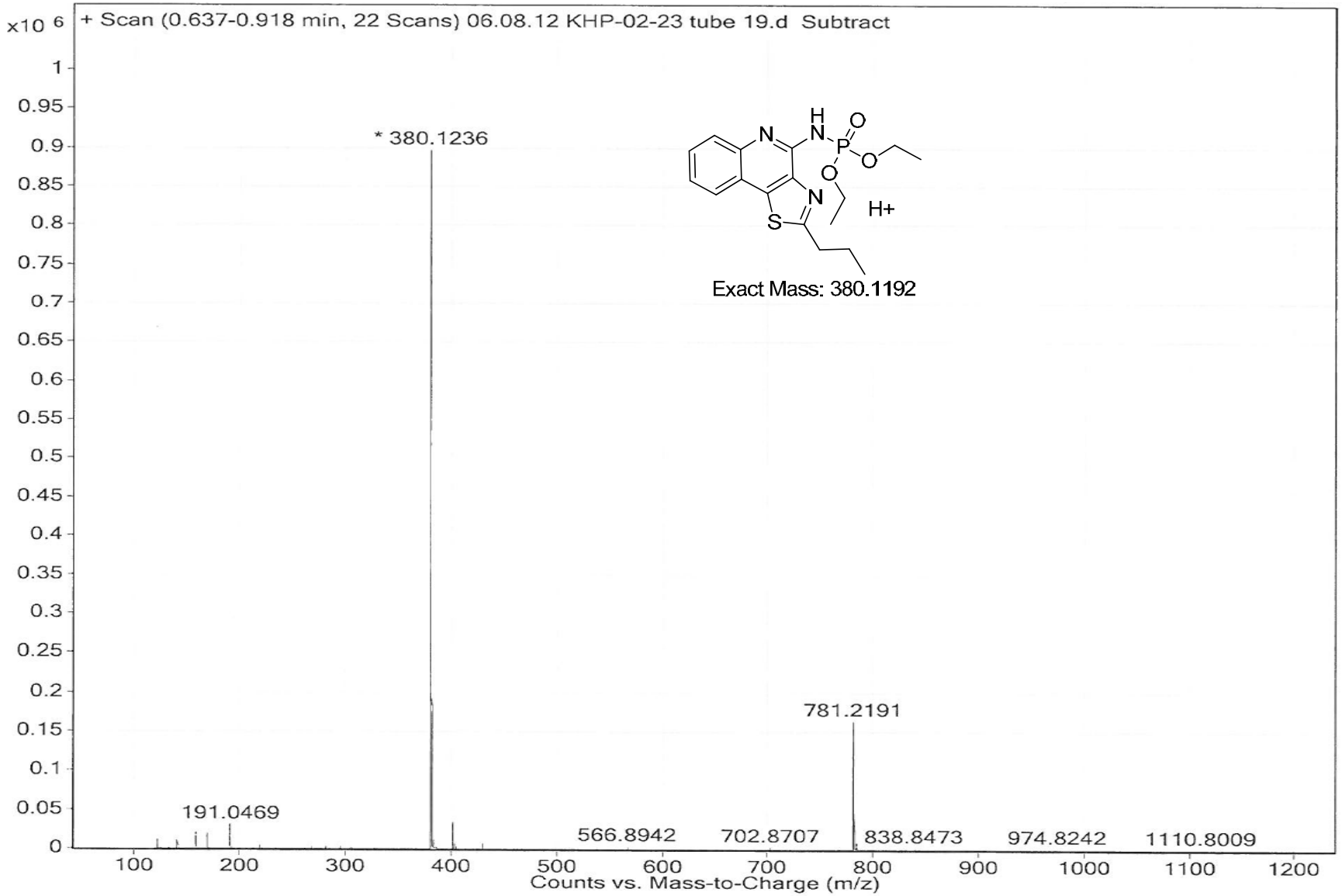
15w ^{1}H NMR



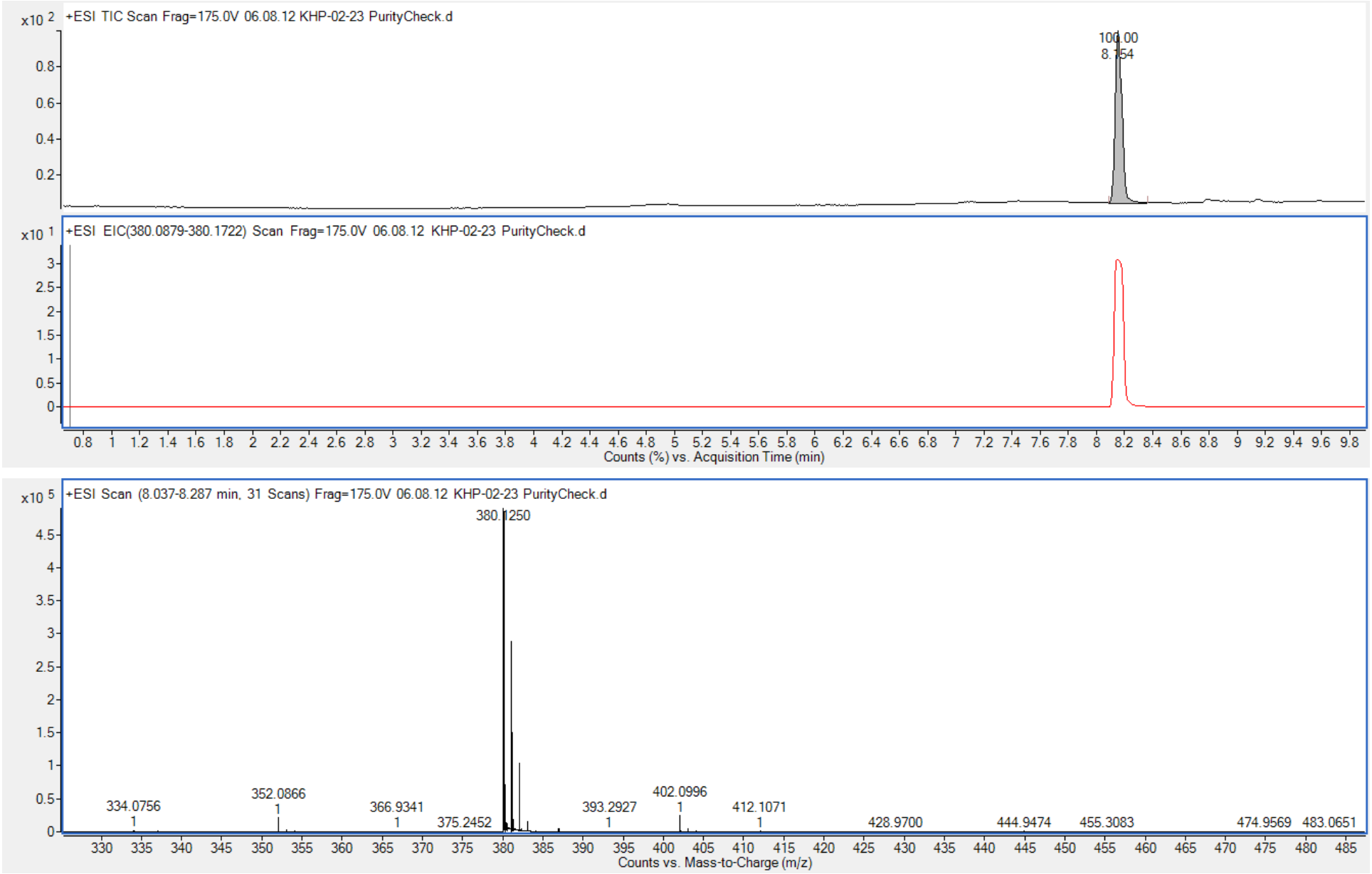
15w ^{13}C NMR



