Supporting Information

Contents:

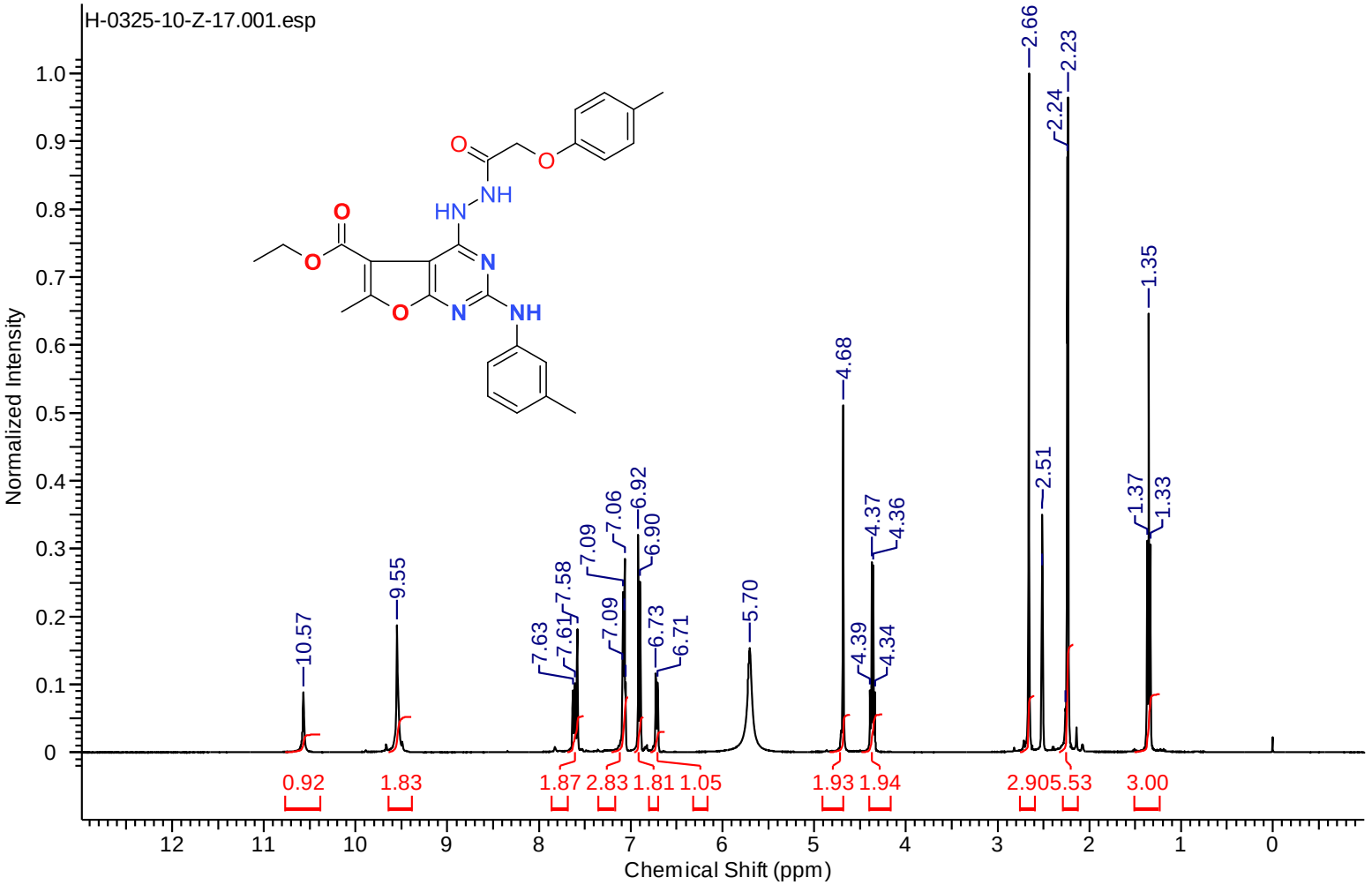
1. CCK8 assay the compounds **5a-5l, 6a-6j** and **7** were test their antitumor activity using the CCK8 assay as described previously. HepG2 cells were cultivated in a density in 96-well plates (5000 cells/well). After incubation for 24 h, cells were treated with compounds for 48 h at a final compound concentration of 0.1-50 μmol/L. Observing the absorbance at 490 nm with a microplate reader, the cell inhibition rate = ((1-A experiment)/A control) × 100%, and calculating the IC_{50} subsequently.

2. Compound **5d** induces apoptosis in HepG2 cells the apoptotic effect of compound **5d** was carried out with propidium iodide (PI) and FITC-annexin-V stain. According to previously reported method and guidance of instructions, HepG2 cells were treated with compound **5d** at 0, 5.0, 10.0, 15.0μmol/L, respectively, for 48 h, and then analyzed by flow cytometry assay.

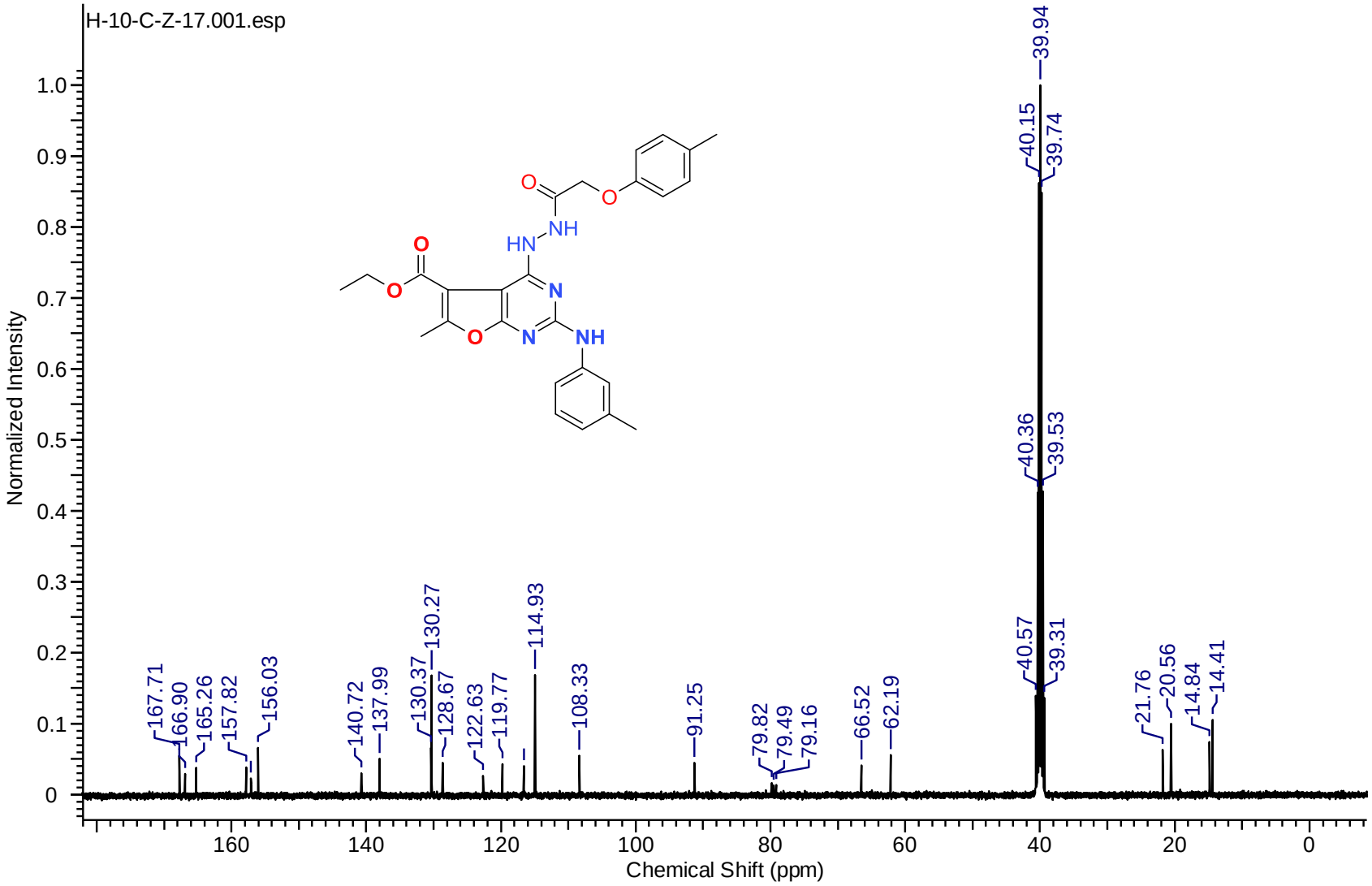
3. Molecular Docking Study

The three-dimension (3D) structures of all compounds were prepared by SYBYL 7.0 followed by 2,000-steps steepest descent minimization and 2,000-sreps conjugate gradient minimization, respectively. The crystal structure of EGFR in complex with Erlotinib (FDA approved drug) was obtained from Protein Data Bank (PDB ID: 1M17). The Erlotinib was deleted from the complex structure and the location of it was used to define the active site. The hydrogen of the receptor were added by using Discovery Studio 4.0. The GOLD 3.0 was used to dock compound **5d** into the active center. The radius of active site was set to 10 Å by using a genetic algorithm (GA) with 300 runs. The top rank conformation of the two compounds were selected as the representative. The docking score is calculated using Autodock Score and expressed in terms of binding free energies (ΔGcal, Kcal/mol). The experimental binding free energies (ΔGexp, Kcal/mol) using the equation $\Delta G = RT\ln IC_{50}$.

4. ^{1}H NMR spectra, ^{13}C NMR, IR and HRMS spectra of compounds **5a-5l**, **6a-6j** and **7a, 7b**

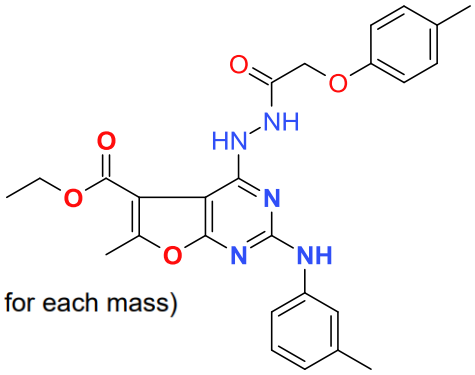


^{1}H NMR **5a**


H-10-C-Z-17.001.esp
Normalized Intensity
Chemical Shift (ppm)
167.71
166.90
165.26
157.82
156.03
140.72
137.99
130.37
130.27
128.67
122.63
119.77
114.93
108.33
91.25
79.82
79.49
79.16
66.52
62.19
40.57
40.36
40.15
39.94
39.74
39.53
39.31
21.76
20.56
14.84
14.41

^{13}C NMR **5a**

Elemental Composition Report



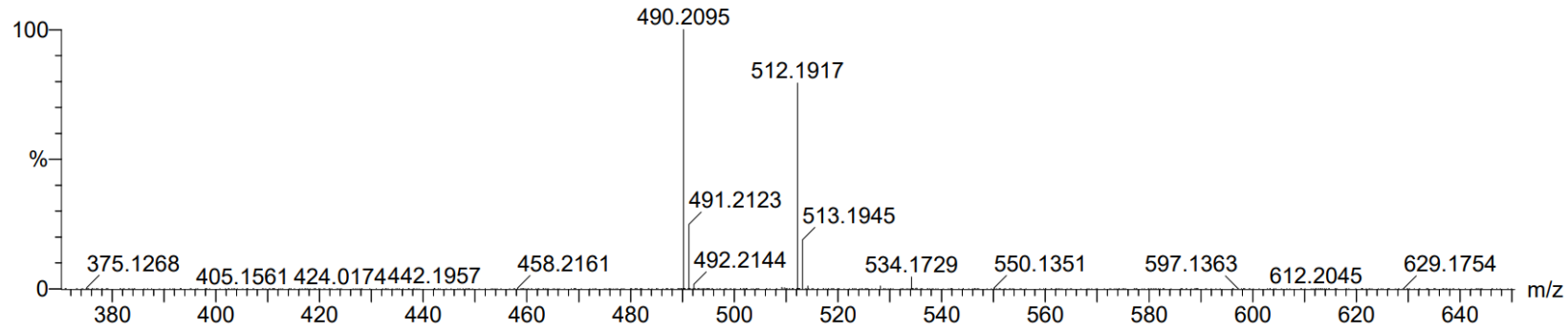
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
972 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 26-26 H: 28-28 N: 0-100 O: 0-100 Na: 0-1

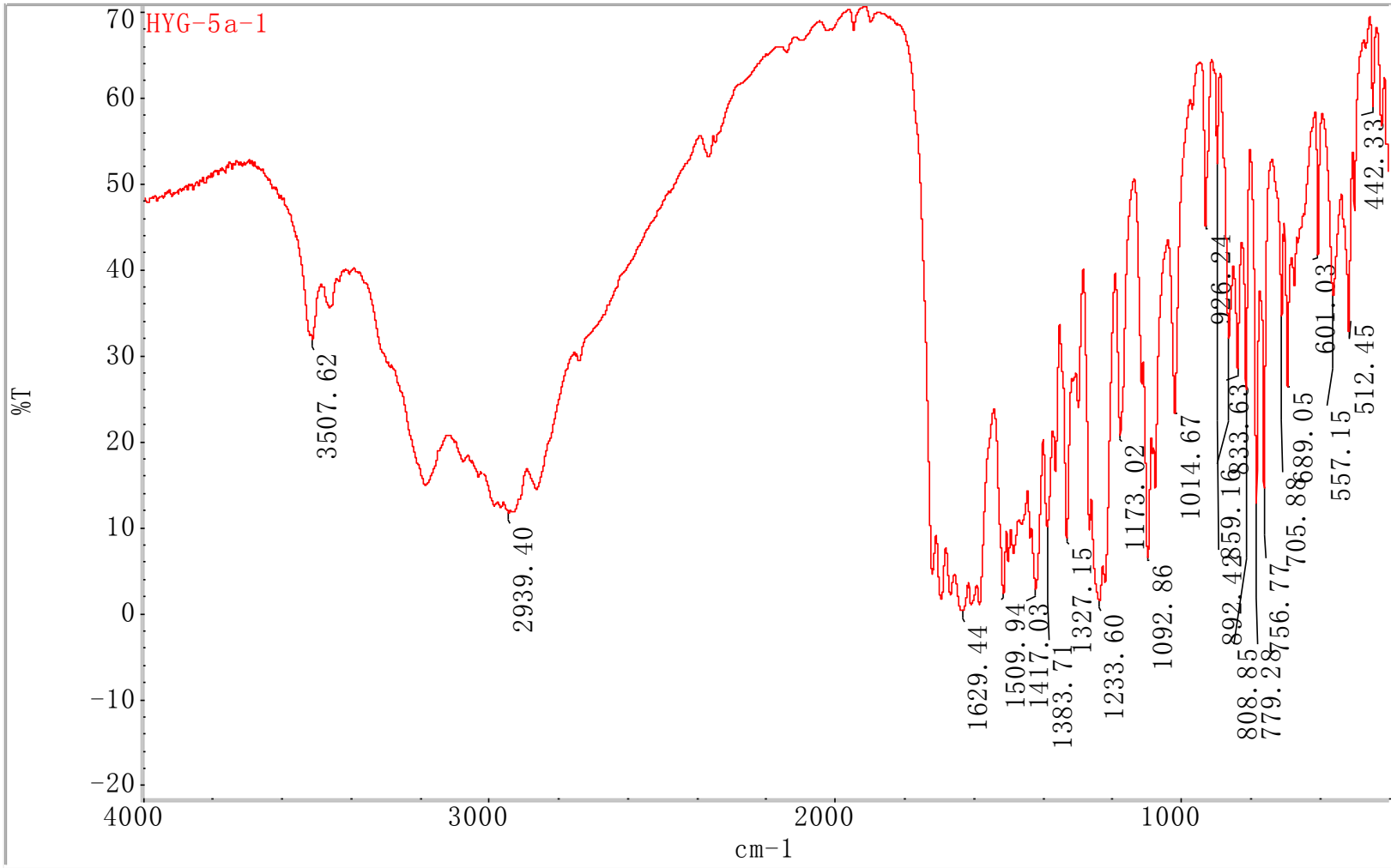
7
240331-2-8-8 11 (0.076)

1: TOF MS ES+
2.01e+005

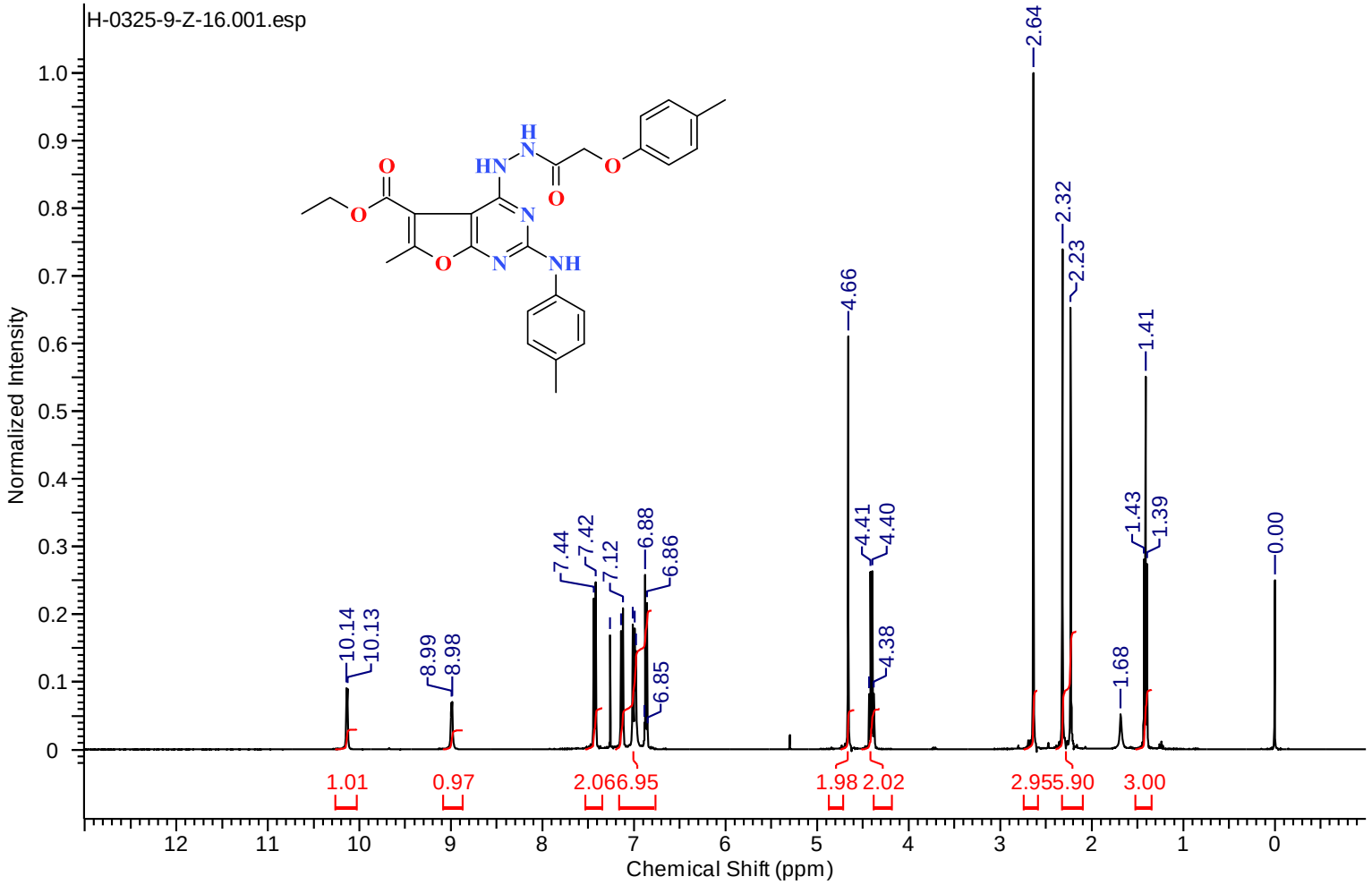


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
490.2095	490.2090	0.5	1.0	15.5	163.9	n/a	n/a	C26 H28 N5 O5

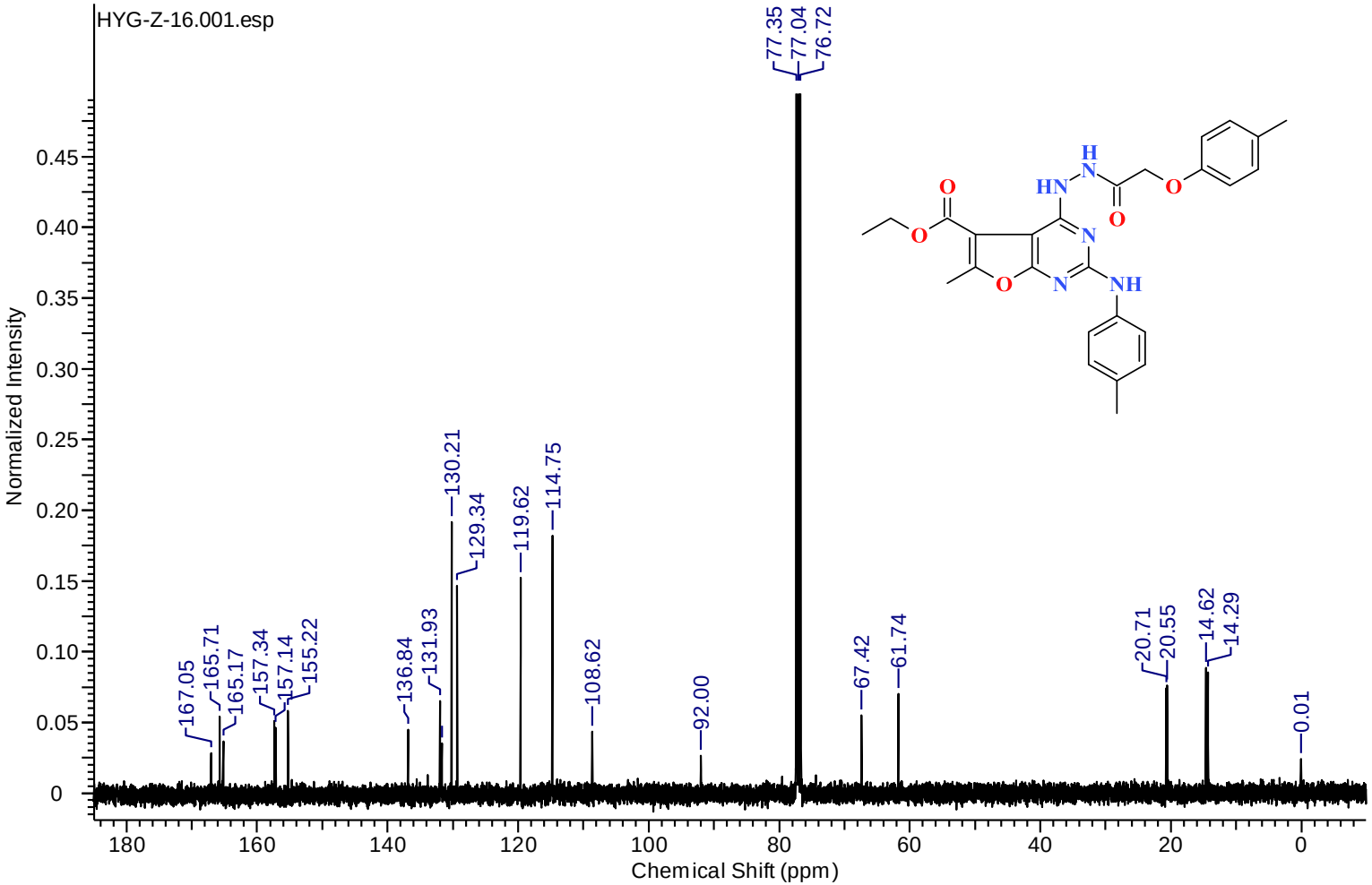
HRMS m/z **5a**


HYG-5a-1
%T
70
60
50
40
30
20
10
0
-10
-20
4000
3000
2000
1000
cm-1
3507.62
2939.40
1629.44
1509.94
1417.03
1383.71
1327.15
1233.60
1173.02
1092.86
1014.67
926.24
892.42
859.16
833.63
808.85
779.28
756.77
705.88
689.05
601.03
557.15
512.45
442.33

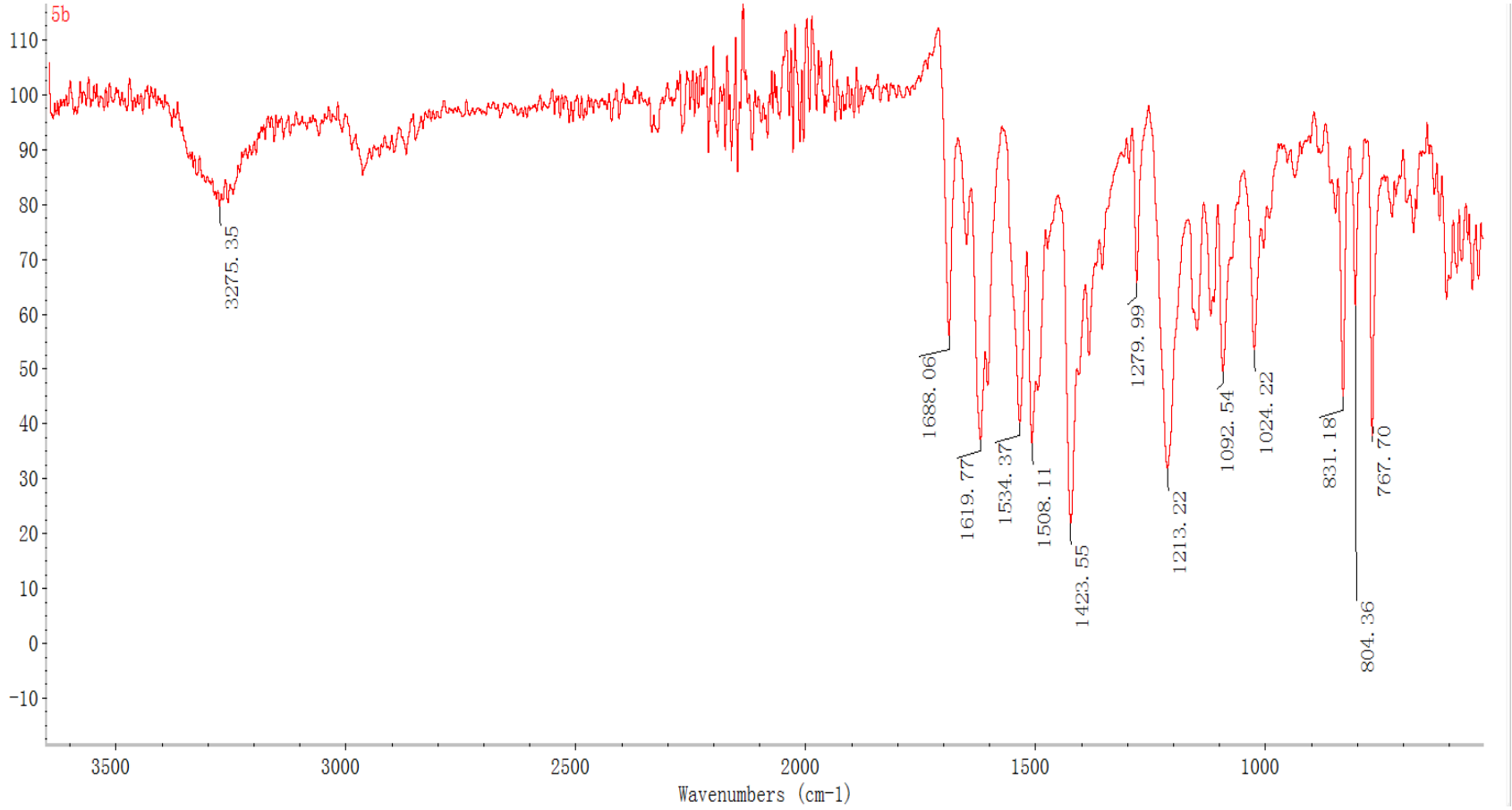
4. ^{1}H NMR spectra, ^{13}C NMR and HRMS spectra of compounds **5a-5l**, **6a-6j** and **7a-7b**.



^{1}H NMR **5b**


HYG-Z-16.001.esp
Normalized Intensity
Chemical Shift (ppm)
77.35
77.04
76.72
167.05
165.71
165.17
157.34
157.14
155.22
136.84
131.93
130.21
129.34
119.62
114.75
108.62
92.00
67.42
61.74
20.71
20.55
14.62
14.29
0.01

^{13}C NMR **5b**


5b
110
100
90
80
70
60
50
40
30
20
10
0
-10
3500
3000
2500
2000
1500
1000
Wavenumbers (cm-1)
3275.35
1688.06
1619.77
1534.37
1508.11
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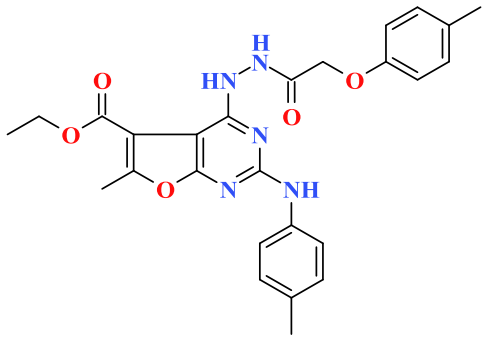
1092.54
1024.22
831.18
804.36
767.70

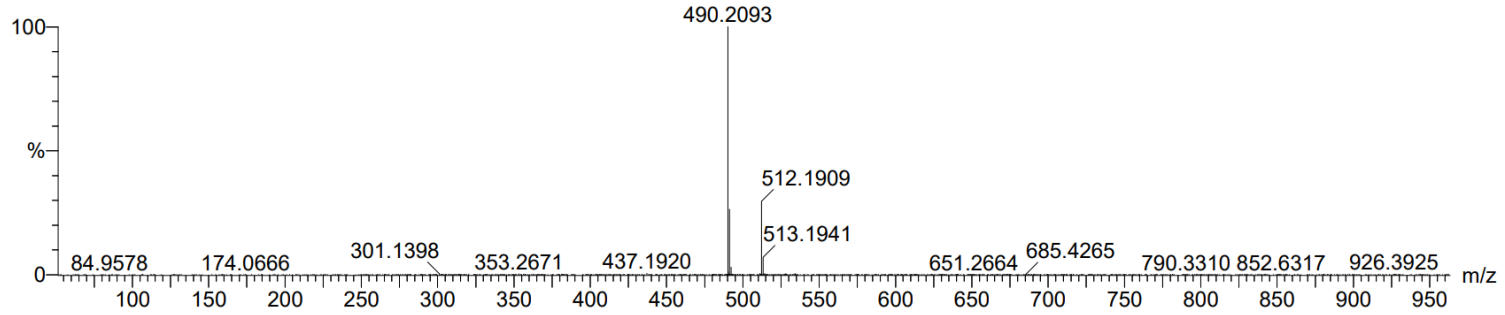


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

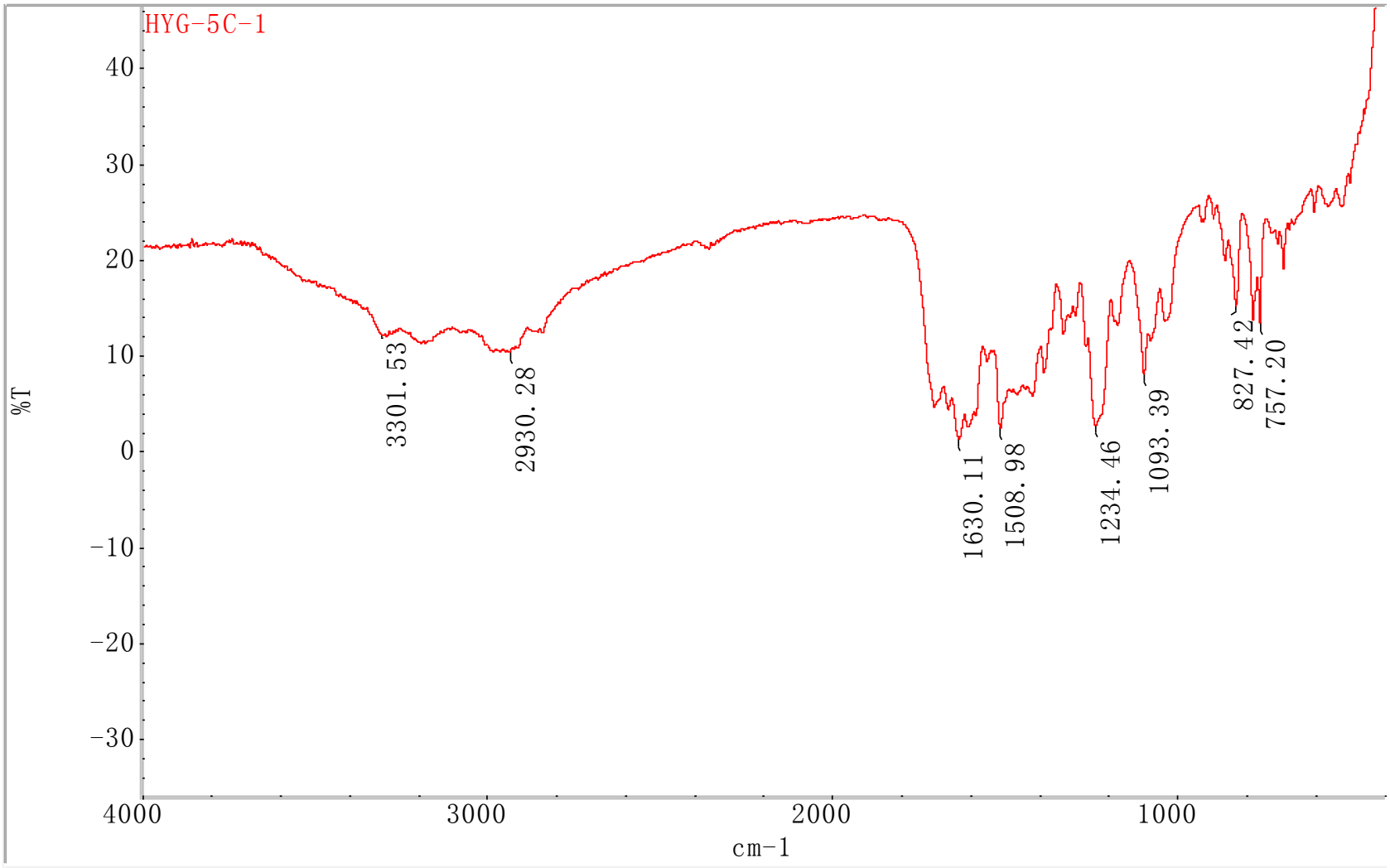
Monoisotopic Mass, Even Electron Ions
972 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 26-26 H: 28-28 N: 0-100 O: 0-100 Na: 0-1
7
240331-2-8-7 13 (0.083)

1: TOF MS ES+
4.96e+005



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
490.2093	490.2090	0.3	0.6	15.5	193.7	n/a	n/a	C26 H28 N5 O5

HRMS m/z **5b**


HYG-5C-1
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30
20
10
0
-10
-20
-30
%T
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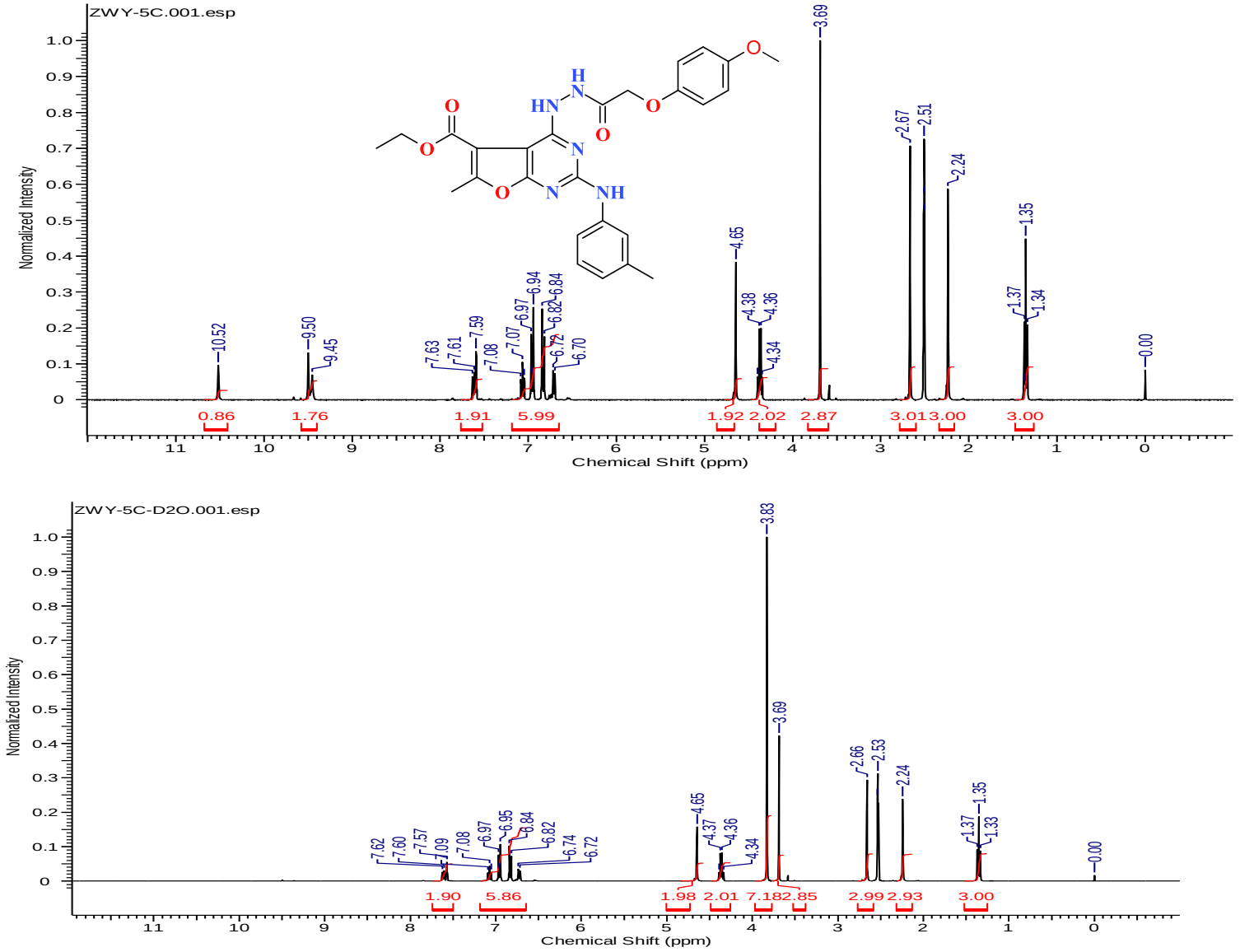
1508.98
1234.46
1093.39
827.42
757.20
4000
3000
2000
1000
cm-1


ZWY-5C.001.esp
Normalized Intensity
Chemical Shift (ppm)
10.52
9.50
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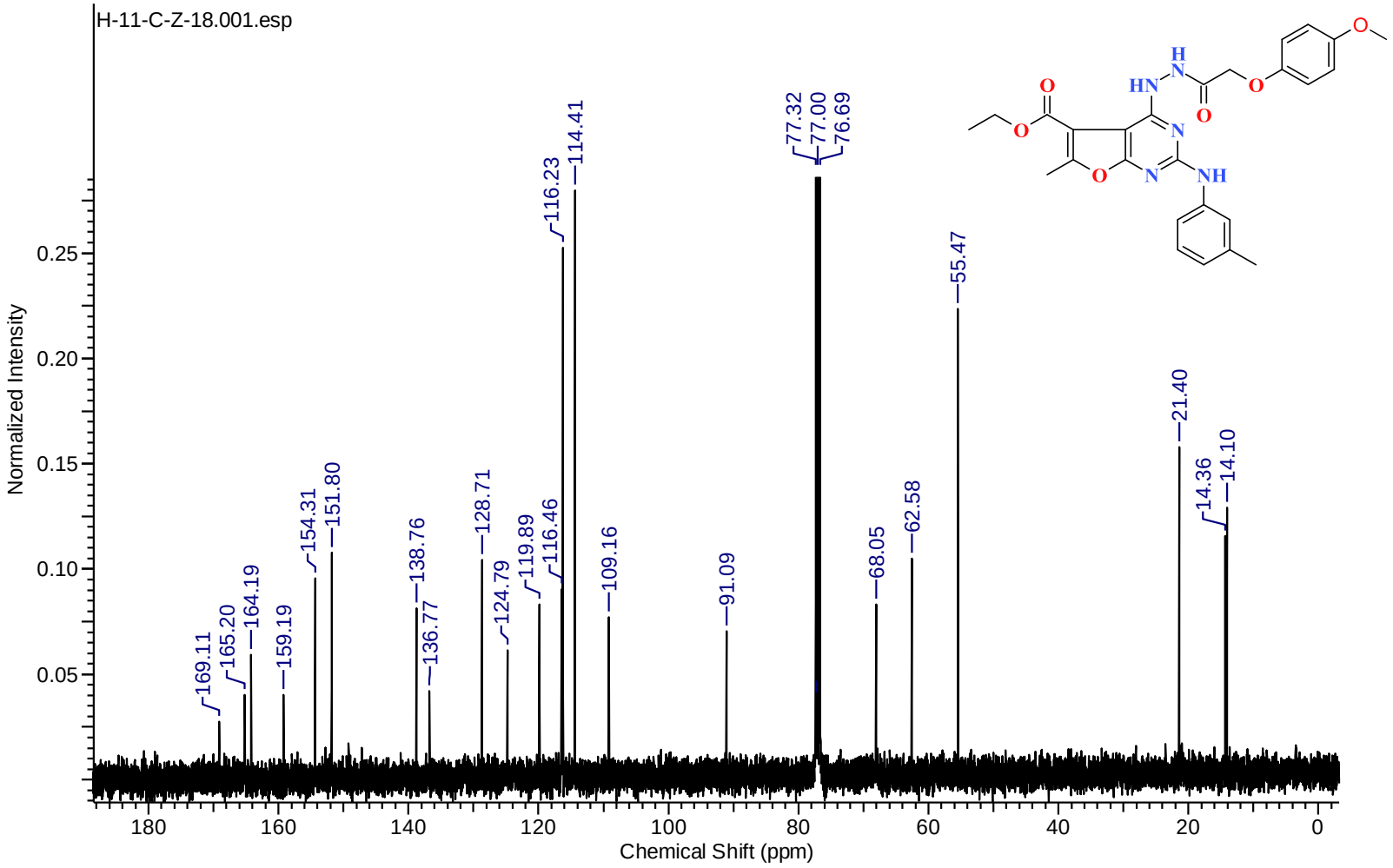
7.61
7.59
7.08
7.07
6.97
6.94
6.84
6.82
6.72
6.70
4.65
4.38
4.36
4.34
3.69
2.67
2.51
2.24
1.37
1.35
1.34
0.00
0.86
1.76
1.91
5.99
1.92
2.02
2.87
3.01
3.00
3.00
ZWY-5C-D2O.001.esp
Normalized Intensity
Chemical Shift (ppm)
7.62
7.60
7.57
7.09
7.08
6.97
6.95
6.84
6.82
6.74
6.72
4.65
4.37
4.36
4.34
3.83
3.69
2.66
2.53
2.24
1.37
1.35
1.33
0.00
1.90
5.86
1.98
2.01
7.18
2.85
2.99
2.93
3.00

^{1}H NMR **5c**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Normalized Intensity
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0.05
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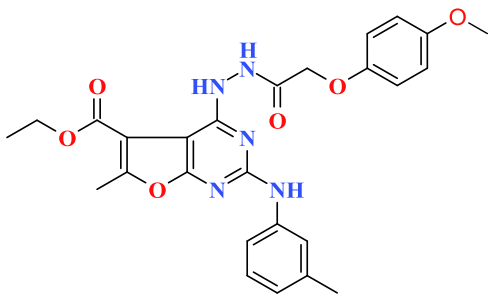
164.19
159.19
154.31
151.80
138.76
136.77
128.71
124.79
119.89
116.46
116.23
114.41
109.16
91.09
77.32
77.00
76.69
68.05
62.58
55.47
21.40
14.36
14.10
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
O
O
O
O
HN
H
N
N
N
NH
O
O

