Supporting Information

SYNTHESIS AND BIOLOGICAL ACTIVITY OF AMINOISOQUINOLINE SCHIFF BASE

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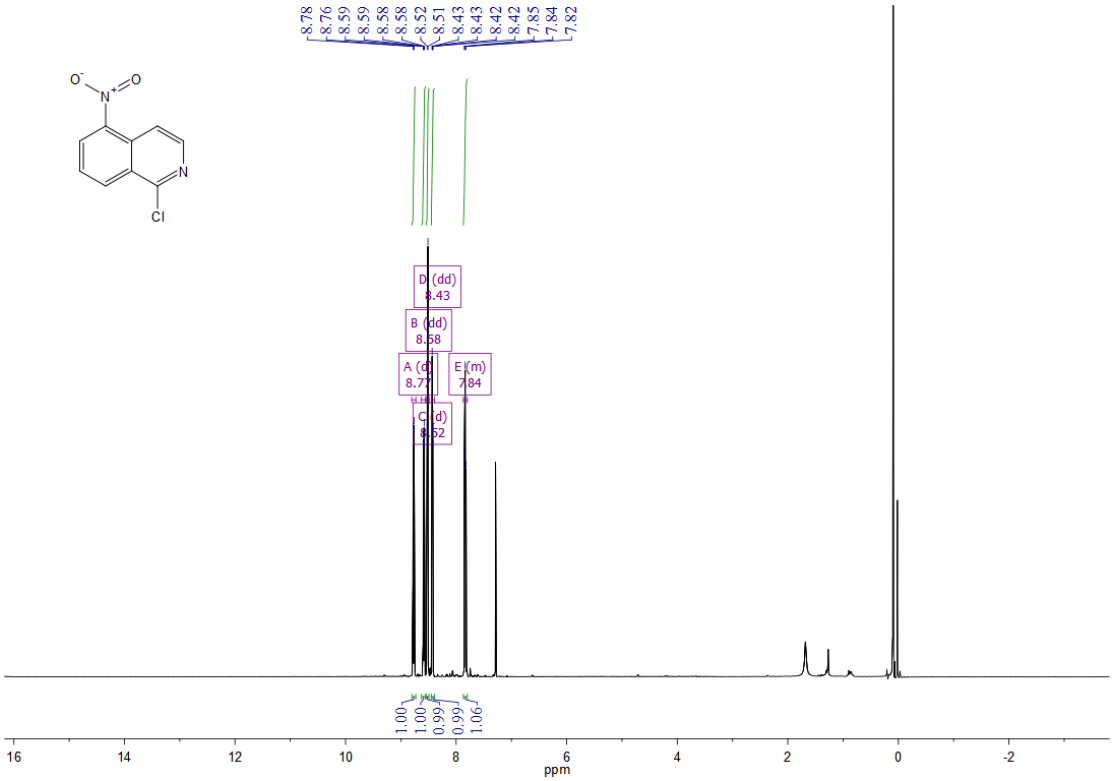
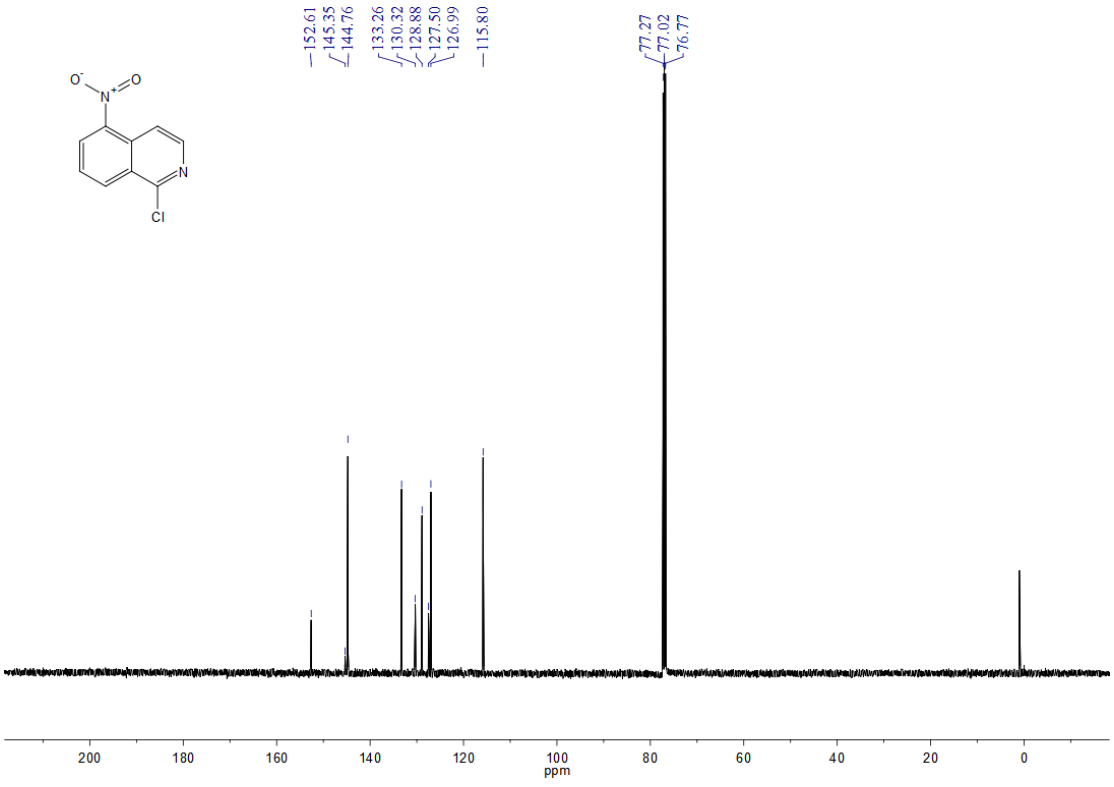
Compound 1

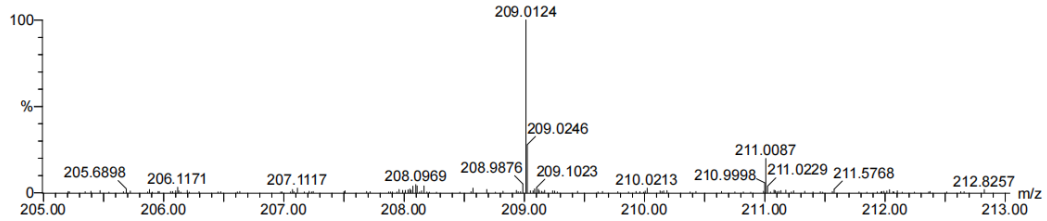

8.78
8.76
8.59
8.59
8.58
8.58
8.52
8.51
8.43
8.43
8.42
8.42
7.85
7.84
7.82
D (dd)
8.43
B (dd)
8.58
A (d)
8.77
E (m)
7.84
C (d)
8.52
1.00
1.00
0.99
0.99
1.06
16
14
12
10
8
6
4
2
0
-2
ppm


152.61
145.35
144.76
133.26
130.32
128.88
127.50
126.99
115.80
77.27
77.02
76.77
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

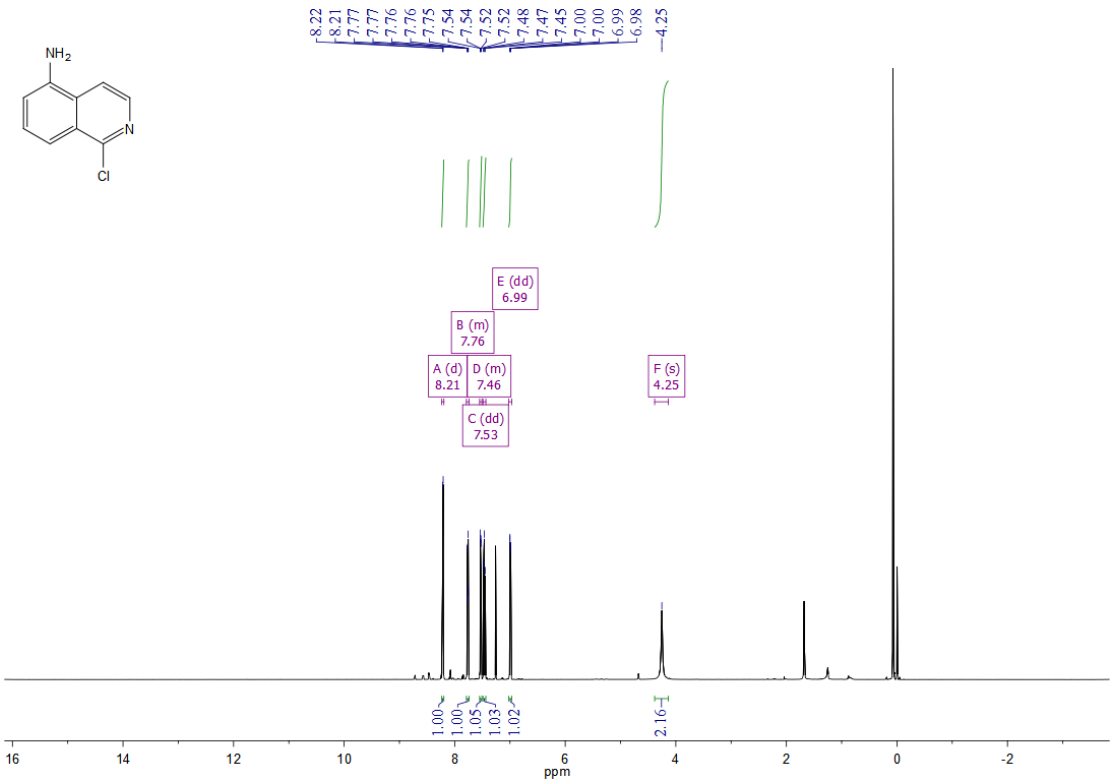
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

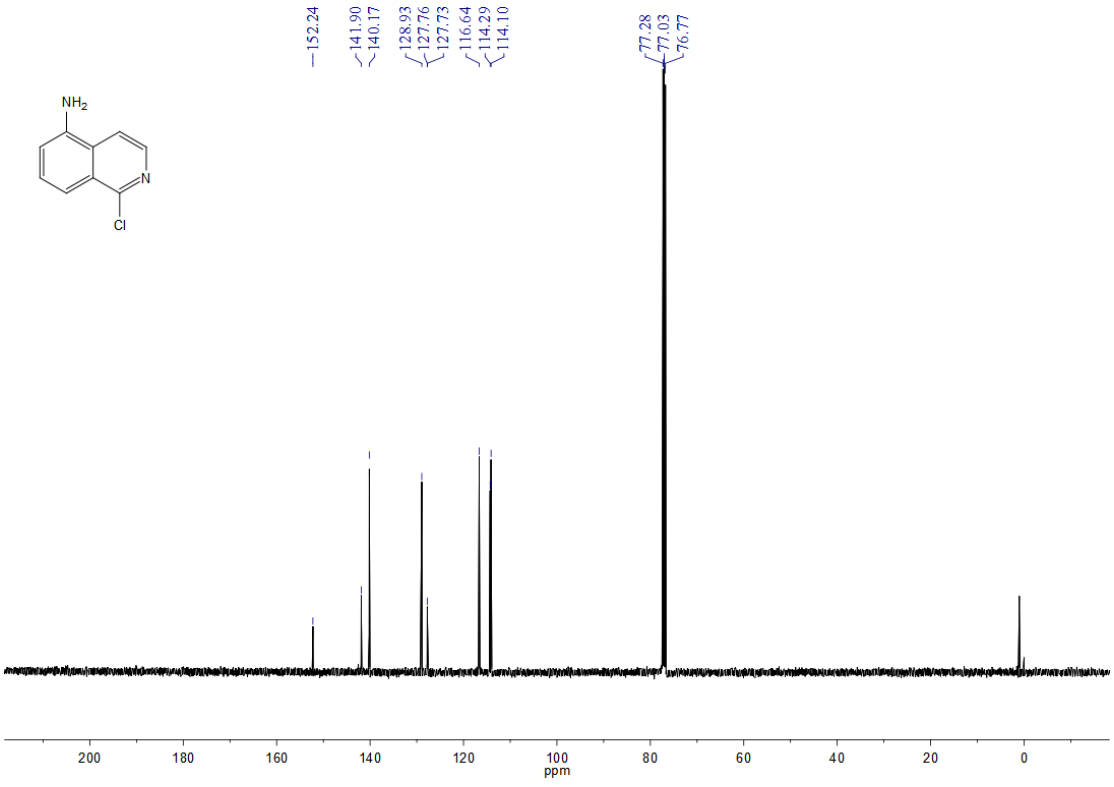
Monoisotopic Mass, Even Electron Ions
152 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 9-9 H: 6-6 N: 0-8 O: 0-20 Cl: 1-4
5
0729-5-14 39 (0.262) 1: TOF MS ES+
6.34e+003