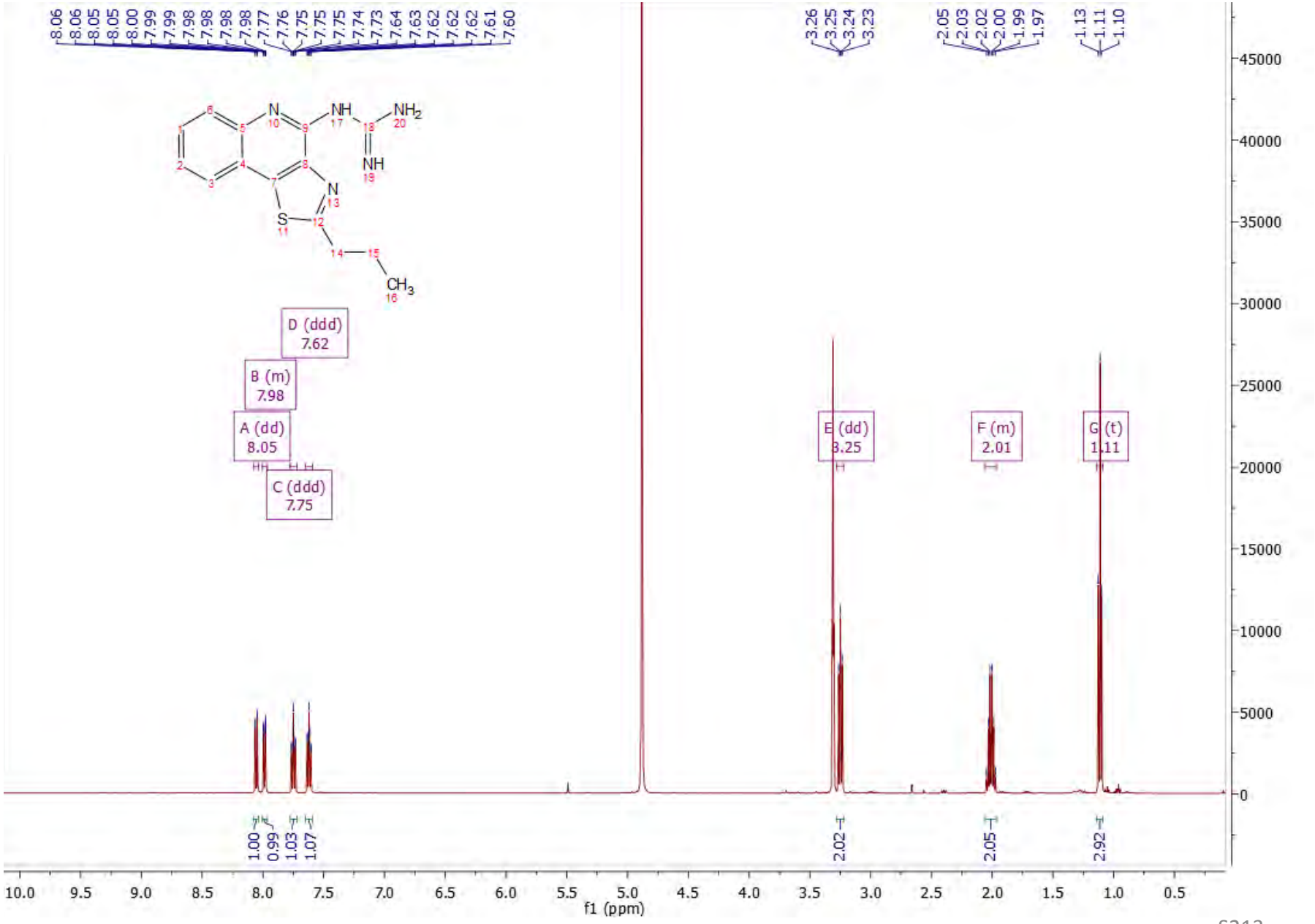
15w MS



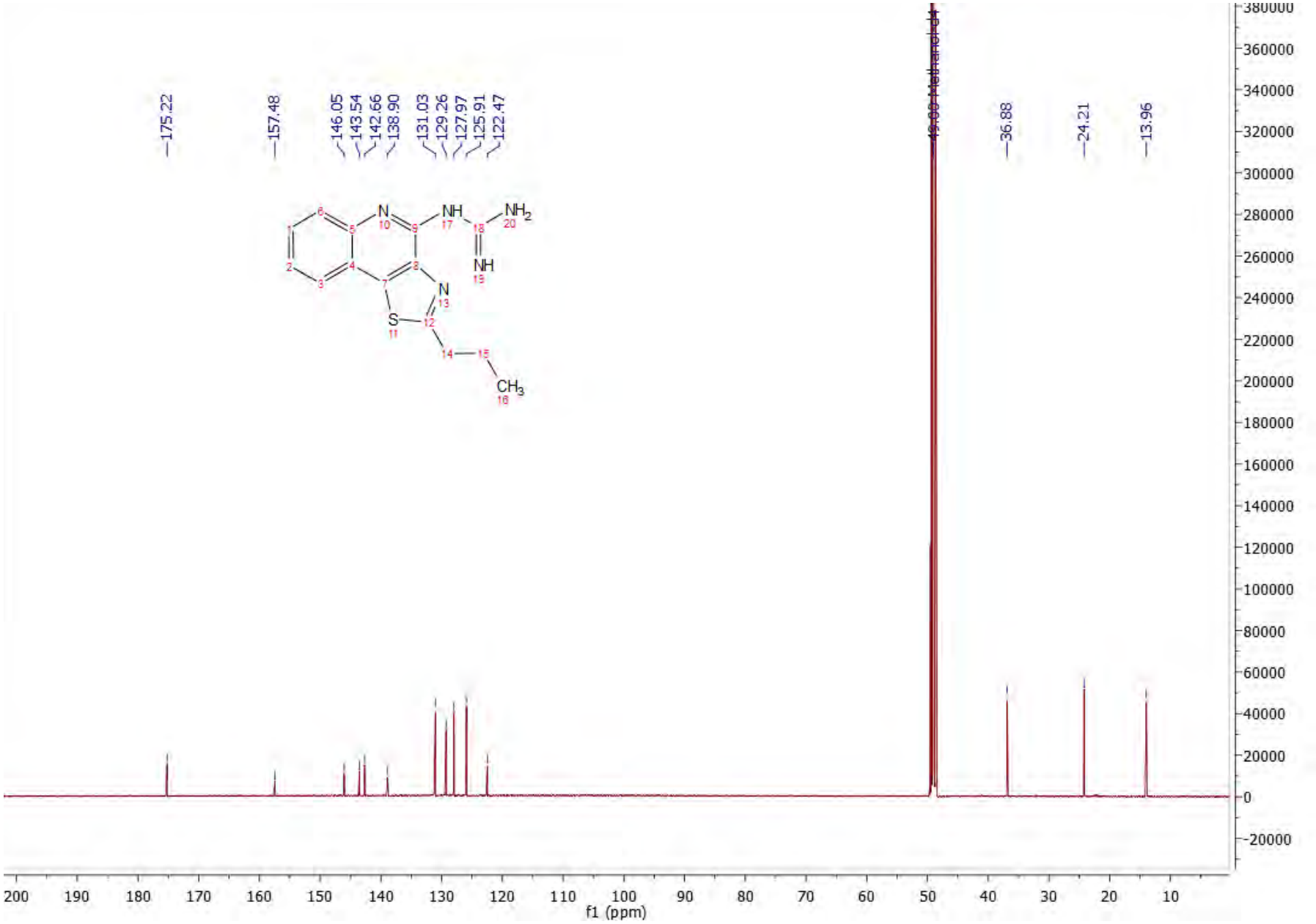
15w LC-MS



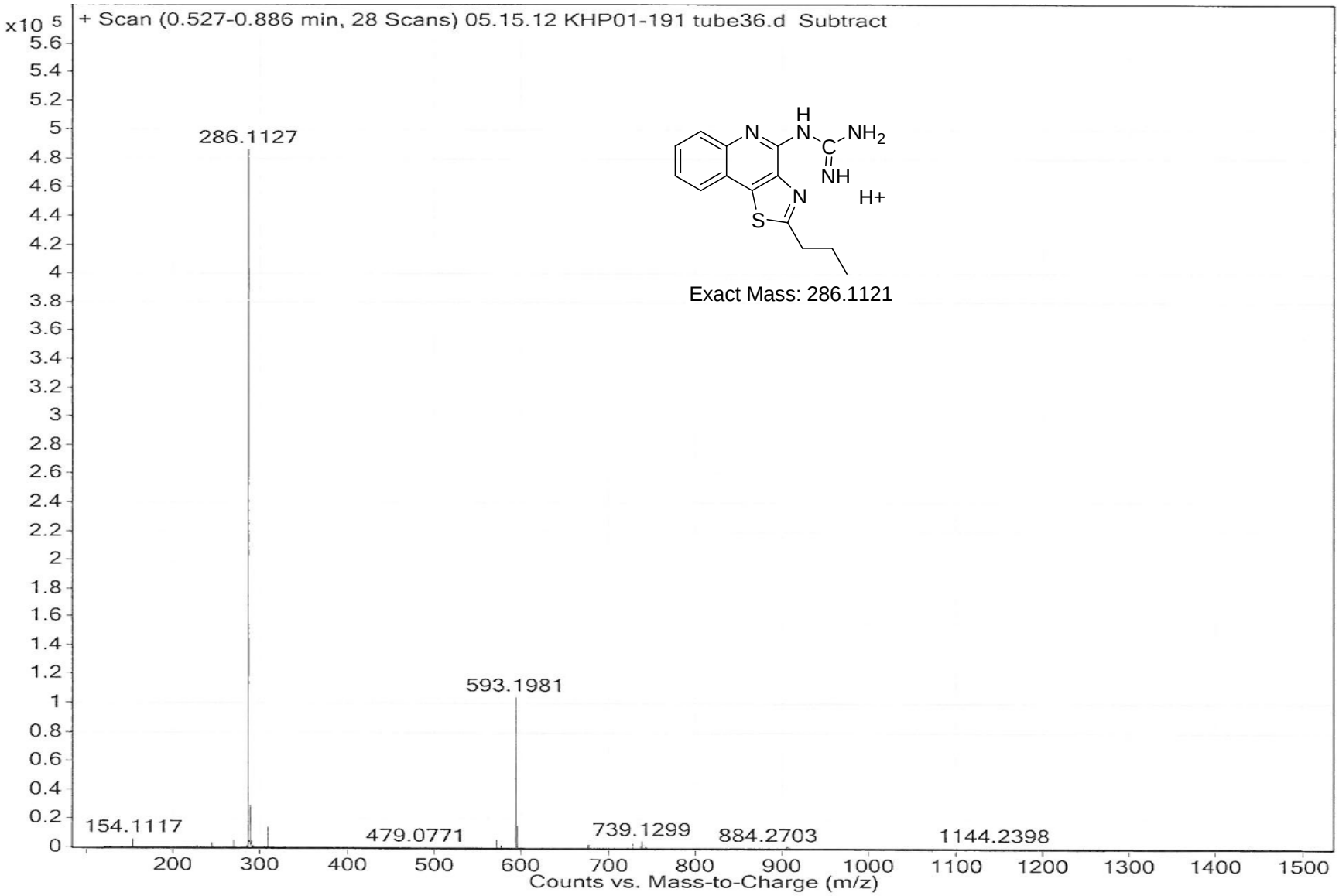