^{13}C NMR **5c**



Elemental Composition Report

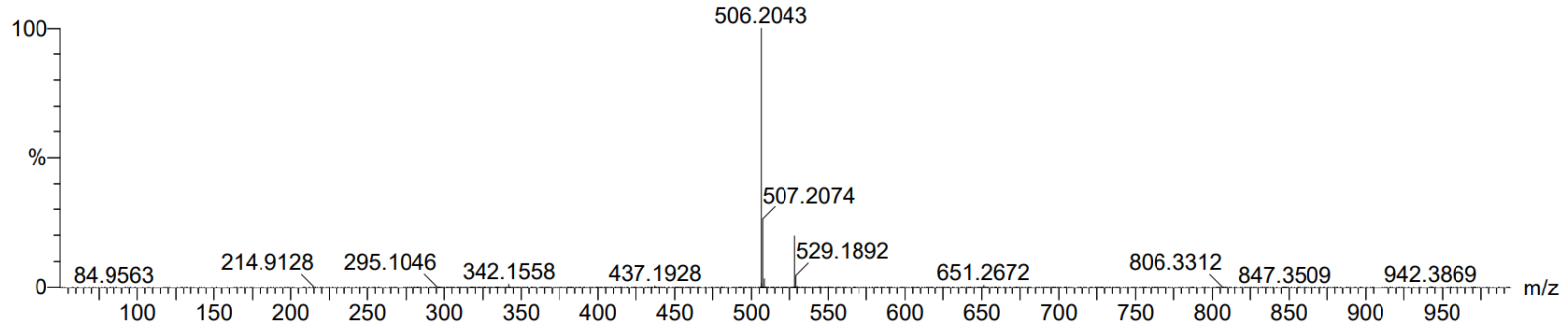
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1030 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 26-26 H: 28-28 N: 0-100 O: 0-100 Na: 0-1

7
240331-2-8-9 10 (0.072)

1: TOF MS ES+
5.80e+005



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Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
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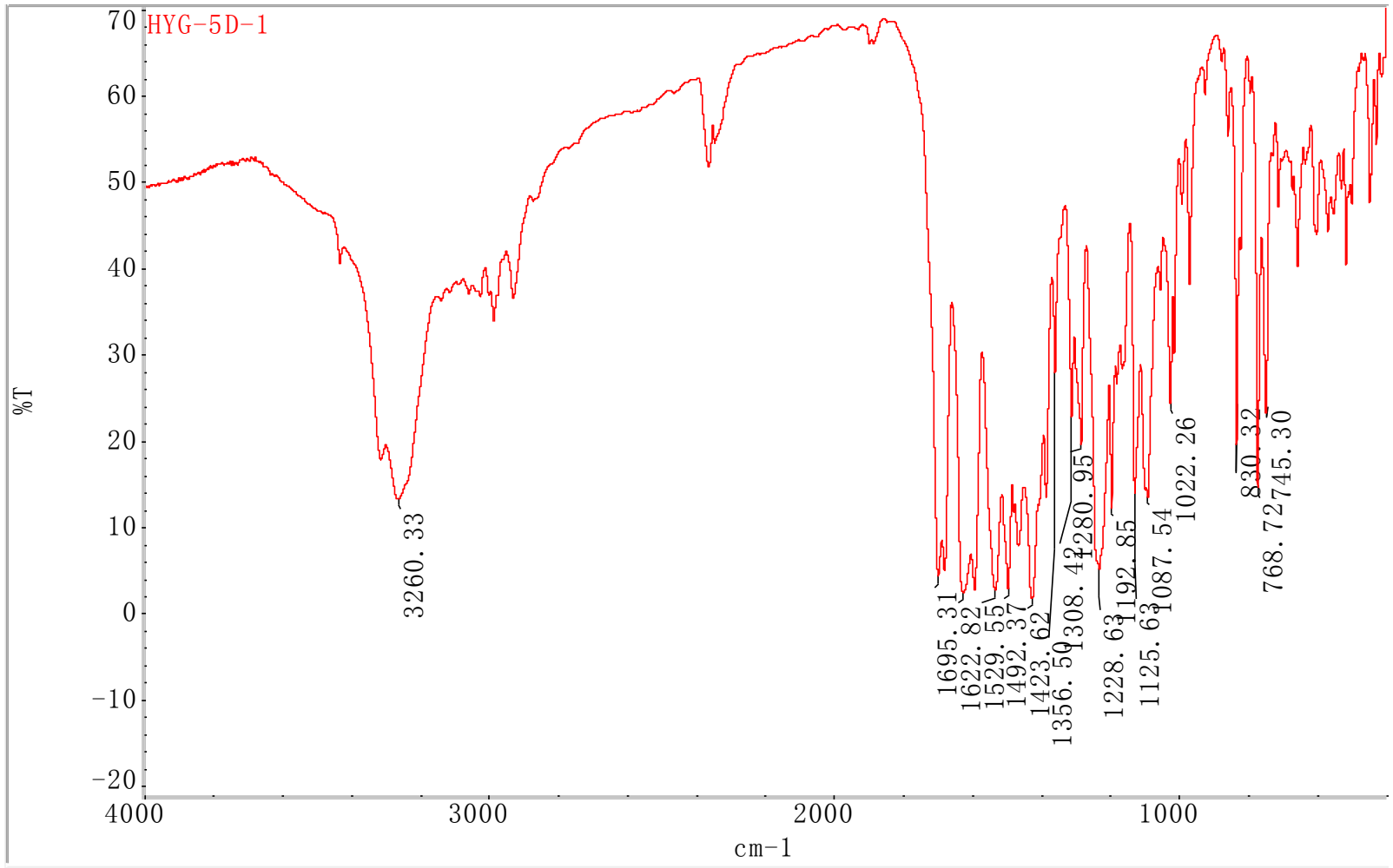
HRMS m/z **5c**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%T
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60
50
40
30
20
10
0
-10
-20
4000
3000
2000
1000
cm-1
3260.33
1695.31
1622.82
1529.55
1492.37
1423.62
1356.50
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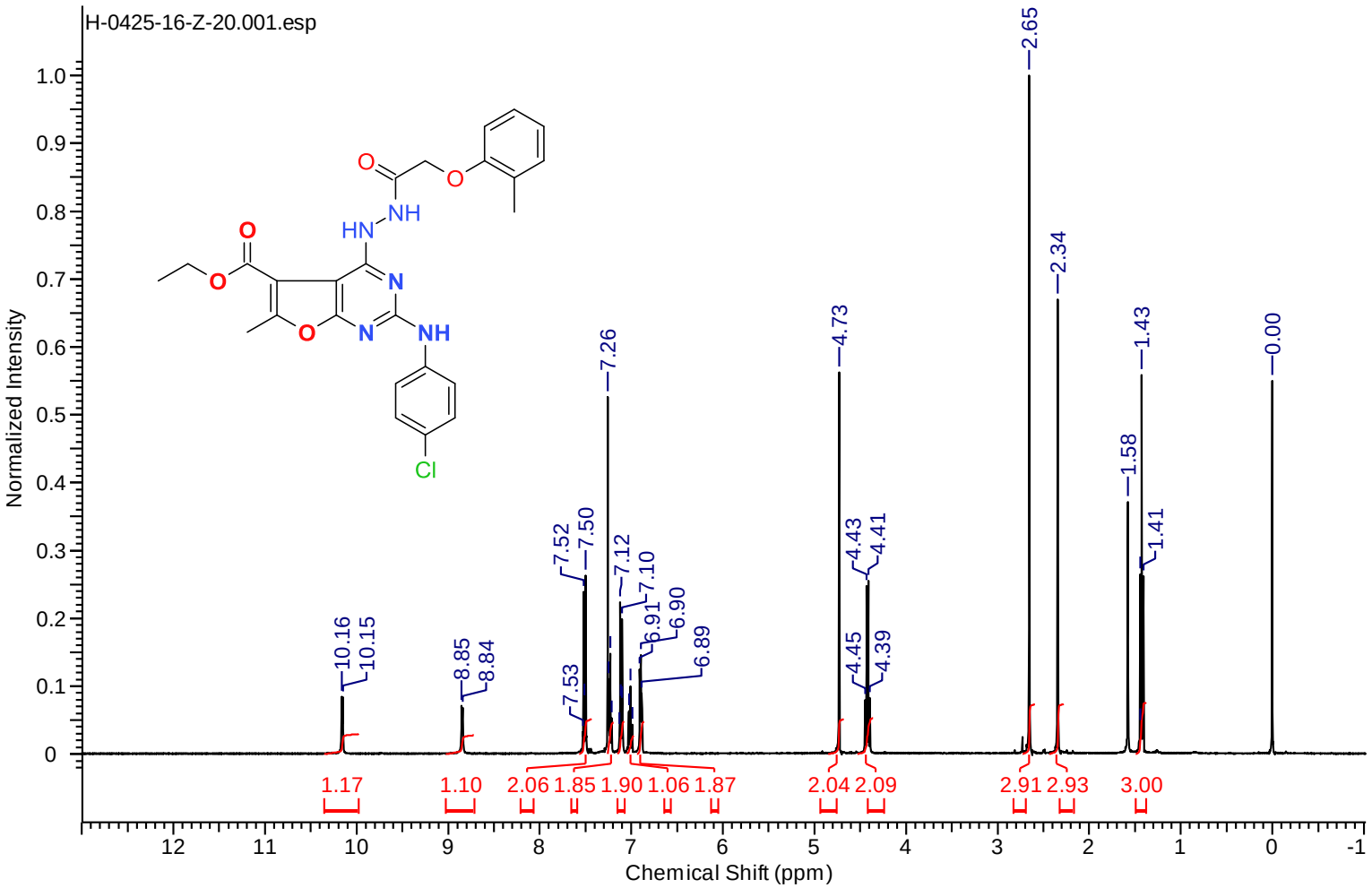
1125.63
1087.54
1022.26
830.32
768.72
745.30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7.52
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7.10
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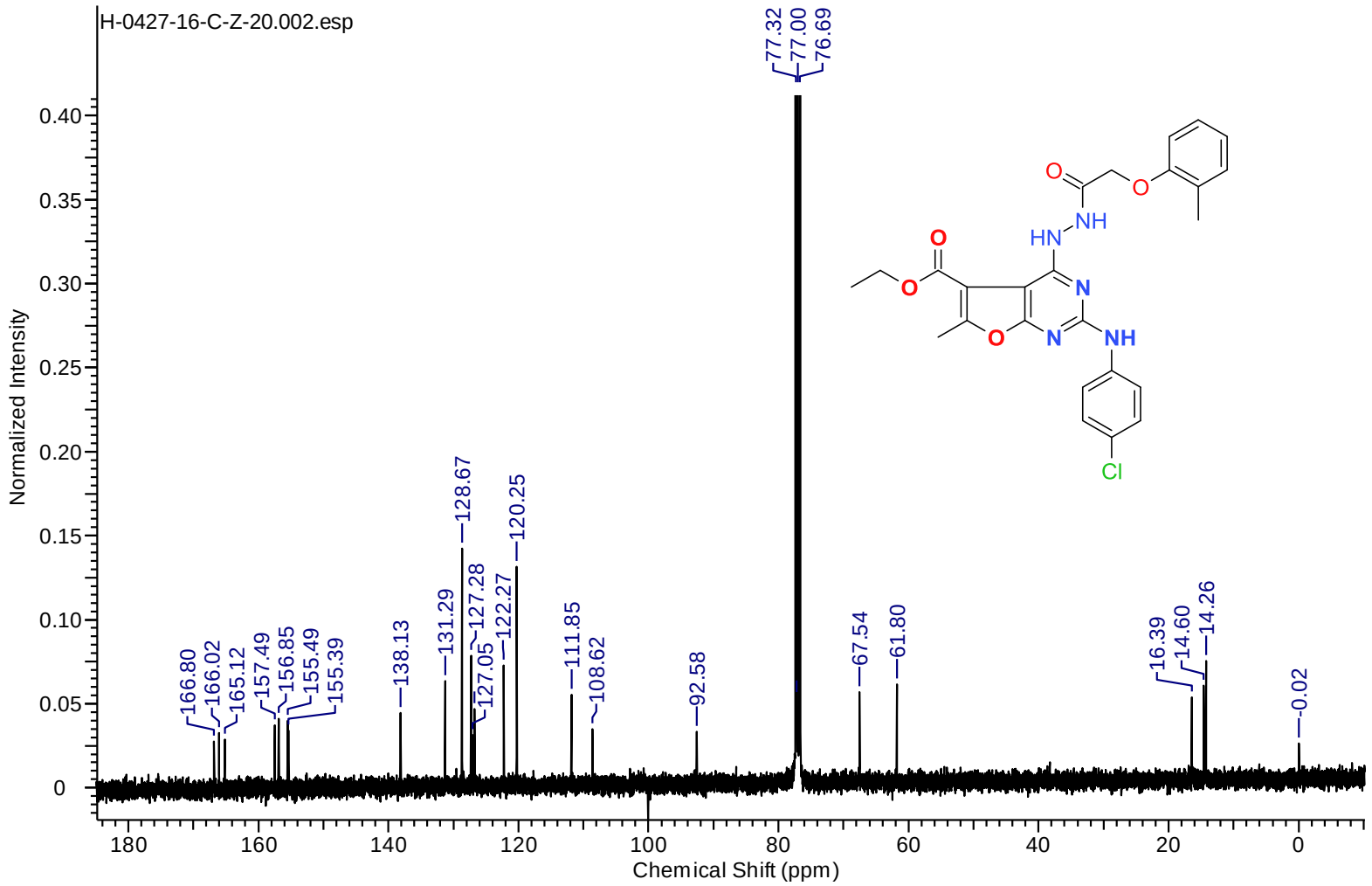
6.90
6.89
4.73
4.45
4.43
4.41
4.39
2.65
2.34
1.58
1.43
1.41
0.00
1.17
1.10
2.06
1.85
1.90
1.06
1.87
2.04
2.09
2.91
2.93
3.00
O
O
HN
NH
N
O
N
NH
Cl

^{1}H NMR **5d**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Normalized Intensity
Chemical Shift (ppm)
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76.69
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128.67
127.28
127.05
122.27
120.25
111.85
108.62
92.58
67.54
61.80
16.39
14.60
14.26
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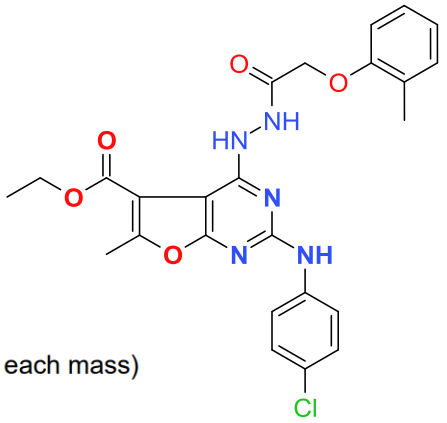
O
NH
HN
N
NH
Cl

^{13}C NMR **5d**

Elemental Composition Report



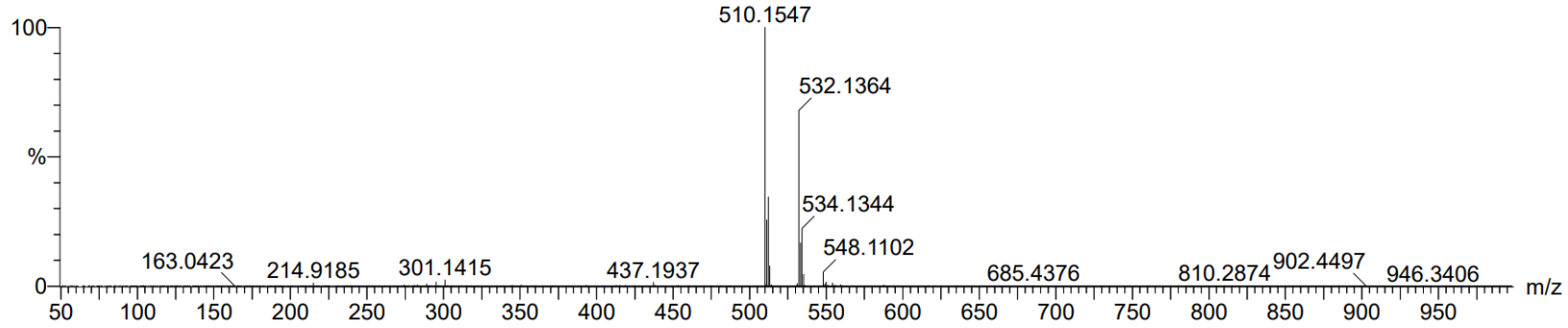
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3587 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 25-25 H: 5-25 N: 0-100 O: 0-100 Na: 0-2 Cl: 1-3

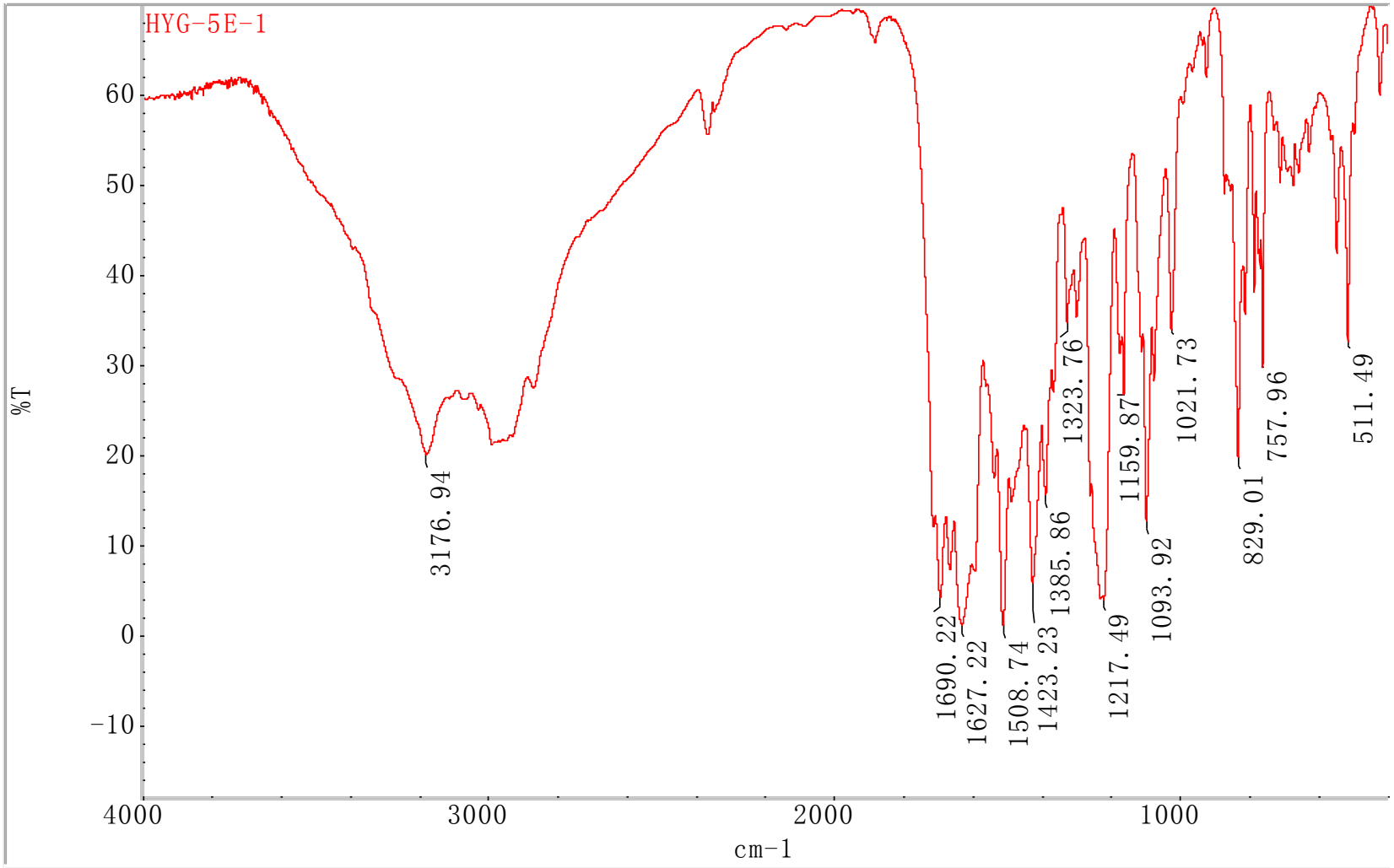
2
240503-3-16 19 (0.196)

1: TOF MS ES+
4.79e+006



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
510.1547	510.1544	0.3	0.6	15.5	651.7	n/a	n/a	C25 H25 N5 O5 Cl

HRMS m/z **5d**


HYG-5E-1
%T
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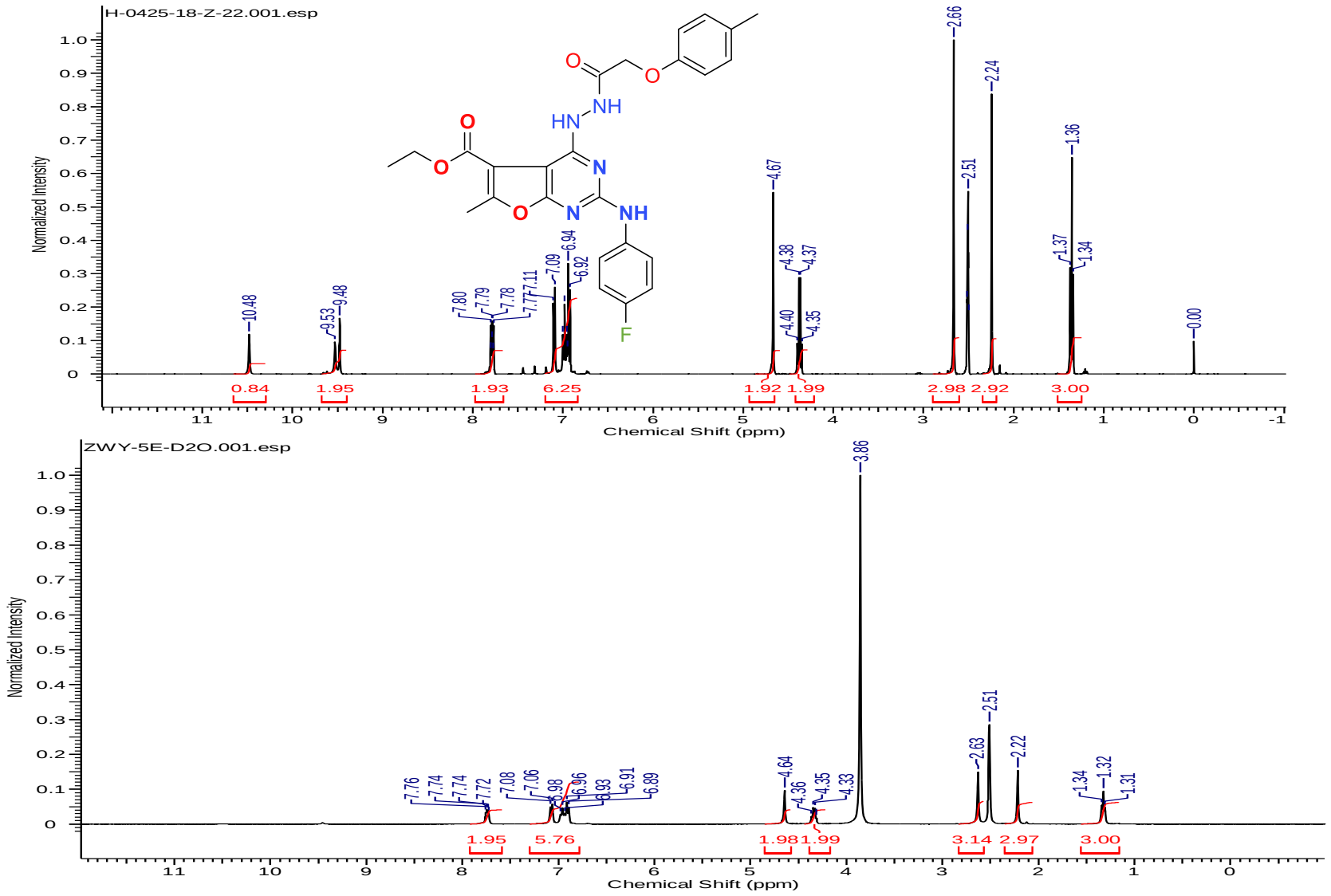
50
40
30
20
10
0
-10
4000
3000
2000
1000
cm-1
3176.94
1690.22
1627.22
1508.74
1423.23
1385.86
1323.76
1217.49
1159.87
1093.92
1021.73
829.01
757.96
511.49


H-0425-18-Z-22.001.esp
Normalized Intensity
Chemical Shift (ppm)
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9.48
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7.79
7.78
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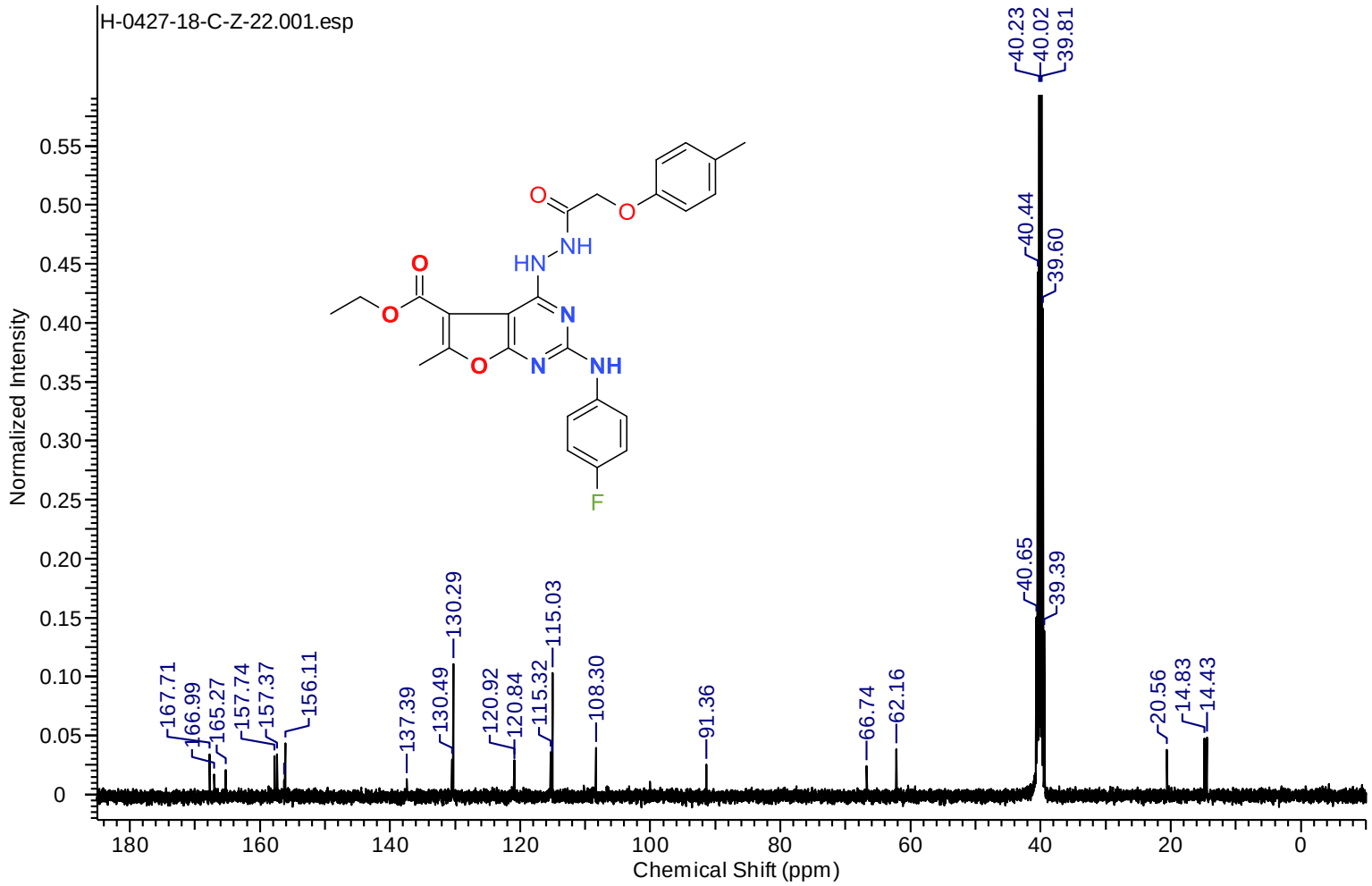
7.11
7.09
6.94
6.92
4.67
4.40
4.38
4.37
4.35
2.66
2.51
2.24
1.37
1.36
1.34
0.00
0.84
1.95
1.93
6.25
1.92
1.99
2.98
2.92
3.00
ZWY-5E-D2O.001.esp
Normalized Intensity
Chemical Shift (ppm)
7.76
7.74
7.74
7.72
7.08
7.06
6.98
6.96
6.93
6.91
6.89
4.64
4.36
4.35
4.33
3.86
2.63
2.51
2.22
1.34
1.32
1.31
1.95
5.76
1.98
1.99
3.14
2.97
3.00

^{1}H NMR **5e**


H-0427-18-C-Z-22.001.esp
Normalized Intensity
Chemical Shift (ppm)
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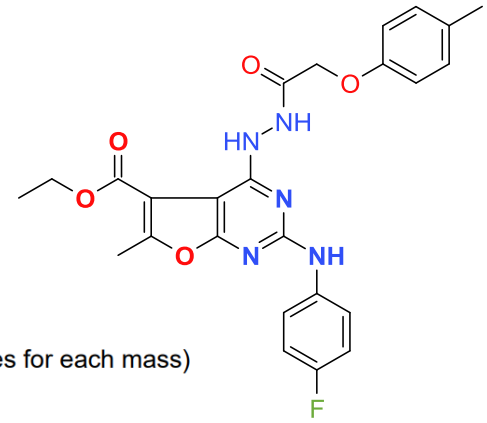
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50
0.55
180
160
140
120
100
80
60
40
20
0
167.71
166.99
165.27
157.74
157.37
156.11
137.39
130.49
130.29
120.92
120.84
115.32
115.03
108.30
91.36
66.74
62.16
40.65
40.44
40.23
40.02
39.81
39.60
39.39
20.56
14.83
14.43
O
O
HN
NH
O
O
N
O
N
NH
F

^{13}C NMR **5e**

Elemental Composition Report



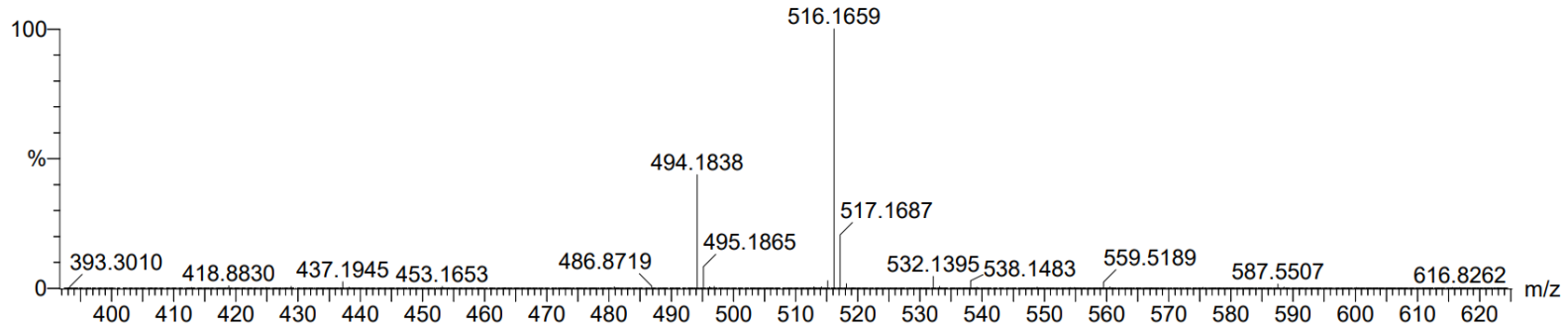
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3996 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 25-25 H: 24-24 N: 0-100 O: 0-100 Na: 0-2 F: 1-3

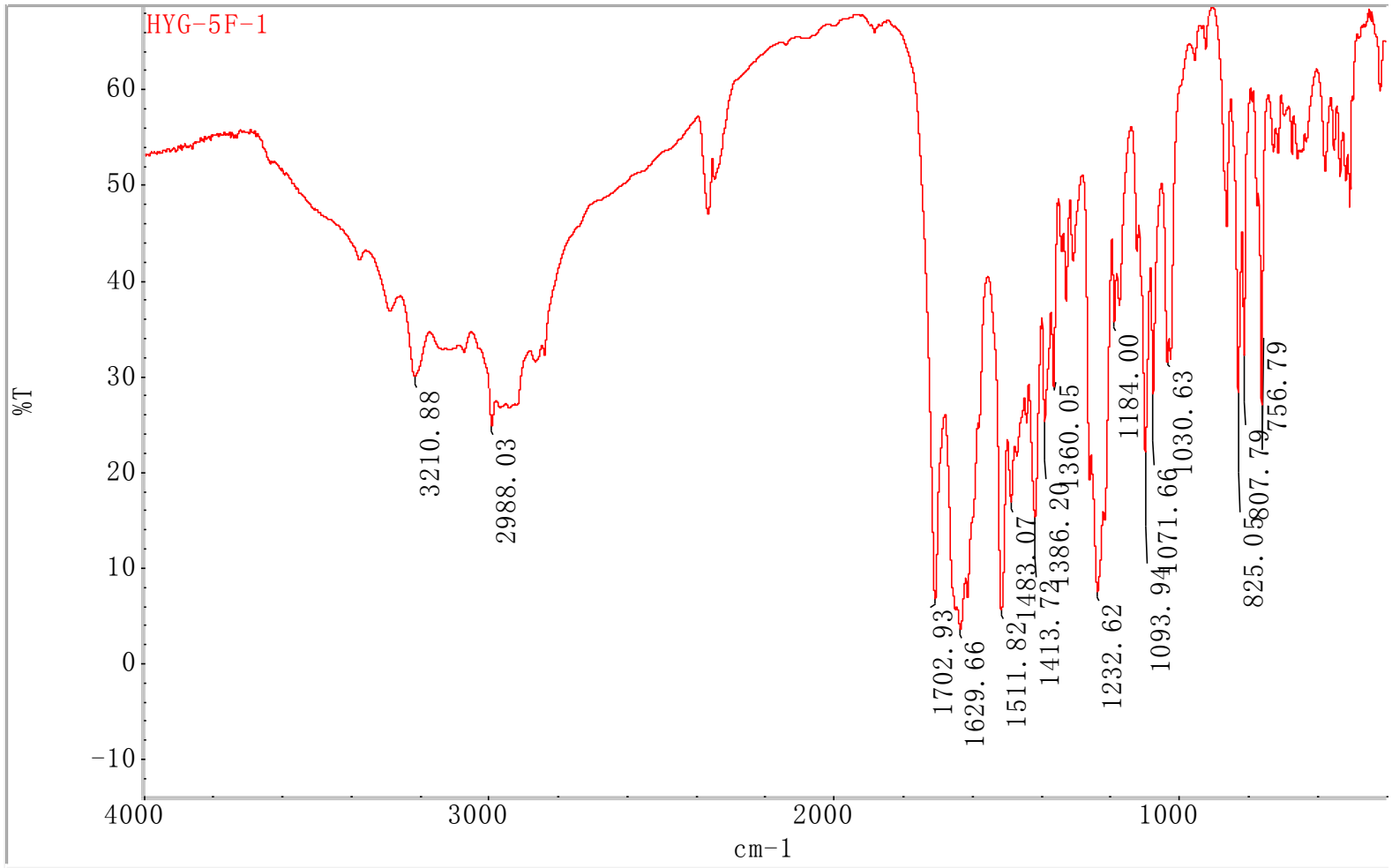
2
240503-3-18 19 (0.196)

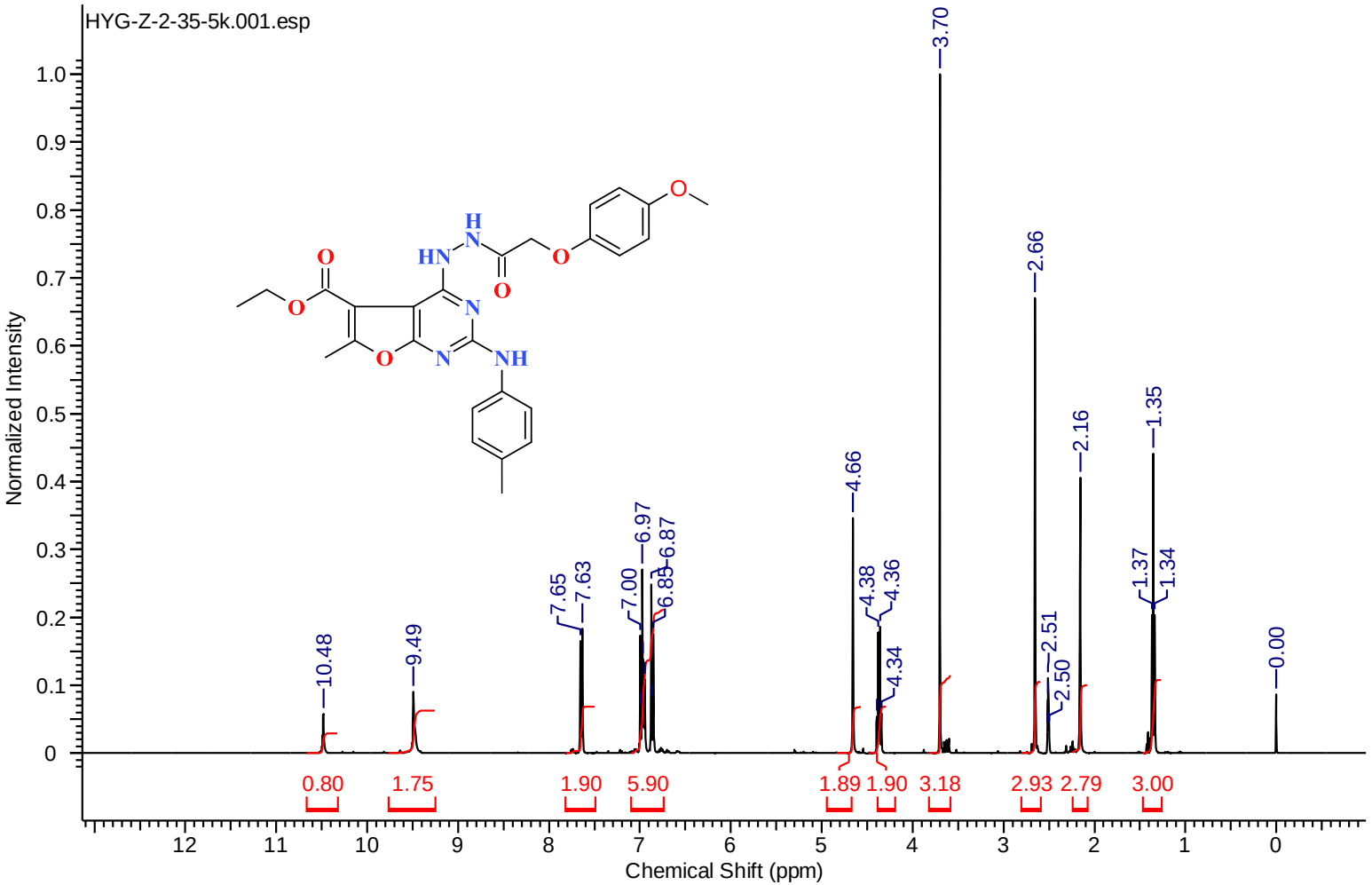
1: TOF MS ES+
9.06e+005



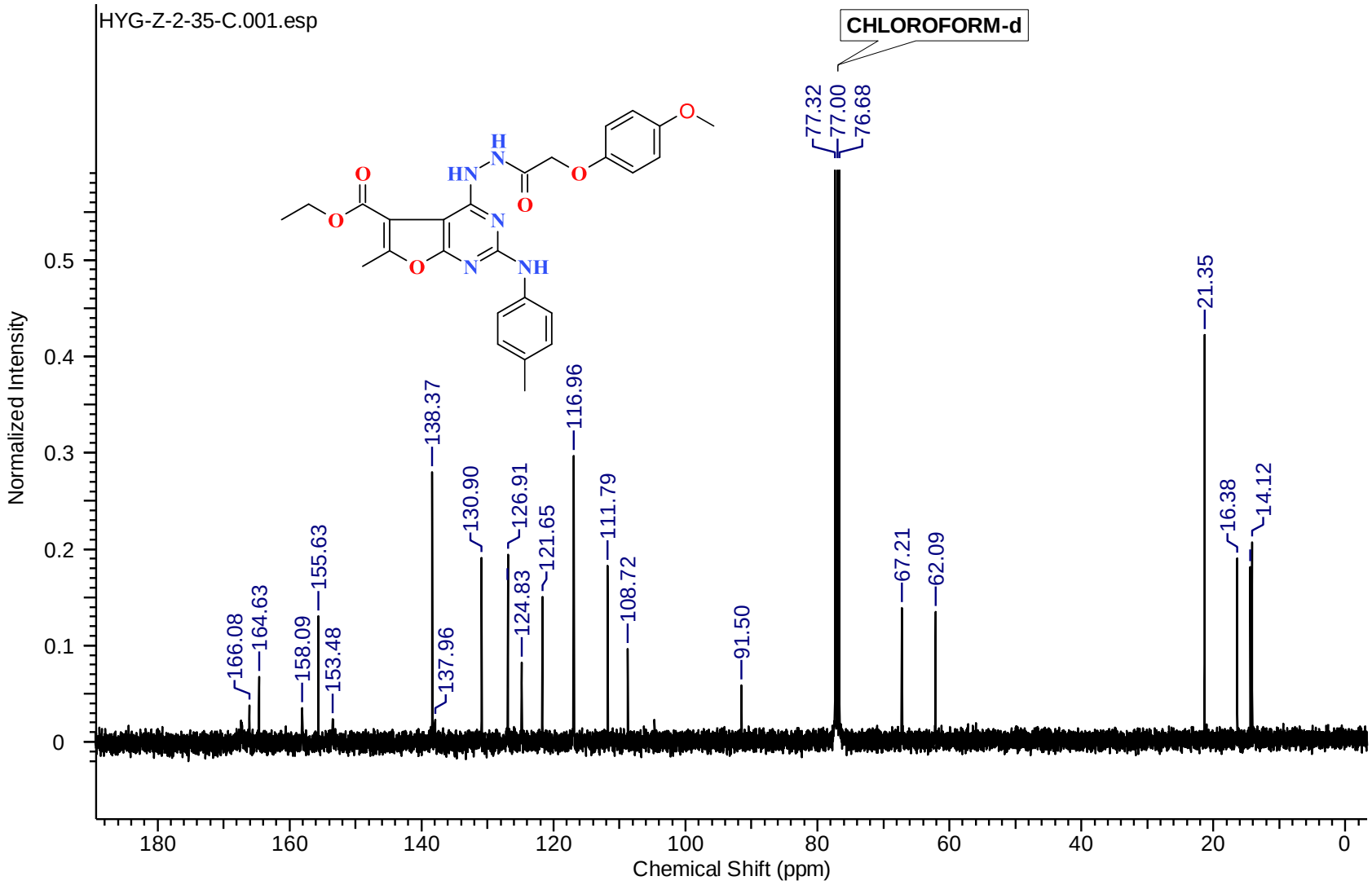
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
516.1659	516.1659	0.0	0.0	15.5	413.2	n/a	n/a	C25 H24 N5 O5 Na F

HRMS m/z **5e**


HYG-5F-1
%T
60
50
40
30
20
10
0
-10
4000
3000
2000
1000
cm-1
3210.88
2988.03
1702.93
1629.66
1511.82
1483.07
1413.74
1386.20
1360.05
1232.62
1184.00
1093.94
1071.66
1030.63
825.05
807.79
756.79