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
209.0124	209.0118	0.6	2.9	7.5	405.3	n/a	n/a	C9 H6 N2 O2 Cl

Compound 2

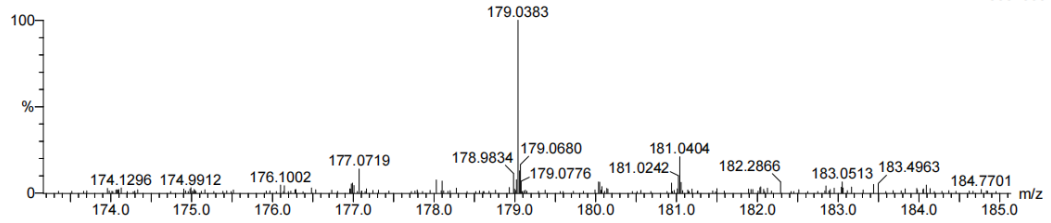

NH2
N
Cl
8.22
8.21
7.77
7.77
7.76
7.76
7.75
7.54
7.54
7.52
7.52
7.48
7.47
7.45
7.00
7.00
6.99
6.98
4.25
E (dd)
6.99
B (m)
7.76
A (d)
8.21
D (m)
7.46
C (dd)
7.53
F (s)
4.25
1.00
1.00
1.05
1.03
1.02
2.16
16
14
12
10
8
6
4
2
0
-2
ppm


NH2
N
Cl
152.24
141.90
140.17
128.93
127.76
127.73
116.64
114.29
114.10
77.28
77.03
76.77
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

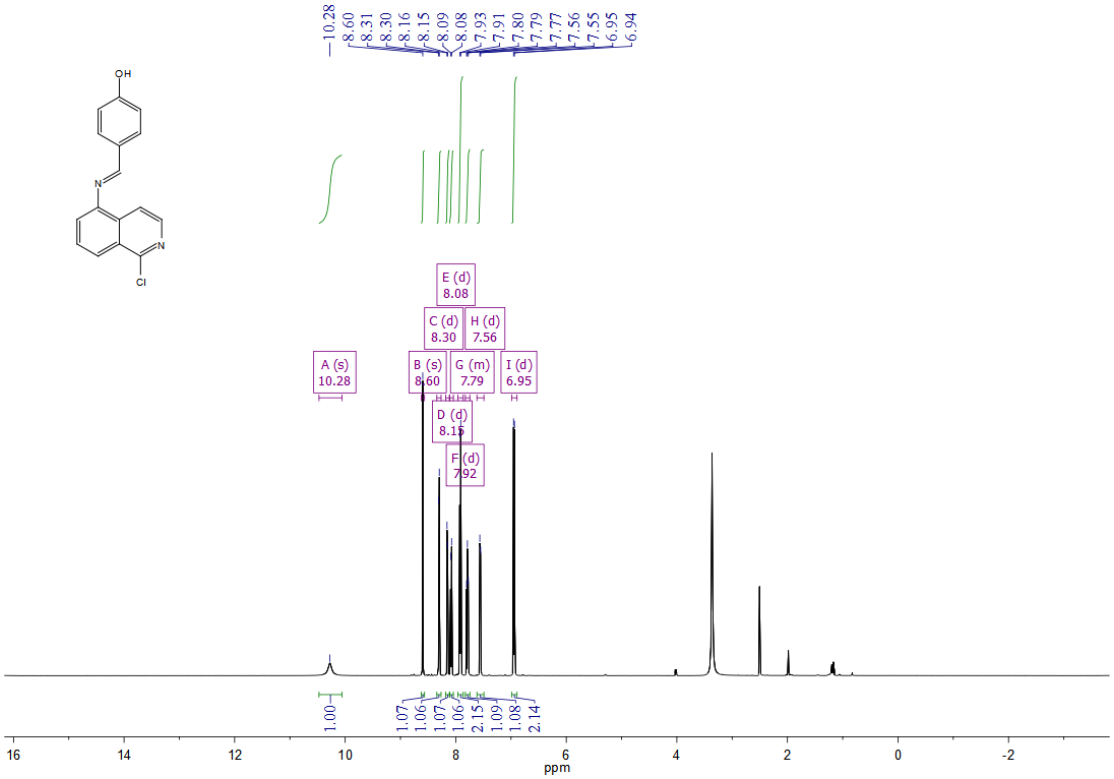
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

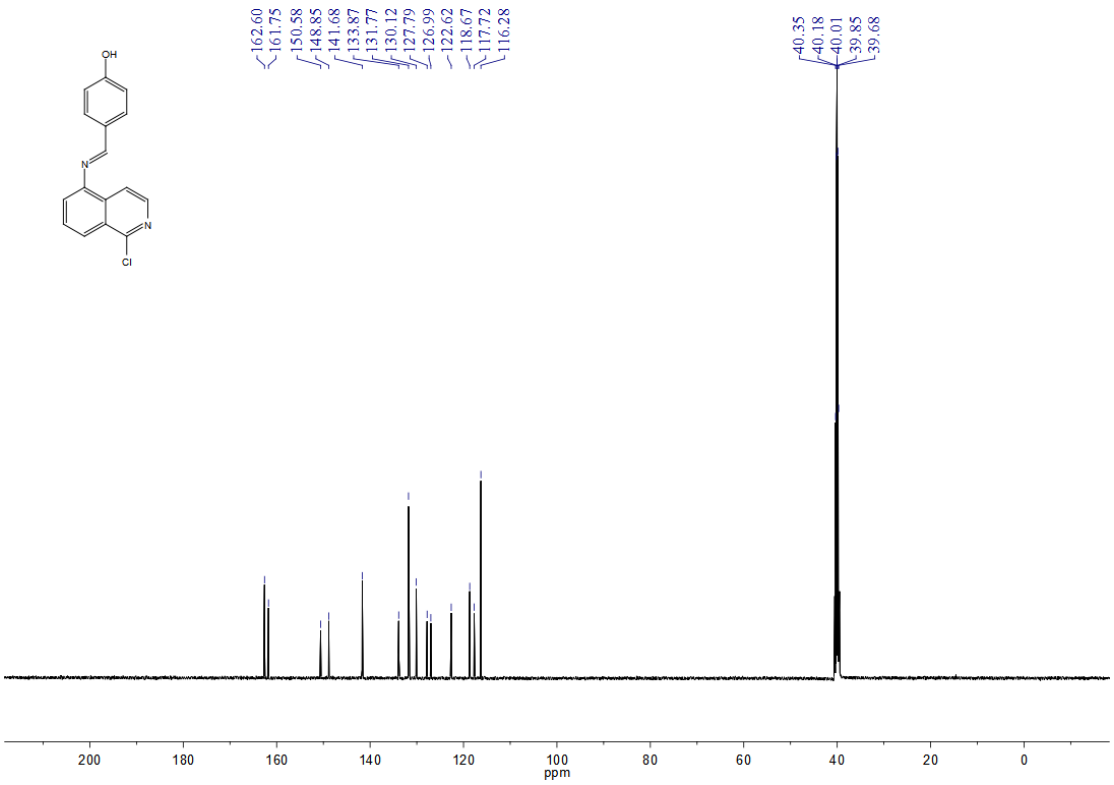
Monoisotopic Mass, Even Electron Ions
107 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 9-9 H: 8-8 N: 0-8 O: 0-20 Cl: 1-4
5
0729-5-13 36 (0.246) 1: TOF MS ES+
2.80e+003



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
179.0383	179.0376	0.7	3.9	6.5	337.2	n/a	n/a	C9 H8 N2 Cl

Compound 3a

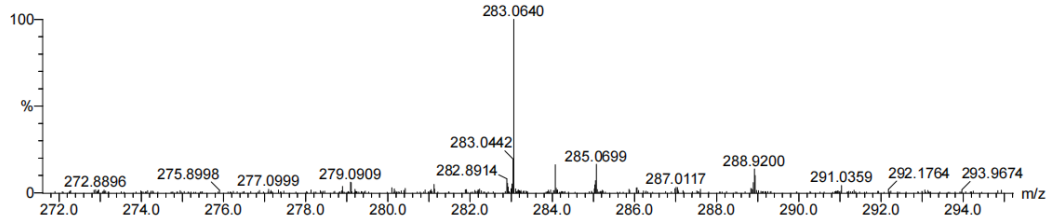

10.28
8.60
8.31
8.30
8.16
8.15
8.09
8.08
7.93
7.91
7.80
7.79
7.77
7.56
7.55
6.95
6.94
OH
N
N
Cl
E (d) 8.08
C (d) 8.30
H (d) 7.56
A (s) 10.28
B (s) 8.60
G (m) 7.79
I (d) 6.95
D (d) 8.15
F (d) 7.92
1.00
1.07
1.06
1.07
1.06
2.15
1.09
1.08
2.14
16
14
12
10
8
6
4
2
0
-2
ppm


162.60
161.75
150.58
148.85
141.68
133.87
131.77
130.12
127.79
126.99
122.62
118.67
117.72
116.28
40.35
40.18
40.01
39.85
39.68
OH
N
N
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

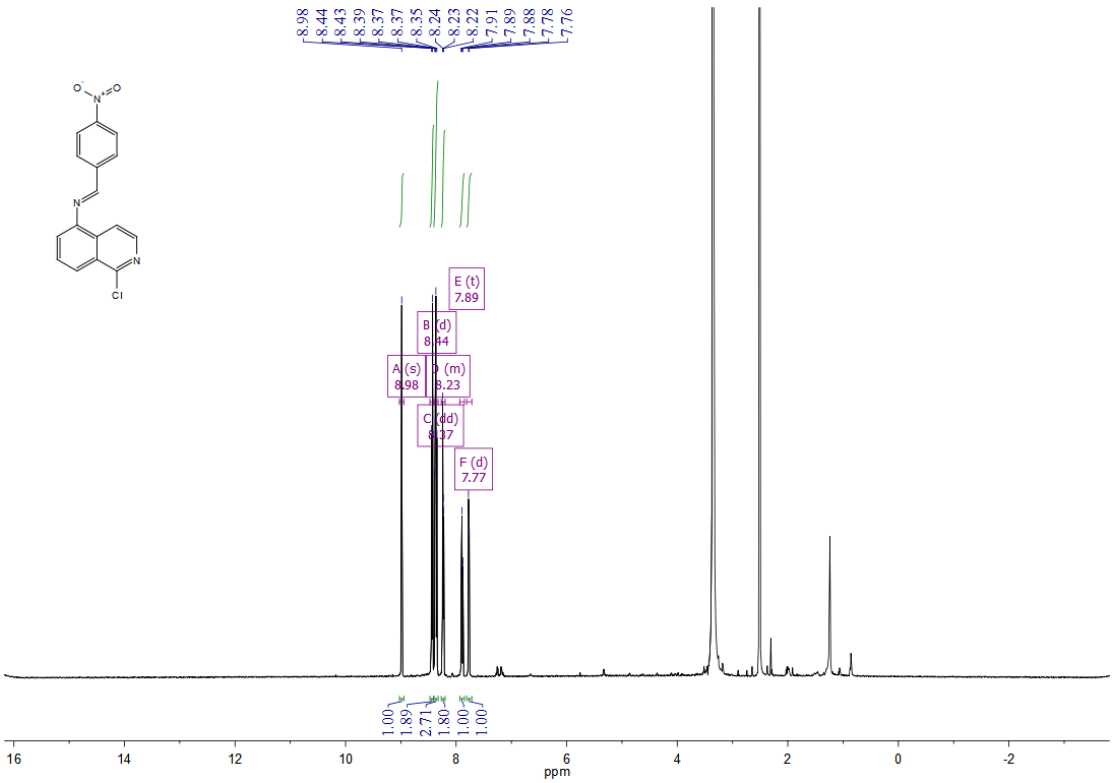
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