17 ^{1}H NMR



17 ^{13}C NMR

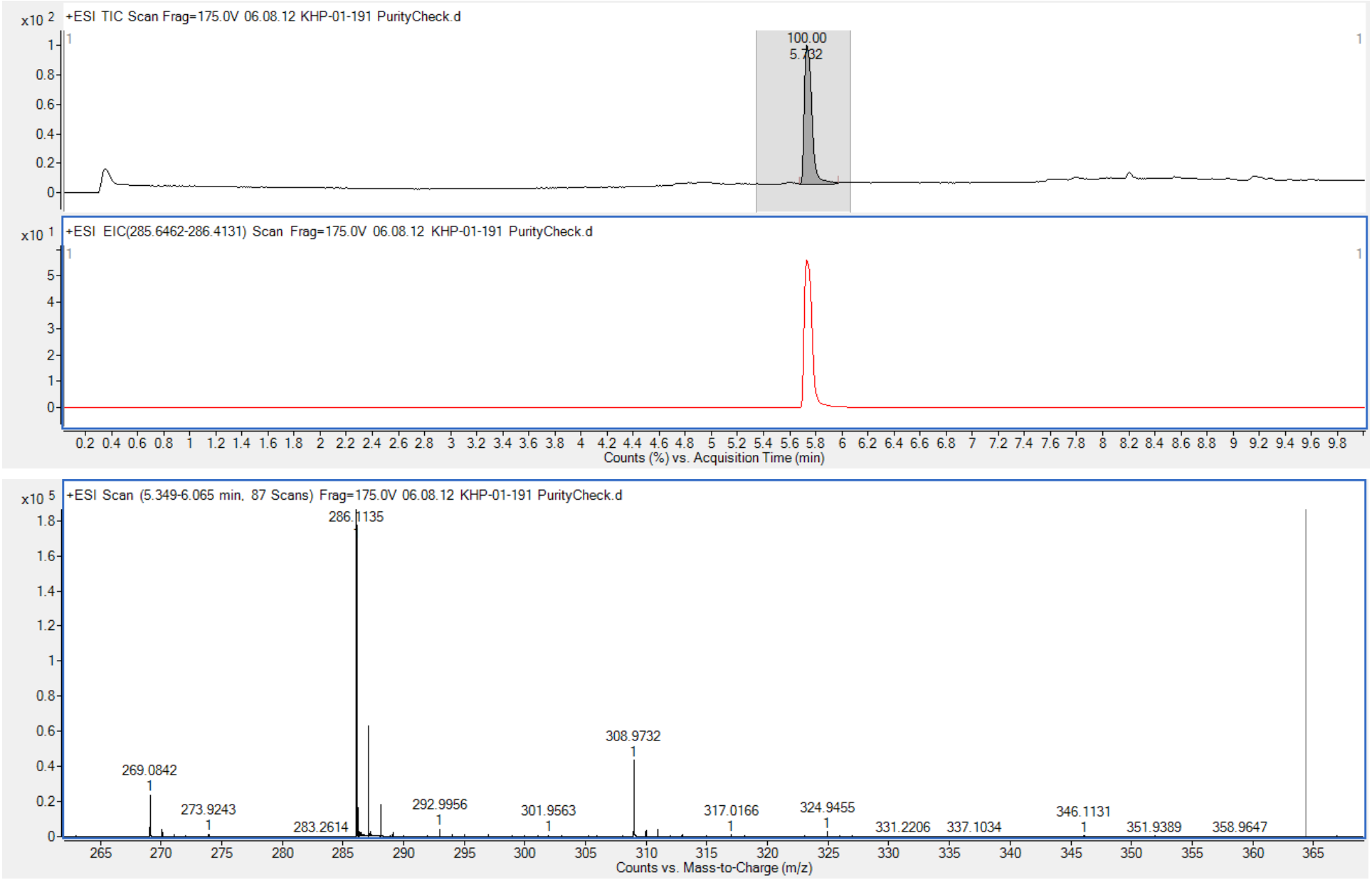


17 MS

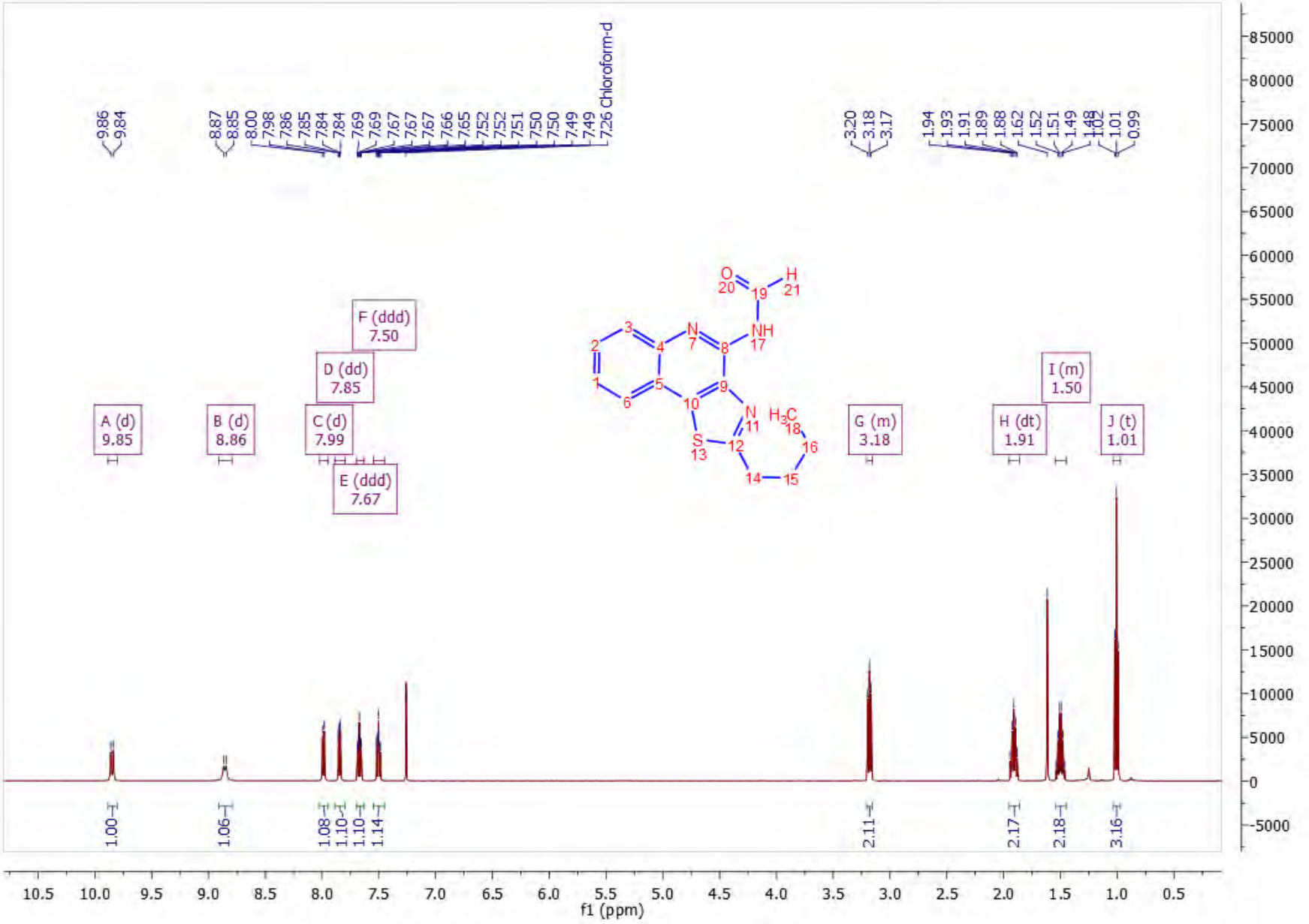