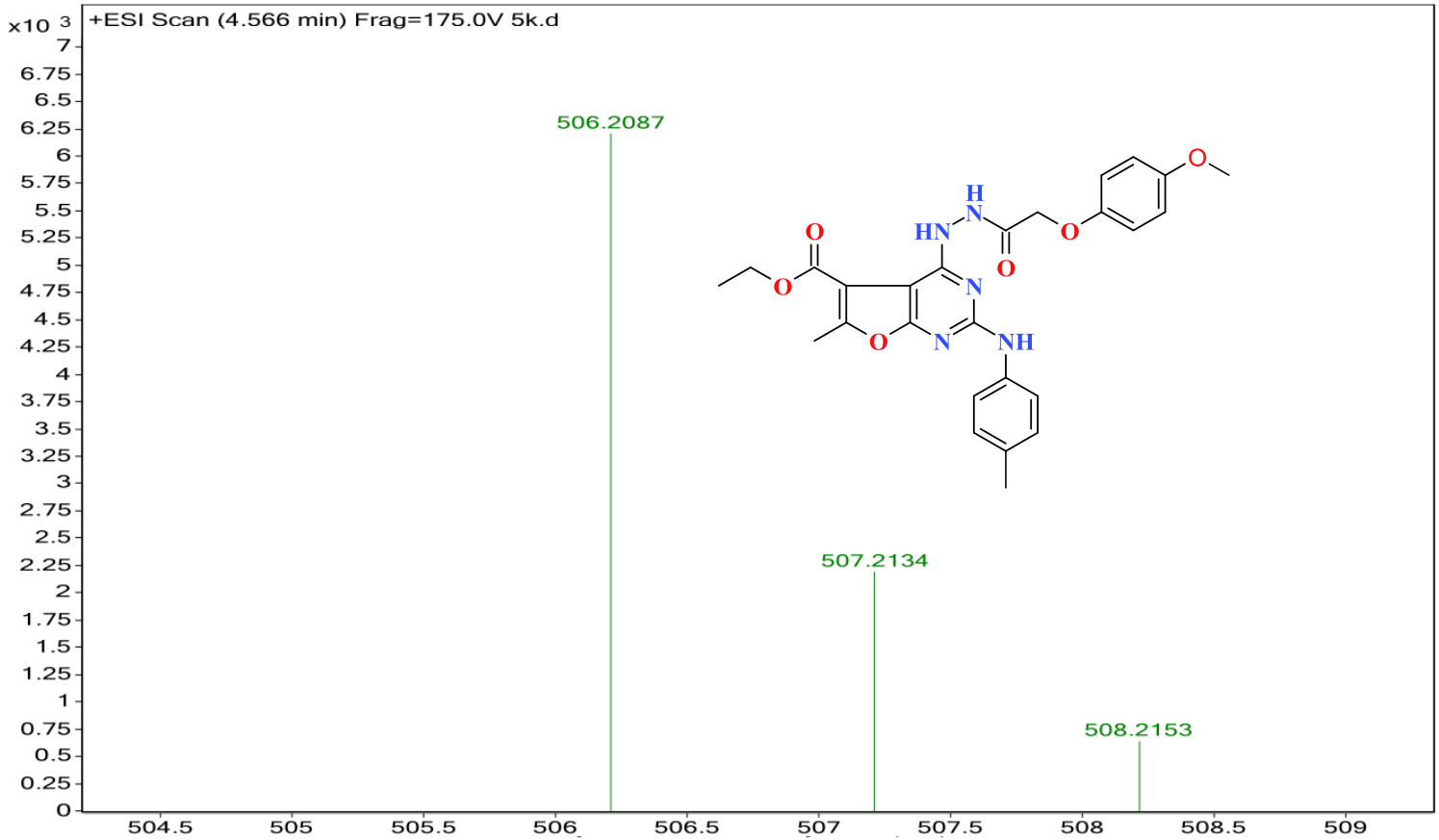

HYG-Z-2-35-5k.001.esp
Normalized Intensity
Chemical Shift (ppm)
10.48
9.49
7.65
7.63
7.00
6.97
6.87
6.85
4.66
4.38
4.36
4.34
3.70
2.66
2.51
2.50
2.16
1.37
1.35
1.34
0.00
0.80
1.75
1.90
5.90
1.89
1.90
3.18
2.93
2.79
3.00

^{1}H NMR **5f**

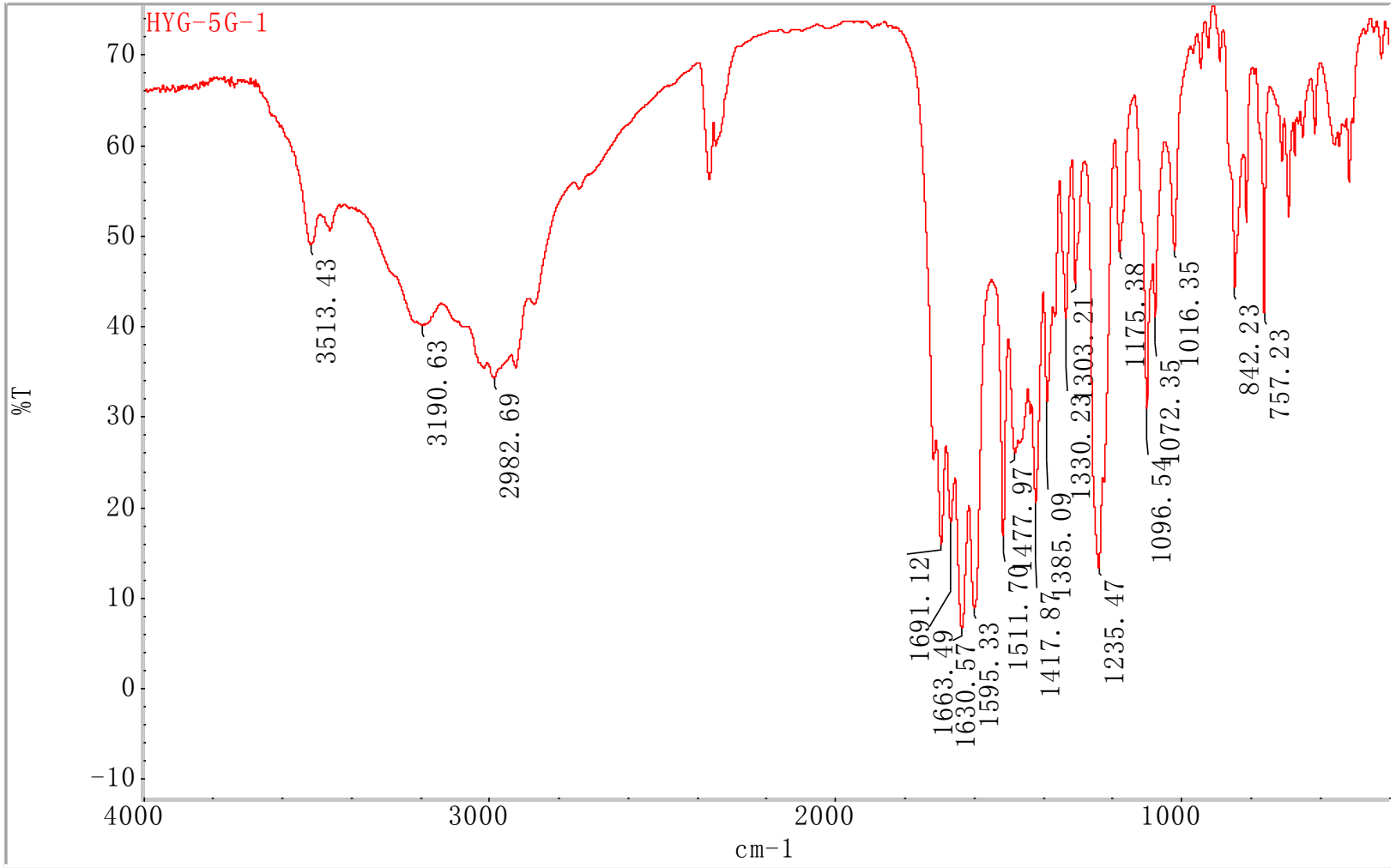

HYG-Z-2-35-C.001.esp
CHLOROFORM-d
77.32
77.00
76.68
21.35
16.38
14.12
138.37
137.96
130.90
126.91
124.83
121.65
116.96
111.79
108.72
91.50
67.21
62.09
166.08
164.63
158.09
155.63
153.48
Normalized Intensity
0
0.1
0.2
0.3
0.4
0.5
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

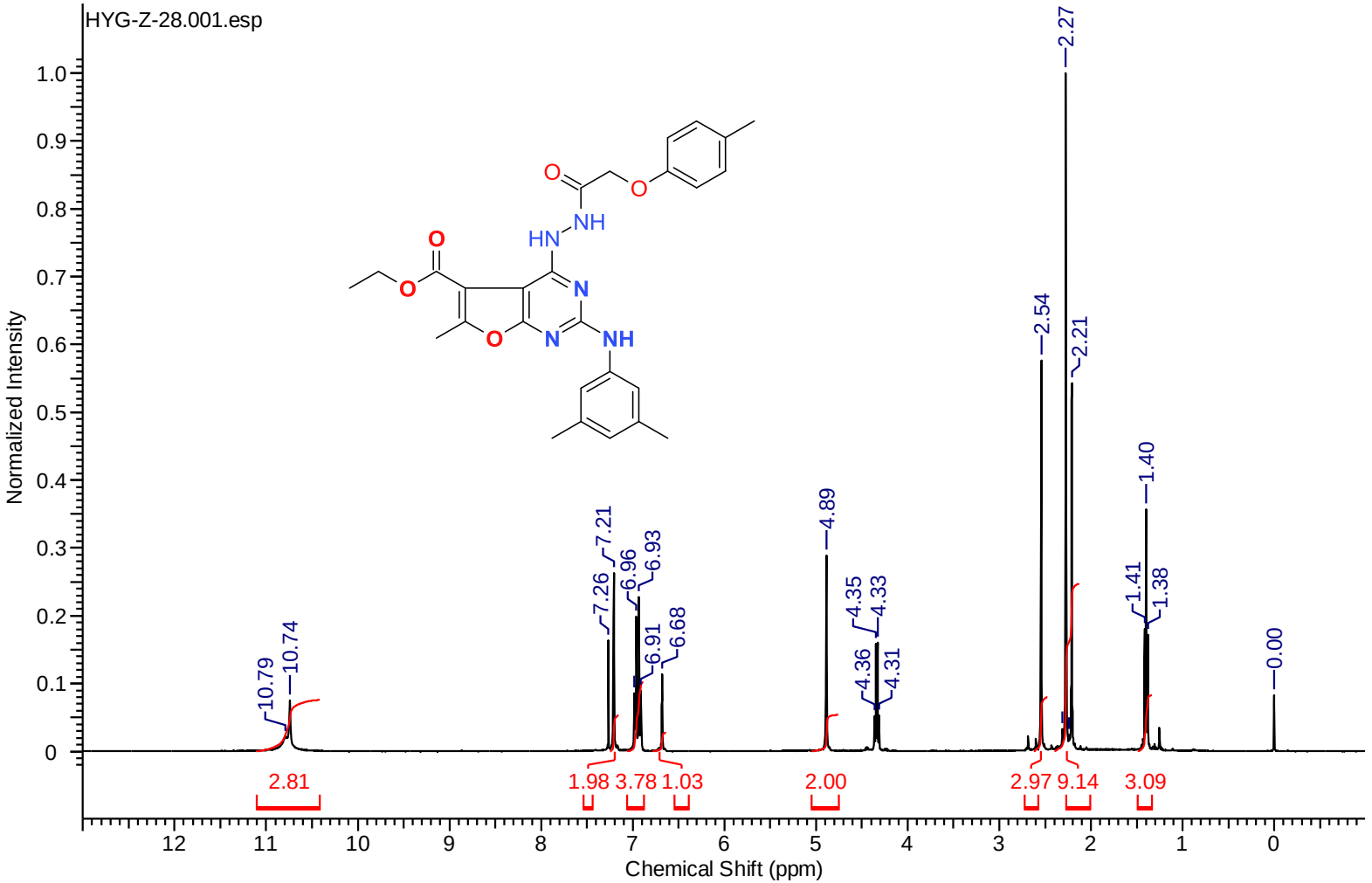
^{13}C NMR **5f**

Sample Name		**Position**	Vial 51	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	5k.d	**ACQ Method**	CYF20201112-NORMAL.m	**Comment**		**Acquired Time**	3/17/2025 11:19:23

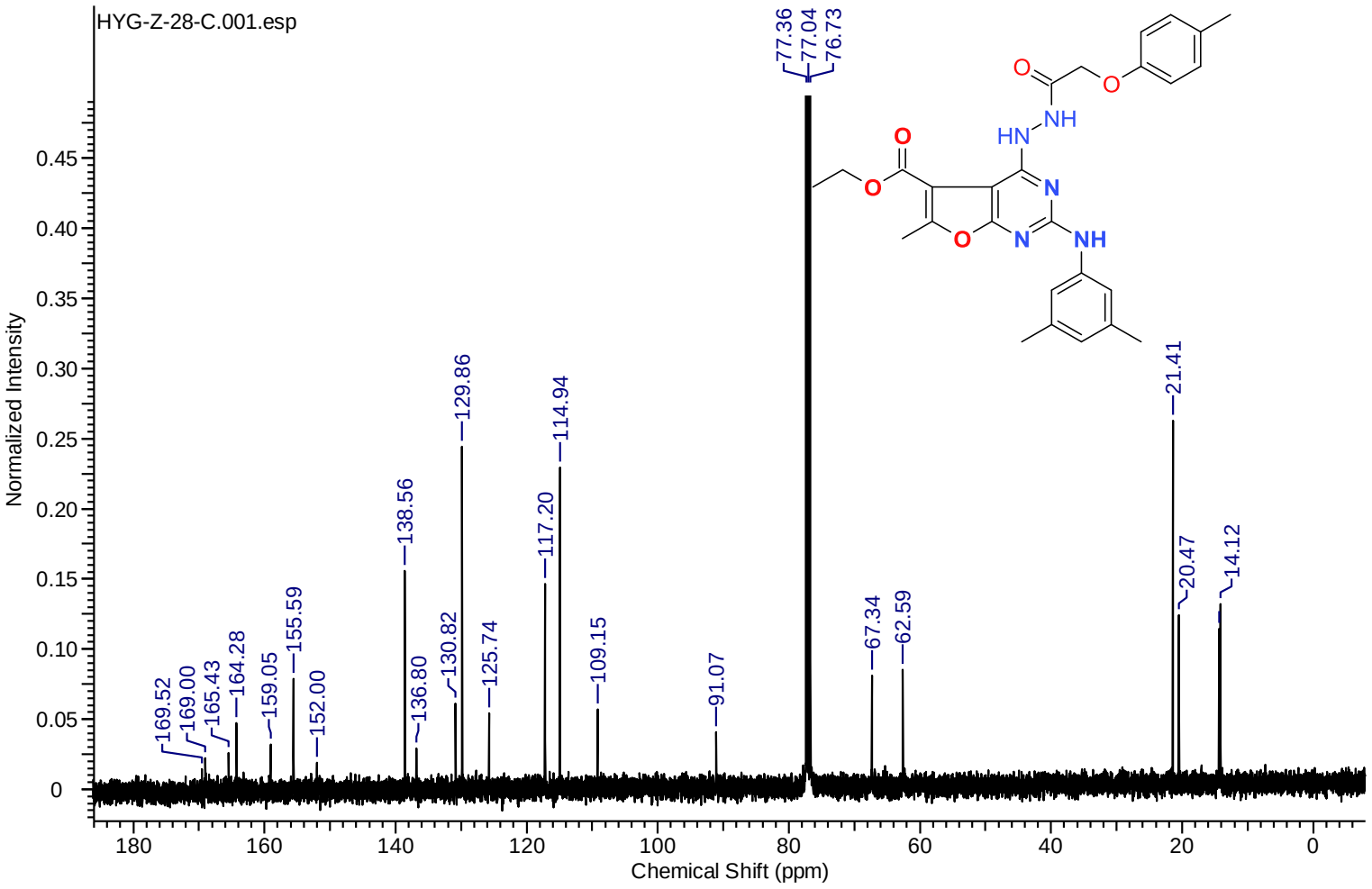


HRMS m/z **5f**


HYG-5G-1
%T
70
60
50
40
30
20
10
0
-10
4000
3000
2000
1000
cm-1
3513.43
3190.63
2982.69
1691.12
1663.49
1630.57
1595.33
1511.70
1477.97
1417.87
1385.09
1330.23
1303.21
1235.47
1175.38
1096.54
1072.35
1016.35
842.23
757.23

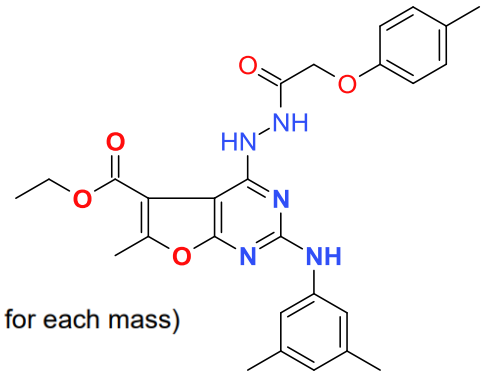

HYG-Z-28.001.esp
Normalized Intensity
Chemical Shift (ppm)
10.79
10.74
7.26
7.21
6.96
6.93
6.91
6.68
4.89
4.36
4.35
4.33
4.31
2.54
2.27
2.21
1.41
1.40
1.38
0.00
2.81
1.98
3.78
1.03
2.00
2.97
9.14
3.09

^{1}H NMR **5g**


HYG-Z-28-C.001.esp
Normalized Intensity
Chemical Shift (ppm)
77.36
77.04
76.73
169.52
169.00
165.43
164.28
159.05
155.59
152.00
138.56
136.80
130.82
129.86
125.74
117.20
114.94
109.15
91.07
67.34
62.59
21.41
20.47
14.12
O
O
HN
NH
O
O
N
O
N
NH

^{13}C NMR **5g**

Elemental Composition Report



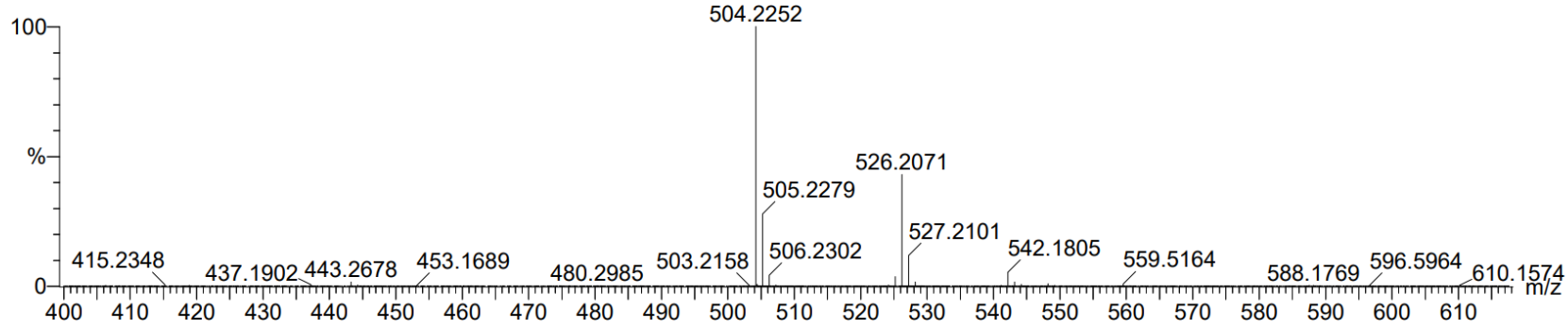
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1902 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 27-27 H: 30-30 N: 0-100 O: 0-100 Na: 0-3

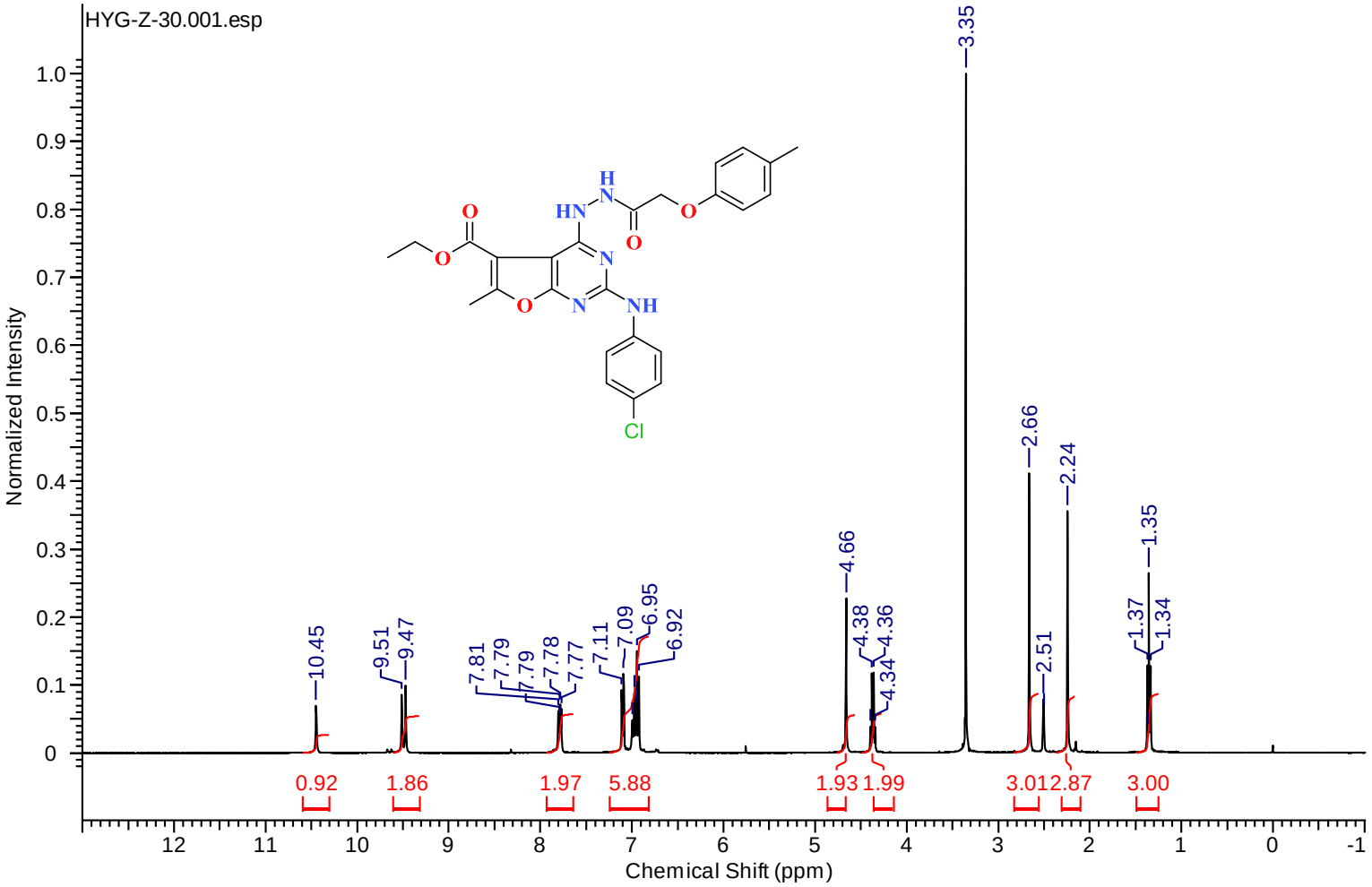
14
240612-1-z-28 21 (0.147)

1: TOF MS ES+
8.79e+005

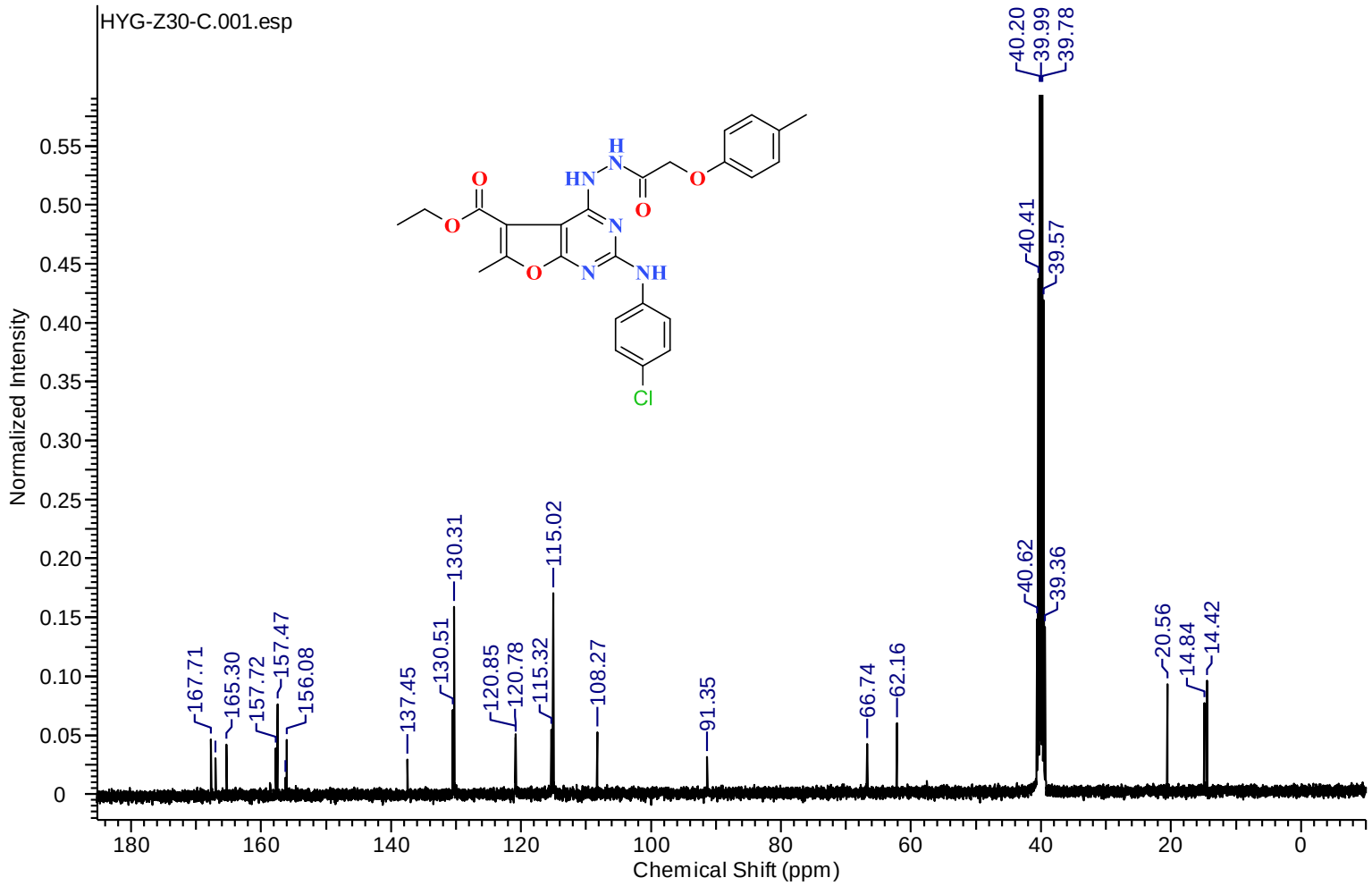


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
504.2252	504.2247	0.5	1.0	15.5	681.2	n/a	n/a	C27 H30 N5 O5

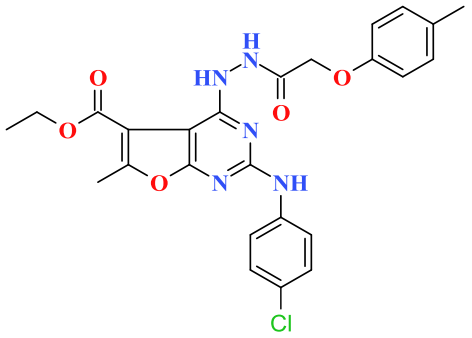
HRMS m/z **5g**


HYG-Z-30.001.esp
Normalized Intensity
Chemical Shift (ppm)
10.45
9.51
9.47
7.81
7.79
7.79
7.78
7.77
7.11
7.09
6.95
6.92
4.66
4.38
4.36
4.34
3.35
2.66
2.51
2.24
1.37
1.35
1.34
0.92
1.86
1.97
5.88
1.93
1.99
3.01
2.87
3.00
Cl

^{1}H NMR **5h**


HYG-Z30-C.001.esp
Normalized Intensity
Chemical Shift (ppm)
167.71
165.30
157.72
157.47
156.08
137.45
130.51
130.31
120.85
120.78
115.32
115.02
108.27
91.35
66.74
62.16
40.62
40.41
40.20
39.99
39.78
39.57
39.36
20.56
14.84
14.42
Cl

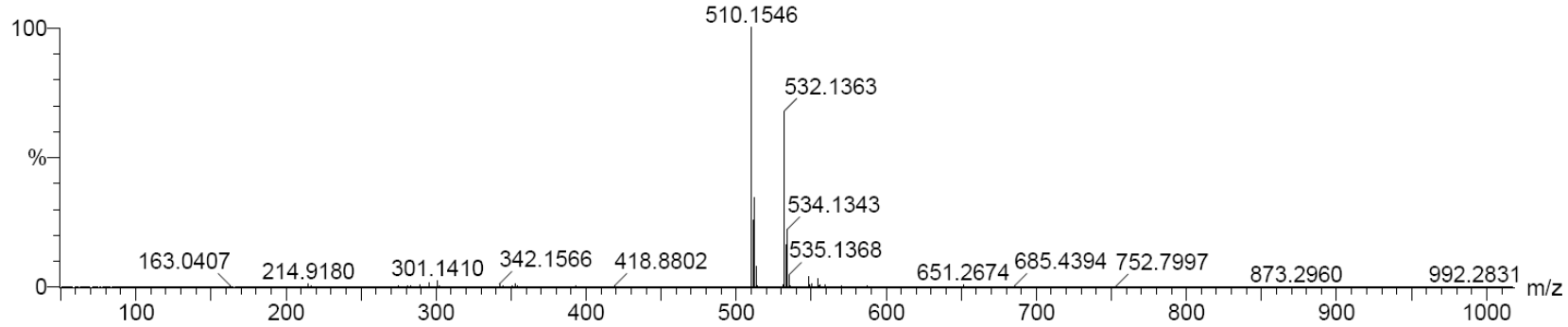
^{13}C NMR **5h**



Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

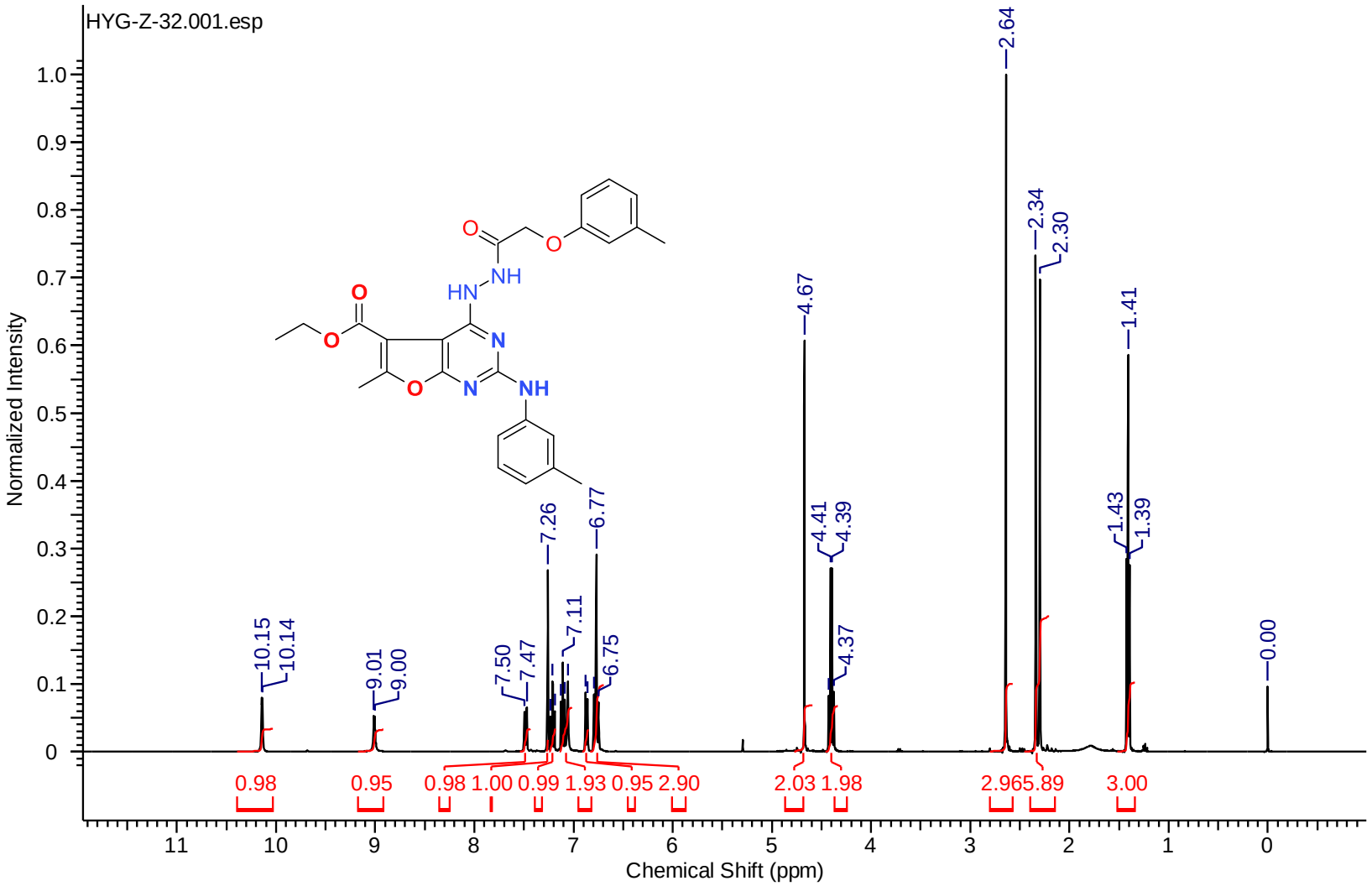
Monoisotopic Mass, Even Electron Ions
3587 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 25-25 H: 5-25 N: 0-100 O: 0-100 Na: 0-2 Cl: 1-3
2
240503-3-15 22 (0.222)

1: TOF MS ES+
4.76e+006

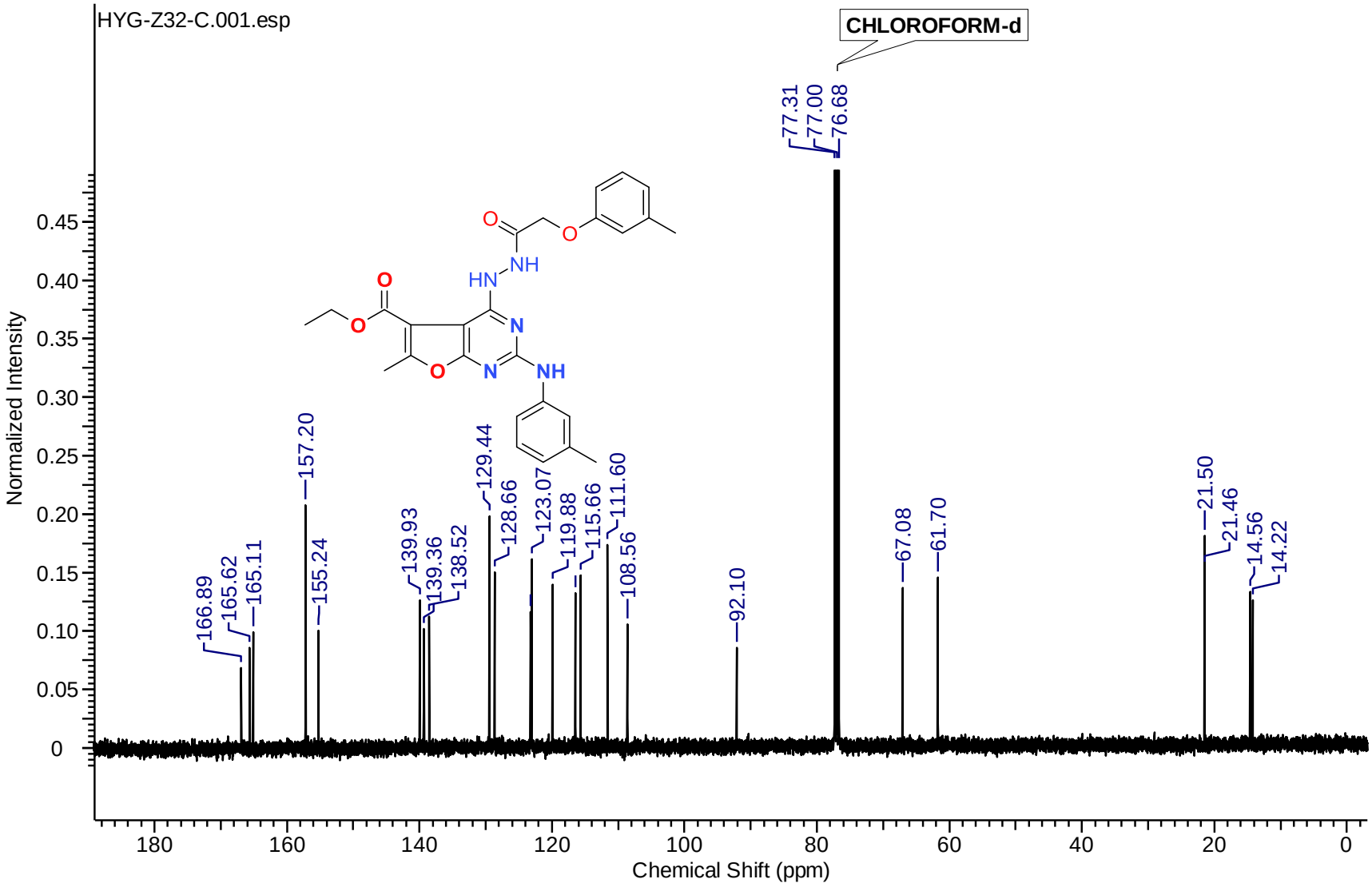


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
510.1546	510.1544	0.2	0.4	15.5	694.8	n/a	n/a	C25 H25 N5 O5 Cl

HRMS m/z **5h**

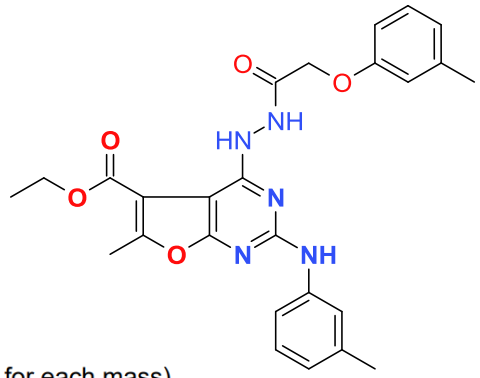

HYG-Z-32.001.esp
Normalized Intensity
Chemical Shift (ppm)
10.15
10.14
9.01
9.00
7.50
7.47
7.26
7.11
6.77
6.75
4.67
4.41
4.39
4.37
2.64
2.34
2.30
1.43
1.41
1.39
0.00
0.98
0.95
0.98
1.00
0.99
1.93
0.95
2.90
2.03
1.98
2.96
5.89
3.00

^{1}H NMR **5i**


HYG-Z32-C.001.esp
CHLOROFORM-d
77.31
77.00
76.68
166.89
165.62
165.11
157.20
155.24
139.93
139.36
138.52
129.44
128.66
123.07
119.88
115.66
111.60
108.56
92.10
67.08
61.70
21.50
21.46
14.56
14.22
Normalized Intensity
0
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

^{13}C NMR **5i**

Elemental Composition Report



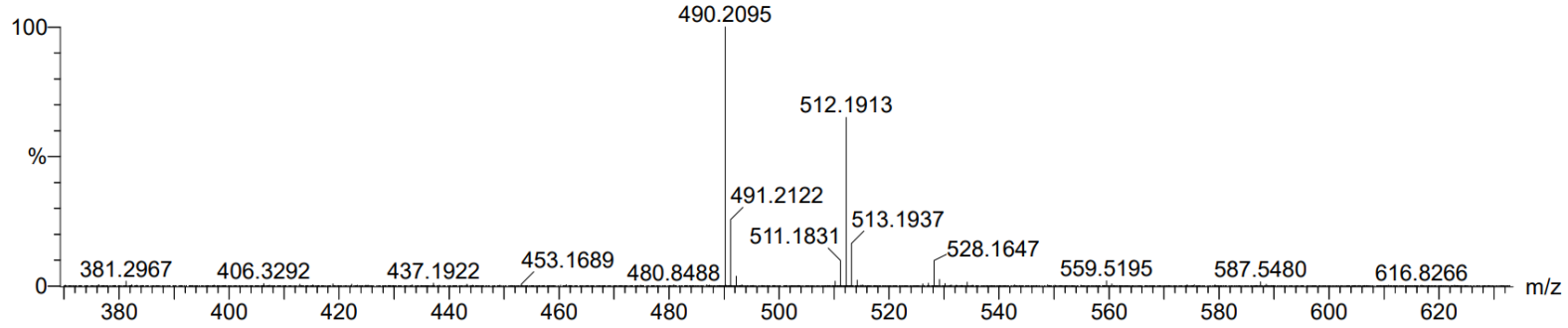
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1790 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 26-26 H: 28-28 N: 0-100 O: 0-100 Na: 0-3

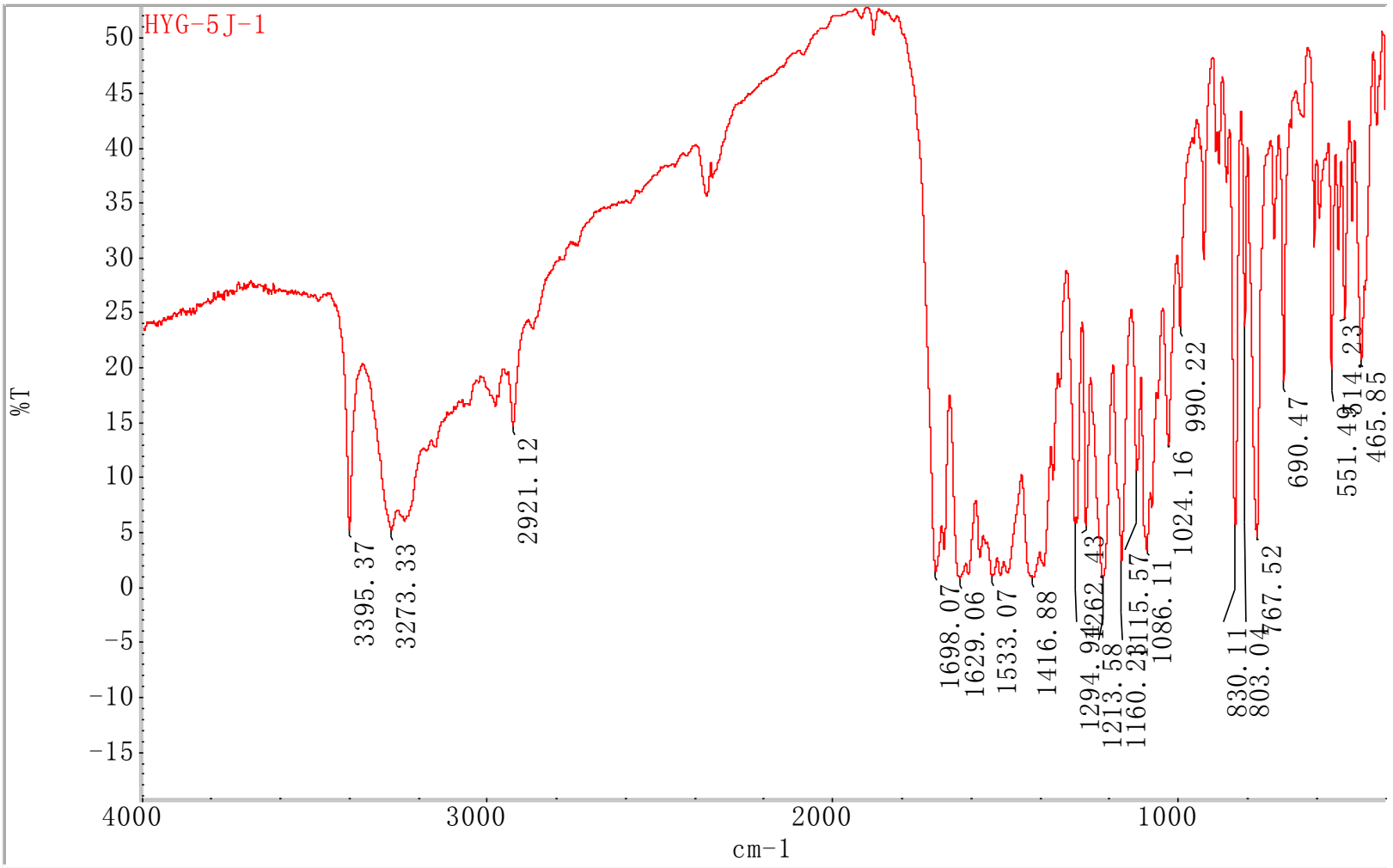
14
240612-1-z-32 29 (0.189)

