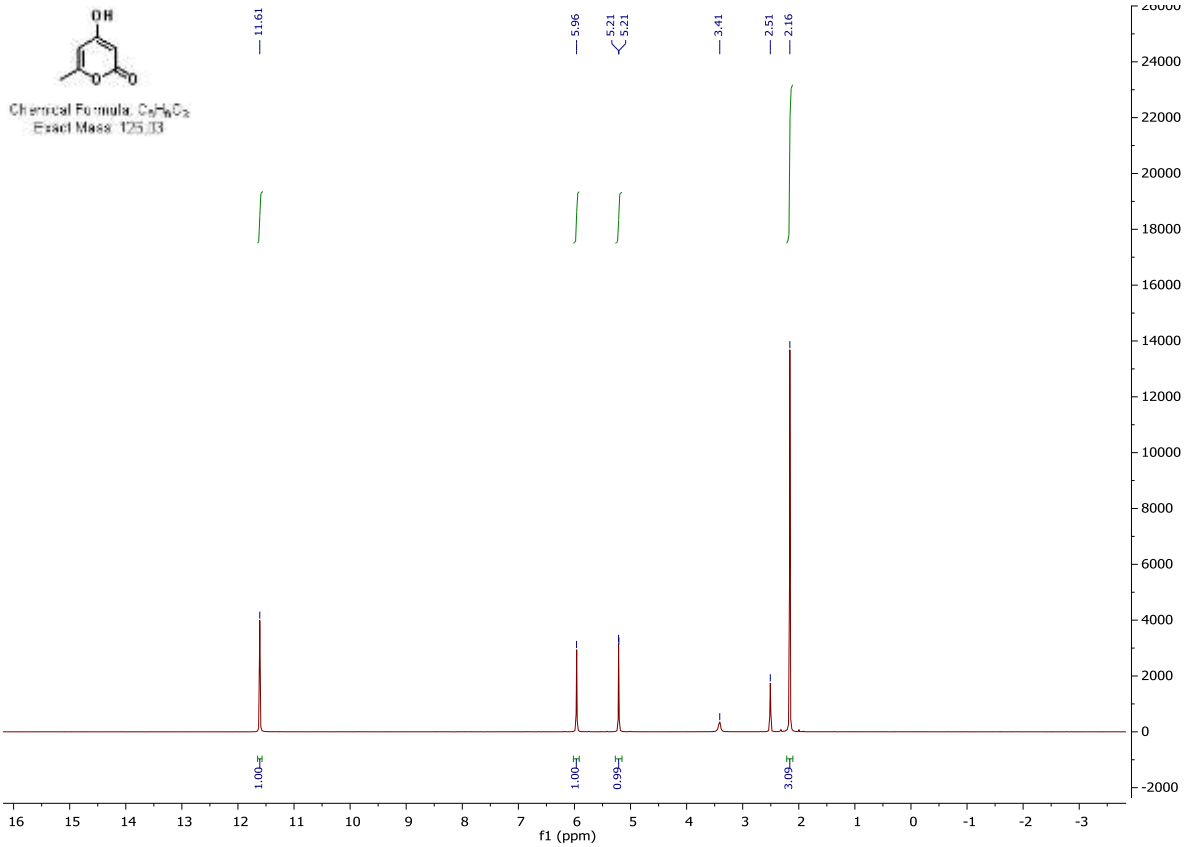
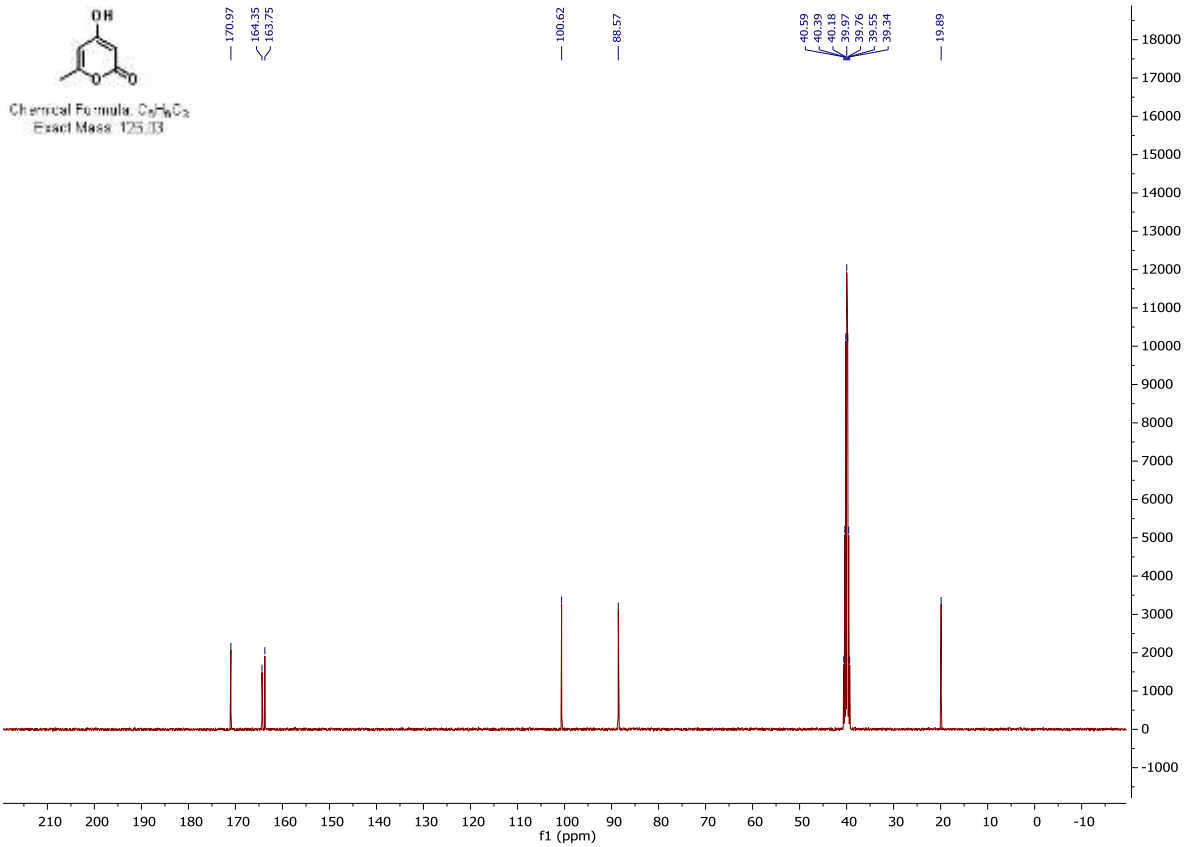
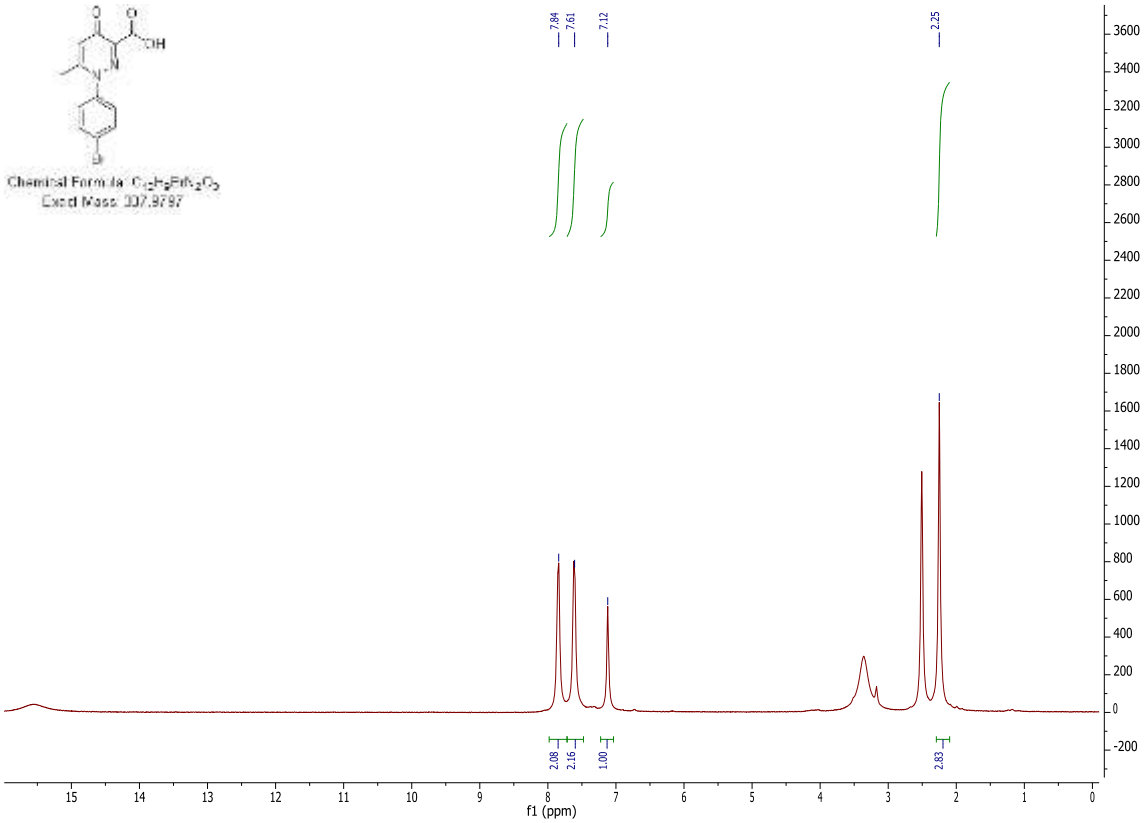
Table of Contents

A. Copies of NMR spectra

A1. Building blocks 1,2



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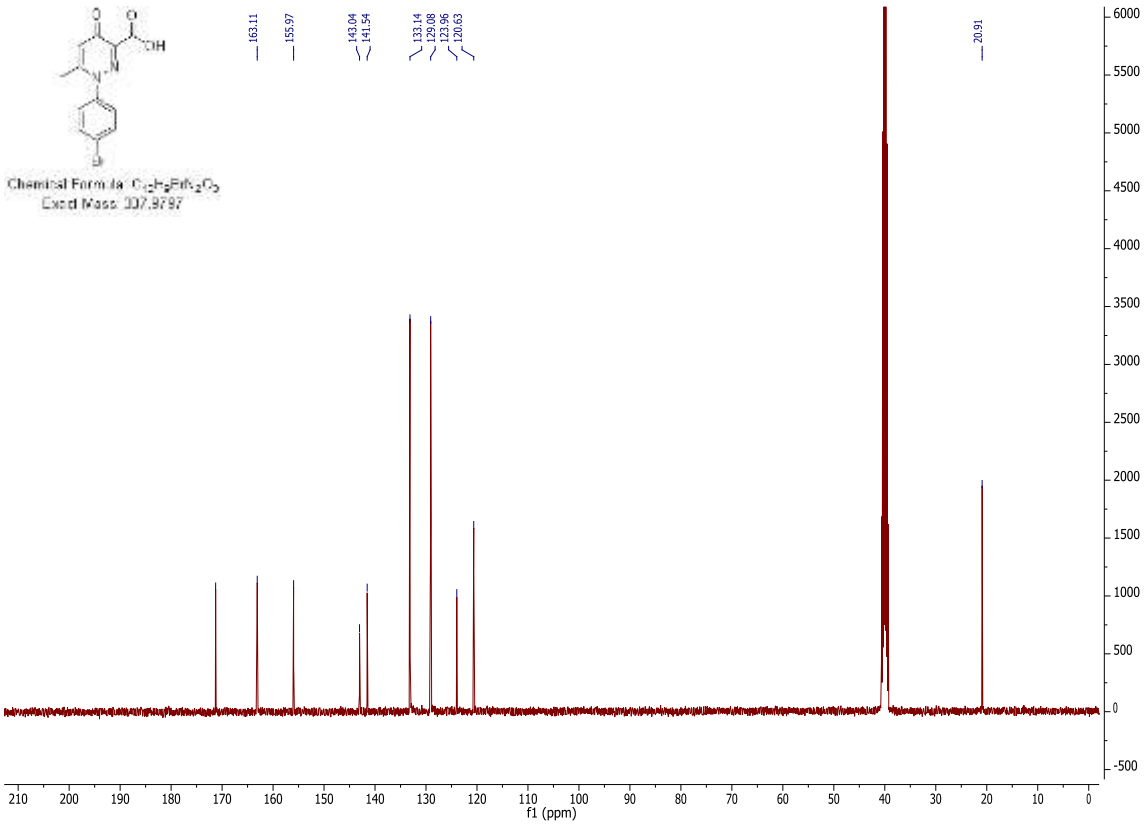
7.12
2.25
2.08
2.16
1.00
2.83
f1 (ppm)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163.11
155.97
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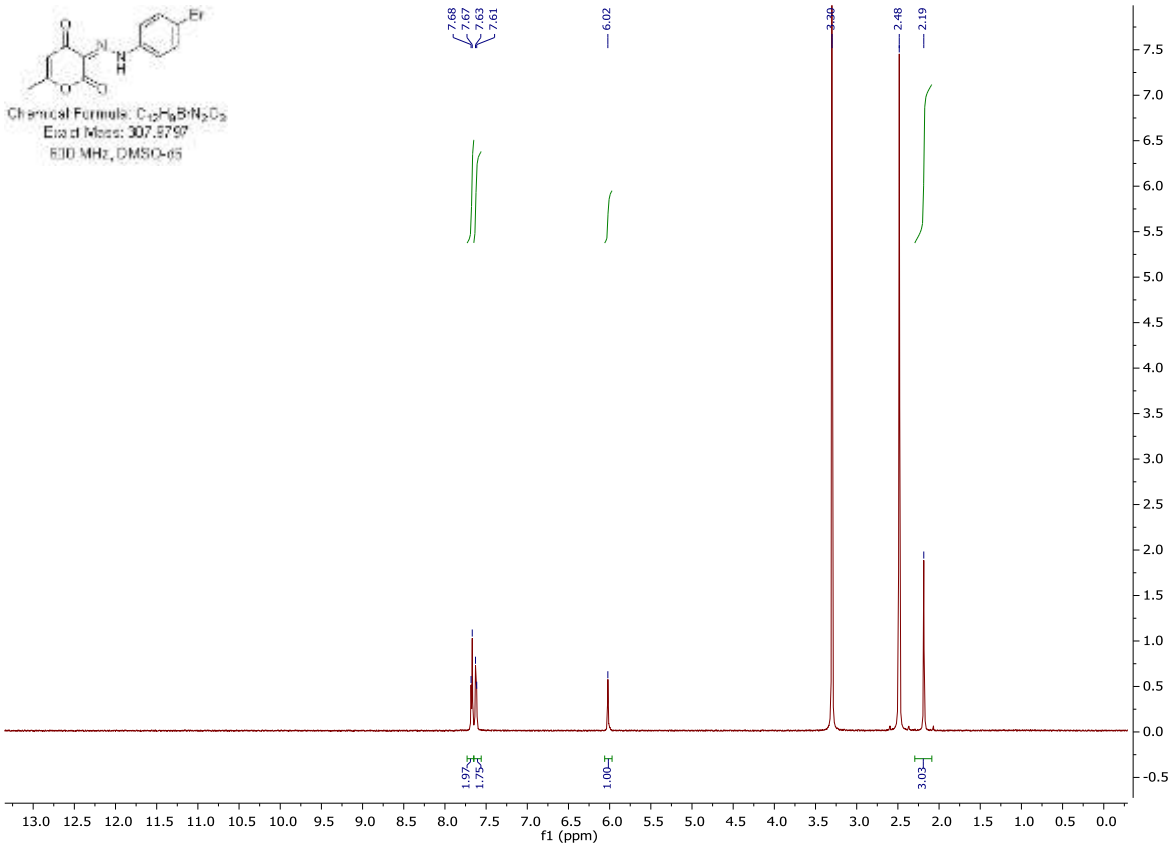
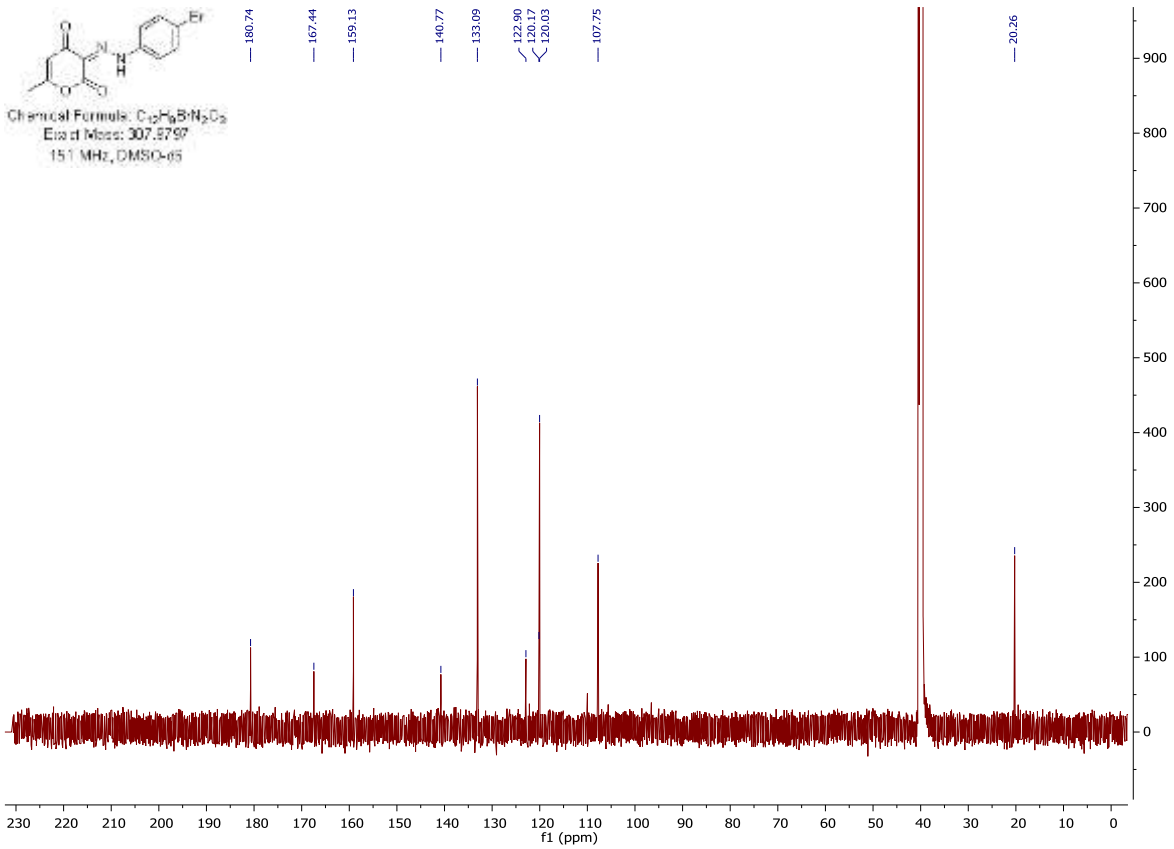
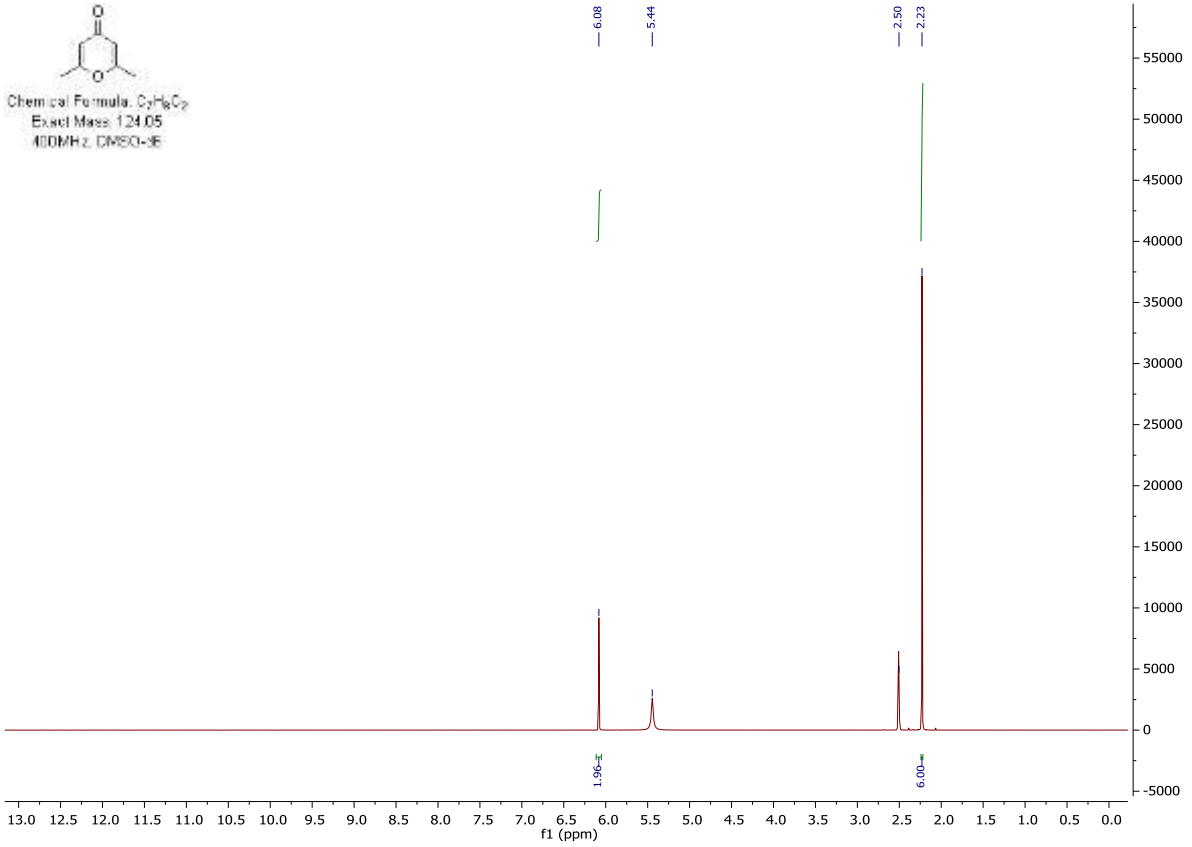
129.08
123.96
120.63
20.91
f1 (ppm)

A2. Compounds 5-7.






Chemical Formula: C7H8O2
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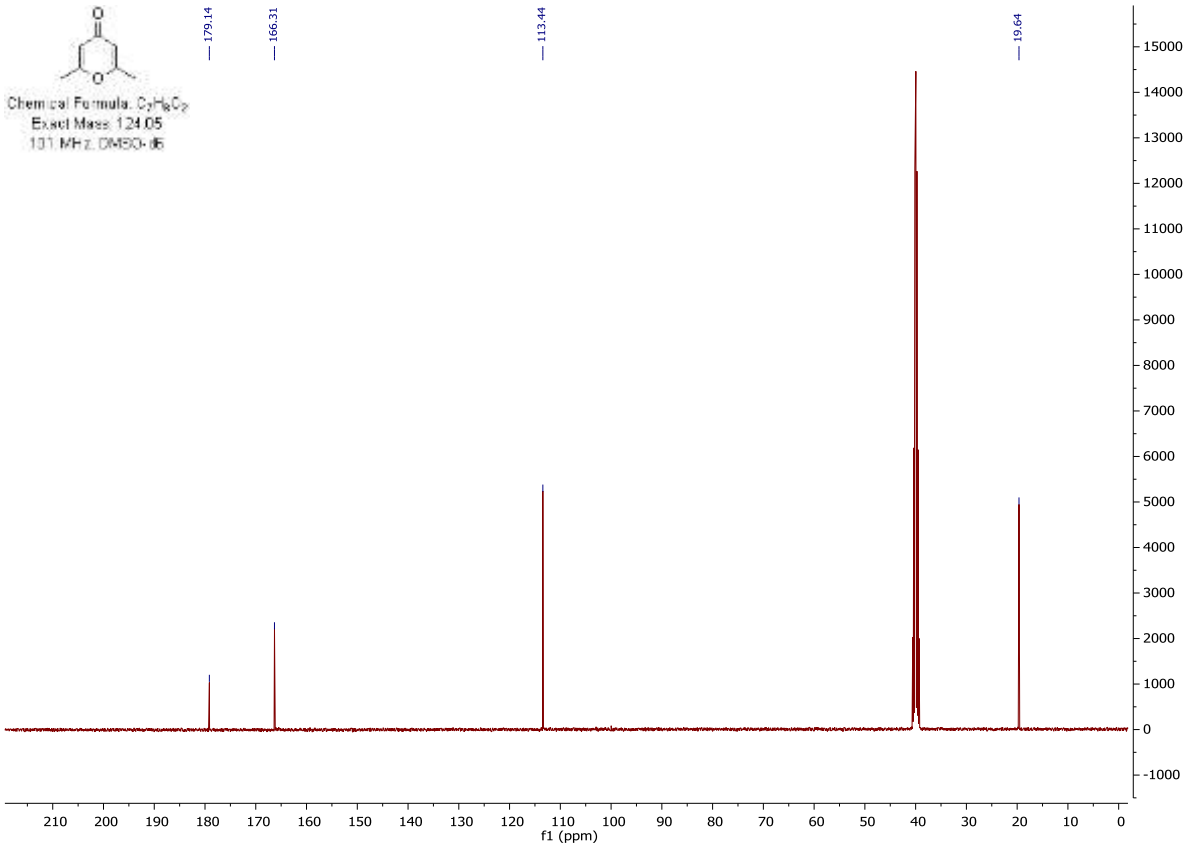
5.44
2.50
2.23
1.96
6.00
f1 (ppm)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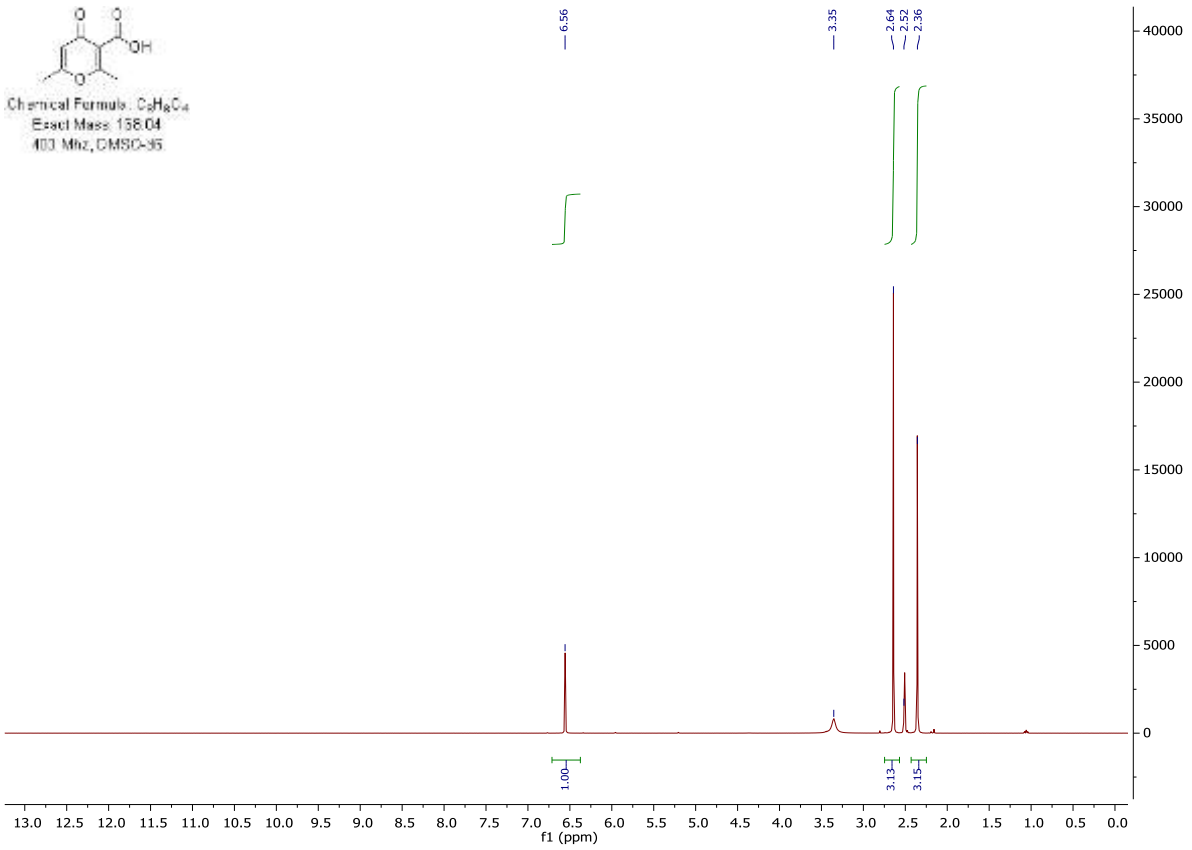
166.31
113.44
19.64
f1 (ppm)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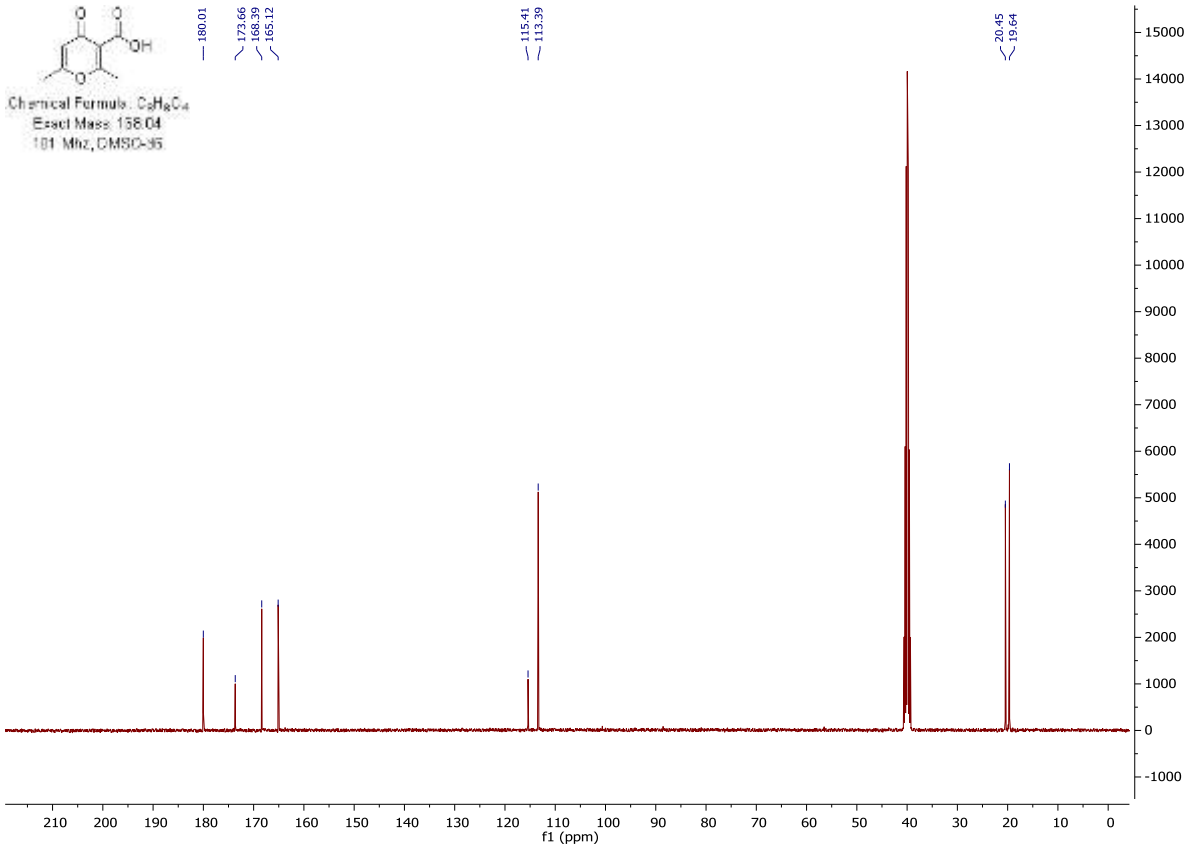
f1 (ppm)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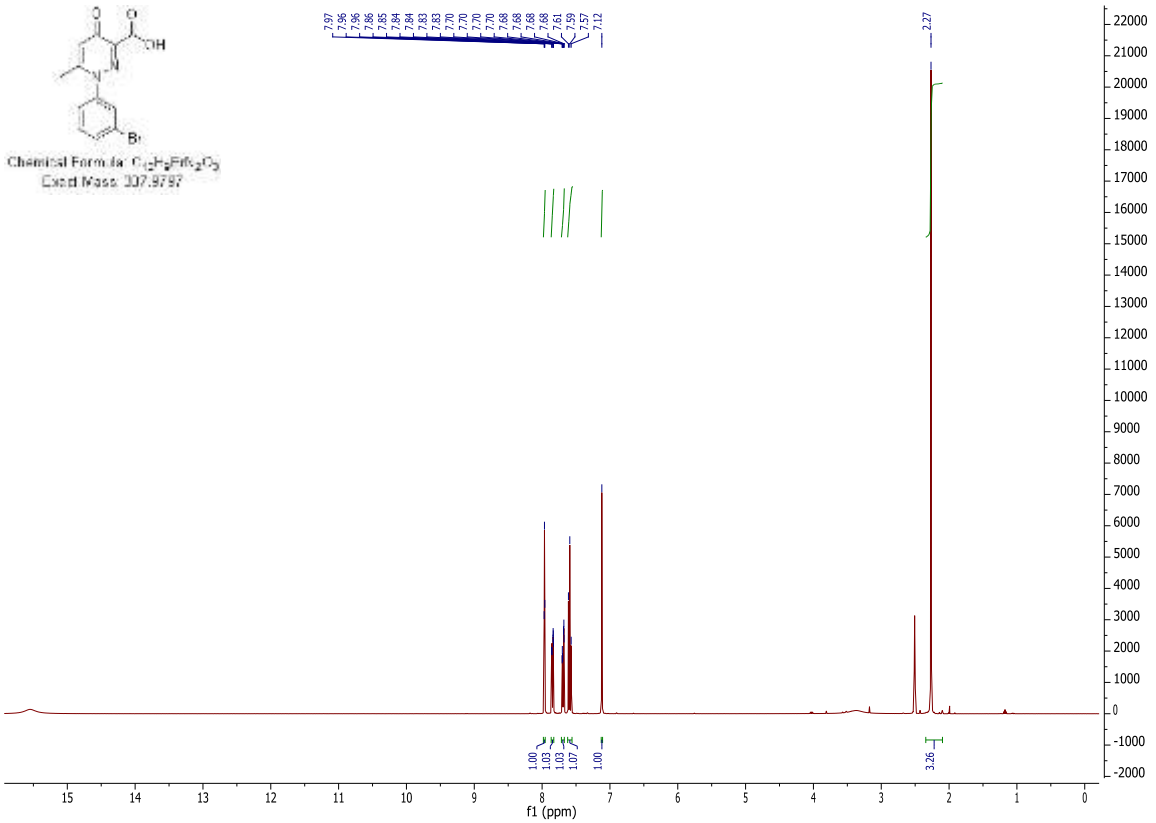
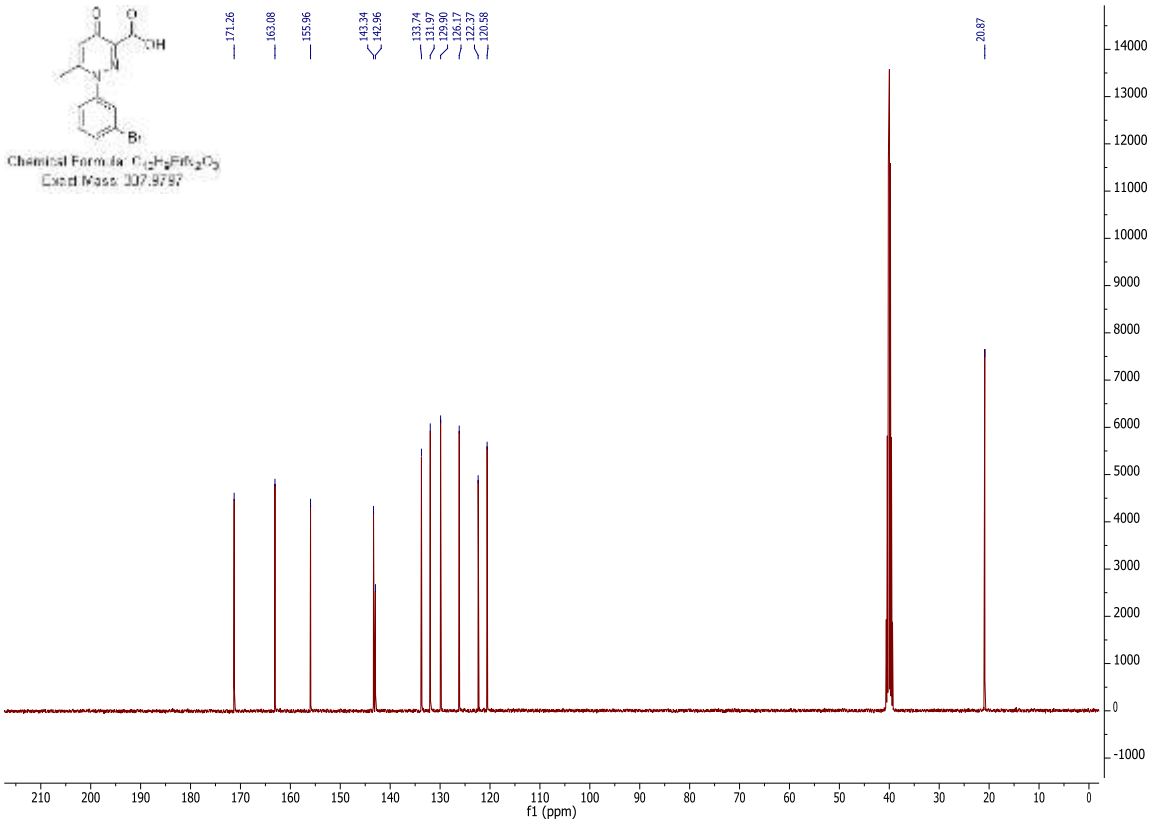
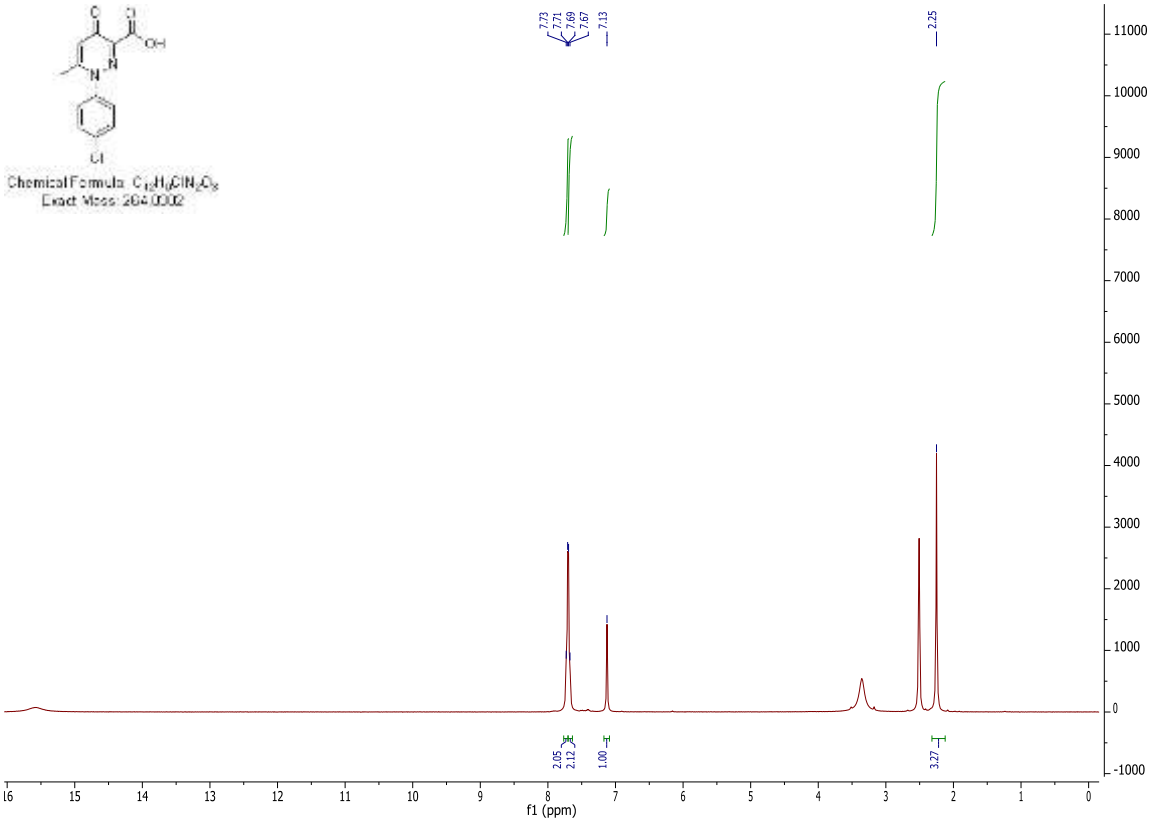
168.39
165.12
115.41
113.39
20.45
19.64
f1 (ppm)