Exact Mass: 286.1121

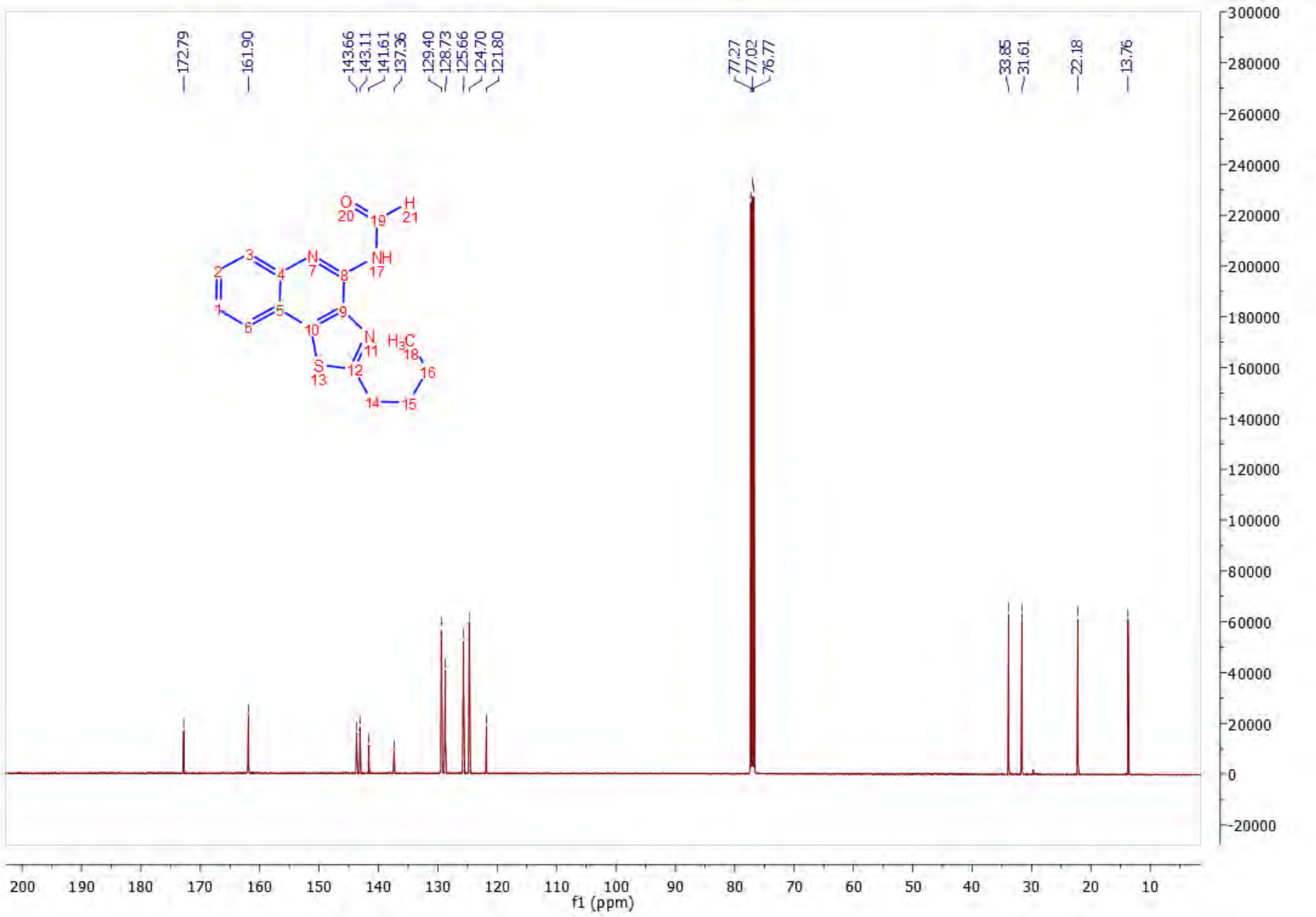
17 LC-MS



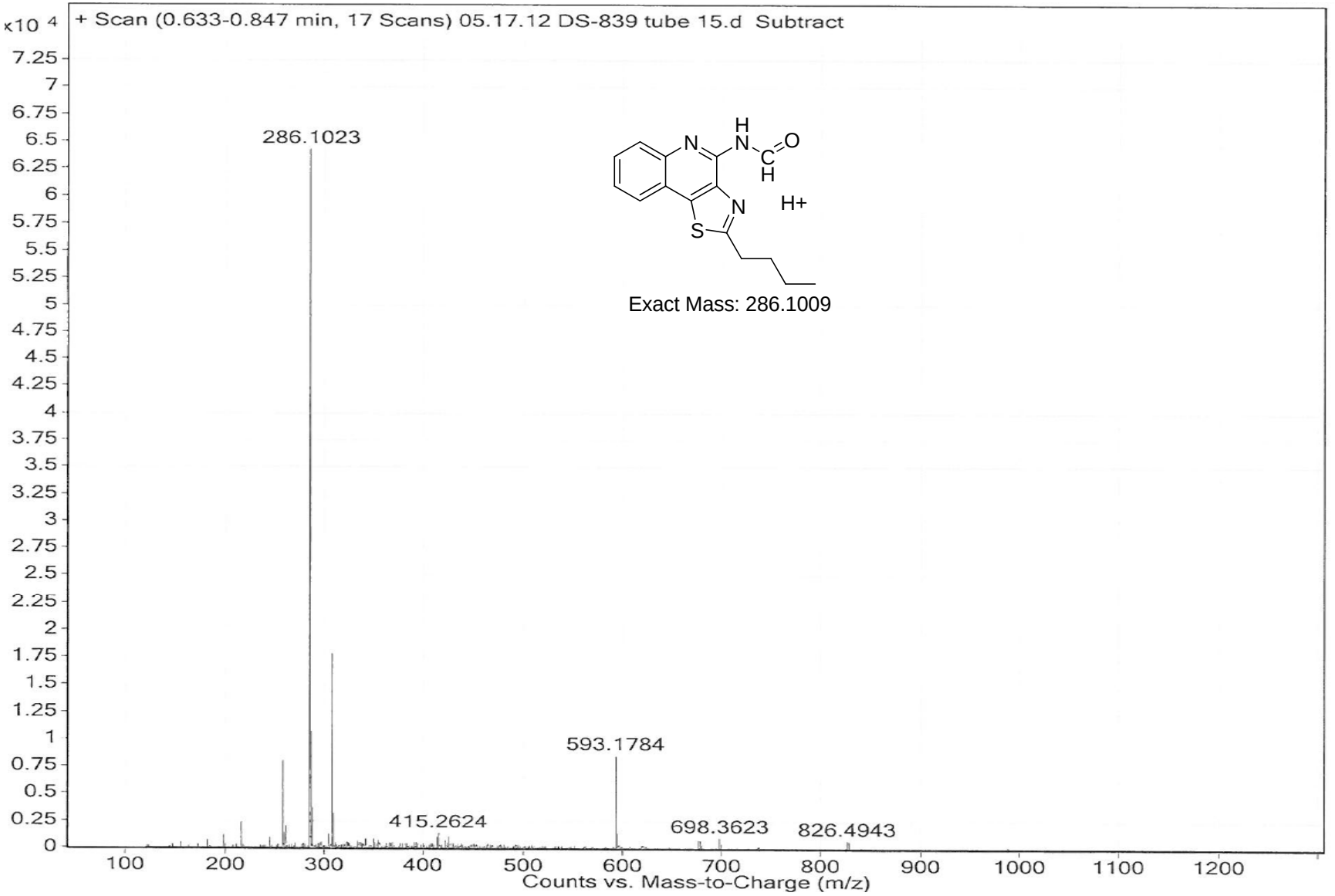
18a ^{1}H NMR