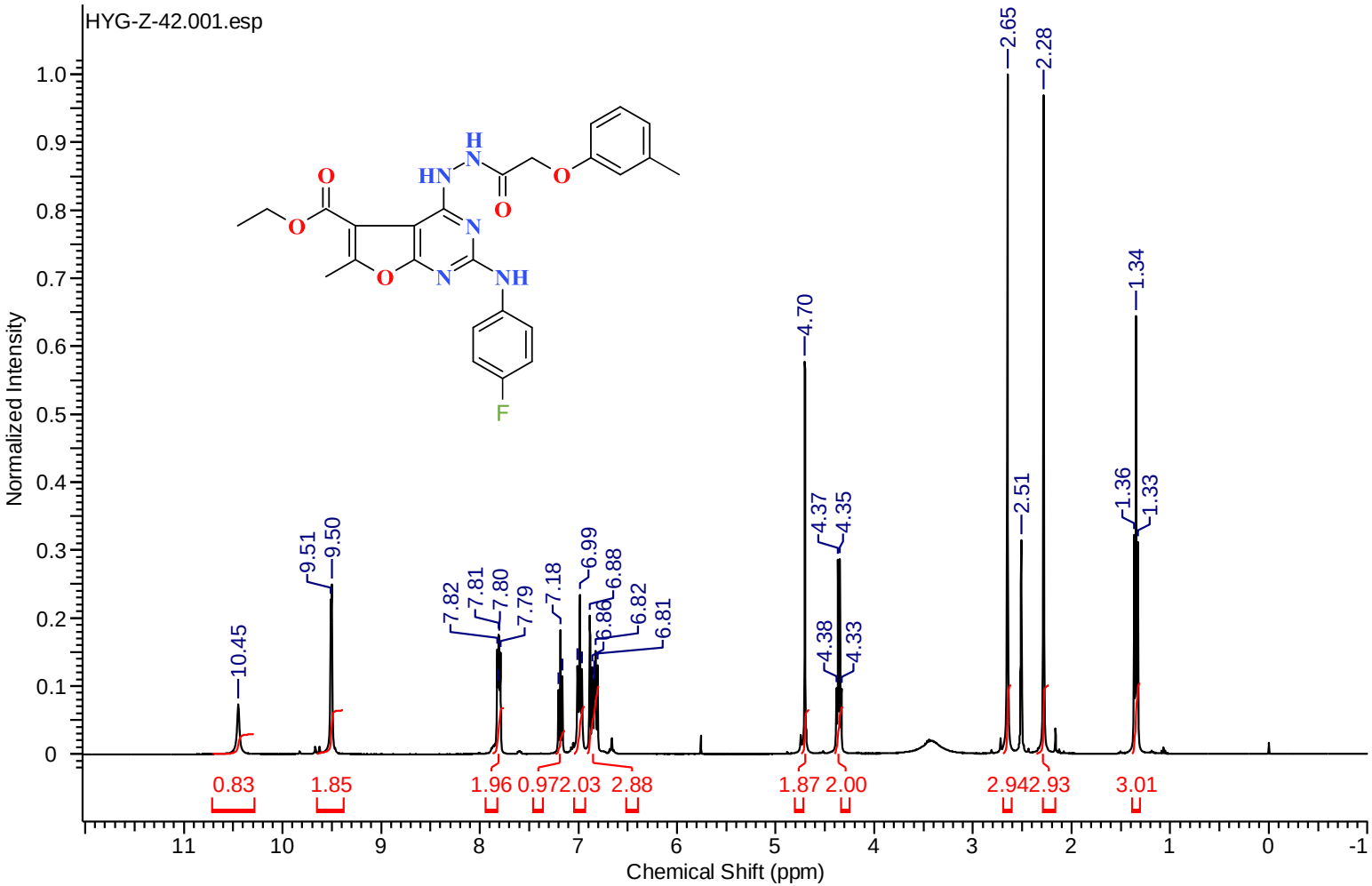
1: TOF MS ES+
2.52e+005



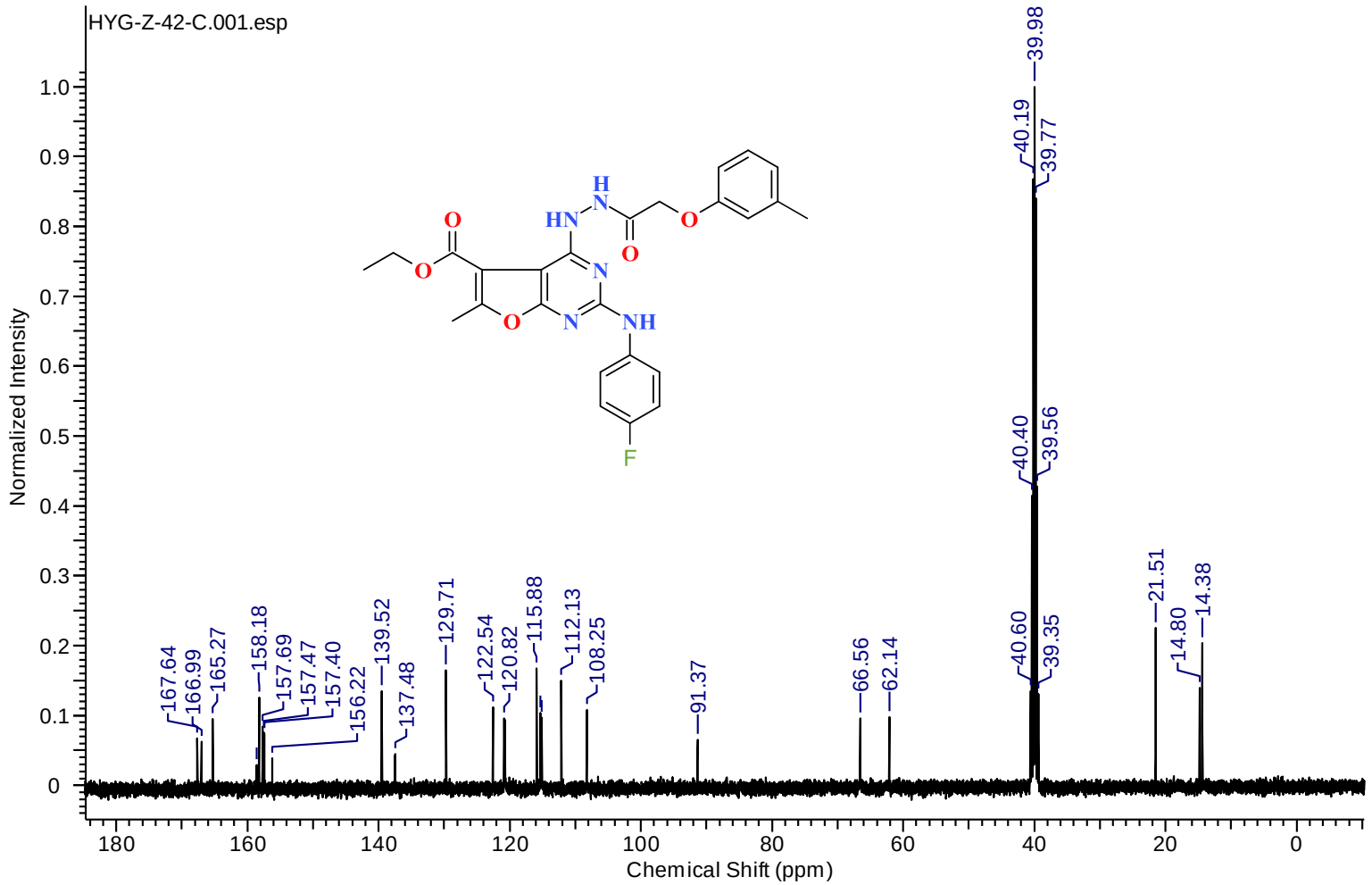
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
490.2095	490.2090	0.5	1.0	15.5	538.2	n/a	n/a	C26 H28 N5 O5

HRMS m/z **5i**


HYG-5J-1
%T
cm-1
4000
3000
2000
1000
50
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
3395.37
3273.33
2921.12
1698.07
1629.06
1533.07
1416.88
1294.94
1262.43
1213.58
1160.28
1115.57
1086.11
1024.16
990.22
830.11
803.04
767.52
690.47
551.49
514.23
465.85

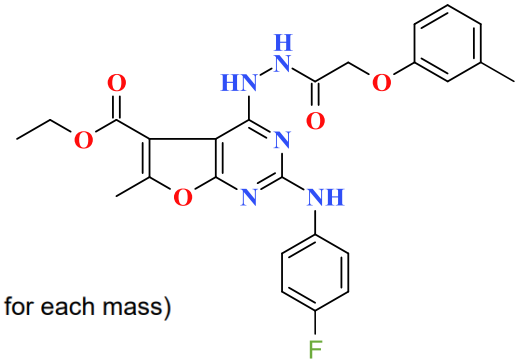

HYG-Z-42.001.esp
Normalized Intensity
Chemical Shift (ppm)
10.45
9.51
9.50
7.82
7.81
7.80
7.79
7.18
6.99
6.88
6.86
6.82
6.81
4.70
4.37
4.35
4.38
4.33
2.65
2.28
2.51
1.36
1.34
1.33
0.83
1.85
1.96
0.97
2.03
2.88
1.87
2.00
2.94
2.93
3.01

^{1}H NMR **5j**


HYG-Z-42-C.001.esp
Normalized Intensity
Chemical Shift (ppm)
167.64
166.99
165.27
158.18
157.69
157.47
157.40
156.22
139.52
137.48
129.71
122.54
120.82
115.88
112.13
108.25
91.37
66.56
62.14
40.60
40.40
40.19
39.98
39.77
39.56
39.35
21.51
14.80
14.38
H
N
HN
O
O
O
O
N
N
O
N
NH
F

^{13}C NMR **5j**

Elemental Composition Report



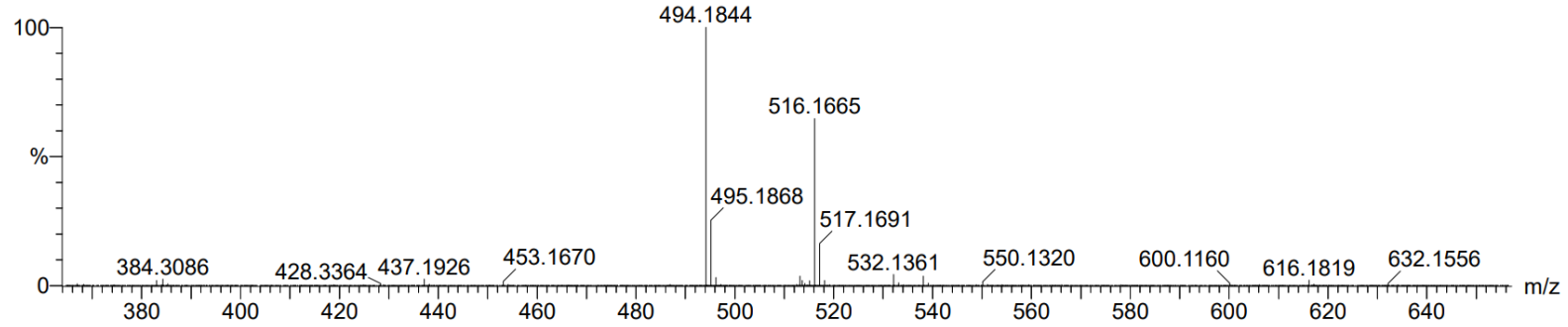
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
913 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 25-25 H: 25-25 N: 0-100 O: 0-100 Na: 0-1 F: 1-1

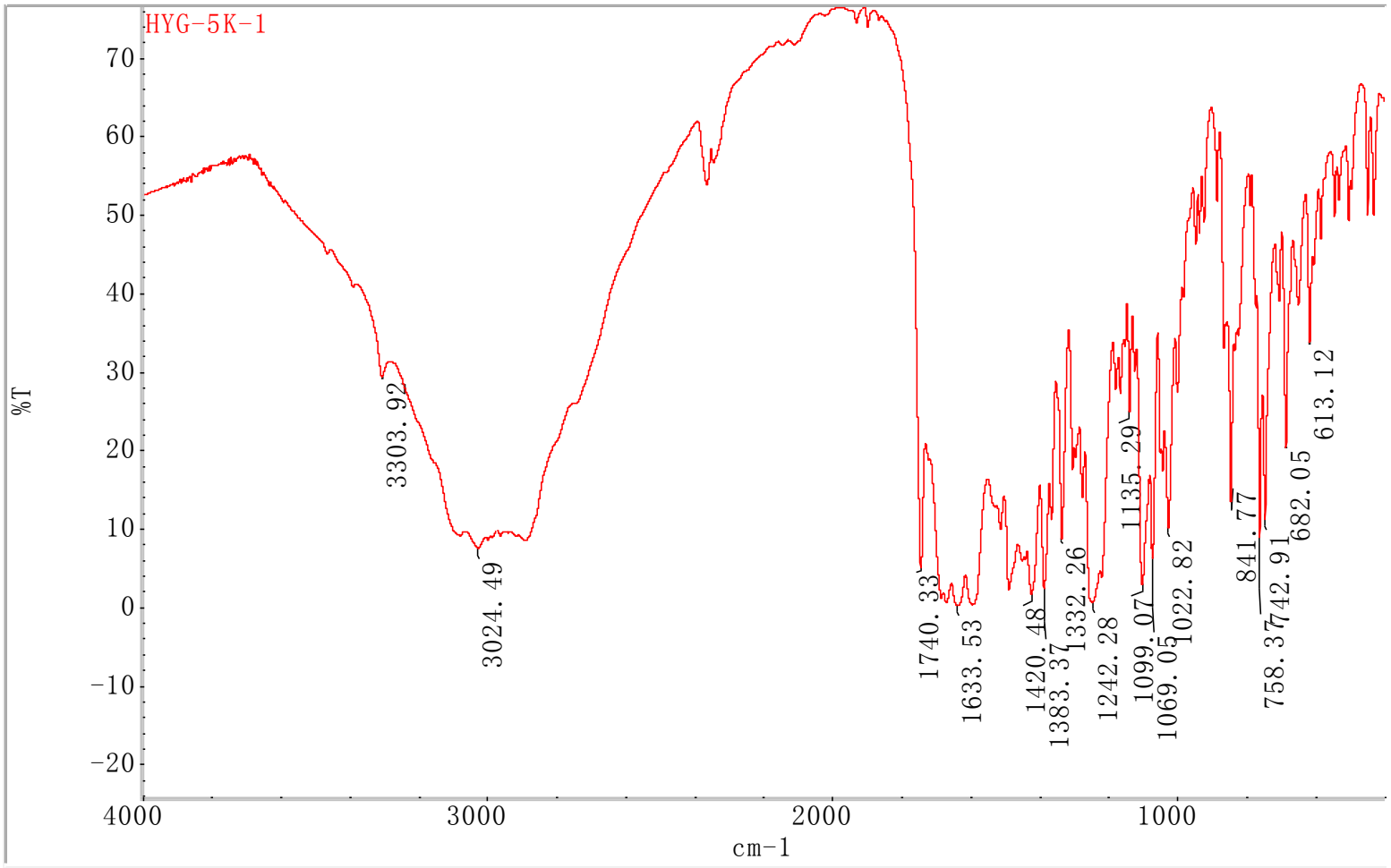
9
240629-4-17 10 (0.089)

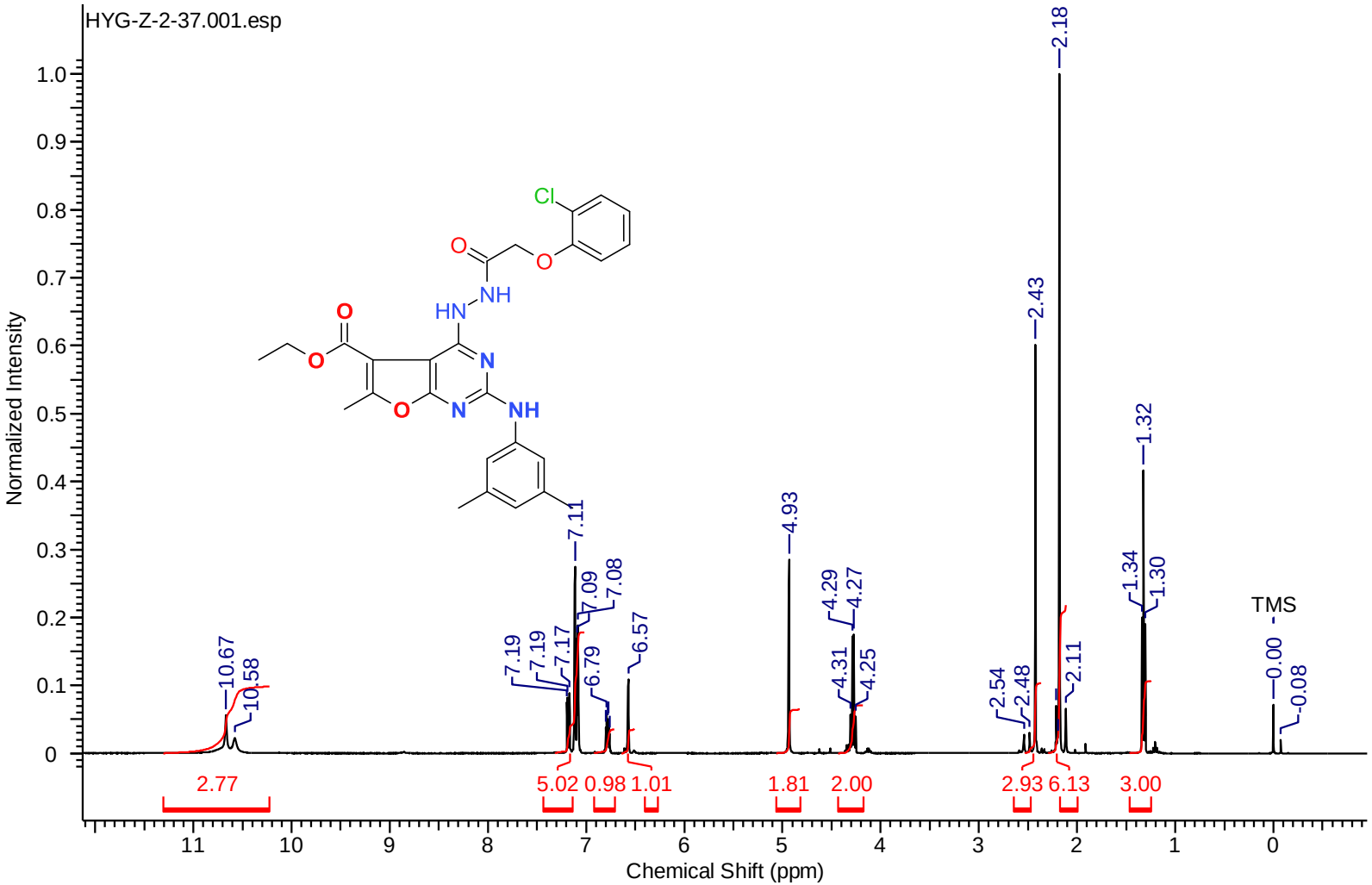
1: TOF MS ES+
3.23e+005



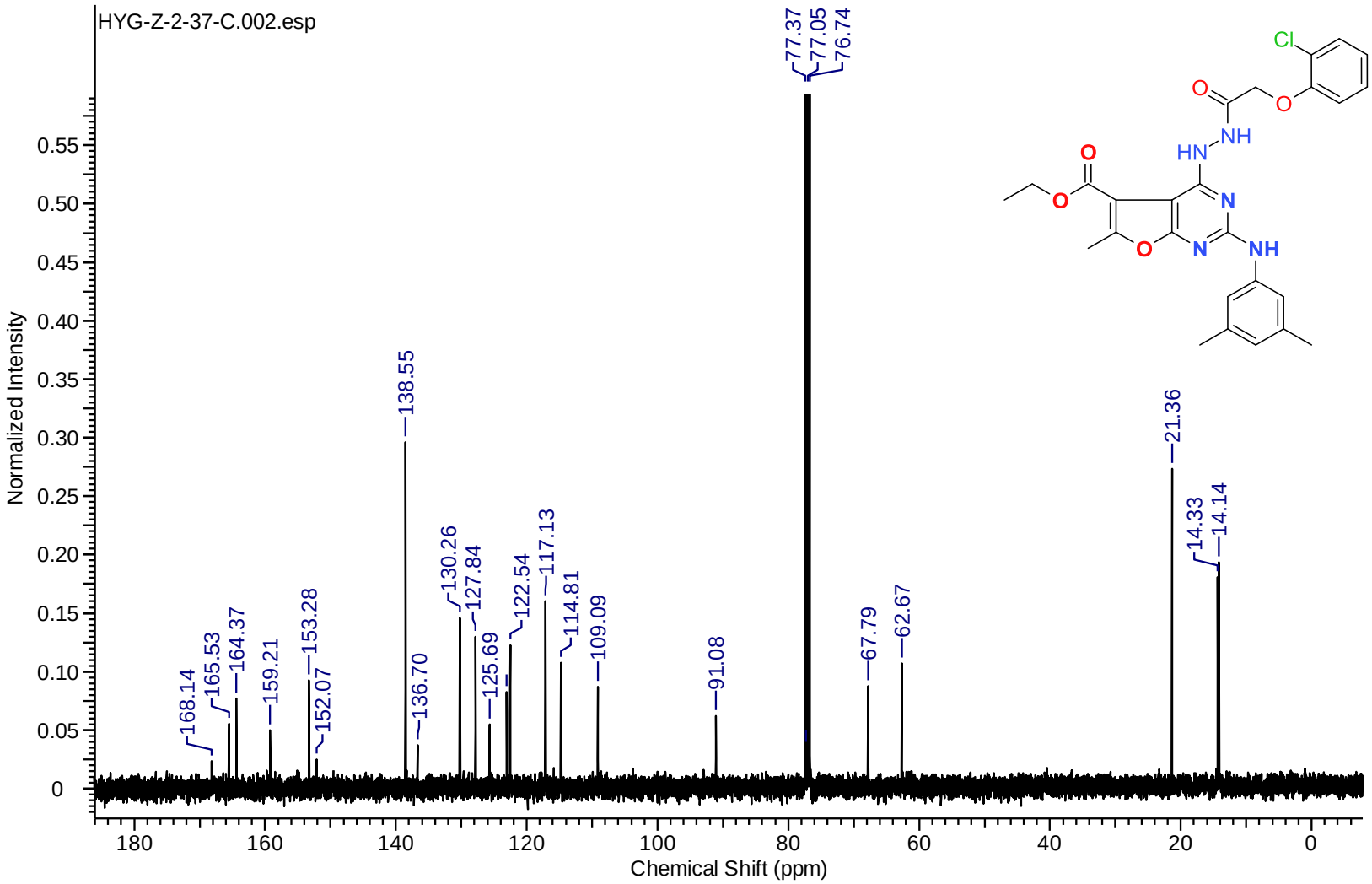
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
494.1844	494.1840	0.4	0.8	15.5	468.8	n/a	n/a	C25 H25 N5 O5 F

HRMS m/z **5j**

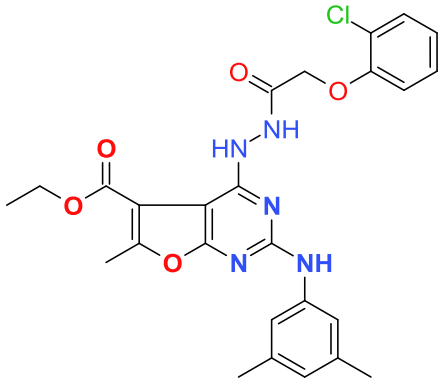

HYG-5K-1
%T
70
60
50
40
30
20
10
0
-10
-20
4000
3000
2000
1000
cm-1
3303.92
3024.49
1740.33
1633.53
1420.48
1383.37
1332.26
1242.28
1135.29
1099.07
1069.05
1022.82
841.77
758.37
742.91
682.05
613.12


HYG-Z-2-37.001.esp
Normalized Intensity
Chemical Shift (ppm)
Cl
O
O
NH
HN
O
O
N
O
N
NH
10.67
10.58
7.19
7.19
7.17
7.11
7.09
7.08
6.79
6.57
4.93
4.29
4.27
4.31
4.25
2.54
2.48
2.43
2.18
2.11
1.34
1.32
1.30
TMS
0.00
-0.08
2.77
5.02
0.98
1.01
1.81
2.00
2.93
6.13
3.00

^{1}H NMR **5k**

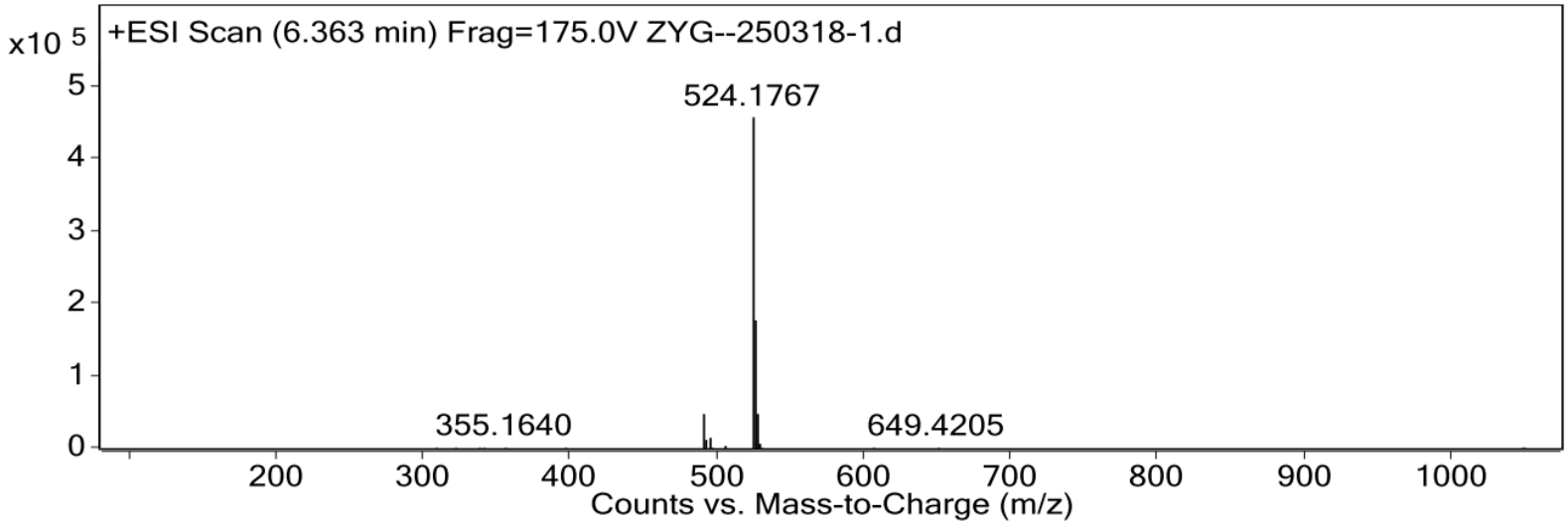

HYG-Z-2-37-C.002.esp
Normalized Intensity
Chemical Shift (ppm)
77.37
77.05
76.74
168.14
165.53
164.37
159.21
153.28
152.07
138.55
136.70
130.26
127.84
125.69
122.54
117.13
114.81
109.09
91.08
67.79
62.67
21.36
14.33
14.14
Cl
O
O
NH
HN
O
O
N
N
NH

^{13}C NMR **5k**

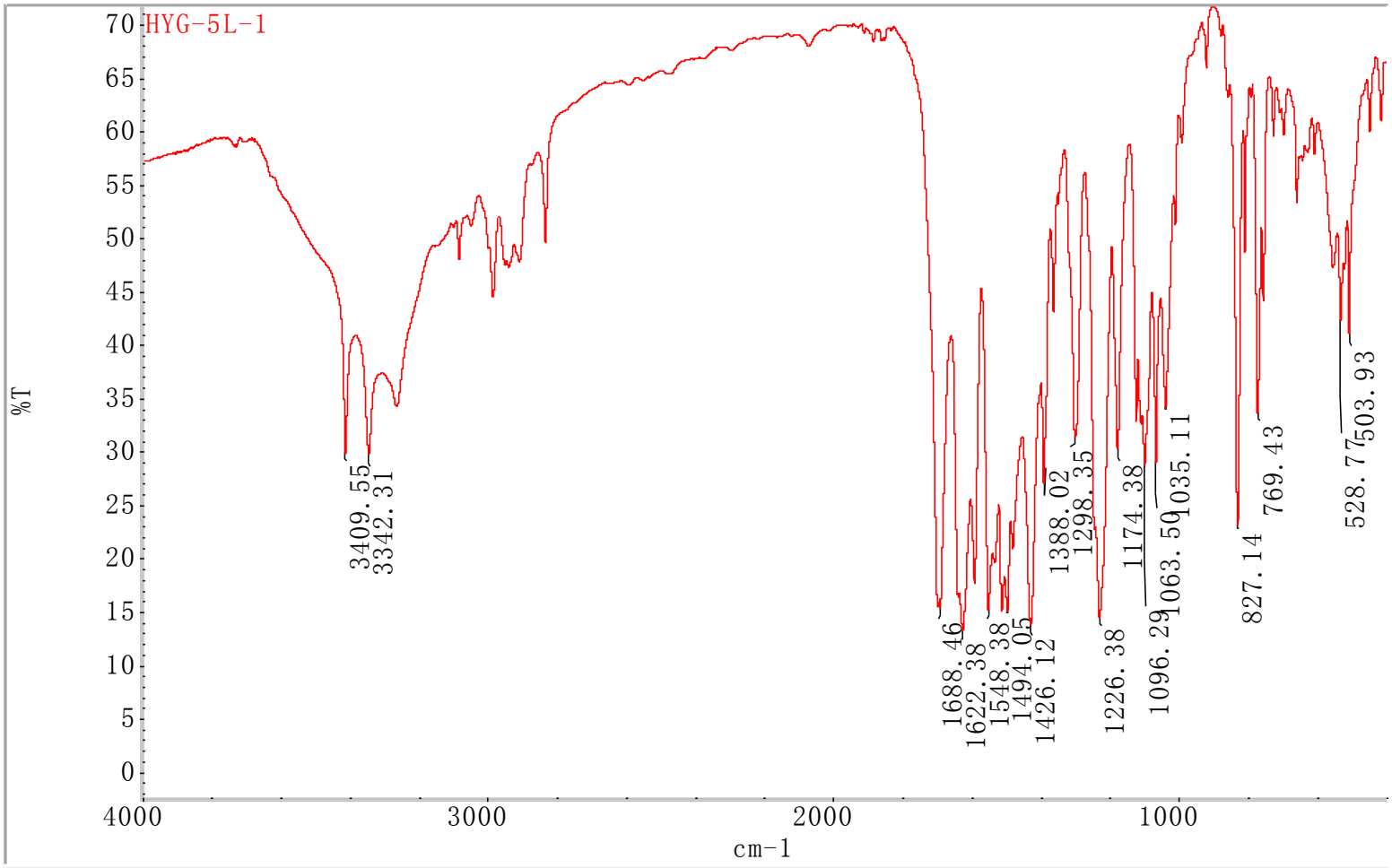


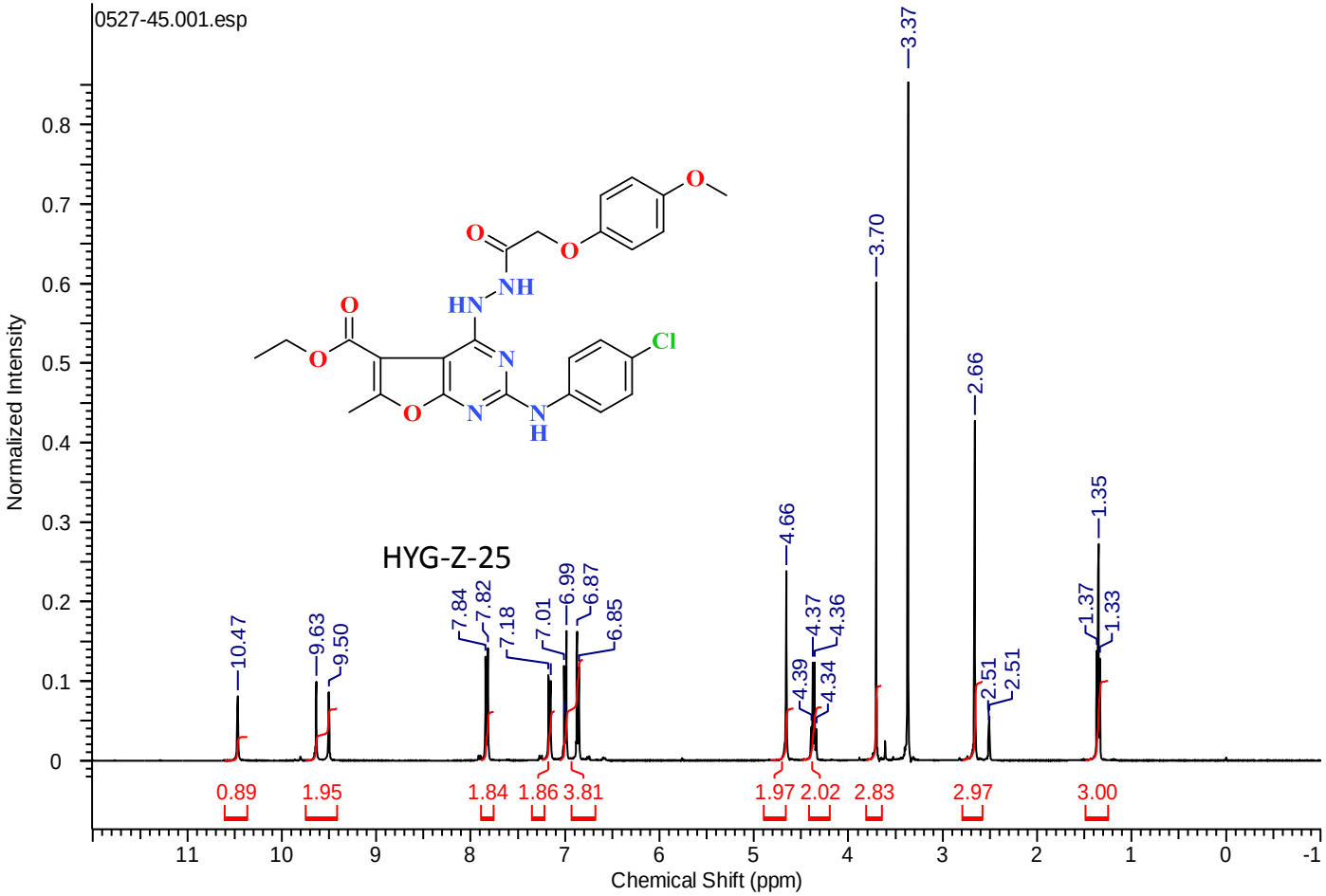
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

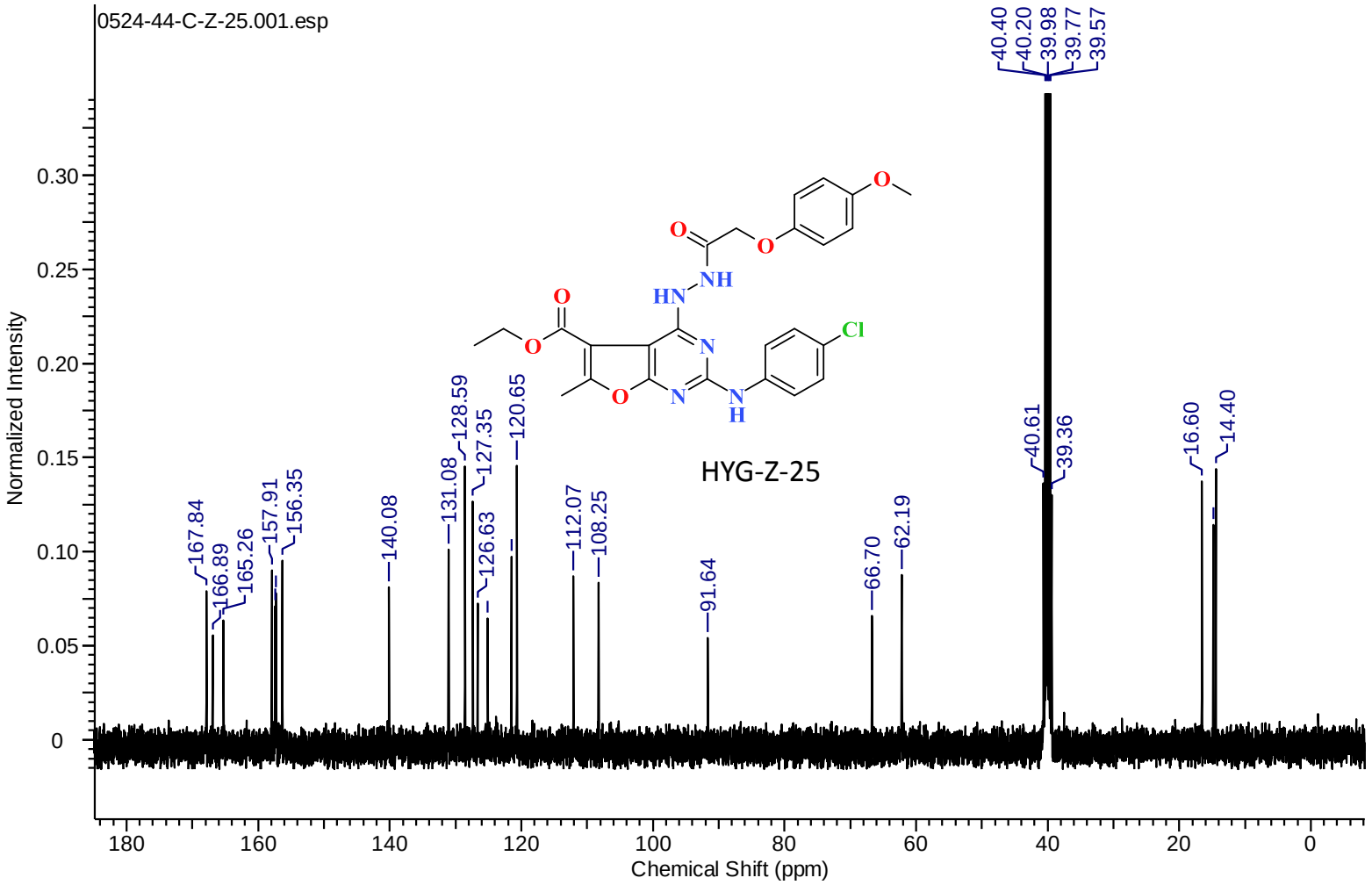


HRMS m/z **5k**


HYG-5L-1
%T
cm-1
4000
3000
2000
1000
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
3409.55
3342.31
1688.46
1622.38
1548.38
1494.05
1426.12
1388.02
1298.35
1226.38
1174.38
1096.29
1063.50
1035.11
827.14
769.43
528.77
503.93

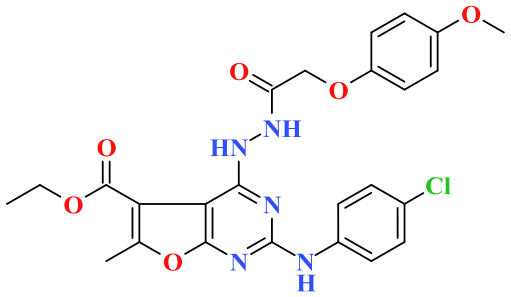

0527-45.001.esp
HYG-Z-25
Normalized Intensity
Chemical Shift (ppm)
10.47
9.63
9.50
7.84
7.82
7.18
7.01
6.99
6.87
6.85
4.66
4.39
4.37
4.36
4.34
3.70
3.37
2.66
2.51
2.51
1.37
1.35
1.33
0.89
1.95
1.84
1.86
3.81
1.97
2.02
2.83
2.97
3.00
Cl

^{1}H NMR **5l**


0524-44-C-Z-25.001.esp
Normalized Intensity
0.30
0.25
0.20
0.15
0.10
0.05
0
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
167.84
166.89
165.26
157.91
156.35
140.08
131.08
128.59
127.35
126.63
120.65
112.07
108.25
91.64
66.70
62.19
40.61
39.36
16.60
14.40
40.40
40.20
39.98
39.77
39.57
HYG-Z-25
O
O
O
NH
HN
O
O
N
N
N
H
Cl
O

^{13}C NMR **5l**

Elemental Composition Report

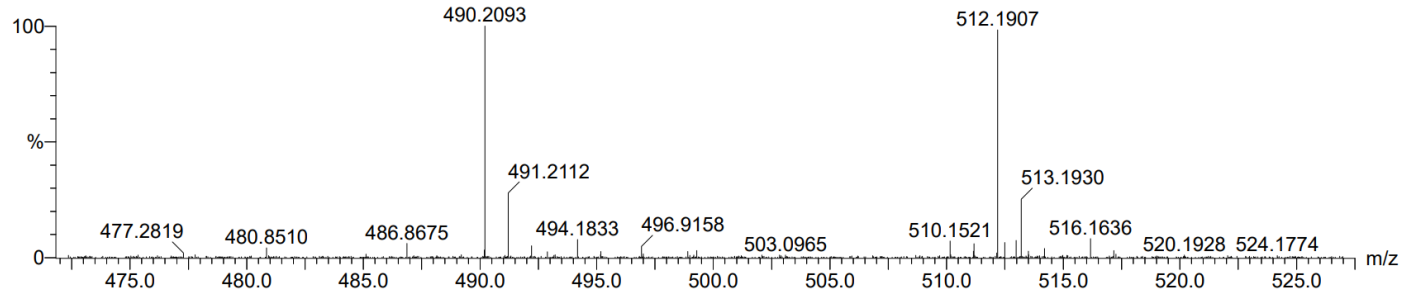


Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
972 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 26-26 H: 28-28 N: 0-100 O: 0-100 Na: 0-1

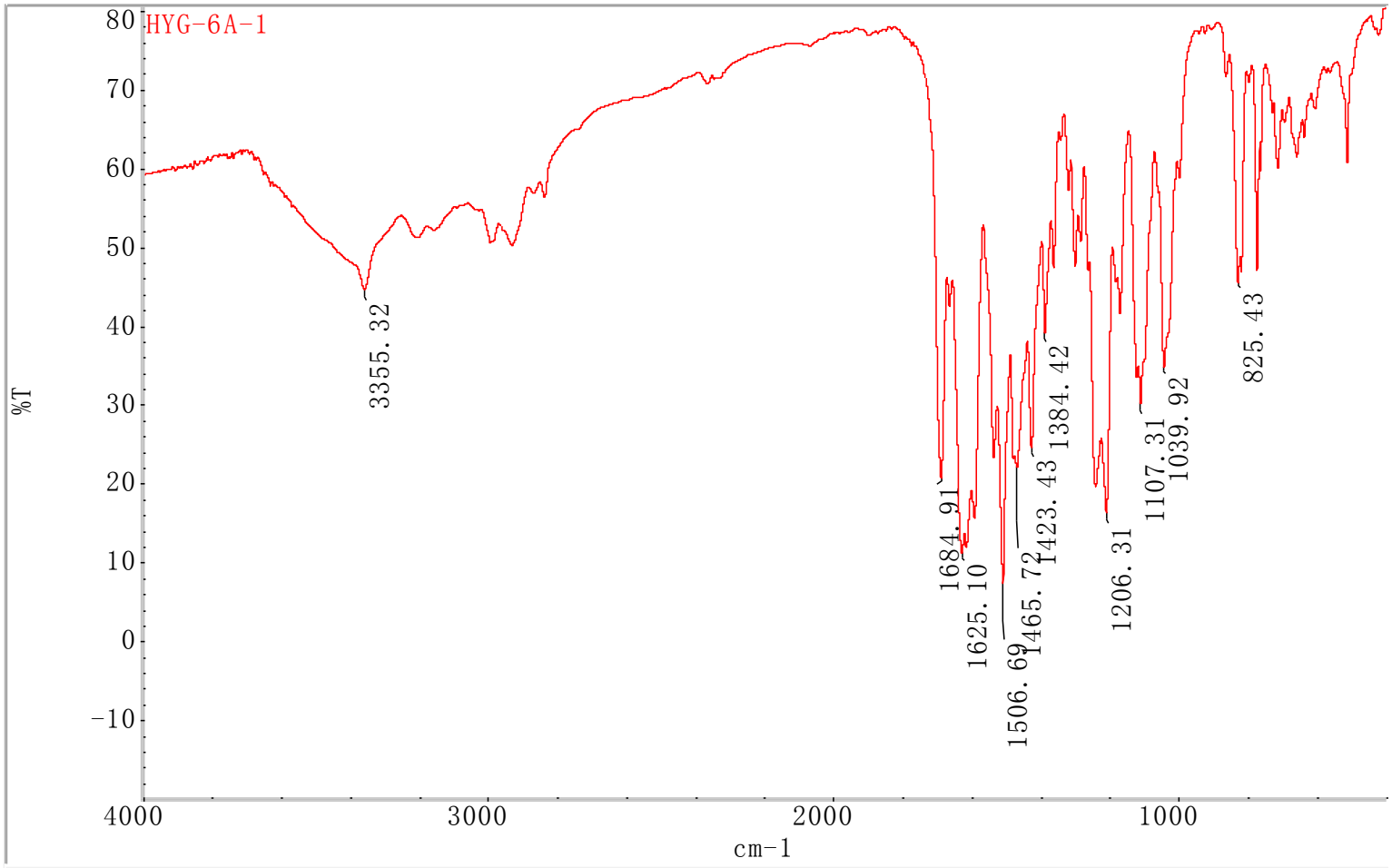
9
240629-4-18 12 (0.100)