A3. Serie A derivatives 8-14



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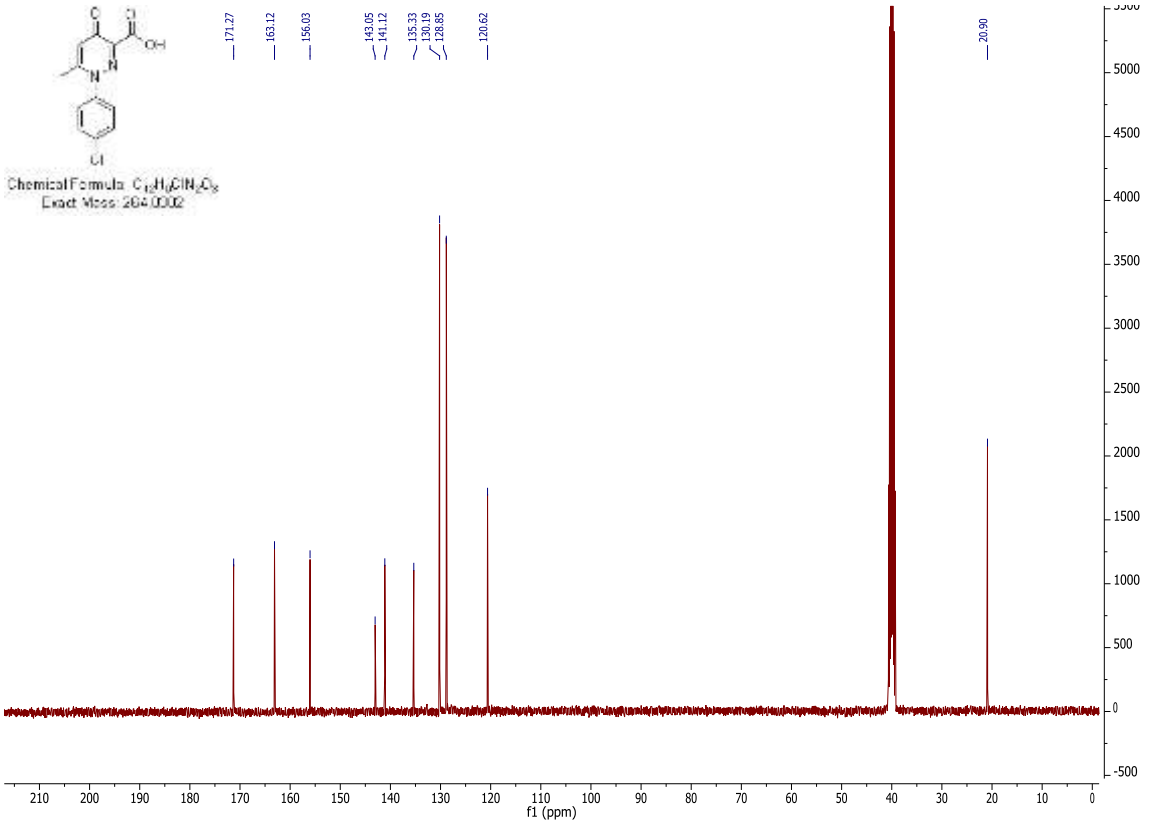
7.69
7.67
7.13
2.25
2.05
2.12
1.00
3.27
f1 (ppm)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163.12
156.03
143.05
141.12
135.33
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128.85
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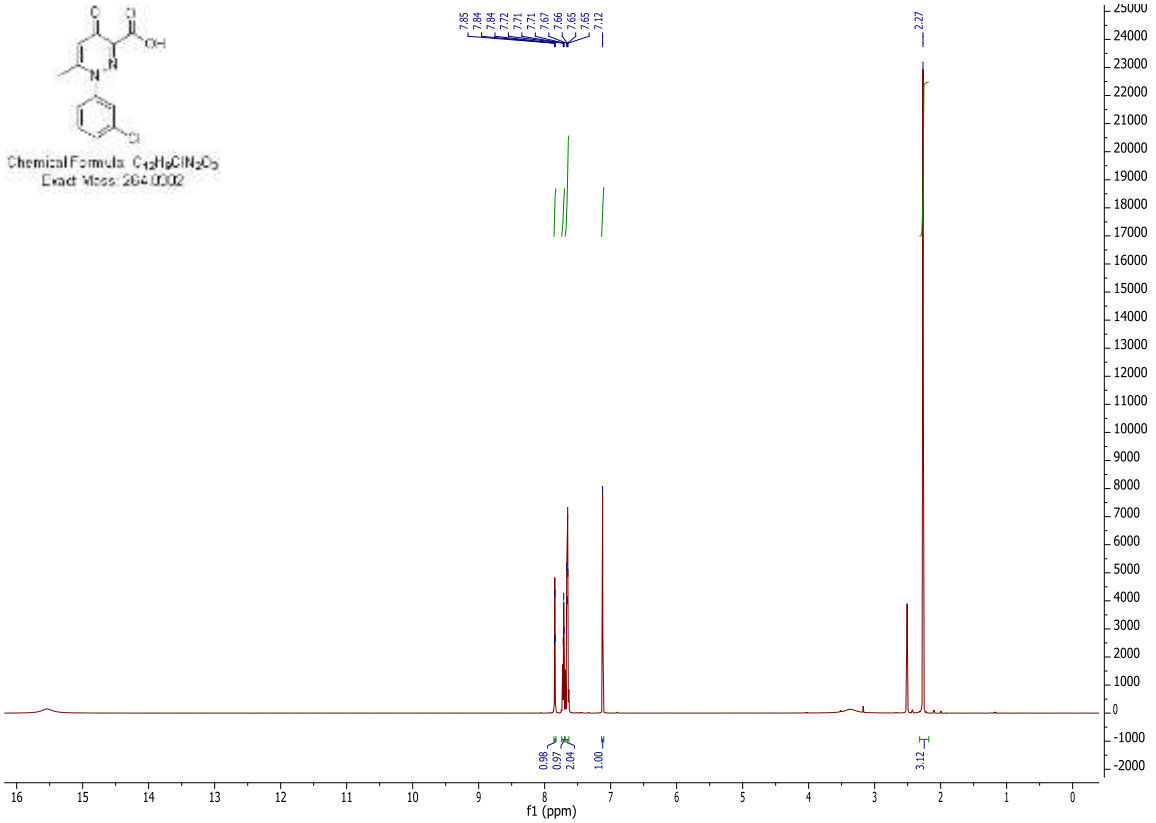
20.90
f1 (ppm)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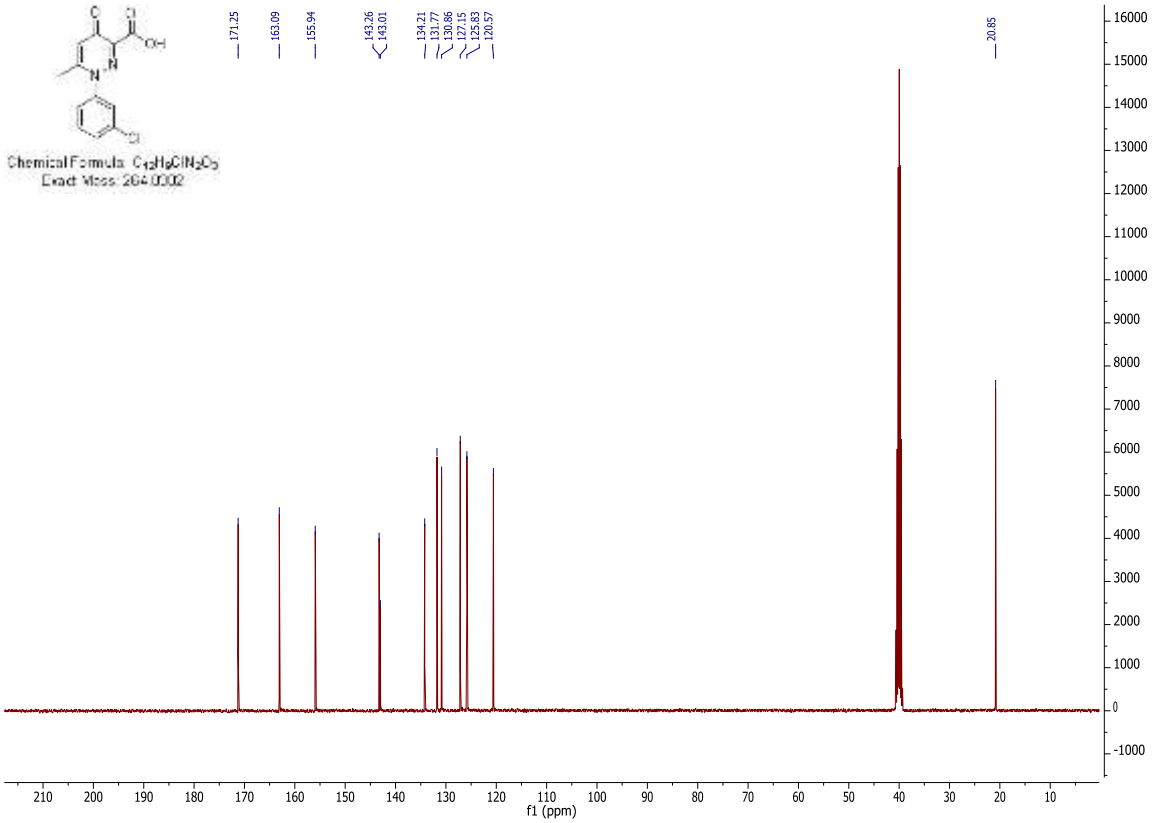
0.98
0.97
2.04
1.00
3.12
f1 (ppm)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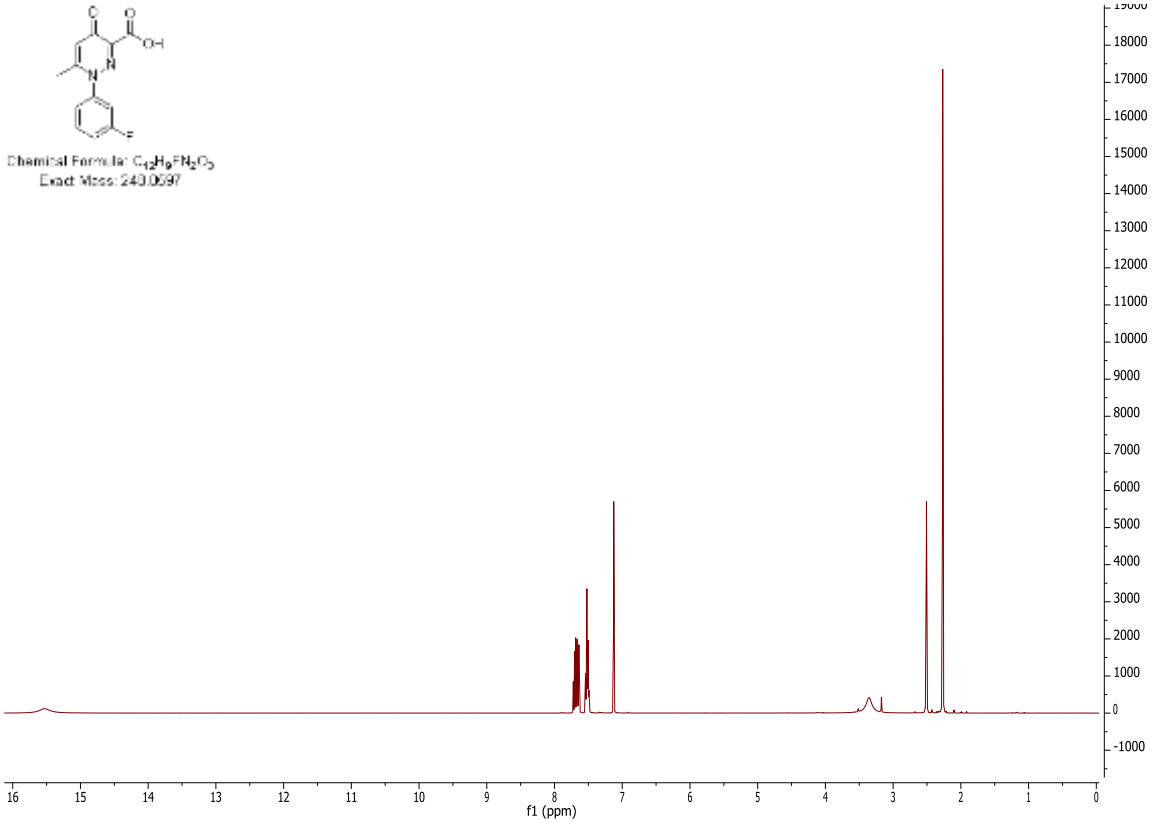
127.15
125.83
120.57
20.85
f1 (ppm)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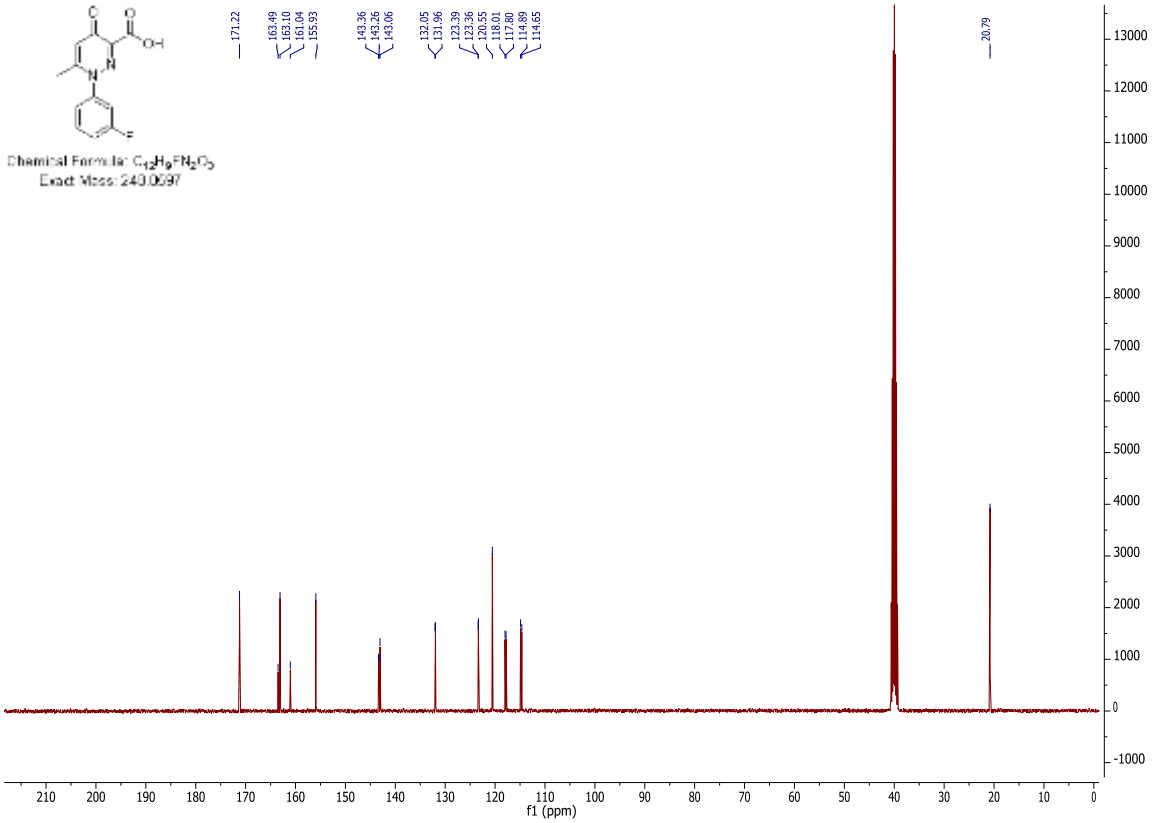
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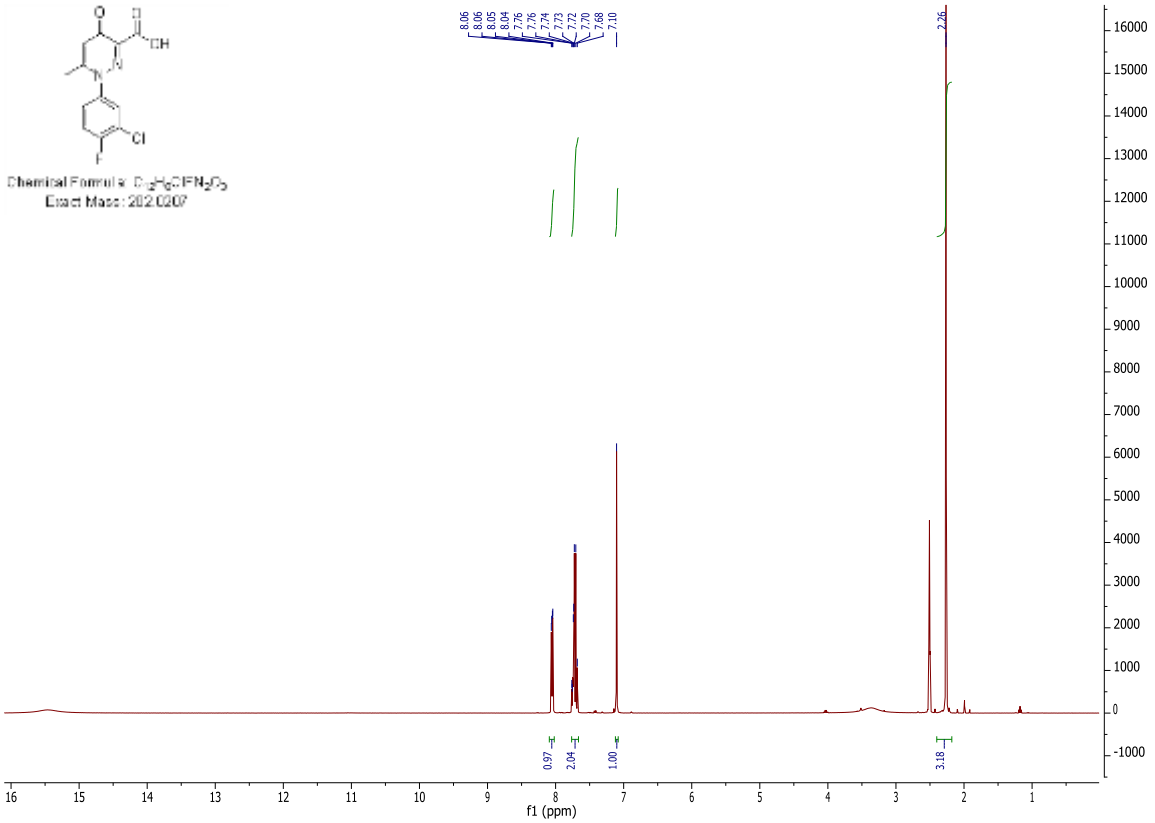
163.49
163.10
161.04
155.93
143.36
143.26
143.06
132.05
131.96
123.39
123.36
120.55
118.01
117.80
114.89
114.65
20.79
Chemical Formula: C12H9FN2O3
Exact Mass: 240.0597
f1 (ppm)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8.06
8.05
8.04
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7.70
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7.10
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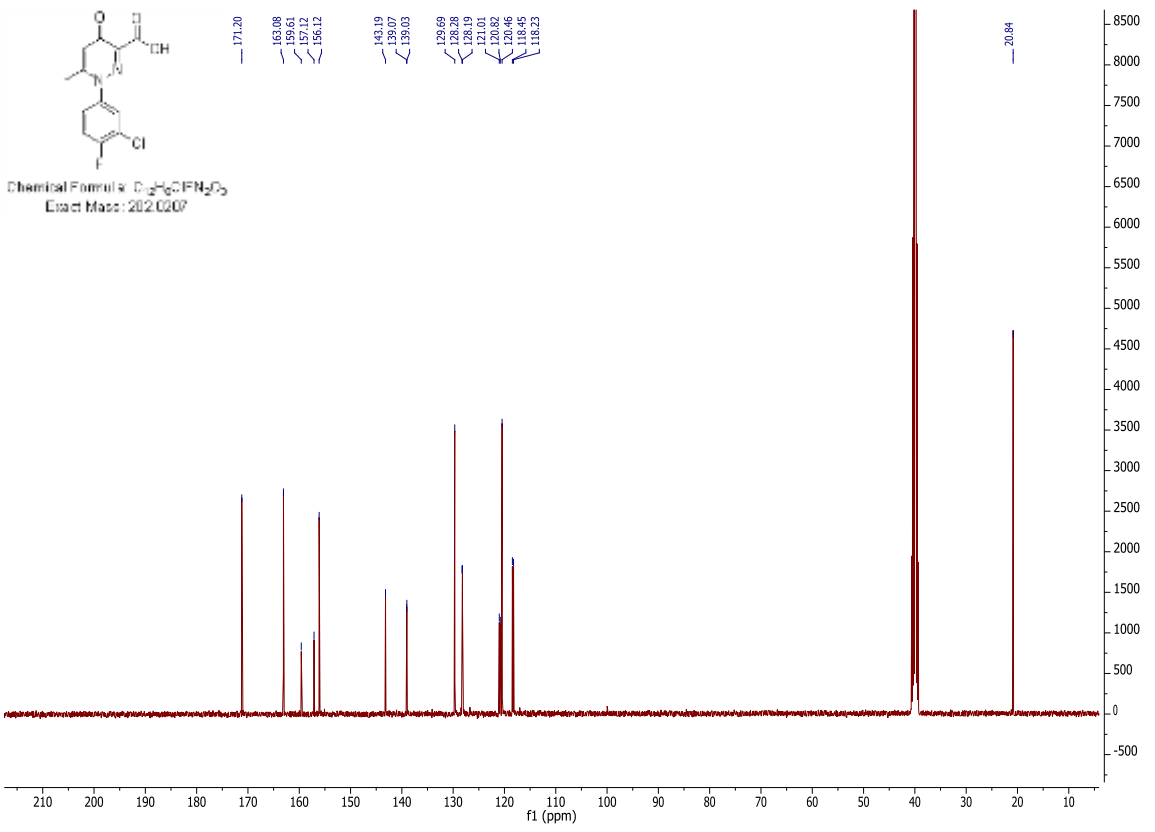
0.97
2.04
1.00
3.18
f1 (ppm)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143.19
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128.28
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121.01
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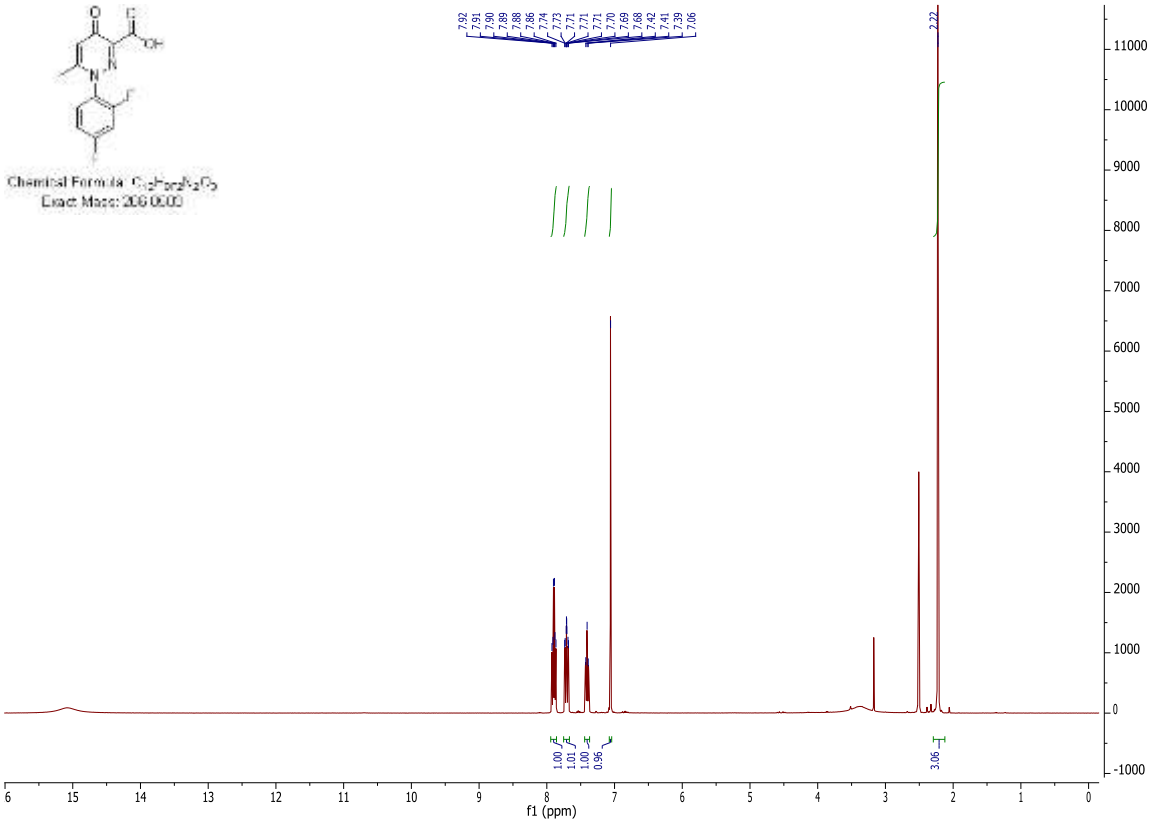
120.46
118.45
118.23
20.84
f1 (ppm)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7.88
7.86
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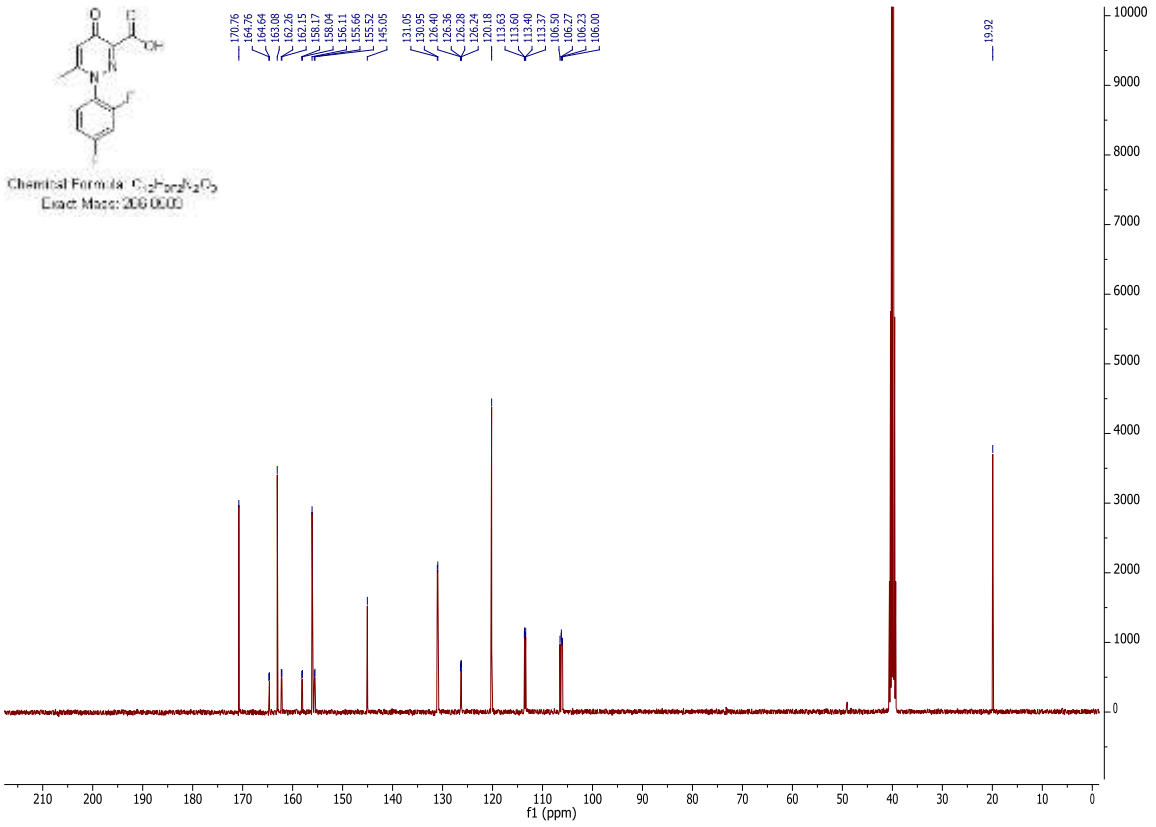
7.73
7.71
7.71
7.71
7.70
7.69
7.68
7.42
7.41
7.39
7.06
2.22
1.00
1.01
1.00
0.98
3.06
f1 (ppm)


Chemical Formula: C12H8F2N2O3
Exact Mass: 266.05
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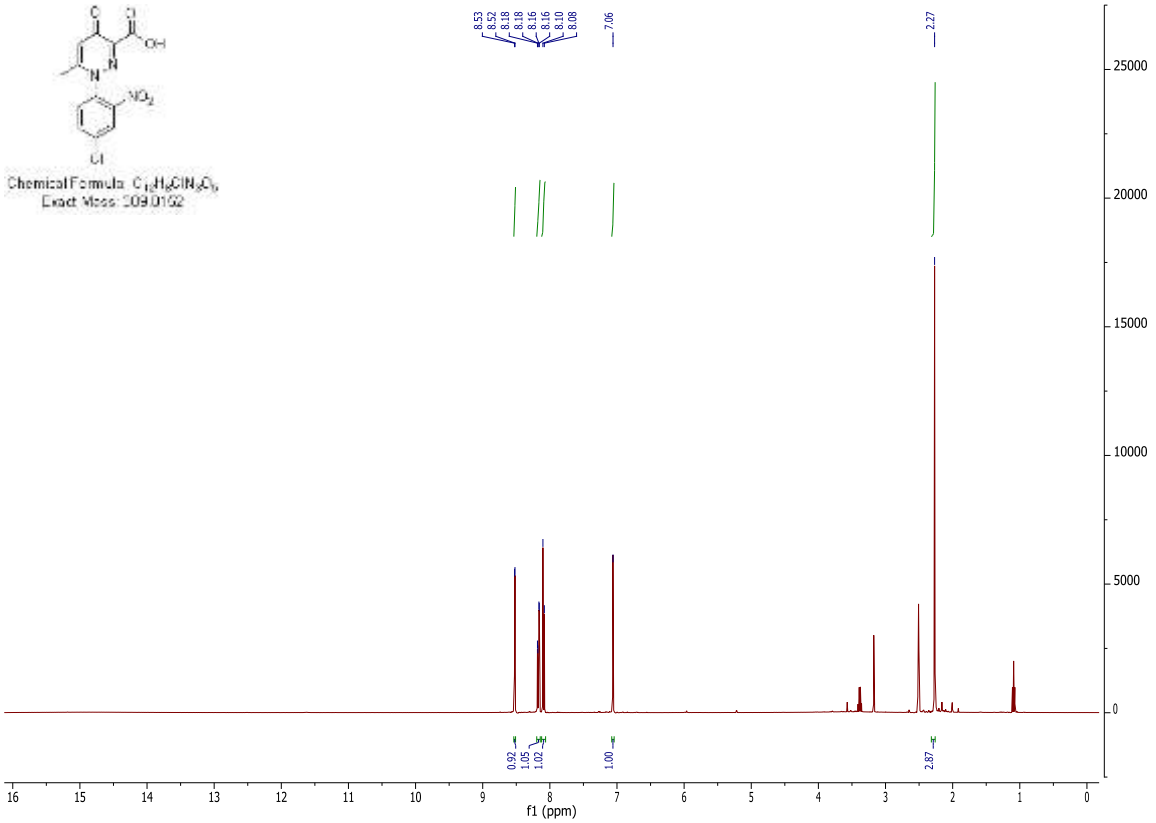
164.76
164.64
163.08
162.26
162.15
158.17
158.04
156.11
155.66
155.52
145.05
131.05
130.95
126.40
126.36
126.28
126.24
120.18
113.63
113.60
113.40
113.37
106.50
106.27
106.23
106.00
19.92
f1 (ppm)


Chemical Formula: C12H8ClN3O5
Exact Mass: 309.0152
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8.52
8.18
8.18
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8.16
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8.08
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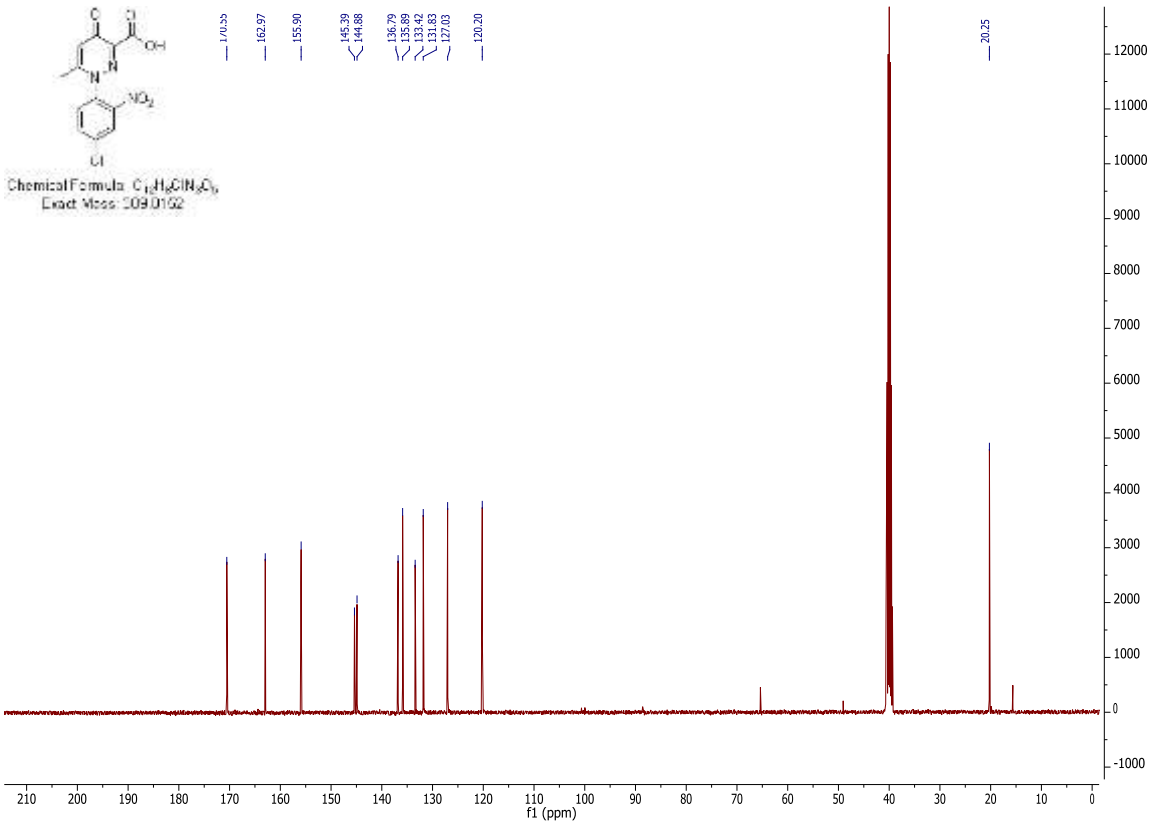
2.27
0.92
1.05
1.02
1.00
2.87
f1 (ppm)


Chemical Formula: C12H8ClN3O5
Exact Mass: 309.0152
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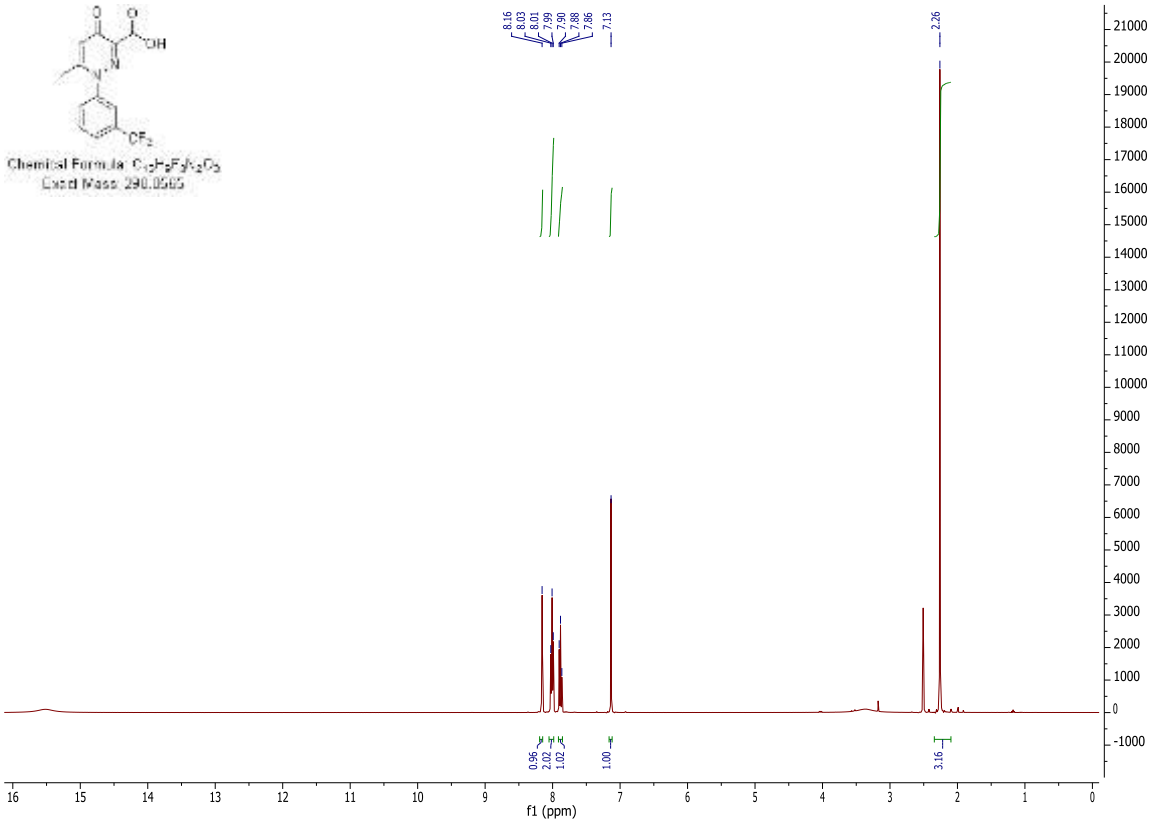
133.42
131.83
127.03
120.20
20.25
f1 (ppm)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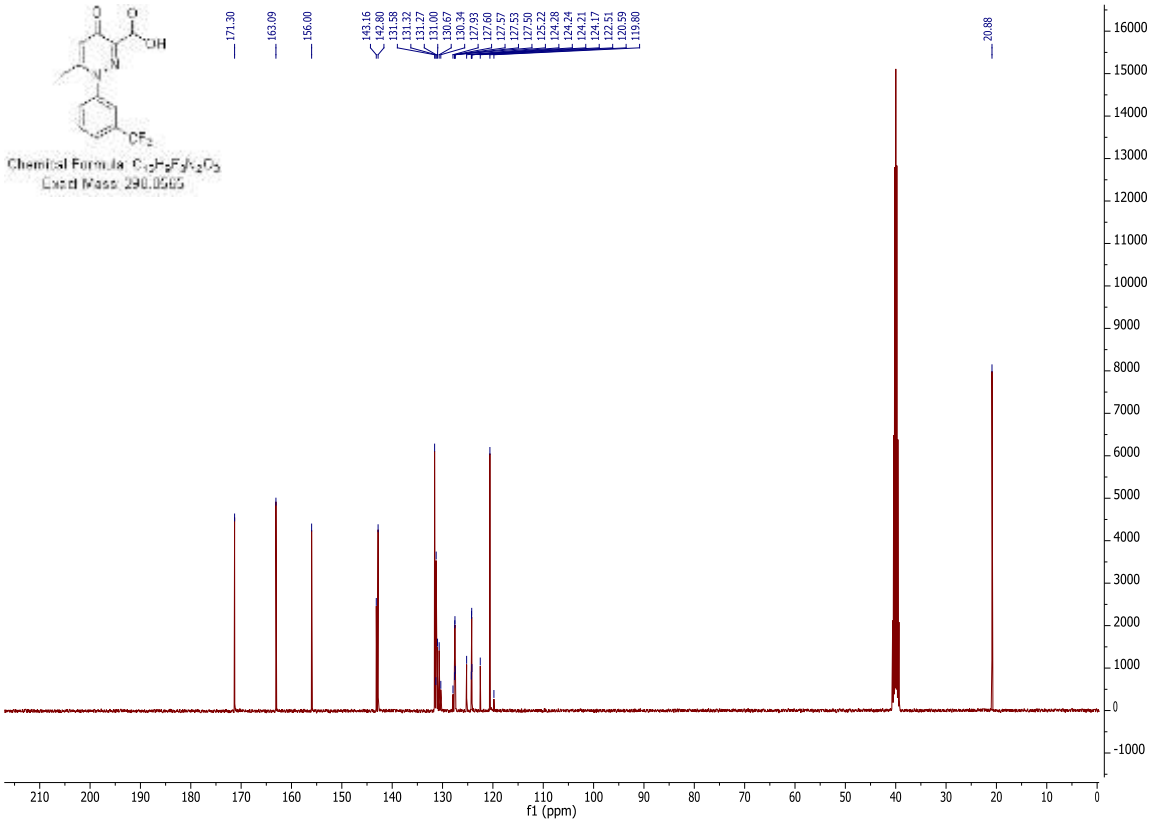
0.96
2.02
1.02
1.00
3.16
f1 (ppm)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131.27
131.00
130.67
130.34
127.93
127.60
127.57
127.53
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124.28
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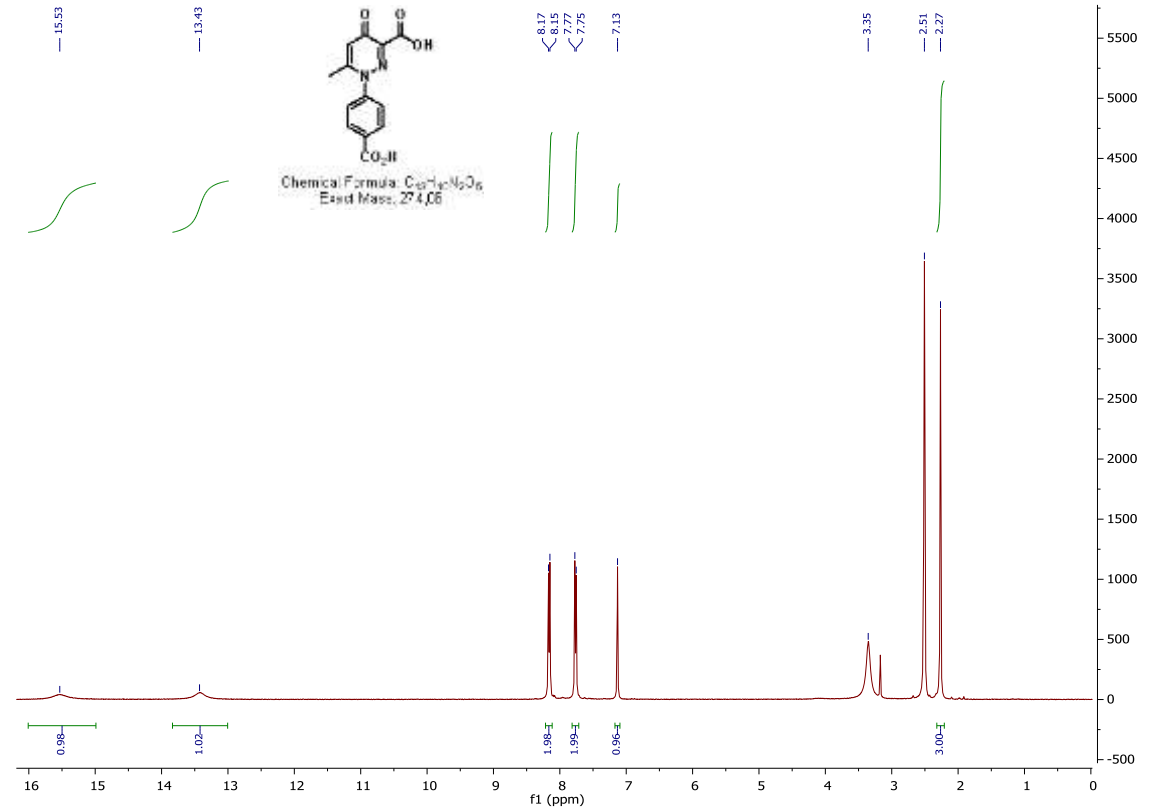
124.21
124.17
123.51
120.59
119.80
20.88
f1 (ppm)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8.17
8.15
7.77
7.75
7.13
3.35
2.51
2.27
Chemical Formula: C13H10N2O5
Exact Mass: 274.06
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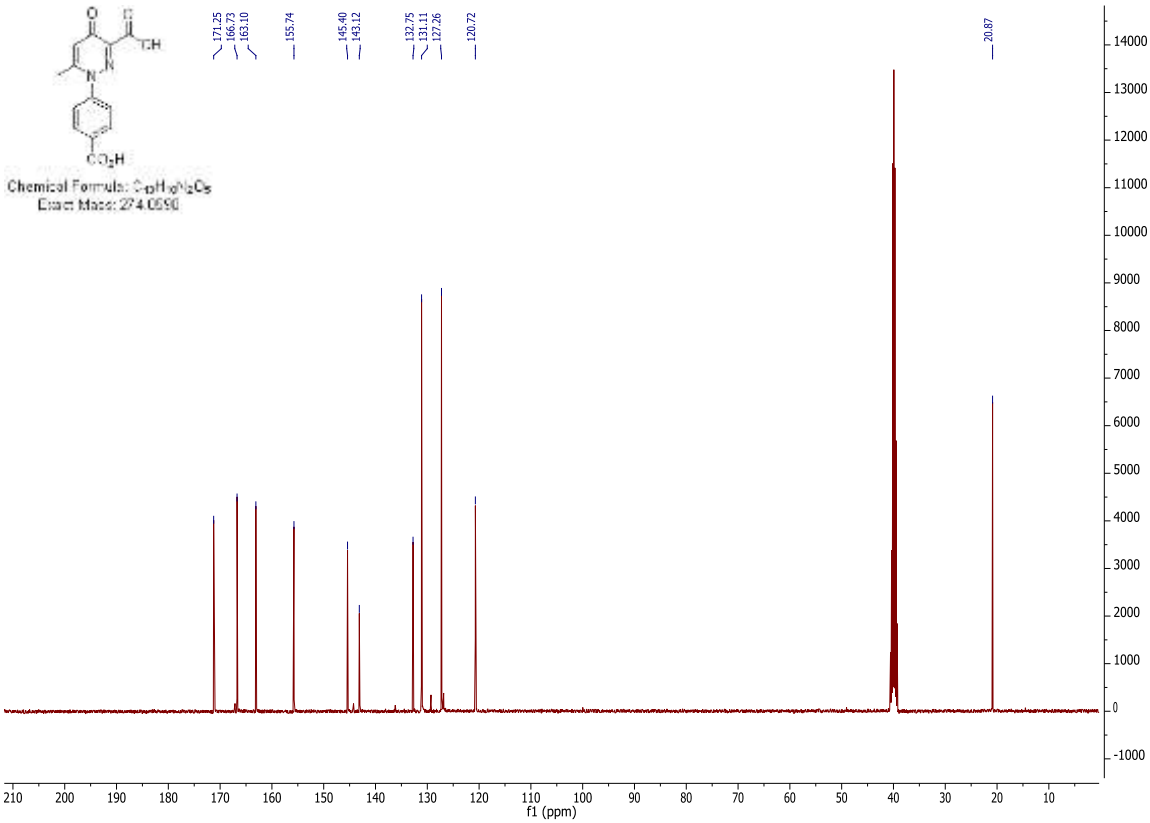
1.02
1.98
1.99
0.96
3.00
f1 (ppm)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166.73
163.10
155.74
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143.12
132.75
131.11
127.26
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20.87
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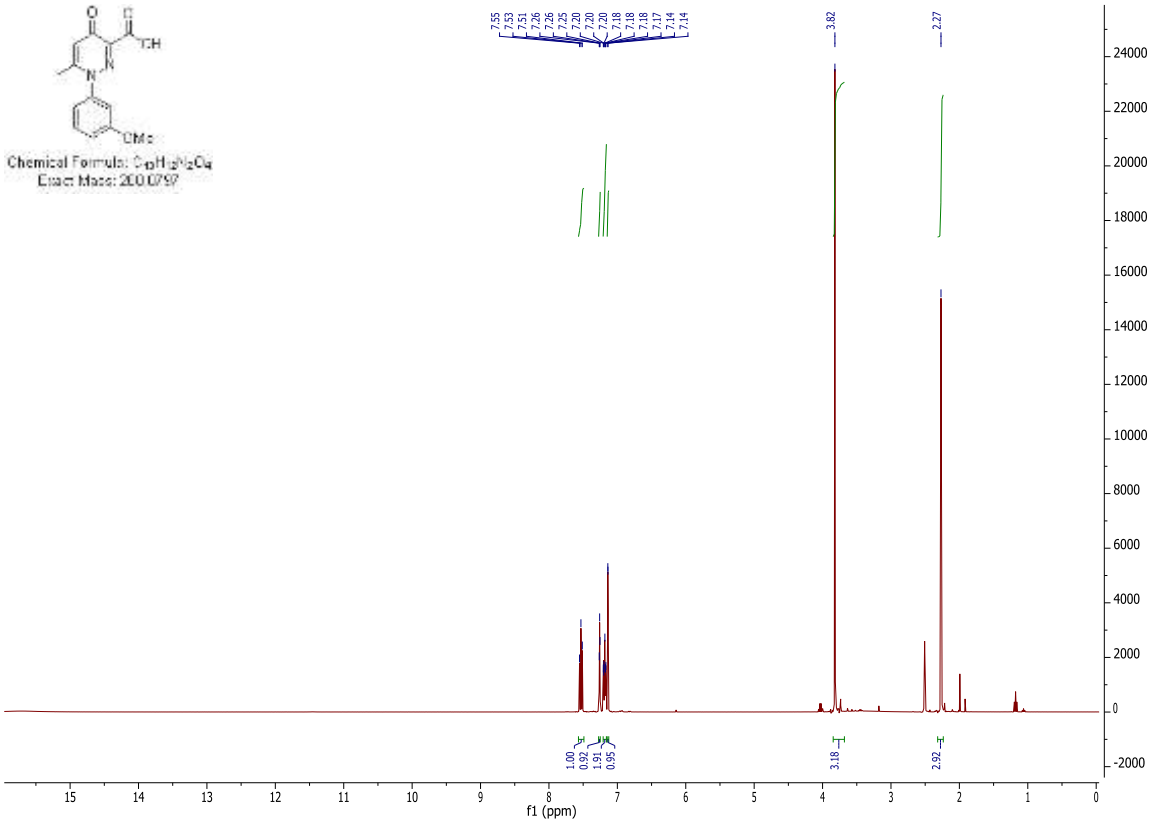
f1 (ppm)


Chemical Formula: C13H12N2O4
Exact Mass: 260.0797
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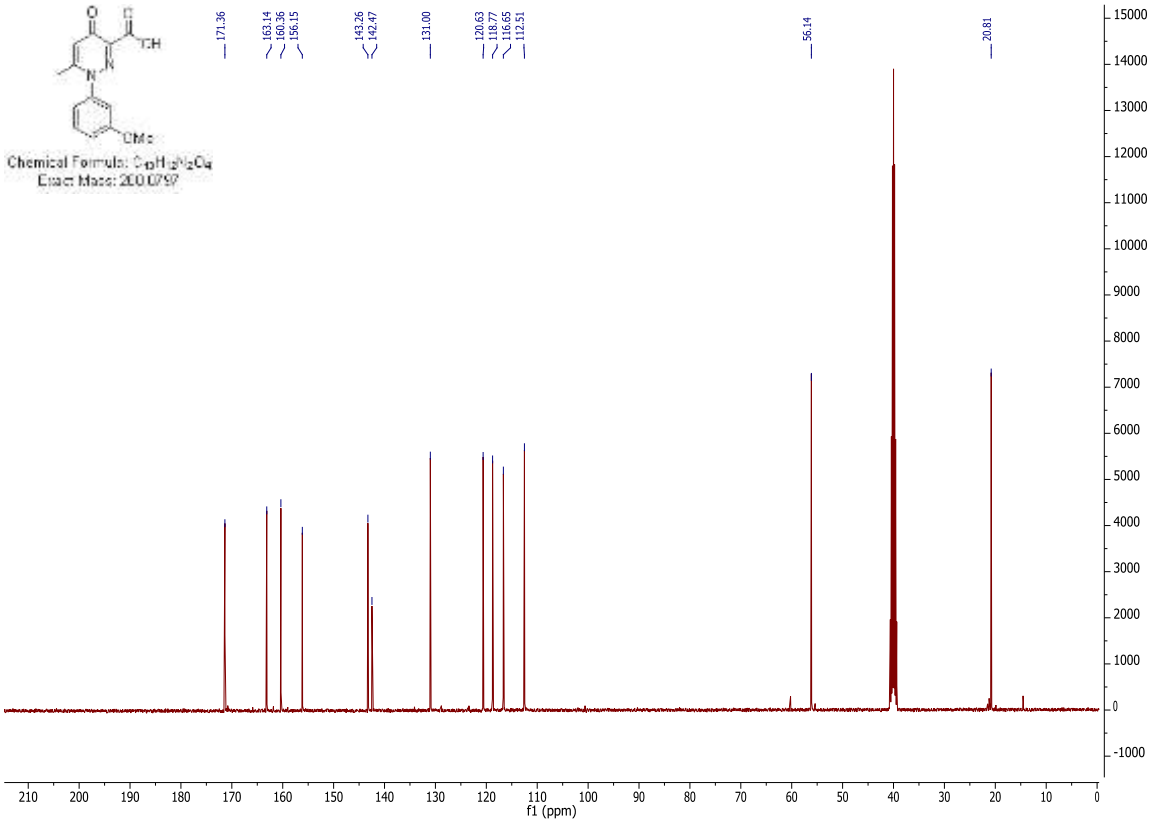
7.53
7.51
7.26
7.26
7.25
7.20
7.20
7.20
7.18
7.18
7.18
7.17
7.14
7.14
3.82
2.27
1.00
0.92
1.91
0.95
3.18
2.92
f1 (ppm)


Chemical Formula: C13H12N2O4
Exact Mass: 260.0797
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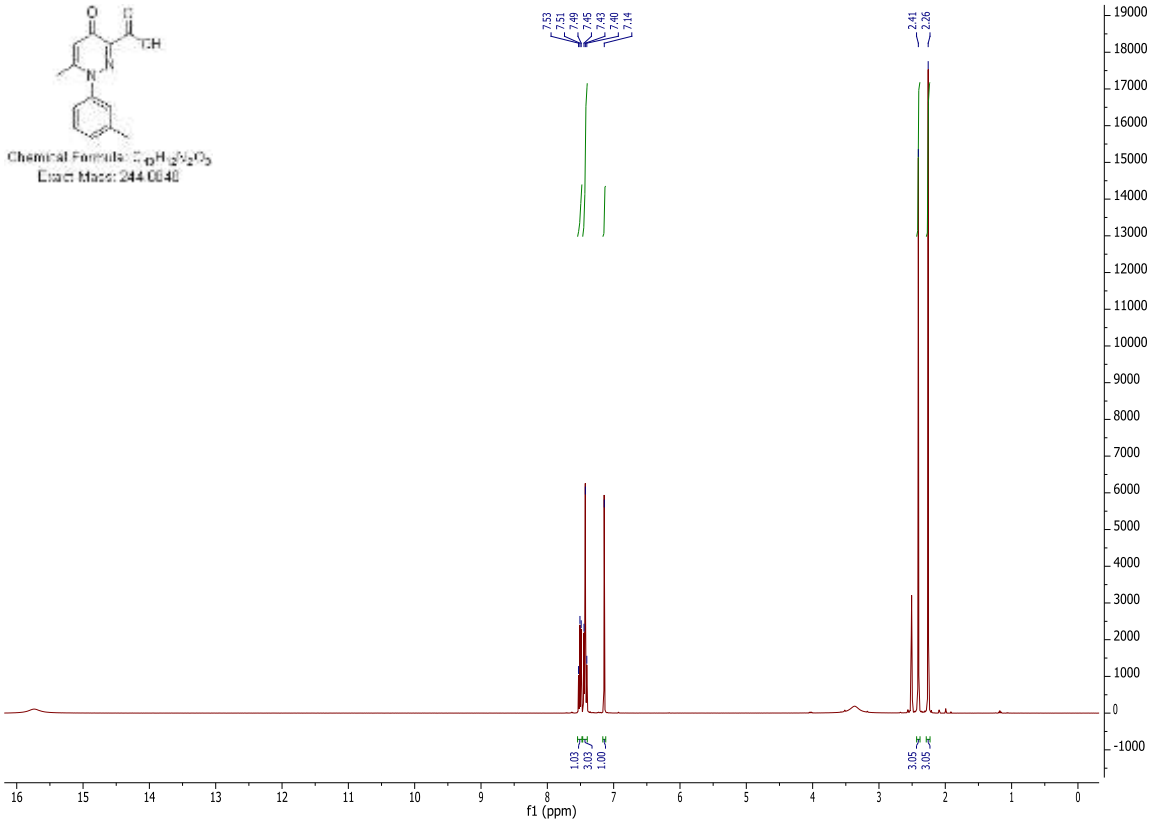
112.51
56.14
20.81
f1 (ppm)


Chemical Formula: C12H12N2O3
Exact Mass: 244.0848
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7.45
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7.14
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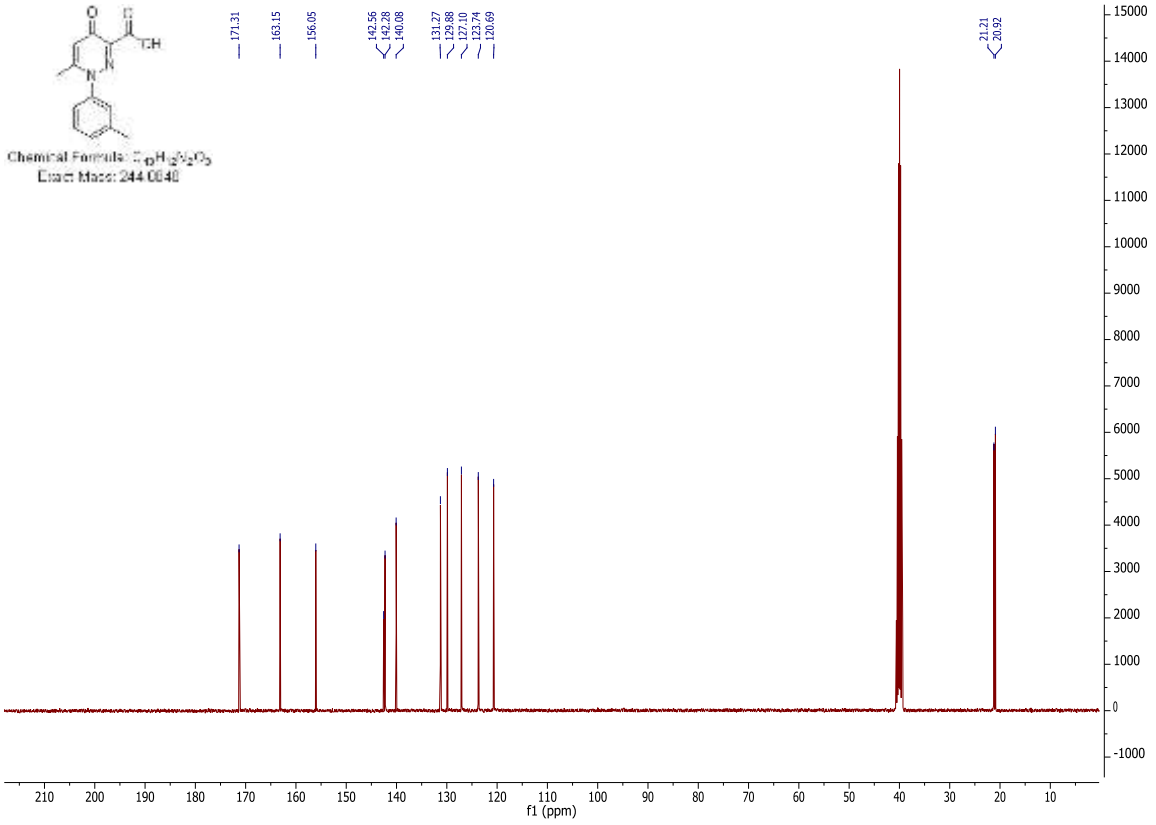
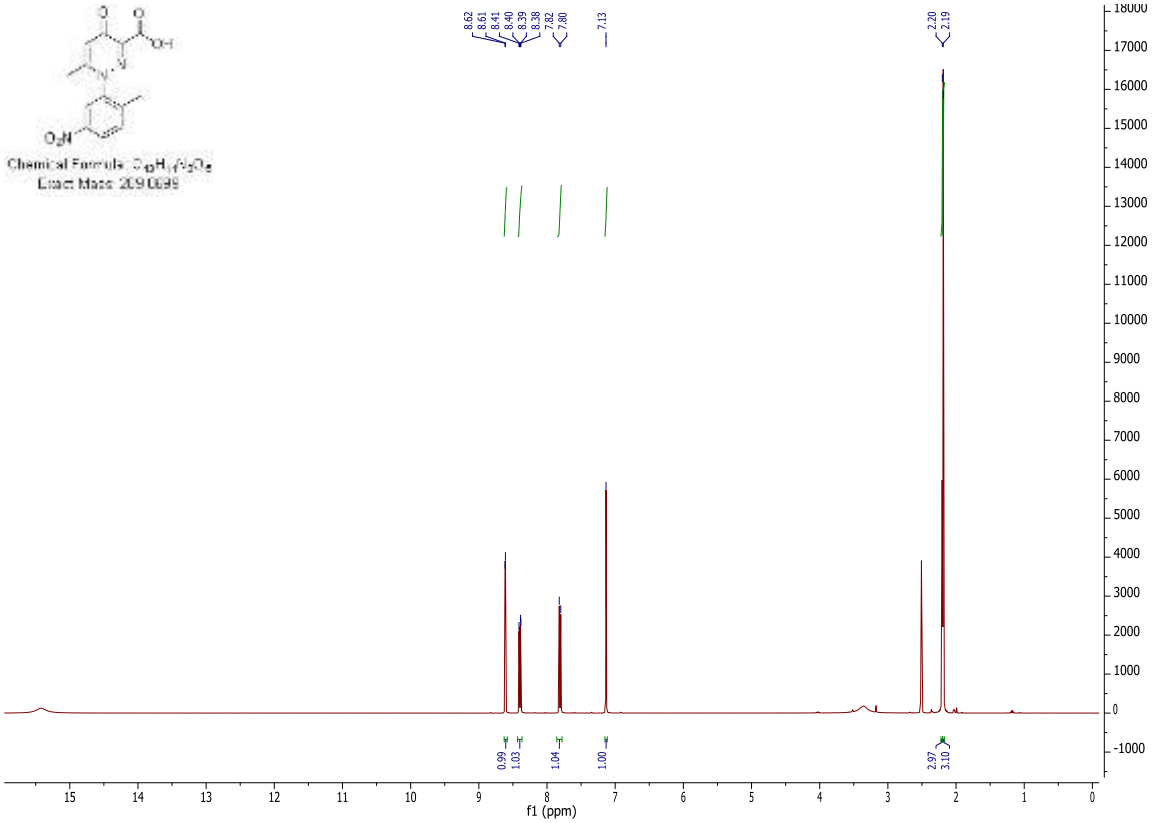
3.03
1.00
3.05
3.05
f1 (ppm)