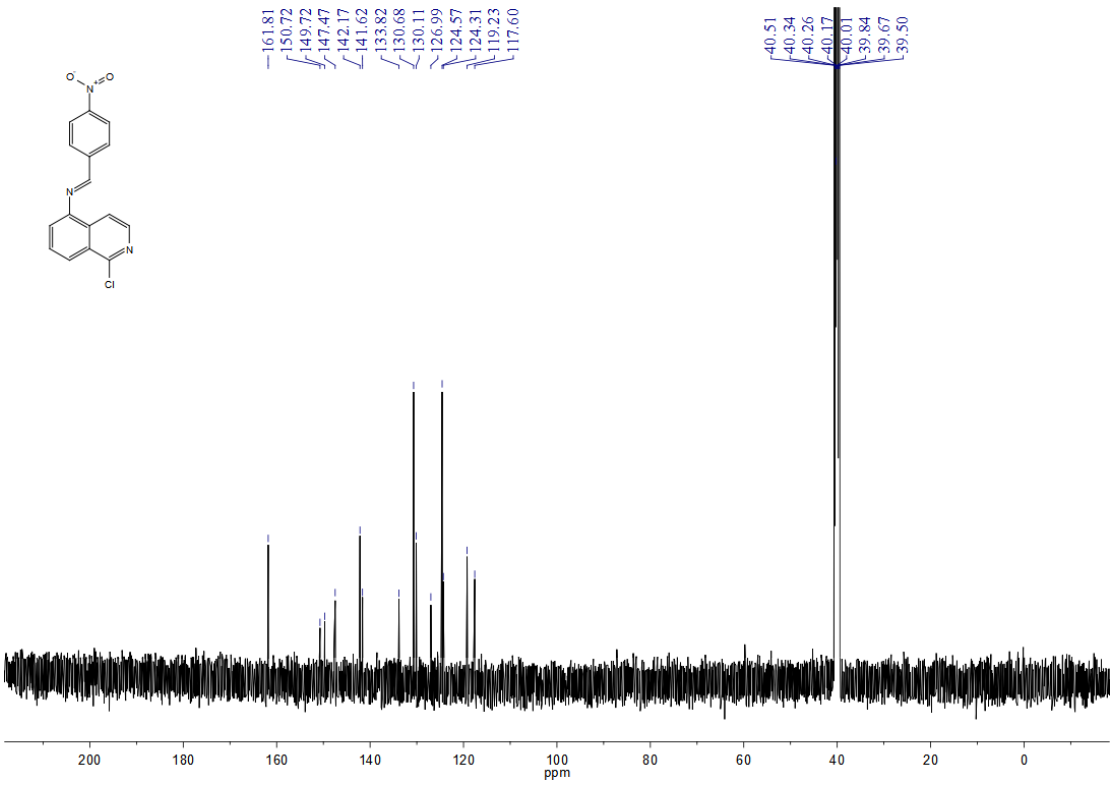
Monoisotopic Mass, Even Electron Ions
318 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 12-12 N: 0-8 O: 0-20 Cl: 1-4
5
0729-5-1 63 (0.412) 1: TOF MS ES+
6.77e+003



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
283.0640	283.0638	0.2	0.7	11.5	428.9	n/a	n/a	C16 H12 N2 O Cl

Compound 3b

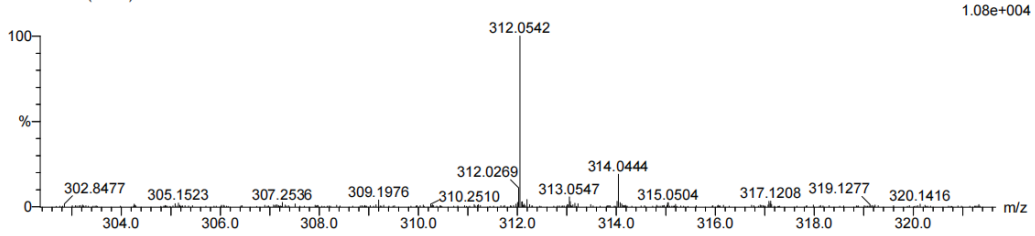

8.98
8.44
8.43
8.39
8.37
8.37
8.35
8.24
8.23
8.22
7.91
7.89
7.88
7.78
7.76
E (t)
7.89
B (d)
8.44
A (s)
8.98
D (m)
8.23
C (dd)
8.37
F (d)
7.77
1.00
1.89
2.71
1.80
1.00
1.00
16
14
12
10
8
6
4
2
0
-2
ppm


161.81
150.72
149.72
147.47
142.17
141.62
133.82
130.68
130.11
126.99
124.57
124.31
119.23
117.60
40.51
40.34
40.26
40.17
40.01
39.84
39.67
39.50
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

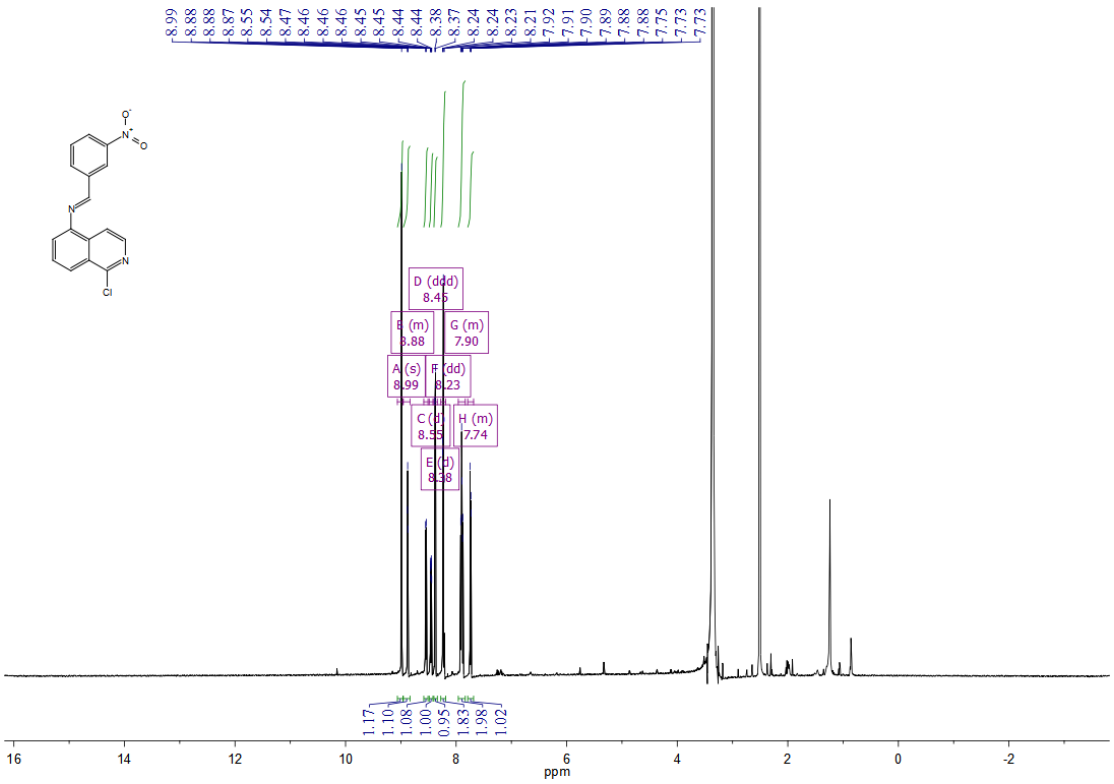
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

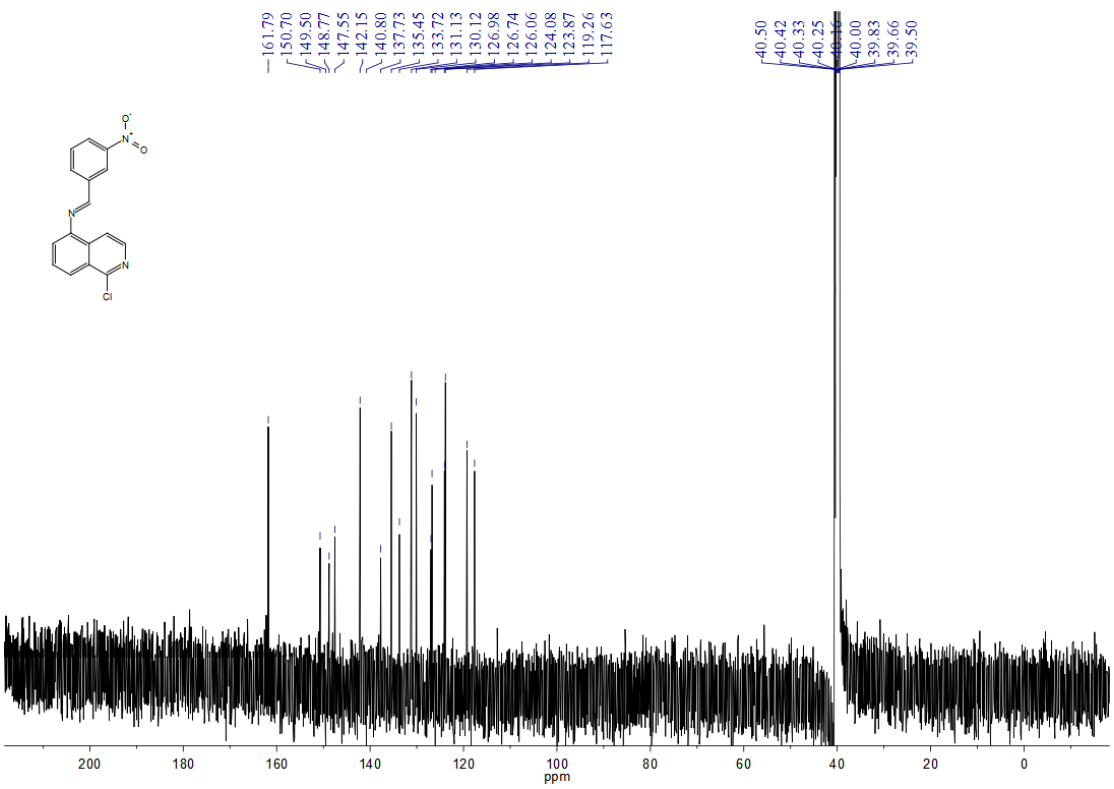
Monoisotopic Mass, Even Electron Ions
366 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 11-11 N: 0-8 O: 0-20 Cl: 1-4
5
0729-5-2 71 (0.462) 1: TOF MS ES+
1.08e+004



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
312.0542	312.0540	0.2	0.6	12.5	427.1	n/a	n/a	C16 H11 N3 O2 Cl

Compound 3c

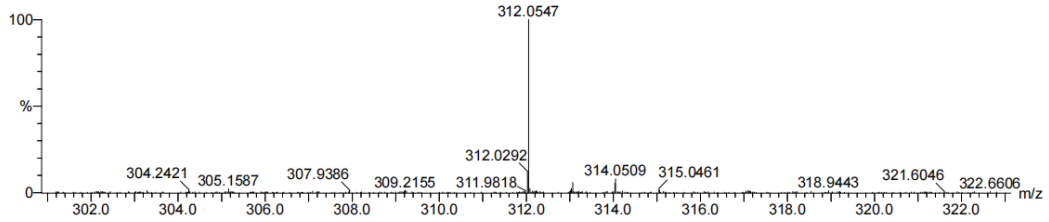

8.99
8.88
8.88
8.87
8.55
8.54
8.47
8.46
8.46
8.46
8.45
8.45
8.44
8.44
8.38
8.37
8.24
8.24
8.23
8.21
7.92
7.91
7.90
7.89
7.88
7.88
7.75
7.73
7.73
D (ddd) 8.45
B (m) 8.88
G (m) 7.90
A (s) 8.99
F (dd) 8.23
C (d) 8.55
H (m) 7.74
E (d) 8.38
1.17
1.10
1.08
1.00
0.95
1.83
1.98
1.02
16
14
12
10
8
6
4
2
0
-2
ppm


161.79
150.70
149.50
148.77
147.55
142.15
140.80
137.73
135.45
133.72
131.13
130.12
126.98
126.74
126.06
124.08
123.87
119.26
117.63
40.50
40.42
40.33
40.25
40.16
40.00
39.83
39.66
39.50
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

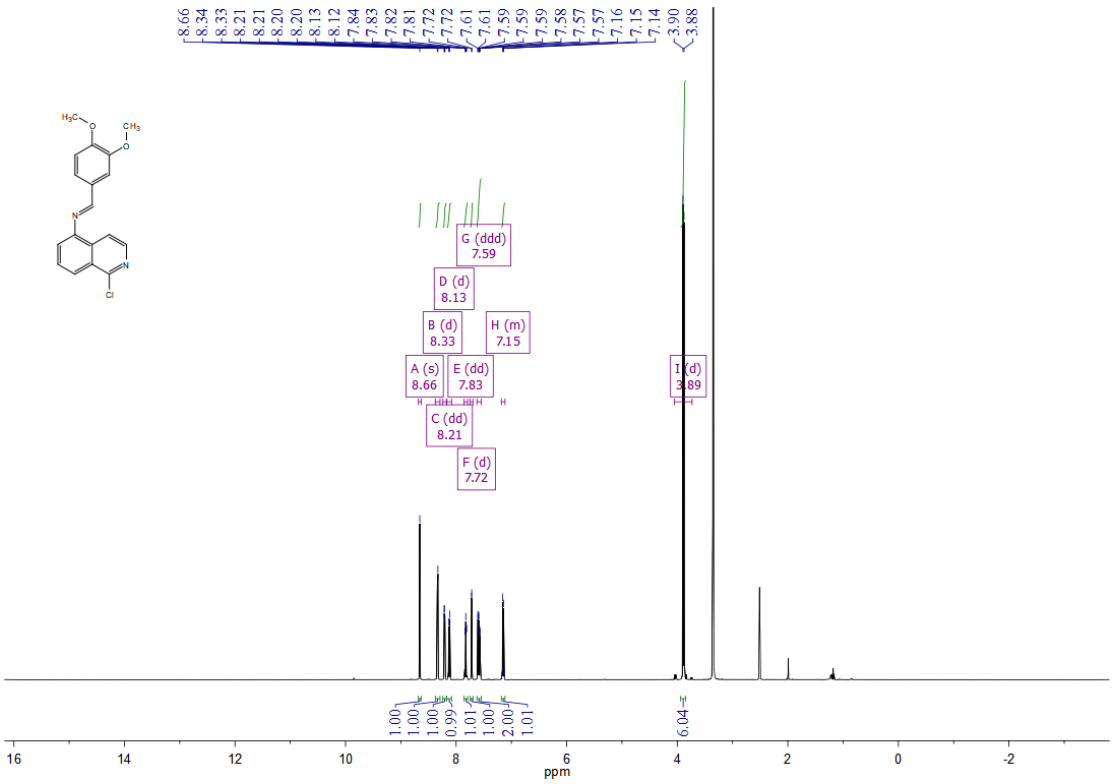
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