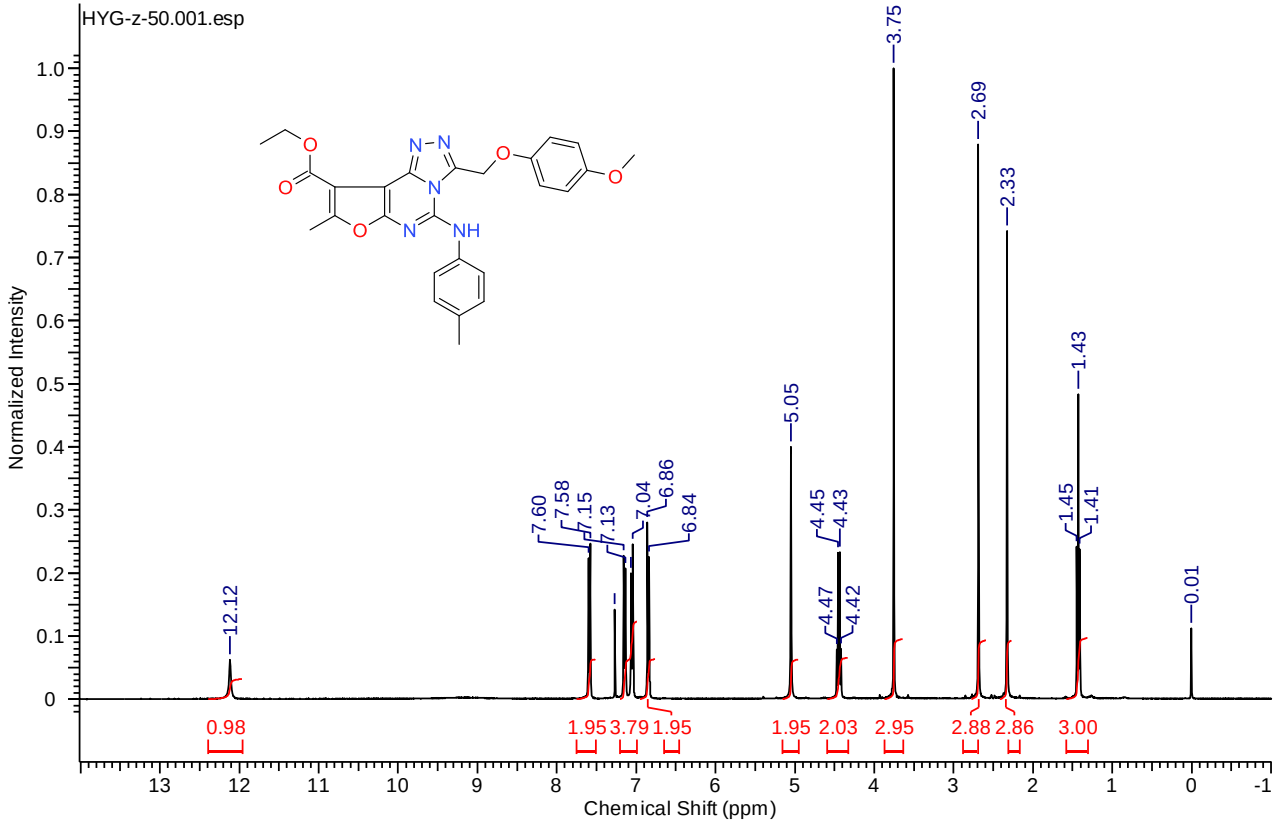
1: TOF MS ES+
1.67e+004



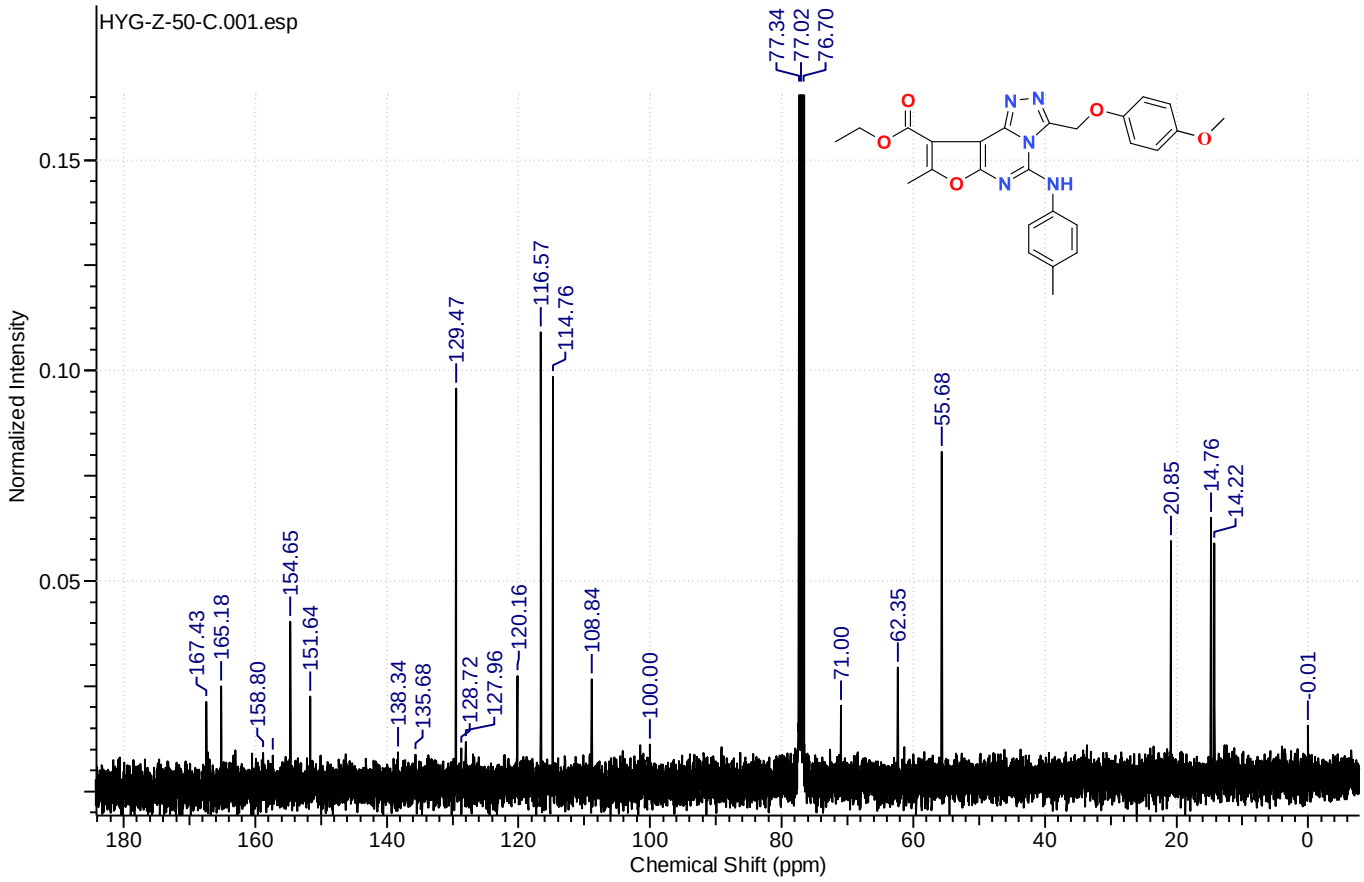
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
490.2093	490.2090	0.3	0.6	15.5	305.6	n/a	n/a	C26 H28 N5 O5

HRMS m/z **5l**


HYG-6A-1
%T
80
70
60
50
40
30
20
10
0
-10
4000
3000
2000
1000
cm-1
3355.32
1684.91
1625.10
1506.69
1465.72
1423.43
1384.42
1206.31
1107.31
1039.92
825.43

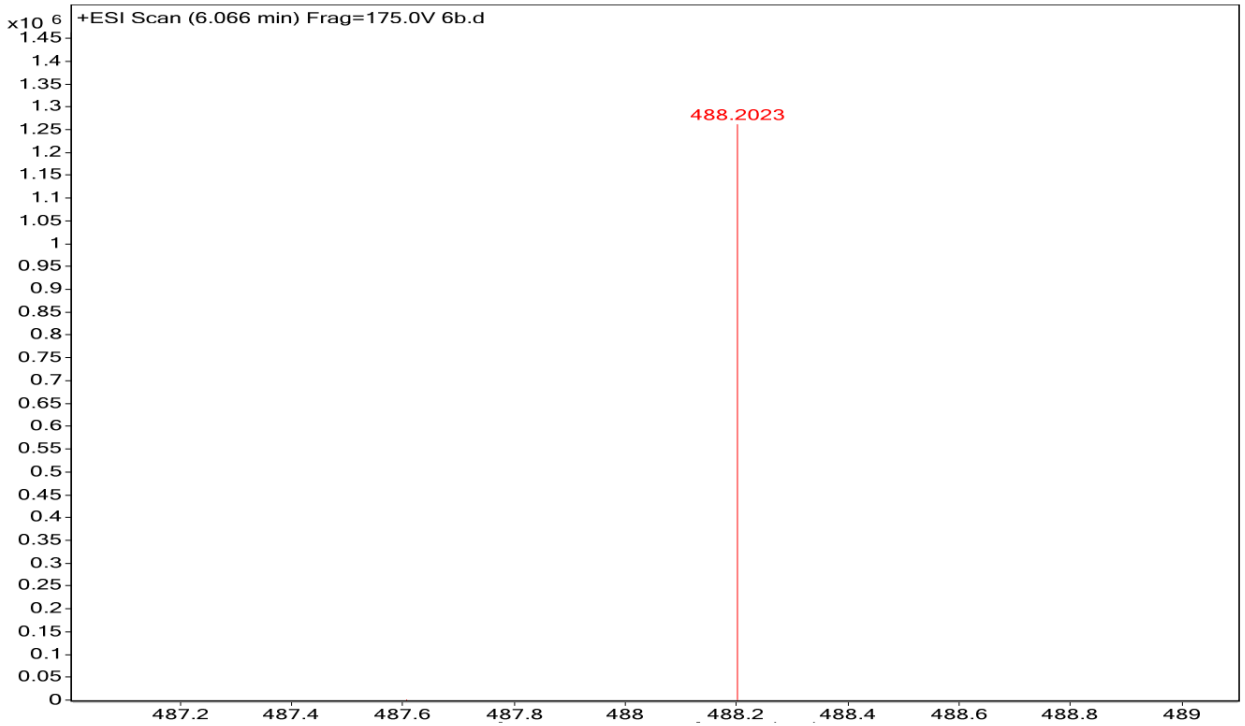

HYG-z-50.001.esp
Normalized Intensity
Chemical Shift (ppm)
12.12
7.60
7.58
7.15
7.13
7.04
6.86
6.84
5.05
4.47
4.45
4.43
4.42
3.75
2.69
2.33
1.45
1.43
1.41
0.01
0.98
1.95
3.79
1.95
1.95
2.03
2.95
2.88
2.86
3.00

^{1}H NMR **6a**

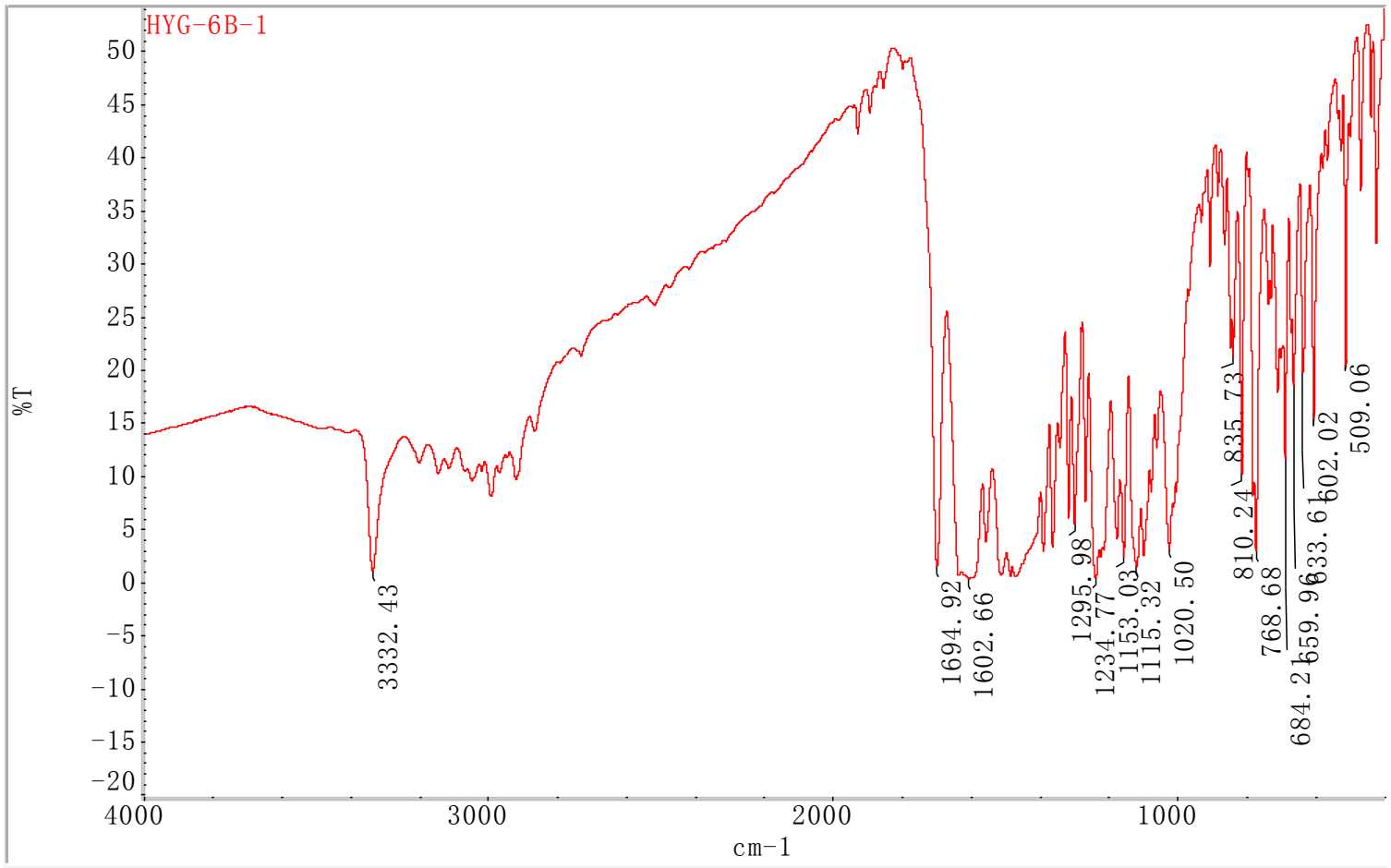

HYG-Z-50-C.001.esp
Normalized Intensity
0.15
0.10
0.05
77.34
77.02
76.70
167.43
165.18
158.80
154.65
151.64
138.34
135.68
129.47
128.72
127.96
120.16
116.57
114.76
108.84
100.00
71.00
62.35
55.68
20.85
14.76
14.22
-0.01
O
O
N-N
N
O
O
N
N
NH
O
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

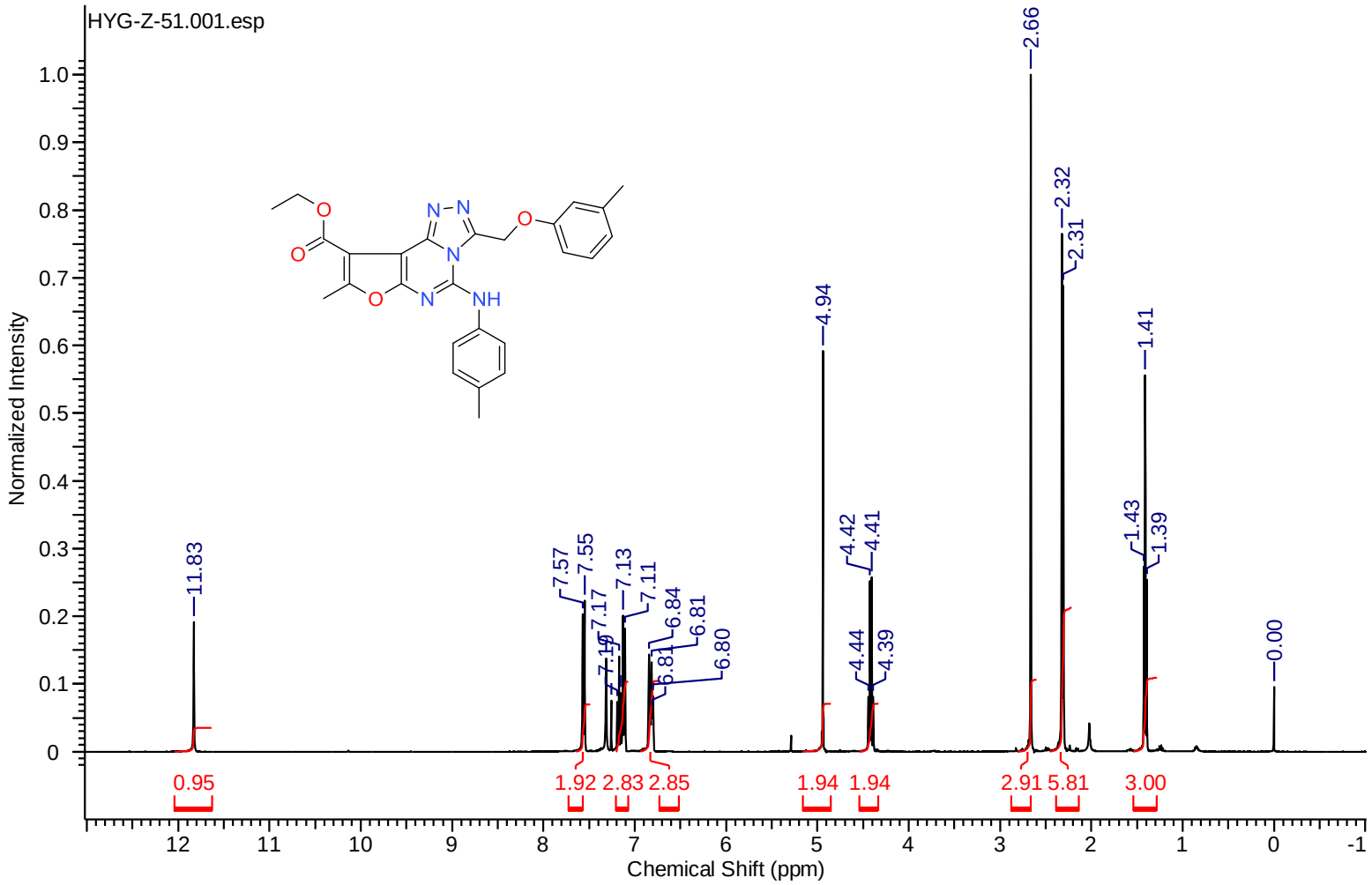
^{13}C NMR **6a**

Sample Name		**Position**	Vial 51	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	6b.d	**ACQ Method**	CYF20201112-NORMAL.m	**Comment**		**Acquired Time**	3/14/2025 4:59:54 P

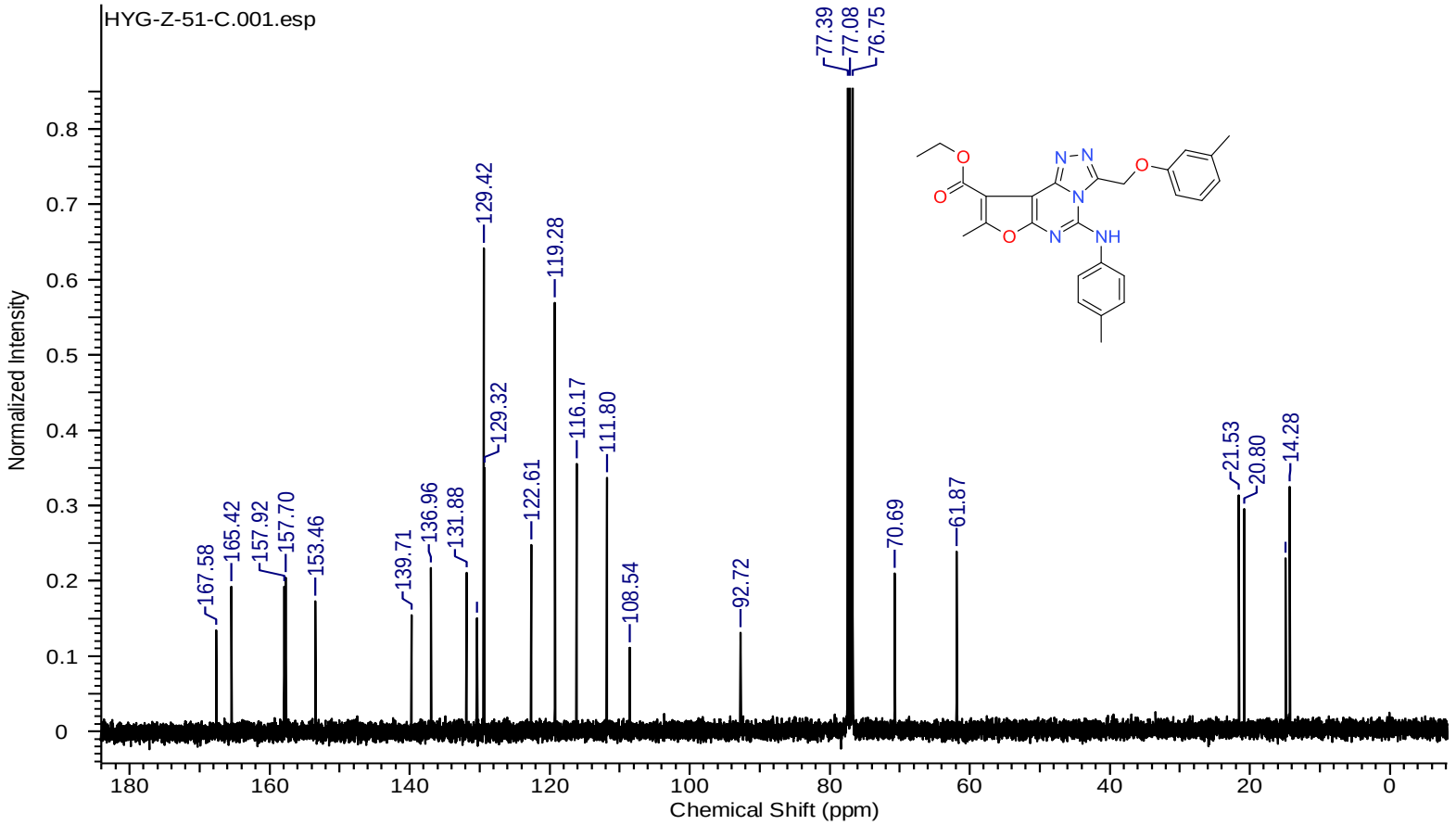


HRMS m/z **6a**

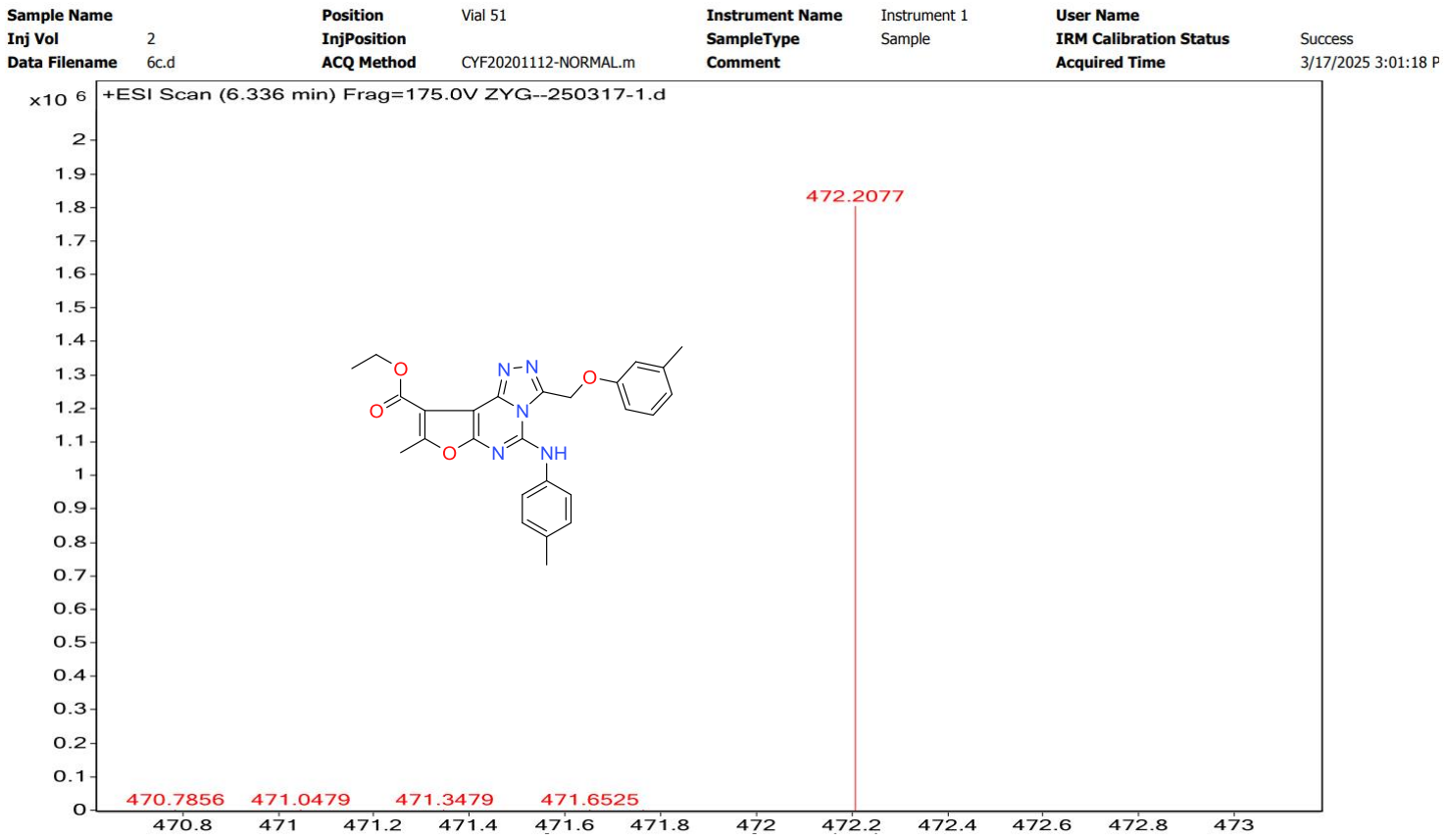

HYG-6B-1
%T
50
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
4000
3000
2000
1000
cm-1
3332.43
1694.92
1602.66
1295.98
1234.77
1153.03
1115.32
1020.50
835.73
810.24
768.68
684.21
659.96
633.61
602.02
509.06


HYG-Z-51.001.esp
Normalized Intensity
Chemical Shift (ppm)
11.83
7.57
7.55
7.17
7.13
7.11
6.84
6.81
6.81
6.80
4.94
4.42
4.41
4.44
4.39
2.66
2.32
2.31
1.43
1.41
1.39
0.00
0.95
1.92
2.83
2.85
1.94
1.94
2.91
5.81
3.00
O
O
N
N
N
O
O
N
NH

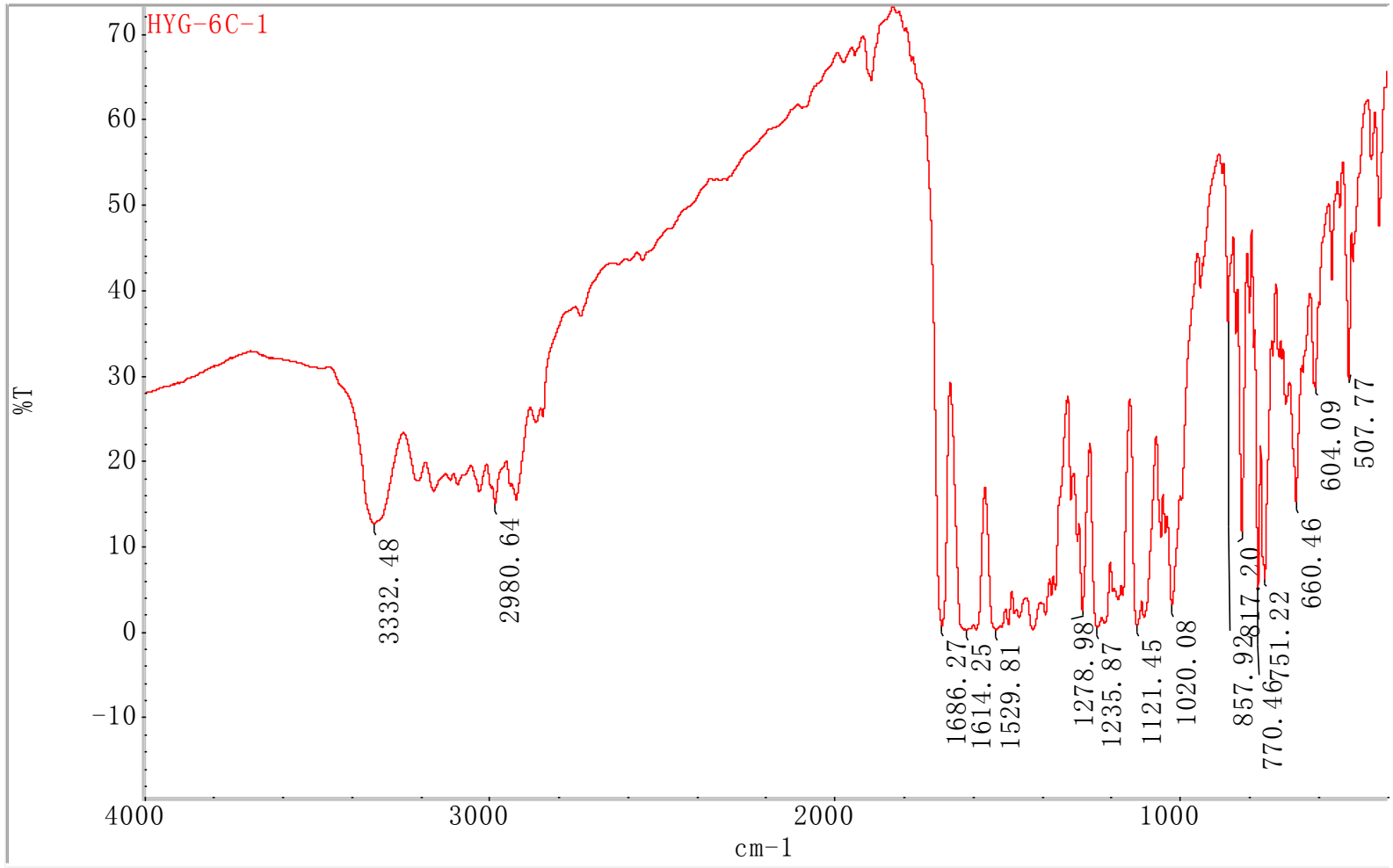
^{1}H NMR **6b**

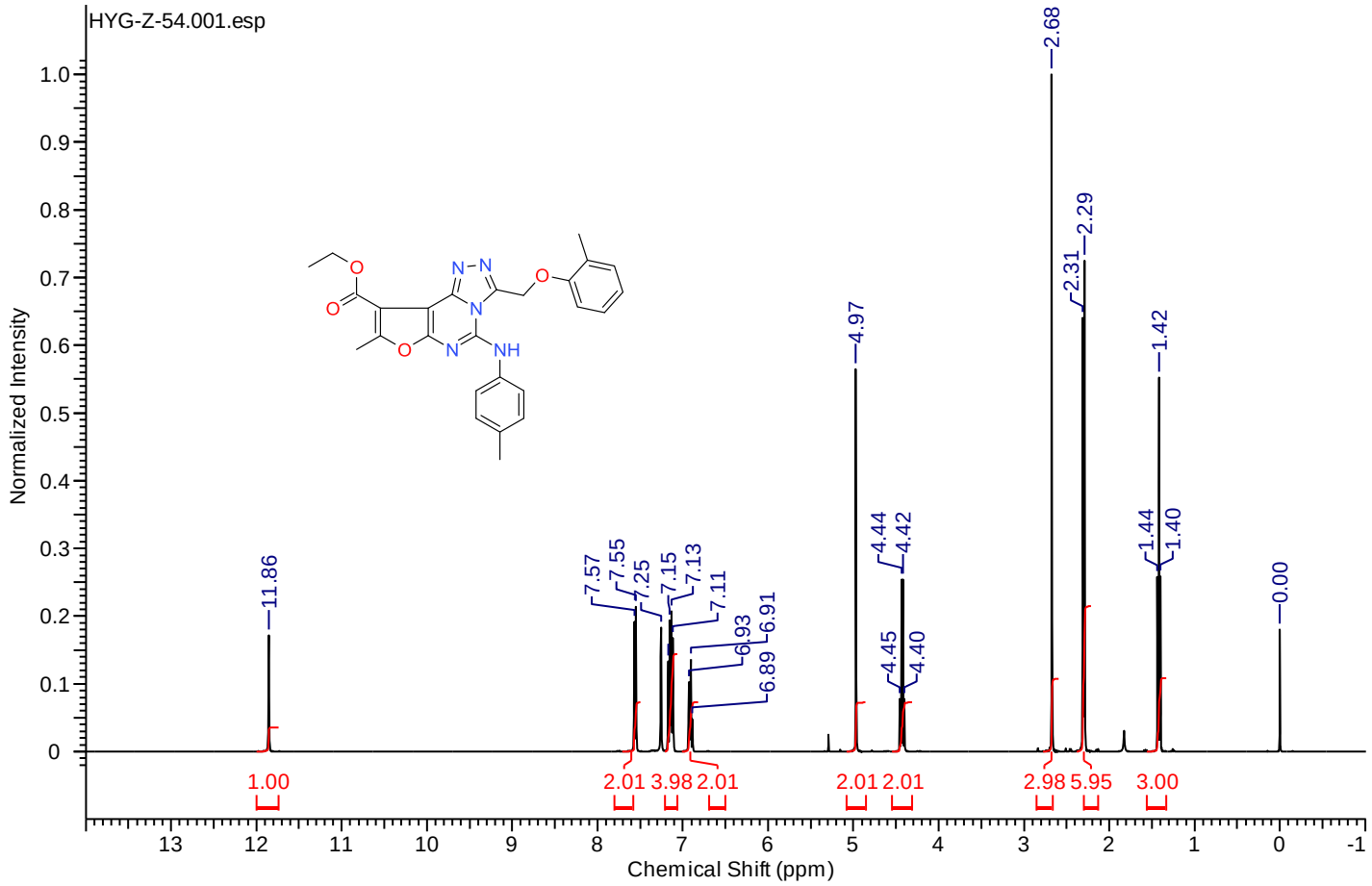

HYG-Z-51-C.001.esp
Normalized Intensity
Chemical Shift (ppm)
167.58
165.42
157.92
157.70
153.46
139.71
136.96
131.88
129.42
129.32
122.61
119.28
116.17
111.80
108.54
92.72
77.39
77.08
76.75
70.69
61.87
21.53
20.80
14.28
O
O
N
N
N
O
N
NH
O

^{13}C NMR **6b**

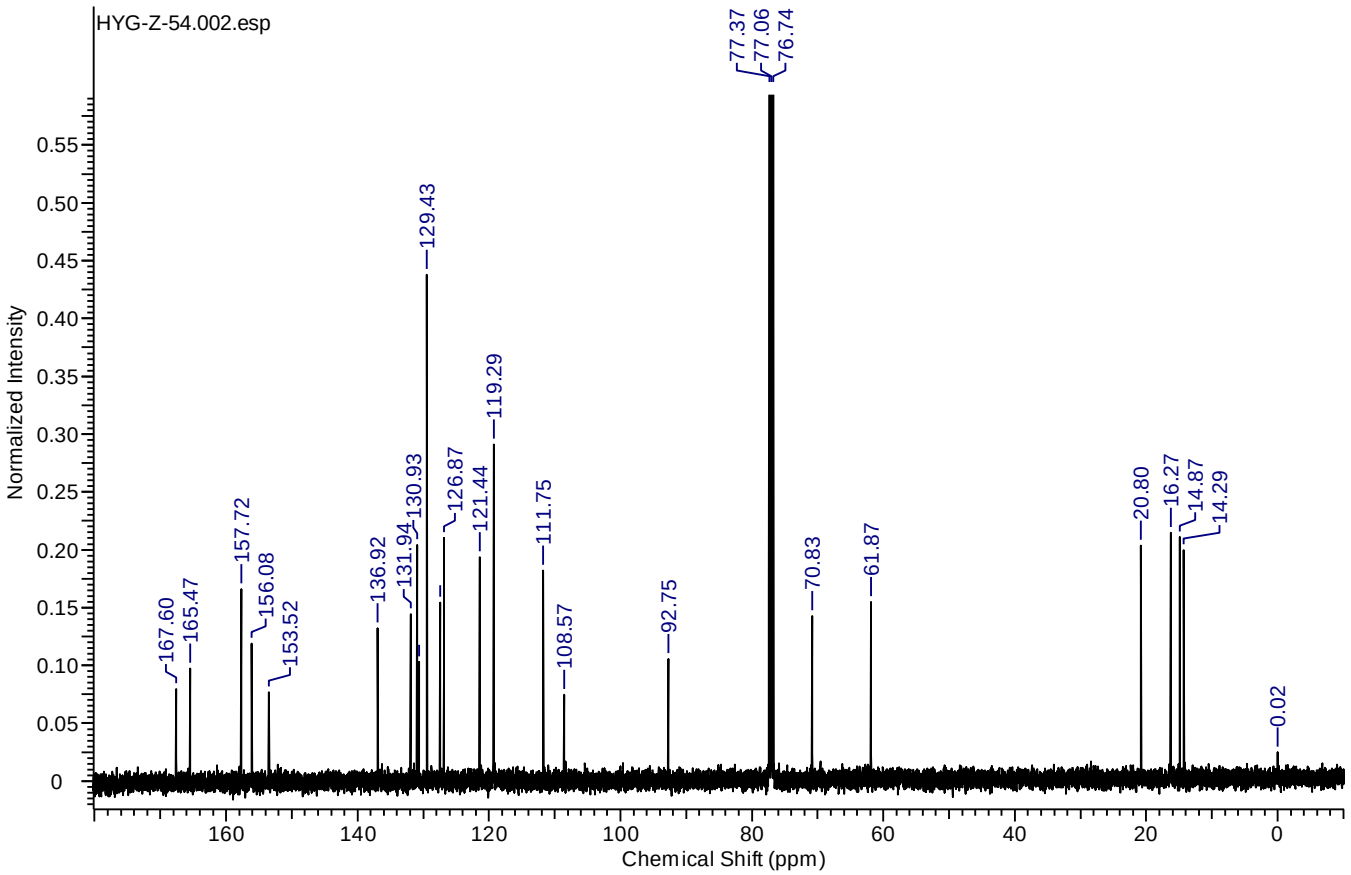

Sample Name
Position Vial 51
Instrument Name Instrument 1
User Name
Inj Vol 2
InjPosition
SampleType Sample
IRM Calibration Status Success
Data Filename 6c.d
ACQ Method CYF20201112-NORMAL.m
Comment
Acquired Time 3/17/2025 3:01:18 P
+ESI Scan (6.336 min) Frag=175.0V ZYG--250317-1.d
x10 6
472.2077
470.7856
471.0479
471.3479
471.6525
O
O
N
N
N
O
O
N
NH

HRMS m/z **6b**


HYG-6C-1
%T
70
60
50
40
30
20
10
0
-10
4000
3000
2000
1000
cm-1
3332.48
2980.64
1686.27
1614.25
1529.81
1278.98
1235.87
1121.45
1020.08
857.92
817.20
770.46
751.22
660.46
604.09
507.77


HYG-Z-54.001.esp
Normalized Intensity
Chemical Shift (ppm)
11.86
7.57
7.55
7.25
7.15
7.13
7.11
6.93
6.91
6.89
4.97
4.44
4.42
4.45
4.40
2.68
2.31
2.29
1.44
1.42
1.40
0.00
1.00
2.01
3.98
2.01
2.01
2.01
2.98
5.95
3.00

^{1}H NMR **6c**


HYG-Z-54.002.esp
Normalized Intensity
0
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50
0.55
167.60
165.47
157.72
156.08
153.52
136.92
131.94
130.93
129.43
126.87
121.44
119.29
111.75
108.57
92.75
77.37
77.06
76.74
70.83
61.87
20.80
16.27
14.87
14.29
0.02
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

^{13}C NMR **6c**

Elemental Composition Report **Page 1**

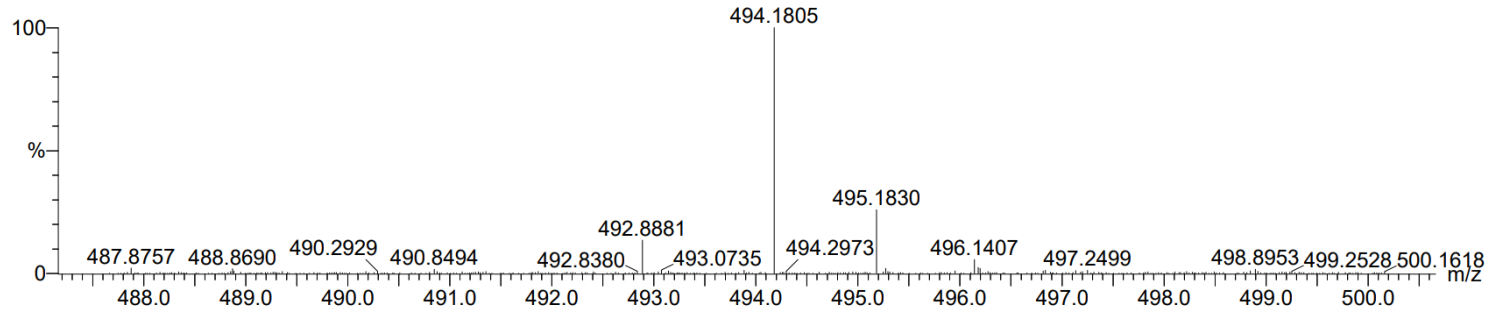
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5652 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 26-26 H: 25-25 N: 0-100 O: 0-100 Na: 0-4 K: 0-2

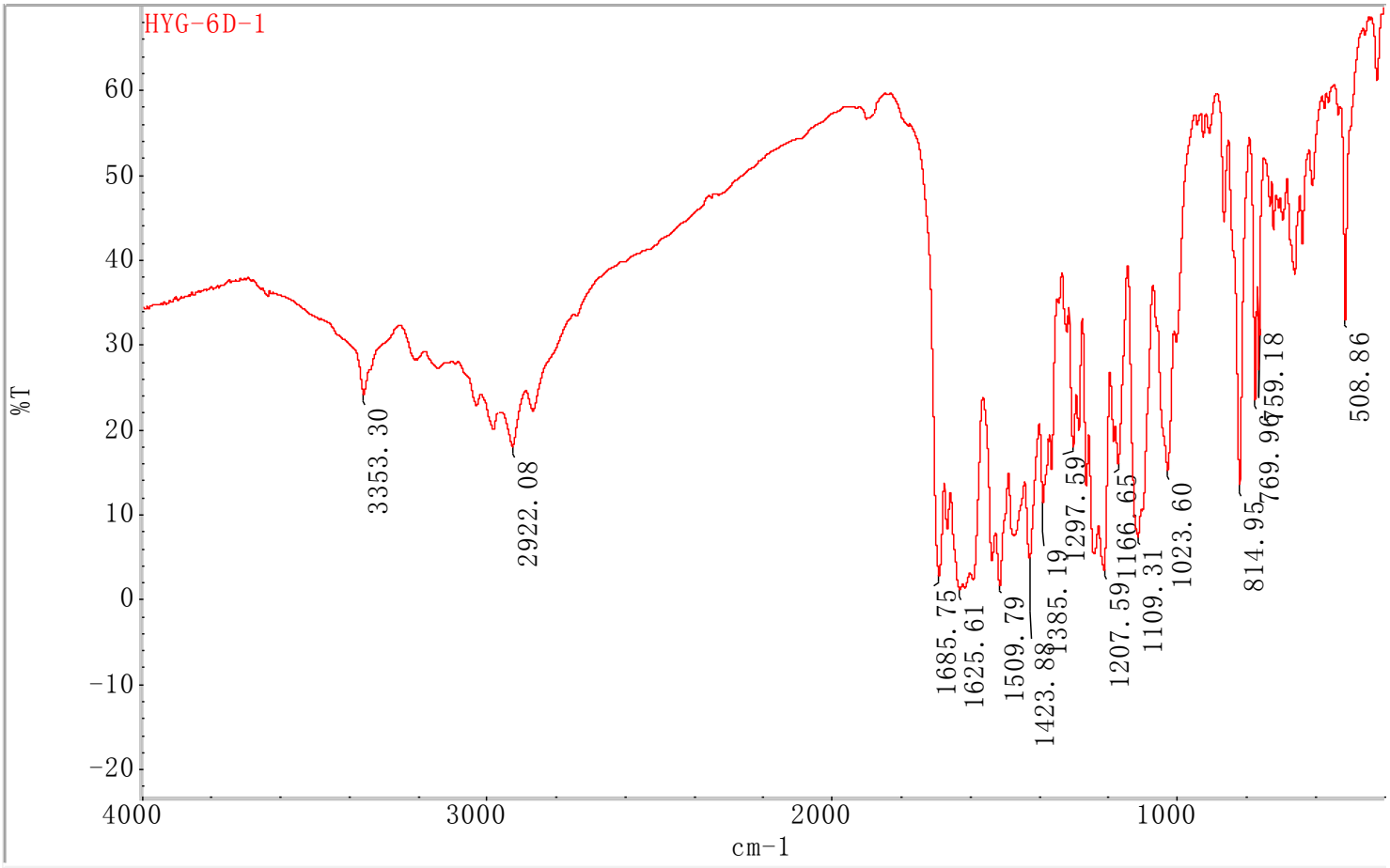
1
240905-6-HYG-Z-54 31 (0.219)