Chemical Formula: C12H12N2O3
Exact Mass: 244.0848
171.31
163.15
156.05
142.56
142.28
140.08
131.27
129.88
127.10
123.74
120.69
21.21
20.92
f1 (ppm)


8.62
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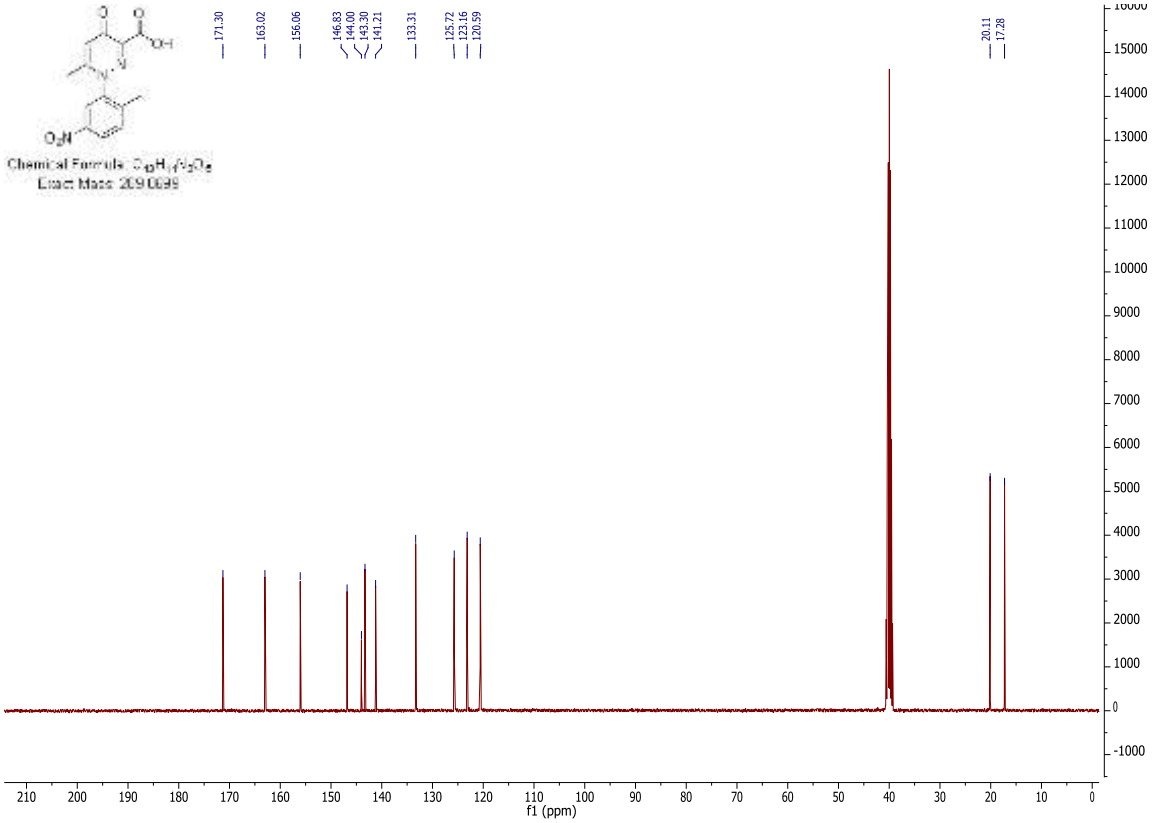
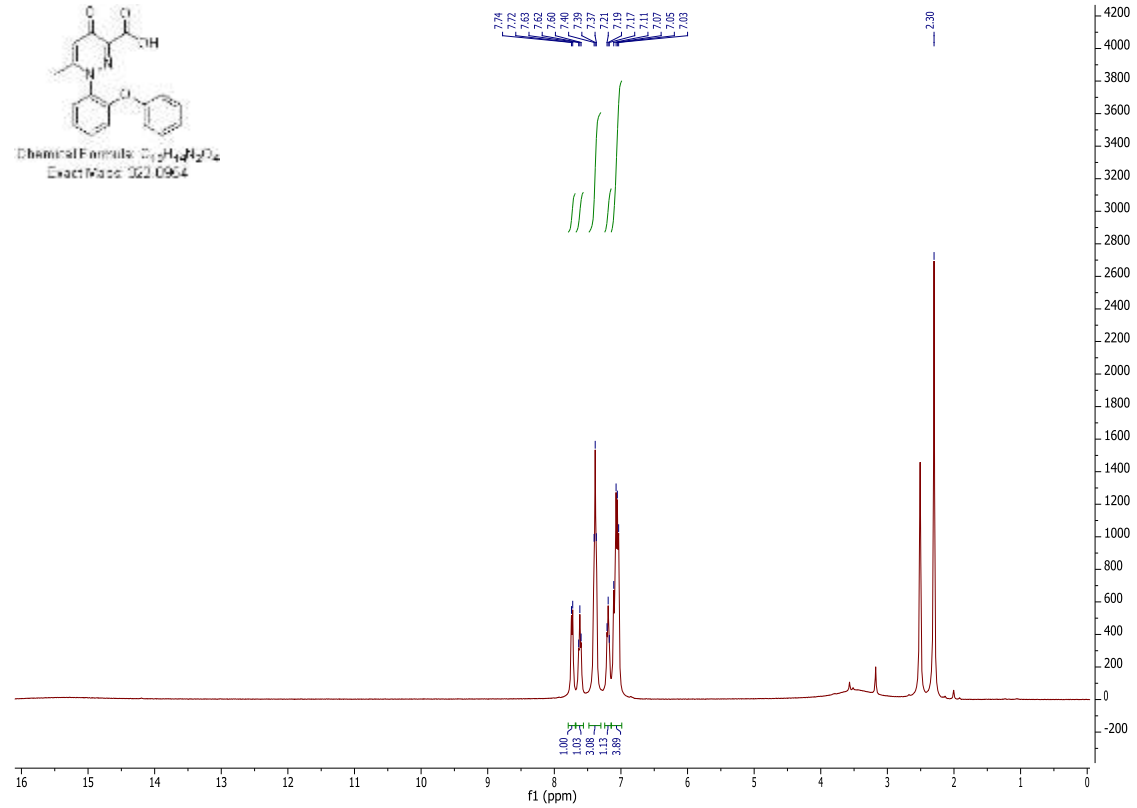
8.41
8.40
8.39
8.38
7.82
7.80
7.13
2.20
2.19
0.99
1.03
1.04
1.00
2.97
3.10
f1 (ppm)


171.30
163.02
156.06
146.83
144.00
143.30
141.21
133.31
125.72
123.16
120.59
20.11
17.28
f1 (ppm)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7.19
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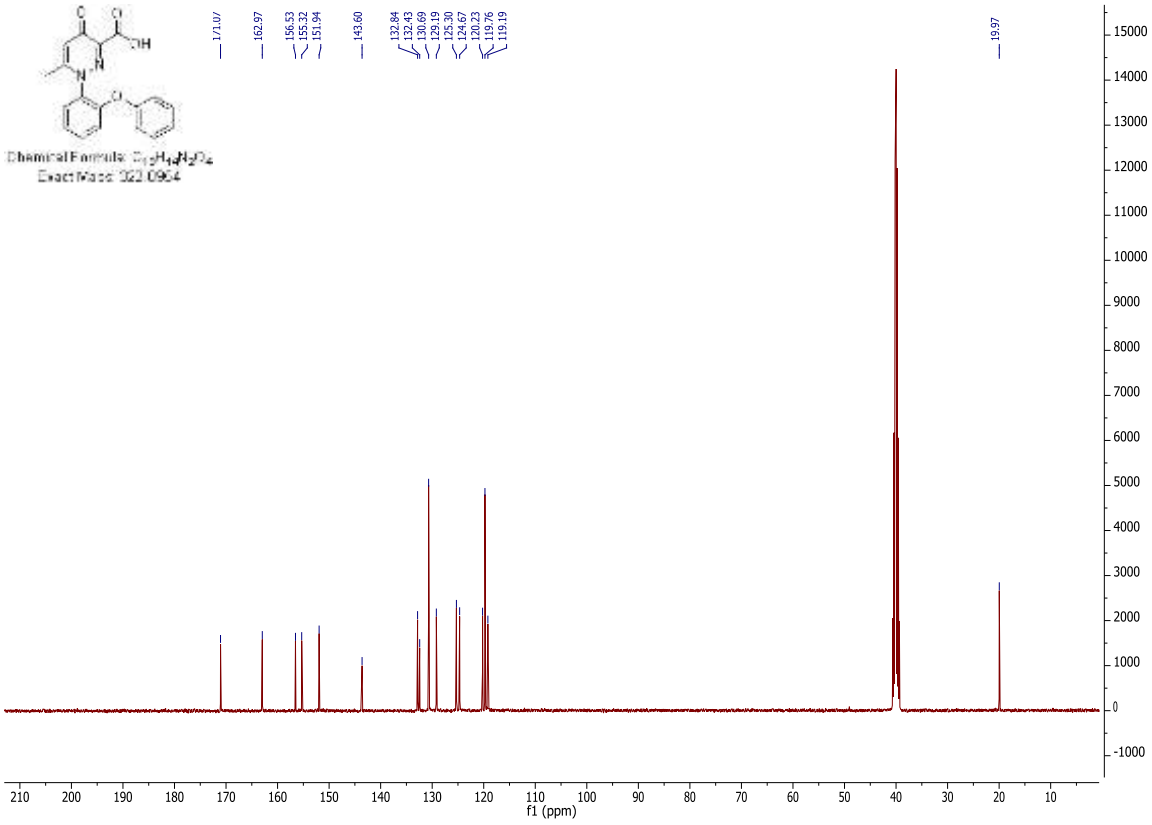
7.05
7.03
2.30
1.00
1.03
3.08
1.13
3.89
f1 (ppm)


Chemical Formula: C16H14N2O4
Exact Mass: 322.0954
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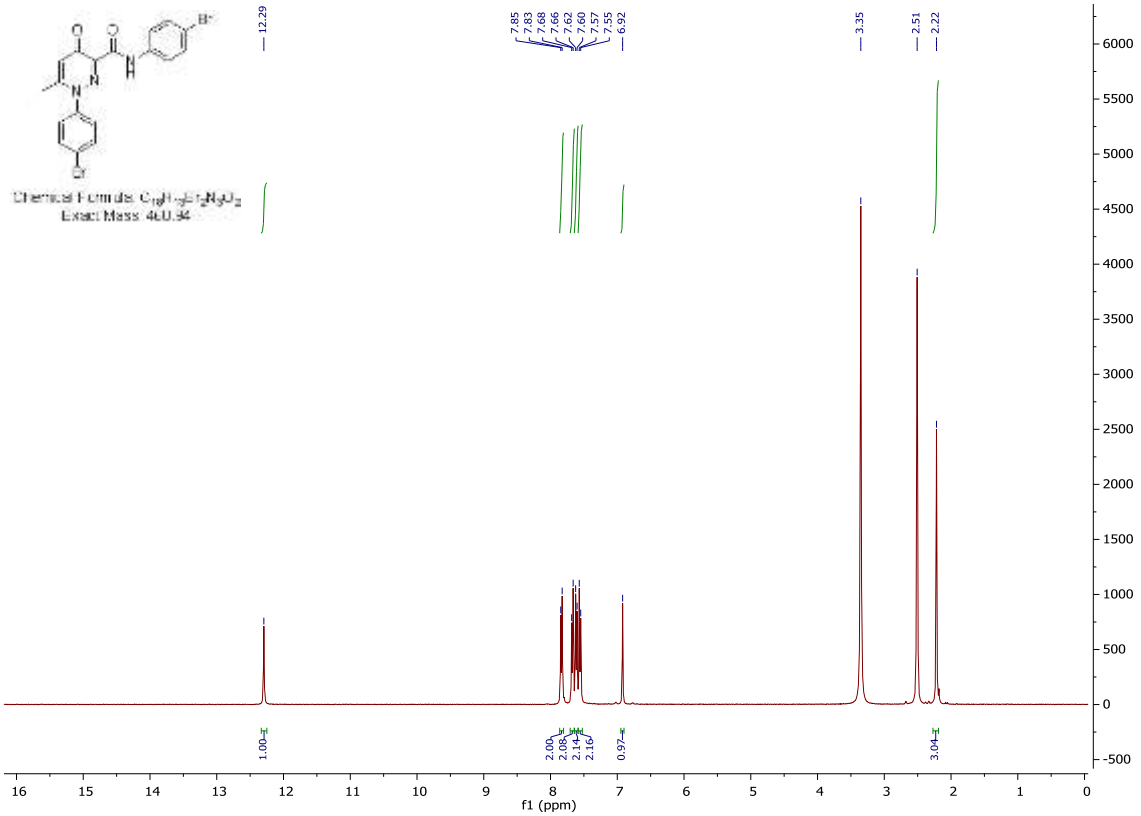
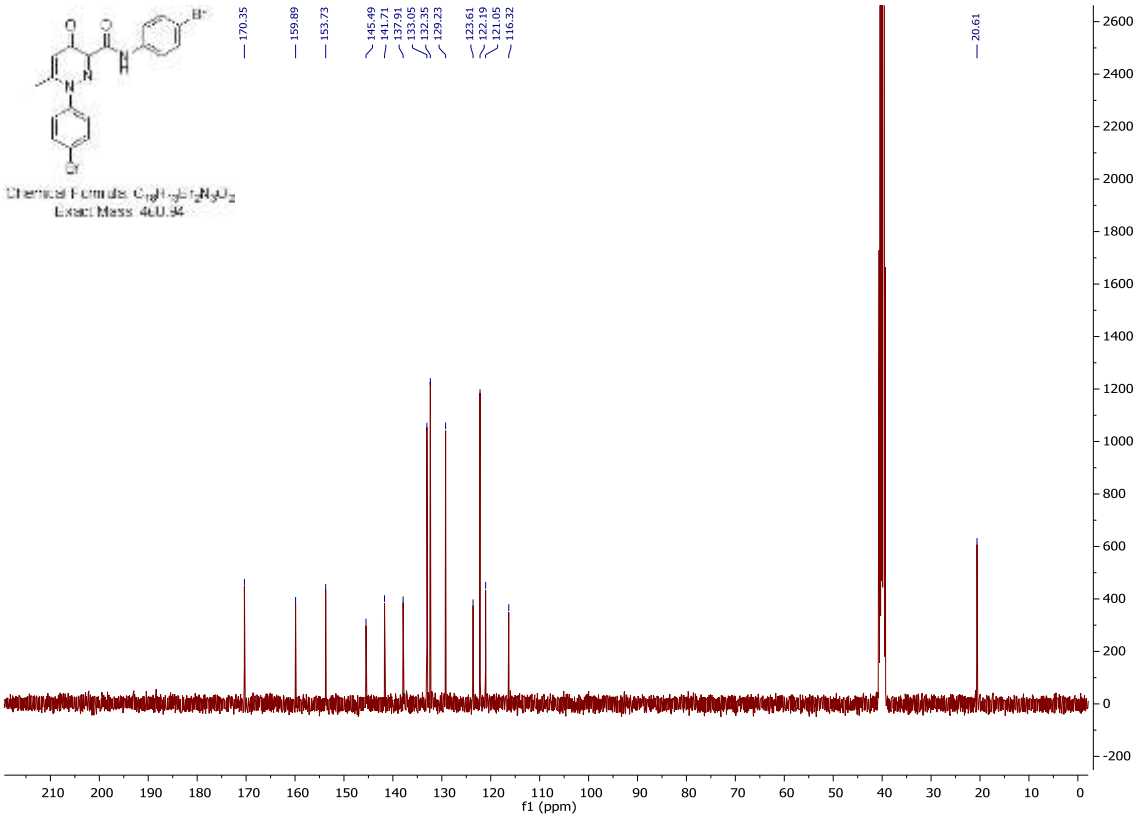
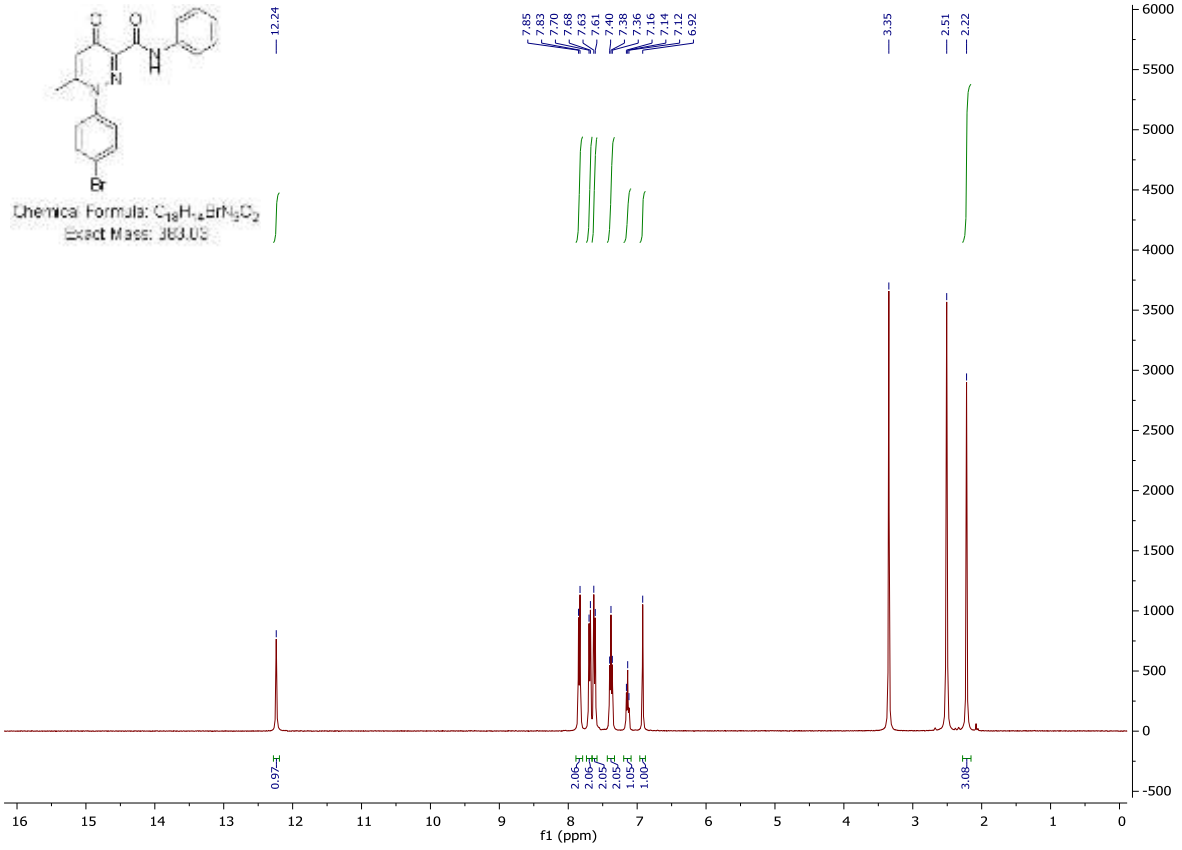
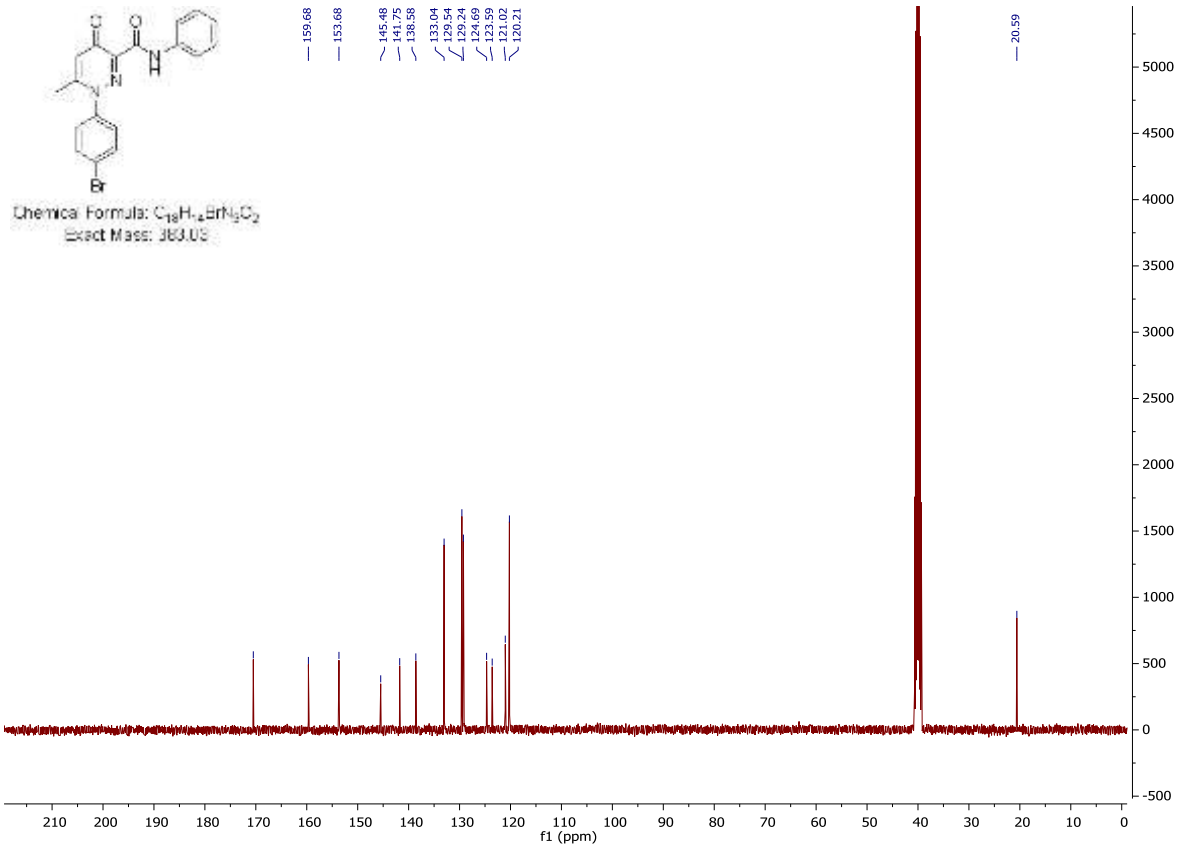
162.97
156.53
155.32
151.94
143.60
132.84
132.43
130.69
129.19
125.30
124.67
120.23
119.76
119.19
19.97
f1 (ppm)

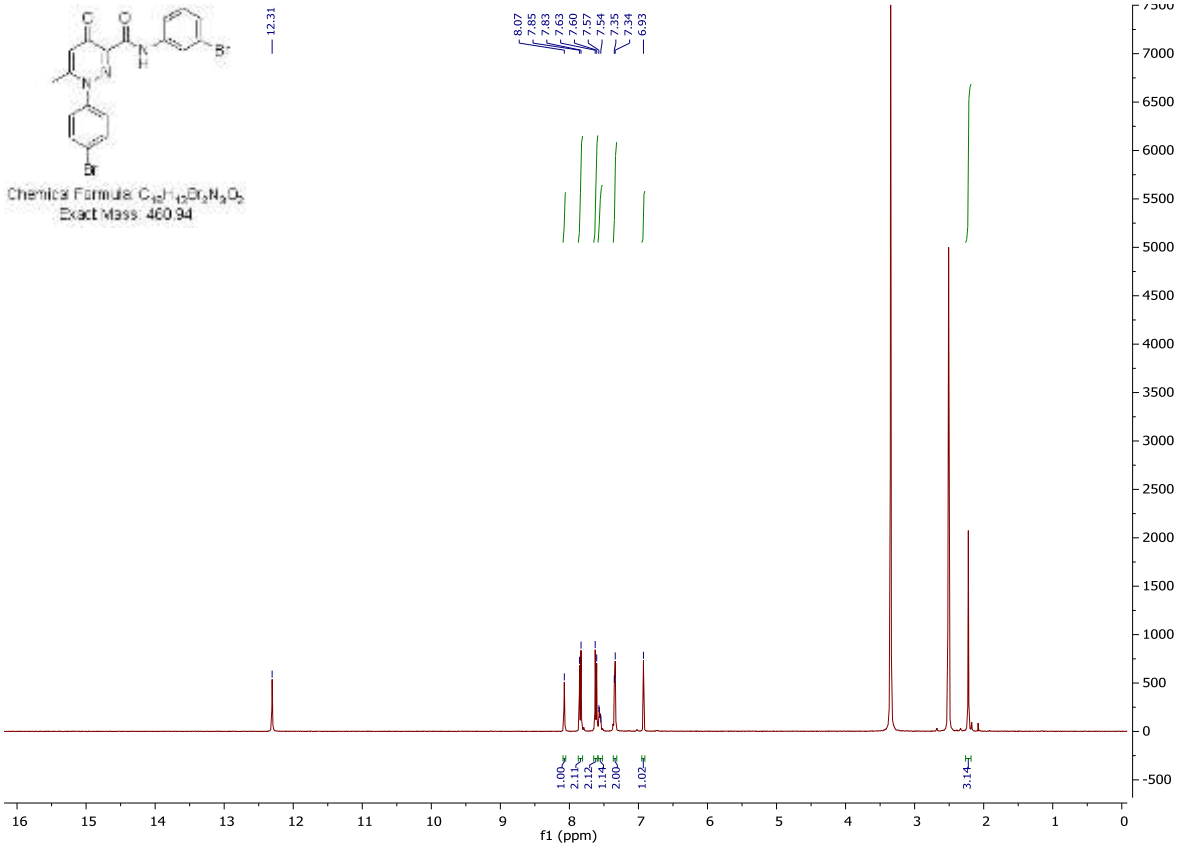
A3. Serie B derivatives 15-23

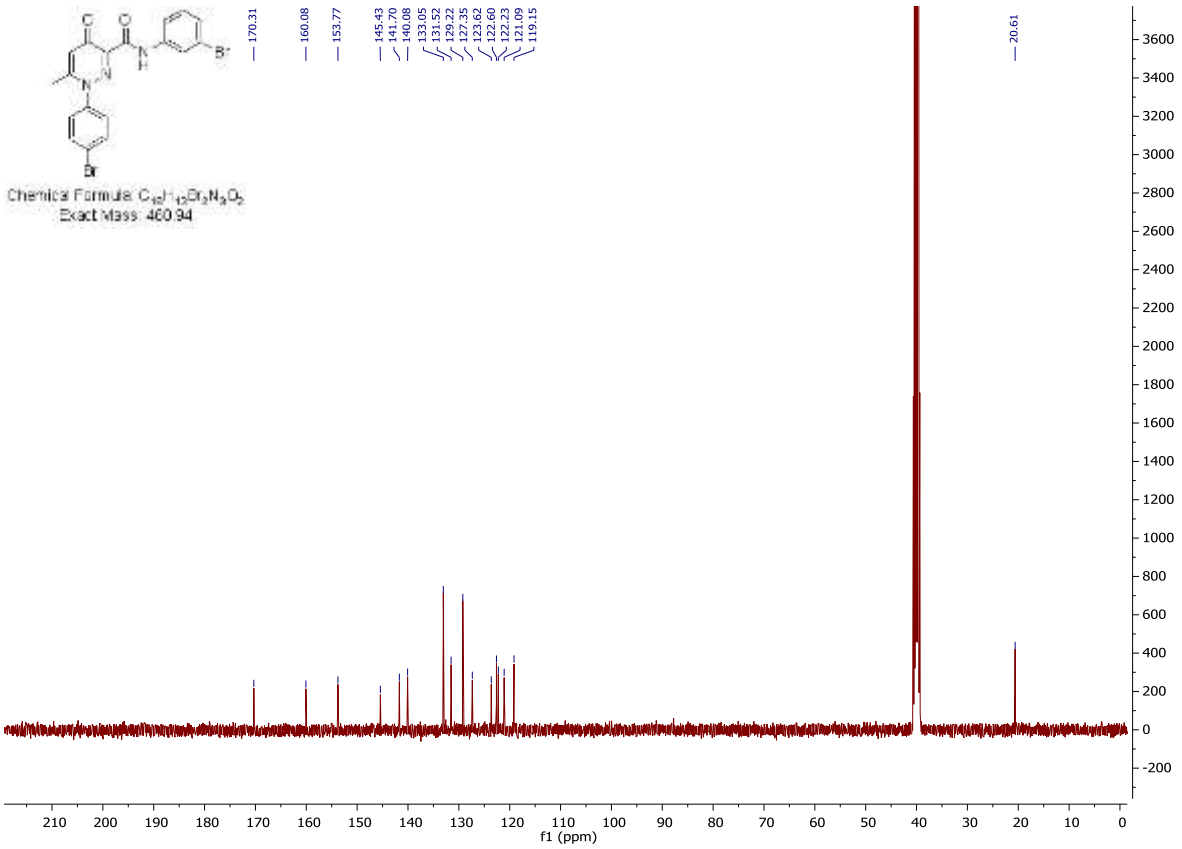


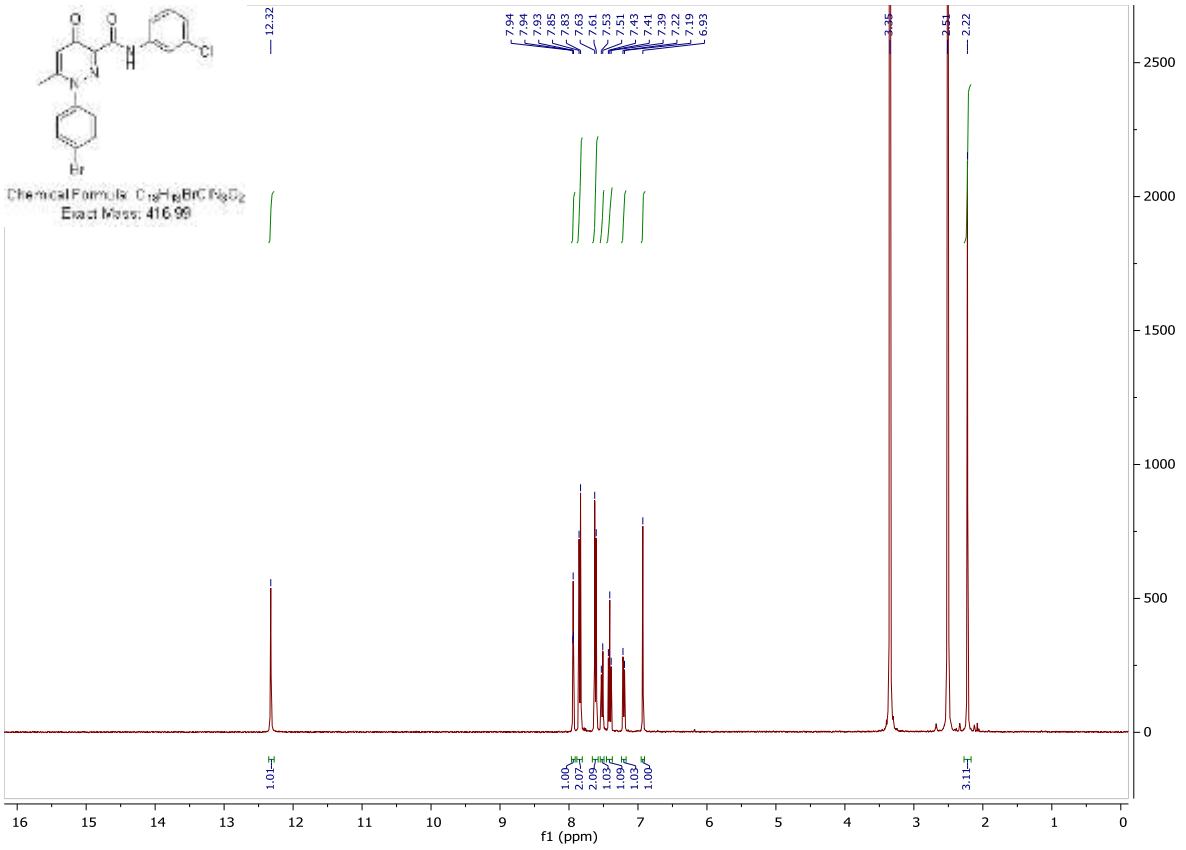


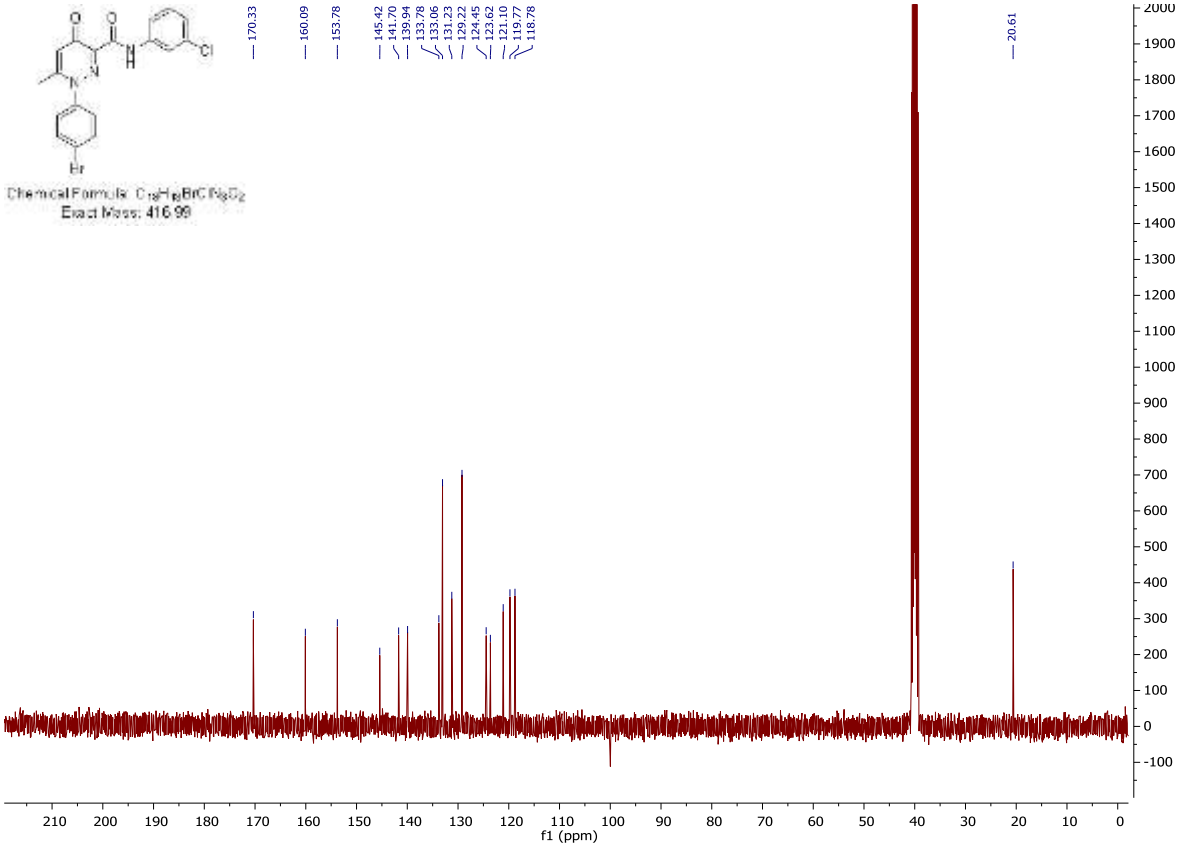

Chemical Formula: C18H14BrN3O2
Exact Mass: 383.03
12.24
7.85
7.83
7.70
7.68
7.63
7.61
7.40
7.38
7.36
7.16
7.14
7.12
6.92
3.35
2.51
2.22
0.97
2.06
2.06
2.05
2.05
1.05
1.00
3.08
f1 (ppm)

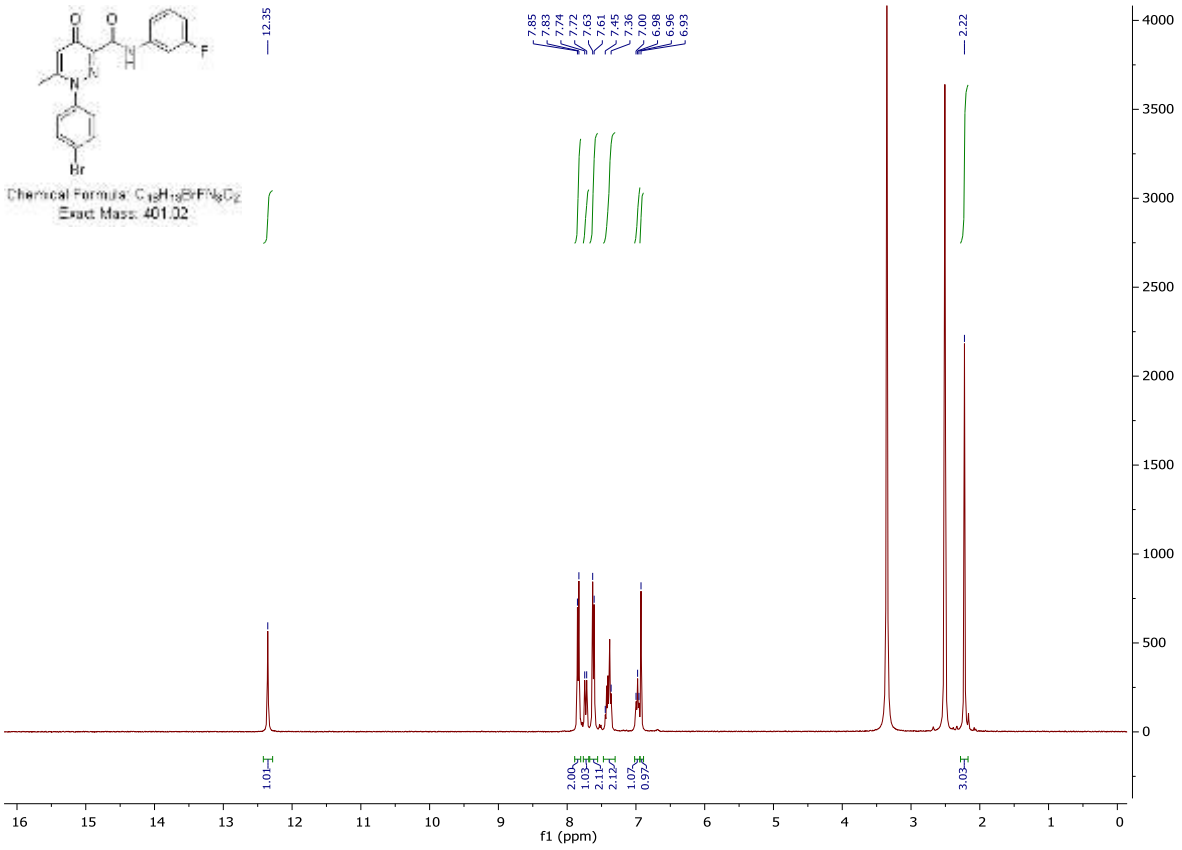

Chemical Formula: C18H14BrN3O2
Exact Mass: 383.03
159.68
153.68
145.48
141.75
138.58
133.04
129.54
129.24
124.69
123.59
121.02
120.21
20.59
f1 (ppm)

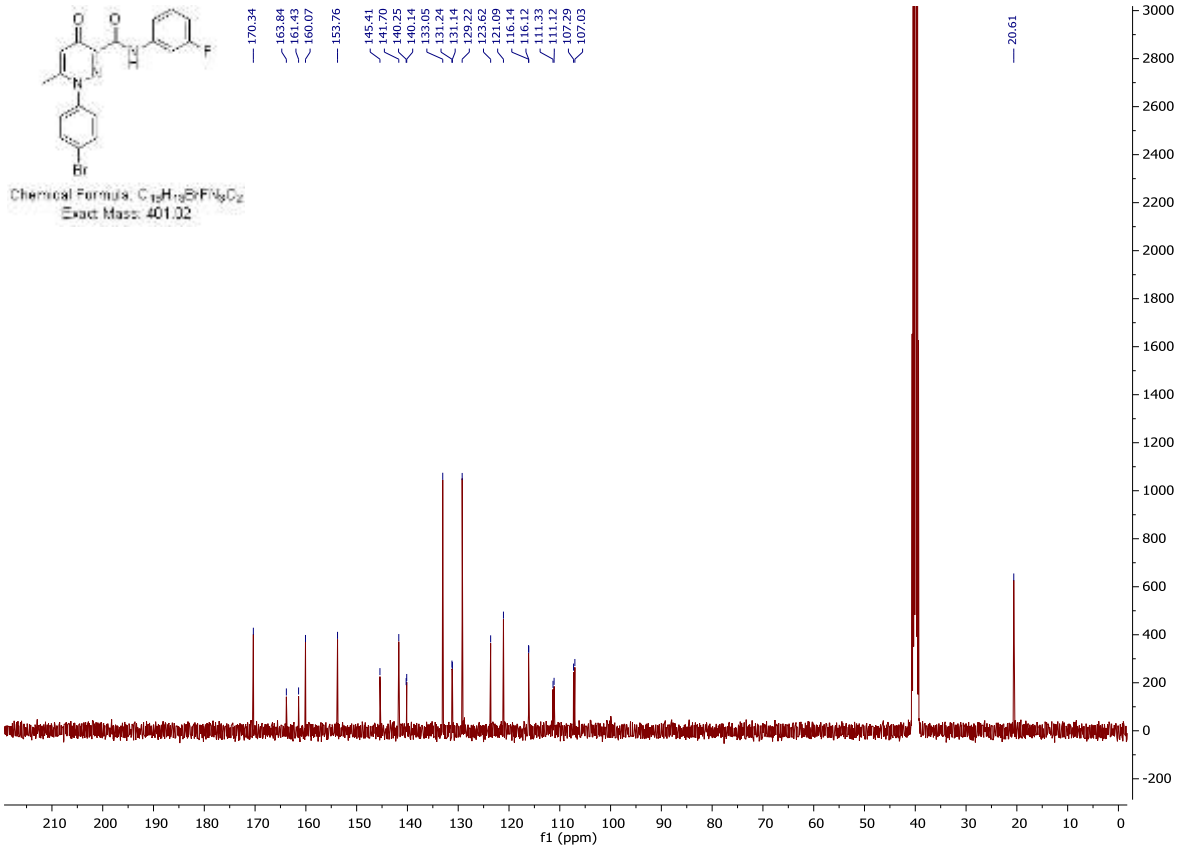

Chemical Formula: C12H10Br2N2O2
Exact Mass: 460.94
12.31
8.07
7.85
7.83
7.63
7.60
7.57
7.54
7.35
7.34
6.93
1.00
2.11
2.12
1.14
2.00
1.02
3.14
f1 (ppm)

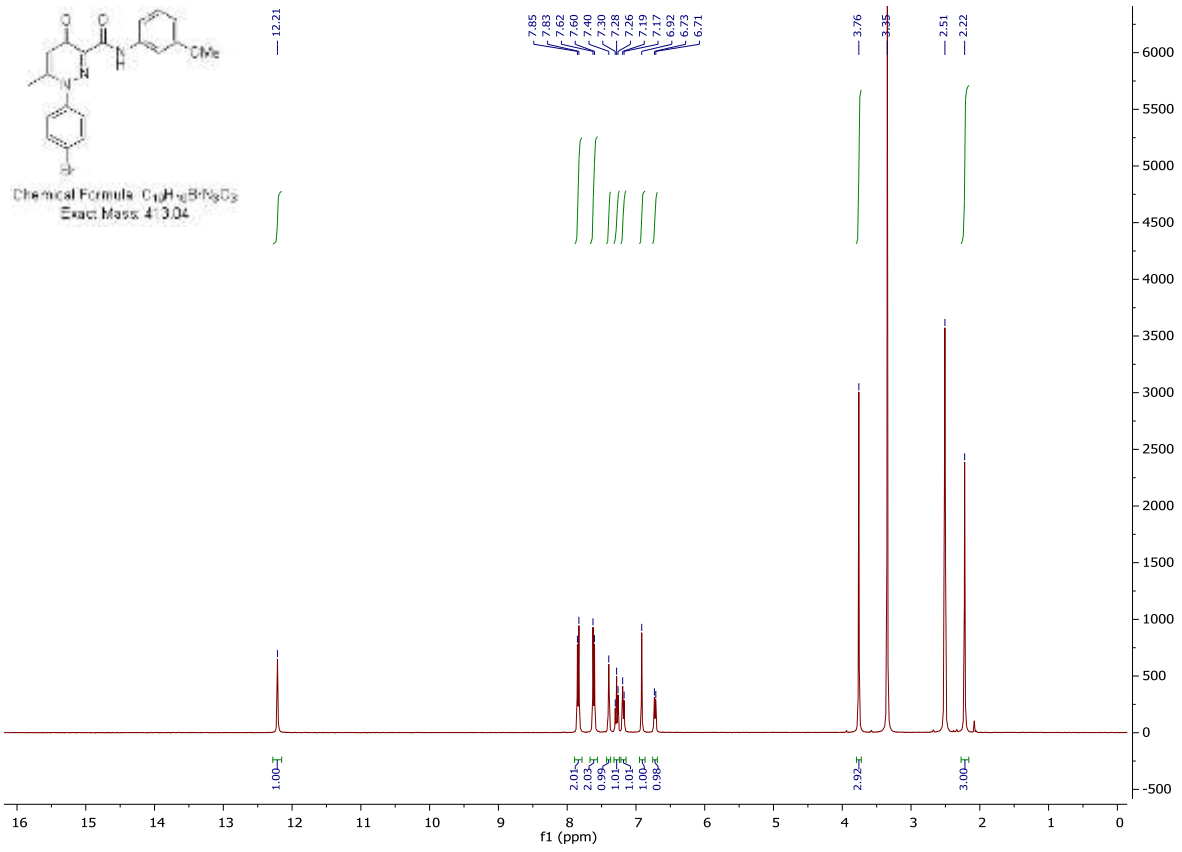

Chemical Formula: C12H10Br2N2O2
Exact Mass: 460.94
170.31
160.08
153.77
145.43
141.70
140.08
133.05
131.52
129.22
127.35
123.62
122.60
122.23
121.09
119.15
20.61
f1 (ppm)

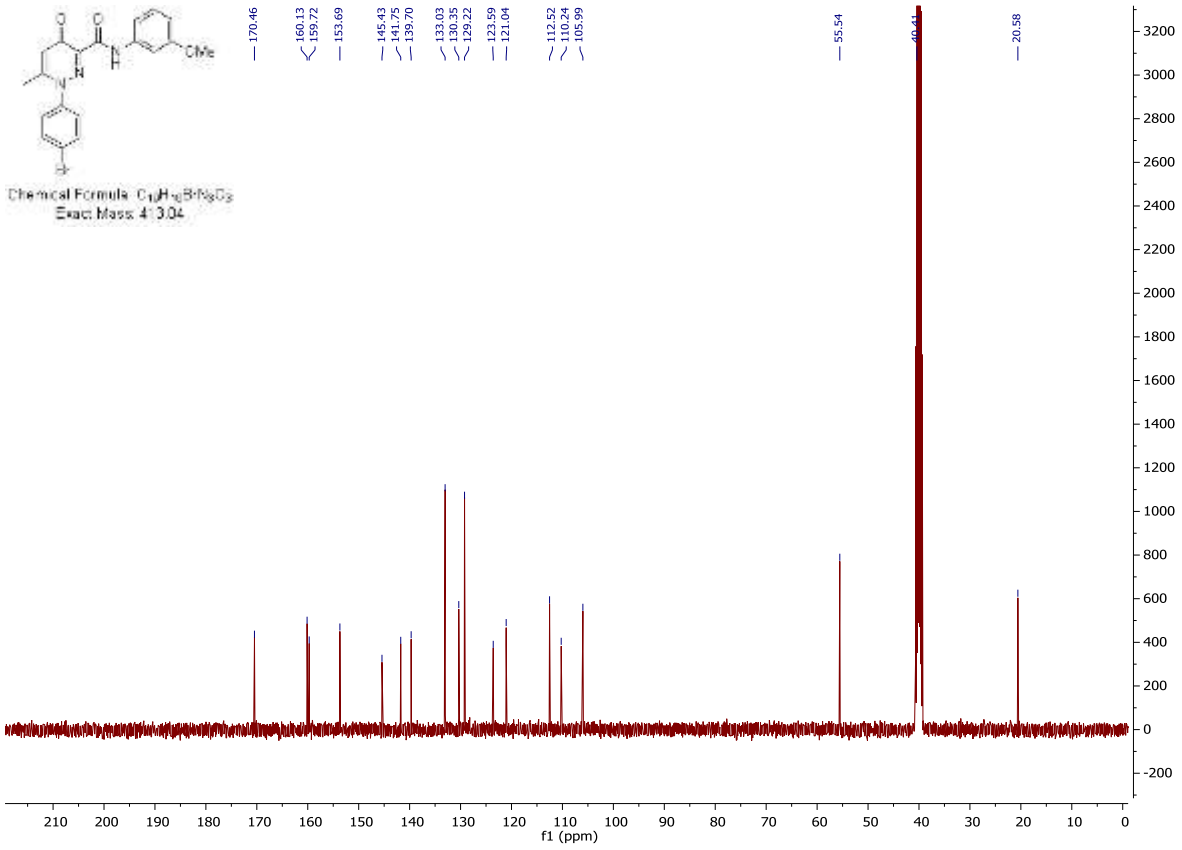

Chemical Formula: C18H13BrClN3O2
Exact Mass: 416.99
12.32
7.94
7.94
7.93
7.85
7.83
7.63
7.61
7.53
7.51
7.43
7.41
7.39
7.22
7.19
6.93
3.36
2.51
2.22
1.01
1.00
2.07
2.09
1.03
1.09
1.03
1.00
3.11
f1 (ppm)