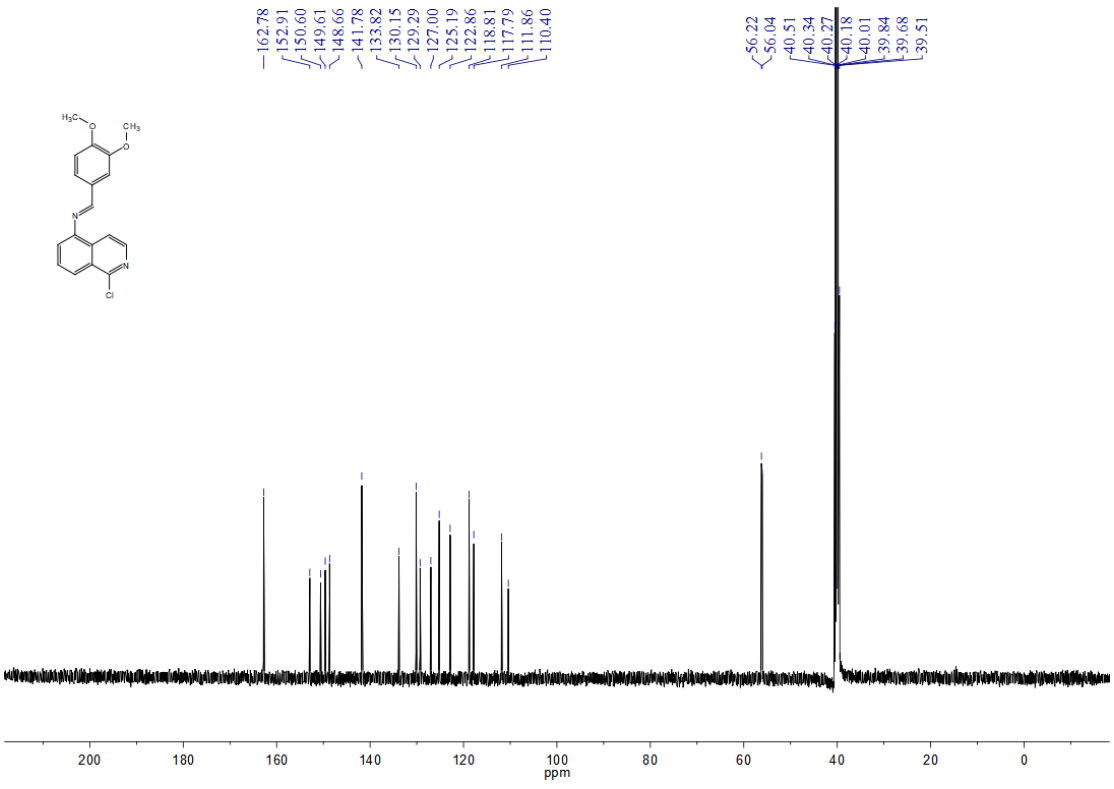
Monoisotopic Mass, Even Electron Ions
366 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 11-11 N: 0-8 O: 0-20 Cl: 1-4
5
0729-5-3 67 (0.441) 1: TOF MS ES+
2.12e+004



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
312.0547	312.0540	0.7	2.2	12.5	433.5	n/a	n/a	C16 H11 N3 O2 Cl

Compound 3d

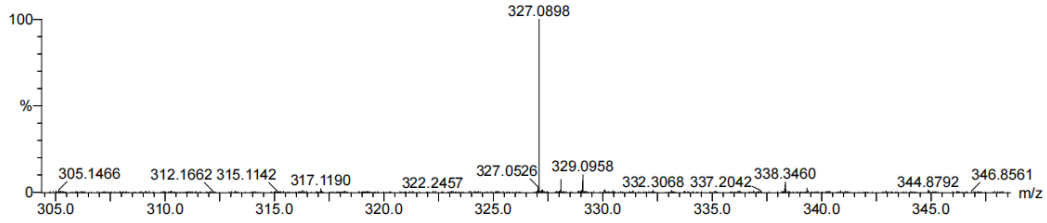

8.66
8.34
8.33
8.21
8.21
8.20
8.20
8.13
8.12
7.84
7.83
7.82
7.81
7.72
7.72
7.61
7.61
7.59
7.59
7.59
7.58
7.57
7.57
7.16
7.15
7.14
3.90
3.88
G (ddd) 7.59
D (d) 8.13
B (d) 8.33
H (m) 7.15
A (s) 8.66
E (dd) 7.83
I (d) 3.89
C (dd) 8.21
F (d) 7.72
1.00
1.00
1.00
0.99
1.01
1.00
2.00
1.01
6.04
ppm


162.78
152.91
150.60
149.61
148.66
141.78
133.82
130.15
129.29
127.00
125.19
122.86
118.81
117.79
111.86
110.40
56.22
56.04
40.51
40.34
40.27
40.18
40.01
39.84
39.68
39.51
ppm

Elemental Composition Report **Page 1**

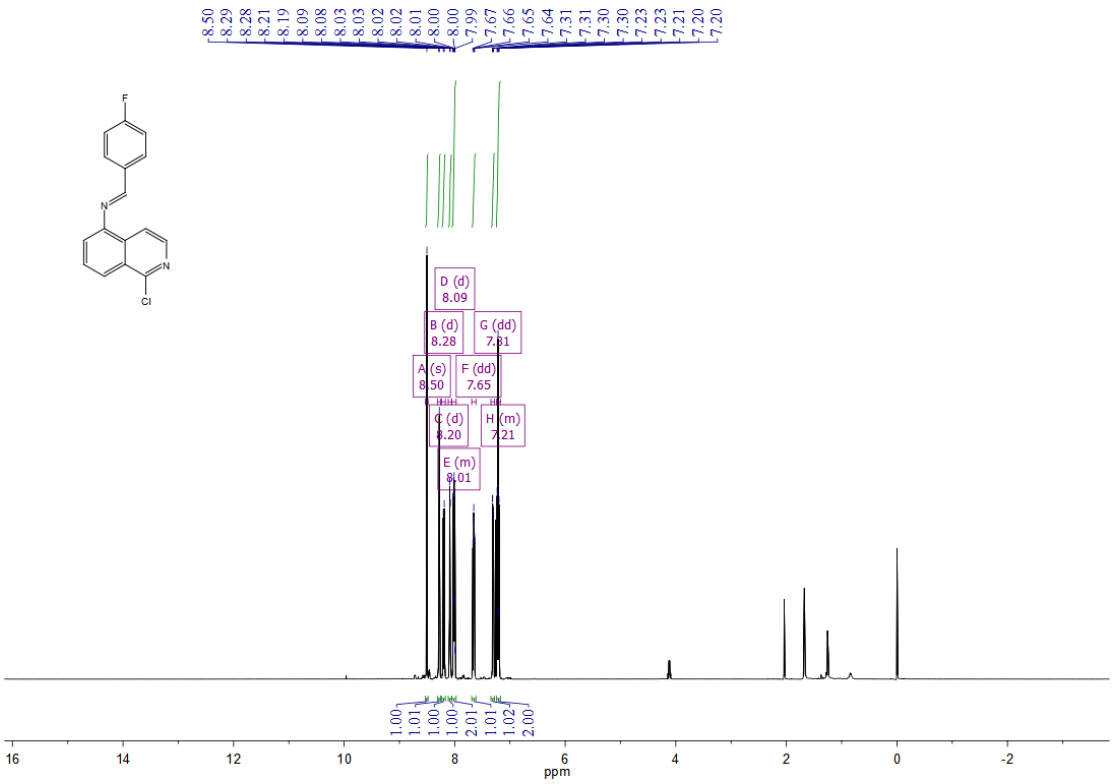
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

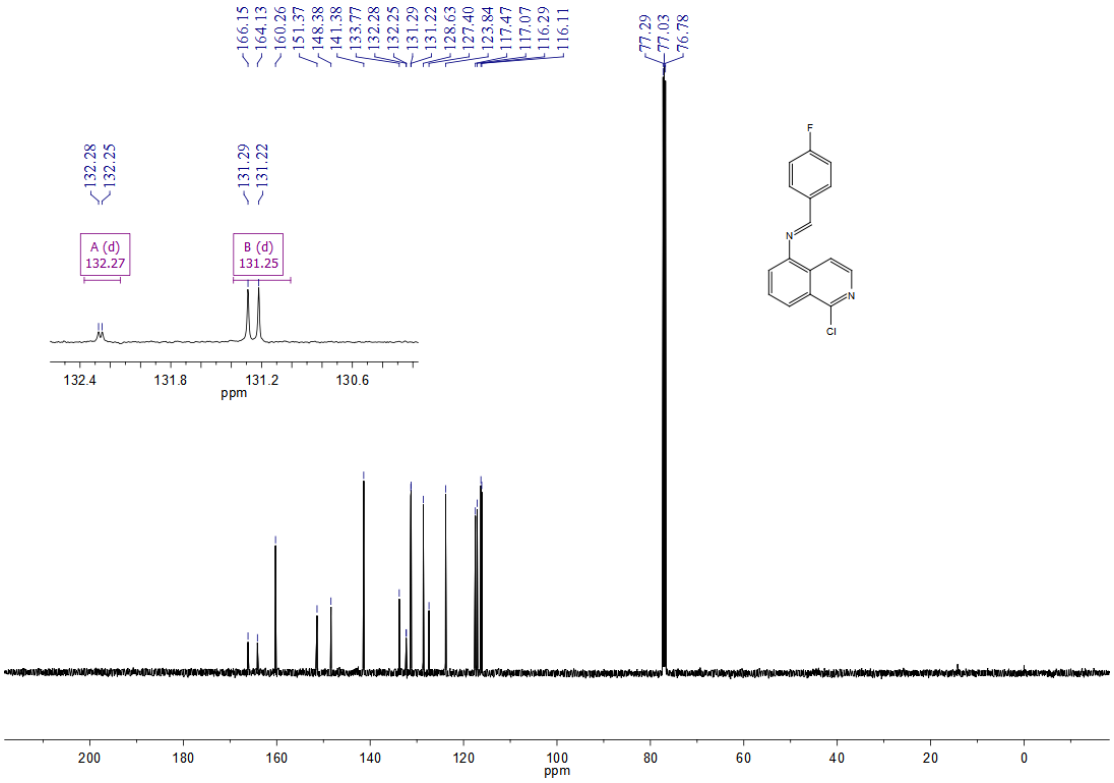
Monoisotopic Mass, Even Electron Ions
405 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 18-18 H: 16-16 N: 0-8 O: 0-20 Cl: 1-4
5
0729-5-4 78 (0.507) 1: TOF MS ES+
2.48e+004



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
327.0898	327.0900	-0.2	-0.6	11.5	454.9	n/a	n/a	C18 H16 N2 O2 Cl

Compound 3e


8.50
8.29
8.28
8.21
8.19
8.09
8.08
8.03
8.03
8.02
8.02
8.01
8.00
8.00
7.99
7.67
7.66
7.65
7.64
7.31
7.31
7.30
7.30
7.23
7.23
7.21
7.20
7.20
F
N
N
Cl
D (d)
8.09
B (d)
8.28
G (dd)
7.81
A (s)
8.50
F (dd)
7.65
C (d)
8.20
H (m)
7.21
E (m)
8.01
1.00
1.01
1.00
1.00
2.01
1.01
1.02
2.00
16
14
12
10
8
6
4
2
0
-2
ppm


166.15
164.13
160.26
151.37
148.38
141.38
133.77
132.28
132.25
131.29
131.22
128.63
127.40
123.84
117.47
117.07
116.29
116.11
77.29
77.03
76.78
132.28
132.25
131.29
131.22
A (d)
132.27
B (d)
131.25
132.4
131.8
131.2
130.6
ppm
F
N
N
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