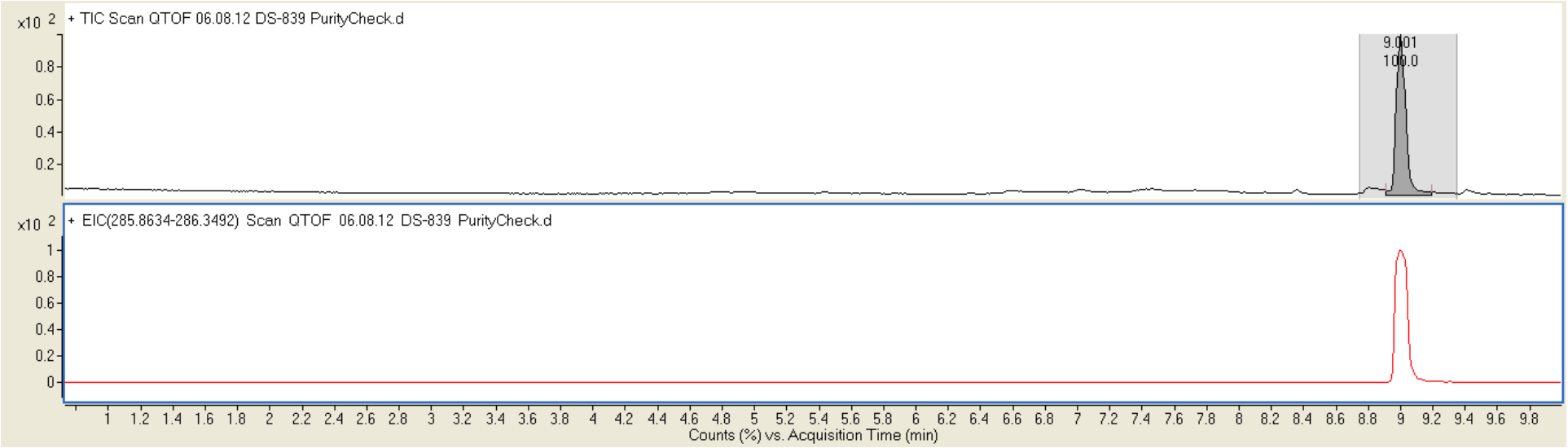
18a ^{13}C NMR

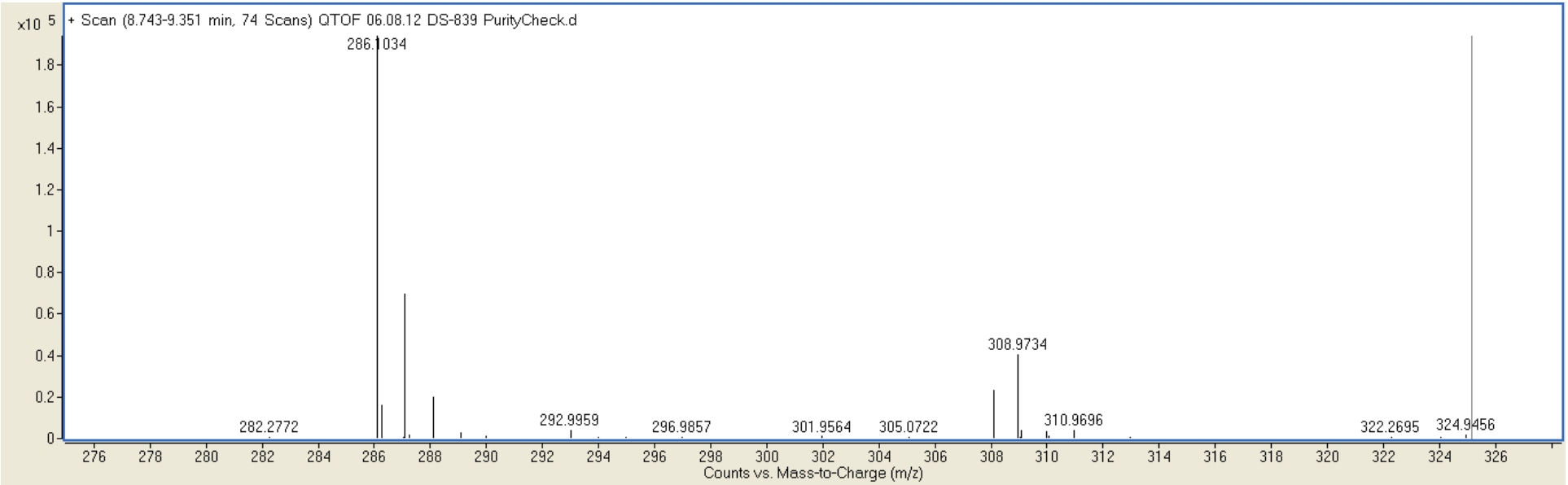


18a MS

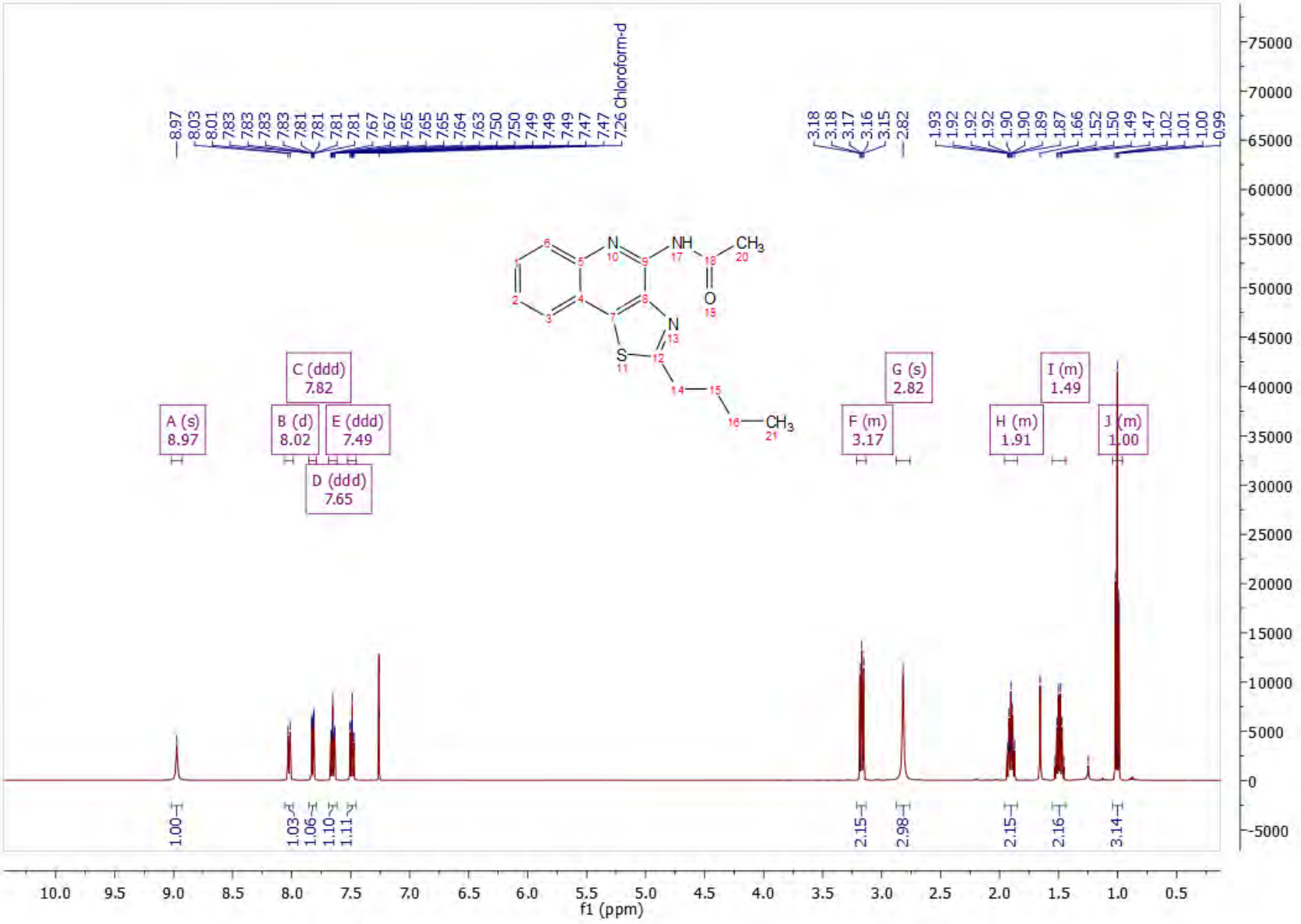