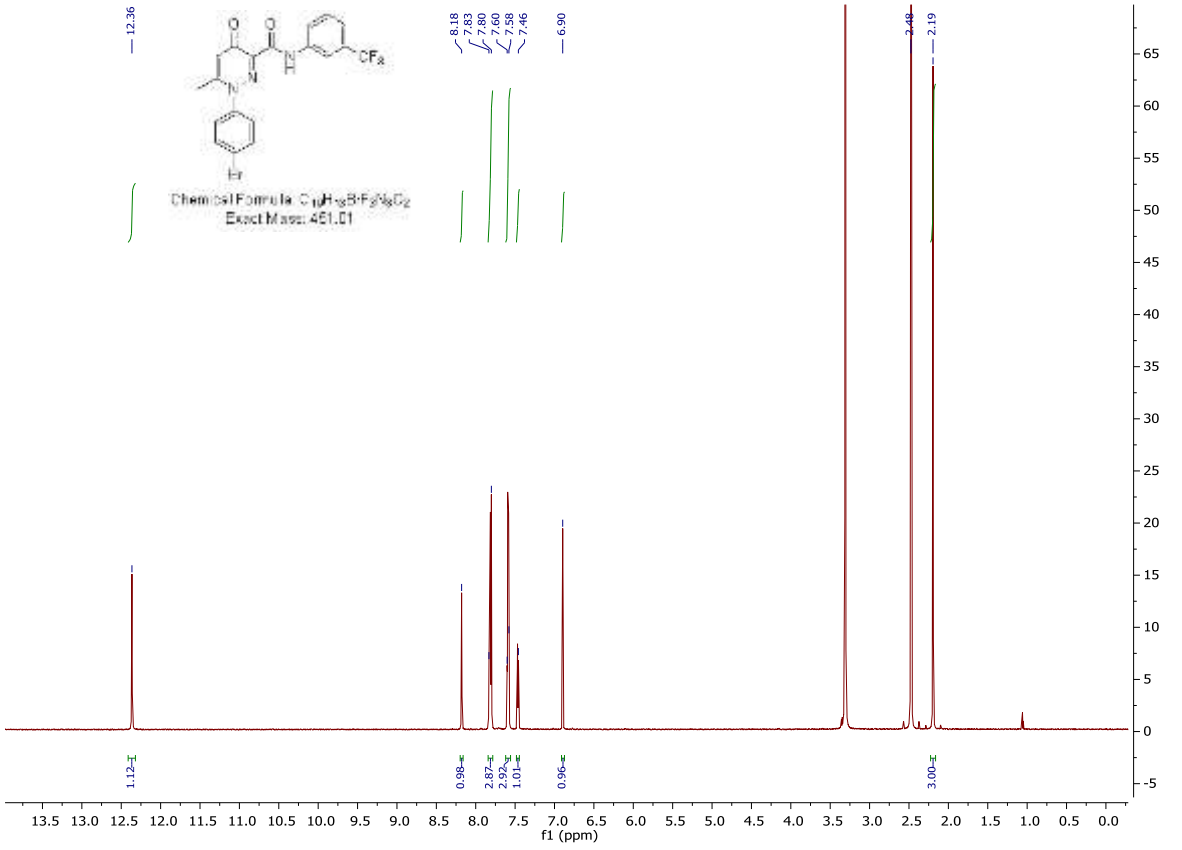

Chemical Formula: C18H14BrClN2O2
Exact Mass: 416.99
170.33
160.09
153.78
145.42
141.70
139.94
133.78
133.06
131.23
129.22
124.45
123.62
121.10
119.77
118.78
20.61
f1 (ppm)

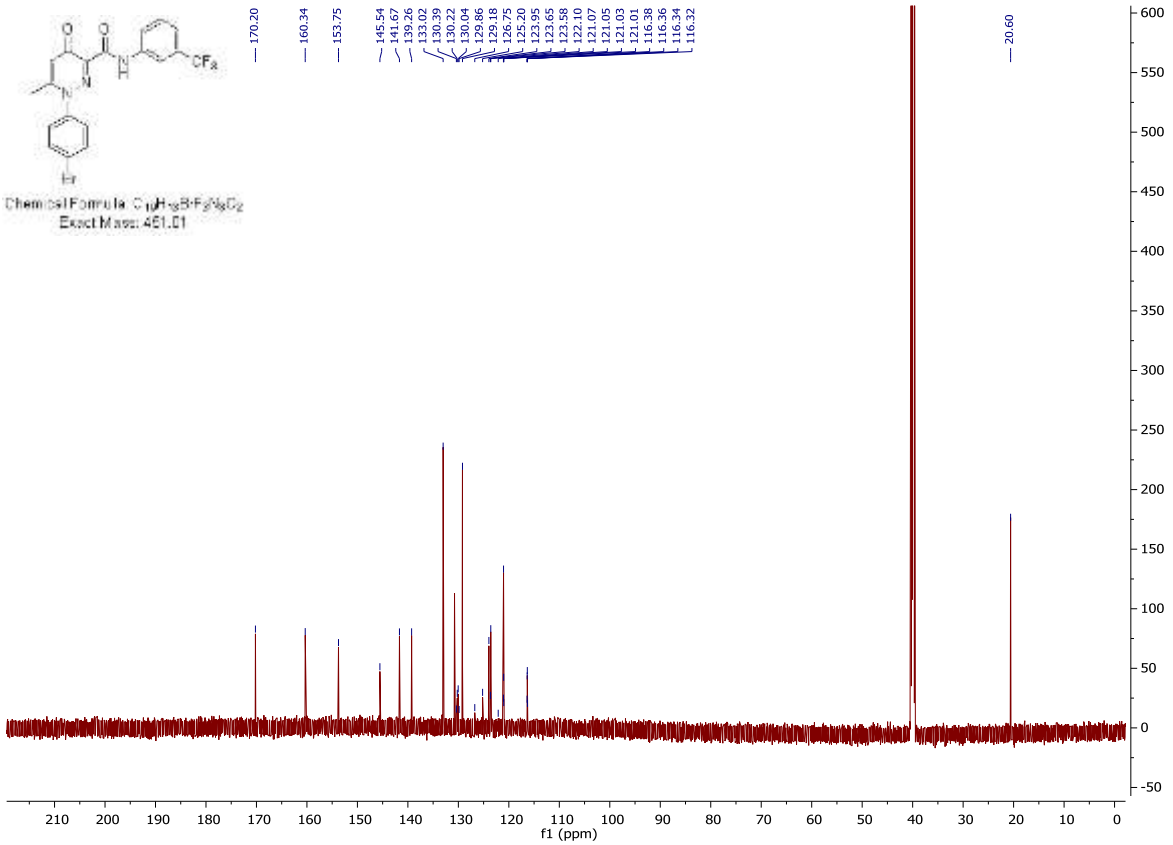

Chemical Formula: C18H14BrFN2O2
Exact Mass: 401.02
12.35
7.85
7.83
7.74
7.72
7.63
7.61
7.45
7.36
7.00
6.98
6.96
6.93
2.22
1.01
2.00
1.03
2.11
2.12
1.07
0.97
3.03
f1 (ppm)

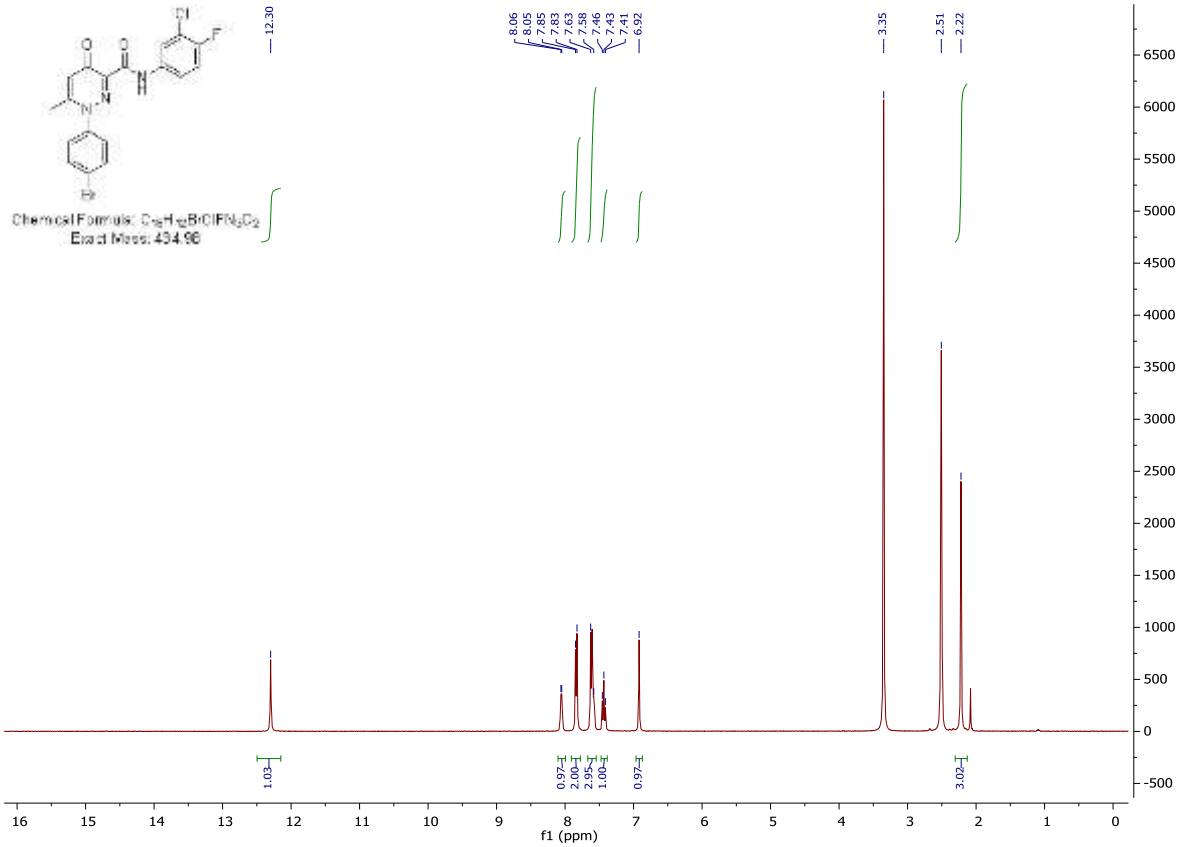

170.34
163.84
161.43
160.07
153.76
145.41
141.70
140.25
140.14
133.05
131.24
131.14
129.22
123.62
121.09
116.14
116.12
111.33
111.12
107.29
107.03
20.61
Br
f1 (ppm)

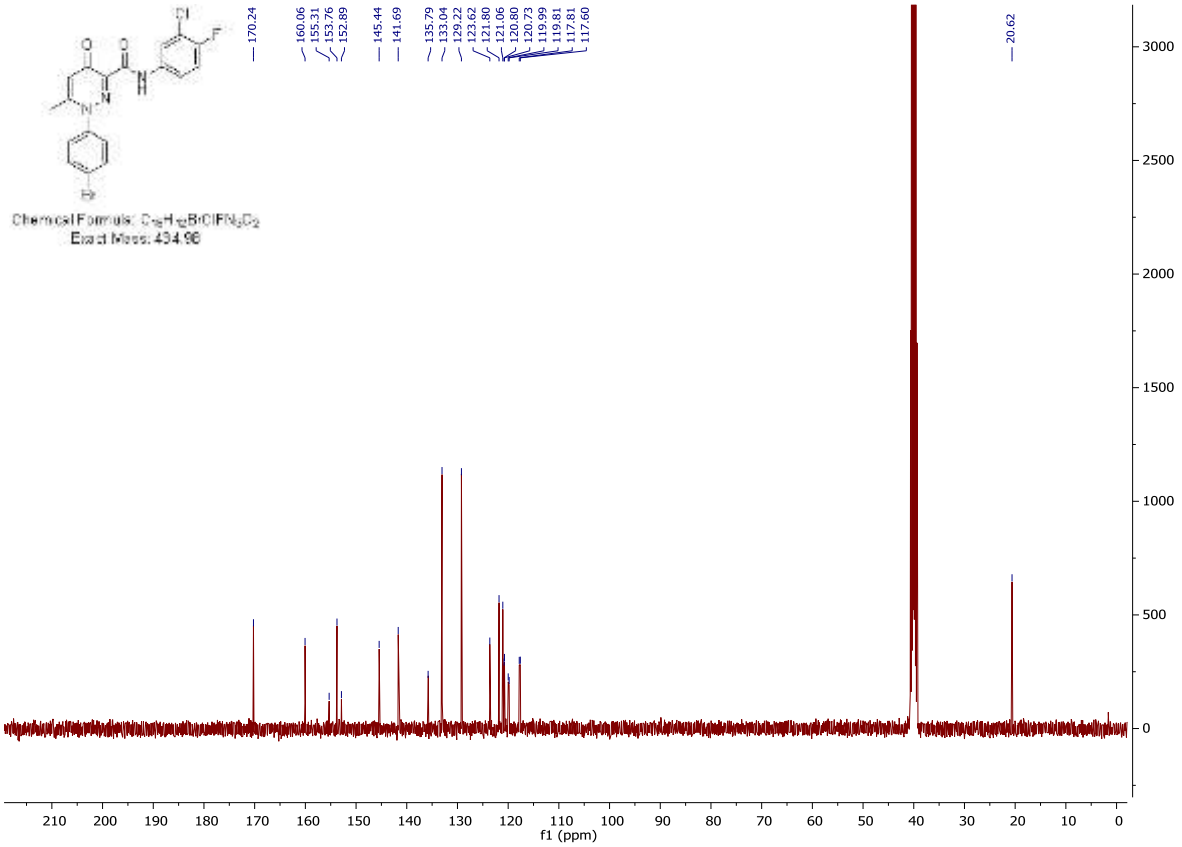

12.21
7.85
7.83
7.62
7.60
7.40
7.30
7.28
7.26
7.19
7.17
6.92
6.73
6.71
3.76
3.35
2.51
2.22
OMe
1.00
2.01
2.03
0.99
1.01
1.01
1.00
0.98
2.92
3.00
f1 (ppm)

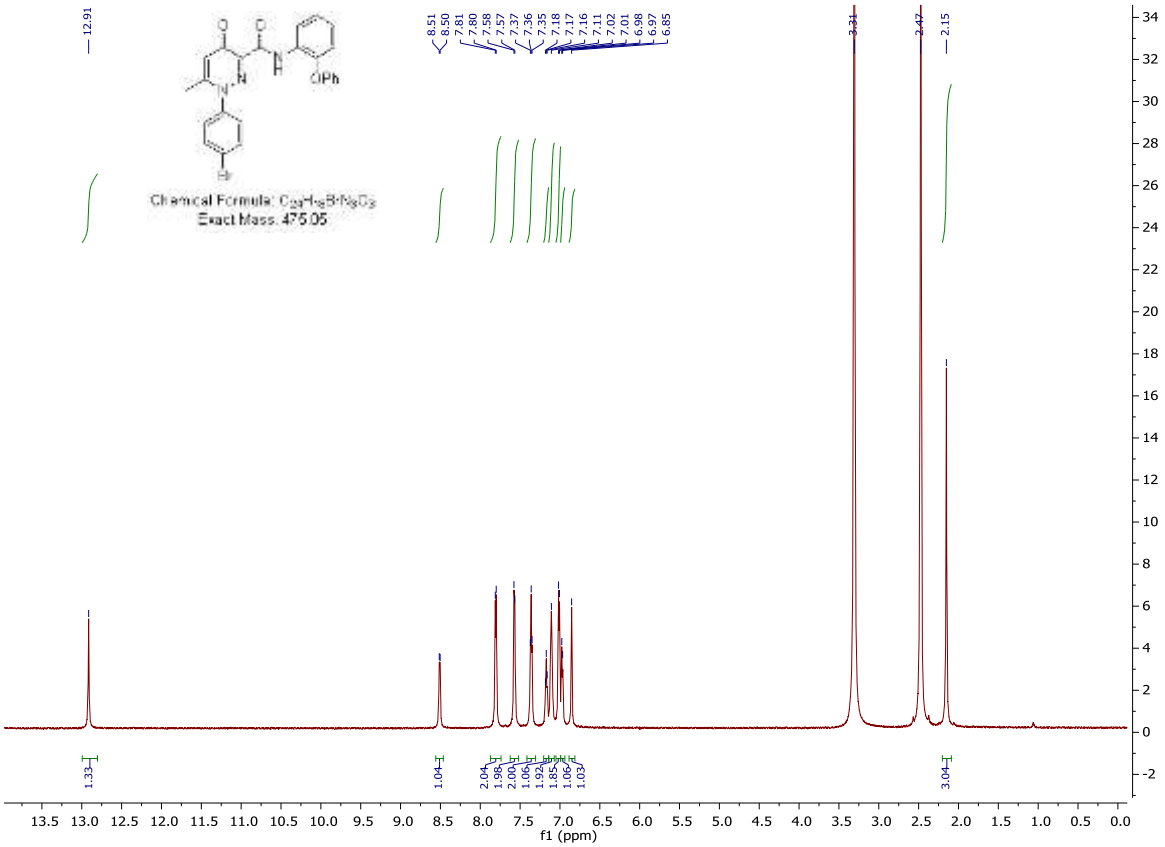

170.46
160.13
159.72
153.69
145.43
141.75
139.70
133.03
130.35
129.22
123.59
121.04
112.52
110.24
105.99
55.54
40.41
20.58
f1 (ppm)

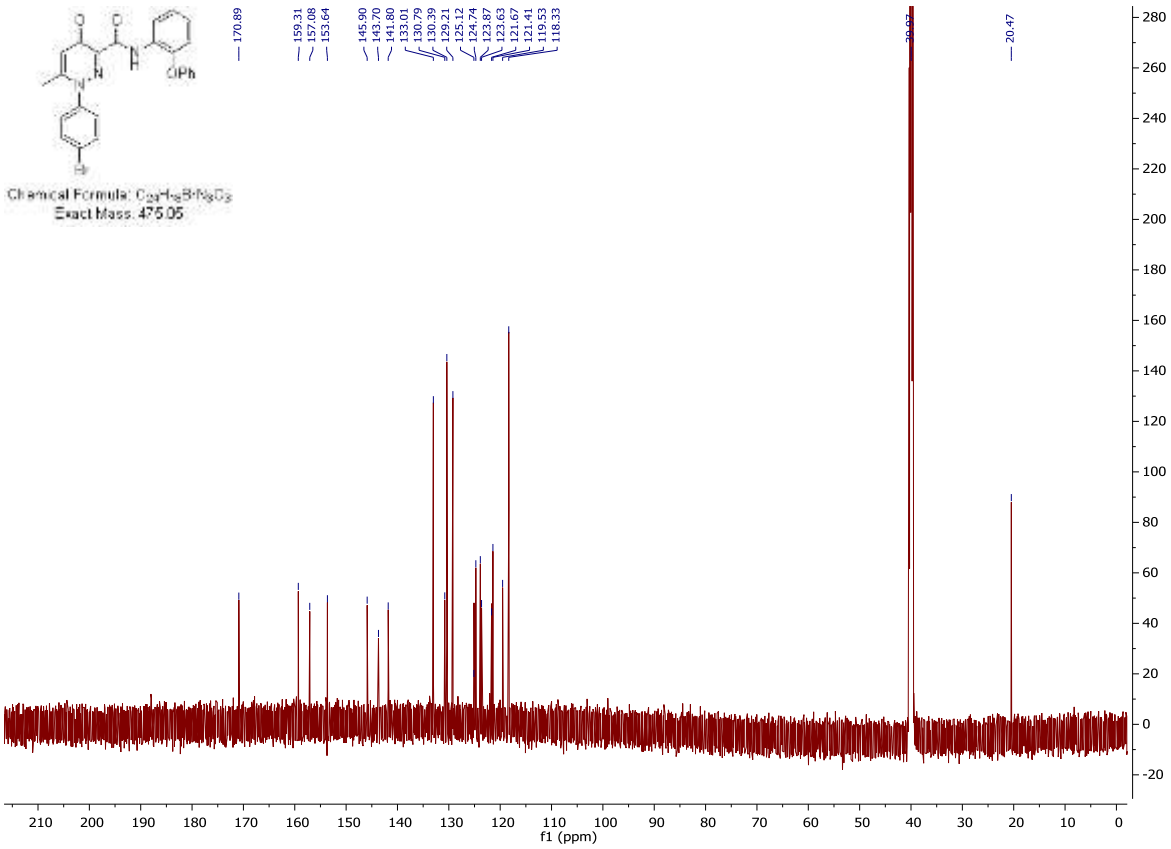

12.36
8.18
7.83
7.80
7.60
7.58
7.46
6.90
2.48
2.19
1.12
0.98
2.87
2.92
1.01
0.96
3.00
f1 (ppm)

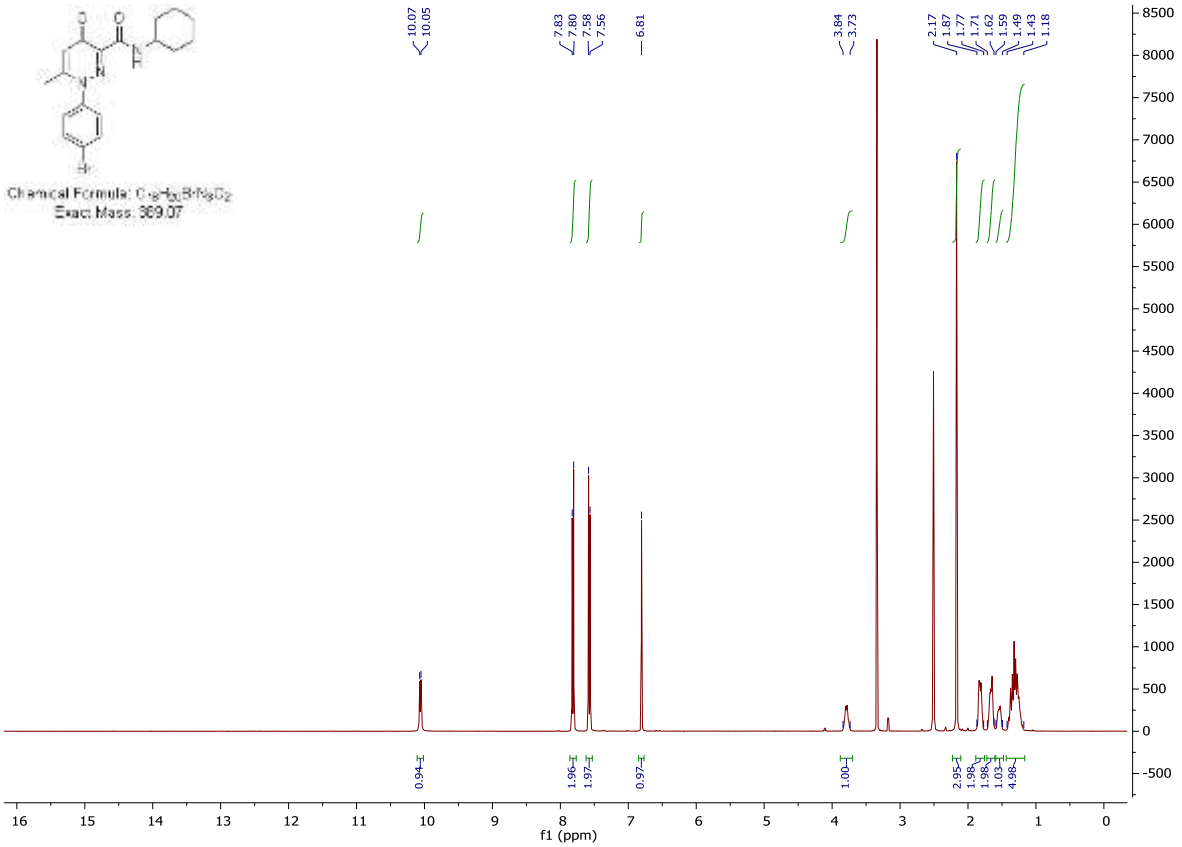

170.20
160.34
153.75
145.54
141.67
139.26
133.02
130.39
130.22
130.04
129.86
129.18
126.75
125.20
123.95
123.65
123.58
122.10
121.07
121.05
121.03
121.01
116.38
116.36
116.34
116.32
20.60
f1 (ppm)

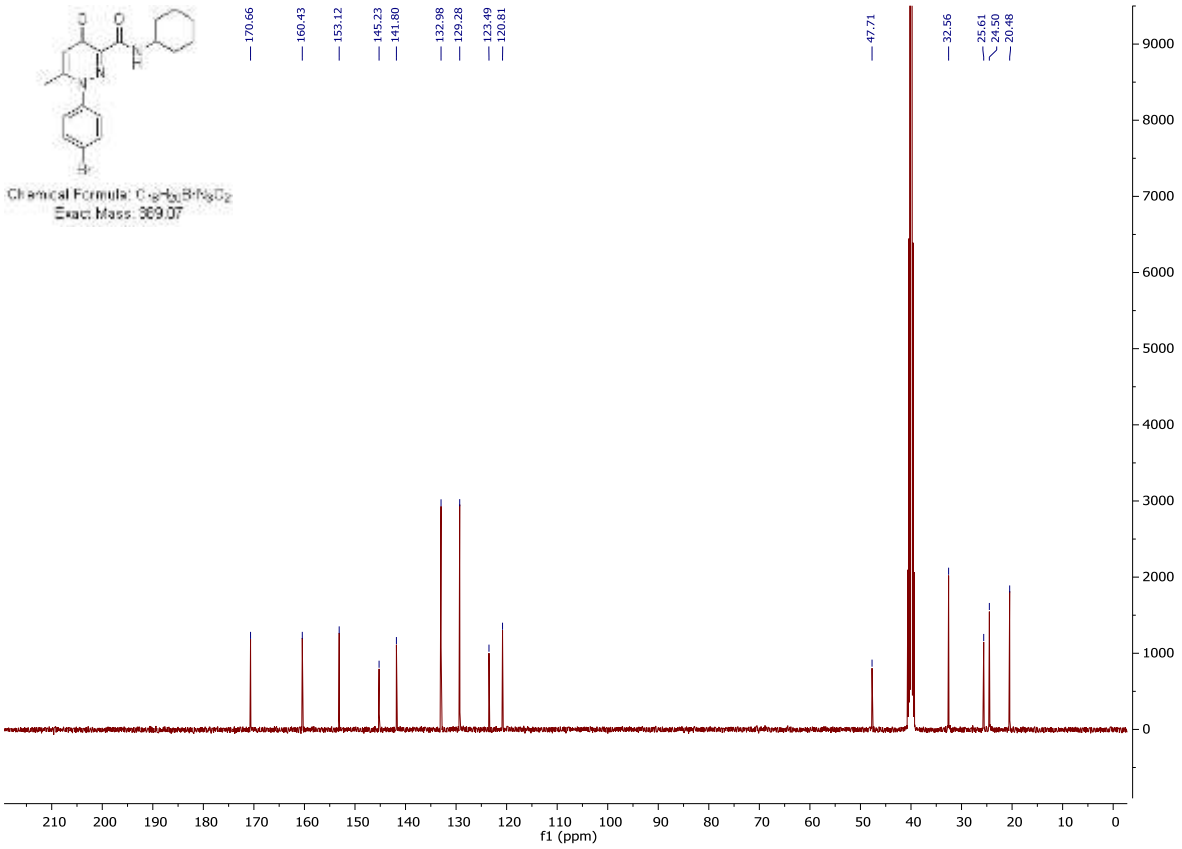

Chemical Formula: C18H12BrClFN3O2
Exact Mass: 434.98
12.30
8.06
8.05
7.85
7.83
7.63
7.58
7.46
7.43
7.41
6.92
3.35
2.51
2.22
1.03
0.97
2.00
2.95
1.00
0.97
3.02
f1 (ppm)

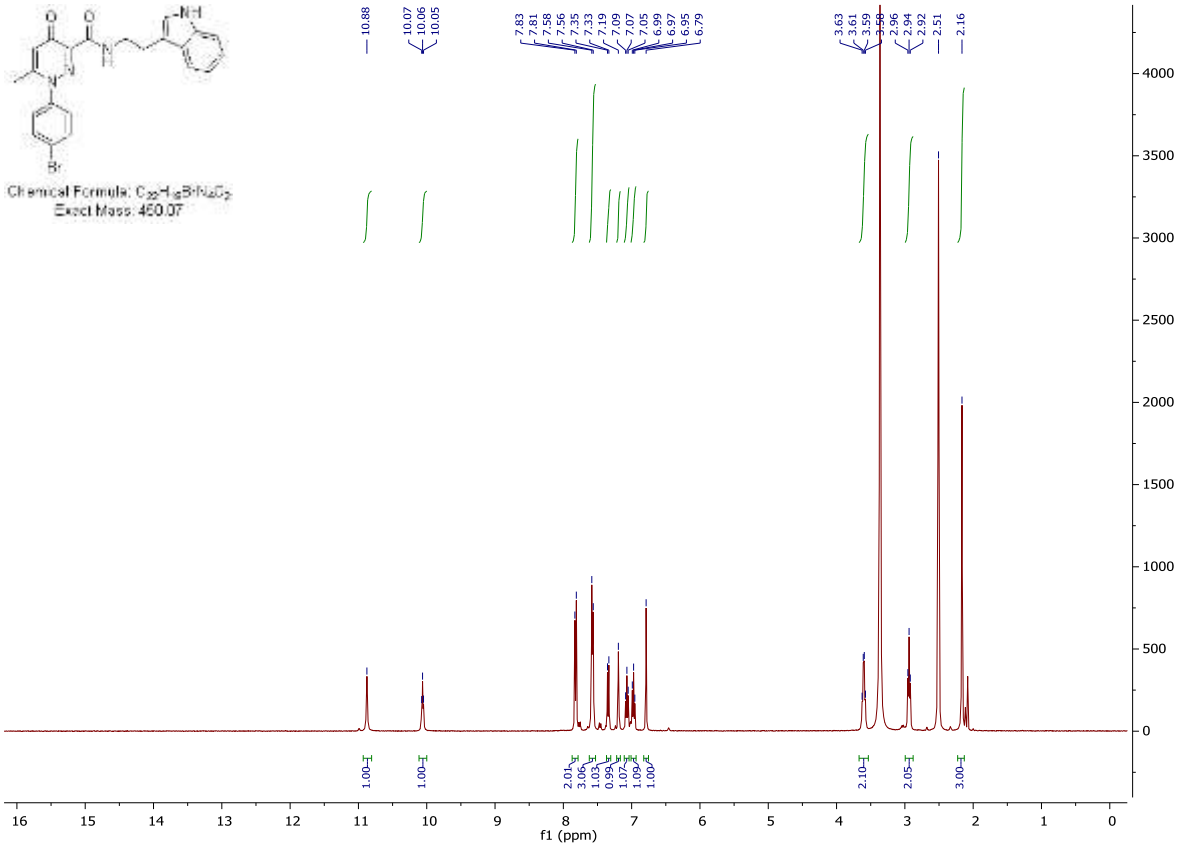

Chemical Formula: C18H12BrClFN3O2
Exact Mass: 434.98
170.24
160.06
155.31
153.76
152.89
145.44
141.69
135.79
133.04
129.22
123.62
121.80
121.06
120.80
120.73
119.99
119.81
117.81
117.60
20.62
f1 (ppm)

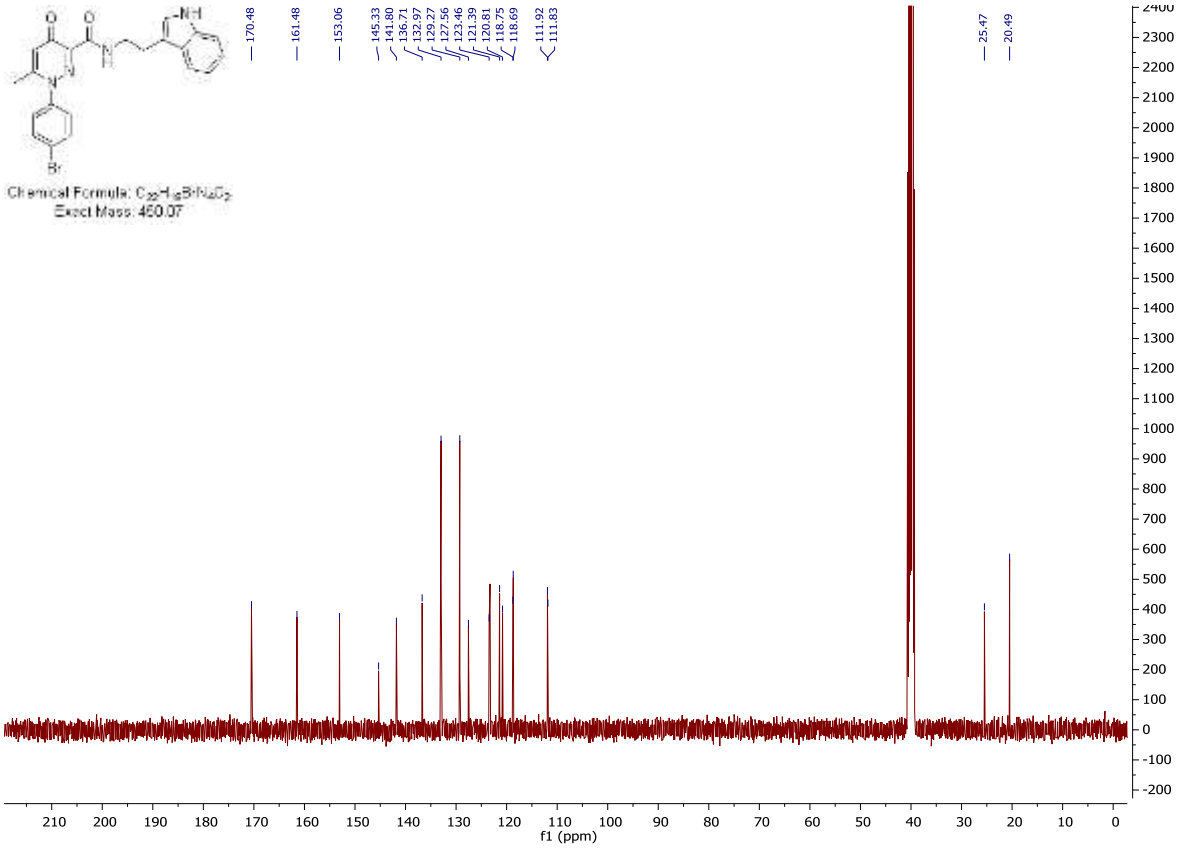

12.91
8.51
8.50
7.81
7.80
7.58
7.57
7.37
7.36
7.35
7.18
7.17
7.16
7.11
7.02
7.01
6.98
6.97
6.85
3.31
2.47
2.15
OPh
Chemical Formula: C23H19BrN2O3
Exact Mass: 475.05
1.33
1.04
2.04
1.98
2.00
1.92
1.85
1.06
1.03
3.04
f1 (ppm)

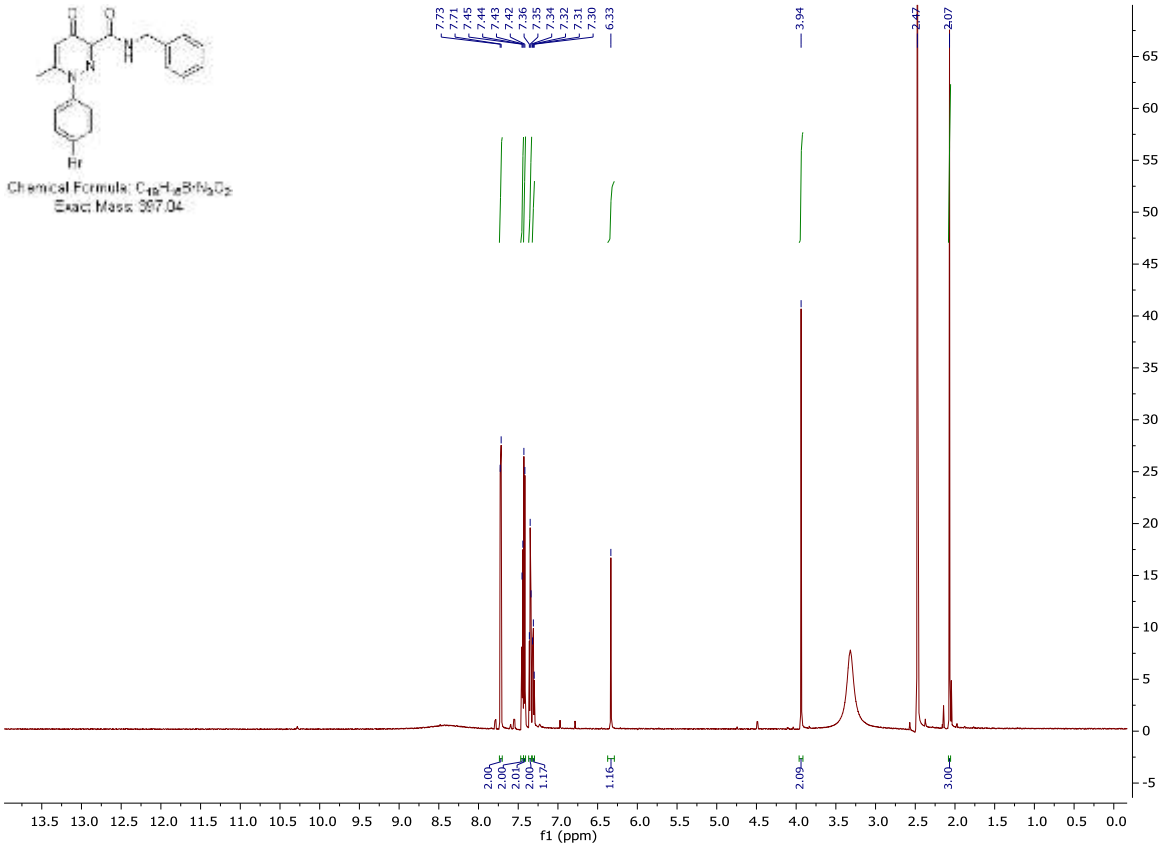

170.89
159.31
157.08
153.64
145.90
143.70
141.80
133.01
130.79
130.39
129.21
125.12
124.74
123.87
123.63
121.67
121.41
119.53
118.33
39.97
20.47
OPh
Chemical Formula: C23H19BrN2O3
Exact Mass: 475.05
f1 (ppm)

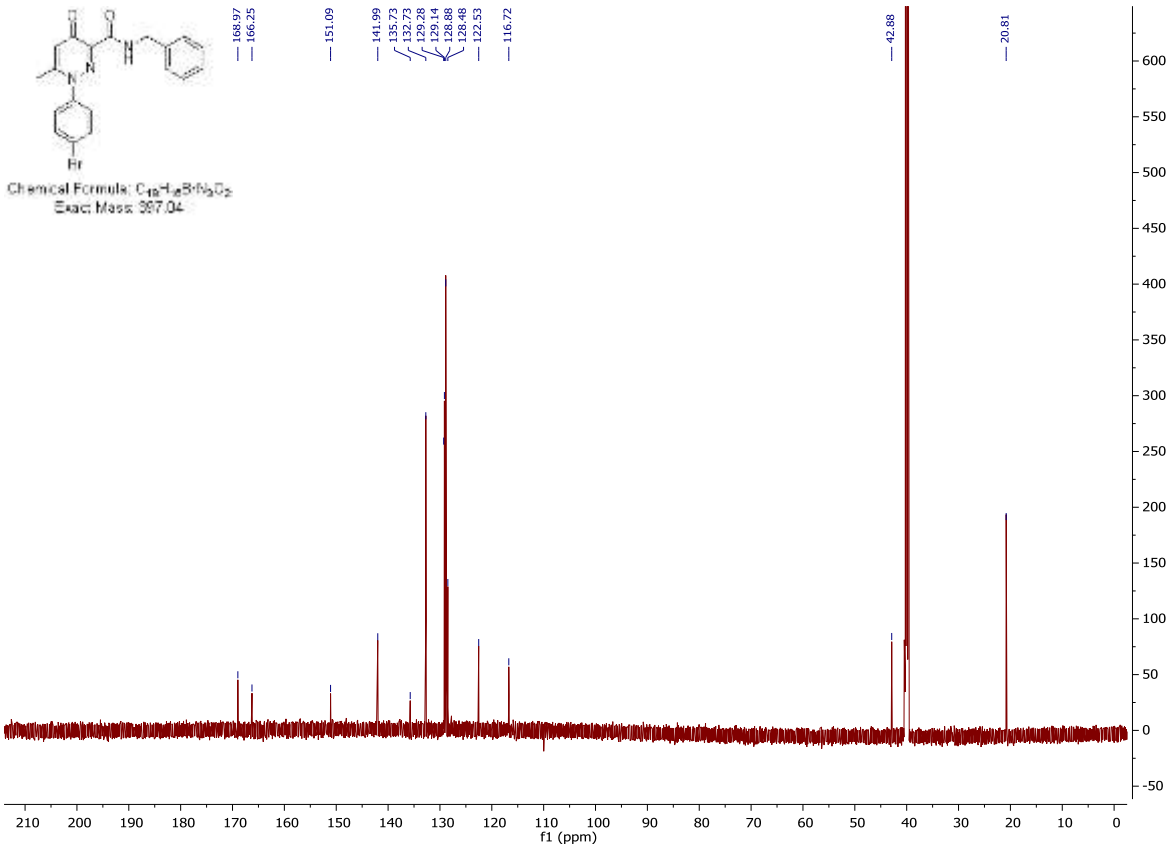

Chemical Formula: C19H16BrN3O2
Exact Mass: 389.07
10.07
10.05
7.83
7.80
7.58
7.56
6.81
3.84
3.73
2.17
1.87
1.77
1.71
1.62
1.59
1.49
1.43
1.18
0.94
1.96
1.97
0.97
1.00
2.95
1.98
1.98
1.03
4.98
f1 (ppm)

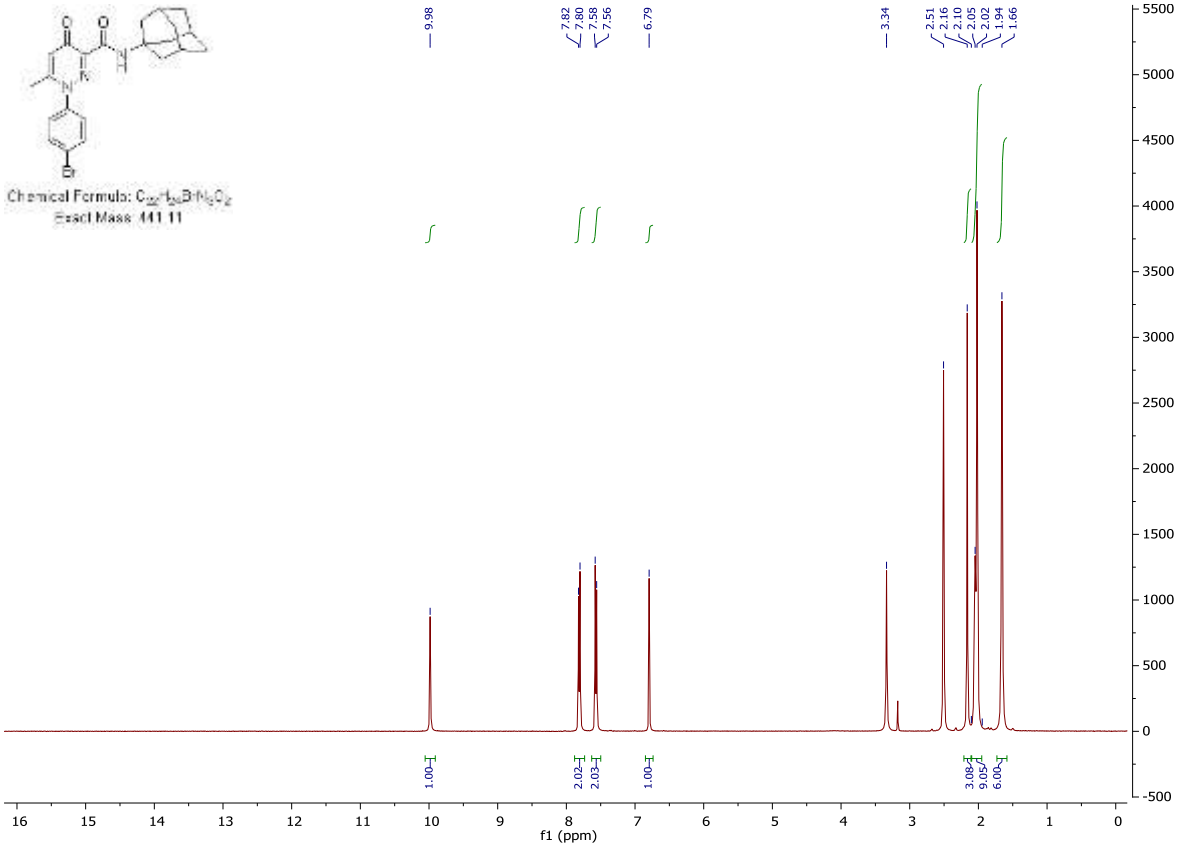

Chemical Formula: C19H16BrN3O2
Exact Mass: 389.07
170.66
160.43
153.12
145.23
141.80
132.98
129.28
123.49
120.81
47.71
32.56
25.61
24.50
20.48
f1 (ppm)

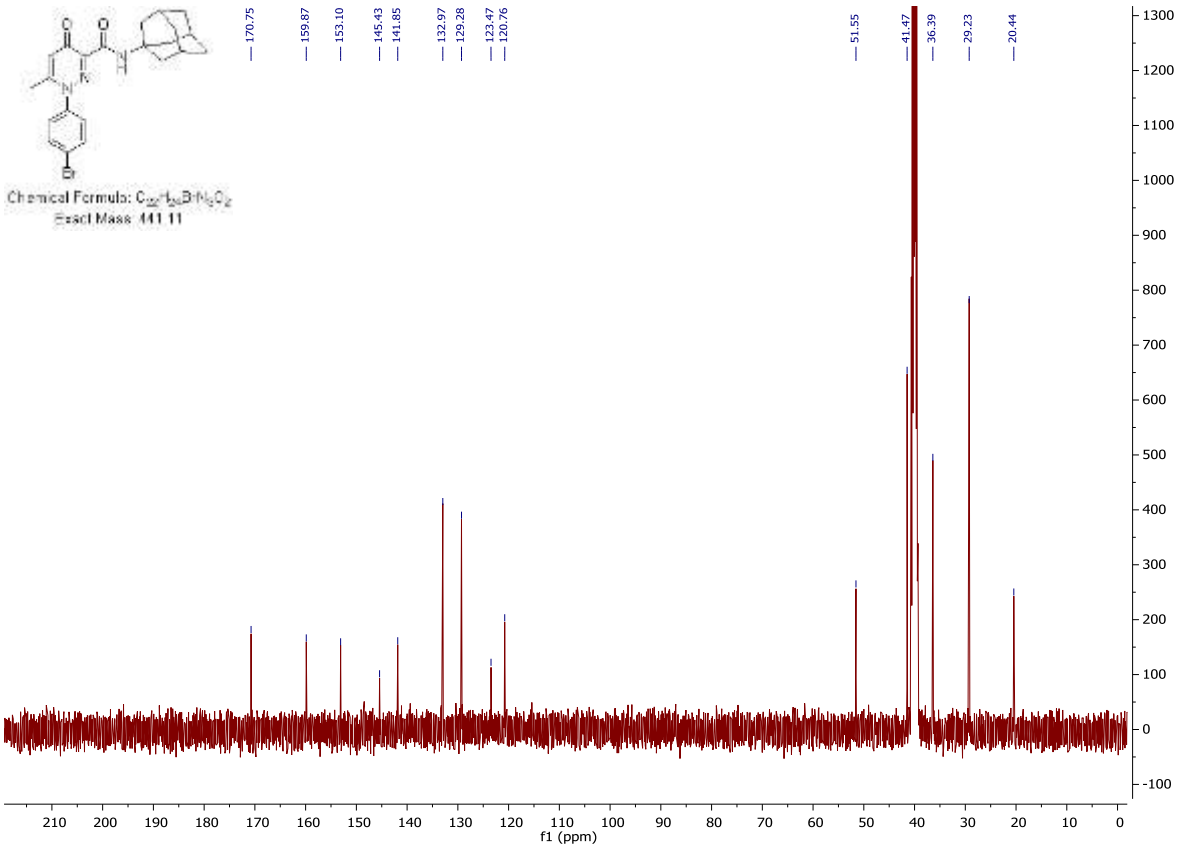

Chemical Formula: C22H18BrN3O2
Exact Mass: 460.07
10.88
10.07
10.06
10.05
7.83
7.81
7.58
7.56
7.35
7.33
7.19
7.09
7.07
7.05
6.99
6.97
6.95
6.79
3.63
3.61
3.59
3.58
2.96
2.94
2.92
2.51
2.16
1.00
1.00
2.01
3.06
1.03
0.99
1.07
1.09
1.00
2.10
2.05
3.00
f1 (ppm)

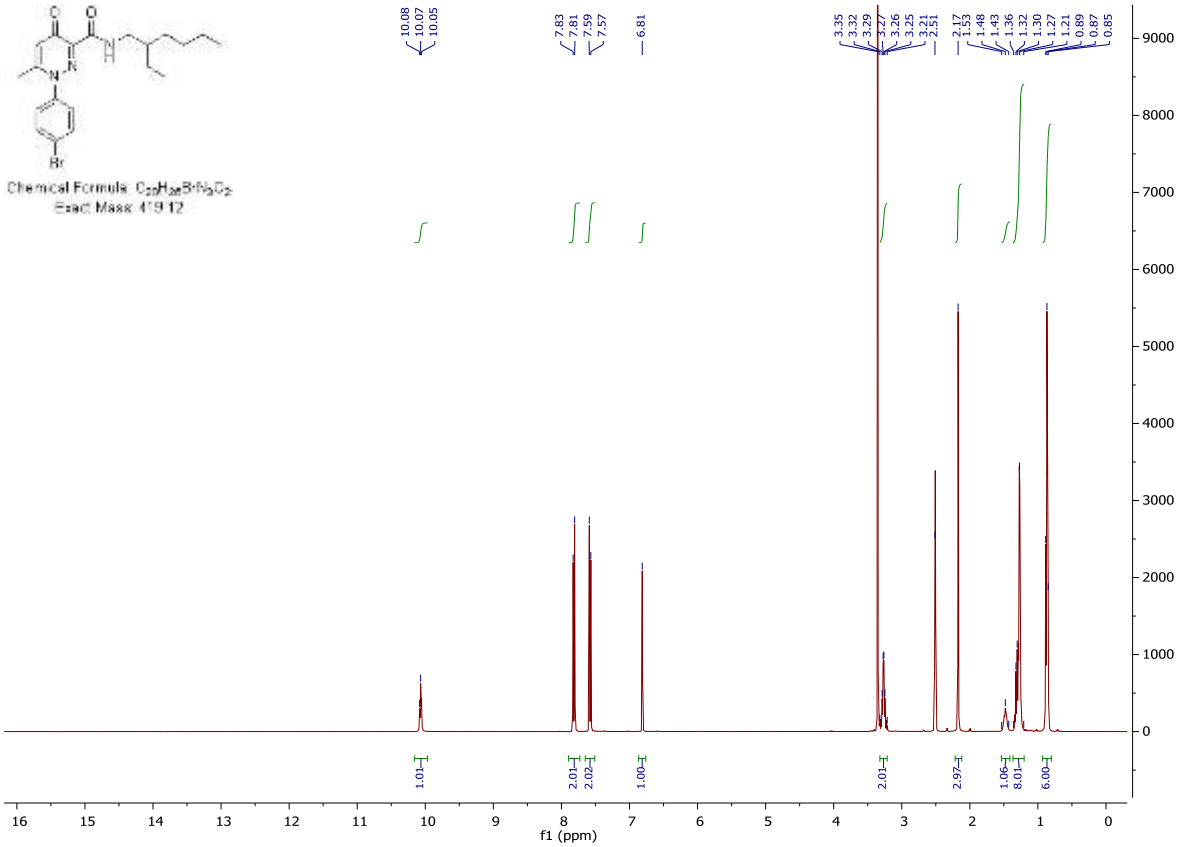

Chemical Formula: C22H18BrN3O2
Exact Mass: 460.07
170.48
161.48
153.06
145.33
141.80
136.71
132.97
129.27
127.56
123.46
121.39
120.81
118.75
118.69
111.92
111.83
25.47
20.49
f1 (ppm)