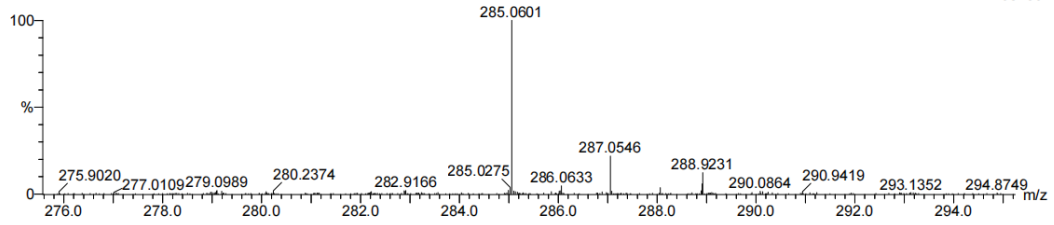
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
230 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 11-11 N: 0-8 Cl: 1-4 F: 1-9

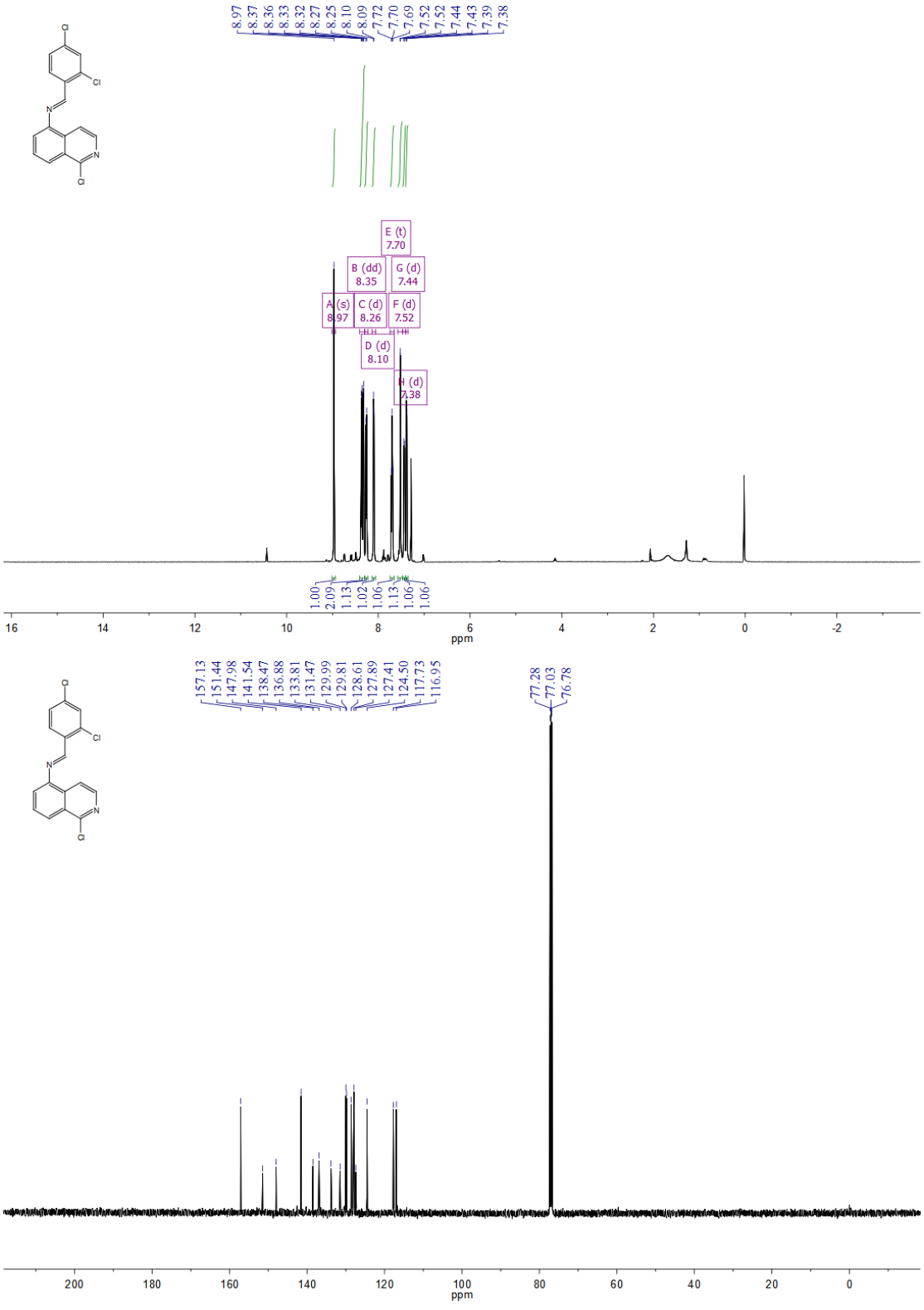
5
0729-5-5 78 (0.507)

1: TOF MS ES+
1.46e+004



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
285.0601	285.0595	0.6	2.1	11.5	389.7	n/a	n/a	C16 H11 N2 Cl F

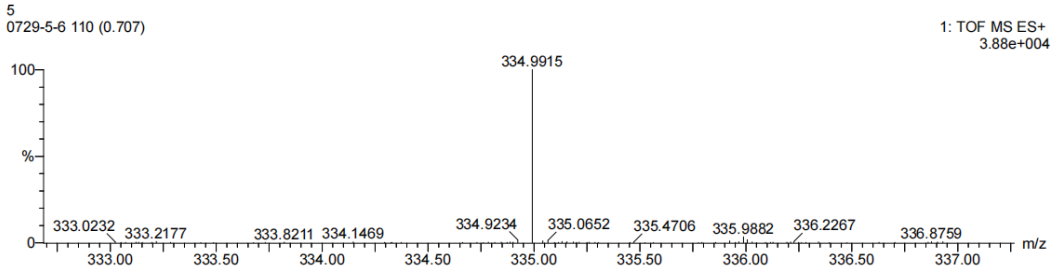
Compound 3f


8.97
8.37
8.36
8.33
8.32
8.27
8.25
8.10
8.09
7.72
7.70
7.69
7.52
7.52
7.44
7.43
7.39
7.38
E (t) 7.70
B (dd) 8.35
G (d) 7.44
A (s) 8.97
C (d) 8.26
F (d) 7.52
D (d) 8.10
H (d) 7.38
1.00
2.09
1.13
1.02
1.06
1.13
1.06
1.06
16
14
12
10
8
6
4
2
0
-2
ppm
157.13
151.44
147.98
141.54
138.47
136.88
133.81
131.47
129.99
129.81
128.61
127.89
127.41
124.50
117.73
116.95
77.28
77.03
76.78
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

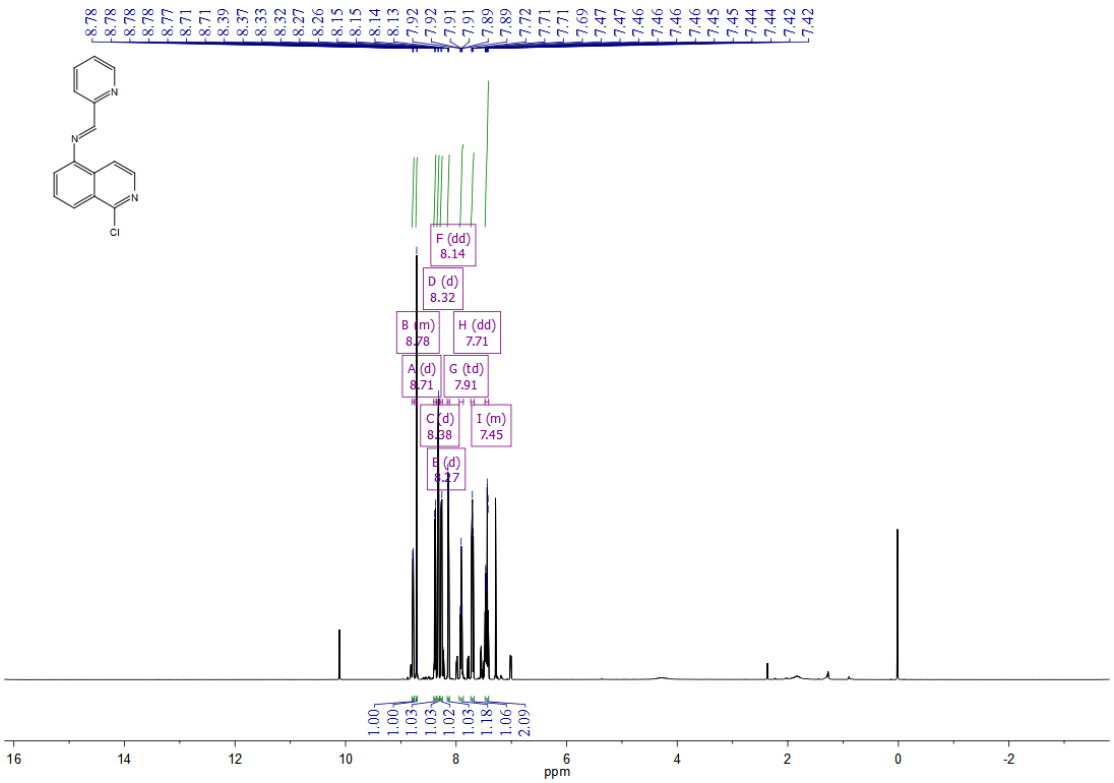
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

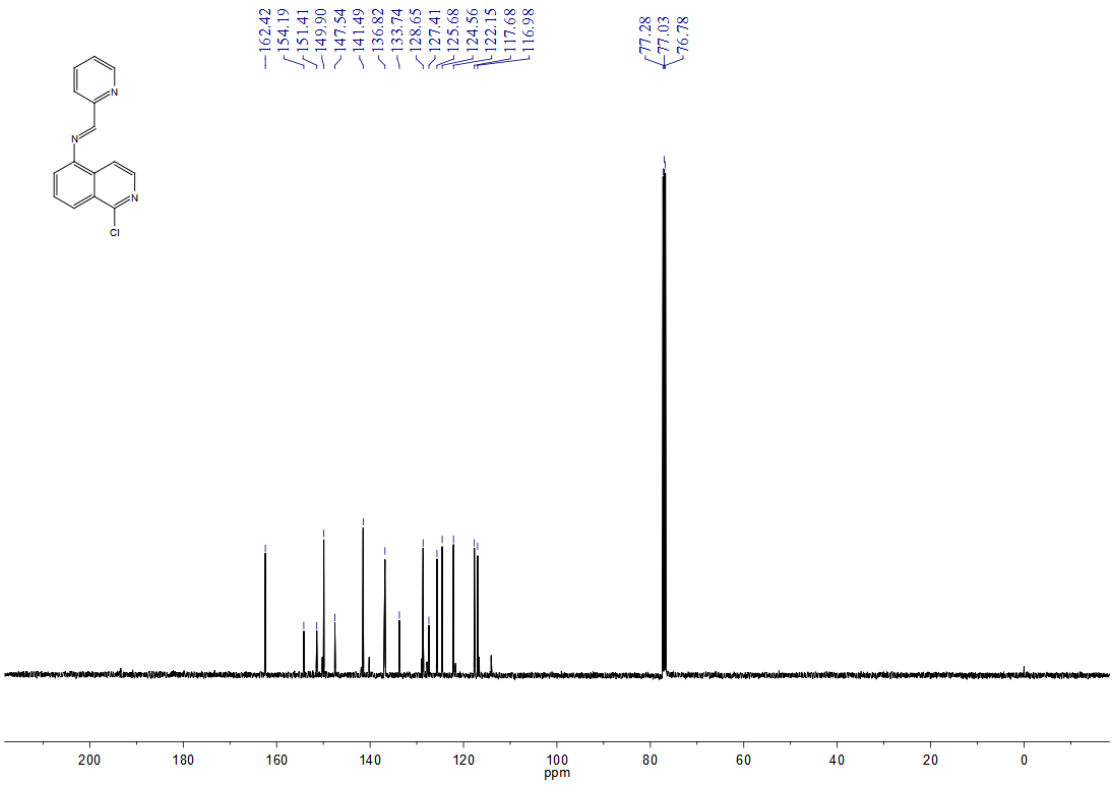
Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 10-10 N: 0-8 Cl: 1-4
5
0729-5-6 110 (0.707)



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
334.9915	334.9910	0.5	1.5	11.5	410.8	n/a	n/a	C16 H10 N2 Cl3