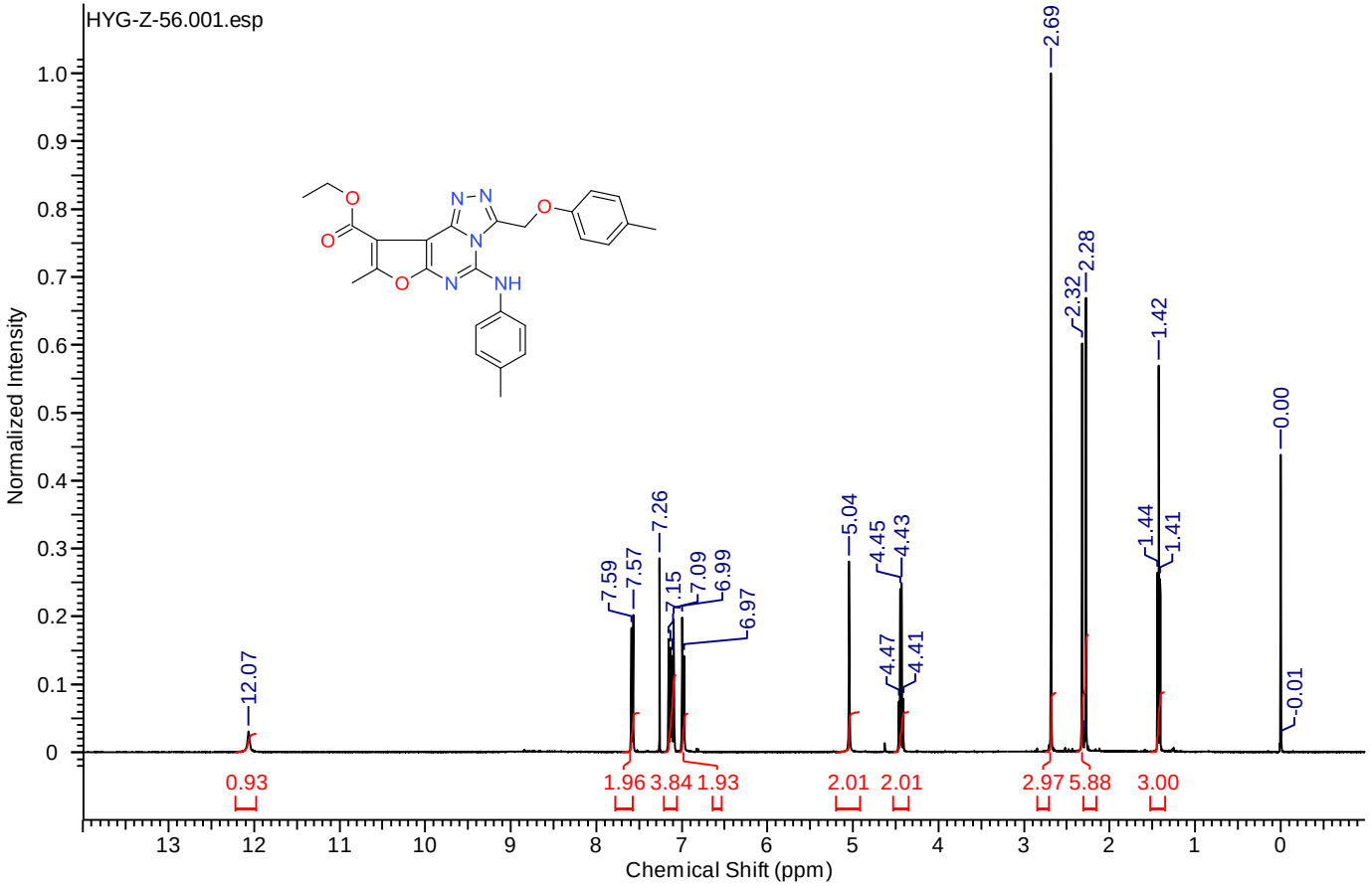
1: TOF MS ES+
6.22e+004



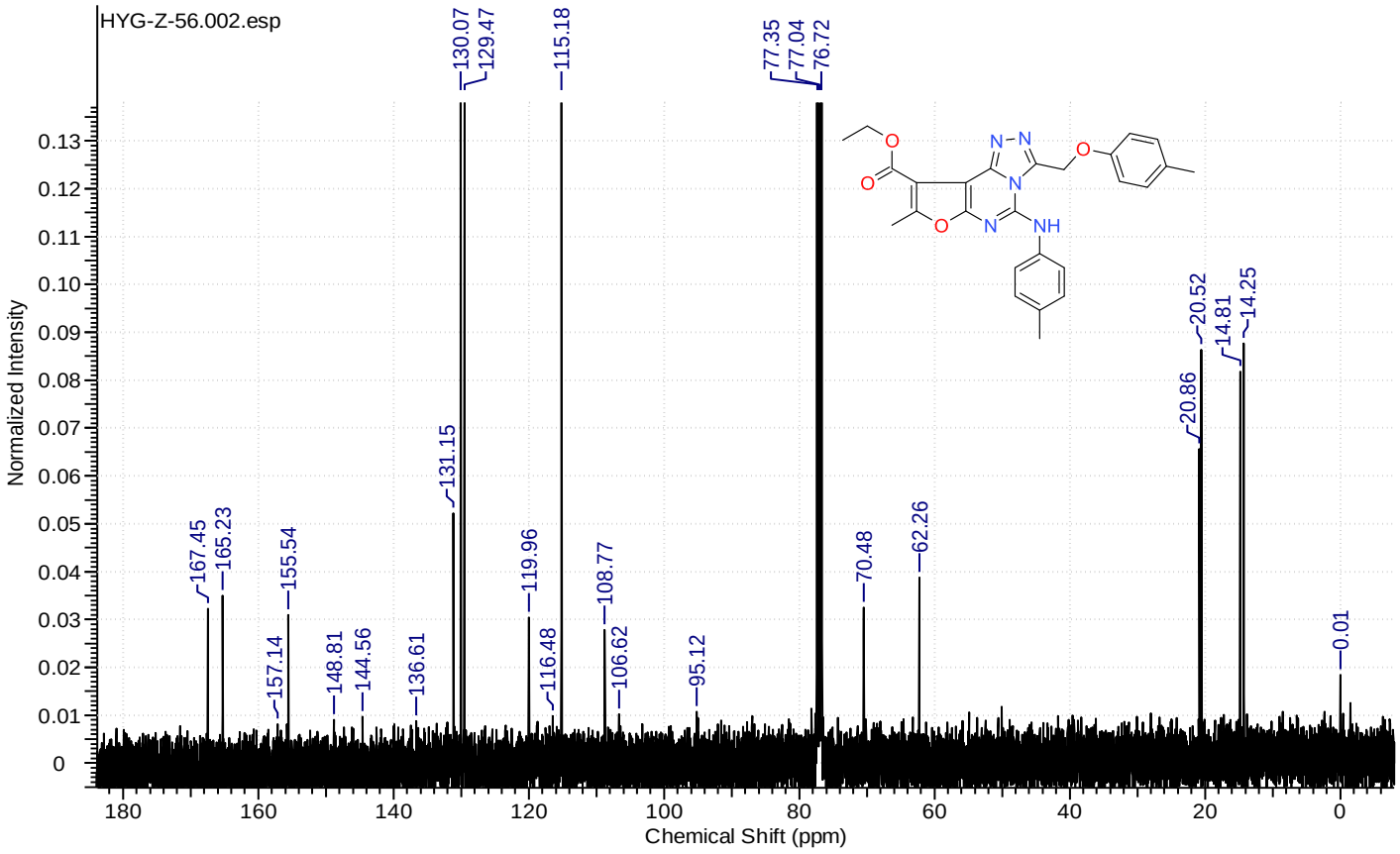
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
494.1805	494.1804	0.1	0.2	16.5	666.4	n/a	n/a	C26 H25 N5 O4 Na

HRMS m/z **6c**


HYG-6D-1
%T
60
50
40
30
20
10
0
-10
-20
4000
3000
2000
1000
cm-1
3353.30
2922.08
1685.75
1625.61
1509.79
1423.88
1385.19
1297.59
1207.59
1166.65
1109.31
1023.60
814.95
769.96
759.18
508.86


HYG-Z-56.001.esp
Normalized Intensity
Chemical Shift (ppm)
12.07
7.59
7.57
7.26
7.15
7.09
6.99
6.97
5.04
4.45
4.43
4.47
4.41
2.69
2.32
2.28
1.44
1.42
1.41
0.00
-0.01
0.93
1.96
3.84
1.93
2.01
2.01
2.97
5.88
3.00

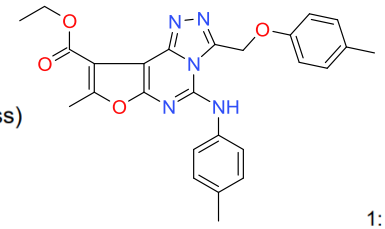
^{1}H NMR **6d**


HYG-Z-56.002.esp
Normalized Intensity
Chemical Shift (ppm)
167.45
165.23
157.14
155.54
148.81
144.56
136.61
131.15
130.07
129.47
119.96
116.48
115.18
108.77
106.62
95.12
77.35
77.04
76.72
70.48
62.26
20.86
20.52
14.81
14.25
0.01
O
O
N-N
N
O
O
N
NH

^{13}C NMR **6d**

Single Mass Analysis

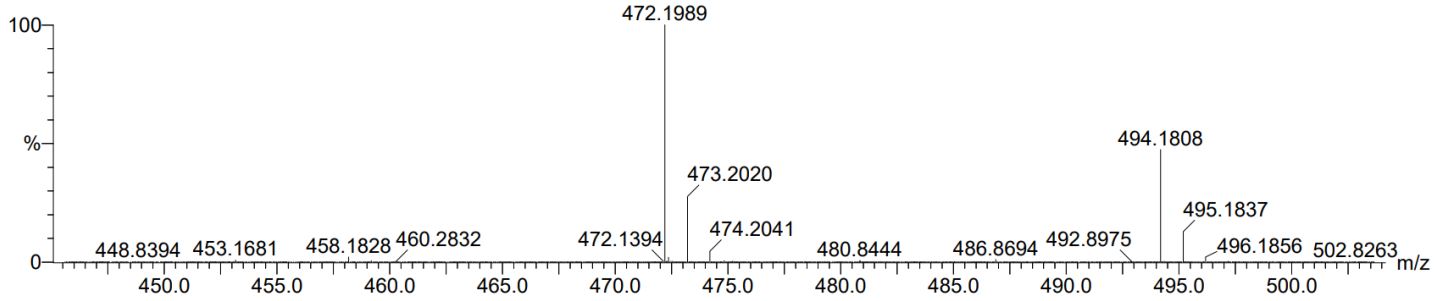
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions
5158 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 26-26 H: 26-26 N: 0-100 O: 0-100 Na: 0-4 K: 0-2

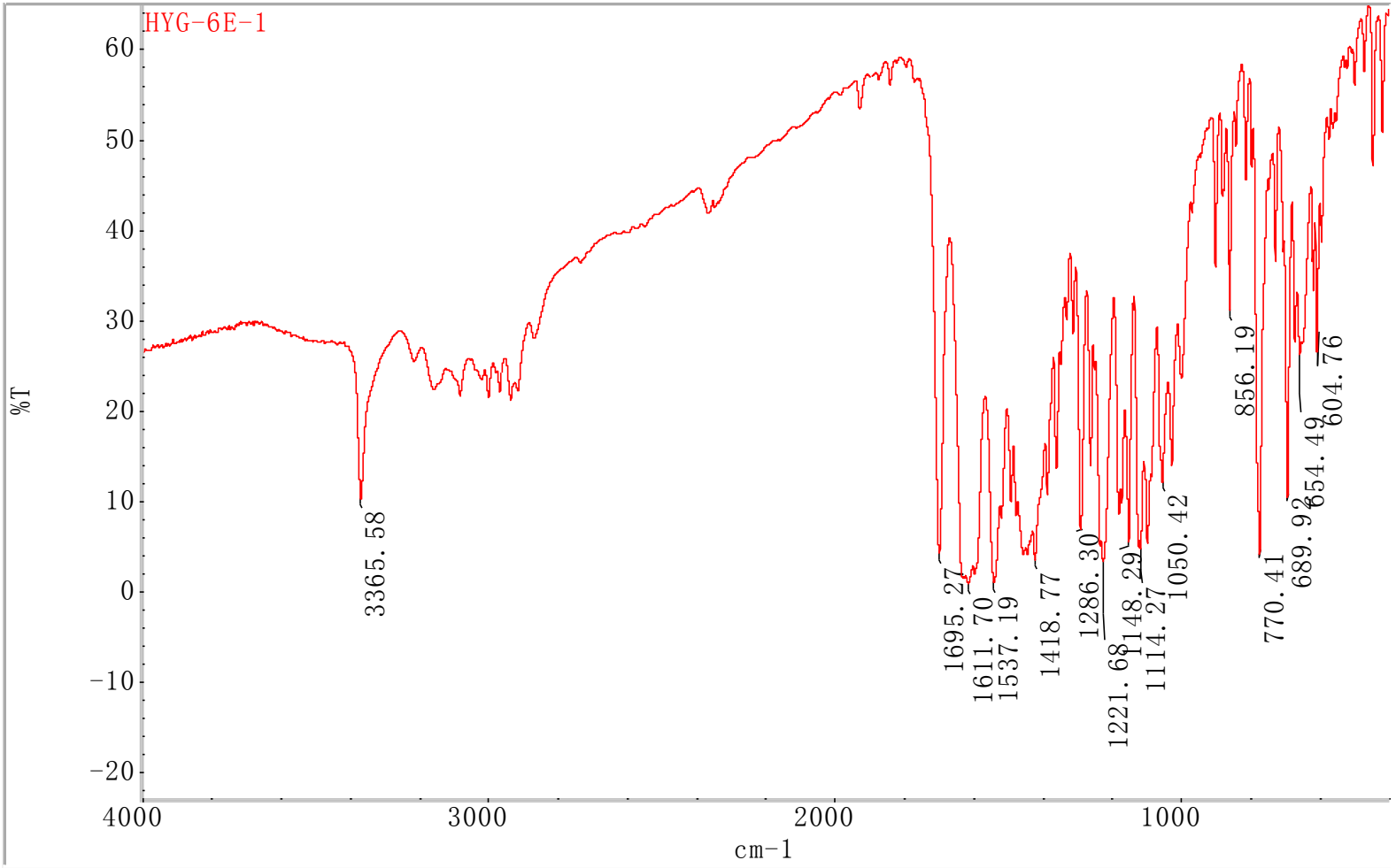
1
240905-6-HYG-Z-55 11 (0.094)

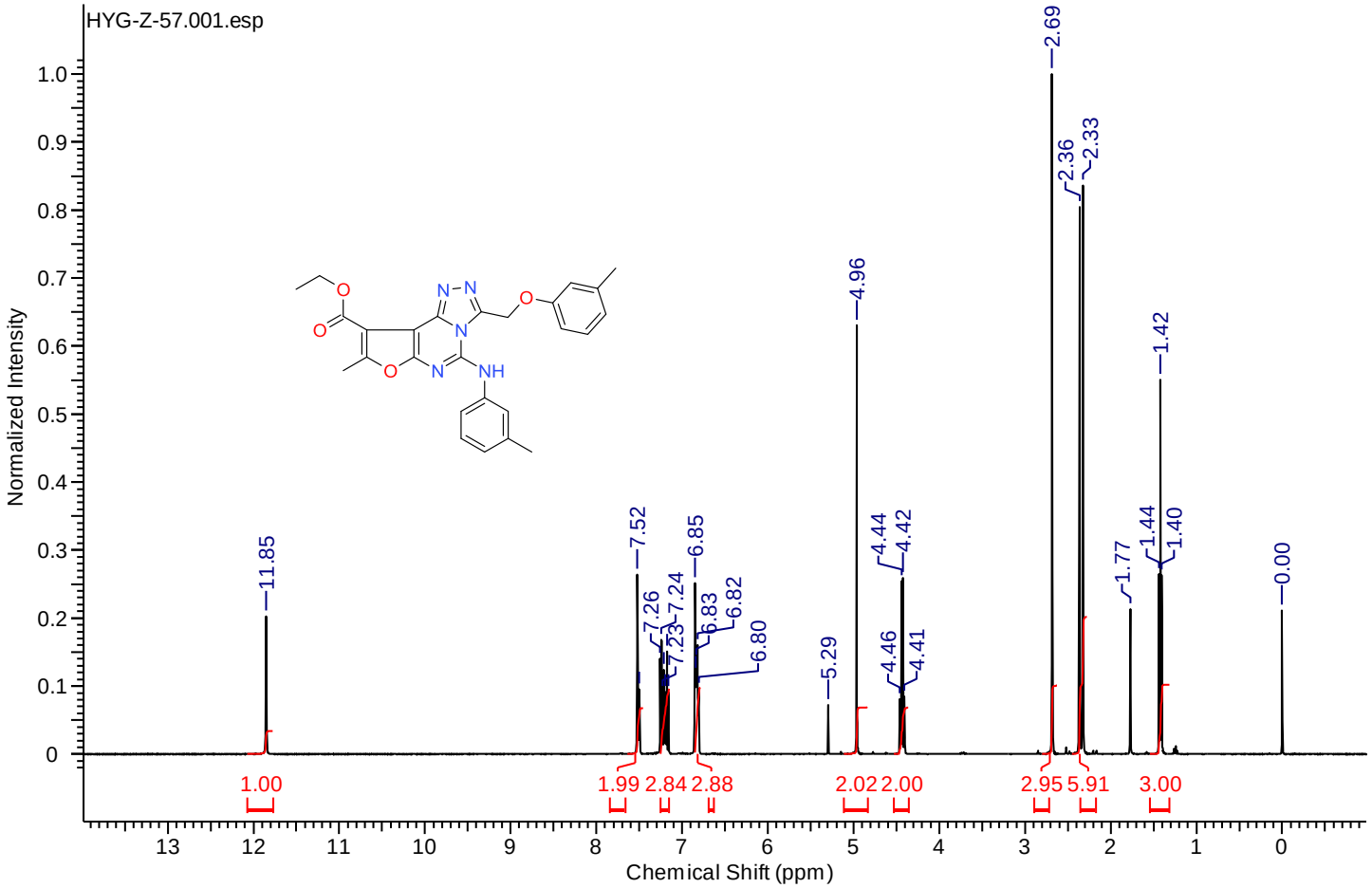
1: TOF MS ES+
1.77e+006



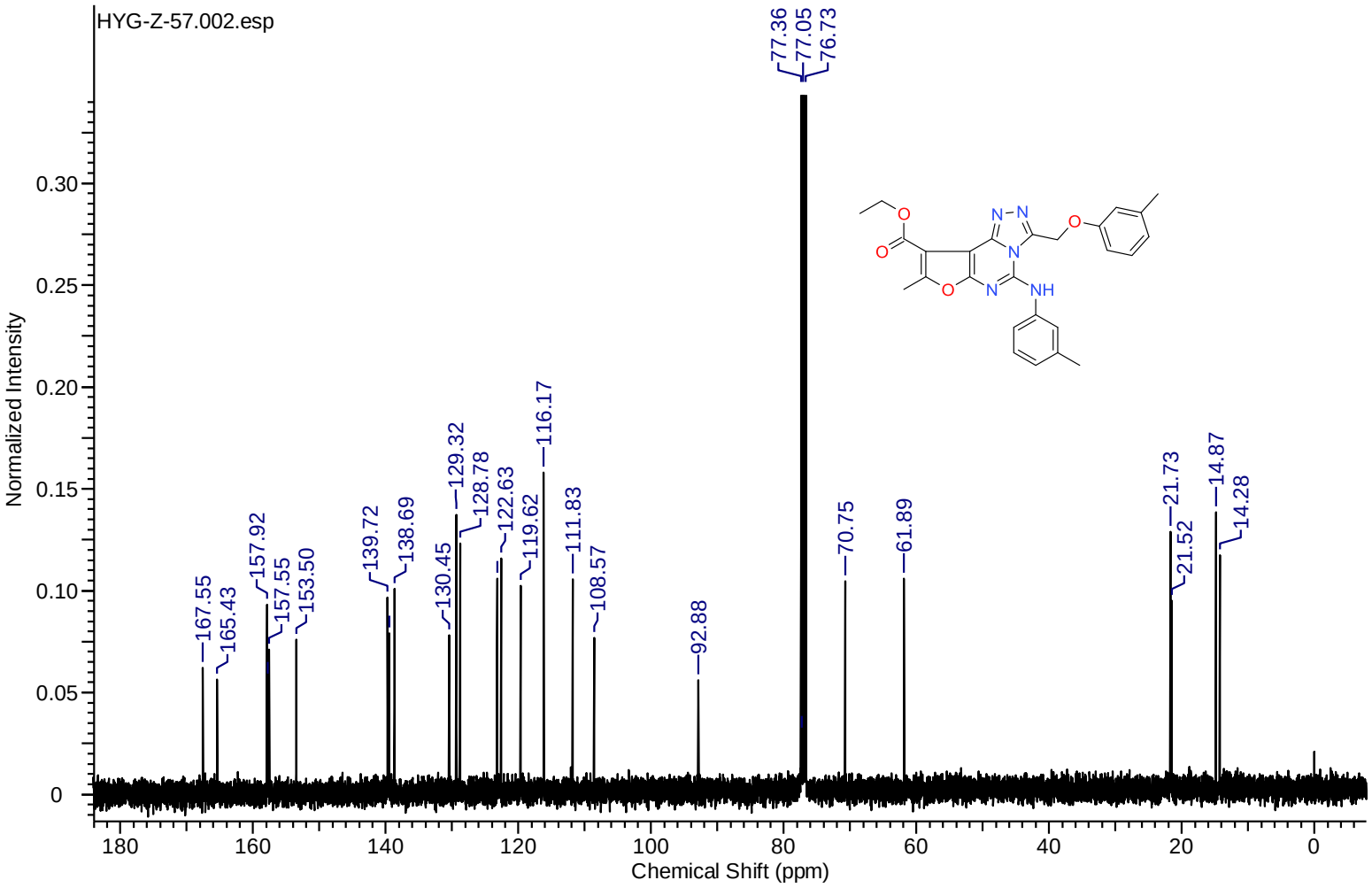
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
472.1989	472.1985	0.4	0.8	16.5	988.9	n/a	n/a	C26 H26 N5 O4

HRMS m/z **6d**


HYG-6E-1
%T
60
50
40
30
20
10
0
-10
-20
4000
3000
2000
1000
cm-1
3365.58
1695.27
1611.70
1537.19
1418.77
1286.30
1221.68
1148.29
1114.27
1050.42
856.19
770.41
689.92
654.49
604.76

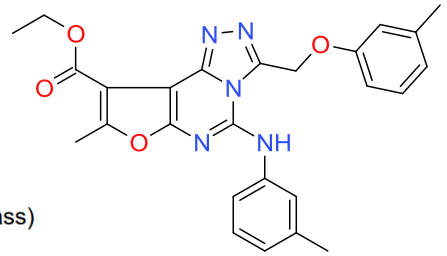

HYG-Z-57.001.esp
Normalized Intensity
Chemical Shift (ppm)
11.85
7.52
7.26
7.24
7.23
6.85
6.83
6.82
6.80
5.29
4.96
4.44
4.42
4.46
4.41
2.69
2.36
2.33
1.77
1.44
1.42
1.40
0.00
1.00
1.99
2.84
2.88
2.02
2.00
2.95
5.91
3.00
O
O
N-N
N
O
O
N
NH

^{1}H NMR **6e**


HYG-Z-57.002.esp
Normalized Intensity
0.30
0.25
0.20
0.15
0.10
0.05
0
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
167.55
165.43
157.92
157.55
153.50
139.72
138.69
130.45
129.32
128.78
122.63
119.62
116.17
111.83
108.57
92.88
77.36
77.05
76.73
70.75
61.89
21.73
21.52
14.87
14.28
O
O
N-N
N
O
O
N
NH

^{13}C NMR **6e**

Elemental Composition Report

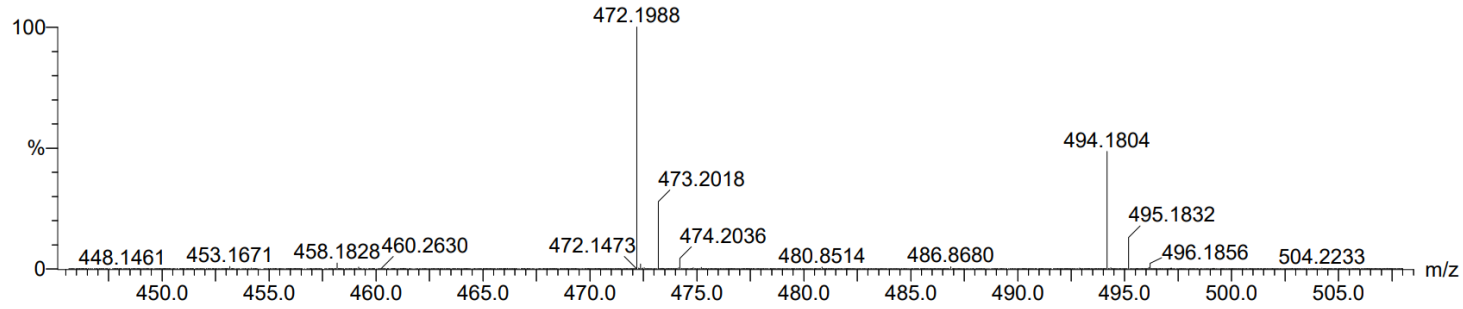


Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5158 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 26-26 H: 26-26 N: 0-100 O: 0-100 Na: 0-4 K: 0-2

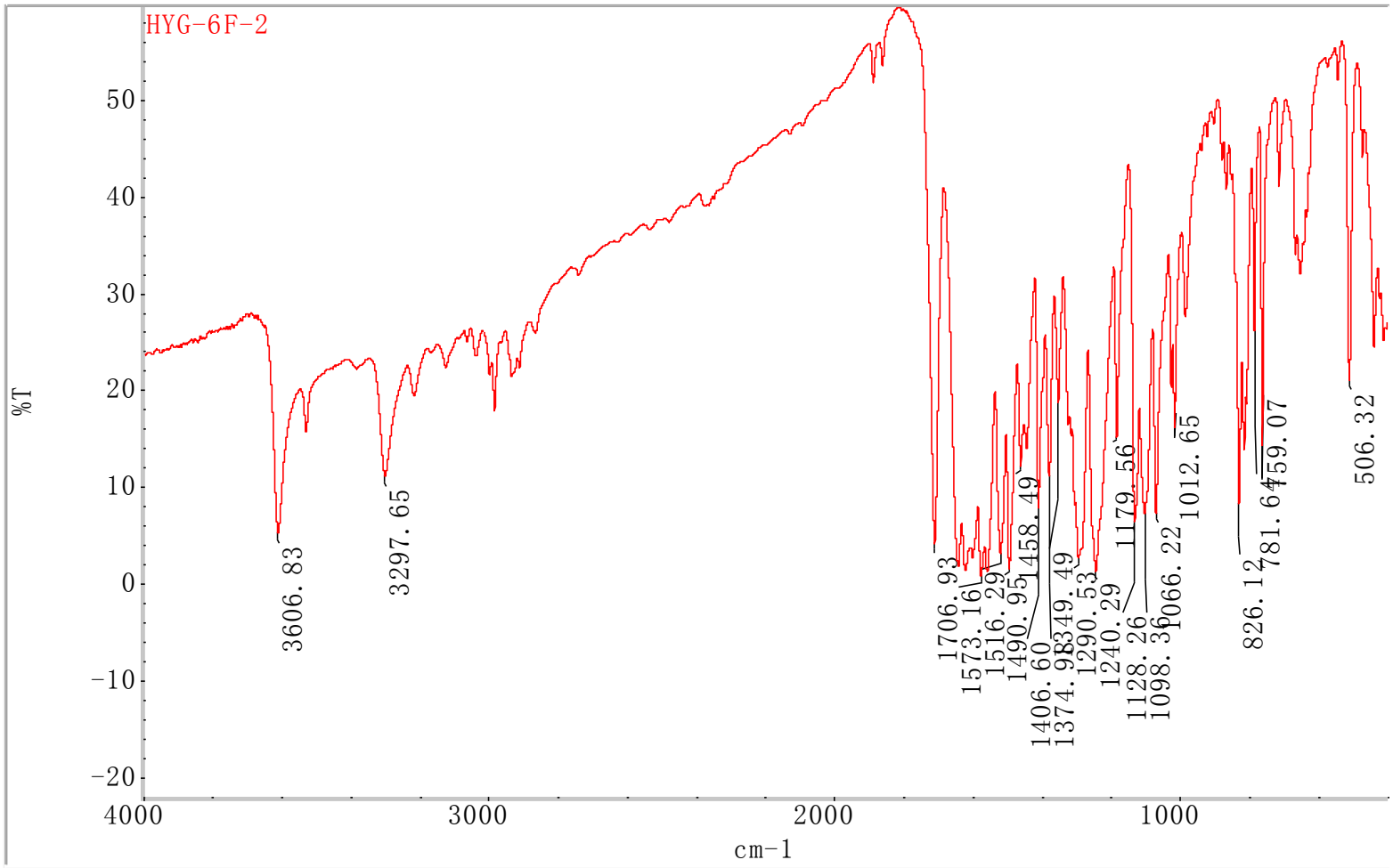
1
240905-6-HYG-Z-57 12 (0.100)

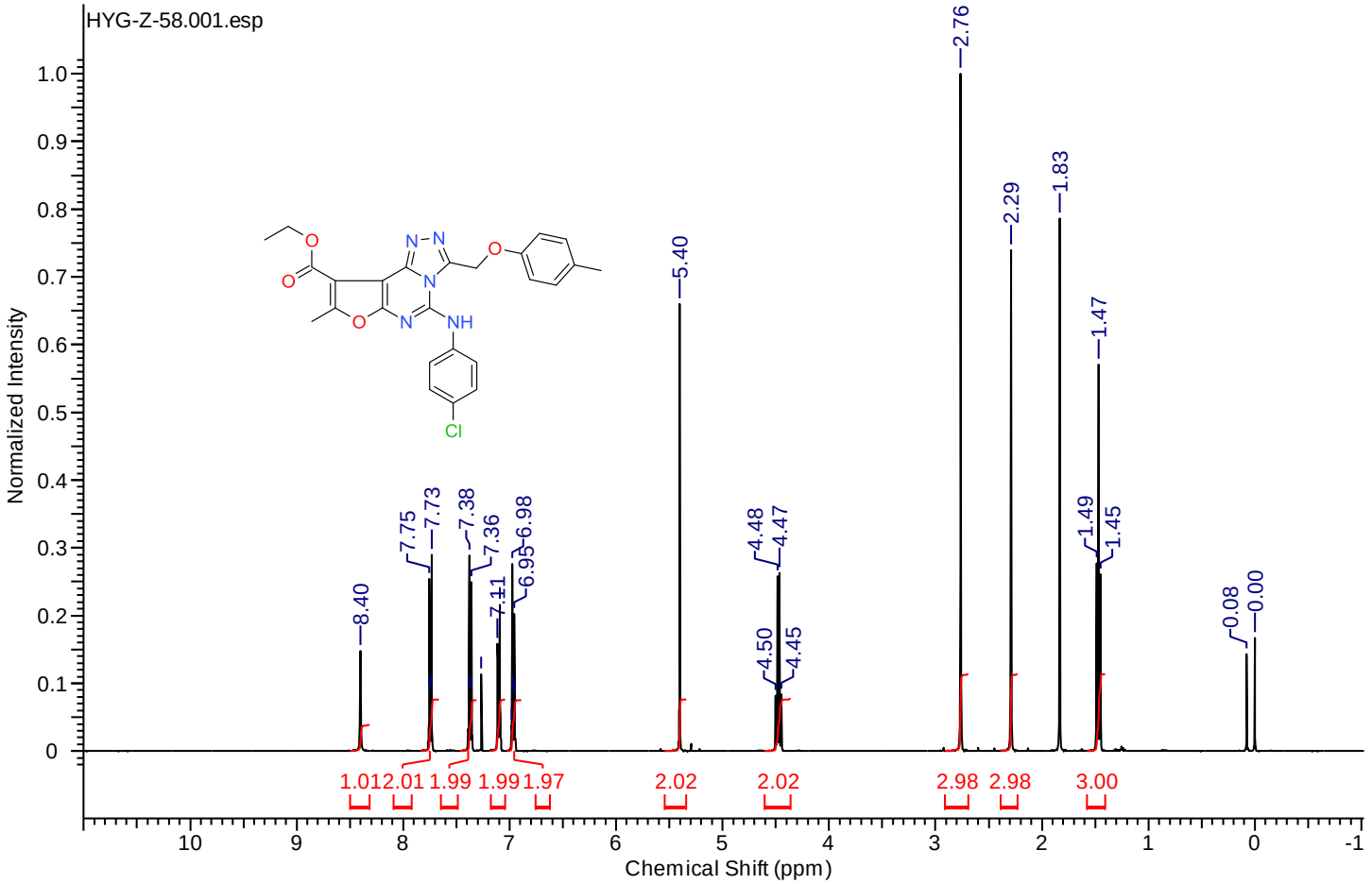
1: TOF MS ES+
2.07e+006



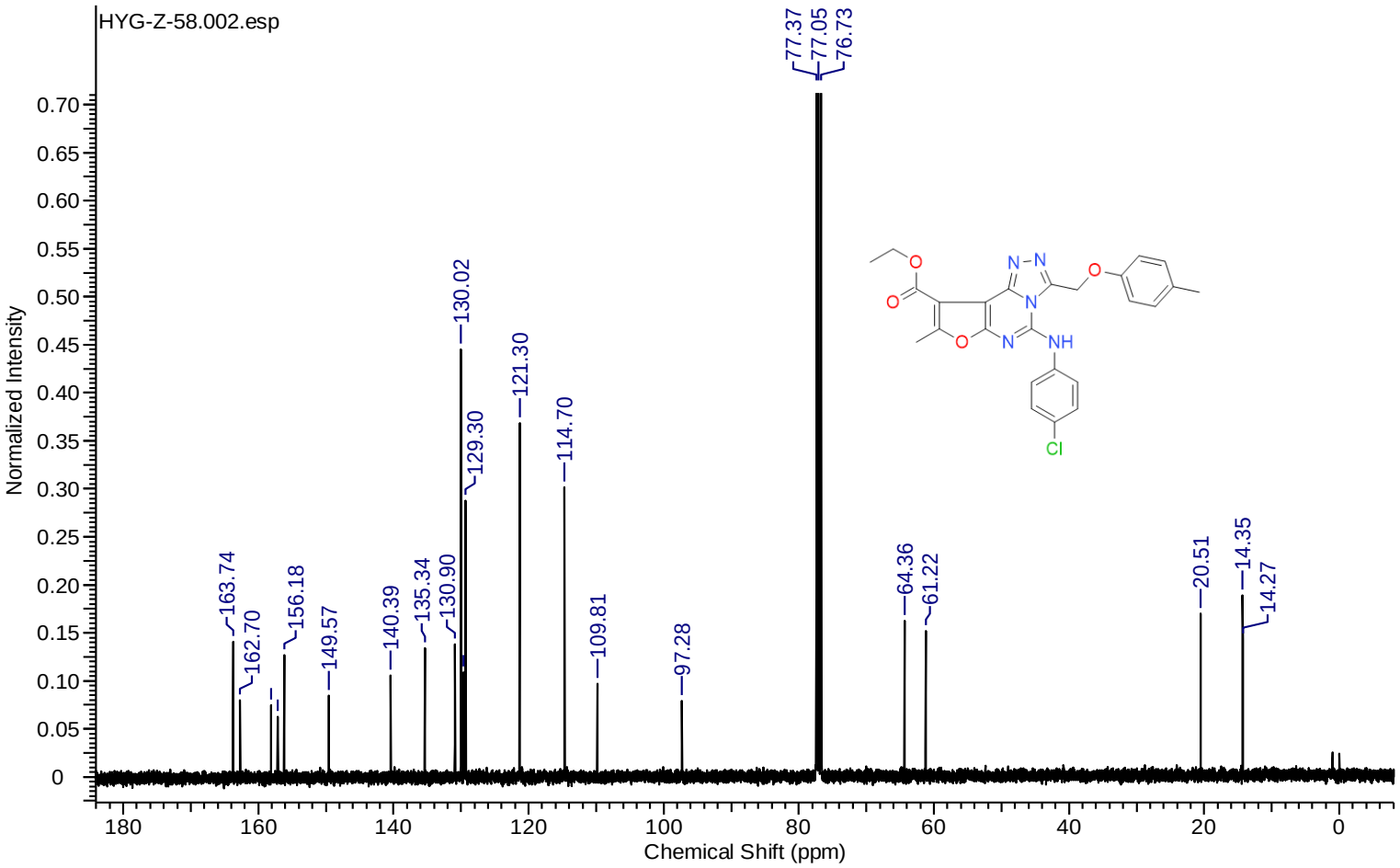
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
472.1988	472.1985	0.3	0.6	16.5	993.4	n/a	n/a	C26 H26 N5 O4

HRMS m/z **6e**


HYG-6F-2
%T
50
40
30
20
10
0
-10
-20
4000
3000
2000
1000
cm-1
3606.83
3297.65
1706.93
1573.16
1516.29
1490.95
1458.49
1406.60
1374.98
1349.49
1290.53
1240.29
1179.56
1128.26
1098.36
1066.22
1012.65
826.12
781.64
759.07
506.32

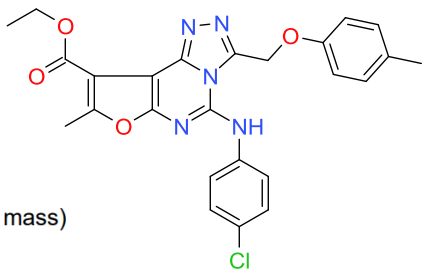

HYG-Z-58.001.esp
Normalized Intensity
Chemical Shift (ppm)
8.40
7.75
7.73
7.38
7.36
7.11
6.98
6.95
5.40
4.48
4.47
4.50
4.45
2.76
2.29
1.83
1.49
1.47
1.45
0.08
0.00
1.01 2.01 1.99 1.99 1.97 2.02 2.02 2.98 2.98 3.00
O
O
N-N
N
O
N
NH
Cl

^{1}H NMR **6f**


HYG-Z-58.002.esp
Normalized Intensity
Chemical Shift (ppm)
77.37
77.05
76.73
130.02
129.30
121.30
114.70
163.74
162.70
156.18
149.57
140.39
135.34
130.90
109.81
97.28
64.36
61.22
20.51
14.35
14.27
O
N
NH
Cl

^{13}C NMR **6f**

Elemental Composition Report **Page 1**

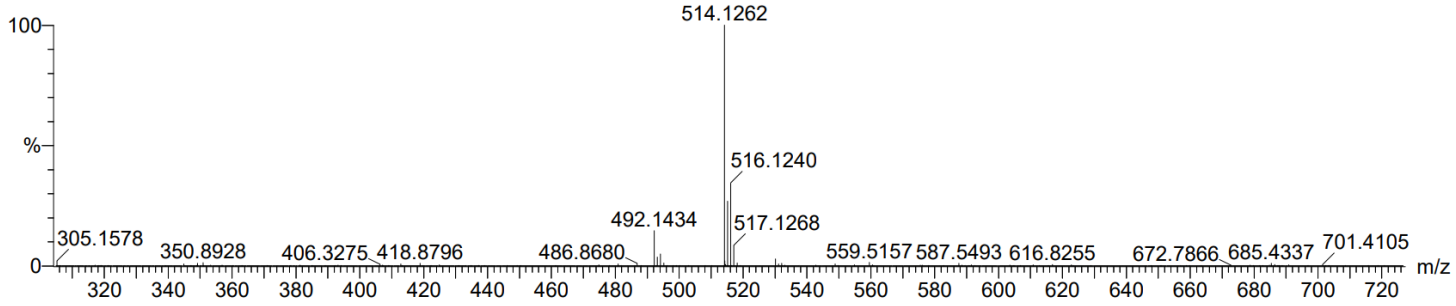


Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
9777 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 25-25 H: 22-22 N: 0-100 O: 0-100 Na: 0-4 Cl: 1-2 K: 0-2

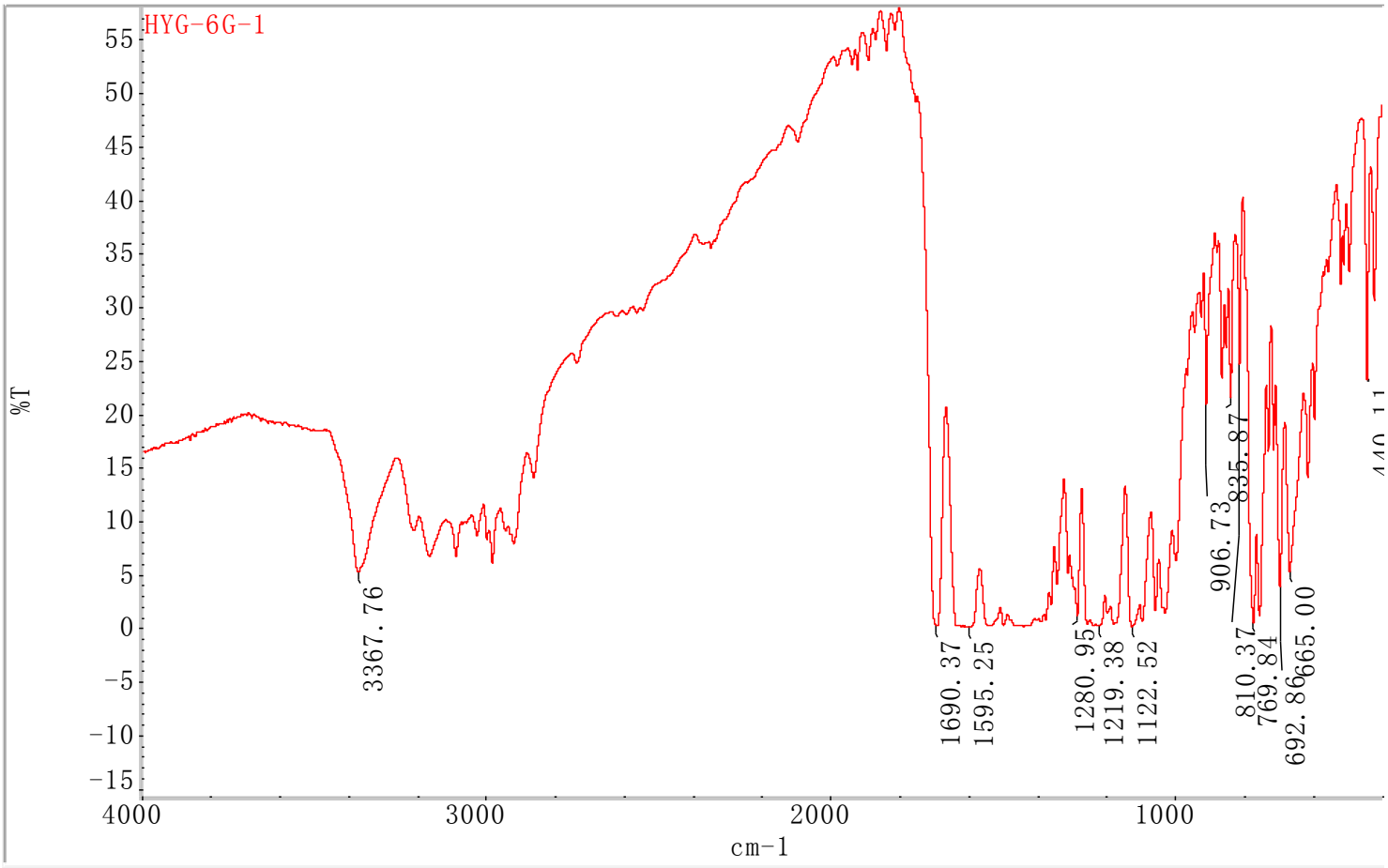
1
240905-6-HYG-Z-58 23 (0.157)