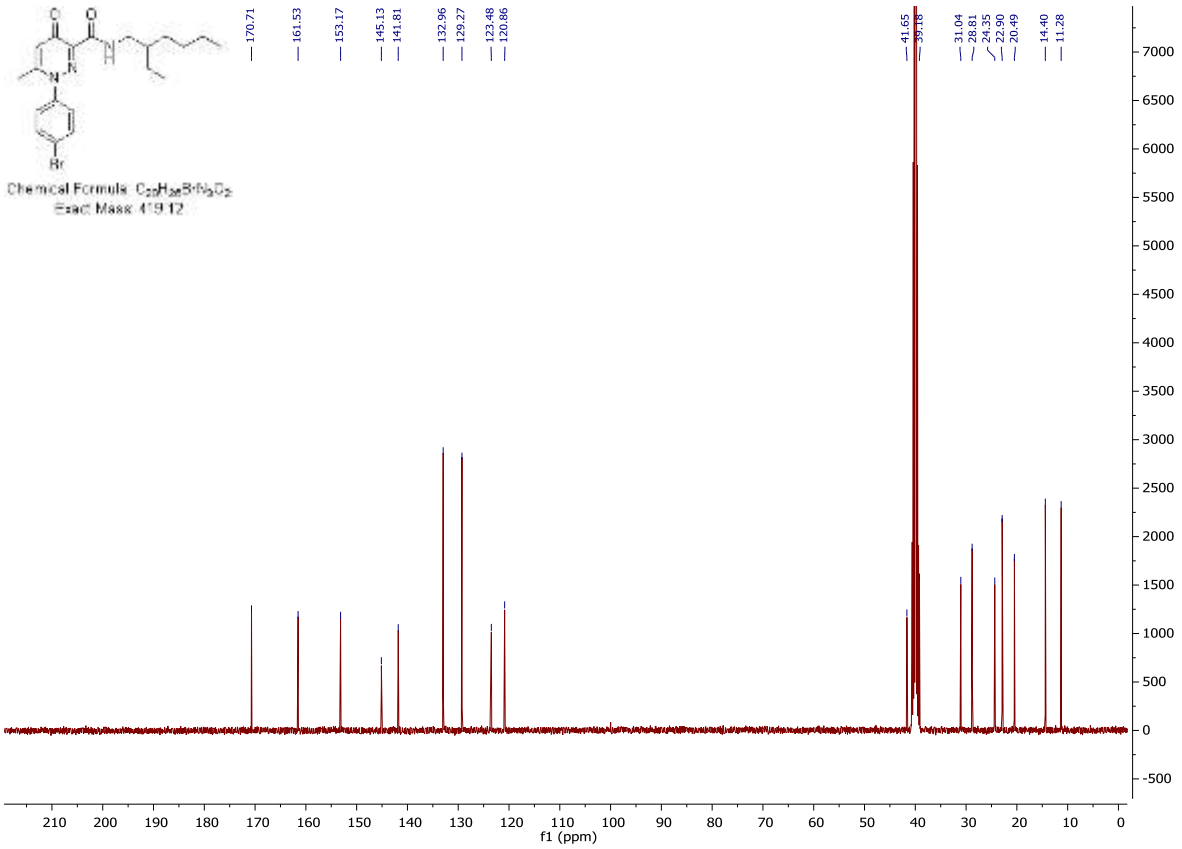

Chemical Formula: C18H15BrN2O2
Exact Mass: 367.04
7.73
7.71
7.45
7.44
7.43
7.42
7.36
7.35
7.34
7.32
7.31
7.30
6.33
3.94
3.47
2.07
2.00
2.00
2.01
2.00
1.17
1.16
2.09
3.00
f1 (ppm)


Chemical Formula: C18H15BrN2O2
Exact Mass: 367.04
168.97
166.25
151.09
141.99
135.73
132.73
129.28
129.14
128.88
128.48
122.53
116.72
42.88
20.81
f1 (ppm)

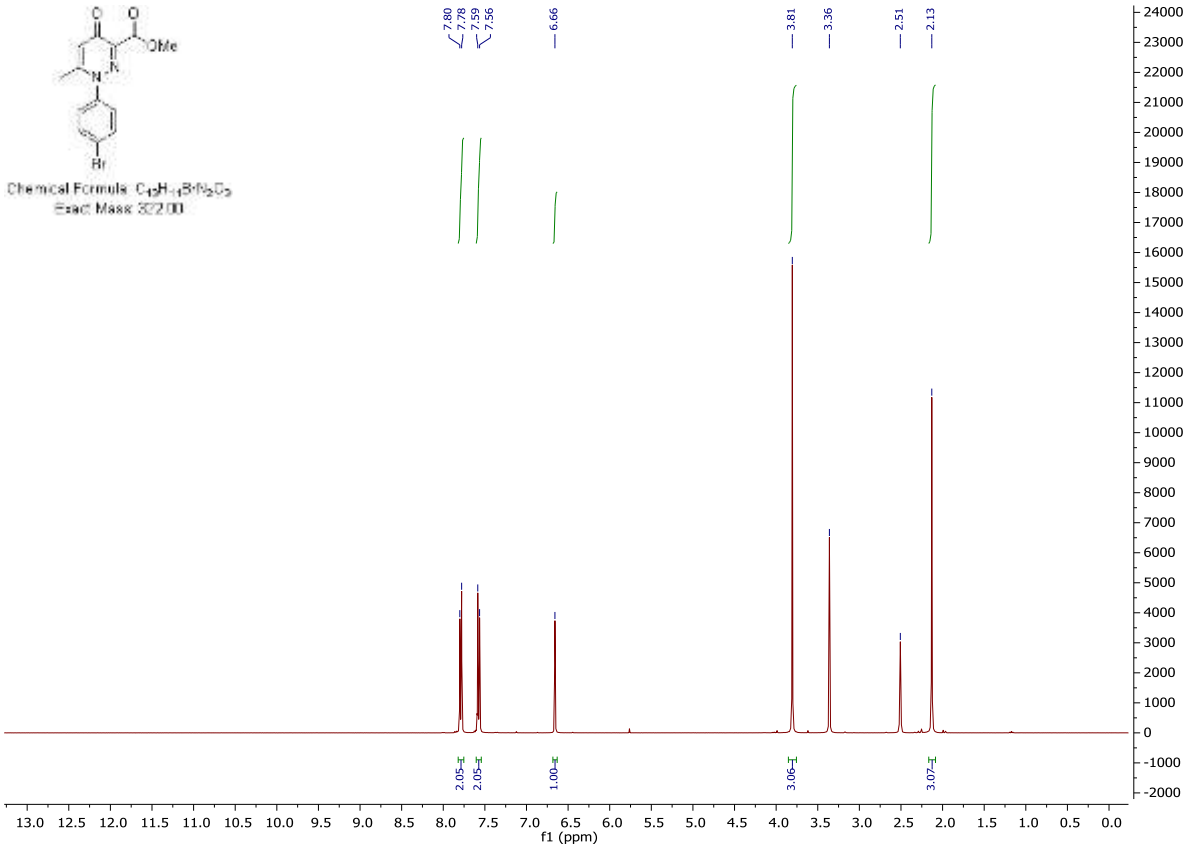

Chemical Formula: C22H24BrN3O2
Exact Mass: 441.11
9.98
7.82
7.80
7.58
7.56
6.79
3.34
2.51
2.16
2.10
2.05
2.02
1.94
1.66
1.00
2.02
2.03
1.00
3.08
9.05
6.00
f1 (ppm)

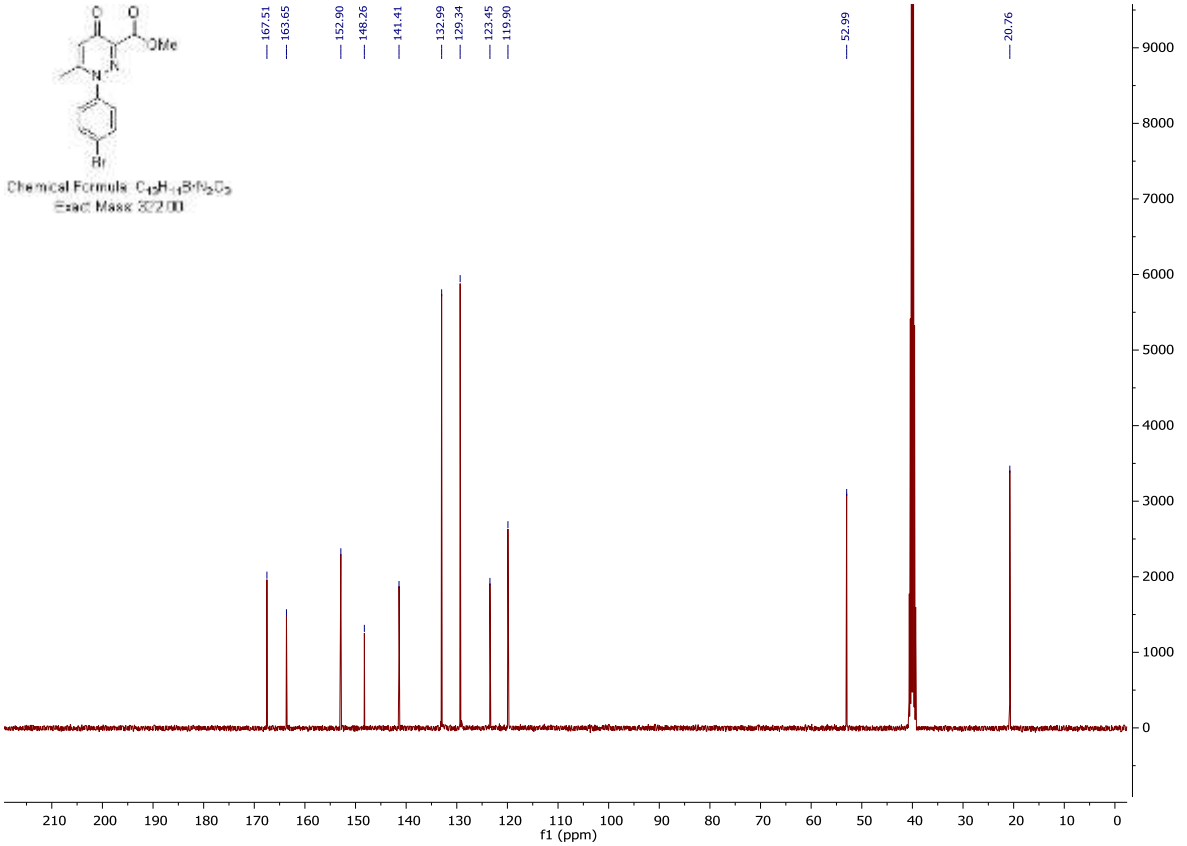

Chemical Formula: C22H24BrN3O2
Exact Mass: 441.11
170.75
159.87
153.10
145.43
141.85
132.97
129.28
123.47
120.76
51.55
41.47
36.39
29.23
20.44
f1 (ppm)

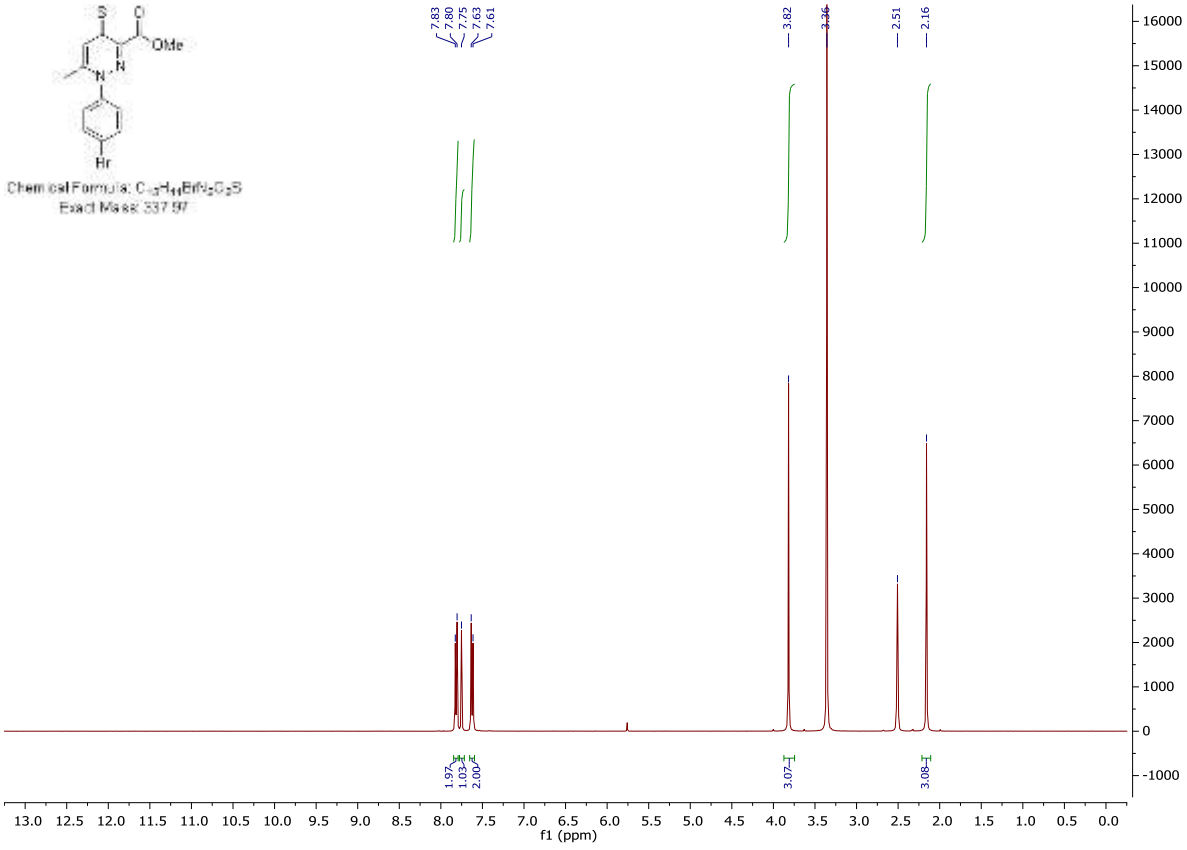

Chemical Formula: C20H28BrN3O2
Exact Mass: 421.12
10.08
10.07
10.05
7.83
7.81
7.59
7.57
6.81
3.35
3.32
3.29
3.27
3.26
3.25
3.21
2.51
2.17
1.53
1.48
1.43
1.36
1.32
1.30
1.27
1.21
0.89
0.87
0.85
1.01
2.01
2.02
1.00
2.01
2.97
1.06
8.01
6.00
f1 (ppm)

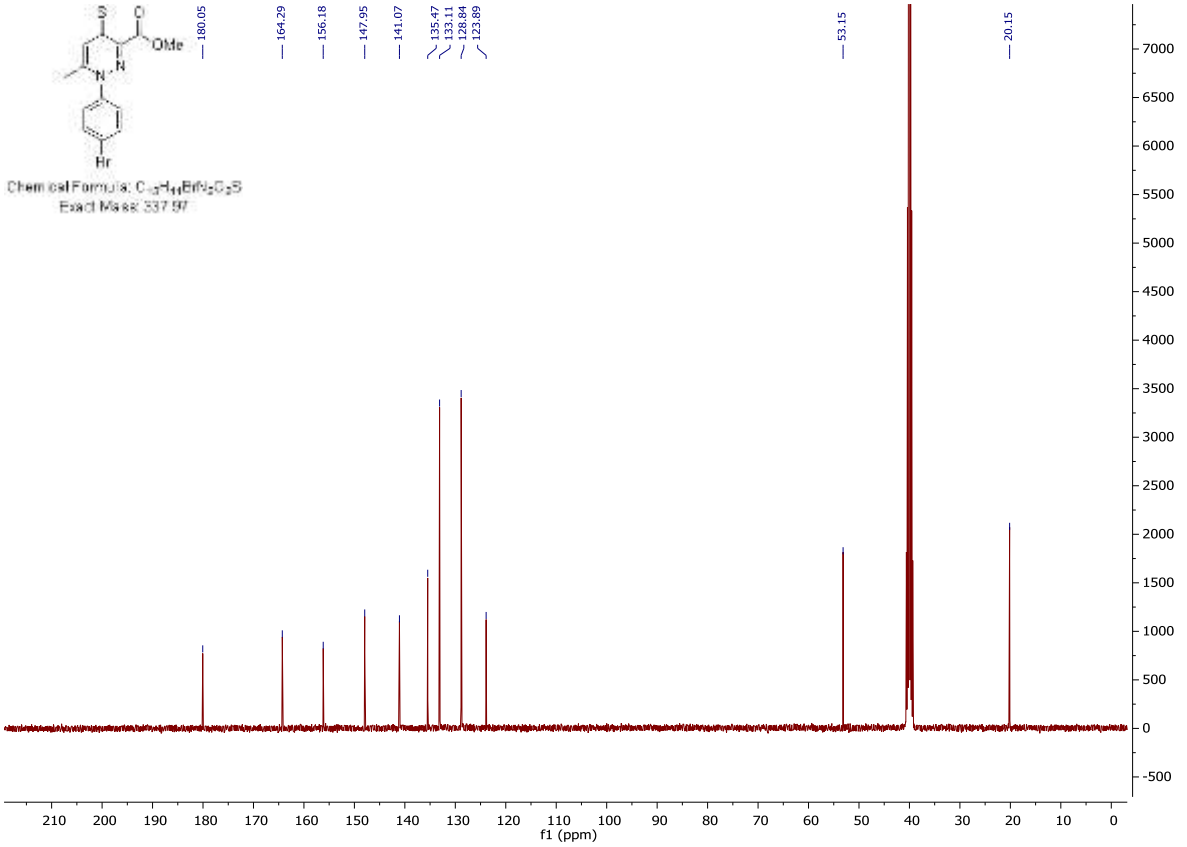

Chemical Formula: C20H28BrN3O2
Exact Mass: 421.12
170.71
161.53
153.17
145.13
141.81
132.96
129.27
123.48
120.86
41.65
39.18
31.04
28.81
24.35
22.90
20.49
14.40
11.28
f1 (ppm)

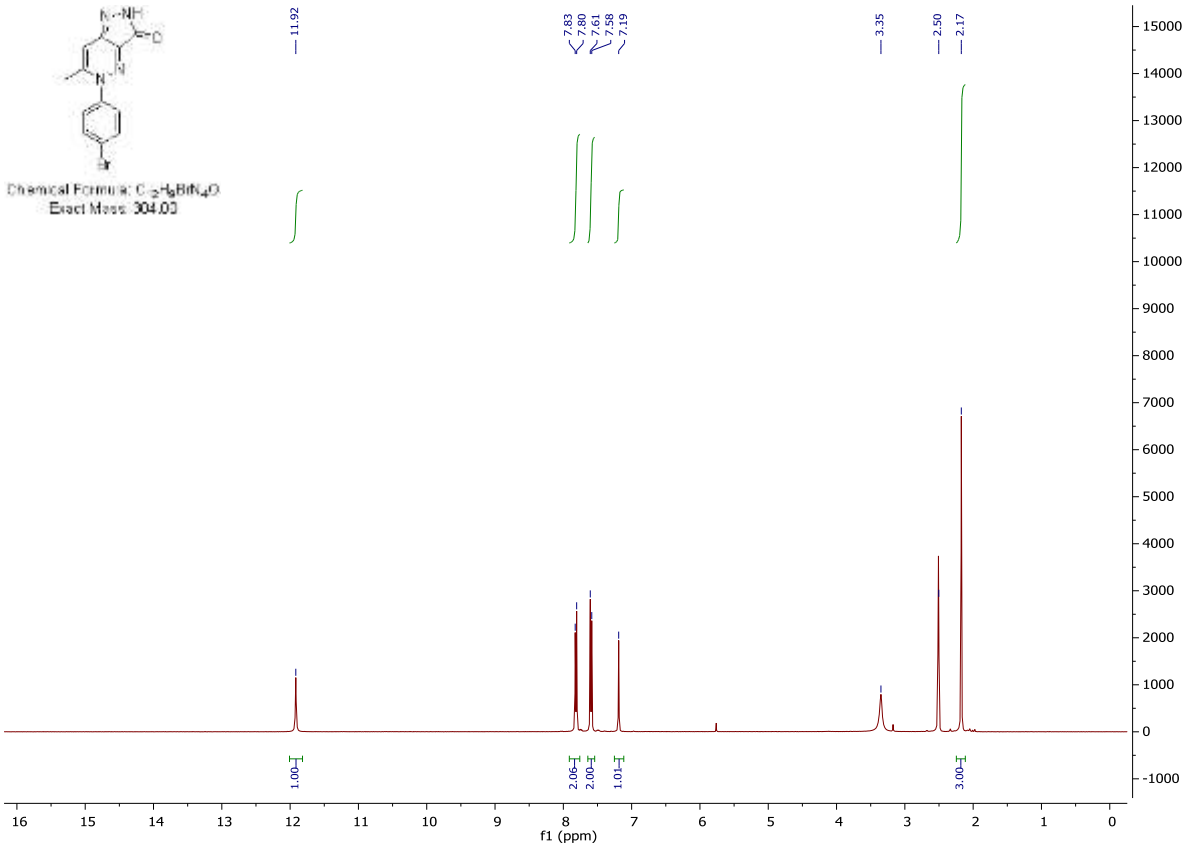
A3. Intermediates 24-26 and C derivatives 27-31

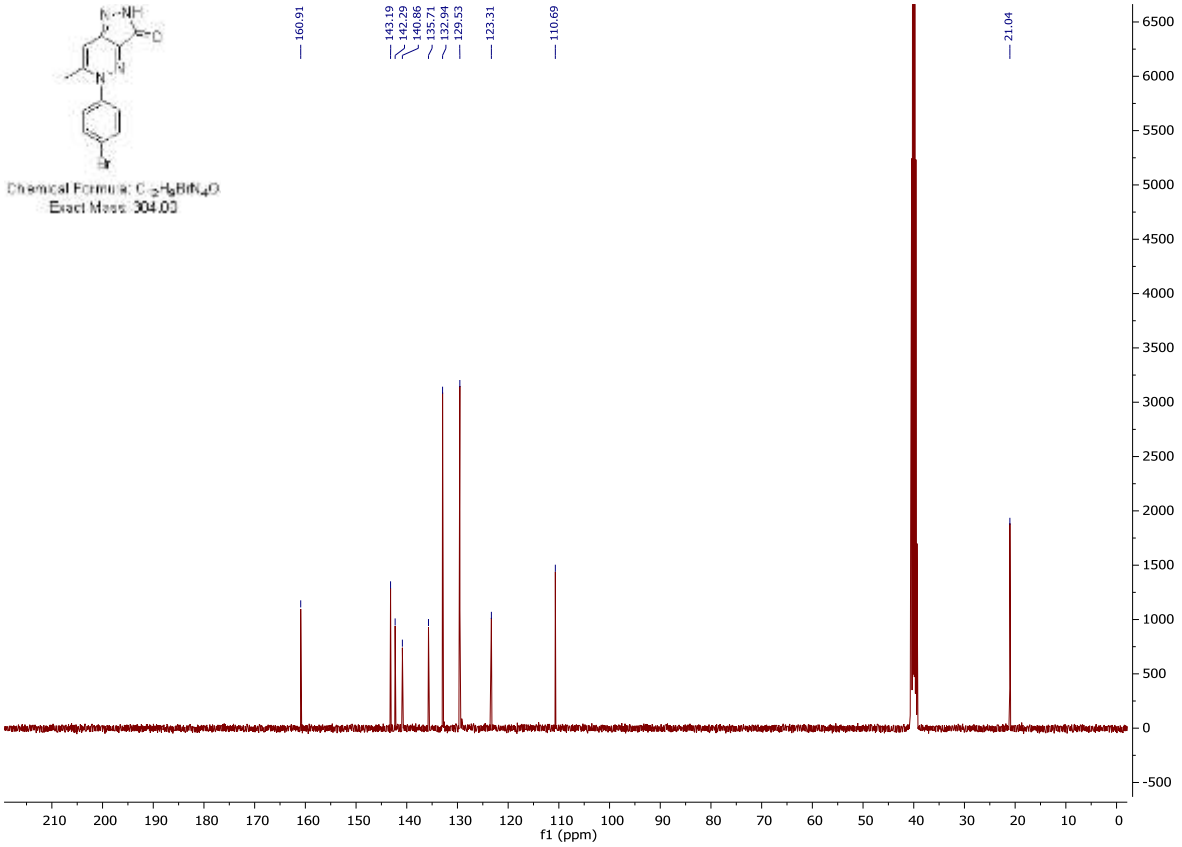


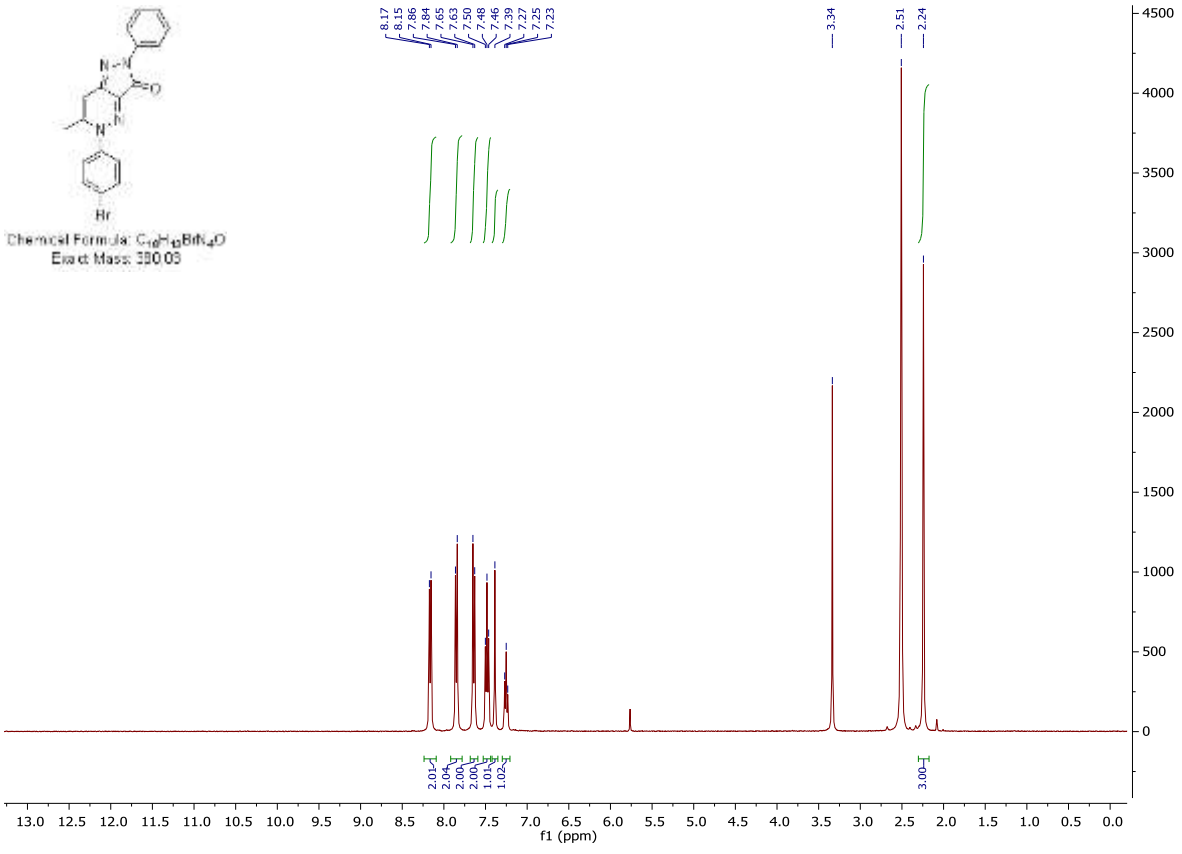

Chemical Formula: C13H11BrN2O3
Exact Mass: 322.00
167.51
163.65
152.90
148.26
141.41
132.99
129.34
123.45
119.90
52.99
20.76
f1 (ppm)

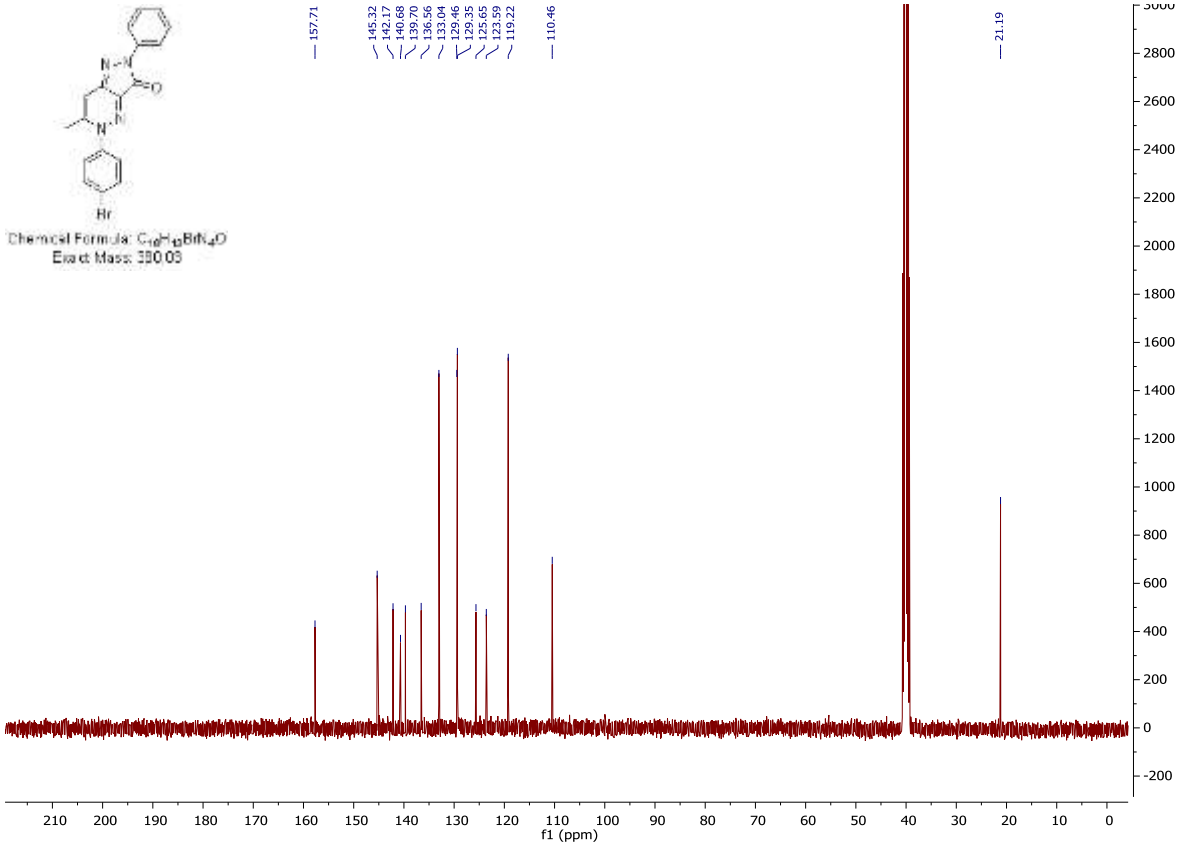

Chemical Formula: C13H11BrN2O3S
Exact Mass: 337.97
7.83
7.80
7.75
7.63
7.61
3.82
2.51
2.16
1.97
1.03
2.00
3.07
3.08
f1 (ppm)

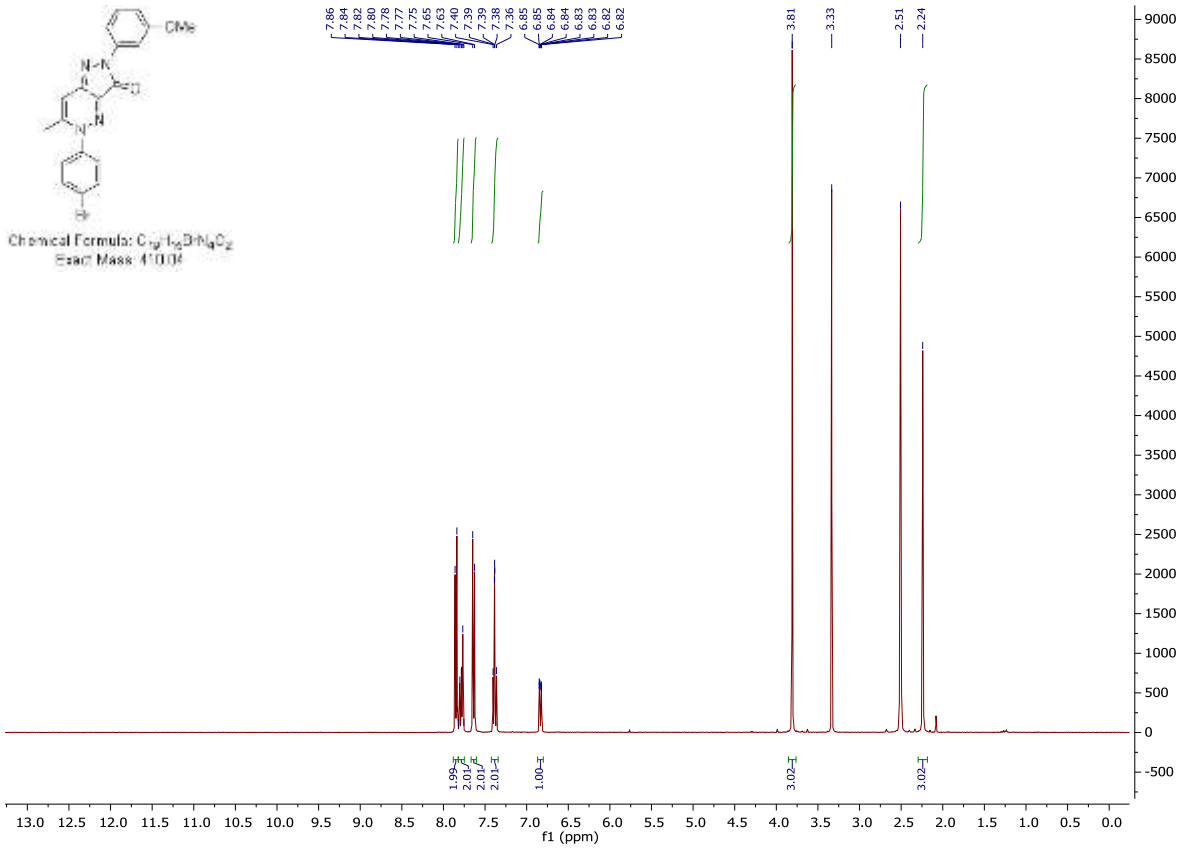

180.05
164.29
156.18
147.95
141.07
135.47
133.11
128.84
123.89
53.15
20.15
OMe
Br
f1 (ppm)


11.92
7.83
7.80
7.61
7.58
7.19
3.35
2.50
2.17
1.00
2.06
2.00
1.01
3.00
f1 (ppm)


Chemical Formula: C12H9BrN4O
Exact Mass: 304.00
160.91
143.19
142.29
140.86
135.71
132.94
129.53
123.31
110.69
21.04
f1 (ppm)


Chemical Formula: C18H13BrN4O
Exact Mass: 380.03
8.17
8.15
7.86
7.84
7.65
7.63
7.50
7.48
7.46
7.39
7.27
7.25
7.23
3.34
2.51
2.24
2.01
2.04
2.00
2.00
1.01
1.02
3.00
f1 (ppm)


Br
Chemical Formula: C16H13BrN4O
Exact Mass: 356.03
157.71
145.32
142.17
140.68
139.70
136.56
133.04
129.46
129.35
125.65
123.59
119.22
110.46
21.19
f1 (ppm)


OMe
Chemical Formula: C17H15BrN4O2
Exact Mass: 410.04
7.86
7.84
7.82
7.80
7.78
7.77
7.75
7.65
7.63
7.40
7.39
7.39
7.38
7.36
6.85
6.85
6.84
6.84
6.83
6.83
6.82
6.82
3.81
3.33
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2.24
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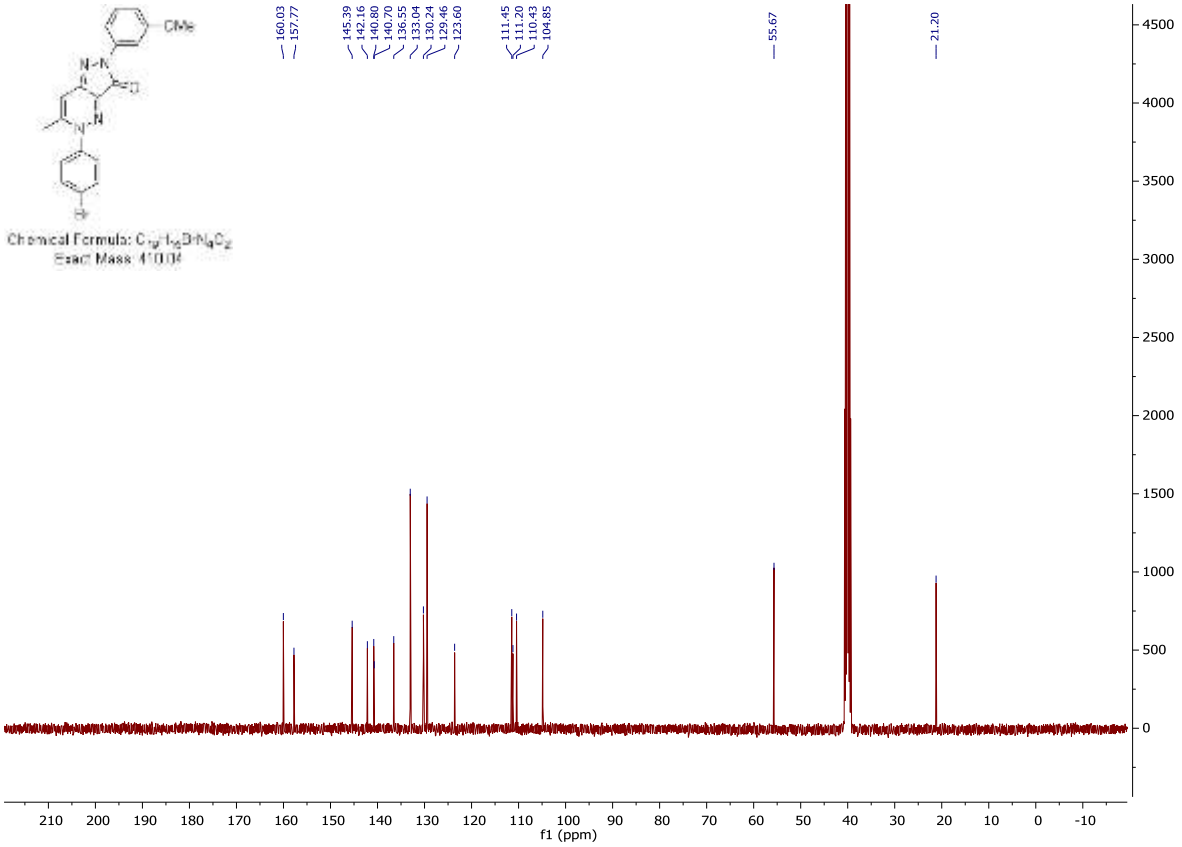
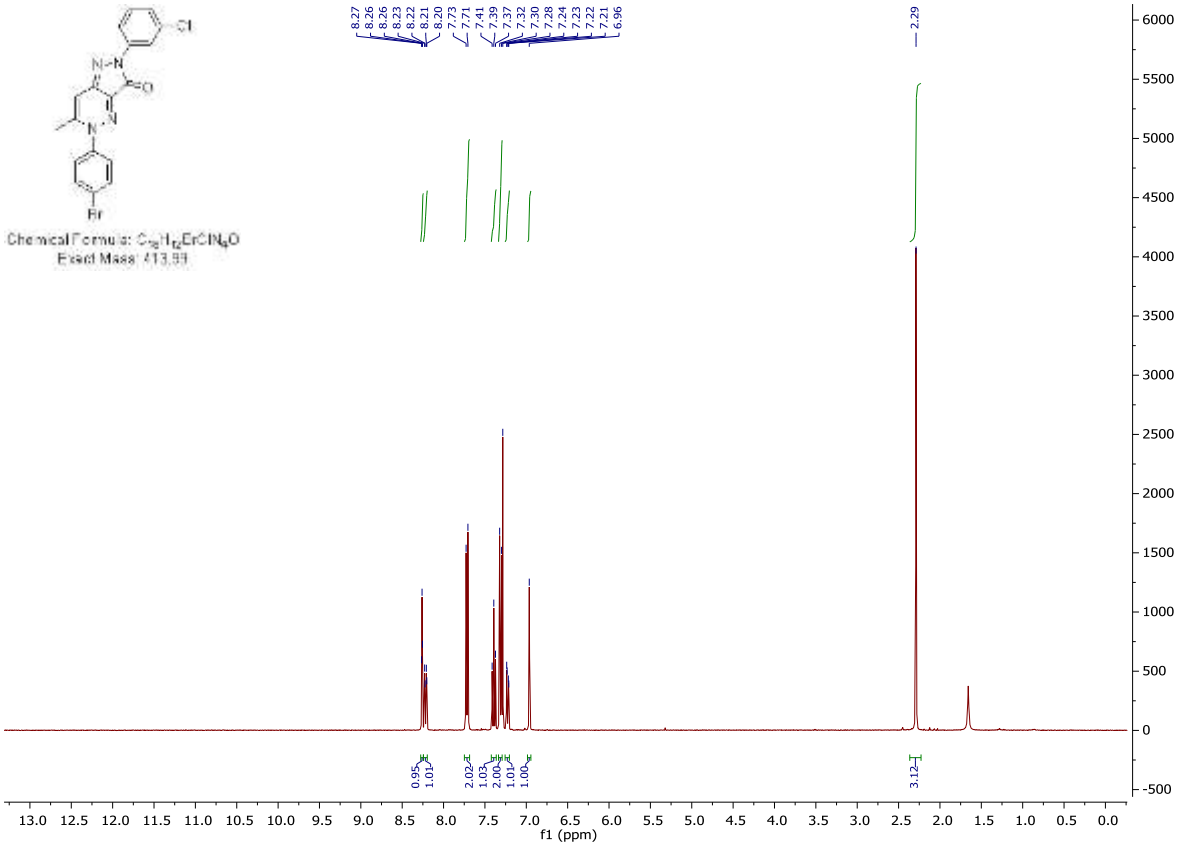
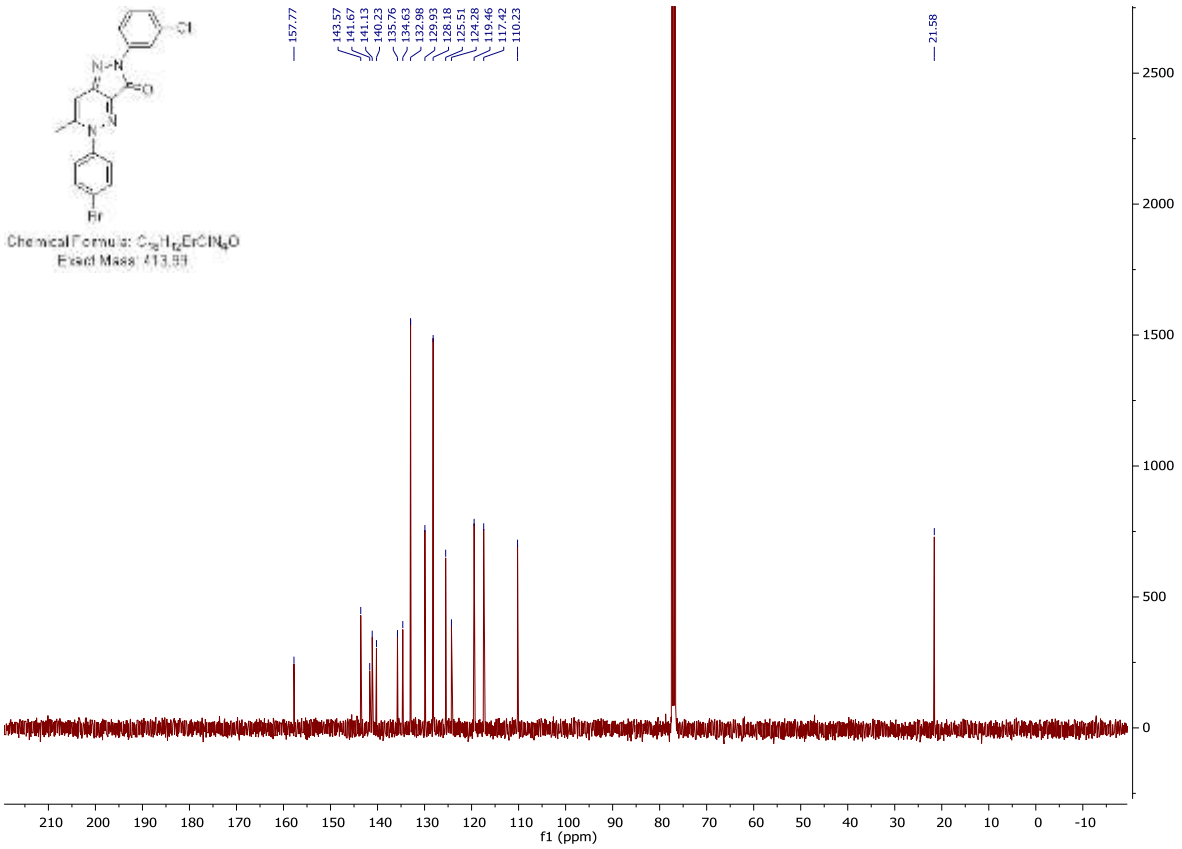
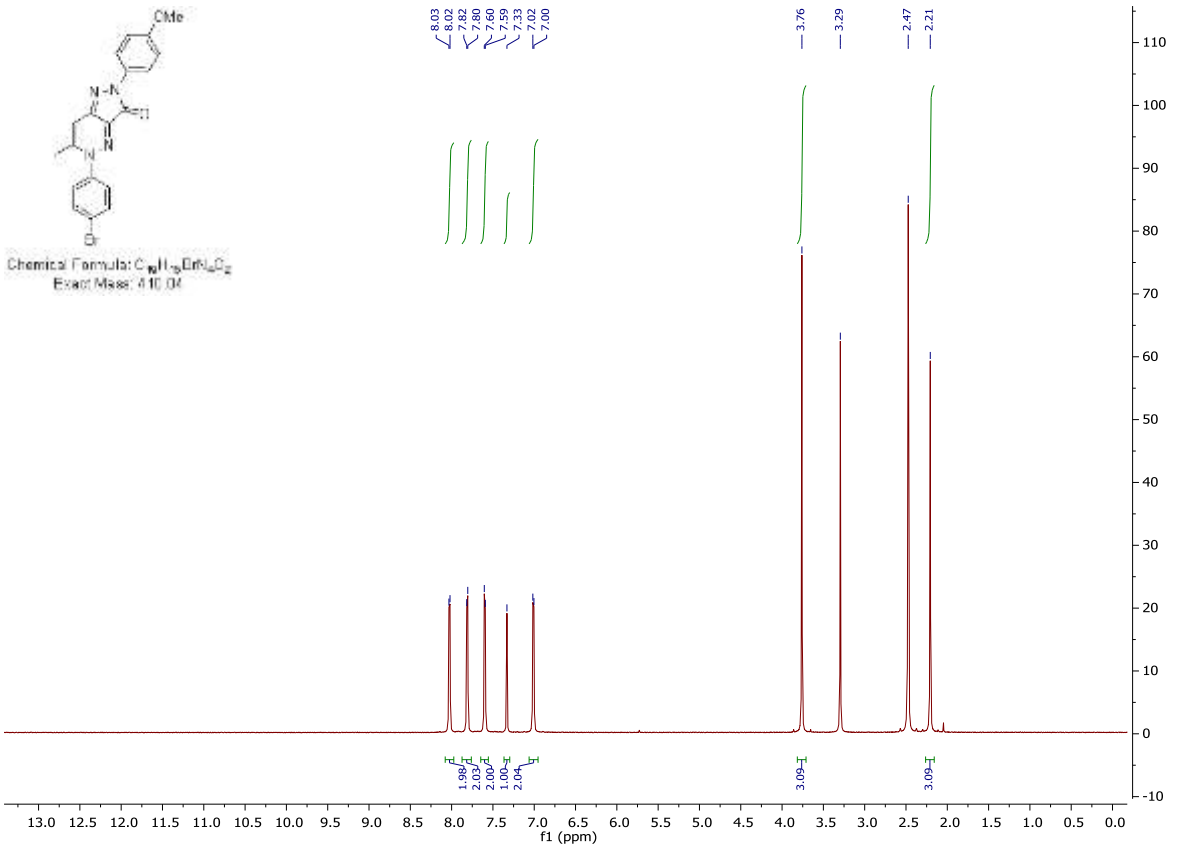
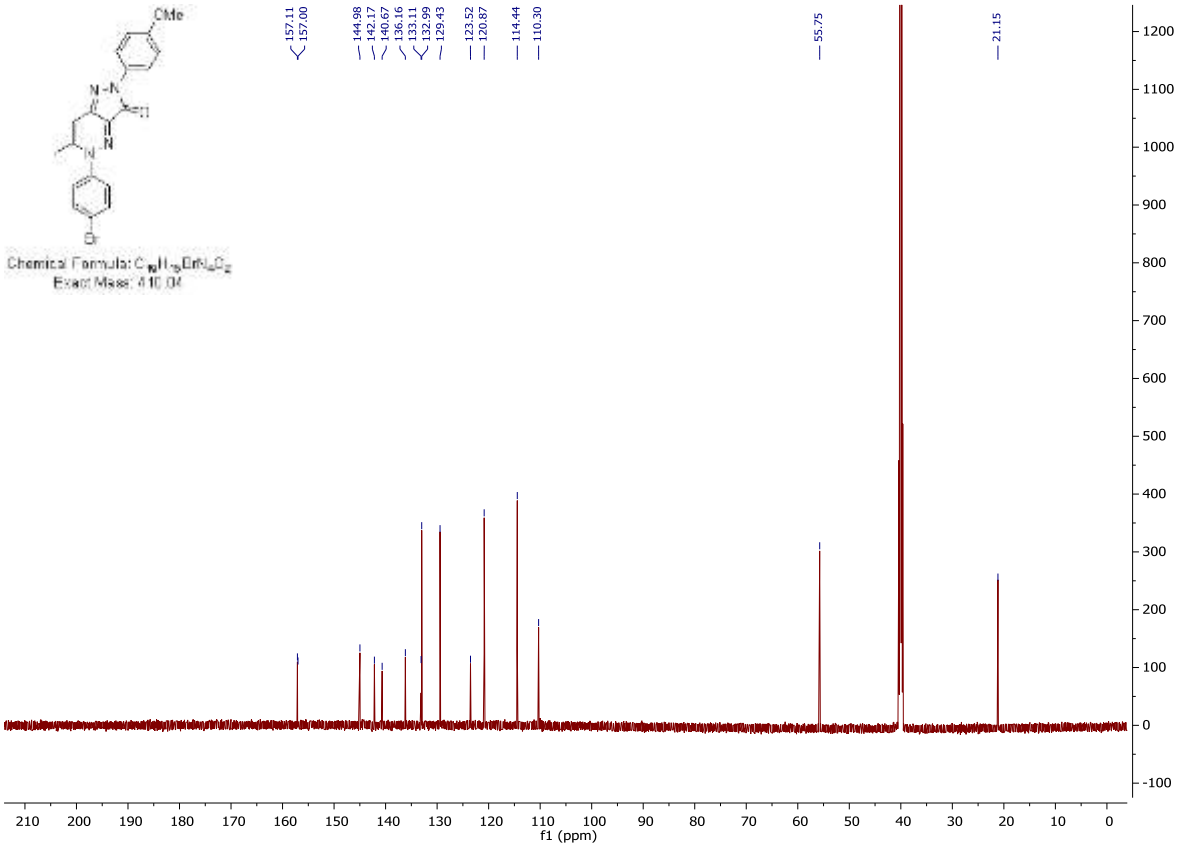
2.01
2.01
1.00
3.02
3.02
f1 (ppm)