Compound 3g

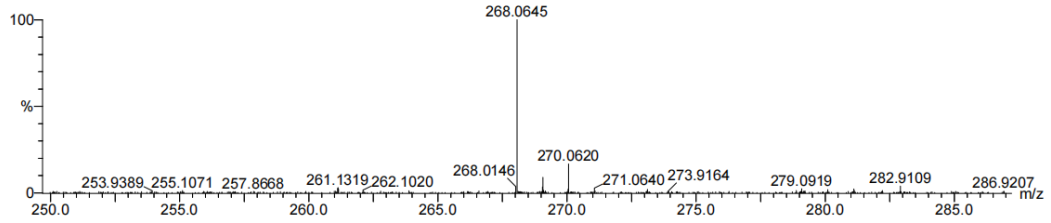

8.78 8.78 8.78 8.78 8.77 8.71 8.71 8.39 8.37 8.33 8.32 8.27 8.26 8.15 8.14 8.13 7.92 7.92 7.91 7.91 7.89 7.89 7.72 7.71 7.71 7.69 7.47 7.47 7.46 7.46 7.46 7.45 7.45 7.44 7.44 7.42 7.42
F (dd) 8.14
D (d) 8.32
B (m) 8.78
H (dd) 7.71
A (d) 8.71
G (td) 7.91
C (d) 8.38
I (m) 7.45
E (d) 8.27
1.00 1.00 1.03 1.03 1.02 1.03 1.18 1.06 2.09
16 14 12 10 8 6 4 2 0 -2
ppm


162.42 154.19 151.41 149.90 147.54 141.49 136.82 133.74 128.65 127.41 125.68 124.56 122.15 117.68 116.98
77.28 77.03 76.78
200 180 160 140 120 100 80 60 40 20 0
ppm

Elemental Composition Report **Page 1**

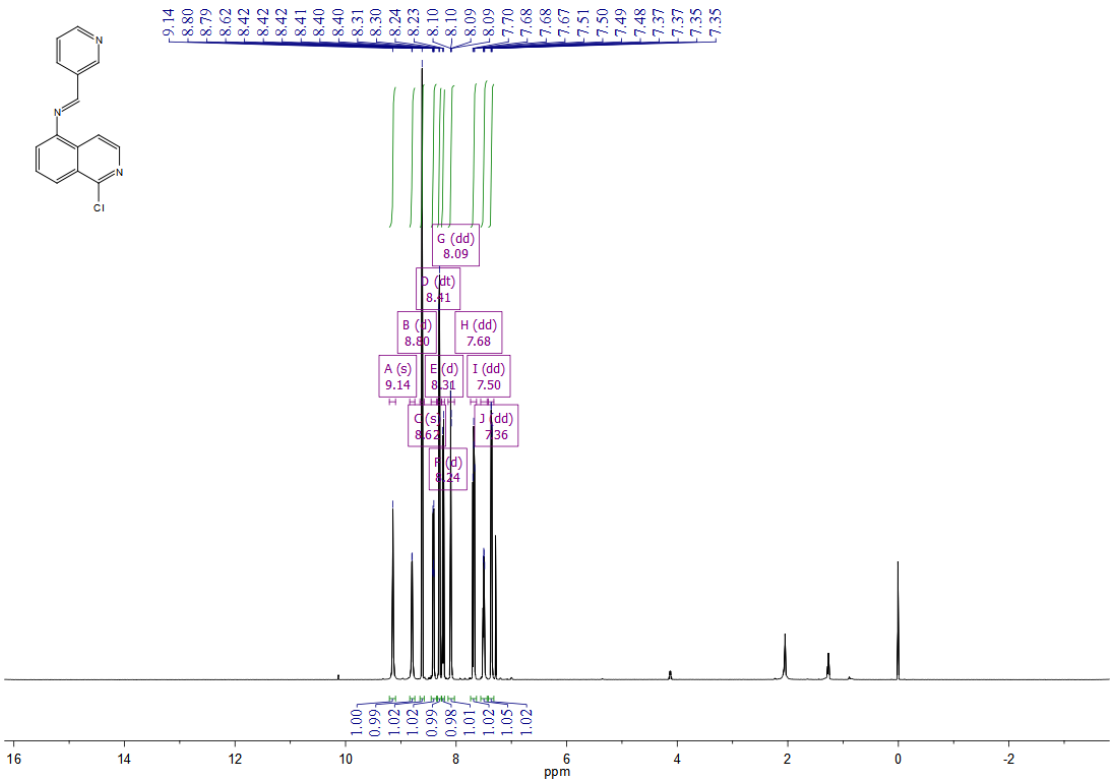
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

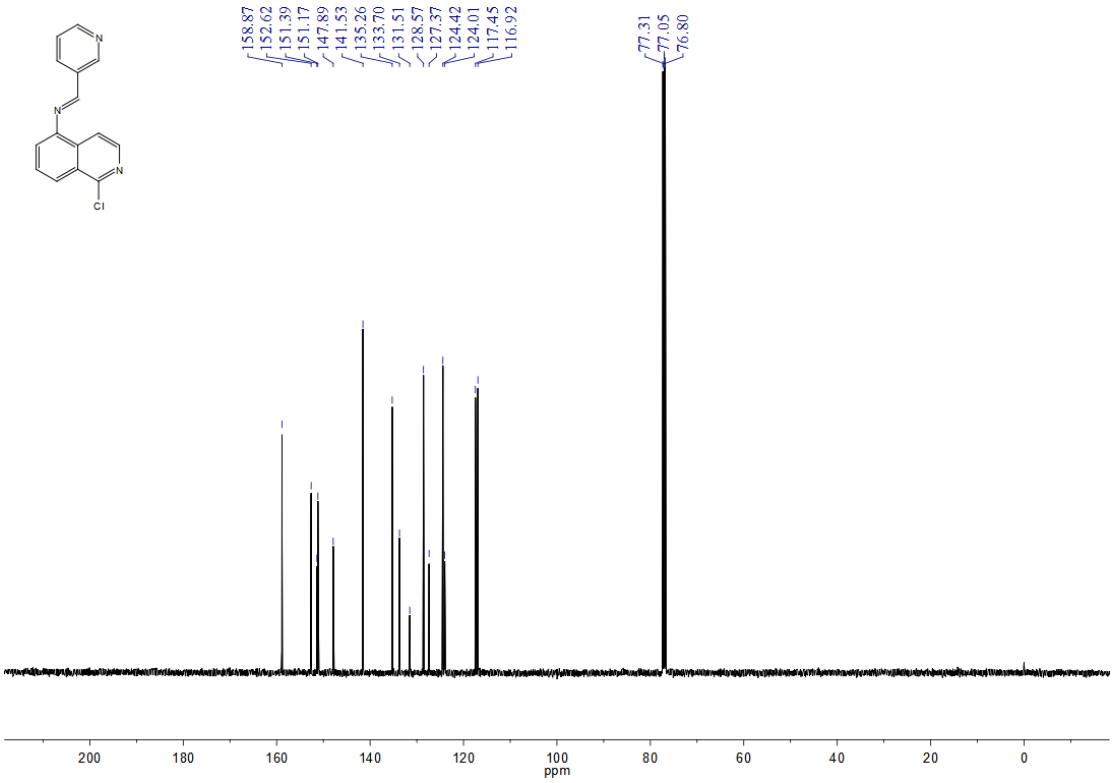
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 15-15 H: 11-11 N: 0-8 Cl: 1-4
5
0729-5-8 62 (0.407) 1: TOF MS ES+
1.70e+004



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
268.0645	268.0642	0.3	1.1	11.5	458.2	n/a	n/a	C15 H11 N3 Cl

Compound 3h

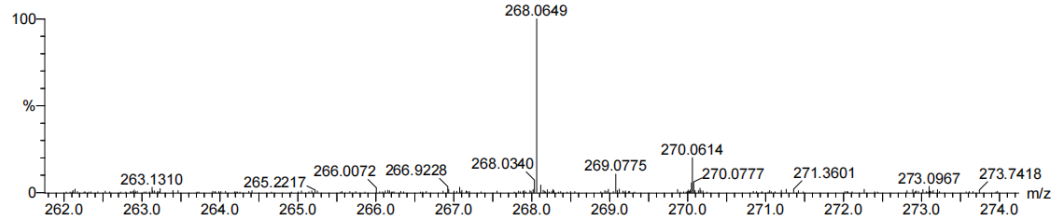

9.14
8.80
8.79
8.62
8.42
8.42
8.42
8.41
8.40
8.40
8.31
8.30
8.24
8.23
8.10
8.10
8.09
8.09
7.70
7.68
7.68
7.67
7.51
7.50
7.49
7.48
7.37
7.37
7.35
7.35
G (dd) 8.09
D (dt) 8.41
B (d) 8.80
H (dd) 7.68
A (s) 9.14
E (d) 8.31
I (dd) 7.50
C (s) 8.62
J (dd) 7.36
F (d) 8.24
1.00
0.99
1.02
1.02
0.99
0.98
1.01
1.02
1.05
1.02
16
14
12
10
8
6
4
2
0
-2
ppm


158.87
152.62
151.39
151.17
147.89
141.53
135.26
133.70
131.51
128.57
127.37
124.42
124.01
117.45
116.92
77.31
77.05
76.80
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

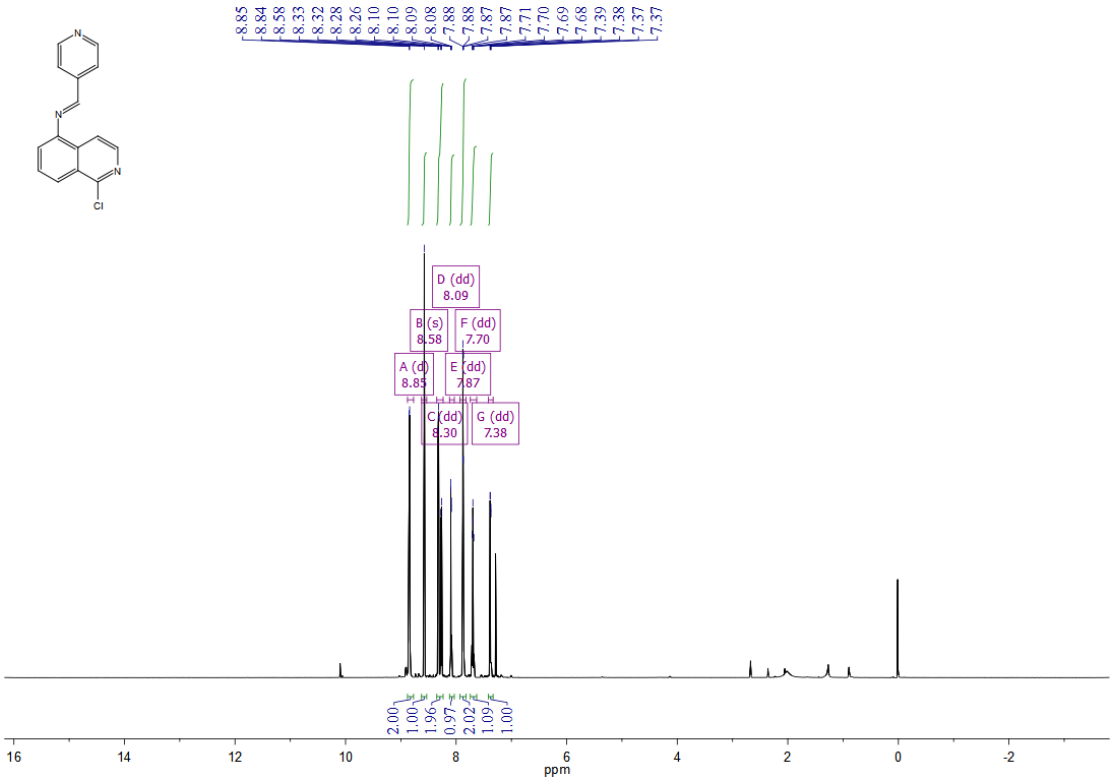
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

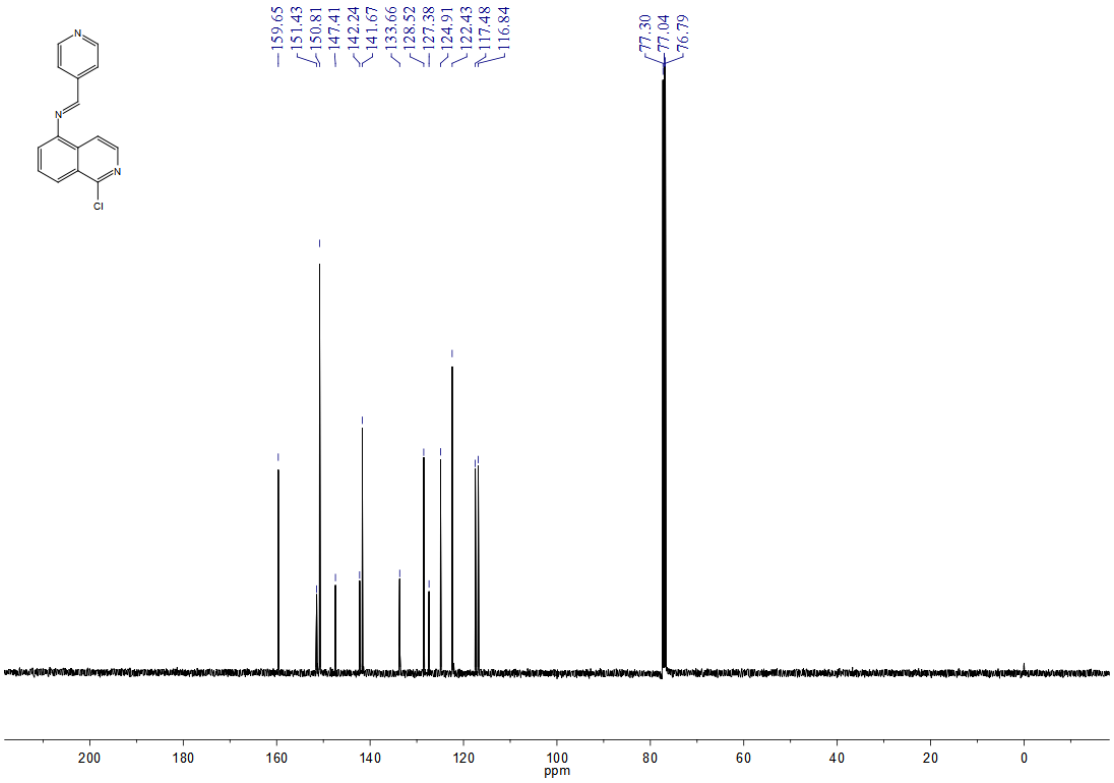
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 15-15 H: 11-11 N: 0-8 Cl: 1-4
5
0729-5-9 74 (0.486) 1: TOF MS ES+
7.17e+003