18a LC-MS

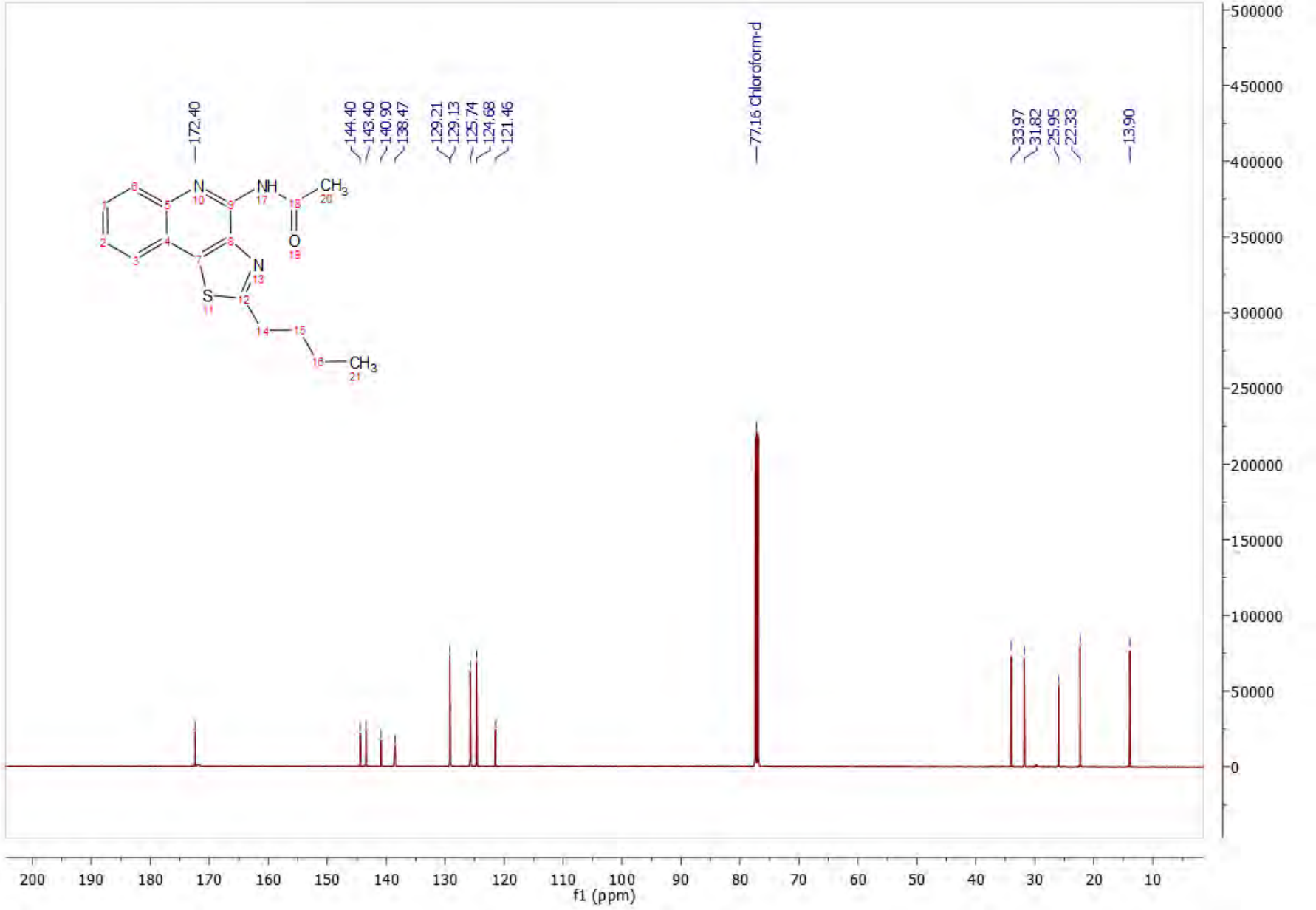




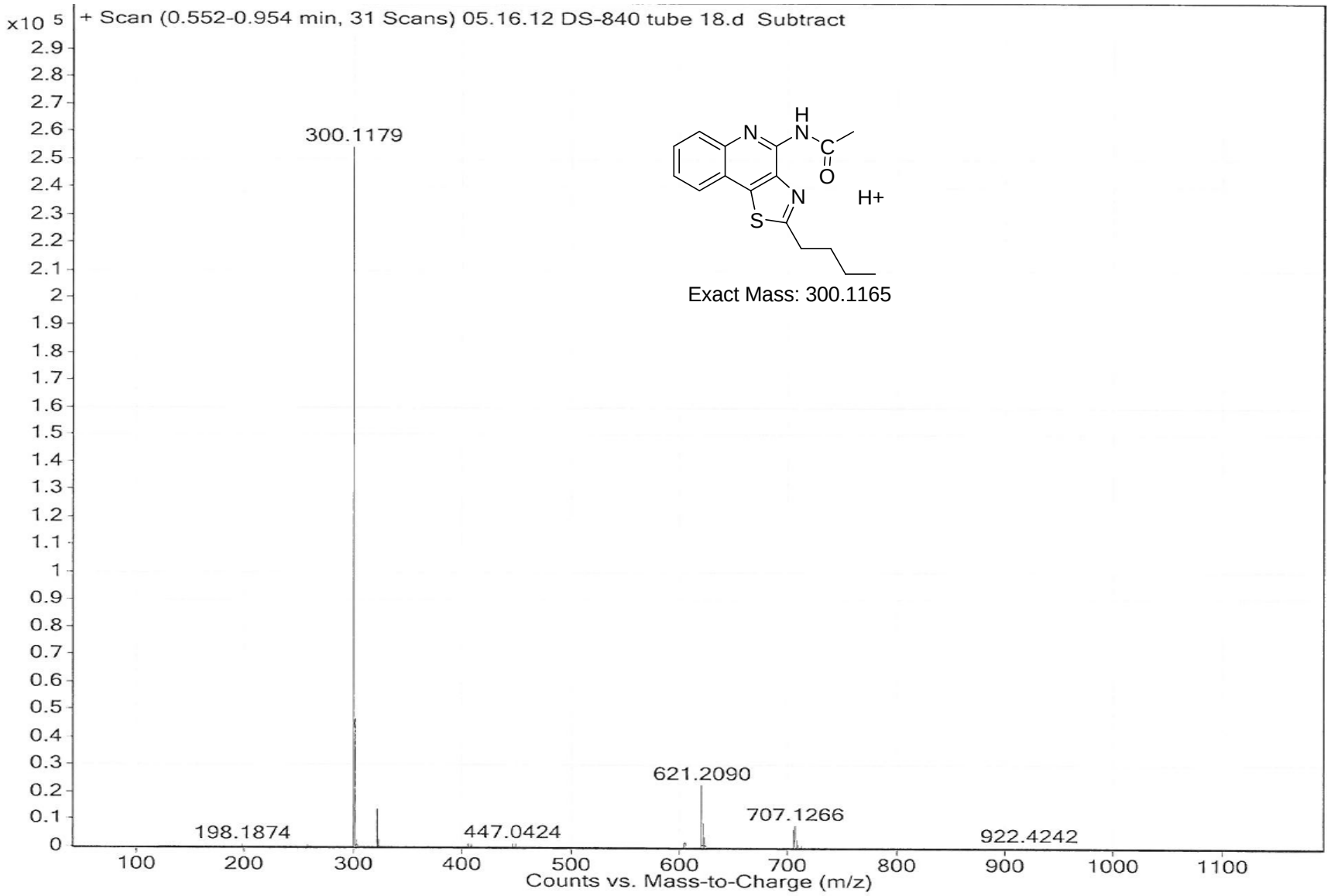
18b ^{1}H NMR