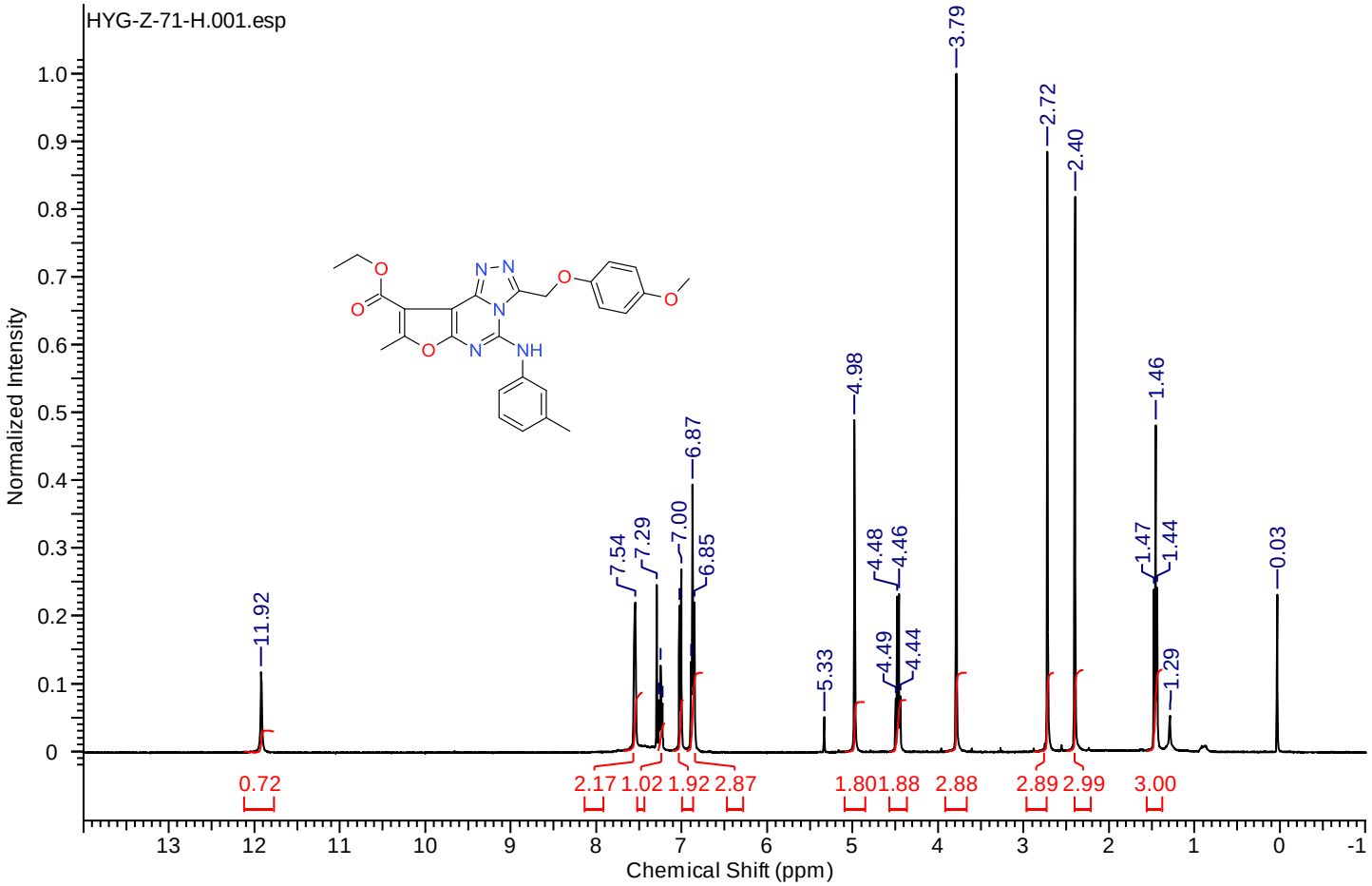
1: TOF MS ES+
2.37e+006



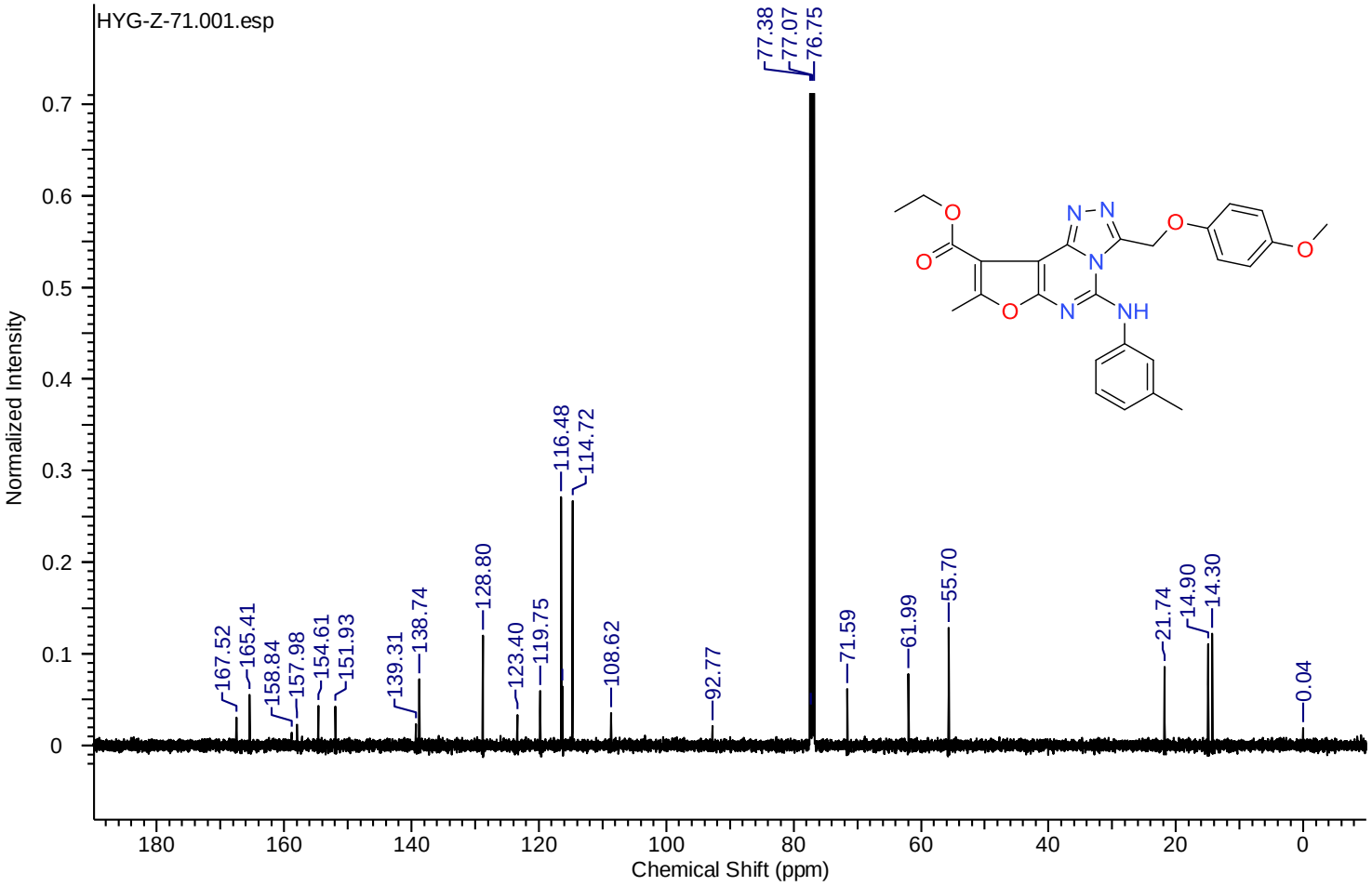
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
514.1262	514.1258	0.4	0.8	16.5	978.5	n/a	n/a	C25 H22 N5 O4 Na Cl

HRMS m/z **6f**

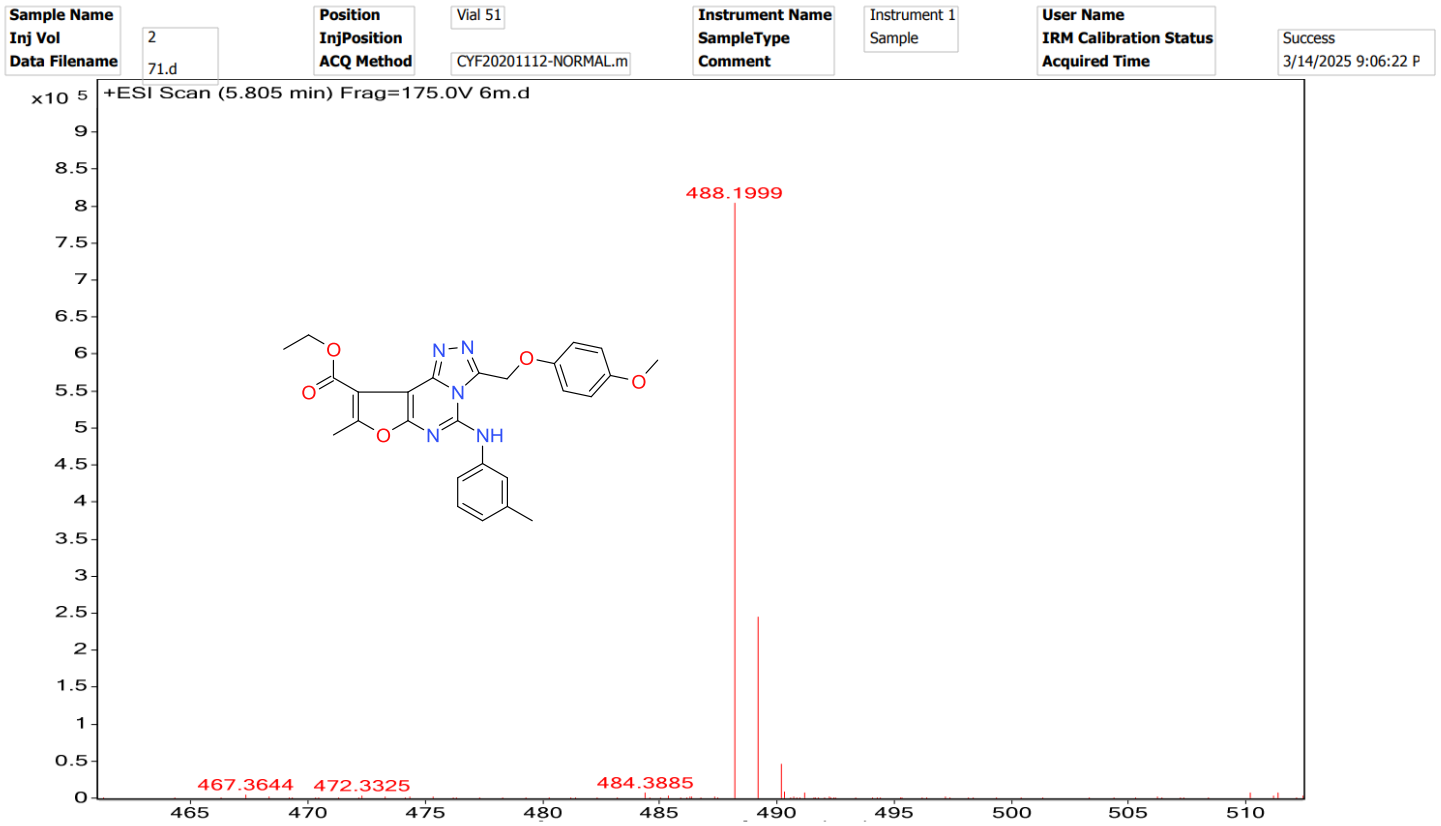

HYG-6G-1
%T
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
4000
3000
2000
1000
cm-1
3367.76
1690.37
1595.25
1280.95
1219.38
1122.52
906.73
835.87
810.37
769.84
692.86
665.00


HYG-Z-71-H.001.esp
Normalized Intensity
Chemical Shift (ppm)
11.92
7.54
7.29
7.00
6.87
6.85
5.33
4.98
4.49
4.48
4.46
4.44
3.79
2.72
2.40
1.47
1.46
1.44
1.29
0.03
0.72
2.17
1.02
1.92
2.87
1.80
1.88
2.88
2.89
2.99
3.00
O
N-N
N
NH
O

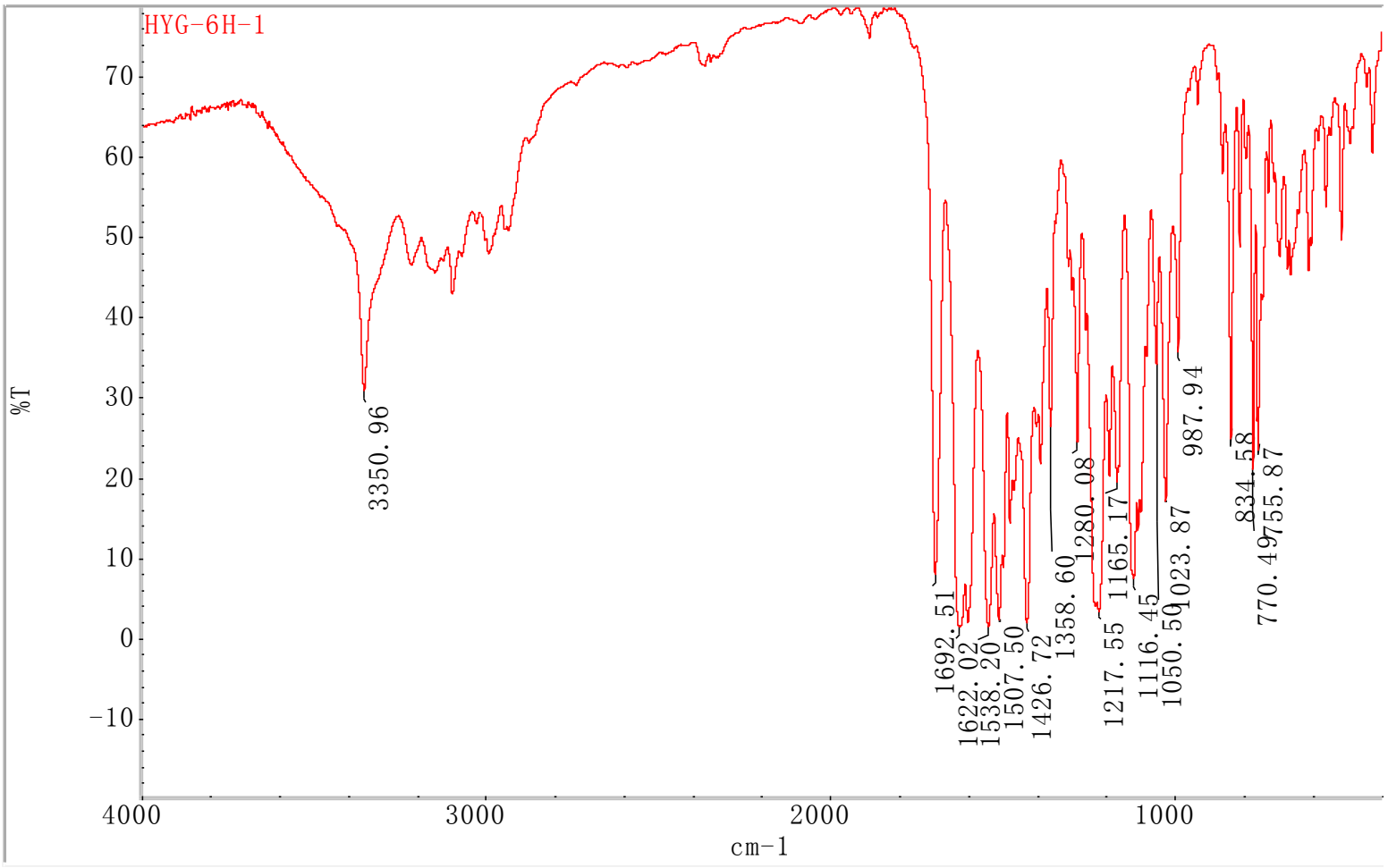
^{1}H NMR **6g**

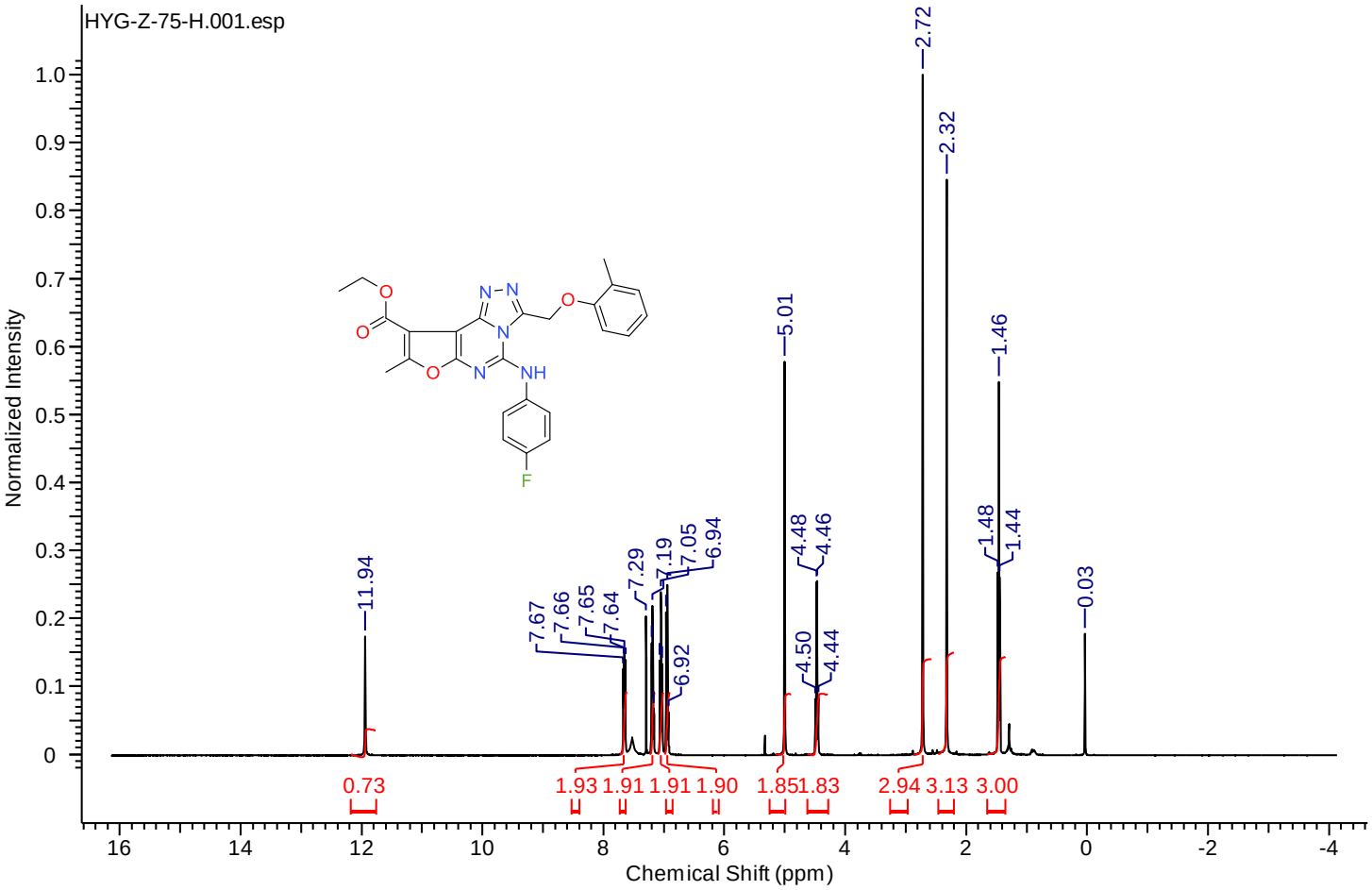

HYG-Z-71.001.esp
Normalized Intensity
Chemical Shift (ppm)
77.38
77.07
76.75
167.52
165.41
158.84
157.98
154.61
151.93
139.31
138.74
128.80
123.40
119.75
116.48
114.72
108.62
92.77
71.59
61.99
55.70
21.74
14.90
14.30
0.04
O
O
N
N
N
O
O
O
N
NH

^{13}C NMR **6g**

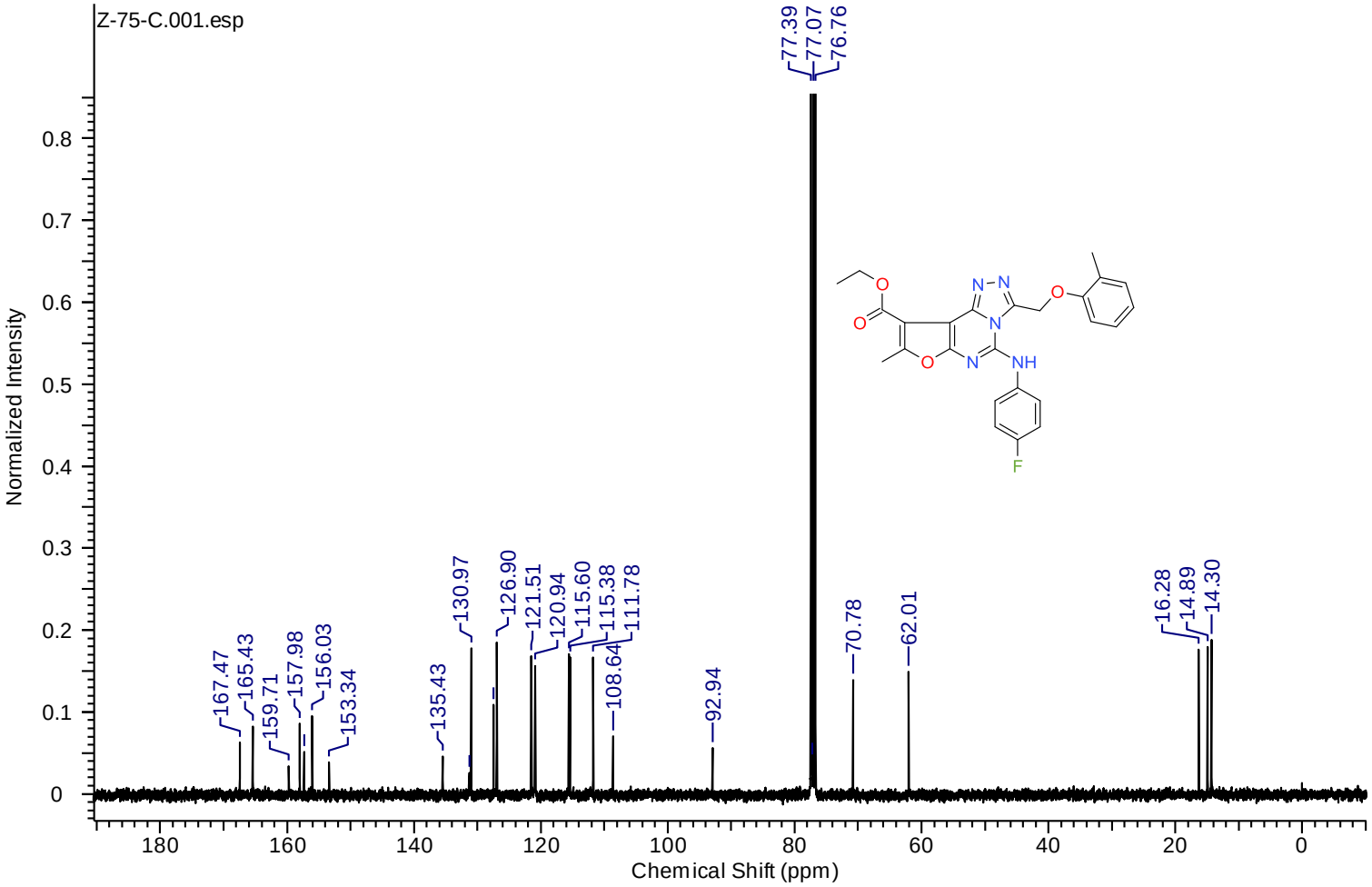

Sample Name
Inj Vol
Data Filename
2
71.d
Position
InjPosition
ACQ Method
Vial 51
CYF20201112-NORMAL.m
Instrument Name
SampleType
Comment
Instrument 1
Sample
User Name
IRM Calibration Status
Acquired Time
Success
3/14/2025 9:06:22 P
+ESI Scan (5.805 min) Frag=175.0V 6m.d
x10 5
488.1999
467.3644
472.3325
484.3885
O
O
N
N
N
O
O
N
NH
O

HRMS m/z **6g**

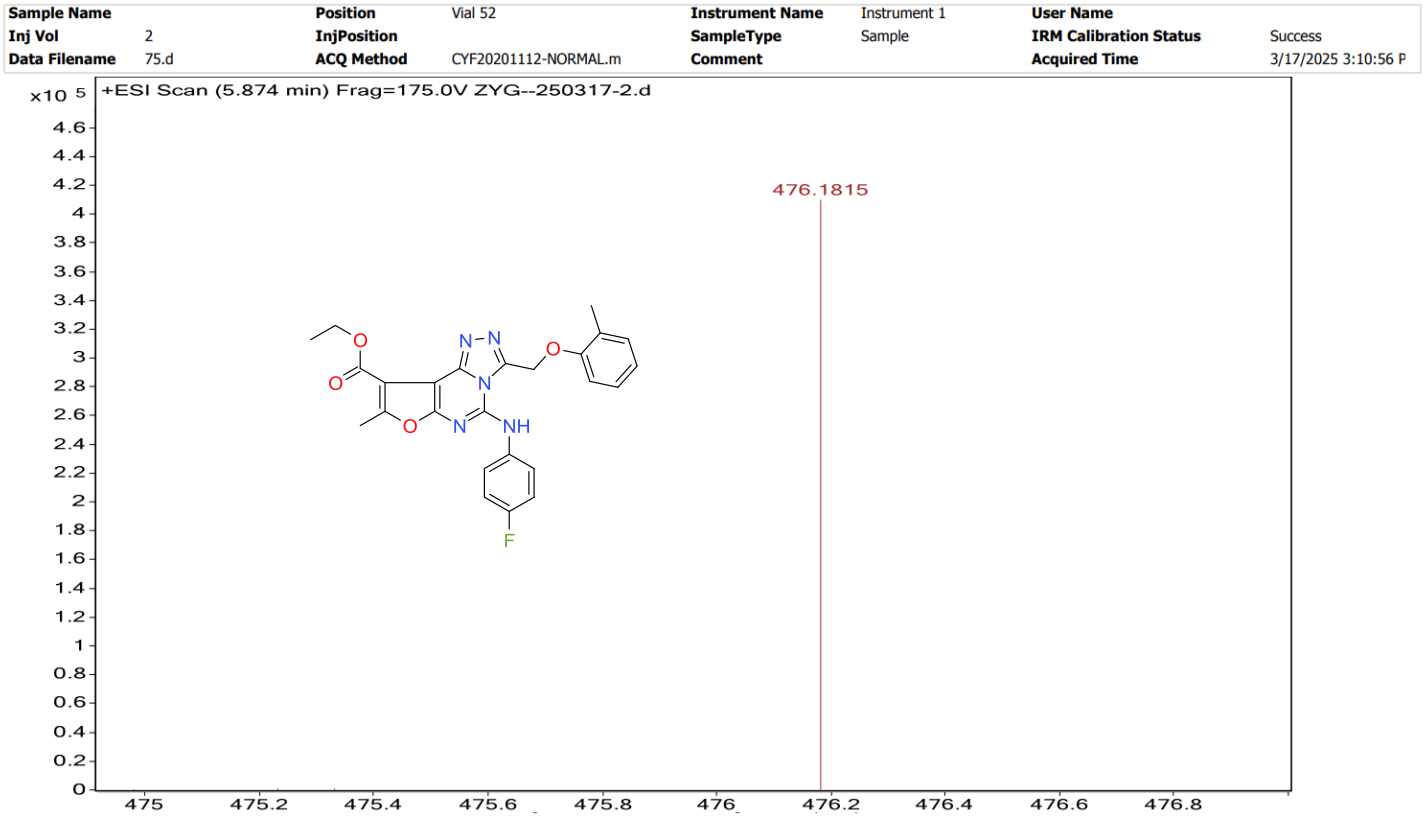

HYG-6H-1
%T
70
60
50
40
30
20
10
0
-10
4000
3000
2000
1000
cm-1
3350.96
1692.51
1622.02
1538.20
1507.50
1426.72
1358.60
1280.08
1217.55
1165.17
1116.45
1050.50
1023.87
987.94
834.58
770.49
755.87


HYG-Z-75-H.001.esp
Normalized Intensity
Chemical Shift (ppm)
11.94
7.67
7.66
7.65
7.64
7.29
7.19
7.05
6.94
6.92
5.01
4.48
4.46
4.50
4.44
2.72
2.32
1.46
1.48
1.44
0.03
0.73
1.93
1.91
1.91
1.90
1.85
1.83
2.94
3.13
3.00
O
O
N
N
N
O
N
NH
F

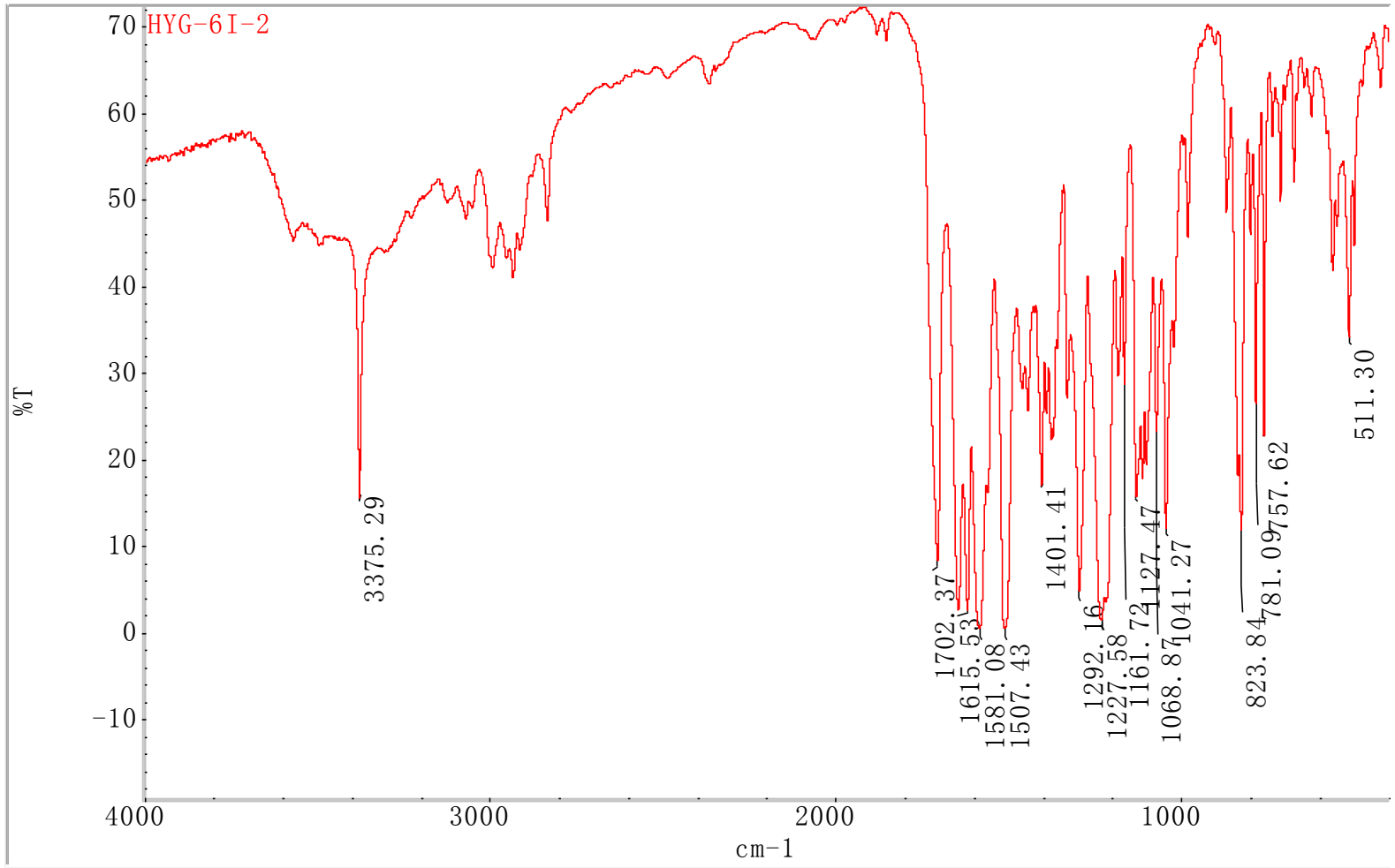
^{1}H NMR **6h**


Z-75-C.001.esp
Normalized Intensity
Chemical Shift (ppm)
77.39
77.07
76.76
167.47
165.43
159.71
157.98
156.03
153.34
135.43
130.97
126.90
121.51
120.94
115.60
115.38
111.78
108.64
92.94
70.78
62.01
16.28
14.89
14.30
NH
F

^{13}C NMR **6h**


Sample Name
Position
Vial 52
Instrument Name
Instrument 1
User Name
Inj Vol
2
InjPosition
SampleType
Sample
IRM Calibration Status
Success
Data Filename
75.d
ACQ Method
CYF20201112-NORMAL.m
Comment
Acquired Time
3/17/2025 3:10:56 P
+ESI Scan (5.874 min) Frag=175.0V ZYG--250317-2.d
x10 5
476.1815
F

HRMS m/z **6h**


HYG-6I-2
%T
70
60
50
40
30
20
10
0
-10
4000
3000
2000
1000
cm-1
3375.29
1702.37
1615.53
1581.08
1507.43
1401.41
1292.16
1227.58
1161.72
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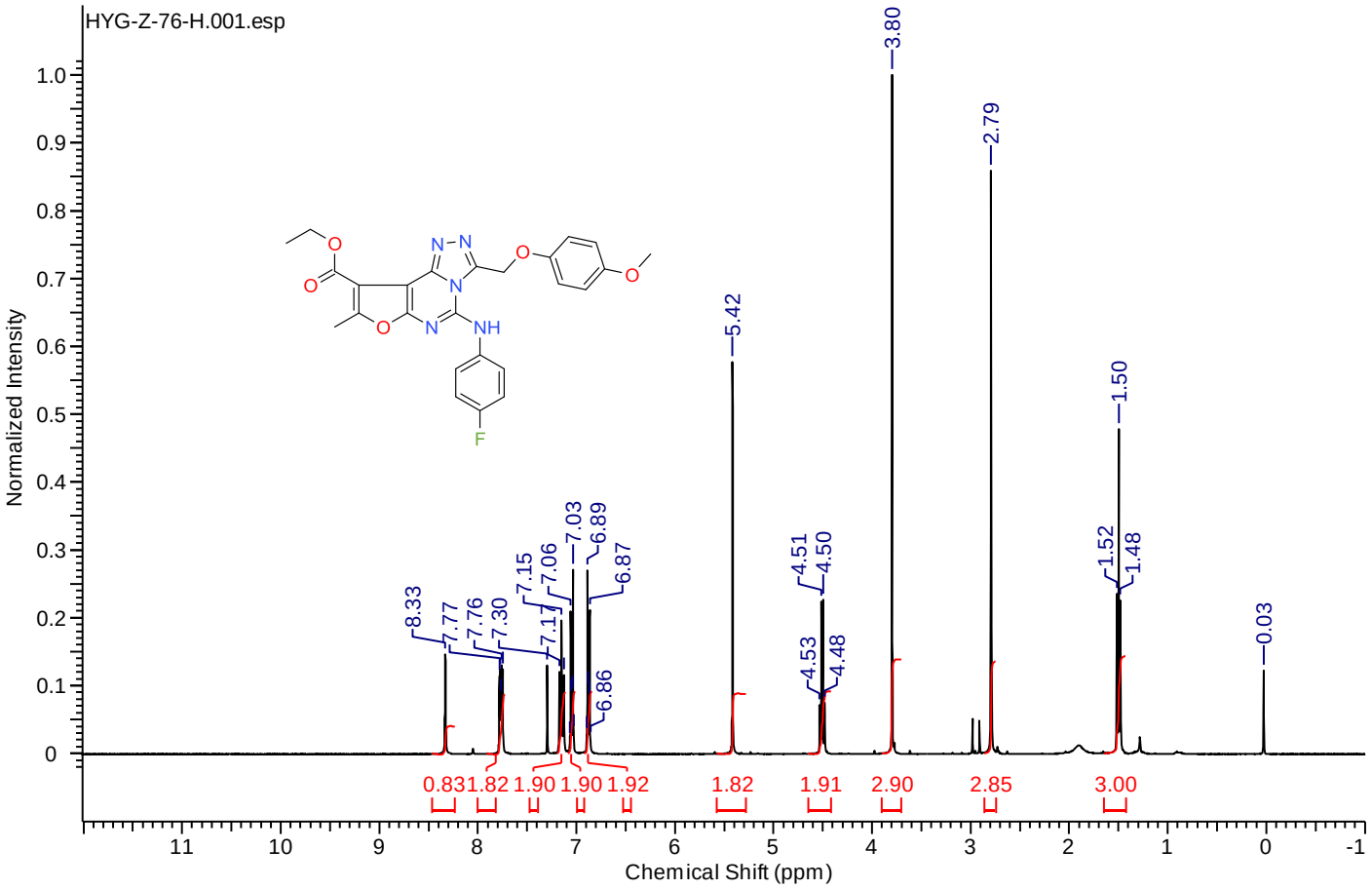
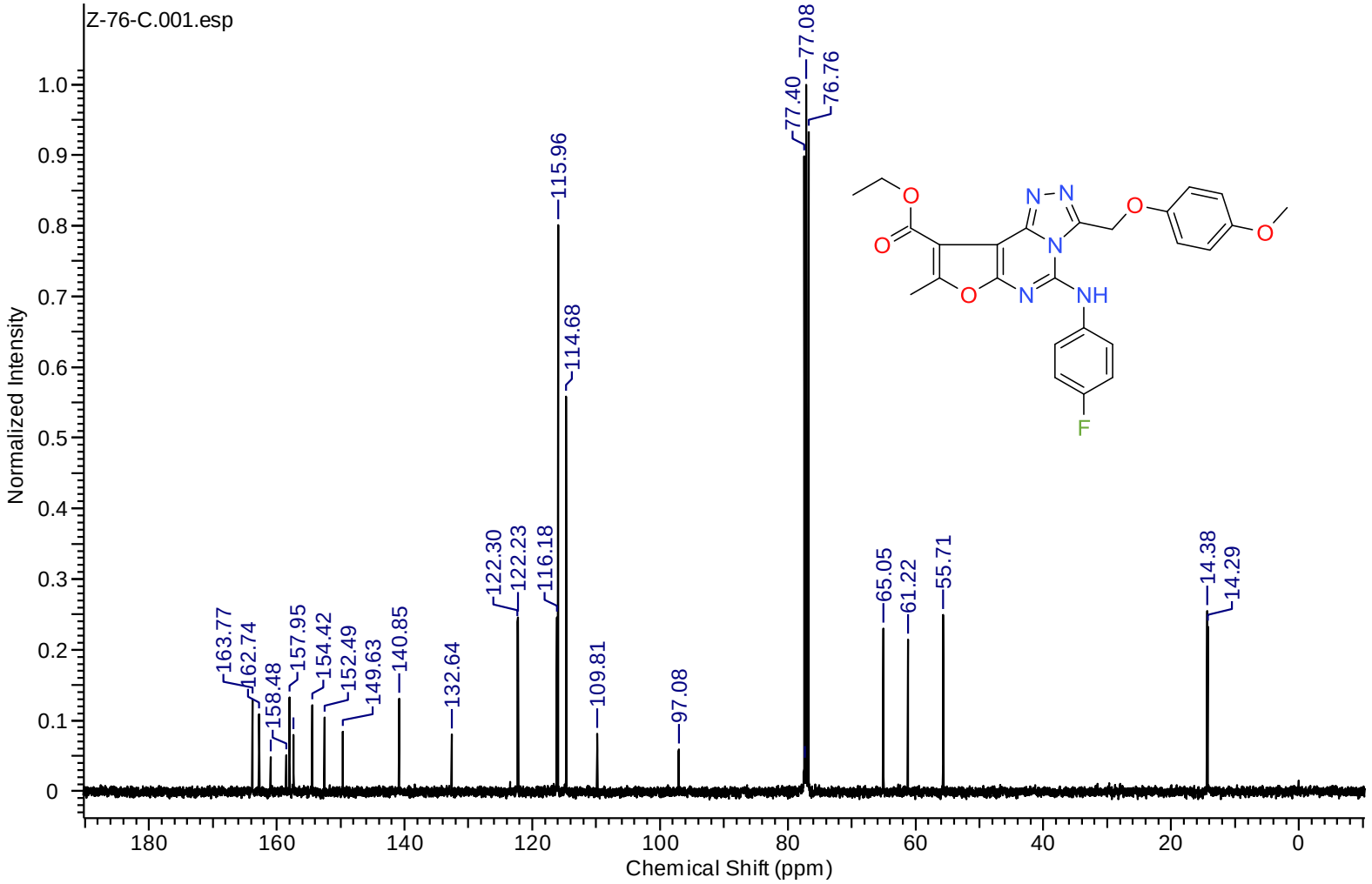
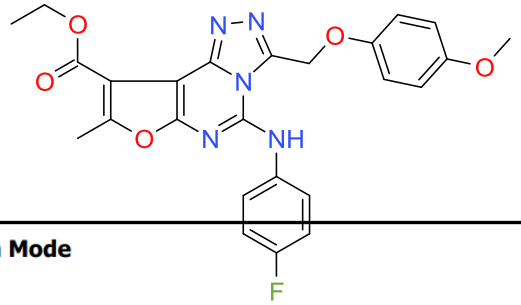
1068.87
1041.27
823.84
781.09
757.62
511.30


HYG-Z-76-H.001.esp
Normalized Intensity
Chemical Shift (ppm)
8.33
7.77
7.76
7.30
7.15
7.11
7.06
7.03
6.89
6.87
6.86
5.42
4.51
4.50
4.53
4.48
3.80
2.79
1.52
1.50
1.48
0.03
0.83
1.82
1.90
1.90
1.92
1.82
1.91
2.90
2.85
3.00

^{1}H NMR **6i**

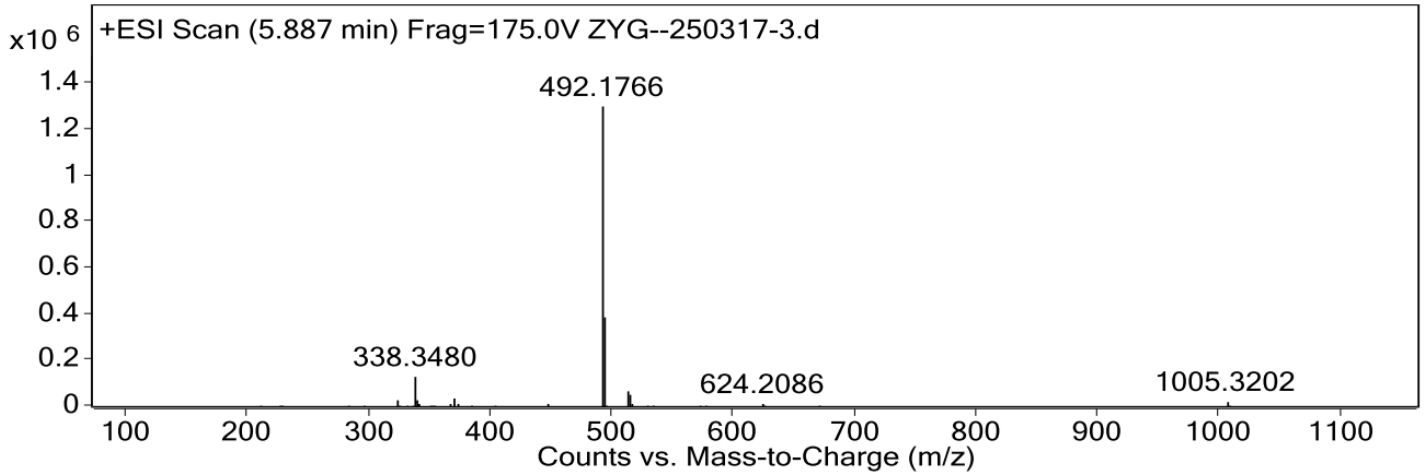

Z-76-C.001.esp
Normalized Intensity
Chemical Shift (ppm)
163.77
162.74
158.48
157.95
154.42
152.49
149.63
140.85
132.64
122.30
122.23
116.18
115.96
114.68
109.81
97.08
77.40
77.08
76.76
65.05
61.22
55.71
14.38
14.29
O
O
N
N
N
O
O
O
N
NH
F