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
268.0649	268.0642	0.7	2.6	11.5	376.0	n/a	n/a	C15 H11 N3 Cl

Compound 3i

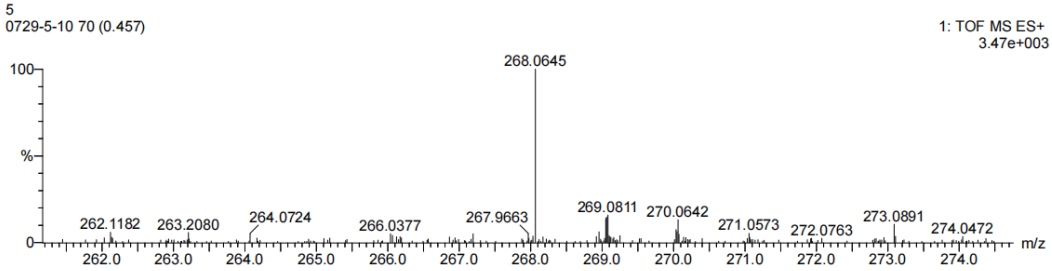

8.85
8.84
8.58
8.33
8.32
8.28
8.26
8.10
8.10
8.09
8.08
7.88
7.88
7.87
7.87
7.71
7.70
7.69
7.68
7.39
7.38
7.37
7.37
D (dd)
8.09
B (s)
8.58
F (dd)
7.70
A (d)
8.85
E (dd)
7.87
C (dd)
8.30
G (dd)
7.38
2.00
1.00
1.96
0.97
2.02
1.09
1.00
16
14
12
10
8
6
4
2
0
-2
ppm


159.65
151.43
150.81
147.41
142.24
141.67
133.66
128.52
127.38
124.91
122.43
117.48
116.84
77.30
77.04
76.79
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

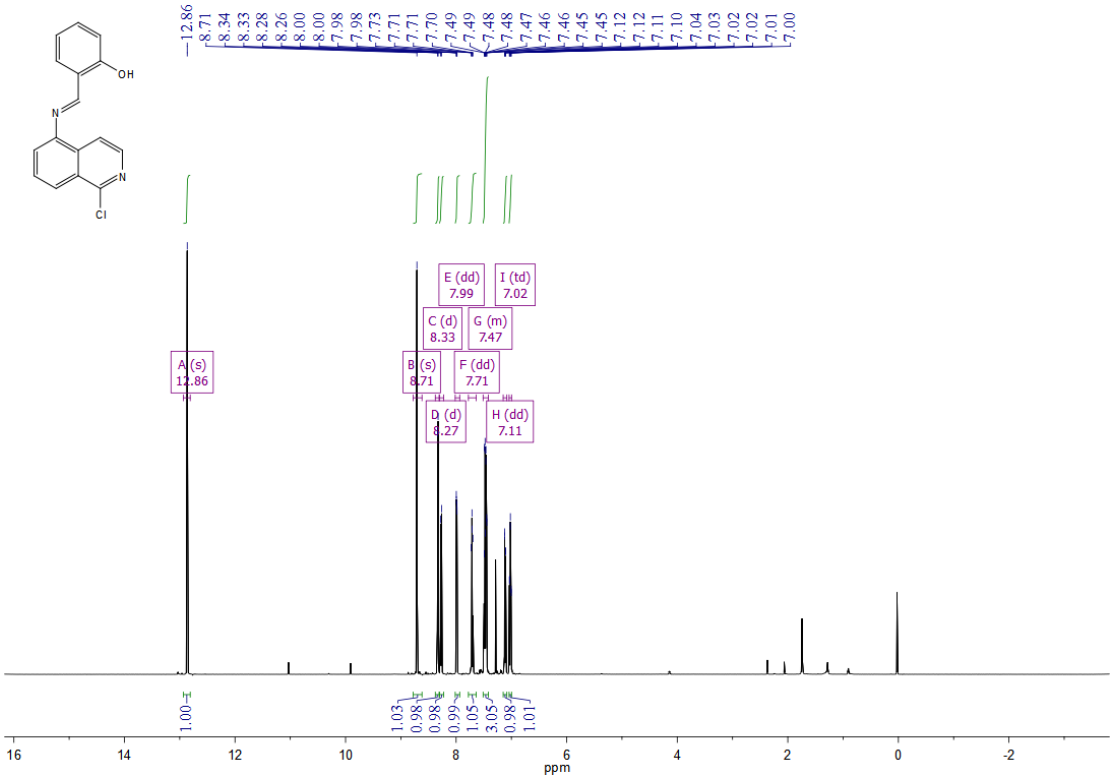
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

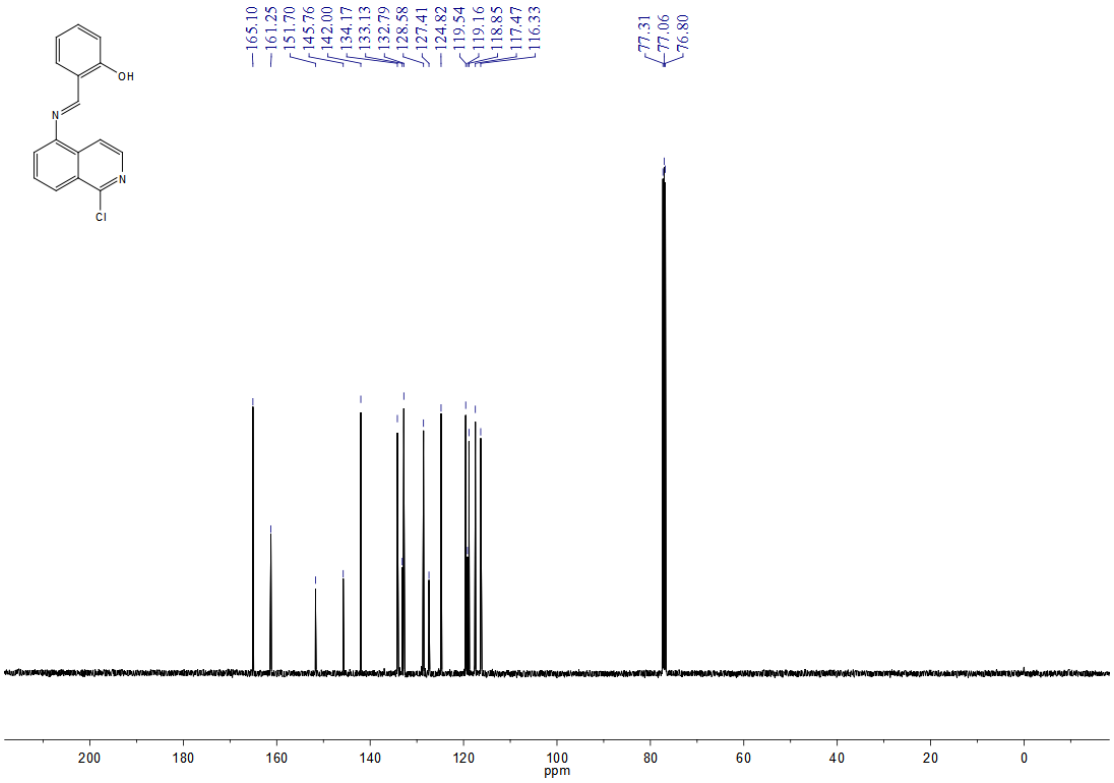
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 15-15 H: 11-11 N: 0-8 Cl: 1-4
5
0729-5-10 70 (0.457)



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
268.0645	268.0642	0.3	1.1	11.5	410.4	n/a	n/a	C15 H11 N3 Cl

Compound 3j


12.86
8.71
8.34
8.33
8.28
8.26
8.00
8.00
7.98
7.98
7.73
7.71
7.71
7.70
7.49
7.49
7.48
7.48
7.47
7.46
7.46
7.45
7.45
7.12
7.12
7.11
7.10
7.04
7.03
7.02
7.02
7.01
7.00
OH
N
N
Cl
A (s) 12.86
B (s) 8.71
C (d) 8.33
D (d) 8.27
E (dd) 7.99
F (dd) 7.71
G (m) 7.47
H (dd) 7.11
I (td) 7.02
1.00
1.03
0.98
0.98
0.99
1.05
3.05
0.98
1.01
16
14
12
10
8
6
4
2
0
-2
ppm

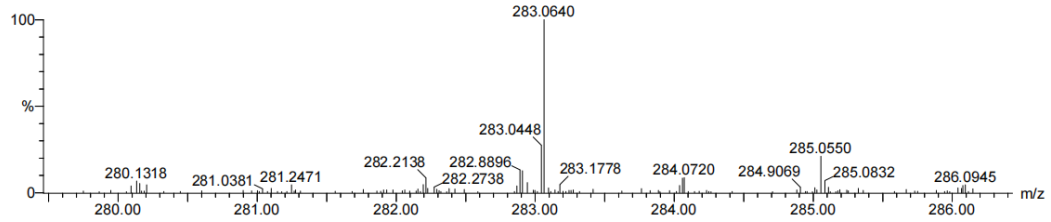

165.10
161.25
151.70
145.76
142.00
134.17
133.13
132.79
128.58
127.41
124.82
119.54
119.16
118.85
117.47
116.33
77.31
77.06
76.80
OH
N
N
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

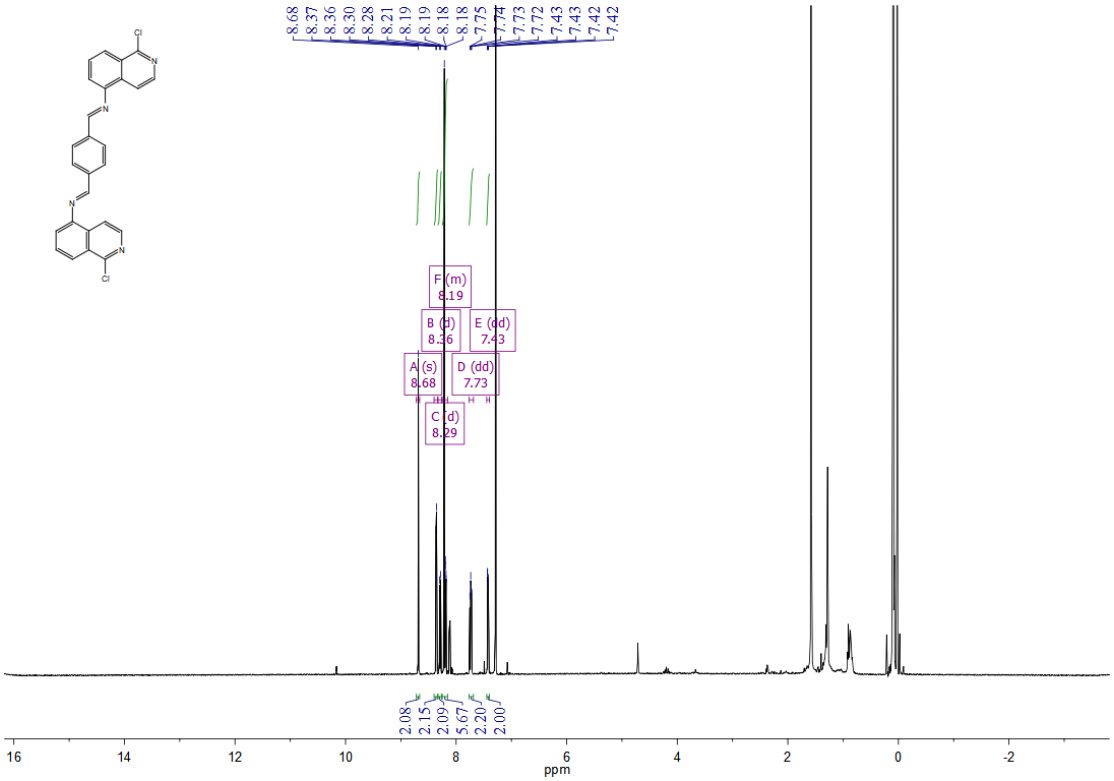
Monoisotopic Mass, Even Electron Ions
318 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 12-12 N: 0-8 O: 0-20 Cl: 1-4
5
0729-5-11 86 (0.557)