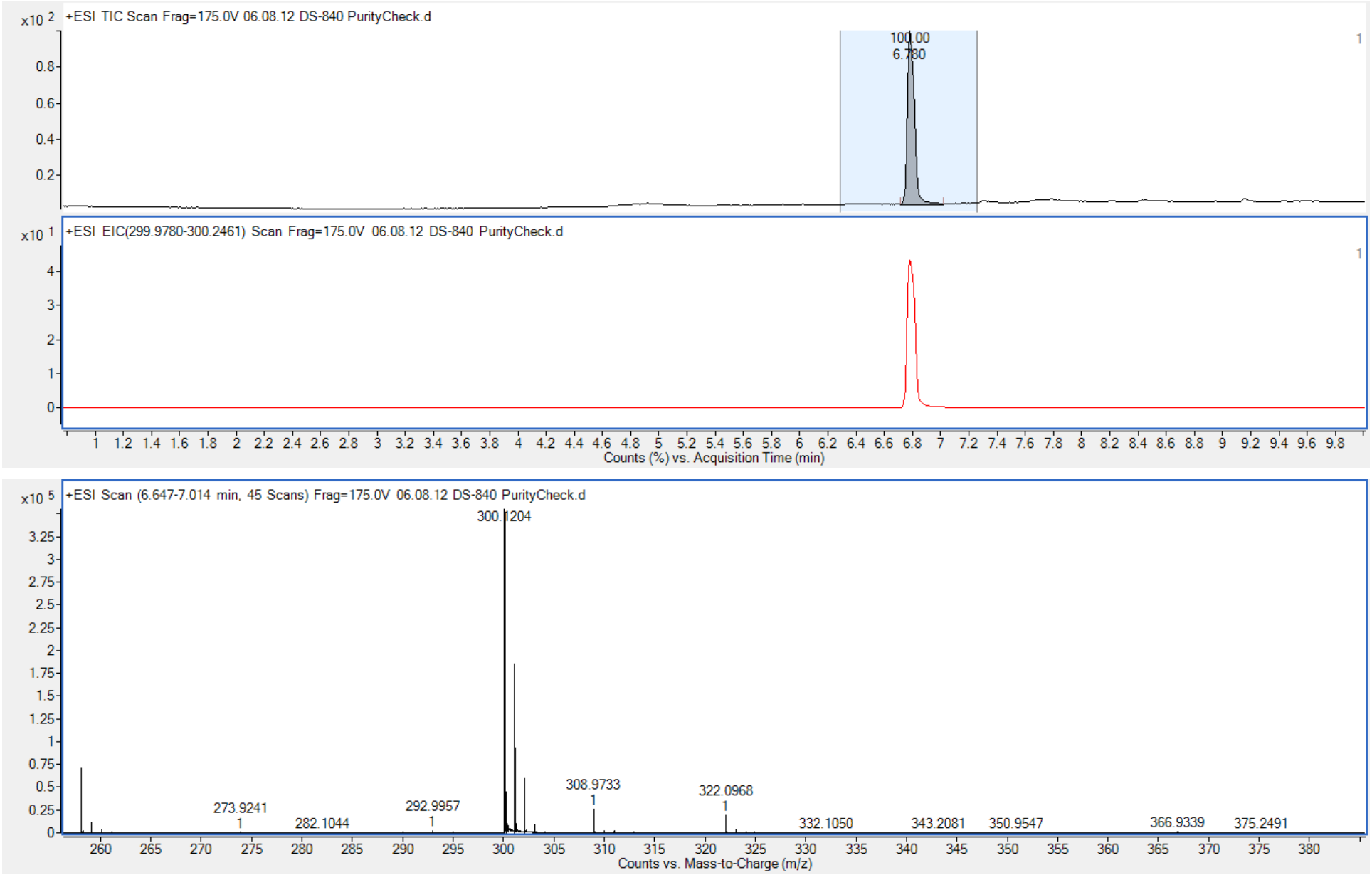
18b ^{13}C NMR



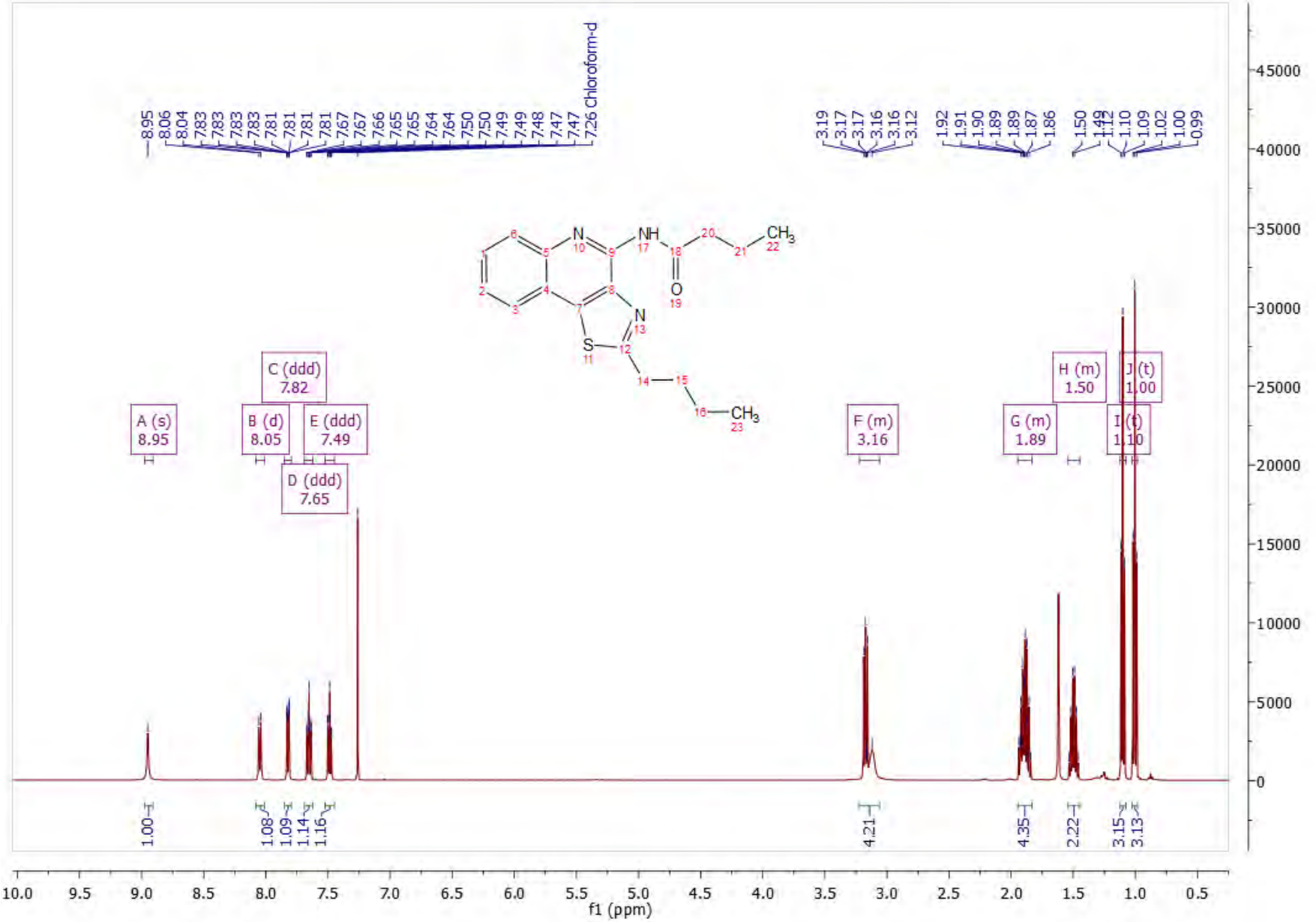
18b MS