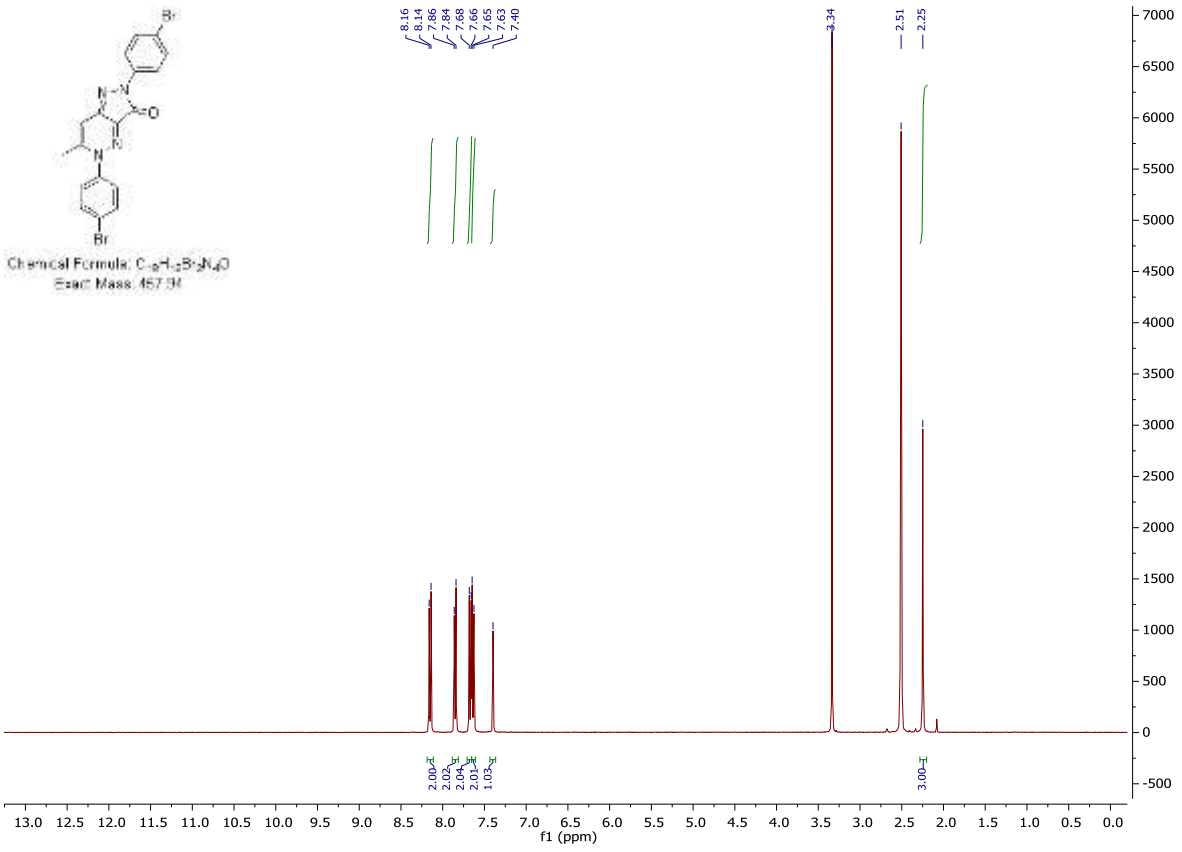

OMe
Br
Chemical Formula: C19H15BrN4O2
Exact Mass: 410.04
160.03
157.77
145.39
142.16
140.80
140.70
136.55
133.04
130.24
129.46
123.60
111.45
111.20
110.43
104.85
55.67
21.20
f1 (ppm)

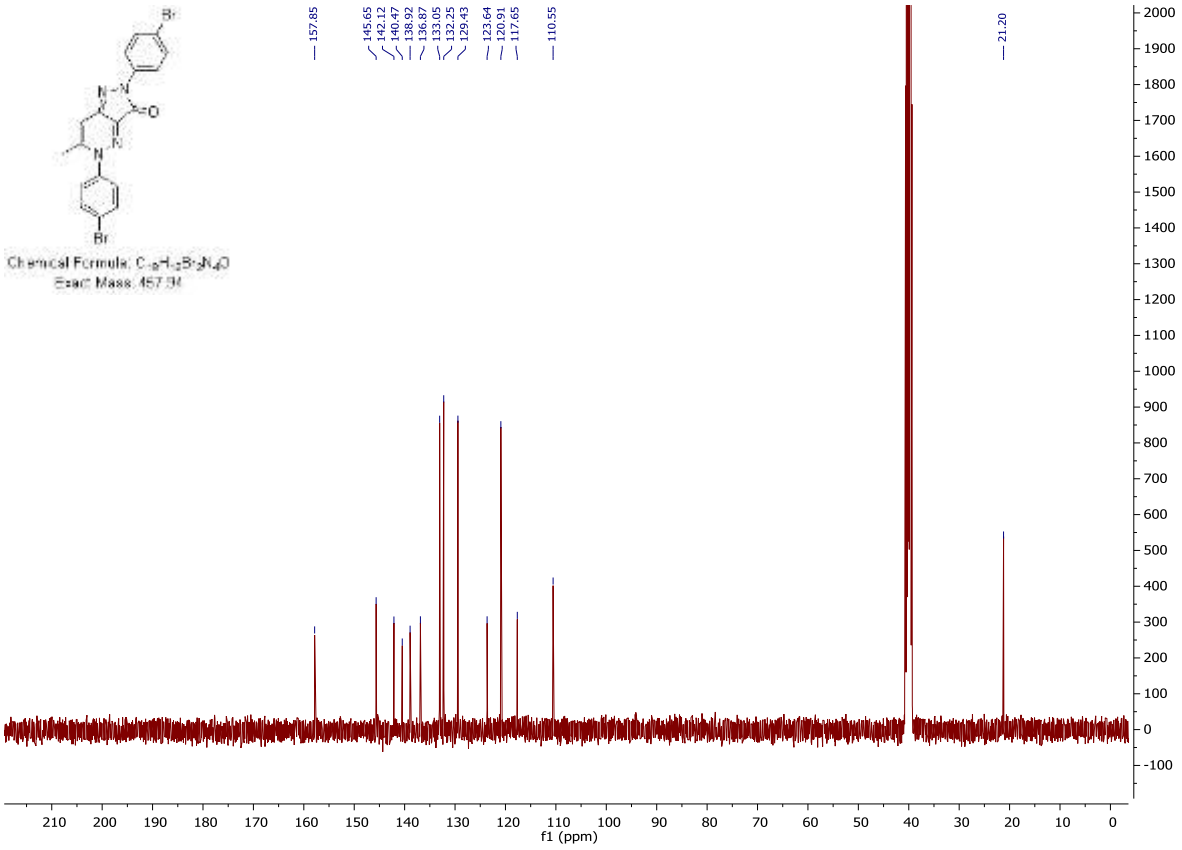

Cl
Br
Chemical Formula: C18H12BrClN4O
Exact Mass: 413.99
8.27
8.26
8.26
8.23
8.22
8.21
8.20
7.73
7.71
7.41
7.39
7.37
7.32
7.30
7.28
7.24
7.23
7.22
7.21
6.96
2.29
0.95
1.01
2.02
1.03
2.00
1.01
1.00
3.12
f1 (ppm)

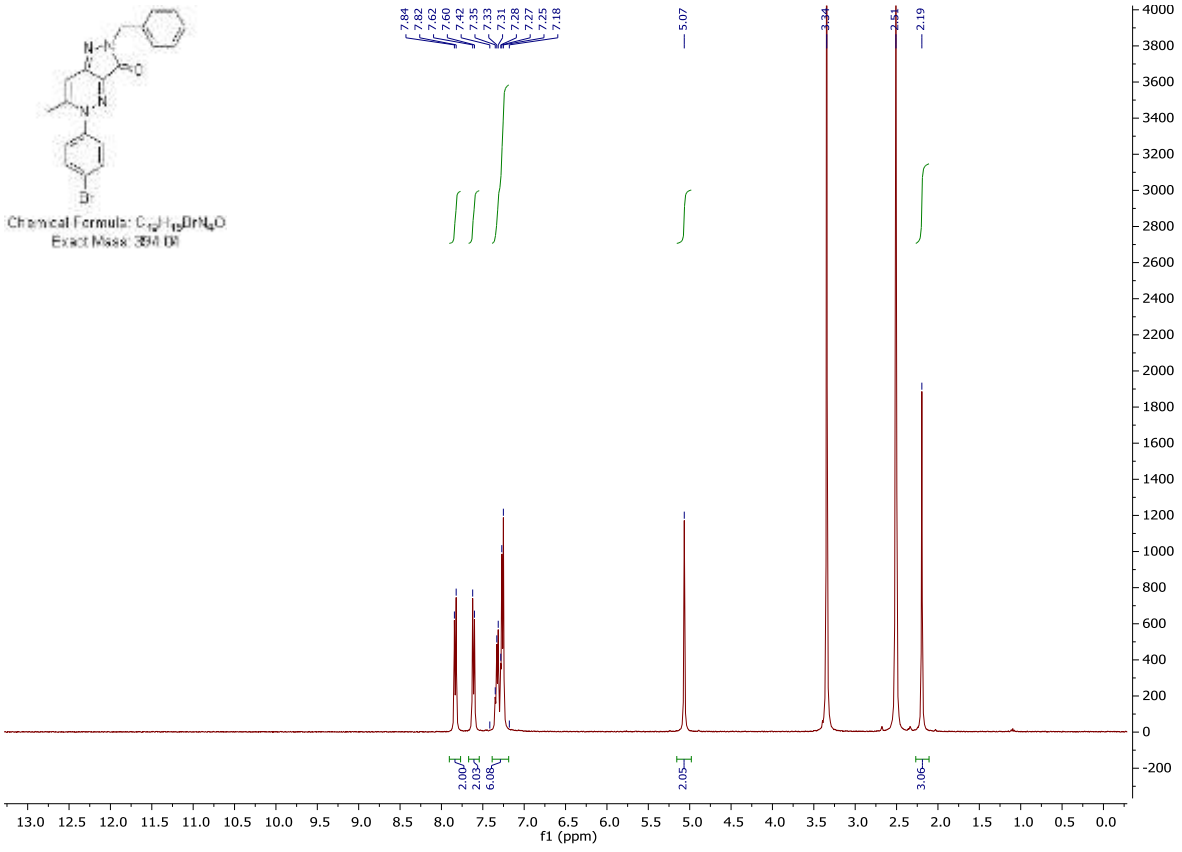

Cl
N-N
O
N
N
Br
Chemical Formula: C16H12BrClN4O
Exact Mass: 413.99
157.77
143.57
141.67
141.13
140.23
135.76
134.63
132.98
129.93
128.18
125.51
124.28
119.46
117.42
110.23
21.58
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

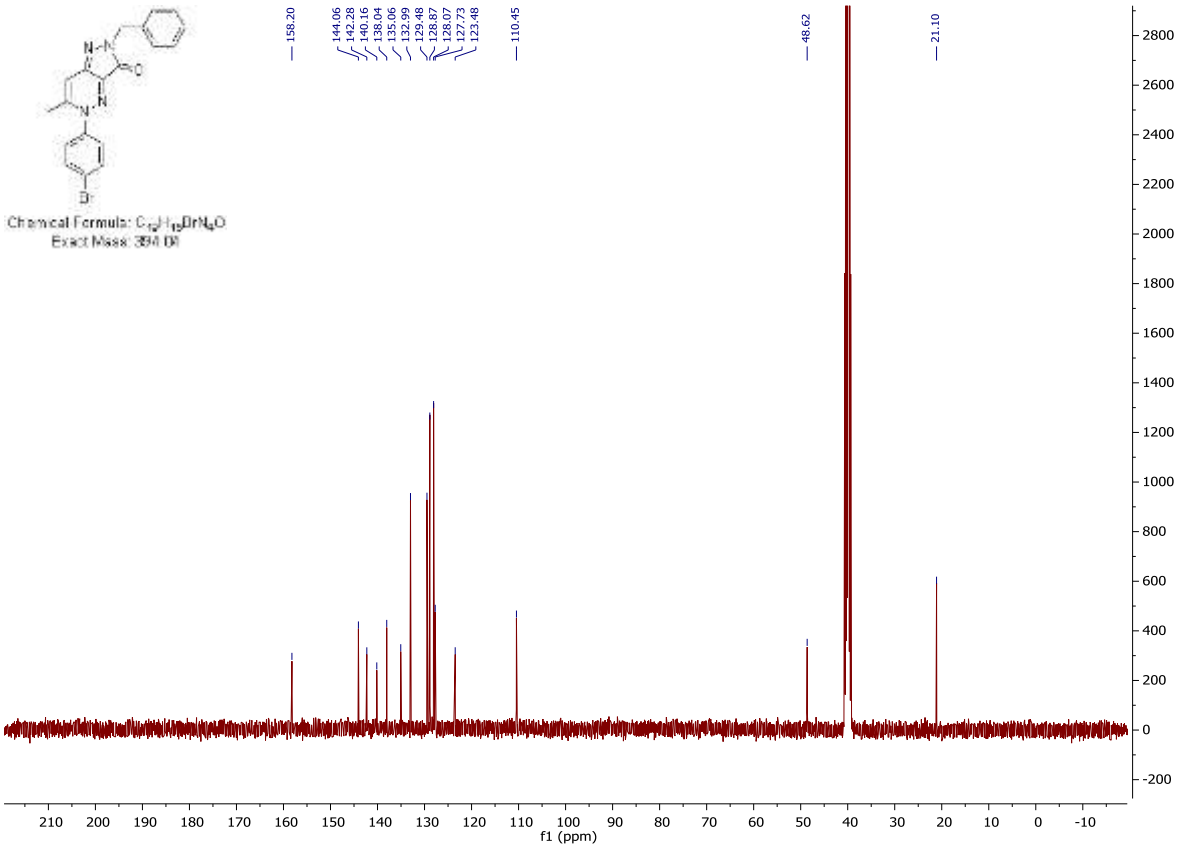

CMe
N-N
O
N
N
Br
Chemical Formula: C17H15BrN4O2
Exact Mass: 410.04
8.03
8.02
7.82
7.80
7.60
7.59
7.33
7.02
7.00
3.76
3.29
2.47
2.21
1.98
2.03
2.00
1.00
2.04
3.09
3.09
110
100
90
80
70
60
50
40
30
20
10
0
-10
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

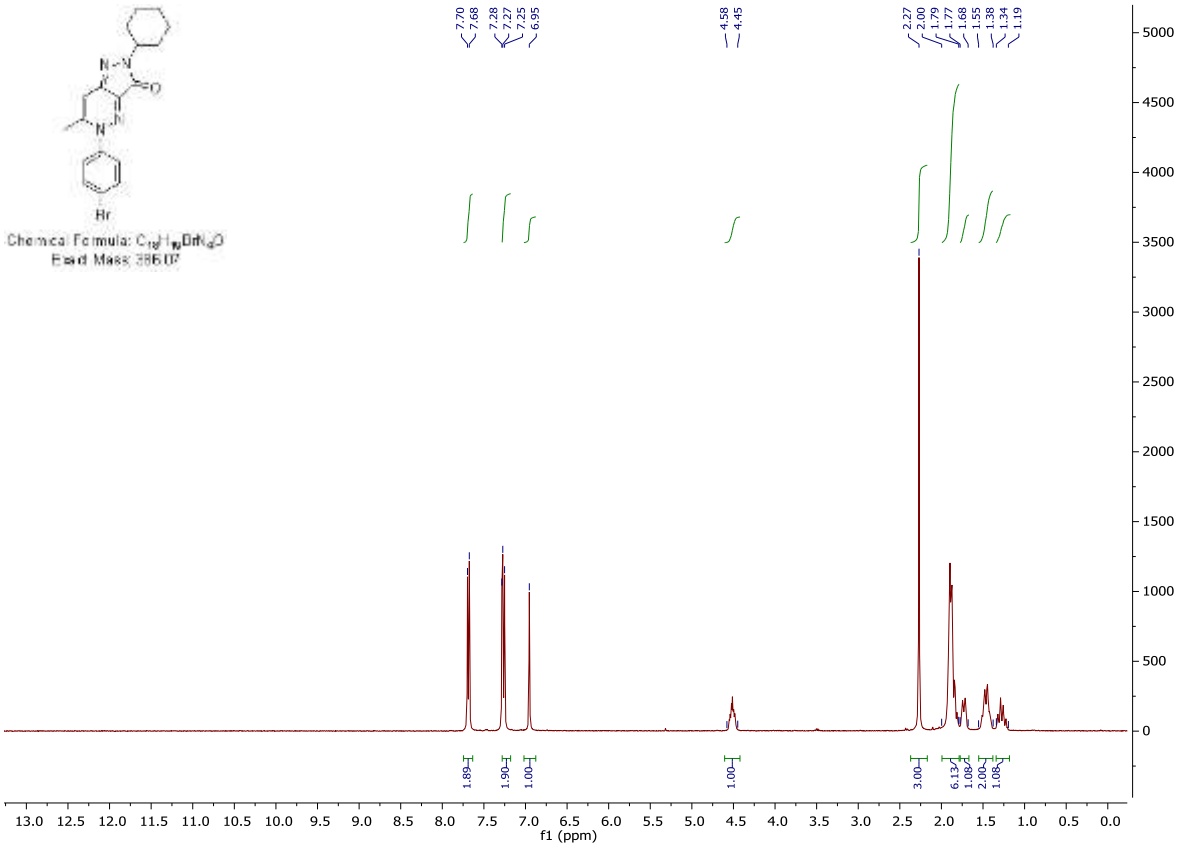

OMe
Br
Chemical Formula: C18H15BrN4O2
Exact Mass: 398.04
157.11
157.00
144.98
142.17
140.67
136.16
133.11
132.99
129.43
123.52
120.87
114.44
110.30
55.75
21.15
f1 (ppm)

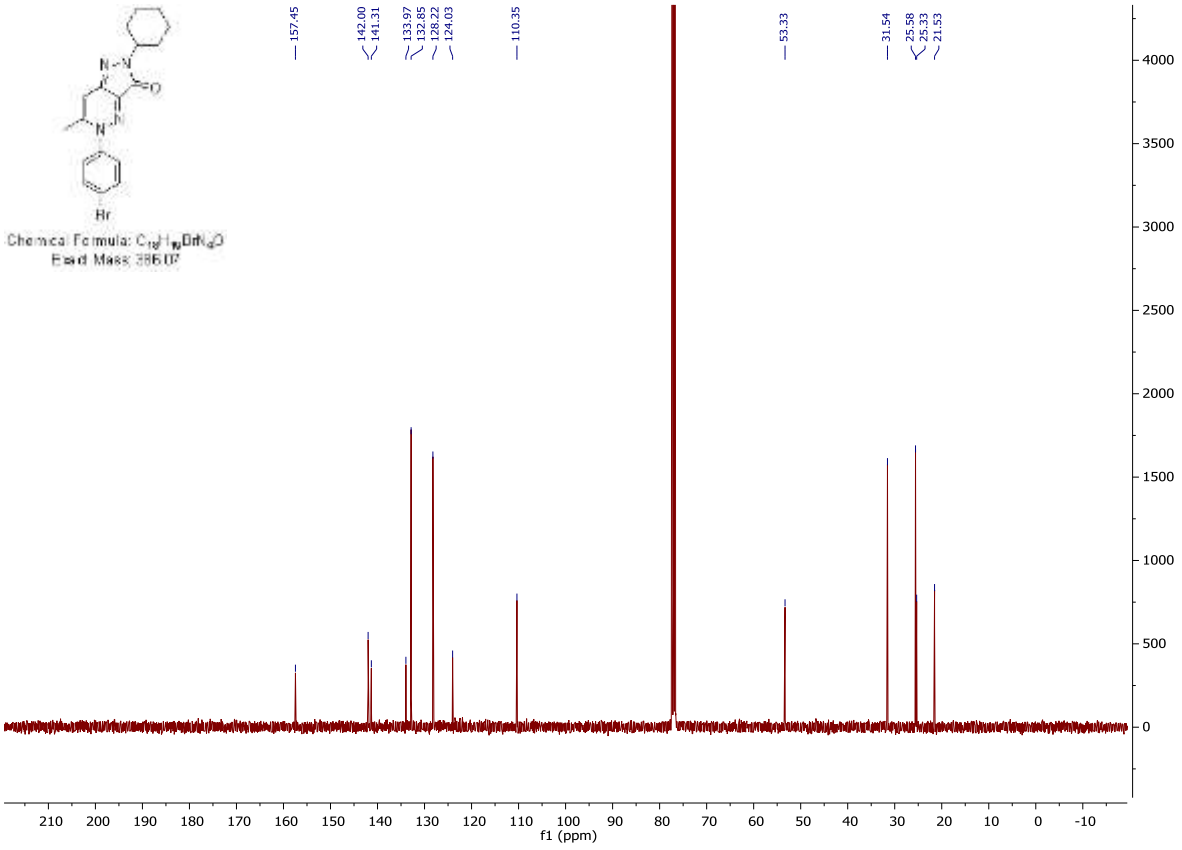

Br
O
Br
Chemical Formula: C18H12Br2N4O
Exact Mass: 457.94
8.16
8.14
7.86
7.84
7.68
7.66
7.65
7.63
7.40
3.34
2.51
2.25
2.00
2.02
2.04
2.01
1.03
3.00
f1 (ppm)

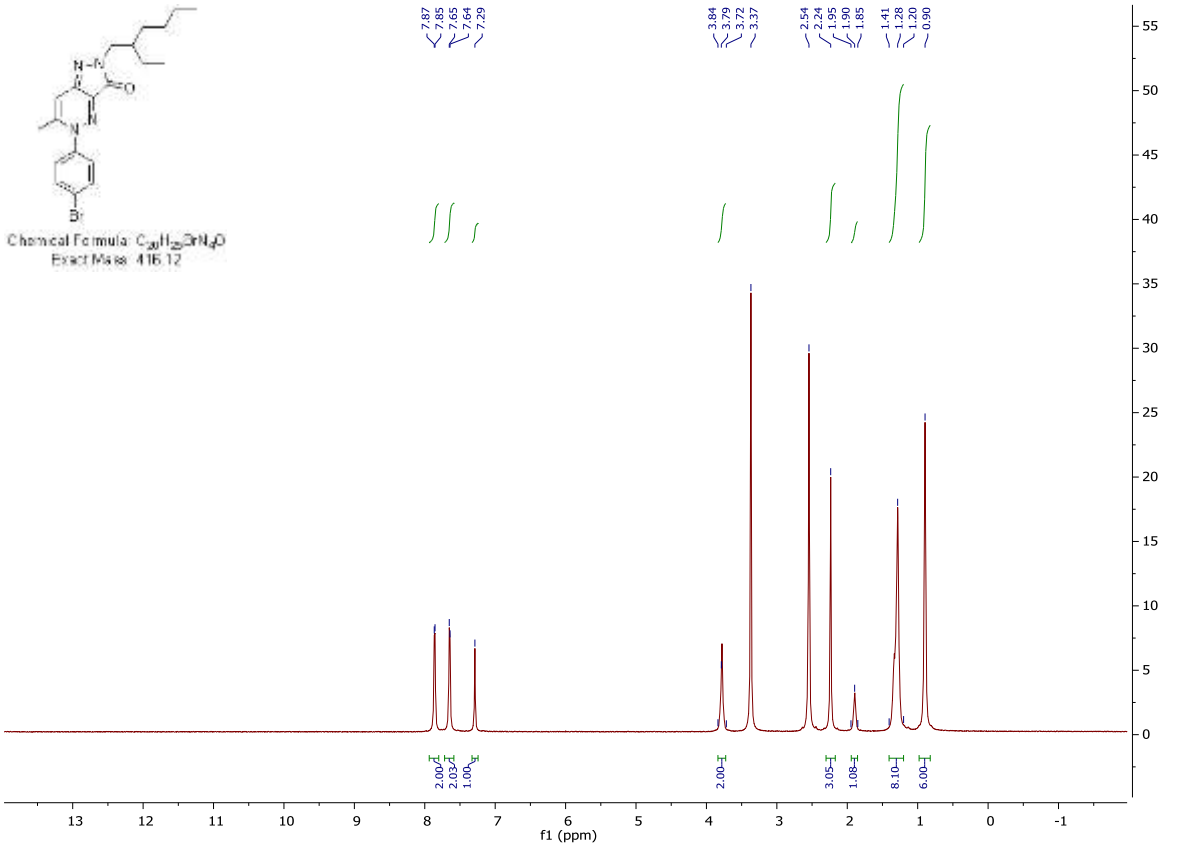

Chemical Formula: C16H12Br2N4O
Exact Mass: 457.94
157.85
145.65
142.12
140.47
138.92
136.87
133.05
132.25
129.43
123.64
120.91
117.65
110.55
21.20
f1 (ppm)

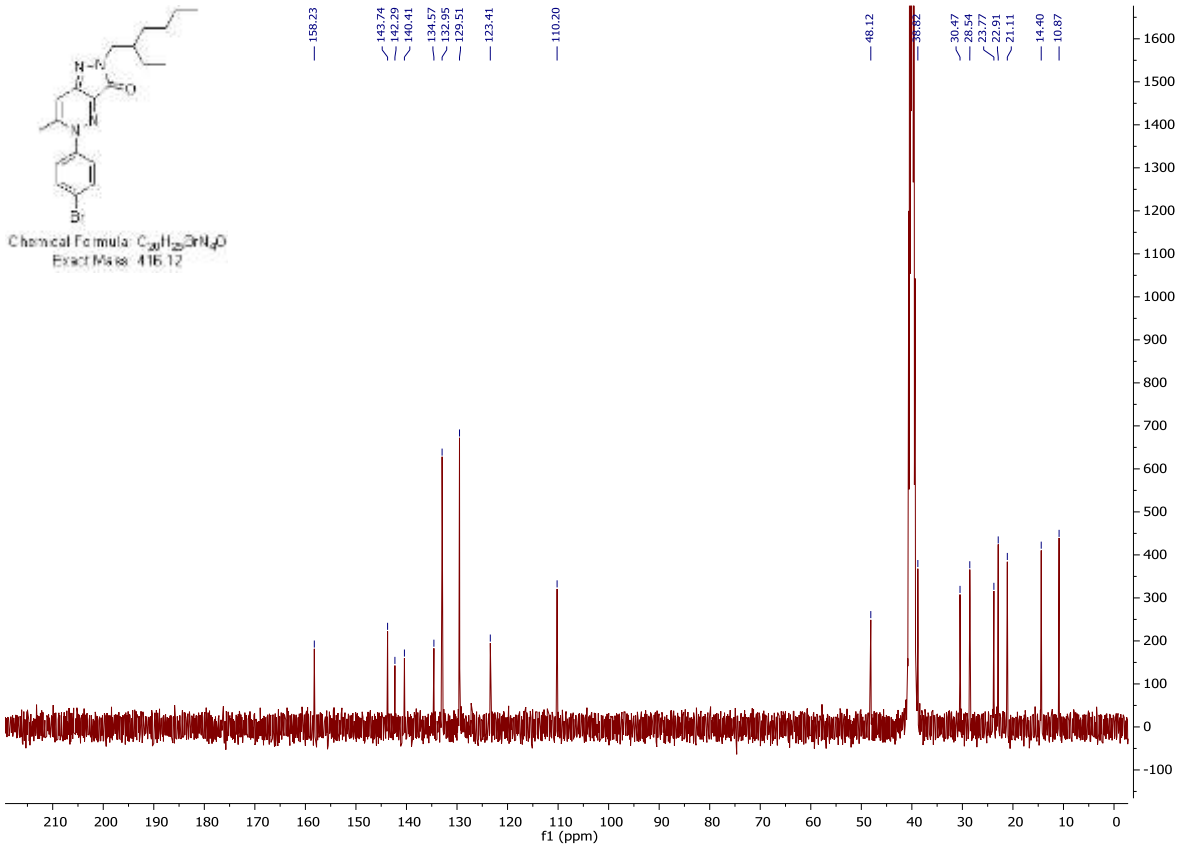

Chemical Formula: C17H15BrN4O
Exact Mass: 394.04
7.84
7.82
7.62
7.60
7.42
7.35
7.33
7.31
7.28
7.27
7.25
7.18
5.07
3.34
2.81
2.19
2.00
2.03
6.08
2.05
3.06
f1 (ppm)


158.20
144.06
142.28
140.16
138.04
135.06
132.99
129.48
128.87
128.07
127.73
123.48
110.45
48.62
21.10
f1 (ppm)


7.70
7.68
7.28
7.27
7.25
6.95
4.58
4.45
2.27
2.00
1.79
1.77
1.68
1.55
1.38
1.34
1.19
1.89
1.90
1.00
1.00
3.00
6.13
1.08
2.00
1.08
f1 (ppm)

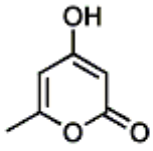

157.45
142.00
141.31
133.97
132.85
128.22
124.03
110.35
53.33
31.54
25.58
25.33
21.53
Chemical Formula: C18H19BrN2O
Exact Mass: 358.07
f1 (ppm)


7.87
7.85
7.65
7.64
7.29
3.84
3.79
3.72
3.37
2.54
2.24
1.95
1.90
1.85
1.41
1.28
1.20
0.90
Chemical Formula: C20H23BrN2O
Exact Mass: 386.10
f1 (ppm)

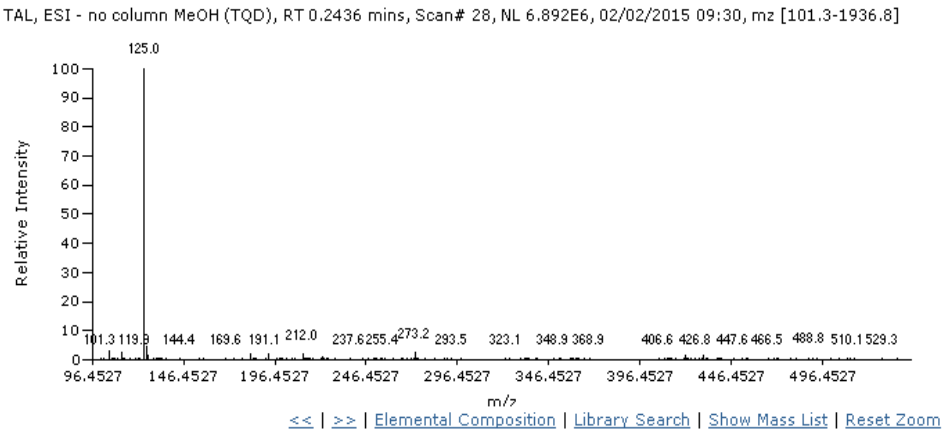

158.23
143.74
142.29
140.41
134.57
132.95
129.51
123.41
110.20
48.12
39.82
30.47
28.54
23.77
22.91
21.11
14.40
10.87
Chemical Formula: C20H25BrN4O
Exact Mass: 416.12
f1 (ppm)

B. Copies of Mass Spectra

B1. Building block 1,2



Chemical Formula: $C_6H_6O_3$
Exact Mass: 126,03

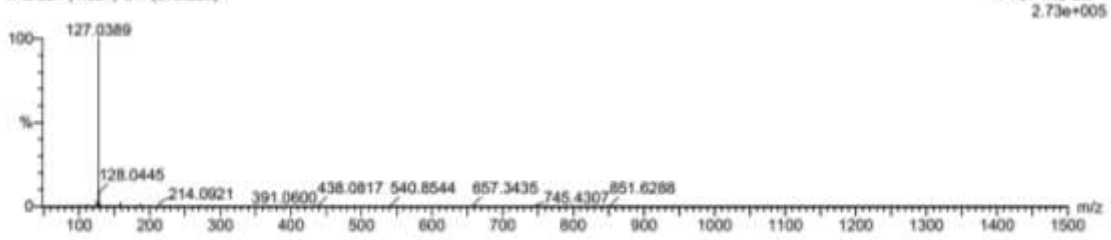


Monoisotopic Mass, Even Electron Ions
145 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-75 H: 0-90 N: 0-10 O: 0-15 S: 0-2

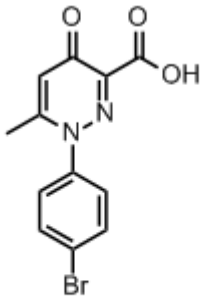
02-Feb-2015
12:16:02
TAL 221 (1.827) Cm (212:229)

QToF Premier
Paolo Filipponi

1: TOF MS ES+
2.73e+005

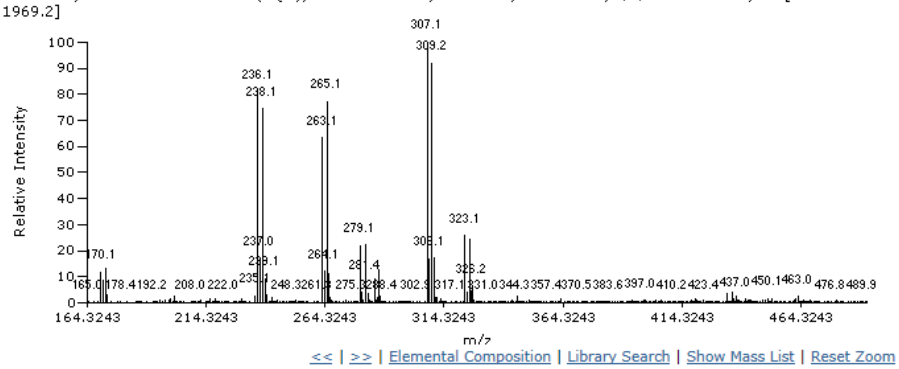


Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
127.0389	127.0395	-0.6	-4.7	3.5	815.4	0.0	C6 H7 O3
	127.0368	2.1	16.5	4.5	822.3	6.9	C2 H3 N6 O
	127.0364	2.5	19.7	-1.5	829.0	13.6	C2 H11 N2 S2
	127.0355	3.4	26.8	-0.5	822.5	7.1	C H7 N2 O5
	127.0429	-4.0	-31.5	-1.5	826.3	10.9	C3 H11 O3 S



Chemical Formula: $C_{12}H_9BrN_2O_3$
Exact Mass: 307.9797

mbs2-4Br, ESI - no column MeOH (TQD), RT 0.3069 mins, Scan# 18, NL 4.773E6, 7/3/2014 1:36 PM, mz [99.9-1969.2]

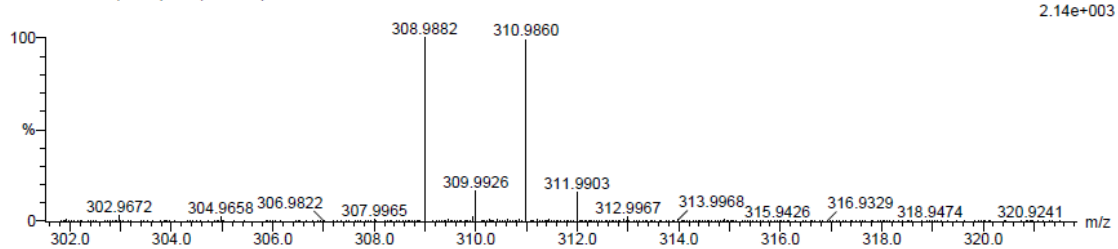


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
9026 formula(e) evaluated with 92 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2 Br: 0-2

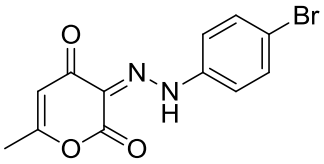
Marcus Baumann
MBS2-4Br 326 (2.686) Cm (321:331)

1: TOF MS ES+
2.14e+003

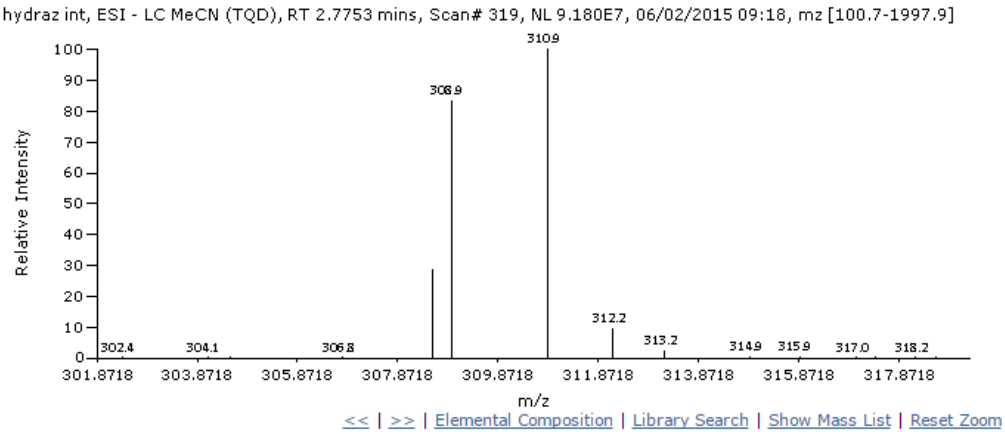


Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
308.9882	308.9875	0.7	2.3	8.5	178.8	0.2	C12 H10 N2 O3 Br
	308.9900	-1.8	-5.8	9.5	181.4	2.8	C10 H7 N6 F Br
	308.9873	0.9	2.9	4.5	181.6	2.9	C10 H12 N2 F2 S Br
	308.9886	-0.4	-1.3	4.5	182.4	3.8	C9 H11 N2 O4 F Br
	308.9884	-0.2	-0.6	0.5	183.8	5.2	C7 H13 N2 O F3 S Br
	308.9909	-2.7	-8.7	3.5	184.2	5.6	C9 H14 N2 O3 S Br
	308.9893	-1.1	-3.6	3.5	184.8	6.2	C11 H15 O3 Cl Br

B2. Compounds 5-7.



Chemical Formula: $C_{12}H_9BrN_2O_3$
Exact Mass: 307.98

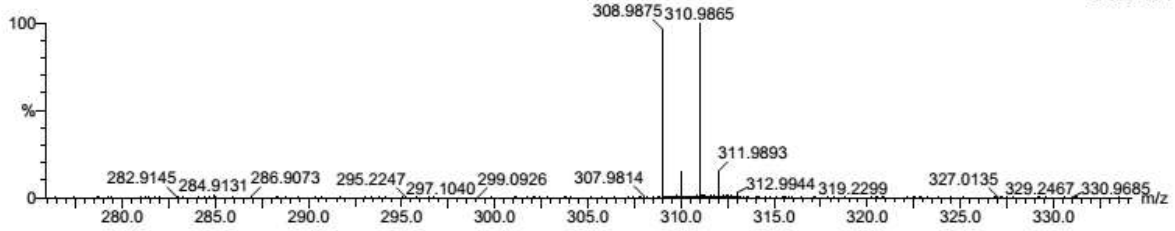


Monoisotopic Mass, Even Electron Ions
1491 formula(e) evaluated with 23 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-75 H: 0-90 N: 0-10 O: 0-15 P: 0-1 Br: 0-2

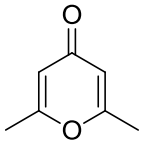
06-Feb-2015
14:13:46
Hydraz int 405 (3.333) Cm (399:417)

QToF Premier
Paolo Filipponi

1: TOF MS ES+
6.52e+004

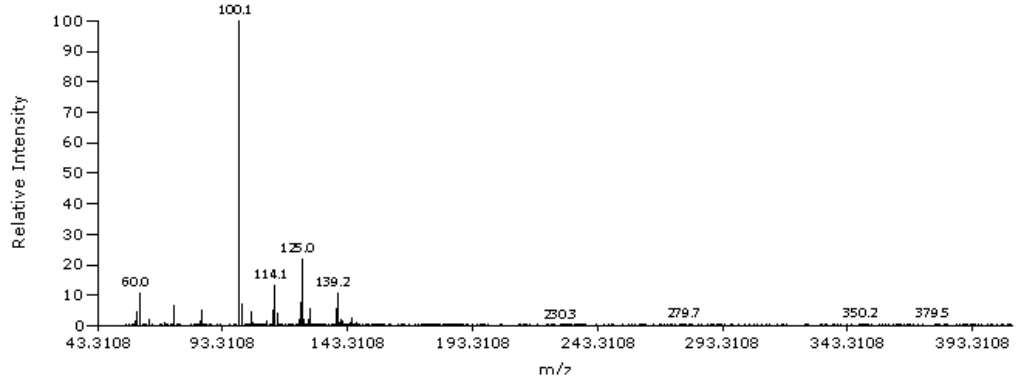


Minimum:				-1.5			
Maximum:		5.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
308.9875	308.9875	0.0	0.0	8.5	561.6	0.5	C12 H10 N2 O3 Br
	308.9872	0.3	1.0	6.5	579.6	18.5	C6 H6 N4 O9 P
	308.9883	-0.8	-2.6	10.5	579.8	18.7	C12 H5 O10
	308.9886	-1.1	-3.6	11.5	579.5	18.4	C7 H2 N8 O5 P
	308.9864	1.1	3.6	4.5	565.4	4.3	C6 H11 N6 O2 P Br
	308.9891	-1.6	-5.2	3.5	565.9	4.8	C10 H15 O4 P Br
	308.9859	1.6	5.2	1.5	579.5	18.4	C5 H10 O13 P



Chemical Formula: $C_7H_8O_2$
Exact Mass: 124.05

3,3-dimethylpyranone, ESI - no column MeOH (TQD), RT 1.0400 mins, Scan# 61, NL 7.038E7, 14/10/2015 08:47, mz [54.7-1997.9]



<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

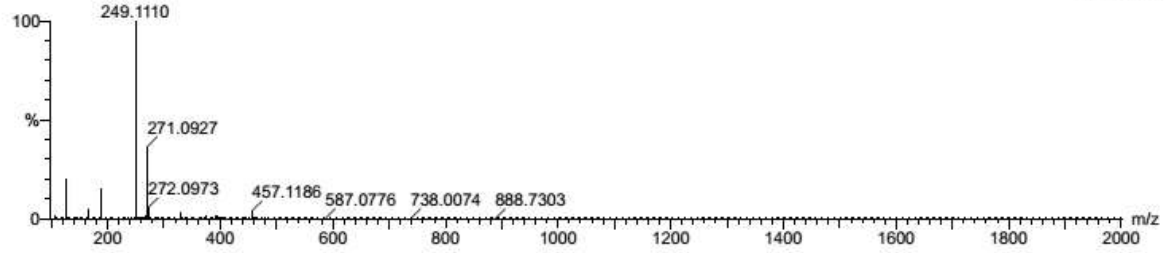
Monoisotopic Mass, Even Electron Ions
79 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-80 N: 0-6 O: 0-6 Br: 0-2

Paolo Filipponi
1: TOF MS ES+

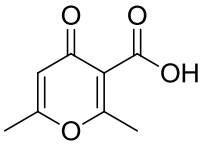
LCT Premier

dimethylpyranone 62 (1.415) Cm (61:64)

3.61e+005

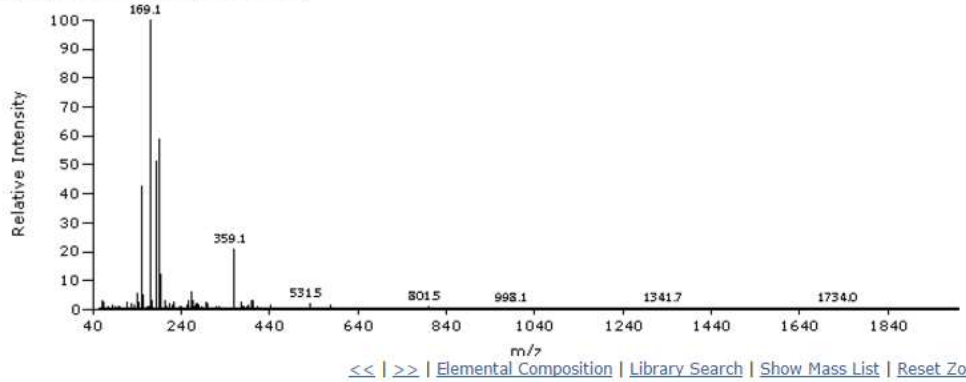


Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
125.0589	125.0603	-1.4	-11.2	3.5	630.6	0.0	C7 H9 O2
	125.0562	2.7	21.6	-0.5	639.9	9.4	C2 H9 N2 O4
	125.0576	1.3	10.4	4.5	641.5	11.0	C3 H5 N6



Chemical Formula: $C_8H_8O_4$
Exact Mass: 168.04

3,5-dimethylpyranone-2-Carboxy, ESI - no column MeOH (TQD), RT 0.3580 mins, Scan# 21, NL 9.423E7, 19/10/2015 13:02, mz [54.9-1999.3]

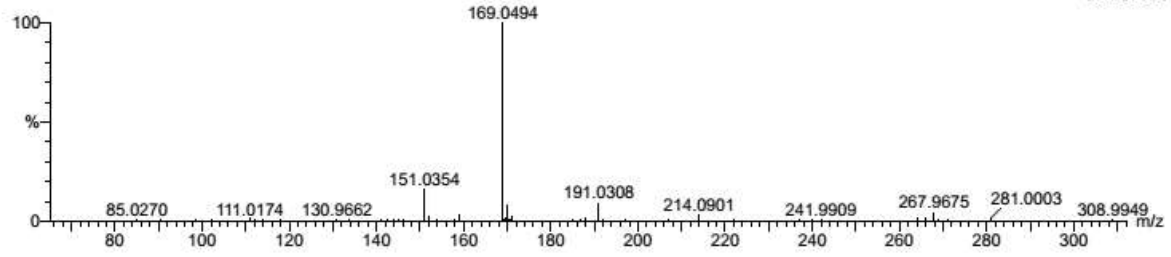


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
520 formula(e) evaluated with 6 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-10 P: 0-1 S: 0-3 96Ru: 0-1

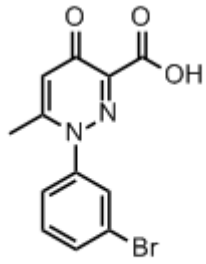
Paolo Filipponi
PF1 201 (1.663) Cm (201:207)

1: TOF MS ES+
5.12e+004

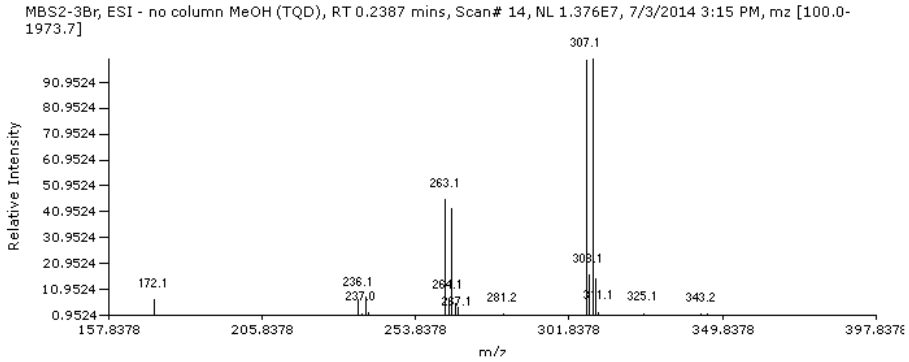


Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
169.0494	169.0501	-0.7	-4.1	4.5	535.6	0.1	C8 H9 O4
	169.0474	2.0	11.8	5.5	538.2	2.7	C4 H5 N6 O2
	169.0514	-2.0	-11.8	9.5	539.0	3.5	C9 H5 N4
	169.0491	0.3	1.8	0.5	540.2	4.7	C2 H10 N4 O3 P
	169.0508	-1.4	-8.3	0.5	542.3	6.8	C H9 N6 O2 S

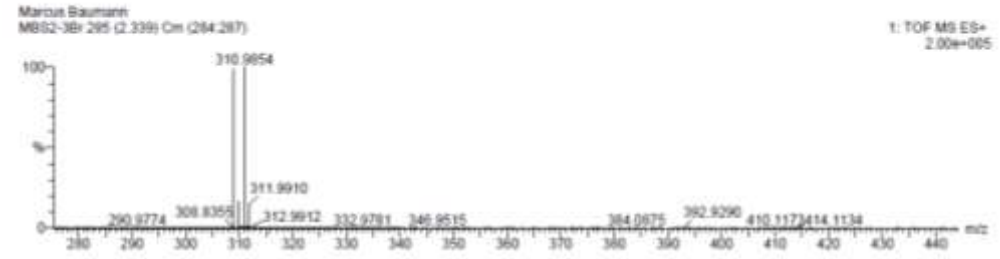
B2. Serie A derivatives 8-14.