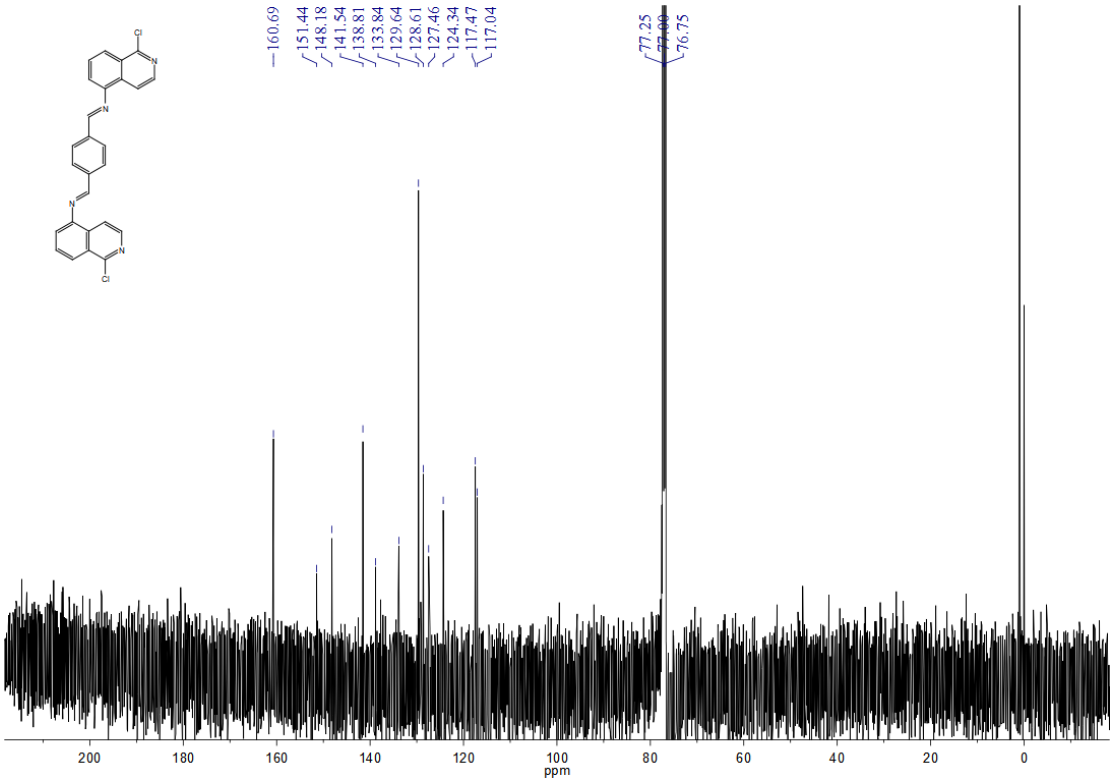
1: TOF MS ES+
3.55e+003



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
283.0640	283.0638	0.2	0.7	11.5	372.9	n/a	n/a	C16 H12 N2 O Cl

Compound 3k


8.68
8.37
8.36
8.30
8.28
8.21
8.19
8.19
8.18
8.18
7.75
7.74
7.73
7.72
7.43
7.43
7.42
7.42
F (m) 8.19
B (d) 8.36
E (dd) 7.43
A (s) 8.68
D (dd) 7.73
C (d) 8.29
2.08
2.15
2.09
5.67
2.20
2.00
16
14
12
10
8
6
4
2
0
-2
ppm

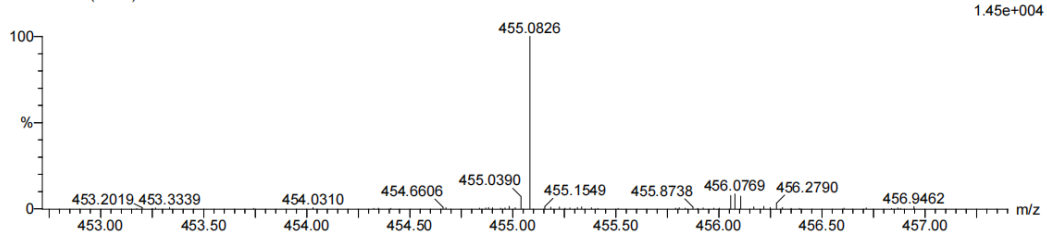

160.69
151.44
148.18
141.54
138.81
133.84
129.64
128.61
127.46
124.34
117.47
117.04
77.25
77.00
76.75
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

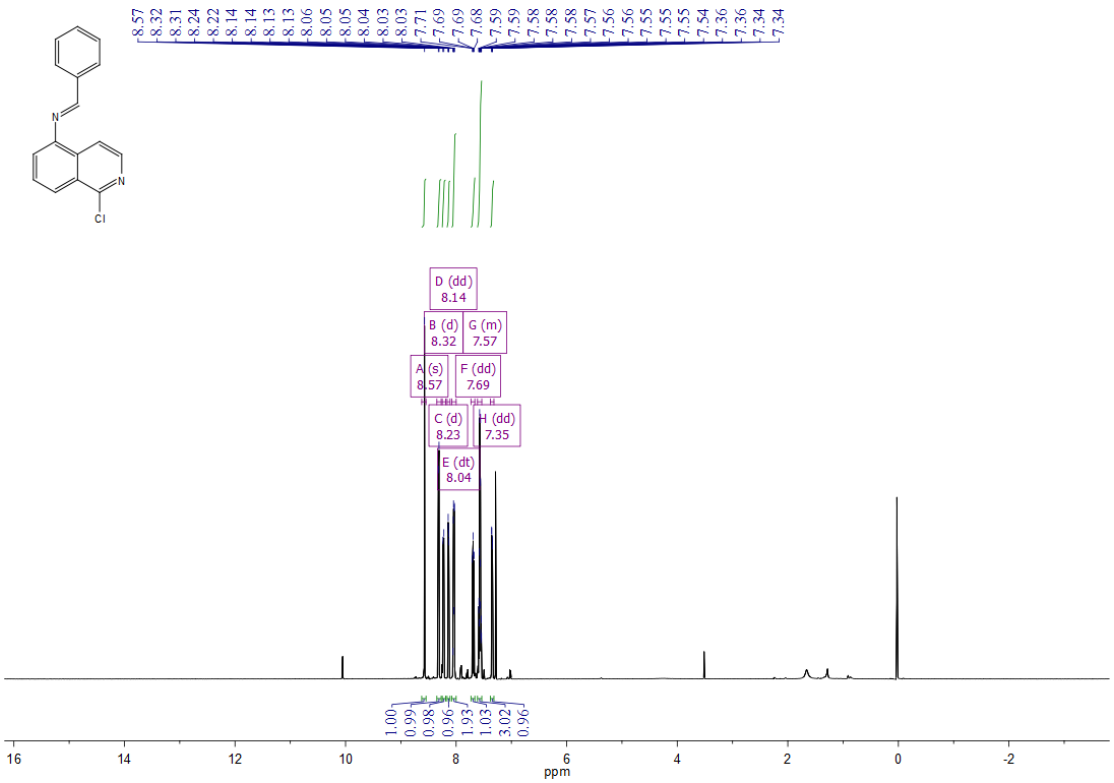
Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 26-26 H: 17-17 N: 0-8 Cl: 1-4
5
0729-5-7 81 (0.531)

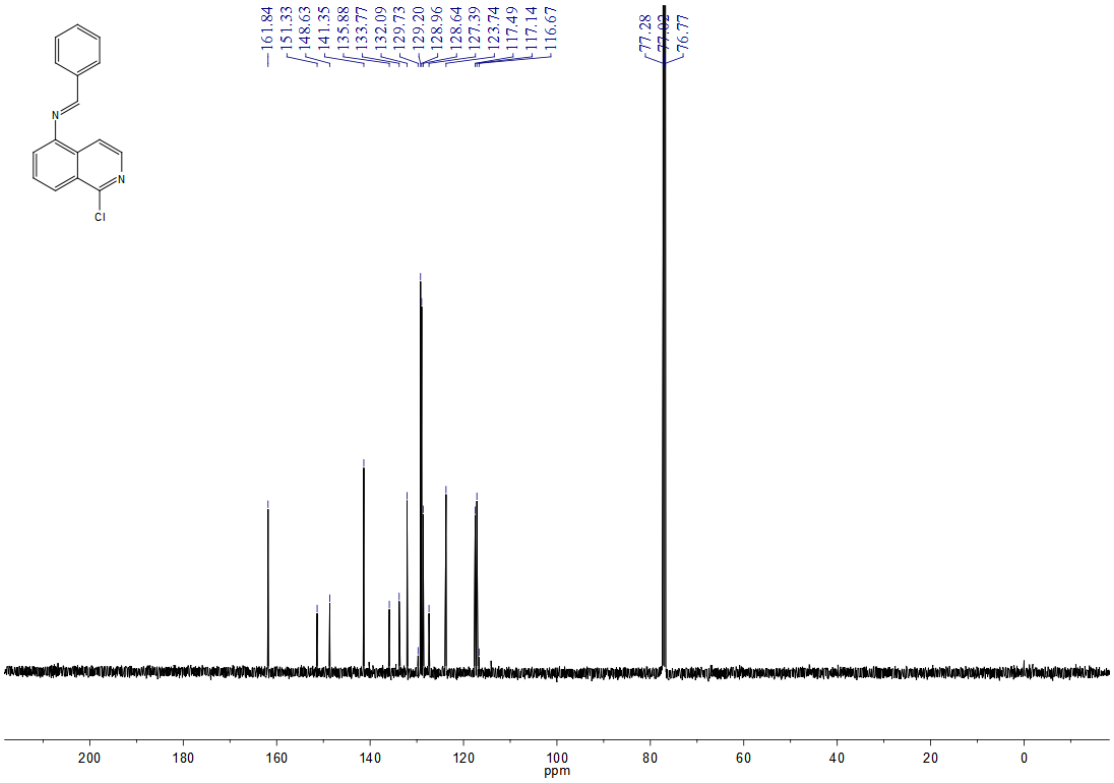
1: TOF MS ES+
1.45e+004



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
455.0826	455.0830	-0.4	-0.9	19.5	322.2	n/a	n/a	C26 H17 N4 Cl2

Compound 3l


8.57
8.32
8.31
8.24
8.22
8.14
8.14
8.13
8.13
8.06
8.05
8.05
8.04
8.03
8.03
7.71
7.69
7.69
7.68
7.59
7.59
7.58
7.58
7.58
7.57
7.56
7.56
7.55
7.55
7.55
7.54
7.36
7.36
7.34
7.34
D (dd) 8.14
B (d) 8.32
G (m) 7.57
A (s) 8.57
F (dd) 7.69
C (d) 8.23
H (dd) 7.35
E (dt) 8.04
1.00
0.99
0.98
0.96
1.93
1.03
3.02
0.96
16
14
12
10
8
6
4
2
0
-2
ppm
N
N
Cl


161.84
151.33
148.63
141.35
135.88
133.77
132.09
129.73
129.20
128.96
128.64
127.39
123.74
117.49
117.14
116.67
77.28
77.02
76.77
200
180
160
140
120
100
80
60
40
20
0
ppm
N
N
Cl

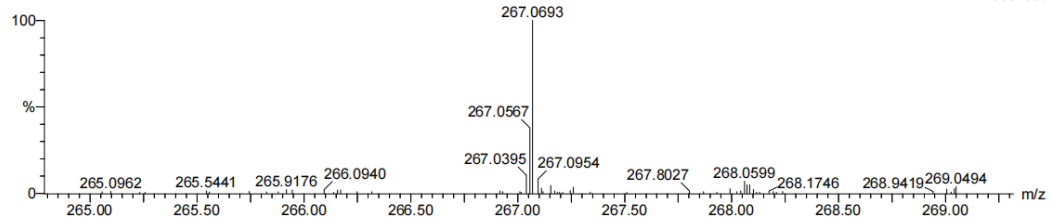
Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
288 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 12-12 N: 0-8 O: 0-20 Cl: 1-4
5
0729-5-12 91 (0.591)

1: TOF MS ES+
4.06e+003



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
267.0693	267.0689	0.4	1.5	11.5	274.6	n/a	n/a	C16 H12 N2 Cl