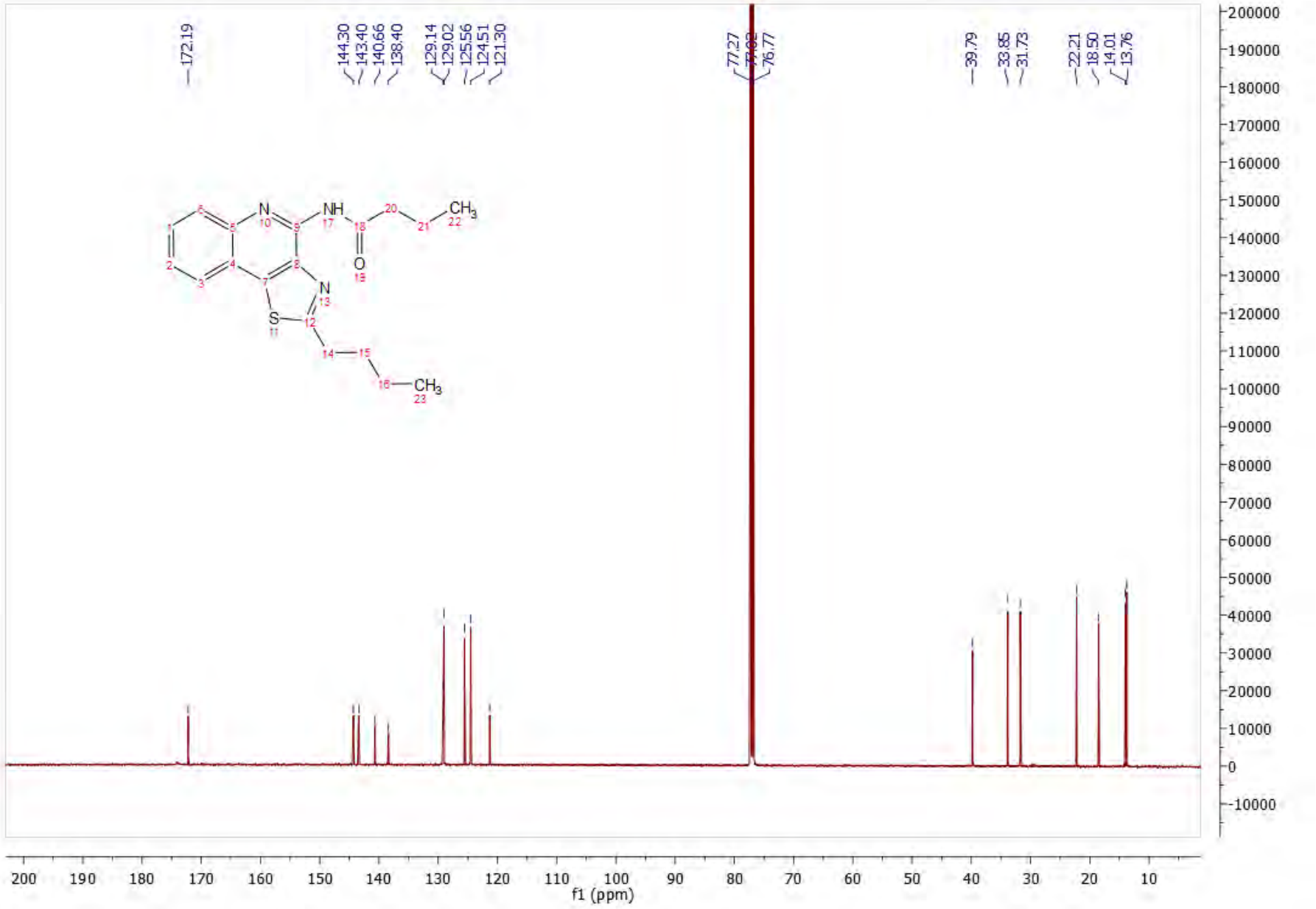
18b LC-MS



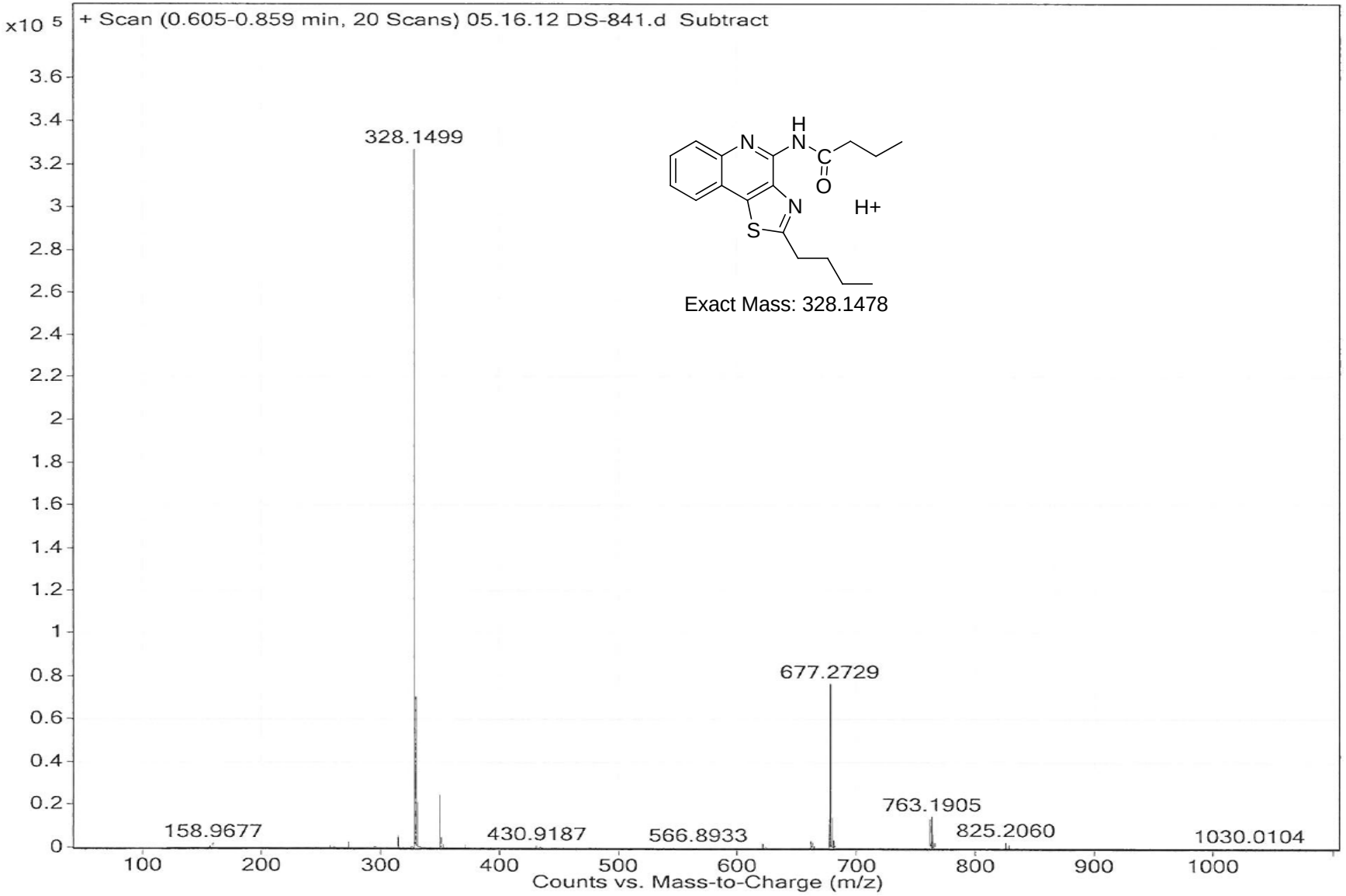
18c ^{1}H NMR



18c ^{13}C NMR



18c MS



18c LC-MS