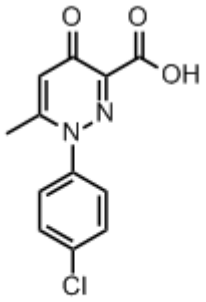
Chemical Formula: $C_{12}H_9BrN_2O_3$
Exact Mass: 307.9797



Monoisotopic Mass, Even Electron Ions
9026 formula(e) evaluated with 92 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2 Br: 0-2

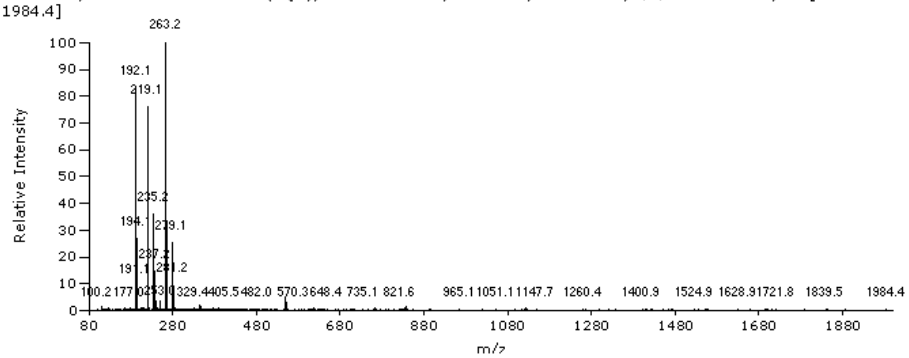


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
300.9871	300.9875	-0.4	-1.3	8.5	579.5	0.3	C12 H10 N2 O3 Br
	300.9900	-2.9	-9.6	9.5	582.7	2.4	C10 H7 N6 F Br
	300.9873	-0.2	-0.6	4.5	582.1	2.9	C10 H12 N2 F2 S Br
	300.9850	2.1	6.9	5.5	582.7	3.4	C10 H9 N2 O F3 Br
	300.9884	-1.5	-4.9	4.5	583.4	4.1	C9 H11 N2 O4 F Br
	300.9843	2.5	7.6	9.5	583.9	4.6	C8 H6 N5 O Br
	300.9904	-3.3	-4.2	0.5	584.3	5.5	C7 H13 N2 O F3 S Br
	300.9857	1.4	4.5	4.5	584.9	5.6	C12 H13 F2 Cl Br
	300.9893	-2.2	-7.1	3.5	585.0	5.7	C11 H15 O3 Cl Br
	300.9869	0.2	0.6	0.5	585.5	6.2	C9 H14 O F3 Cl Br
	300.9898	-2.7	-8.7	0.5	585.5	6.2	C4 H12 N2 O5 F2 Br
	300.9897	-2.6	-8.4	6.5	585.9	6.6	C12 H9 O2 F2 Cl



Chemical Formula: $C_{12}H_9ClN_2O_3$
Exact Mass: 264.0302

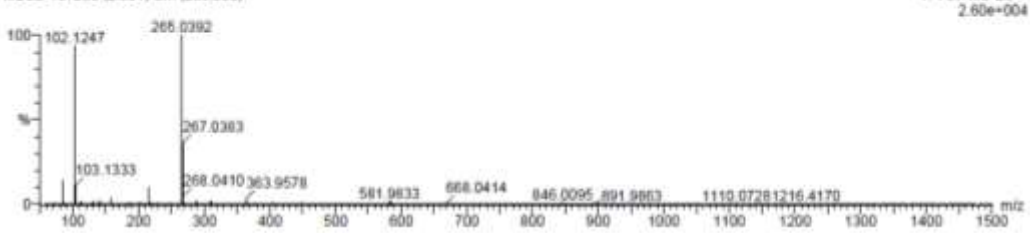
MBS2-4Cl, ESI - no column MeOH (TQD), RT 0.3410 mins, Scan# 20, NL 4.132E6, 7/3/2014 3:16 PM, mz [100.2-1984.4]



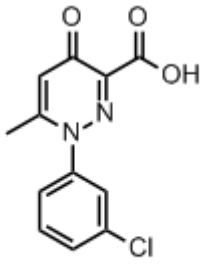
Monoisotopic Mass, Even Electron Ions
5480 formula(e) evaluated with 53 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2 Br: 0-2

Marcus Baumann
MBS2-4Cl 286 (2.351) Cm (286:300)

1: TOF MS ES+
2.60e+004

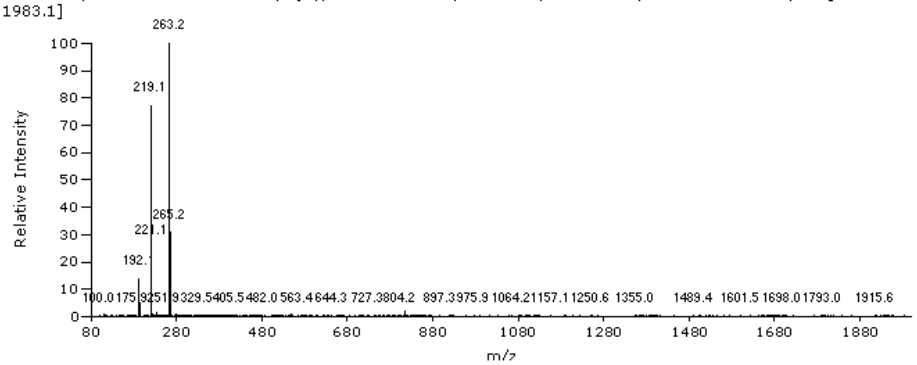


Minimum:			-1.5				
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
265.0392	265.0380	1.2	4.5	8.5	401.8	0.4	C12 H10 N2 O3 Cl
	265.0420	-2.8	-10.6	12.5	403.6	2.2	C17 H10 O Cl
	265.0405	-1.3	-4.9	9.5	403.0	2.4	C10 H7 N6 F Cl
	265.0370	1.4	5.3	4.5	404.3	2.9	C10 H12 N2 F2 S Cl
	265.0414	-2.12	-8.0	3.5	405.1	3.7	C9 H14 N2 O3 S Cl
	265.0391	0.1	0.4	4.5	405.2	3.8	C9 H11 N2 O4 F Cl
	265.0389	0.3	1.1	0.5	407.1	5.7	C7 H13 N2 O F3 S Cl
	265.0416	-2.4	-9.1	5.5	407.1	5.7	C7 H9 N6 O F2 Cl
	265.0403	-1.1	-4.2	0.5	407.4	6.0	C6 H12 N2 O5 F2 Cl
	265.0387	0.5	1.9	4.5	408.5	7.1	C5 H10 N6 O S Cl
	265.0365	2.7	10.2	5.5	408.1	7.7	C5 H7 N8 O2 F Cl
	265.0373	1.9	7.2	-0.5	409.4	9.0	C4 H14 N4 O5 S Cl
	265.0382	1.0	3.8	3.5	409.4	9.0	C9 H13 O7 S
	265.0393	-0.1	-0.4	-0.5	409.5	9.1	C6 H14 O8 F S
	265.0390	-0.8	-2.3	3.5	409.6	9.2	C11 H15 O3 Cl2
	265.0403	-1.1	-4.2	2.5	409.9	9.4	C11 H16 F2 Br
	265.0410	-1.8	-6.8	-0.5	410.0	9.6	C9 H16 O4 F Cl2



Chemical Formula: $C_{12}H_9ClN_2O_3$
Exact Mass: 264.0302

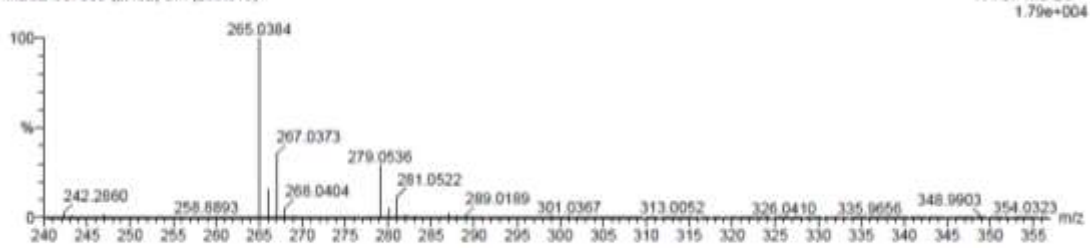
mbs203Cl, ESI - no column MeOH (TQD), RT 0.2728 mins, Scan# 16, NL 2.325E7, 7/3/2014 1:33 PM, mz [100.0-1983.1]



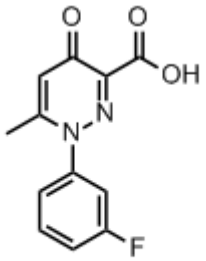
<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
3963 formula(e) evaluated with 50 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2
Marcus Baumann
MBS2-3Cl 303 (2.492) Cm (298:319)

1: TOF MS ES+
1.79e+004

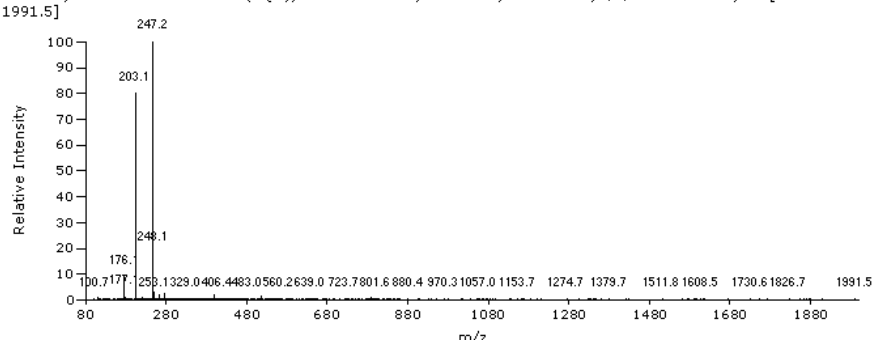


Minimum:			-1.5				
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
265.0384	265.0383	0.1	0.4	0.5	382.0	12.4	C4 H12 N6 O2 F C12
	265.0385	-0.1	-0.4	5.5	384.6	17.0	C7 H7 N4 O5 F2
	265.0386	-0.2	-0.8	14.5	386.5	16.9	C11 H2 N8 F
	265.0382	0.2	0.8	3.5	379.8	10.2	C9 H13 O7 S
	265.0387	-0.3	-1.1	4.5	379.2	8.6	C5 H10 N8 O S Cl
	265.0380	0.4	1.5	0.5	369.7	0.1	C12 H10 N2 O3 Cl
	265.0380	0.4	1.5	0.5	387.6	18.0	C H9 N6 O10
	265.0380	0.4	1.5	5.5	384.2	14.6	C3 N6 N10 O2 F S
	265.0389	-0.5	-1.9	0.5	376.7	7.0	C7 H13 N2 O F3 S Cl
	265.0378	0.6	2.3	4.5	373.7	4.1	C10 H12 N2 F2 S Cl
	265.0391	-0.7	-2.6	1.5	385.9	16.3	H7 N10 O3 F2 S
	265.0391	-0.7	-2.6	4.5	374.5	4.9	C9 H11 N2 O4 F Cl



Chemical Formula: $C_{12}H_{9F}N_2O_3$
Exact Mass: 248.0597

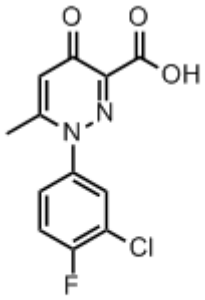
mbs2-3F, ESI - no column MeOH (TQD), RT 0.2728 mins, Scan# 16, NL 1.776E7, 7/3/2014 1:32 PM, mz [100.7-1991.5]



Monoisotopic Mass, Even Electron Ions
3334 formula(e) evaluated with 34 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2
Marcus Baumann
MBS2-3F 240 (1.976) Cm (240:268)

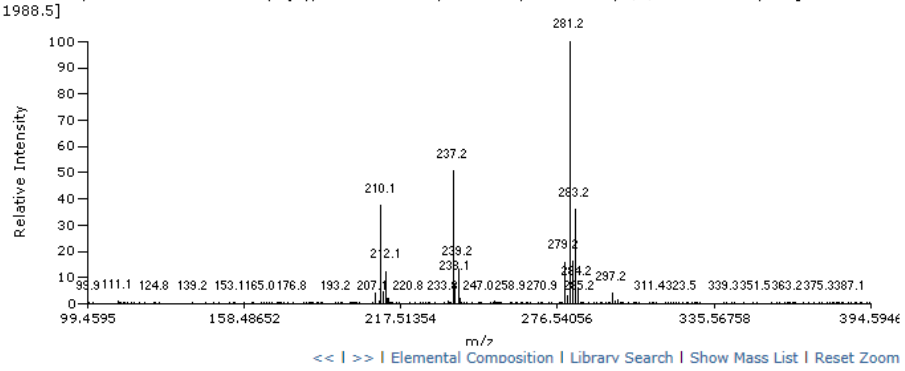
1: TOF MS ES+
1.24e+005

Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
249.0679	249.0670	0.1	0.4	0.5	654.5	15.3	C4 H12 N4 O2 F2 Cl
	249.0682	-0.3	-1.2	7.5	656.4	15.7	C14 H14 O2 Cl
	249.0676	0.3	1.2	-1.5	654.7	16.0	C6 H10 N2 O4 S Cl
	249.0682	-0.3	-1.2	4.5	647.9	9.2	C5 H10 N8 O F S
	249.0683	-0.4	-1.6	-0.5	645.2	6.5	C3 H13 N4 O9
	249.0675	0.4	1.6	0.5	639.1	0.4	C12 H10 N2 O3 F
	249.0674	0.5	2.0	3.5	655.3	16.6	C9 H15 N4 Cl2
	249.0673	0.6	2.4	4.5	647.0	8.3	C10 H12 N2 F3 S
	249.0655	-0.6	-2.4	-0.5	655.6	16.7	C6 H16 N4 O F Cl2
	249.0671	0.0	0.2	0.5	647.1	8.4	C8 H9 N8 S
	249.0687	-0.8	-3.2	4.5	640.8	2.2	C9 H11 N2 O4 F2
	249.0671	0.0	0.2	1.5	644.7	6.0	C2 H8 N8 O3 F3



Chemical Formula: $C_{12}H_8ClFN_2O_3$
Exact Mass: 282.0207

mbs2-3CN, ESI - no column MeOH (TQD), RT 0.2387 mins, Scan# 14, NL 2.266E7, 7/3/2014 1:36 PM, mz [99.9-1988.5]

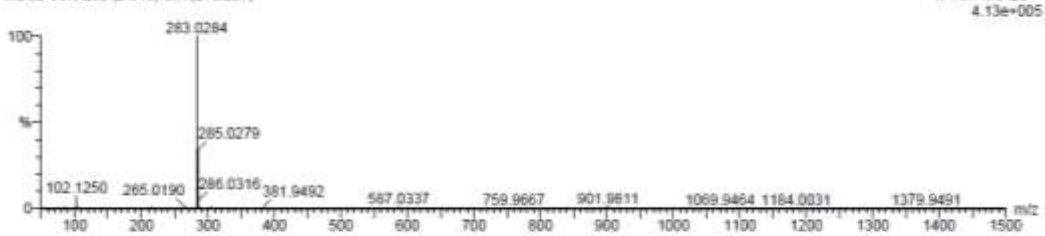


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

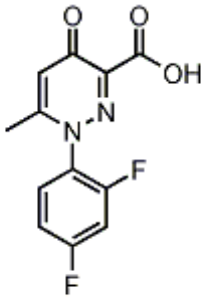
Monoisotopic Mass, Even Electron Ions
6756 formula(e) evaluated with 70 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2 Br: 0-2

Marcus Baumann
MBS2-3CN 285 (2.348) Cm (278:297)

1: TOF MS ES+
4.13e+005

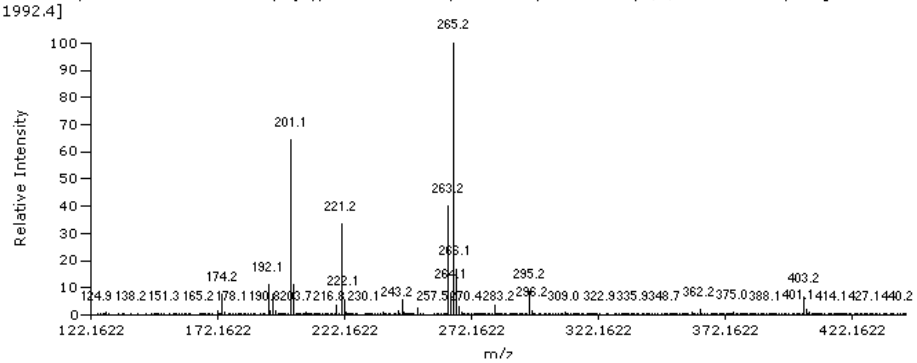


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
283.0284	283.0286	-0.2	-0.7	8.5	696.3	0.0	C12 H8 N2 O3 F Cl
	283.0311	-2.7	-9.5	9.5	700.1	3.8	C10 H6 N6 F2 Cl
	283.0308	-2.4	-8.5	7.5	704.0	7.8	C12 H12 N2 O2 S Cl
	283.0284	0.0	0.0	4.5	704.4	8.2	C10 H11 N2 F3 S Cl
	283.0259	2.5	8.8	9.5	704.6	8.4	C8 H5 N8 O F Cl
	283.0287	-1.3	-4.6	4.5	704.7	8.4	C9 H10 N2 O4 F2 Cl
	283.0274	1.0	3.5	12.5	705.1	8.9	C15 H8 N2 O2 Cl
	283.0261	0.3	1.1	8.5	705.2	8.9	C8 H8 N6 S Cl
	283.0248	1.6	5.7	3.5	707.4	11.1	C7 H12 N4 O4 S Cl
	283.0309	-2.5	-8.8	0.5	707.9	11.7	C6 H11 N2 O5 F3 Cl
	283.0293	-0.9	-3.2	4.5	708.7	12.4	C5 H9 N8 O F S Cl
	283.0270	1.4	4.9	8.5	708.8	12.5	C5 H4 N8 O2 F2 Cl
	283.0254	3.0	10.6	-1.5	708.9	12.6	C6 H16 O6 S Cl
	283.0276	0.8	2.8	7.5	709.3	13.1	C12 H11 O6 S
	283.0306	-2.2	-7.8	4.5	709.5	13.2	C4 H8 N8 O5 Cl
	283.0288	-0.4	-1.4	3.5	709.5	13.2	C9 H12 O7 F S
	283.0279	0.5	1.8	-0.5	709.7	13.4	C4 H13 N4 O5 F S Cl



Chemical Formula: $C_{12}H_{8F2}N_2O_3$
Exact Mass: 266.0503

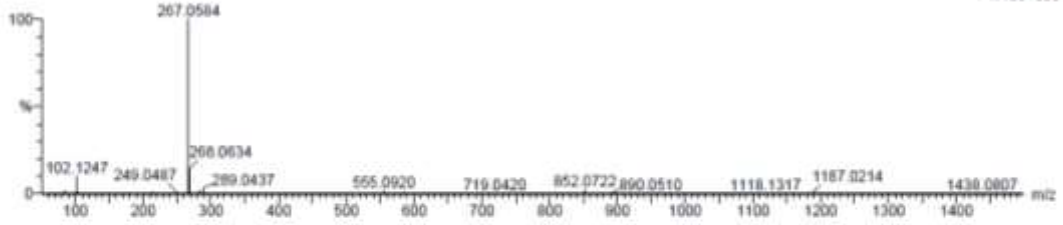
MBS2-24F, ESI - no column MeOH (TQD), RT 0.2728 mins, Scan# 16, NL 2.016E7, 7/3/2014 3:16 PM, mz [100.1-1992.4]



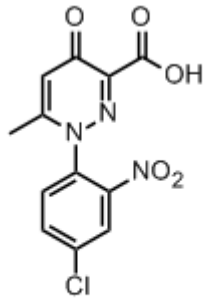
Monoisotopic Mass, Even Electron Ions
5576 formula(e) evaluated with 48 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2 Br: 0-2

Marcus Baumann
MBS2-24F 254 (2.098) Cm (254:262)

1: TOF MS ES+
1.48e+005

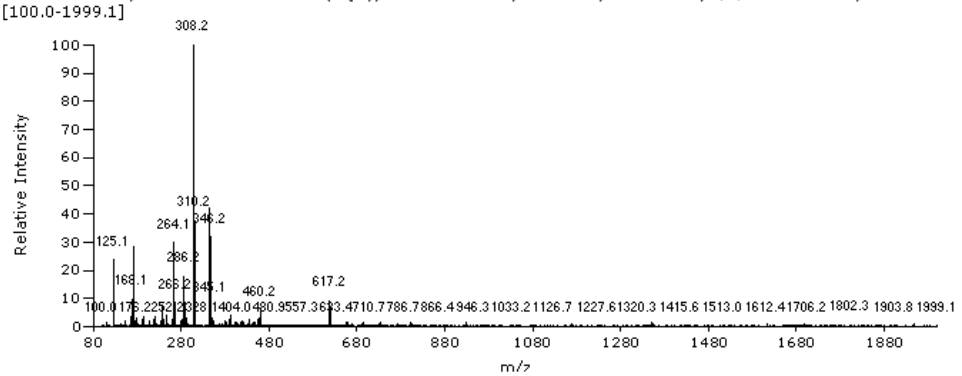


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
267.0584	267.0581	0.3	1.1	8.5	604.2	0.0	C12 H9 N2 O3 F2
	267.0570	1.4	5.2	12.5	610.6	6.4	C15 H5 N2 O2 F
	267.0593	-0.9	-3.4	4.5	611.0	6.7	C9 H10 N2 O4 F3
	267.0606	-2.2	-8.2	9.5	611.1	6.9	C10 H6 N6 F3
	267.0590	-0.6	-2.2	8.5	612.6	8.4	C7 H7 N8 O4
	267.0610	-2.6	-9.7	16.5	612.9	8.6	C20 H5 F
	267.0554	3.0	11.2	9.5	613.0	8.8	C8 H5 N8 O F2
	267.0558	2.6	9.7	16.5	613.2	9.0	C13 H7 N2 O
	267.0577	0.7	2.6	3.5	614.2	9.9	C6 H11 N4 O6
	267.0566	1.8	6.7	8.5	615.8	11.6	C5 H4 N8 O2 F3
	267.0602	-1.8	-6.7	4.5	615.9	11.7	C4 H3 N8 O5 F
	267.0588	-0.4	-1.5	-0.5	616.5	12.3	C3 H12 N4 O9 F
	267.0613	-2.9	-10.9	0.5	618.7	14.5	C H9 N8 O6 F2
	267.0577	0.7	2.6	8.5	620.0	15.7	C8 H3 N8 F 3
	267.0604	-2.0	-7.5	7.5	620.0	15.8	C12 H12 N2 O2 F 3



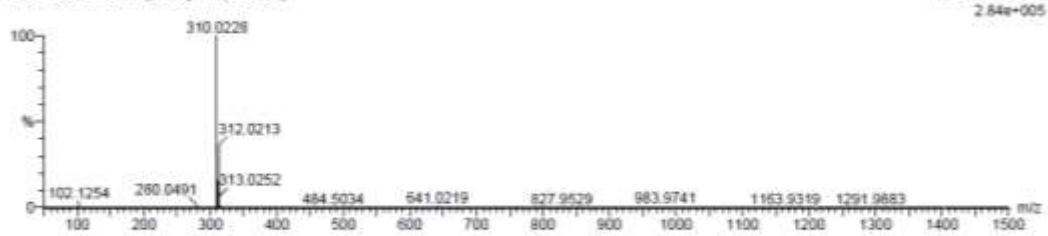
Chemical Formula: $C_{12}H_8ClN_3O_5$
Exact Mass: 309.0152

MBS2-4Cl2nitro, ESI - no column MeOH (TQD), RT 0.2728 mins, Scan# 16, NL 4.407E6, 7/3/2014 3:14 PM, mz [100.0-1999.1]

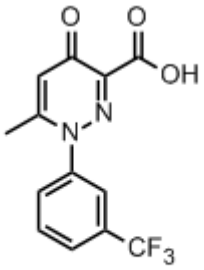


Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2
Marcus Baumann
MBS2-4Cl2nitro 277 (2.282) Cm (275:281)

1: TOF MS ES+
2.84e+005

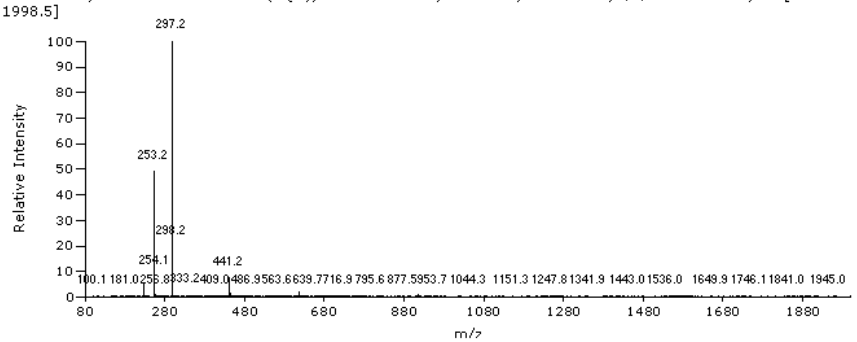


Minimum:				-1.5			
Maximum:		1.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
310.0228	310.0228	0.0	0.0	15.5	625.5	19.4	C16 H3 N3 O F3
	310.0227	0.1	0.3	2.5	619.2	13.1	C2 H7 N9 O5 F2 Cl
	310.0229	-0.1	-0.3	5.5	610.2	4.1	C10 H11 N3 O2 F2 S Cl
	310.0226	0.2	0.6	12.5	624.9	18.0	C14 H9 O
	310.0225	0.3	1.0	1.5	616.9	10.9	C9 H13 N O3 F3 Cl2
	310.0231	-0.3	-1.0	9.5	606.1	0.0	C12 H5 N3 O5 Cl
	310.0224	0.4	1.3	0.5	616.7	10.6	C4 H13 N5 O7 S Cl
	310.0224	0.4	1.3	0.5	617.1	11.0	C15 H14 N S Cl2
	310.0224	0.4	1.3	10.5	624.0	17.7	C10 H5 N5 O4 F
	310.0233	-0.5	-1.6	6.5	617.1	11.0	C9 H12 N O9 S
	310.0222	0.6	1.9	5.5	618.0	11.7	C7 H10 N7 O3 Cl2
	310.0222	0.6	1.9	6.5	619.4	13.1	C8 H7 N5 O3 F3 S
	310.0234	-0.6	-1.9	1.5	619.2	13.1	C4 H11 N7 O4 F Cl2
	310.0235	-0.7	-2.3	6.5	616.4	10.3	C12 H15 N O F S Cl2
	310.0235	-0.7	-2.3	14.5	609.9	3.8	C10 N7 O F2 Cl
	310.0235	-0.7	-2.3	6.5	625.0	18.9	C7 H6 N5 O7 F2
	310.0220	0.8	2.6	1.5	620.2	14.1	C5 H12 N7 F2 S Cl2
	310.0237	-0.9	-2.9	15.5	624.9	18.8	C11 H N9 O2 F
	310.0238	-1.0	-3.2	5.5	615.3	9.3	C5 H9 N9 O3 S Cl



Chemical Formula: $C_{13}H_9F_3N_2O_3$
Exact Mass: 298.0565

MBS2-3CF3, ESI - no column MeOH (TQD), RT 0.2387 mins, Scan# 14, NL 3.610E7, 7/3/2014 3:12 PM, mz [100.1-1998.5]

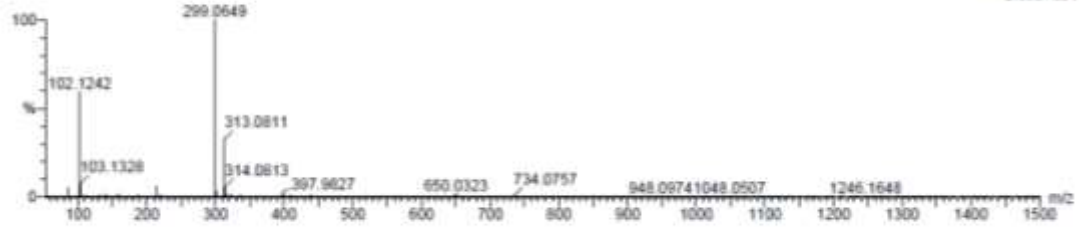


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

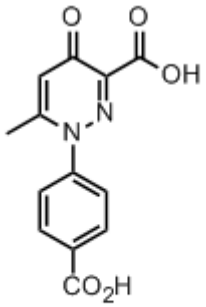
Monoisotopic Mass, Even Electron Ions
8011 formula(e) evaluated with 65 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2 Br: 0-2

Marcus Baumann
MBS2-3CF3 325 (2.670) Cm (323:331)

1: TOF MS ES+
2.59e+004

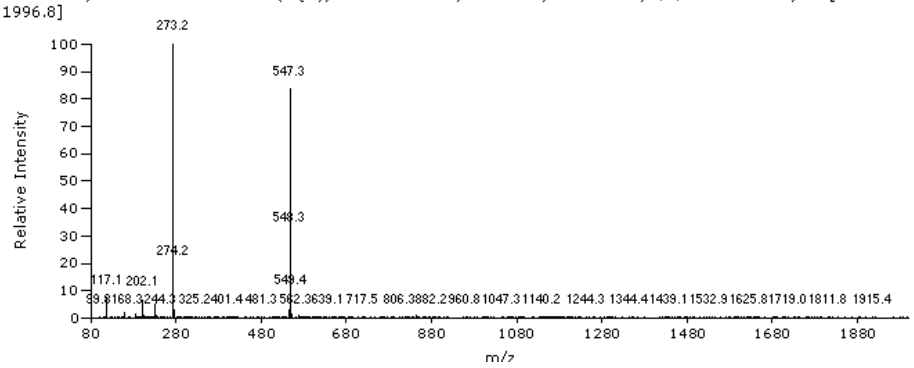


Minimum:			-1.5				
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
299.0649	299.0641	0.8	2.7	12.5	362.5	0.0	C11 H7 N2 O3
	299.0644	0.5	1.7	9.5	363.4	1.7	C13 H10 N2 O3 F3
	299.0628	2.1	7.0	7.5	363.6	2.0	C10 H11 N4 O7
	299.0660	-1.9	-6.4	11.5	363.8	2.1	C15 H11 N2 O5
	299.0653	-0.4	-1.3	3.5	364.5	2.3	C8 H8 N3 O4 F
	299.0632	1.7	5.7	12.5	365.0	3.3	C16 H9 N2 O2 F2
	299.0639	1.0	3.3	3.5	366.3	4.7	C7 H12 N4 O8 F
	299.0664	-1.5	-5.0	4.5	366.5	4.9	C5 H9 N3 O5 F2
	299.0621	2.8	9.4	14.5	367.4	5.7	C19 H8 N2 O F
	299.0651	-0.2	-0.7	-0.5	367.4	5.7	C6 H13 N4 O9 F2
	299.0672	-2.3	-7.7	14.5	368.7	7.0	C21 H9 F2
	299.0675	-2.6	-8.7	0.5	369.0	7.1	C2 H10 N8 O6 F3



Chemical Formula: $C_{13}H_{10}N_2O_5$
Exact Mass: 274.0590

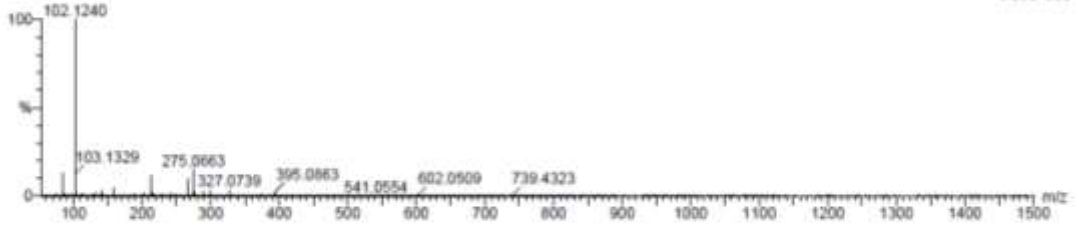
mbs2-4CN, ESI - no column MeOH (TQD), RT 0.3069 mins, Scan# 18, NL 1.614E7, 7/3/2014 1:34 PM, mz [99.8-1996.8]



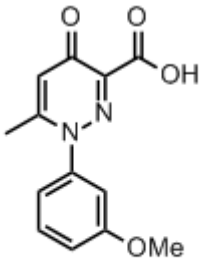
Monoisotopic Mass, Even Electron Ions
6250 formula(e) evaluated with 46 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2 Br: 0-2

Marcus Baumann
MBS2-4CN 251 (2.065) Cm (249:252)

1: TOF MS ES+
6.85e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
275.0663	275.0660	-0.5	-1.8	9.5	124.7	0.8	C13 H11 N2 O5
	275.0666	-0.3	-1.1	5.5	125.7	1.8	C11 H13 N2 O2 F2 S
	275.0654	0.9	3.3	9.5	126.2	2.3	C14 H12 N2 O F S
	275.0681	-1.8	-6.5	14.5	126.9	3.0	C14 N7 N6 O
	275.0679	-1.6	-5.8	5.5	126.9	3.0	C10 H12 N2 O6 F
	275.0677	-1.4	-5.1	1.5	127.4	3.5	C8 H14 N2 O3 F3 S
	275.0684	-2.1	-7.6	10.5	127.4	3.5	C16 H10 O F3
	275.0644	1.9	6.9	6.5	127.6	3.7	C11 H10 N2 O3 F3
	275.0693	-3.0	-10.9	10.5	127.9	4.0	C11 N3 N6 O2 F
	275.0672	-0.9	-3.3	14.5	128.0	4.1	C19 N9 F2
	275.0641	2.2	8.0	10.5	128.1	4.2	C9 N7 N5 O3
	275.0643	2.0	7.3	13.5	128.3	4.4	C17 H11 N2 S

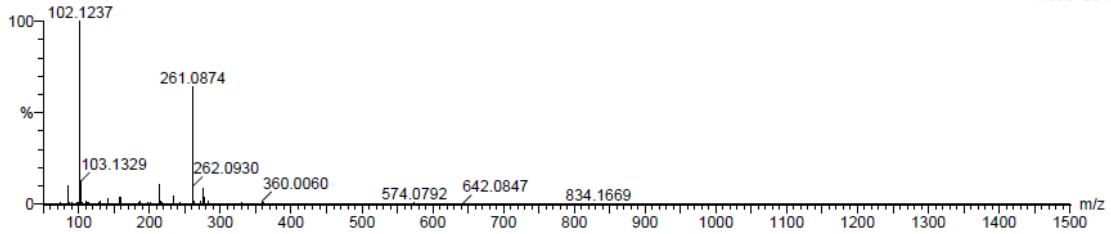


Chemical Formula: $C_{13}H_{12}N_2O_4$
Exact Mass: 260.0797

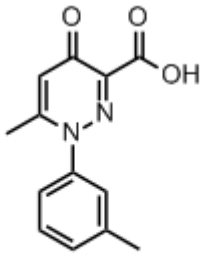
Monoisotopic Mass, Even Electron Ions
3802 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2

Marcus Baumann
MBS2-3OMe 269 (2.215) Cm (269:296)

1: TOF MS ES+
4.89e+004

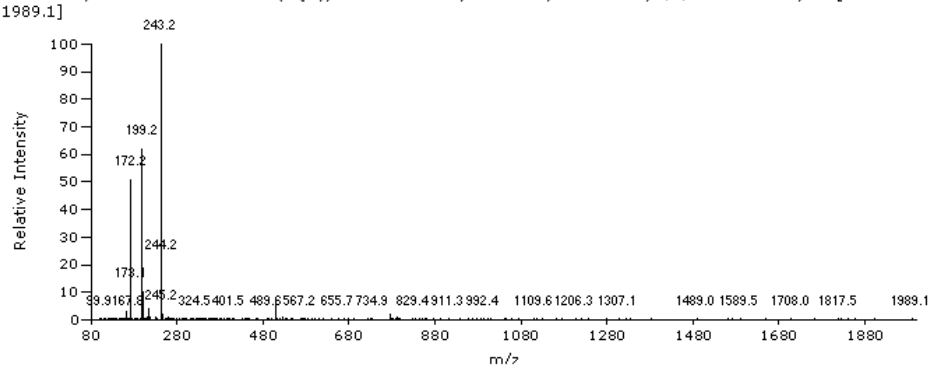


Minimum:				-1.5			
Maximum:		1.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
261.0874	261.0873	0.1	0.4	4.5	448.4	9.3	C11 H15 N2 O F2 S
	261.0875	-0.1	-0.4	8.5	439.0	0.0	C13 H13 N2 O4
	261.0871	0.3	1.1	1.5	449.0	9.9	C3 H11 N8 O4 F2
	261.0878	-0.4	-1.5	0.5	455.6	16.6	C5 H15 N6 O3 F Cl
	261.0869	0.5	1.9	-0.5	450.3	11.3	C5 H17 N4 O6 S
	261.0869	0.5	1.9	0.5	455.4	16.4	C10 H17 O2 F3 Cl
	261.0880	-0.6	-2.3	3.5	455.5	16.4	C13 H19 F S Cl
	261.0867	0.7	2.7	4.5	455.7	16.7	C8 H14 N6 O2 Cl
	261.0882	-0.8	-3.1	4.5	449.4	10.3	C6 H13 N8 O2 S

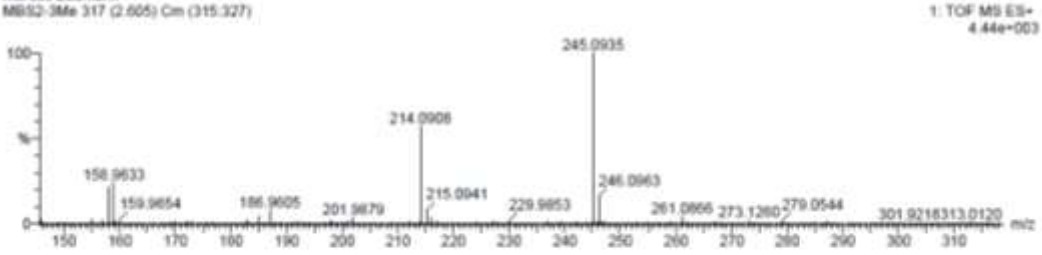


Chemical Formula: $C_{13}H_{12}N_2O_3$
Exact Mass: 244.0848

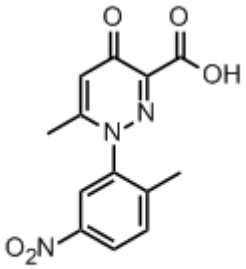
mbs2-3Me, ESI - no column MeOH (TQD), RT 0.3751 mins, Scan# 22, NL 4.862E6, 7/3/2014 1:31 PM, mz [99.9-1989.1]



Monoisotopic Mass, Even Electron Ions
3205 formula(e) evaluated with 23 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2
Marcus Baumann
MBS2-3Me 317 (2.605) Cm (315:327)

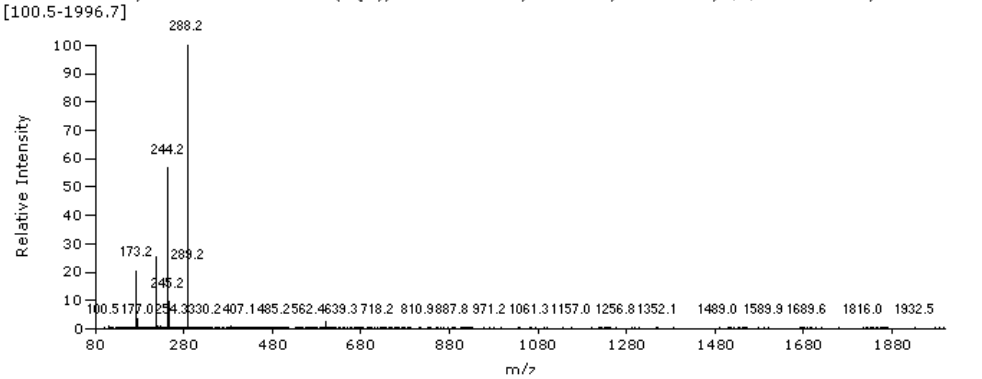


Minimum:			-1.5				
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
245.0935	245.0935	0.0	0.0	0.5	246.9	14.4	C9 H16 N2 O F3 S
	245.0936	-0.1	-0.4	-0.5	253.2	20.7	C7 H19 N4 O C12
	245.0933	0.2	0.8	4.5	247.2	14.7	C6 H13 N3 O S
	245.0938	-0.3	-1.2	4.5	237.1	4.6	C10 H14 N2 O4 F
	245.0929	0.6	2.4	0.5	252.6	20.1	C5 H15 N6 O2 F Cl
	245.0942	-0.7	-2.9	-0.5	252.7	20.2	C10 H20 F2 S Cl
	245.0944	-0.9	-3.7	3.5	252.5	20.0	C12 H18 O3 Cl
	245.0944	-0.9	-3.7	0.5	240.3	15.0	C9 H14 N3 O2 F S
	245.0926	0.9	3.7	0.5	232.5	0.0	C13 H18 N2 O3
	245.0924	1.1	4.5	4.5	246.5	14.0	C11 H15 N2 F2 S
	245.0922	1.3	5.3	1.5	245.4	12.9	C9 H11 N5 O2 F2
	245.0969	-1.4	-5.7	0.5	240.6	9.1	C7 H15 N2 O5 F2
	245.0920	1.5	6.1	0.5	252.7	20.2	C10 H17 O F3 Cl
	245.0920	1.5	6.1	-0.5	247.0	15.3	C5 H17 N4 O5 S
	245.0951	-1.6	-6.5	3.5	237.1	4.6	C11 H10 N6 F
	245.0951	-1.6	-6.5	-0.5	253.0	20.5	C5 H13 N6 O S Cl
	245.0915	1.7	6.9	4.5	252.7	20.2	C9 H14 N6 O Cl
	245.0956	-2.1	-8.6	-0.5	252.8	20.3	C9 H19 O4 F Cl
	245.0950	-2.1	-9.4	0.5	246.1	13.6	C2 H13 N3 O6



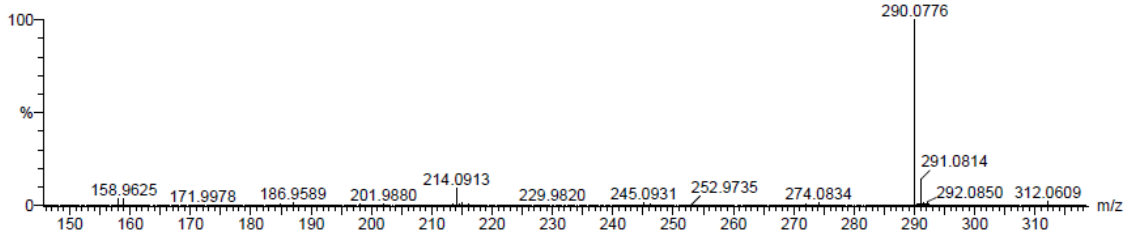
Chemical Formula: $C_{13}H_{11}N_3O_5$
Exact Mass: 289.0699

mbs2-5nitro2Me, ESI - no column MeOH (TQD), RT 0.2387 mins, Scan# 14, NL 2.516E7, 7/3/2014 1:31 PM, mz [100.5-1996.7]

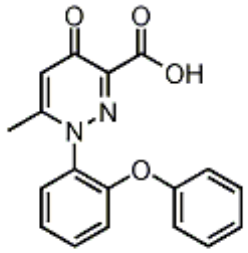


Monoisotopic Mass, Even Electron Ions
4982 formula(e) evaluated with 37 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2
Marcus Baumann
MBS2-5NO2-2Me 263 (2.163) Cm (263:273)

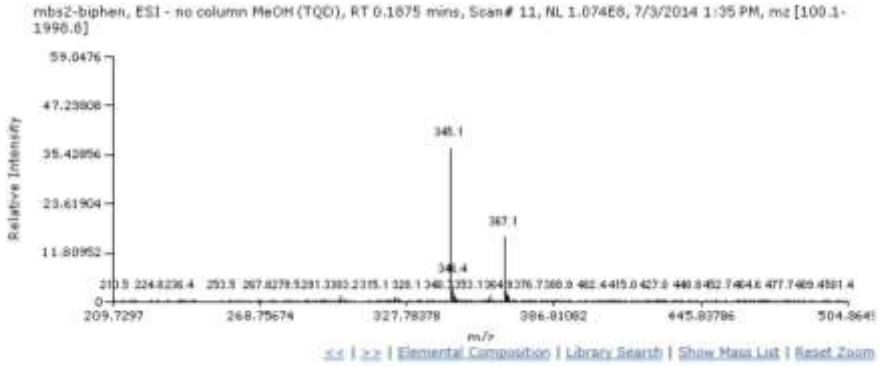
1: TOF MS ES+
1.96e+004



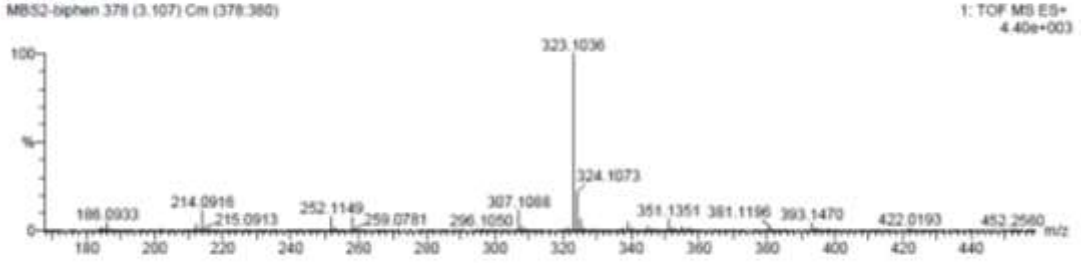
Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
290.0776	290.0777	-0.1	-0.3	9.5	368.2	2.5	C13 H12 N3 O5
	290.0775	0.1	0.3	5.5	379.7	14.0	C11 H14 N3 O2 F2 S
	290.0773	0.3	1.0	2.5	377.2	11.5	C3 H10 N9 O5 F2
	290.0780	-0.4	-1.4	1.5	385.6	19.9	C5 H14 N7 O4 F Cl
	290.0771	0.5	1.7	1.5	385.4	19.7	C10 H16 N O3 F3 Cl
	290.0781	-0.5	-1.7	14.5	371.1	5.4	C19 H10 N F2
	290.0770	0.6	2.1	0.5	380.7	15.0	C5 H16 N5 O7 S
	290.0770	0.6	2.1	8.5	385.5	19.8	C16 H17 N S Cl
	290.0782	-0.6	-2.1	4.5	385.5	19.8	C13 H18 N O F S Cl
	290.0768	0.8	2.8	5.5	385.5	19.8	C8 H13 N7 O3 Cl
	290.0784	-0.8	-2.8	-1.5	380.7	15.0	H11 N9 O6 F3
	290.0784	-0.8	-2.8	5.5	380.3	14.6	C6 H12 N9 O3 S
	290.0766	1.0	3.4	1.5	385.9	20.2	C6 H15 N7 F2 S Cl
	290.0786	-1.0	-3.4	1.5	379.9	14.2	C8 H15 N3 O3 F3 S
	290.0787	-1.1	-3.8	0.5	386.2	20.5	C7 H18 N5 O3 Cl2



Chemical Formula: $C_{18}H_{14}N_2O_4$
Exact Mass: 322.0954

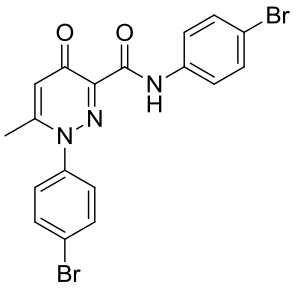


Monoisotopic Mass, Even Electron Ions
5625 formula(e) evaluated with 43 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3 S: 0-1 Cl: 0-2
Marcus Baumann
MBS2-biphen 378 (3.107) Cm (378:380)

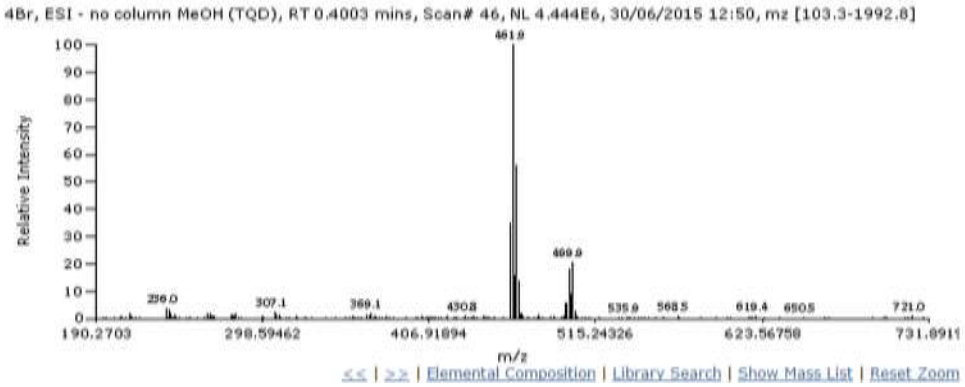


Minimum:			-1.5				
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
307.1088	307.1088	0.0	0.0	-0.5	75.5	5.6	C7 H20 N4 O6 F 5
	307.1090	-0.2	-0.7	1.5	76.4	6.5	C5 H14 N8 O4 F3
	307.1090	-0.2	-0.7	0.5	72.9	3.0	C11 H15 N8 O 5
	307.1096	0.2	0.7	4.5	80.0	10.9	C10 H17 N6 O2 F Cl
	307.1092	-0.4	-1.3	4.5	72.3	2.4	C13 H18 N2 O F3 S
	307.1092	-0.4	-1.3	3.5	81.4	11.7	C12 H21 N4 O Cl2
	307.1083	0.5	1.6	12.5	71.1	1.2	C18 H15 N2 O3
	307.1094	-0.6	-2.0	8.5	71.0	1.9	C15 H16 N2 O4 F
	307.1096	-0.8	-2.0	-1.5	80.0	10.9	C9 H24 N2 O5 S Cl
	307.1081	0.7	2.3	0.5	71.5	1.4	C16 H17 N2 F2 S
	307.1079	0.9	2.9	-1.5	81.9	12.0	C11 H25 O5 Cl2
	307.1076	0.9	2.9	5.5	75.7	5.8	C8 H13 N8 O3 F2
	307.1097	-0.9	-2.9	0.5	80.0	10.9	C7 H18 N6 O3 F2 Cl

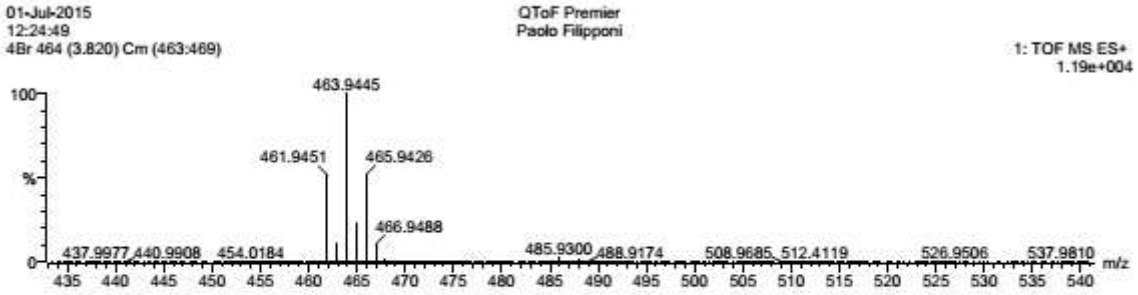
B3. Serie B derivatives 15-23.