^{13}C NMR **6i**

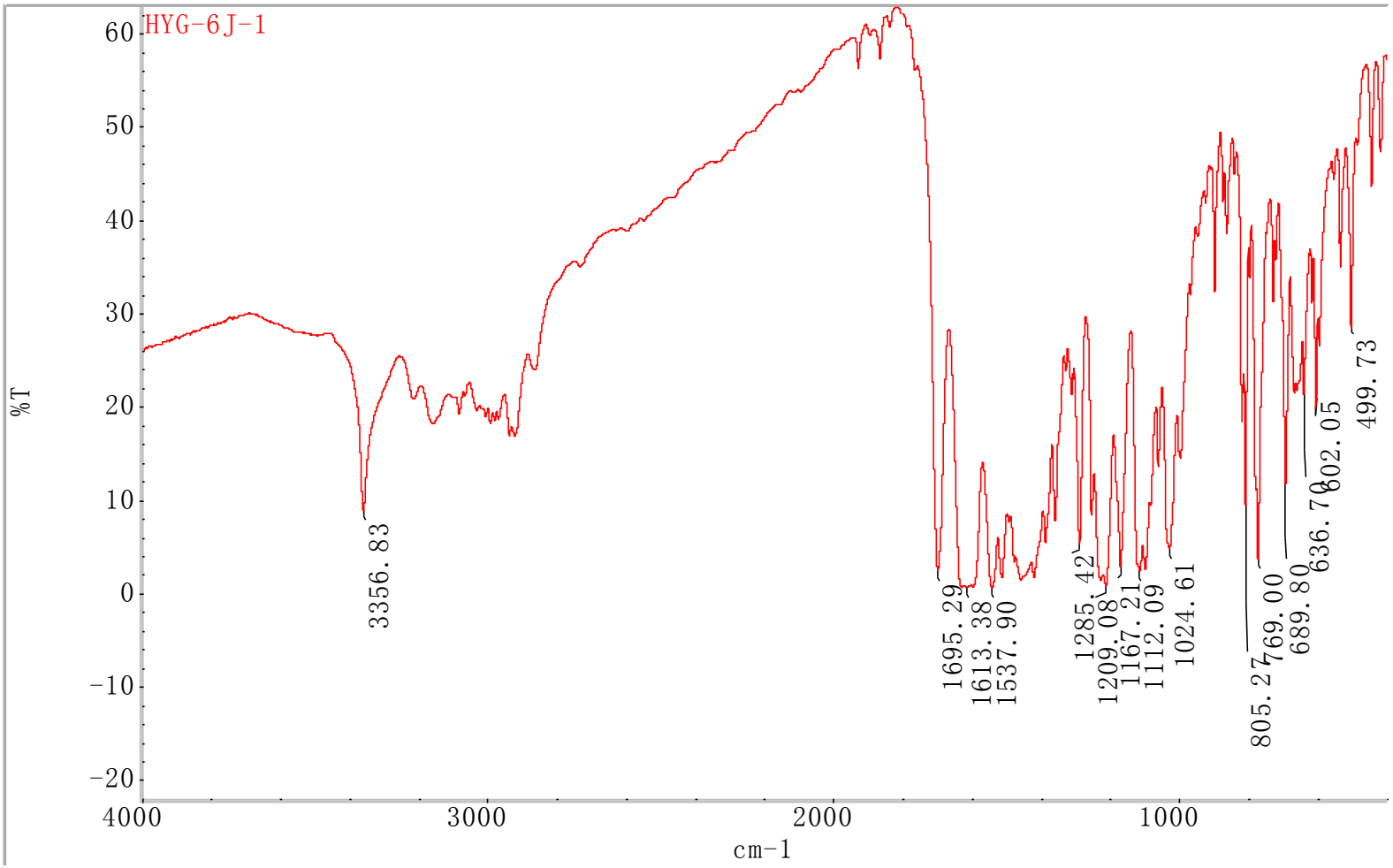


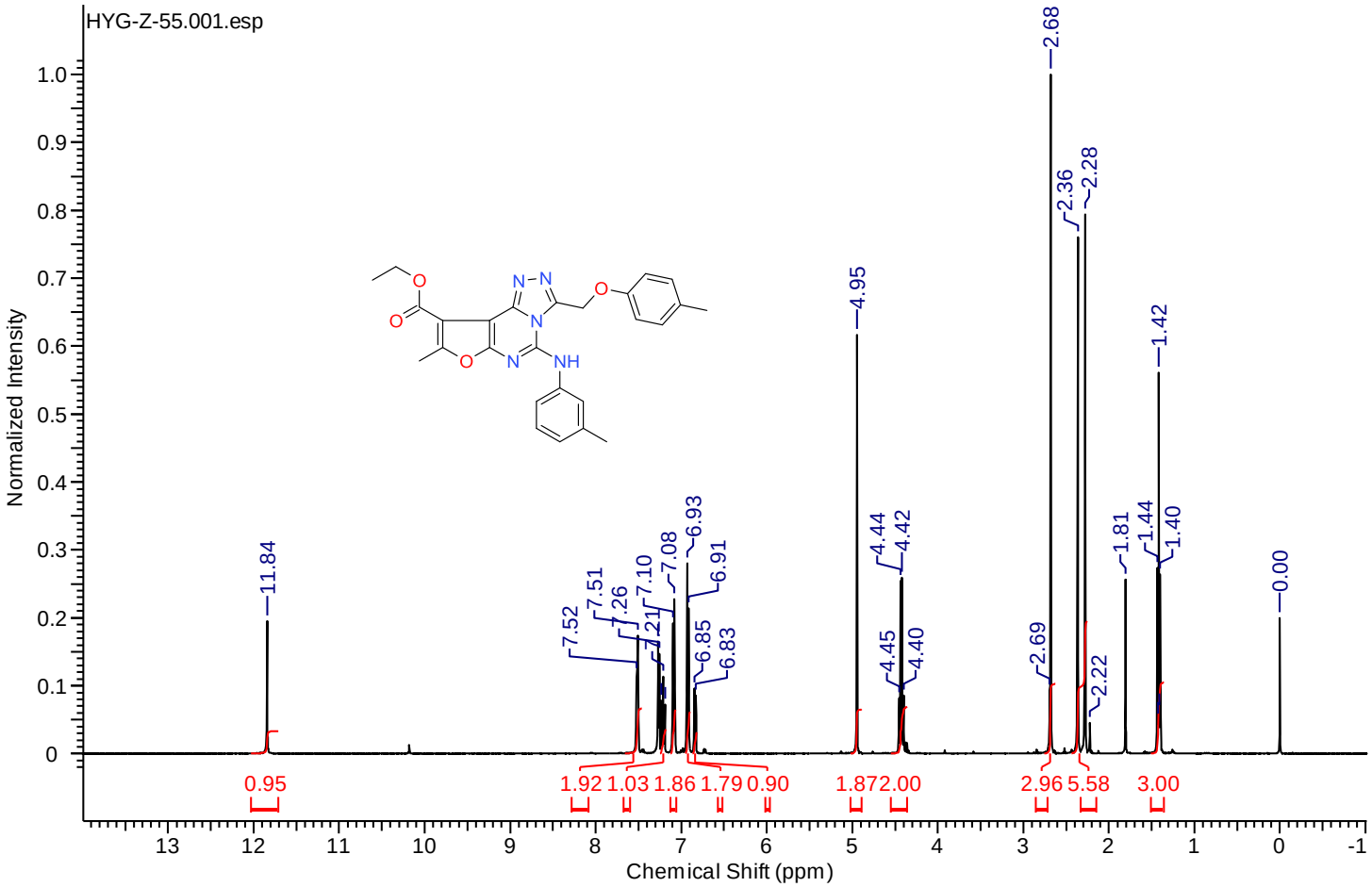
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

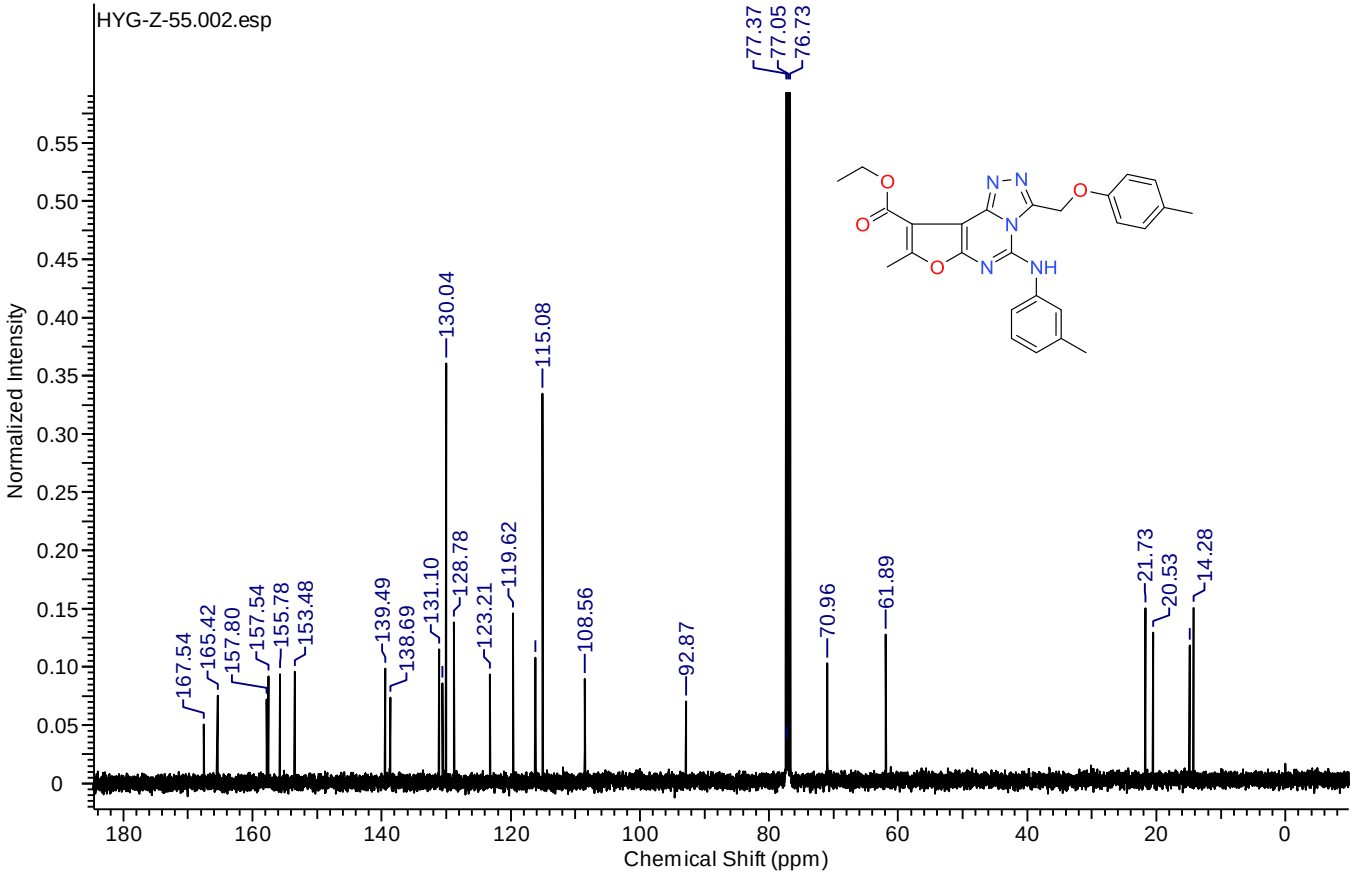


HRMS m/z **6i**


HYG-6J-1
%T
60
50
40
30
20
10
0
-10
-20
4000
3000
2000
1000
cm-1
3356.83
1695.29
1613.38
1537.90
1285.42
1209.08
1167.21
1112.09
1024.61
805.27
769.00
689.80
636.70
602.05
499.73


HYG-Z-55.001.esp
Normalized Intensity
Chemical Shift (ppm)
11.84
7.52
7.51
7.26
7.21
7.10
7.08
6.93
6.91
6.85
6.83
4.95
4.44
4.42
4.45
4.40
2.68
2.69
2.36
2.28
2.22
1.81
1.44
1.42
1.40
0.00
0.95
1.92
1.03
1.86
1.79
0.90
1.87
2.00
2.96
5.58
3.00

^{1}H NMR **6j**


HYG-Z-55.002.esp
Normalized Intensity
Chemical Shift (ppm)
167.54
165.42
157.80
157.54
155.78
153.48
139.49
138.69
131.10
130.04
128.78
123.21
119.62
115.08
108.56
92.87
77.37
77.05
76.73
70.96
61.89
21.73
20.53
14.28
O
O
N-N
N
O
O
N
NH

^{13}C NMR **6j**

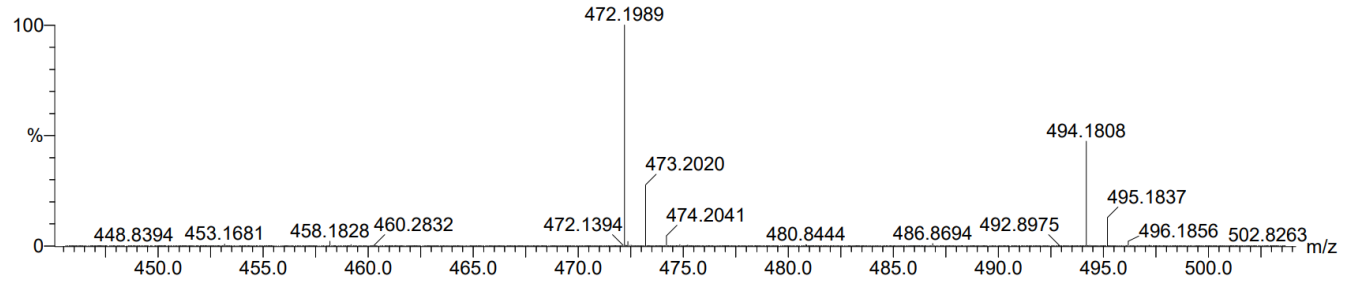
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5158 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 26-26 H: 26-26 N: 0-100 O: 0-100 Na: 0-4 K: 0-2

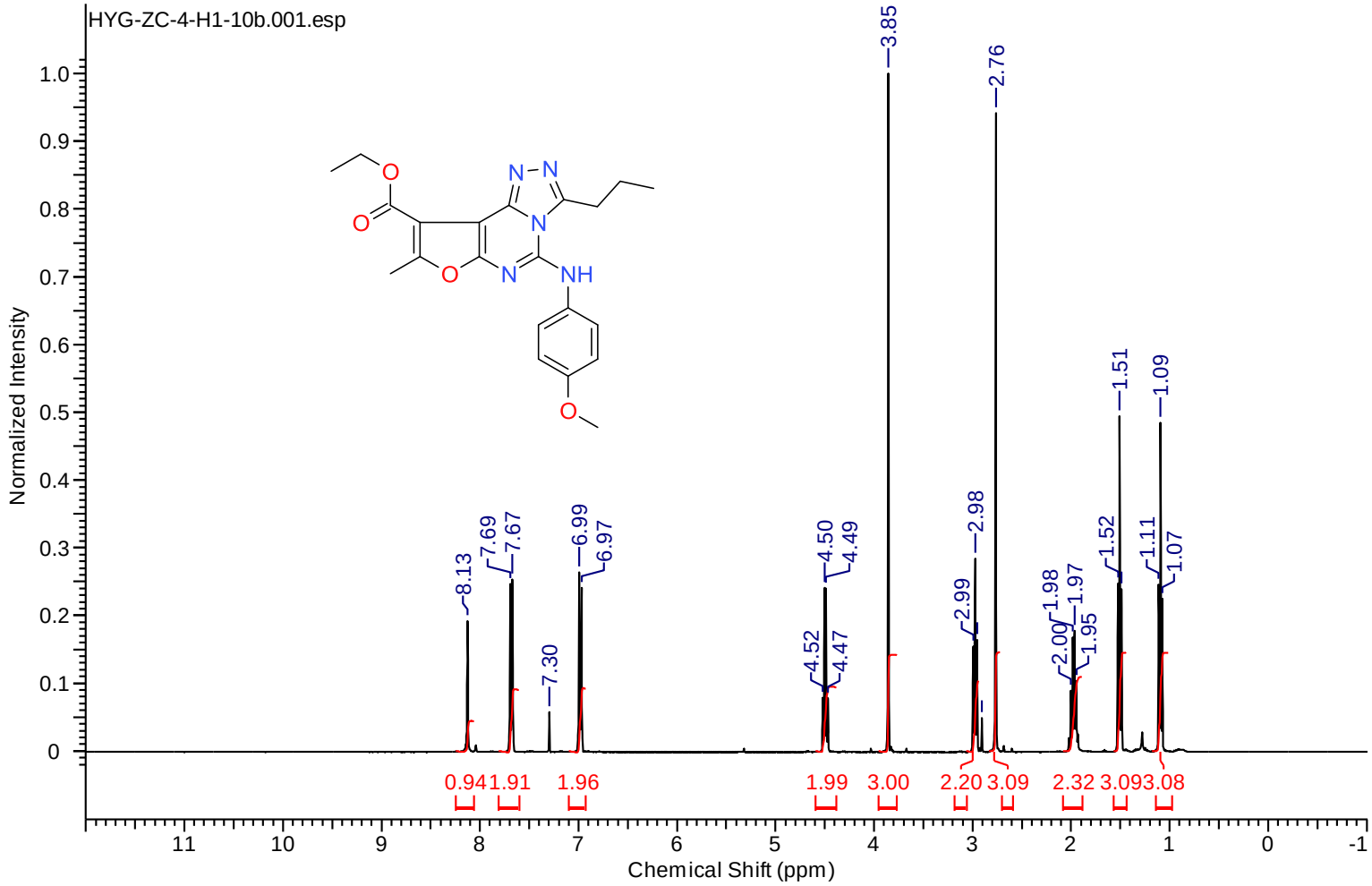
1
240905-6-HYG-Z-55 11 (0.094)

1: TOF MS ES+
1.77e+006

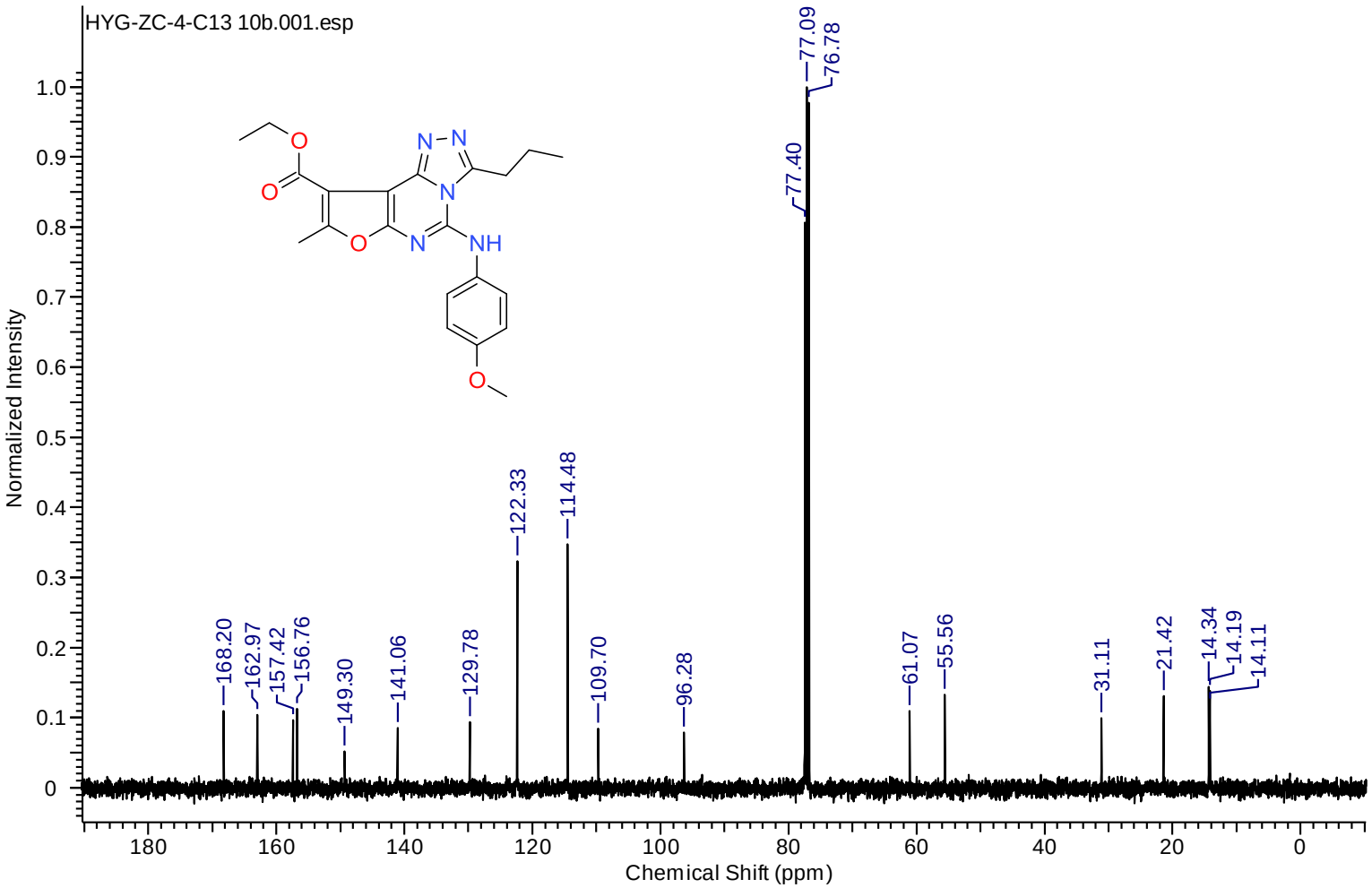


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
472.1989	472.1985	0.4	0.8	16.5	988.9	n/a	n/a	C26 H26 N5 O4

HRMS m/z **6j**


HYG-ZC-4-H1-10b.001.esp
Normalized Intensity
Chemical Shift (ppm)
8.13
7.69
7.67
7.30
6.99
6.97
4.52
4.50
4.49
4.47
3.85
2.99
2.98
2.76
2.00
1.98
1.97
1.95
1.52
1.51
1.11
1.09
1.07
0.94
1.91
1.96
1.99
3.00
2.20
3.09
2.32
3.09
3.08
O
O
O
N
N
N
N
NH
O

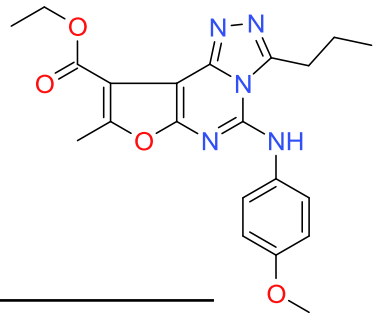
^{1}H NMR **7a**


HYG-ZC-4-C13 10b.001.esp
Normalized Intensity
Chemical Shift (ppm)
168.20
162.97
157.42
156.76
149.30
141.06
129.78
122.33
114.48
109.70
96.28
77.40
77.09
76.78
61.07
55.56
31.11
21.42
14.34
14.19
14.11

^{13}C NMR **7a**

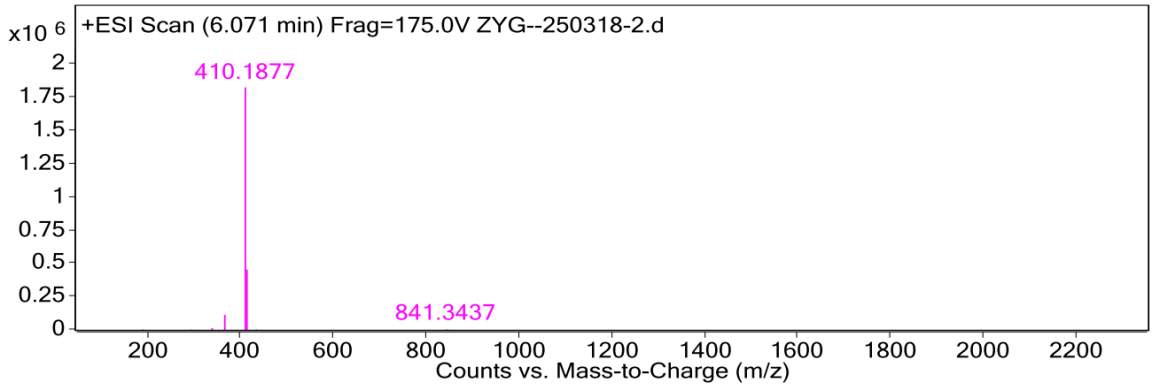
IRM Calibration Status	Success	**DA Method**	TQQ-18-23-20250109.m
Comment			

Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.00 (B5042.2)		

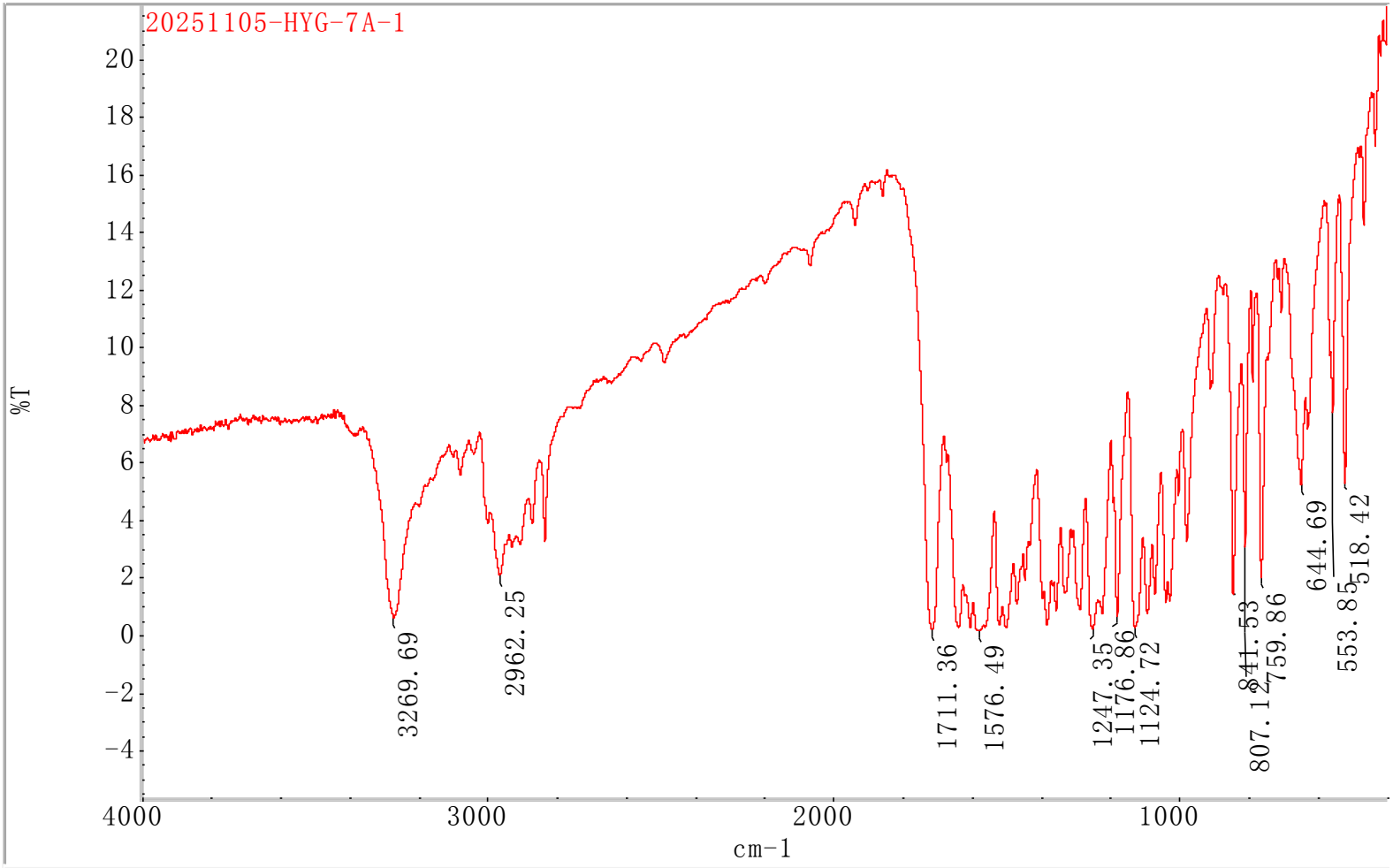


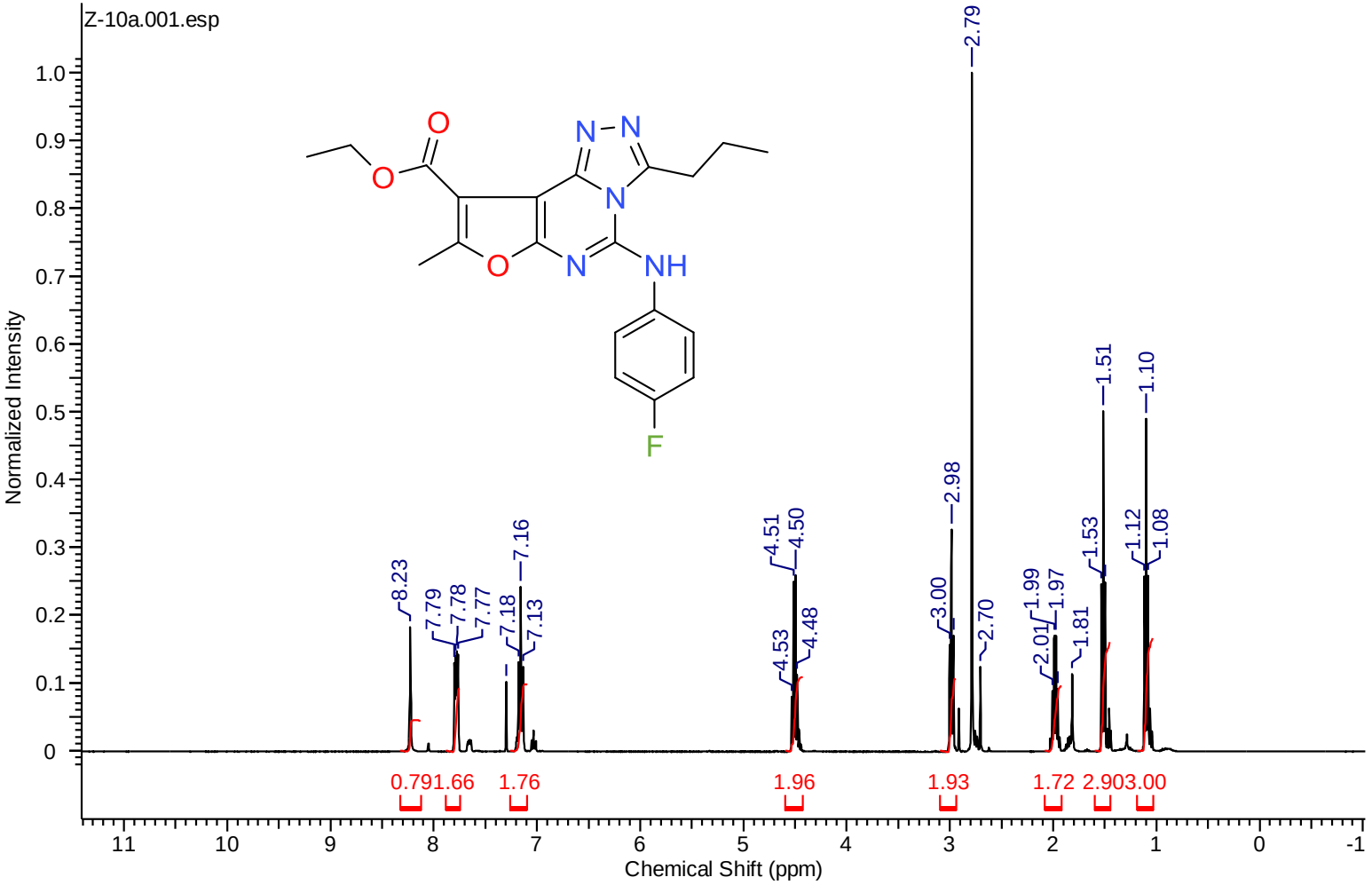
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



HRMS m/z **7a**


20251105-HYG-7A-1
%T
20
18
16
14
12
10
8
6
4
2
0
-2
-4
4000
3000
2000
1000
cm-1
3269.69
2962.25
1711.36
1576.49
1247.35
1176.86
1124.72
841.53
807.12
759.86
644.69
553.85
518.42


Z-10a.001.esp
Normalized Intensity
Chemical Shift (ppm)
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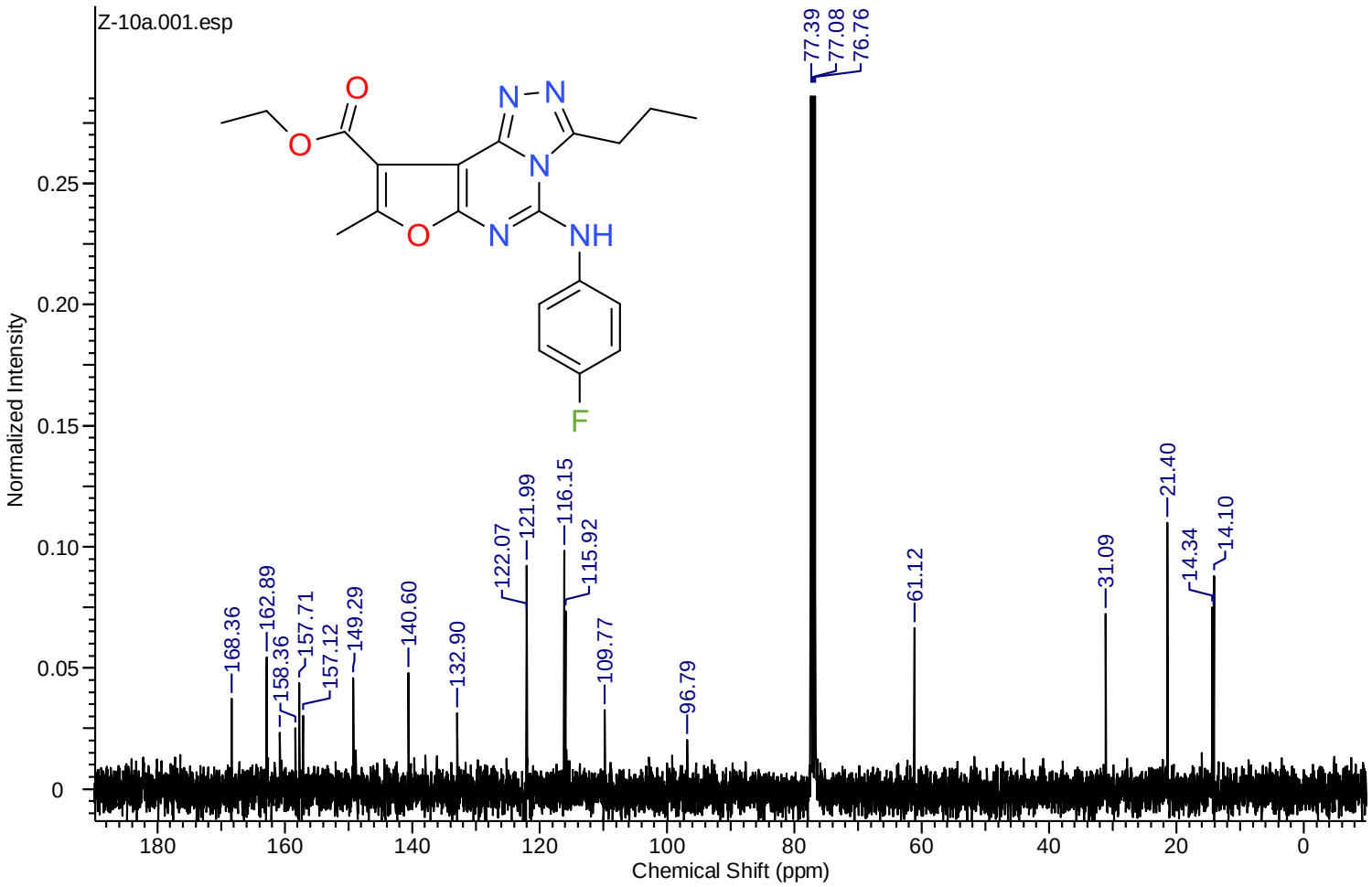
O
N
N
N
O
N
NH
F
8.23
7.79
7.78
7.77
7.18
7.16
7.13
4.53
4.51
4.50
4.48
3.00
2.98
2.79
2.70
2.01
1.99
1.97
1.81
1.53
1.51
1.12
1.10
1.08
0.79
1.66
1.76
1.96
1.93
1.72
2.90
3.00

^{1}H NMR **7b**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Normalized Intensity
Chemical Shift (ppm)
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0.20
0.25
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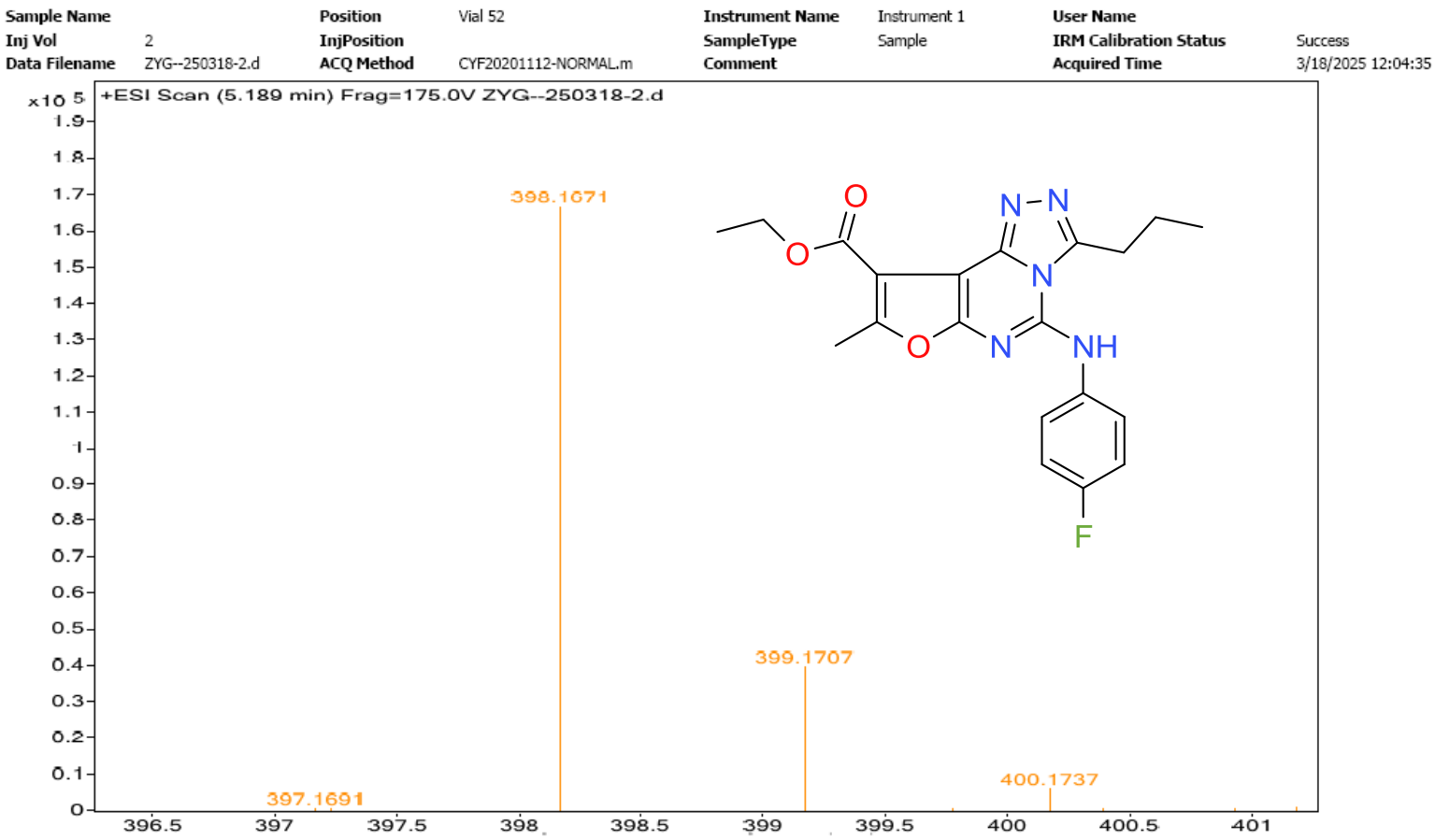
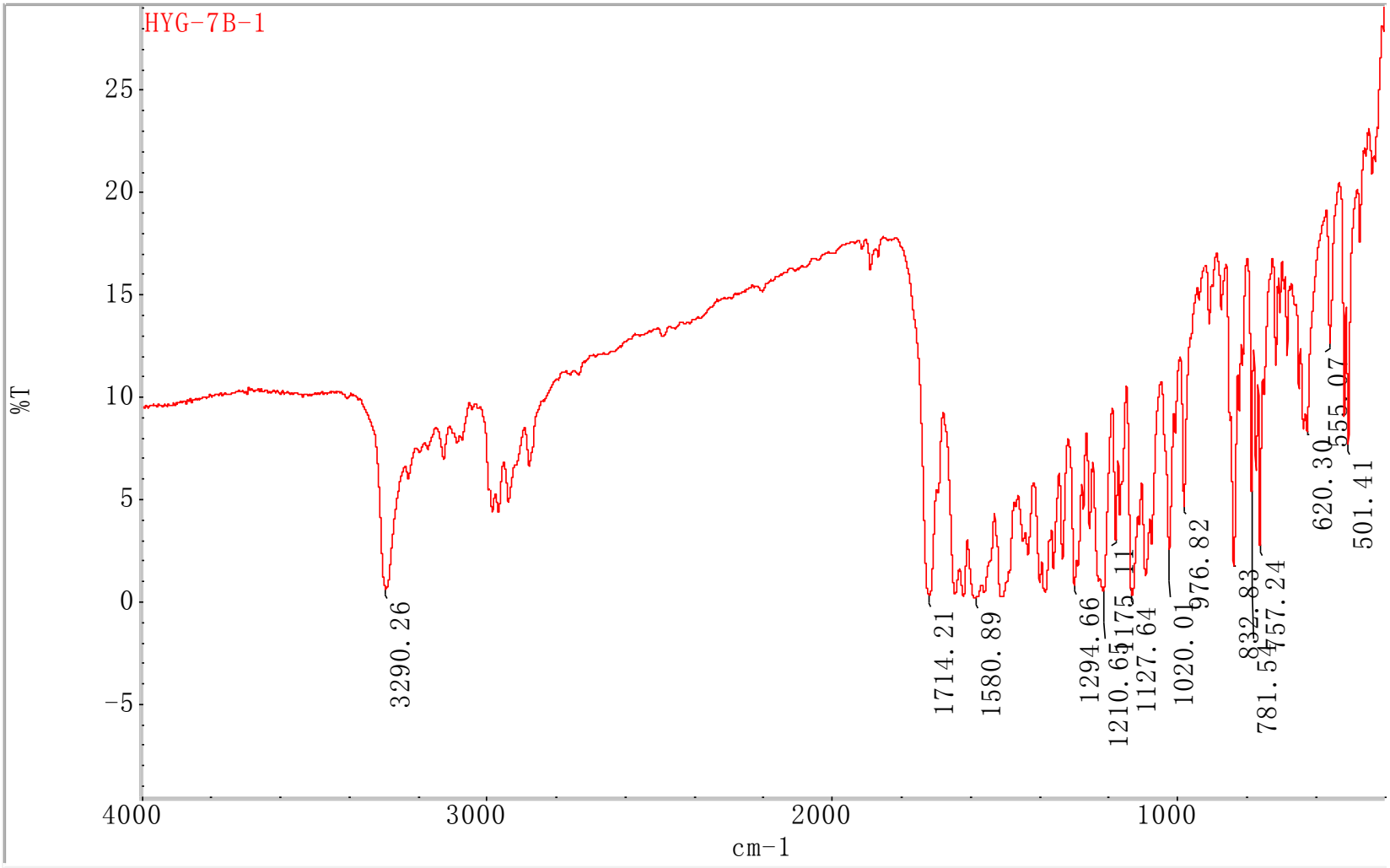
160
140
120
100
80
60
40
20
0
168.36
162.89
158.36
157.71
157.12
149.29
140.60
132.90
122.07
121.99
116.15
115.92
109.77
96.79
77.39
77.08
76.76
61.12
31.09
21.40
14.34
14.10
O
O
N
N
N
O
N
NH
F

^{13}C NMR **7b**


Sample Name
Position
Vial 52
Instrument Name
Instrument 1
User Name
Inj Vol
2
InjPosition
SampleType
Sample
IRM Calibration Status
Success
Data Filename
ZYG--250318-2.d
ACQ Method
CYF20201112-NORMAL.m
Comment
Acquired Time
3/18/2025 12:04:35
+ESI Scan (5.189 min) Frag=175.0V ZYG--250318-2.d
x10 5
398.1671
399.1707
397.1691
400.1737
O
O
N
N
N
O
N
NH
F

HRMS m/z **7b**


HYG-7B-1
%T
25
20
15
10
5
0
-5
4000
3000
2000
1000
cm-1
3290.26
1714.21
1580.89
1294.66
1210.65
1175.11
1127.64
1020.01
976.82
832.83
781.54
757.24
620.30
555.07
501.41