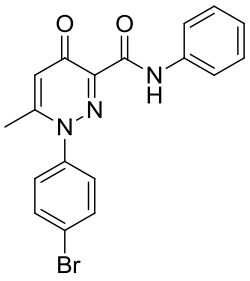
Chemical Formula: $C_{18}H_{13}Br_2N_3O_2$
Exact Mass: 460.94



Monoisotopic Mass, Even Electron Ions
6188 formula(e) evaluated with 59 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-6 Cl: 0-2 Br: 0-2 F: 0-3

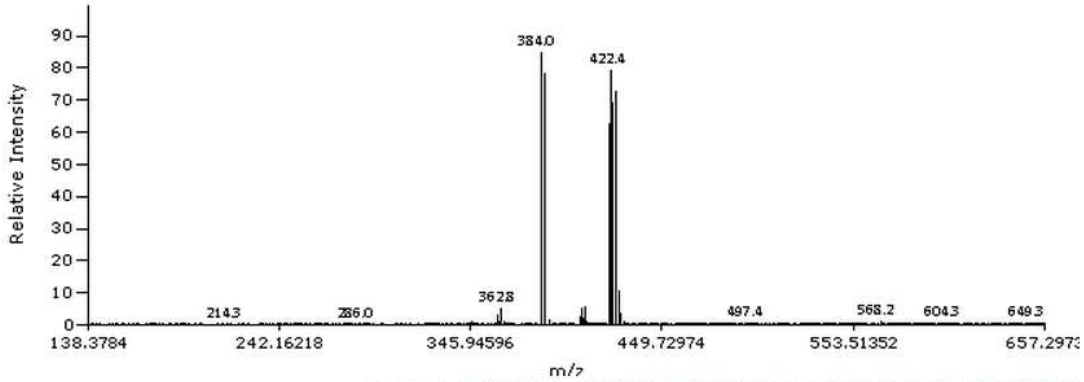


Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
461.9451	461.9453	-0.2	-0.4	12.5	221.3	0.1	C18 H14 N3 O2 Br2
	461.9493	-4.2	-9.1	16.5	224.8	3.5	C23 H14 N Br2
	461.9464	-1.3	-2.8	8.5	225.4	4.2	C15 H15 N3 O3 Br2 F
	461.9428	2.3	5.0	9.5	225.6	4.3	C16 H13 N3 Br2 F3
	461.9475	-2.4	-5.2	10.5	227.5	6.2	C18 H13 N O2 Cl2 Br F2



Chemical Formula: $C_{18}H_{14}BrN_3O_2$
Exact Mass: 383.03

Anil, ESI - no column MeOH (TQD), RT 0.2001 mins, Scan# 23, NL 9.318E7, 03/07/2015 09:10, mz [101.9-1998.3]



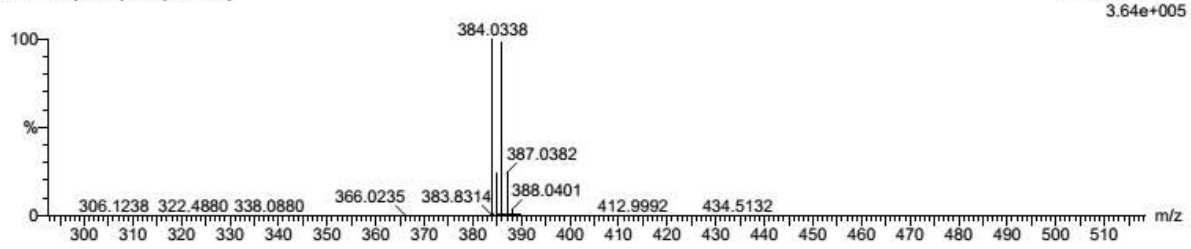
<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
739 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-10 Br: 0-2

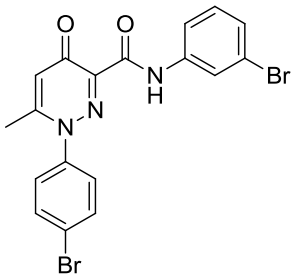
03-Jul-2015
12:55:39
Anil 393 (3.236) Cm (392:395)

QToF Premier
Paolo Filipponi

1: TOF MS ES+
3.64e+005

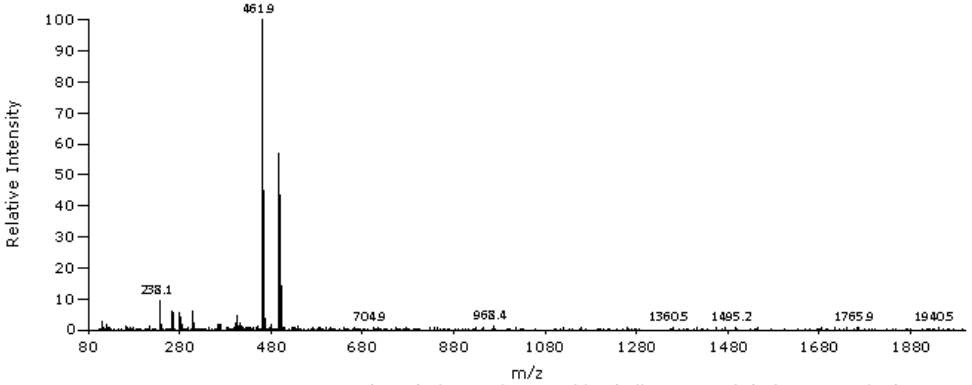


Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
384.0338	384.0348	-1.0	-2.6	12.5	505.6	1.7	C18 H15 N3 O2 Br
	384.0356	-1.8	-4.7	14.5	523.4	19.5	C18 H10 N O9
	384.0310	2.8	7.3	28.5	523.7	19.8	C26 H2 N5
	384.0366	-2.8	-7.3	-0.5	513.9	10.0	C6 H19 N5 O9 Br
	384.0307	3.1	8.1	8.5	510.7	6.8	C13 H15 N5 O4 Br
	384.0369	-3.1	-8.1	19.5	523.5	19.6	C19 H6 N5 O5
	384.0297	4.1	10.7	23.5	523.7	19.8	C25 H6 N O4
	384.0294	4.4	11.5	3.5	511.5	7.6	C12 H19 N O8 Br
	384.0388	-5.0	-13.0	16.5	504.1	0.2	C23 H15 N Br



Chemical Formula: $C_{18}H_{13}Br_2N_3O_2$
Exact Mass: 460.94

3Br, ESI - no column MeOH (TQD), RT 0.3654 mins, Scan# 42, NL 3.900E6, 30/06/2015 12:44, mz [102.4-1994.6]



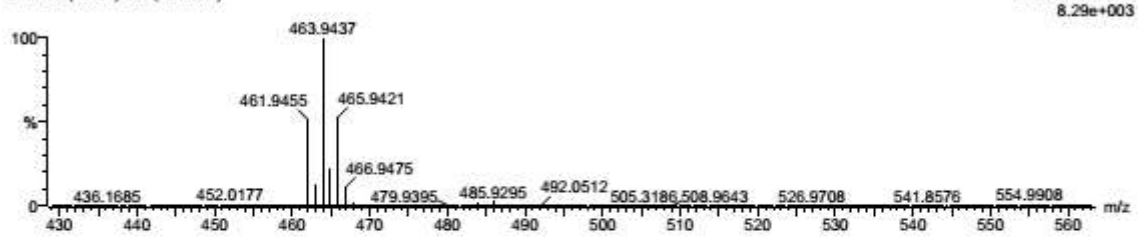
<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
1678 formula(e) evaluated with 15 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-6 Cl: 0-2 Br: 0-2

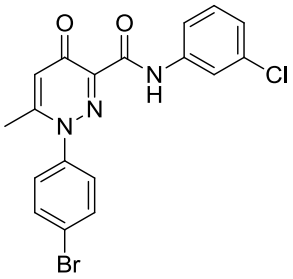
01-Jul-2015
11:45:43
3Br 499 (4.102) Cm (496:506)

QToF Premier
Paolo Filipponi

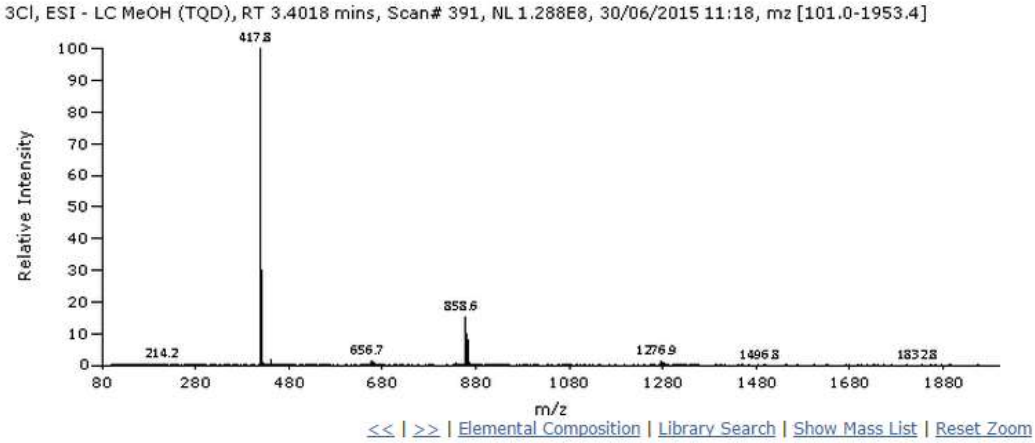
1: TOF MS ES+
8.29e+003



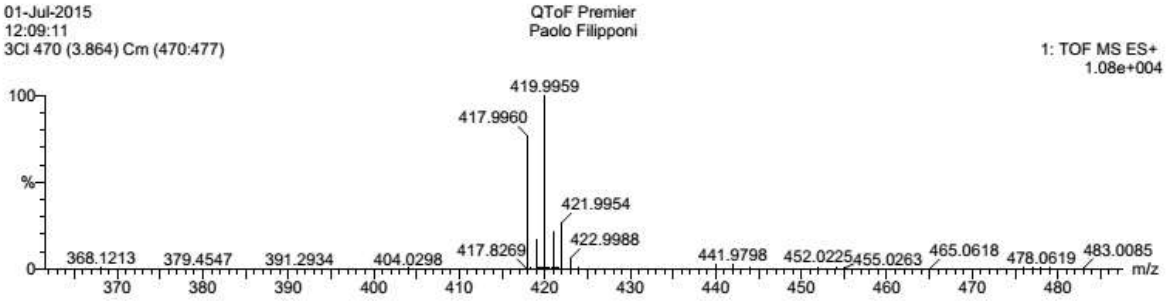
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
461.9455	461.9453	0.2	0.4	12.5	219.4	0.2	C18 H14 N3 O2 Br2
	461.9452	0.3	0.6	18.5	224.5	5.3	C24 H11 N Cl2 Br
	461.9449	0.6	1.3	-1.5	227.1	7.9	C11 H24 N O4 Cl2 Br2
	461.9462	-0.7	-1.5	3.5	227.5	8.3	C12 H20 N5 Cl2 Br2
	461.9471	-1.6	-3.5	7.5	224.5	5.3	C17 H19 N O2 Cl Br2
	461.9473	-1.8	-3.9	25.5	231.1	11.9	C25 H2 N3 O3 Cl2
	461.9474	-1.9	-4.1	19.5	230.0	10.8	C19 H5 N5 O5 Br
	461.9434	2.1	4.5	23.5	228.5	9.3	C25 H6 N3 Cl Br
	461.9433	2.2	4.8	21.5	231.9	12.8	C20 H2 N5 O5 Cl2
	461.9431	2.4	5.2	3.5	226.9	7.7	C12 H19 N3 O4 Cl Br2
	461.9492	-3.7	-8.0	14.5	228.2	9.0	C18 H10 N3 O5 Cl Br
	461.9493	-3.8	-8.2	16.5	220.8	1.6	C23 H14 N Br2
	461.9415	4.0	8.7	28.5	231.6	12.4	C26 H N5 Br
	461.9413	4.2	9.1	8.5	225.9	6.7	C13 H14 N5 O4 Br2
	461.9412	4.3	9.3	14.5	225.7	6.5	C19 H11 N3 O2 Cl2 Br



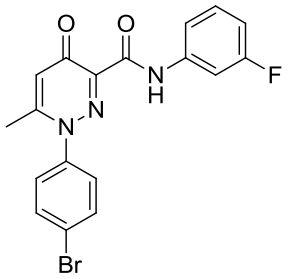
Chemical Formula: $C_{18}H_{13}BrClN_3O_2$
Exact Mass: 416.99



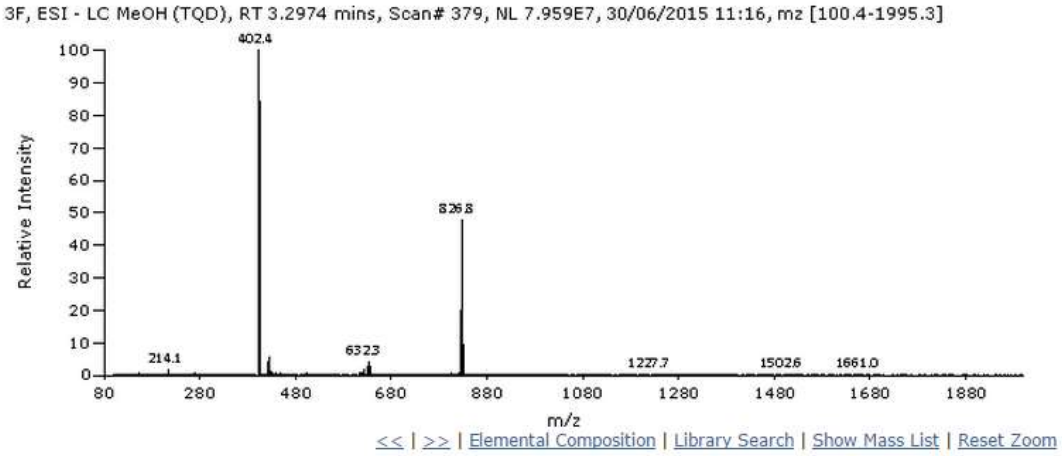
Monoisotopic Mass, Even Electron Ions
5453 formula(e) evaluated with 58 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-6 Cl: 0-2 Br: 0-2 F: 0-3



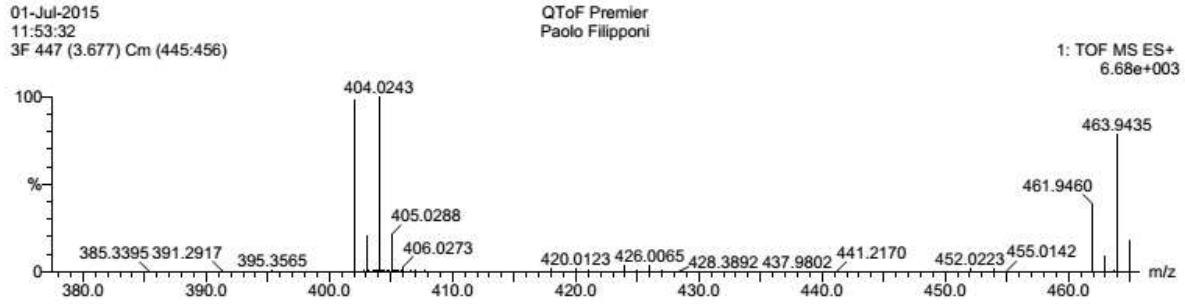
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
417.9960	417.9962	-0.2	-0.5	15.5	266.6	13.7	C19 H8 N3 O2 Cl2 F2
	417.9962	-0.2	-0.5	9.5	262.4	9.5	C13 H11 N5 O4 Br F2
	417.9958	0.2	0.5	12.5	253.1	0.2	C18 H14 N3 O2 Cl Br
	417.9963	-0.3	-0.7	20.5	274.3	21.4	C22 H3 N O5 F3
	417.9955	0.5	1.2	16.5	268.5	15.6	C17 H4 N5 O3 Cl F3
	417.9953	0.7	1.7	-1.5	265.2	12.3	C9 H21 N3 O2 Br2 F3
	417.9952	0.8	1.9	4.5	263.0	10.0	C15 H18 N C12 Br F3
	417.9952	0.8	1.9	24.5	274.4	21.5	C25 H2 N O4 F2
	417.9951	0.9	2.2	13.5	262.4	9.4	C16 H10 N5 O3 Br F
	417.9969	-0.9	-2.2	8.5	258.5	5.5	C15 H15 N3 O3 Cl Br F



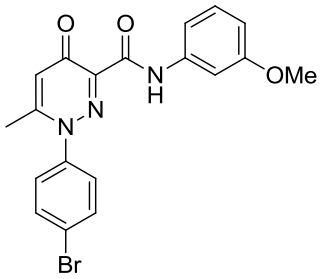
Chemical Formula: $C_{18}H_{13}BrFN_3O_2$
Exact Mass: 401.02



Monoisotopic Mass, Even Electron Ions
5143 formula(e) evaluated with 53 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-6 Cl: 0-2 Br: 0-2 F: 0-3

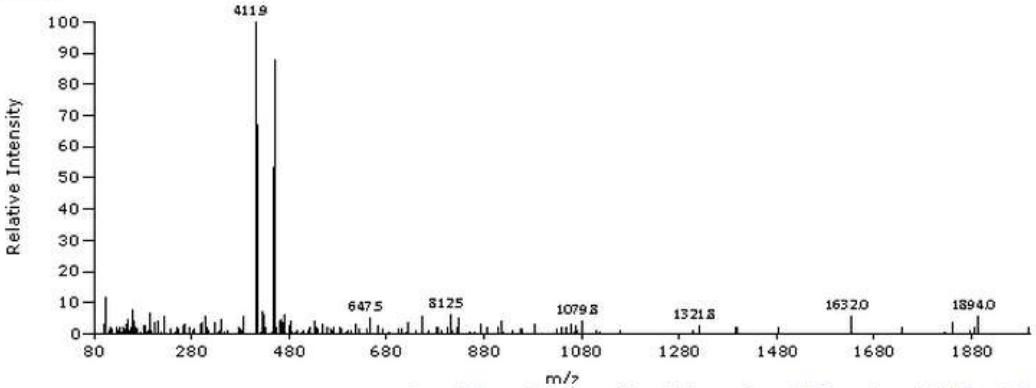


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
402.0259	402.0260	-0.1	-0.2	11.5	276.8	7.4	C20 H18 N O Cl Br
	402.0260	-0.1	-0.2	9.5	279.4	10.1	C15 H14 N3 O6 Cl2
	402.0257	0.2	0.5	15.5	282.3	12.9	C19 H8 N3 O2 Cl F3
	402.0263	-0.4	-1.0	3.5	280.6	11.2	C12 H20 N5 Cl2 Br F
	402.0263	-0.4	-1.0	23.5	292.0	22.6	C22 H4 N5 O4
	402.0264	-0.5	-1.2	14.5	279.4	10.1	C21 H12 N O Cl2 F2
	402.0253	0.6	1.5	18.5	280.0	10.6	C24 H11 N Cl2 F
	402.0253	0.6	1.5	12.5	269.4	0.1	C18 H14 N3 O2 Br F
	402.0265	-0.6	-1.5	8.5	271.9	2.5	C15 H15 N3 O3 Br F2
	402.0250	0.9	2.2	-1.5	280.4	11.1	C11 H24 N O4 Cl2 Br F



Chemical Formula: $C_{19}H_{16}BrN_3O_3$
Exact Mass: 413.04

3OMe, ESI - no column MeOH (TQD), RT 0.1740 mins, Scan# 20, NL 6.919E5, 01/07/2015 13:18, mz [101.2-1997.5]



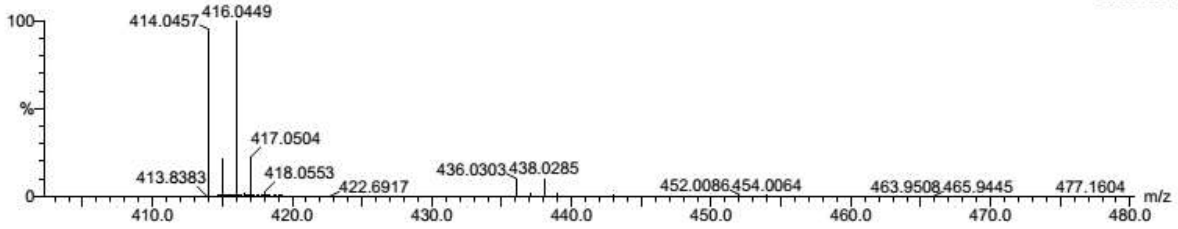
<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
557 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-6 Br: 0-2

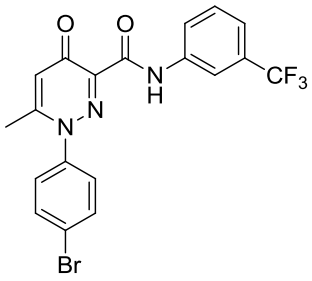
02-Jul-2015
11:52:04
3OMe 421 (3.459) Cm (421:427)

QToF Premier
Paolo Filipponi

1: TOF MS ES+
6.10e+004

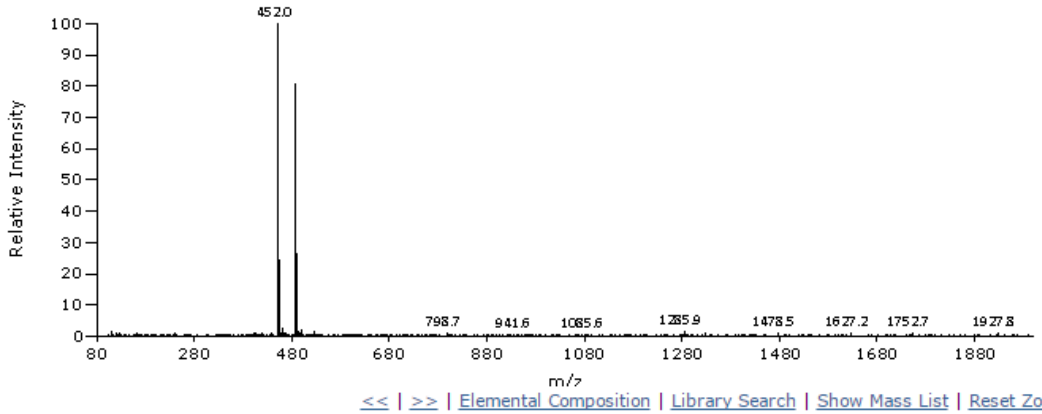


Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
414.0457	414.0453	0.4	1.0	12.5	428.1	0.0	C19 H17 N3 O3 Br
	414.0475	-1.8	-4.3	19.5	446.5	18.4	C20 H8 N5 O6
	414.0432	2.5	6.0	5.5	438.3	10.2	C18 H26 N Br2
	414.0494	-3.7	-8.9	16.5	432.3	4.2	C24 H17 N O Br
	414.0416	4.1	9.9	28.5	446.8	18.7	C27 H4 N5 O
	414.0413	4.4	10.6	8.5	433.0	4.9	C14 H17 N5 O5 Br
	414.0504	-4.7	-11.4	1.5	439.3	11.2	C12 H26 N5 O Br2



Chemical Formula: $C_{19}H_{13}BrF_3N_3O_2$
Exact Mass: 451.01

3CF3, ESI - no column MeOH (TQD), RT 0.4176 mins, Scan# 48, NL 5.740E6, 30/06/2015 12:47, mz [103.6-1990.6]



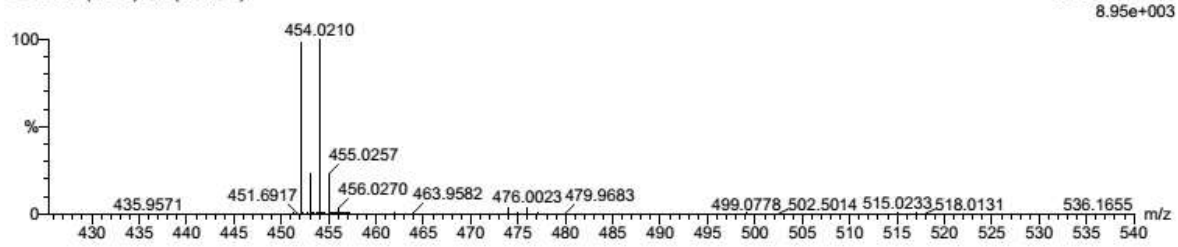
<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
6038 formula(e) evaluated with 58 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-6 Cl: 0-2 Br: 0-2 F: 0-3

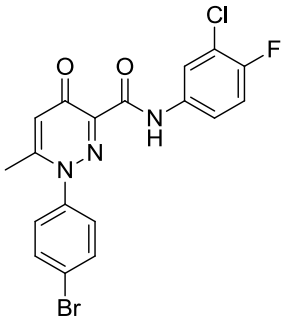
01-Jul-2015
12:01:21
3CF3 485 (3.992) Cm (485:495)

QToF Premier
Paolo Filipponi

1: TOF MS ES+
8.95e+003

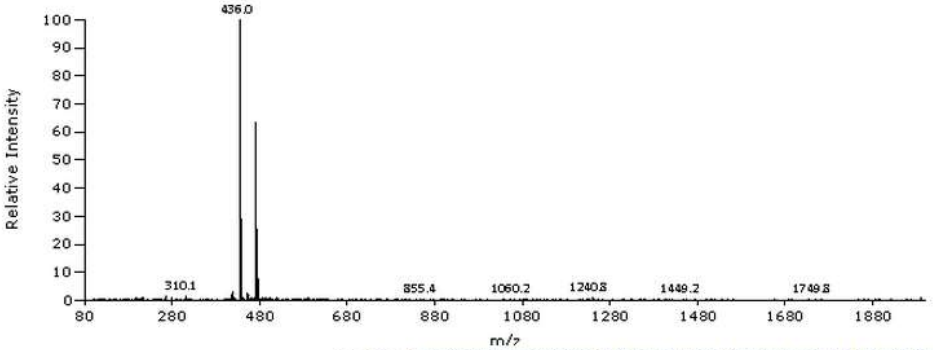


Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
452.0222	452.0221	0.1	0.2	18.5	274.2	11.0	C25 H11 N Cl2 F3
	452.0221	0.1	0.2	12.5	264.3	1.1	C19 H14 N3 O2 Br F3
	452.0224	-0.2	-0.4	6.5	273.1	10.0	C15 H20 N3 O6 Cl Br
	452.0220	0.2	0.4	27.5	285.4	22.2	C26 H3 N5 O3 F
	452.0225	-0.3	-0.7	8.5	275.2	12.1	C20 H24 N O Br2
	452.0218	0.4	0.9	-1.5	275.3	12.1	C12 H24 N O4 Cl2 Br F3



Chemical Formula: $C_{18}H_{12}BrClFN_3O_2$
Exact Mass: 434.98

4F-3Cl, ESI - no column MeOH (TQD), RT 0.1740 mins, Scan# 20, NL 5.455E6, 30/06/2015 12:51, mz [101.1-1989.6]



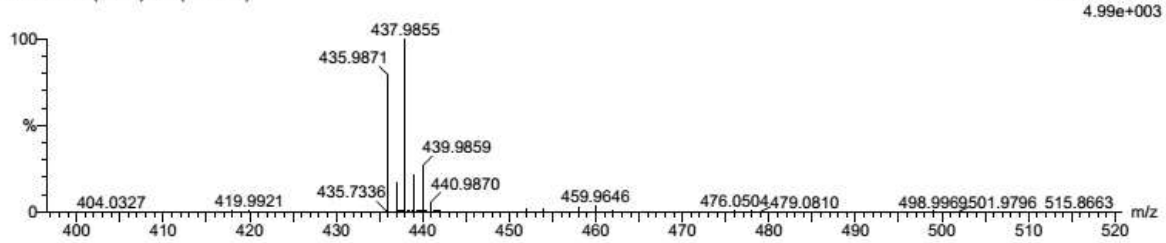
<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
5784 formula(e) evaluated with 59 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-6 Cl: 0-2 Br: 0-2 F: 0-3

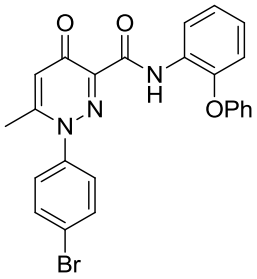
01-Jul-2015
12:17:00
4F-3Cl 476 (3.916) Cm (474:478)

QToF Premier
Paolo Filipponi

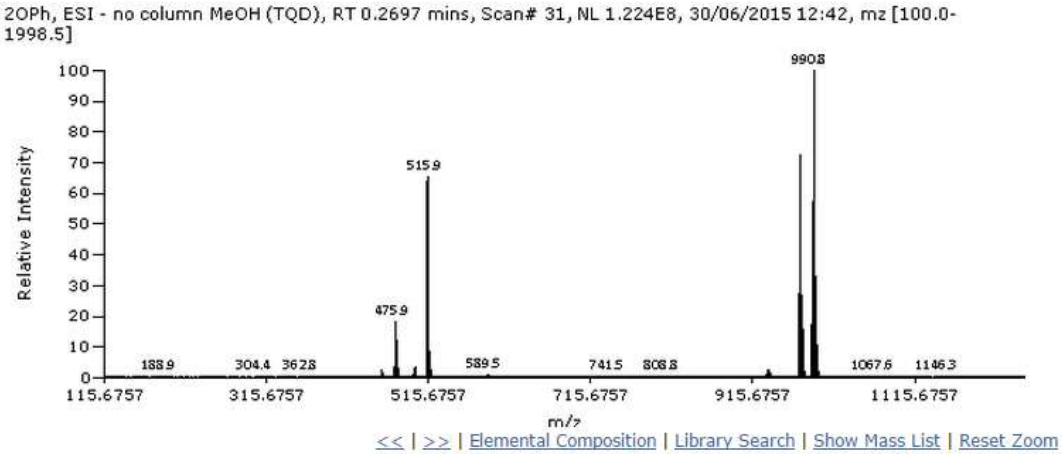
1: TOF MS ES+
4.99e+003



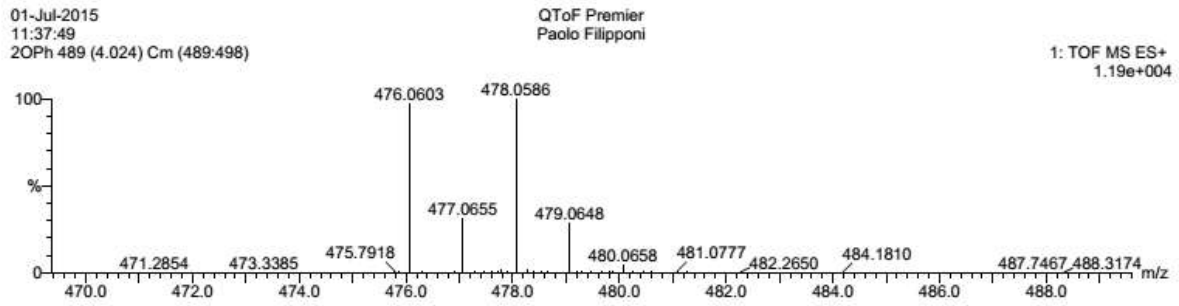
Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
435.9871	435.9871	0.0	0.0	11.5	187.3	6.7	C20 H17 N O Cl2 Br
	435.9871	0.0	0.0	5.5	189.9	9.3	C14 H20 N3 O3 Br2
	435.9868	0.3	0.7	9.5	187.7	7.1	C13 H10 N5 O4 Br F3
	435.9874	-0.3	-0.7	23.5	193.2	12.6	C22 H3 N5 O4 Cl
	435.9875	-0.4	-0.9	8.5	184.0	3.3	C15 H14 N3 O3 Cl Br F2
	435.9867	0.4	0.9	15.5	191.6	11.0	C19 H7 N3 O2 Cl2 F3
	435.9864	0.7	1.6	12.5	180.8	0.2	C18 H13 N3 O2 Cl Br F



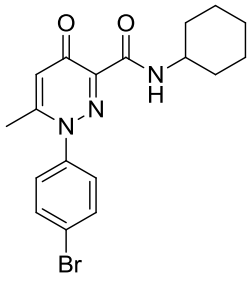
Chemical Formula: $C_{24}H_{18}BrN_3O_3$
Exact Mass: 475.05



Monoisotopic Mass, Even Electron Ions
1713 formula(e) evaluated with 17 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-6 Cl: 0-2 Br: 0-2

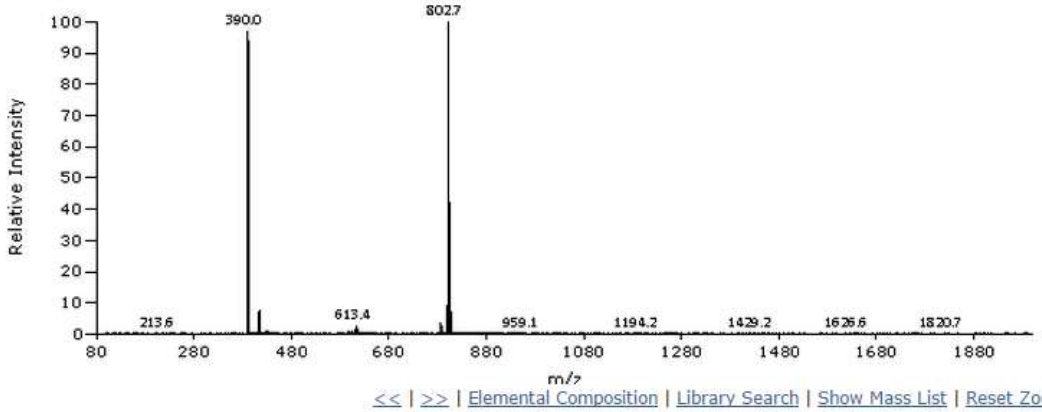


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
476.0603	476.0650	-4.7	-9.9	20.5	260.2	0.0	C29 H19 N O Br
	476.0610	-0.7	-1.5	16.5	263.6	3.4	C24 H19 N3 O3 Br
	476.0570	3.3	6.9	12.5	268.3	8.1	C19 H19 N5 O5 Br
	476.0628	-2.5	-5.3	11.5	268.9	8.7	C23 H24 N O3 Cl Br
	476.0609	-0.6	-1.3	22.5	269.2	9.0	C30 H16 N O Cl2
	476.0588	1.5	3.2	7.5	270.0	9.8	C18 H24 N3 O5 Cl Br
	476.0569	3.4	7.1	18.5	270.6	10.4	C25 H16 N3 O3 Cl2
	476.0606	-0.3	-0.6	2.5	270.8	10.6	C17 H29 N O5 Cl2 Br
	476.0620	-1.7	-3.6	7.5	271.5	11.3	C18 H25 N5 O Cl2 Br



Chemical Formula: $C_{18}H_{20}BrN_3O_2$
Exact Mass: 389.07

CHEX, ESI - no column MeOH (TQD), RT 0.2871 mins, Scan# 33, NL 8.375E7, 10/07/2015 10:30, mz [101.3-1989.6]



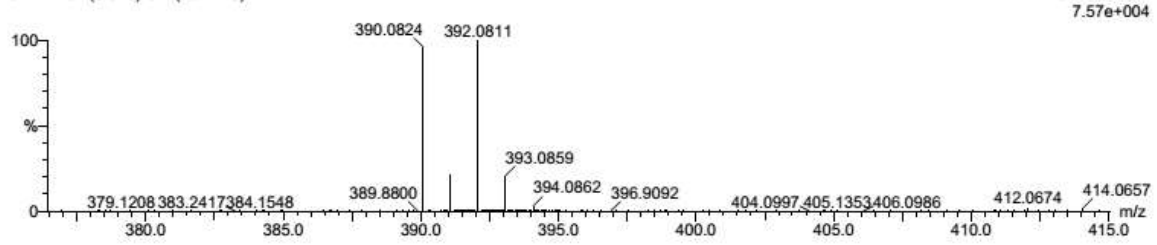
<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
758 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-6 O: 0-10 Br: 0-2

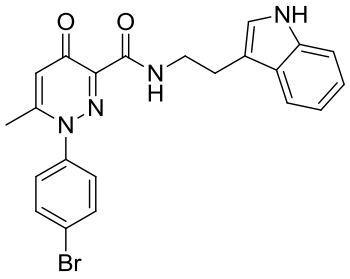
13-Jul-2015
11:00:03
CHEX 402 (3.310) Cm (402:413)

QToF Premier
Paolo Filipponi

1: TOF MS ES+
7.57e+004

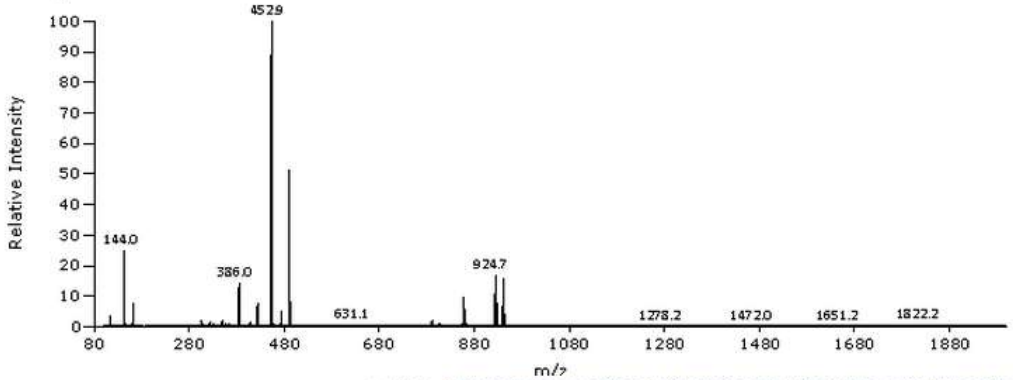


Minimum:				-1.5			
Maximum:		5.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
390.0824	390.0825	-0.1	-0.3	11.5	497.7	21.7	C18 H16 N O9
	390.0817	0.7	1.8	9.5	476.0	0.0	C18 H21 N3 O2 Br
	390.0838	-1.4	-3.6	16.5	497.7	21.8	C19 H12 N5 O5
	390.0857	-3.3	-8.5	13.5	480.3	4.4	C23 H21 N Br
	390.0780	4.4	11.3	25.5	498.1	22.1	C26 H8 N5
	390.0868	-4.4	-11.3	-1.5	488.7	12.7	C11 H30 N5 Br2
	390.0777	4.7	12.0	5.5	483.2	7.2	C13 H21 N5 O4 Br



Chemical Formula: $C_{22}H_{19}BrN_4O_2$
Exact Mass: 450.07

TRYPT, ESI - no column MeOH (TQD), RT 0.2523 mins, Scan# 29, NL 1.324E8, 03/07/2015 09:14, mz [102.1-1998.1]



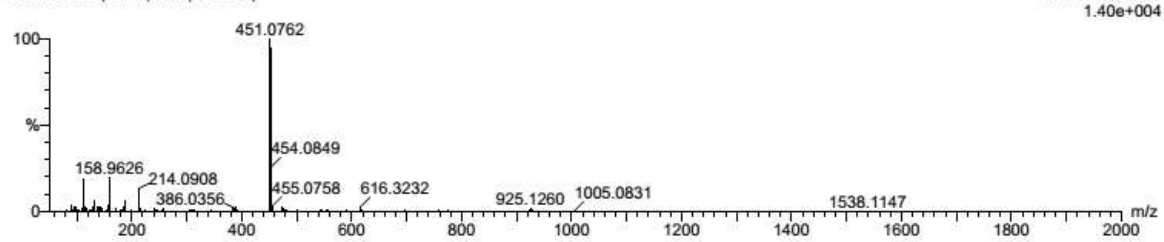
<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
880 formula(e) evaluated with 12 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-10 Br: 0-2

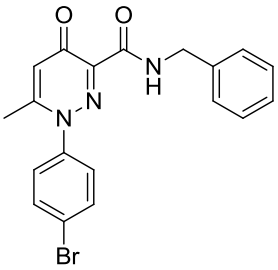
03-Jul-2015
13:03:30
TRYPT 384 (3.161) Cm (384:390)

QToF Premier
Paolo Filipponi

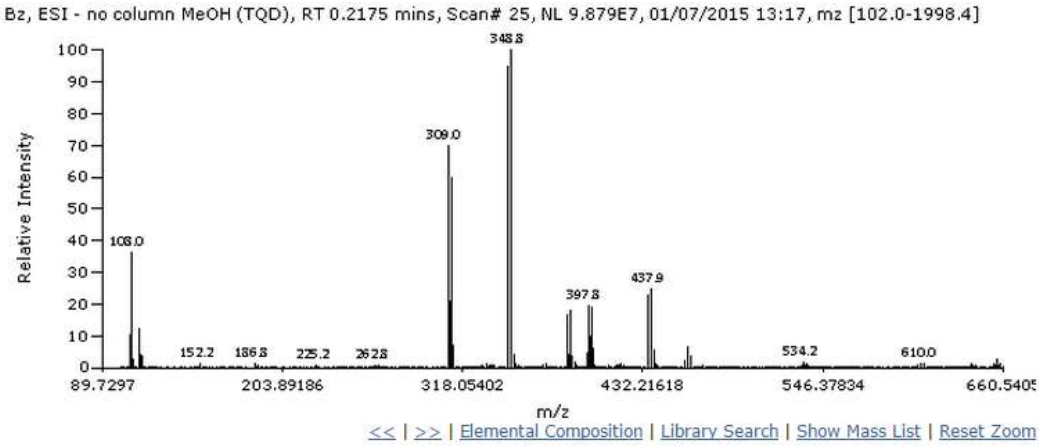
1: TOF MS ES+
1.40e+004



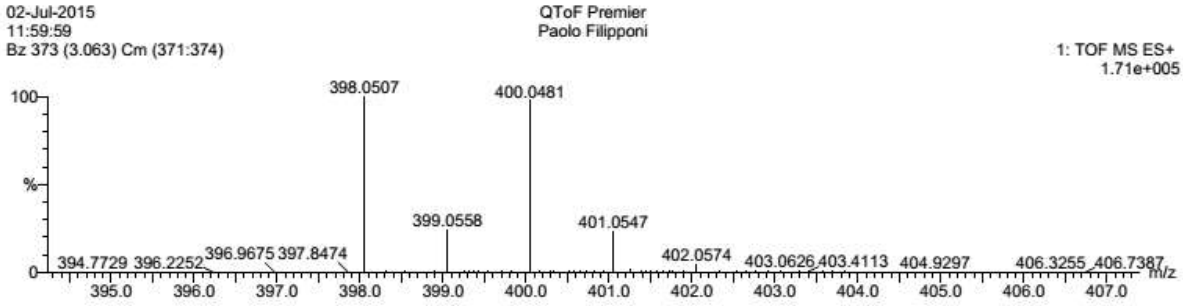
Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
451.0762	451.0759	0.3	0.7	29.5	307.7	14.9	C34 H11 O2
	451.0756	0.6	1.3	9.5	293.6	0.8	C21 H24 O6 Br
	451.0770	-0.8	-1.8	14.5	293.8	1.0	C22 H20 N4 O2 Br
	451.0778	-1.6	-3.5	16.5	307.0	14.2	C22 H15 N2 O9
	451.0788	-2.6	-5.8	1.5	298.7	5.8	C10 H24 N6 O9 Br
	451.0791	-2.9	-6.4	21.5	307.1	14.2	C23 H11 N6 O5
	451.0732	3.0	6.7	30.5	307.2	14.4	C30 H7 N6



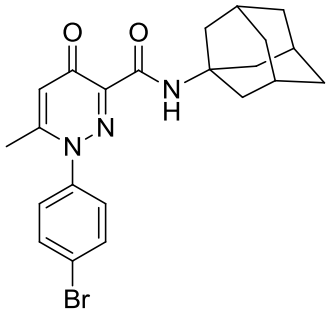
Chemical Formula: $C_{19}H_{16}BrN_3O_2$
Exact Mass: 397.04



Monoisotopic Mass, Even Electron Ions
541 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-6 Br: 0-2

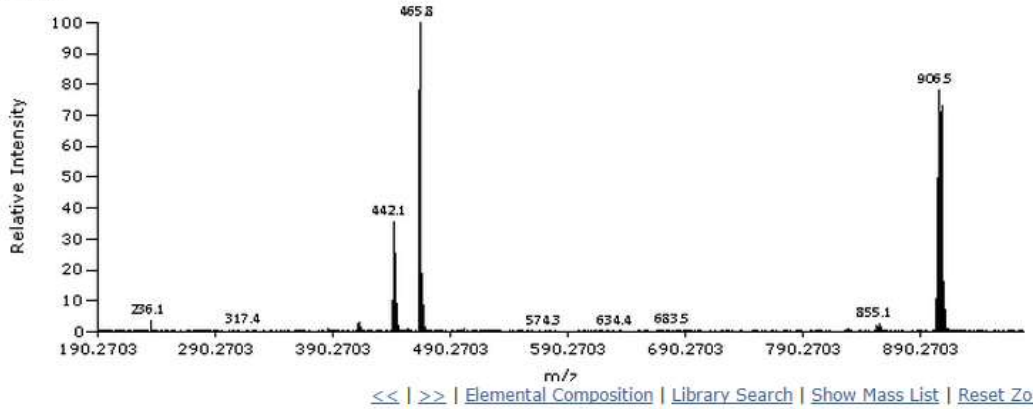


Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
398.0507	398.0504	0.3	0.8	12.5	515.0	0.4	C19 H17 N3 O2 Br
	398.0525	-1.8	-4.5	19.5	532.9	18.3	C20 H8 N5 O5
	398.0544	-3.7	-9.3	16.5	515.7	1.1	C24 H17 N Br
	398.0467	4.0	10.0	28.5	533.1	18.5	C27 H4 N5
	398.0464	4.3	10.8	8.5	520.2	5.6	C14 H17 N5 O4 Br
	398.0555	-4.8	-12.1	1.5	525.8	11.2	C12 H26 N5 Br2



Chemical Formula: $C_{22}H_{24}BrN_3O_2$
Exact Mass: 441.11

ADNT, ESI - no column MeOH (TQD), RT 0.4785 mins, Scan# 55, NL 3.964E7, 10/07/2015 10:34, mz [101.0-1992.5]



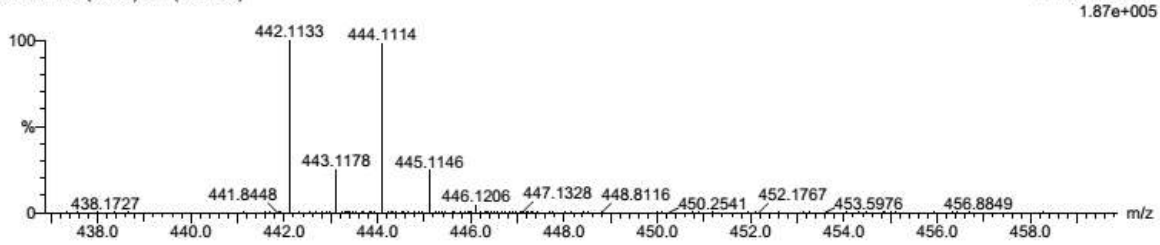
<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

Monoisotopic Mass, Even Electron Ions
853 formula(e) evaluated with 8 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-6 O: 0-10 Br: 0-2

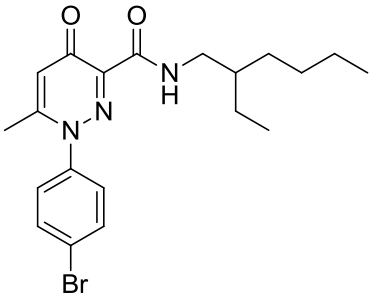
13-Jul-2015
11:08:53
ADNT 473 (3.890) Cm (473:482)

QToF Premier
Paolo Filipponi

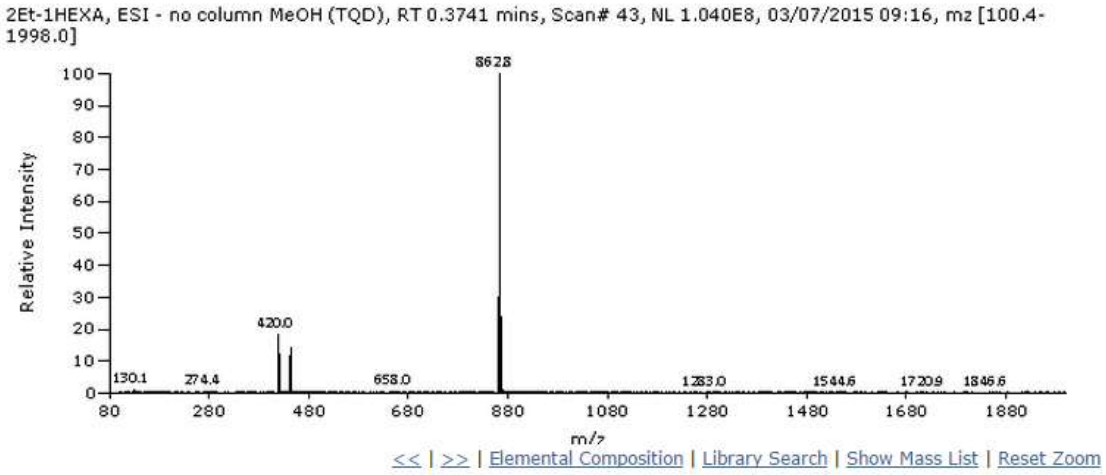
1: TOF MS ES+
1.87e+005



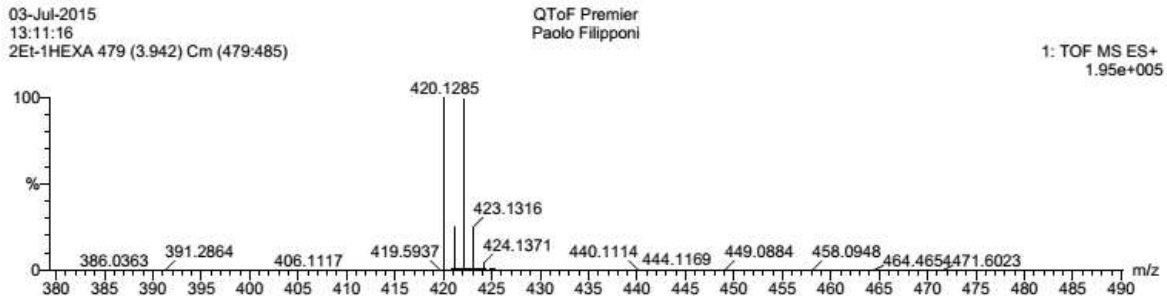
Minimum:				-1.5			
Maximum:		5.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
442.1133	442.1130	0.3	0.7	11.5	512.5	0.0	C22 H25 N3 O2 Br
	442.1138	-0.5	-1.1	13.5	534.6	22.2	C22 H20 N O9
	442.1149	-1.6	-3.6	-1.5	522.7	10.3	C10 H29 N5 O9 Br
	442.1151	-1.8	-4.1	18.5	534.7	22.2	C23 H16 N5 O5
	442.1170	-3.7	-8.4	15.5	518.8	6.4	C27 H25 N Br
	442.1093	4.0	9.0	27.5	534.9	22.5	C30 H12 N5
	442.1090	4.3	9.7	7.5	519.0	6.5	C17 H25 N5 O4 Br
	442.1181	-4.8	-10.9	0.5	526.4	14.0	C15 H34 N5 Br2



Chemical Formula: $C_{20}H_{26}BrN_3O_2$
Exact Mass: 419.12

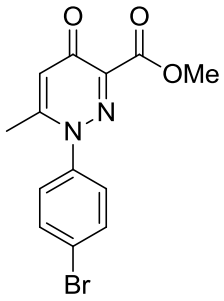


Monoisotopic Mass, Even Electron Ions
819 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-50 N: 0-6 O: 0-10 Br: 0-2



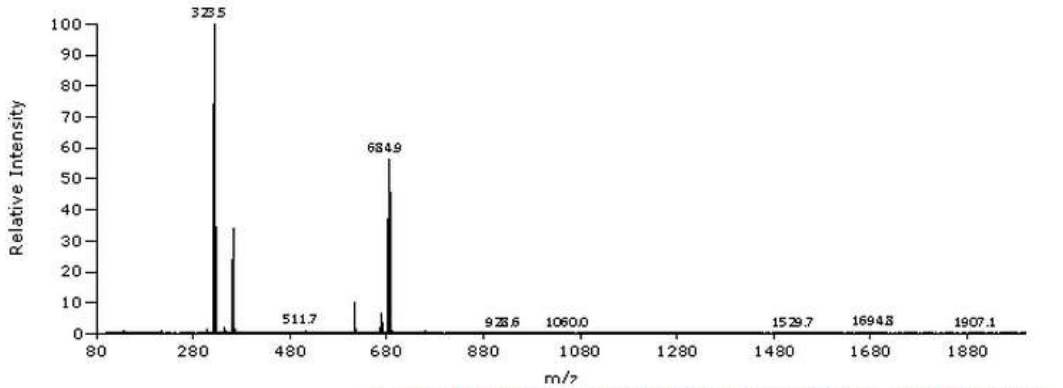
Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
420.1285	420.1287	-0.2	-0.5	8.5	491.7	0.0	C20 H27 N3 O2 Br
	420.1295	-1.0	-2.4	10.5	511.1	19.4	C20 H22 N O9
	420.1308	-2.3	-5.5	15.5	511.2	19.5	C21 H18 N5 O5
	420.1249	3.6	8.6	24.5	511.4	19.7	C28 H14 N5
	420.1246	3.9	9.3	4.5	498.1	6.4	C15 H27 N5 O4 Br
	420.1327	-4.2	-10.0	12.5	494.8	3.1	C25 H27 N Br
	420.1236	4.9	11.7	19.5	511.4	19.7	C27 H18 N O4

B4. Intermediates 24-26 and C derivatives 27-31



Chemical Formula: $C_{13}H_{11}BrN_2O_3$
Exact Mass: 322.00

pyridazone Me-Est, ESI - no column MeOH (TQD), RT 0.0852 mins, Scan# 5, NL 6.594E7, 24/09/2015 14:32, mz [100.6-1998.4]

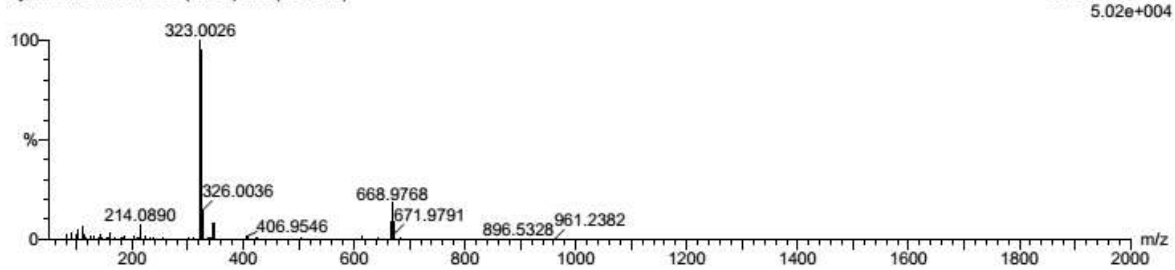


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

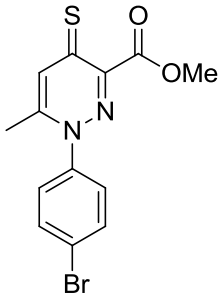
Monoisotopic Mass, Even Electron Ions
9040 formula(e) evaluated with 109 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 S: 0-6 Cl: 0-8 Br: 0-8

Paolo Filipponi
Pyridazone MeEst 336 (2.769) Cm (335:346)

1: TOF MS ES+
5.02e+004

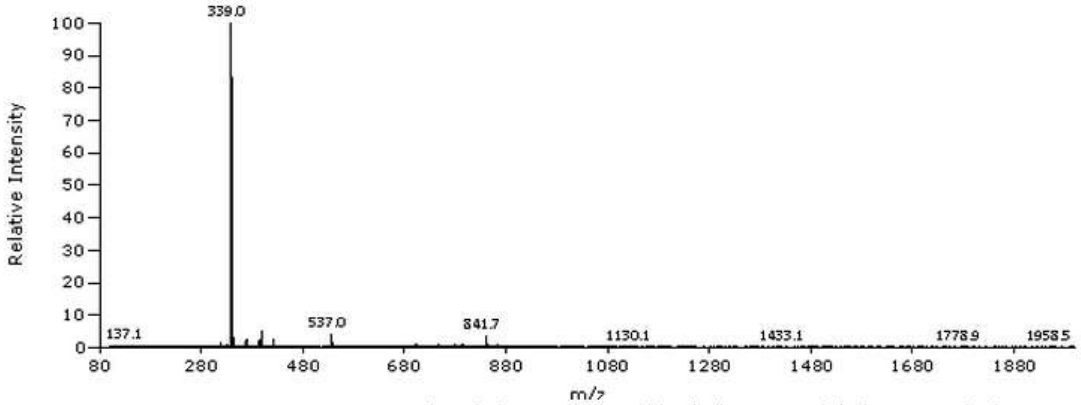


Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
323.0026	323.0031	-0.5	-1.5	8.5	396.6	0.9	C13 H12 N2 O3 Br
	323.0004	2.2	6.8	9.5	397.3	1.7	C9 H8 N8 O Br
	323.0072	-4.6	-14.2	12.5	397.4	1.8	C18 H12 O Br
	323.0038	-1.2	-3.7	4.5	398.3	2.7	C6 H12 N8 O S Br
	323.0009	1.7	5.3	5.5	398.7	3.0	C13 H14 O3 Cl3
	323.0000	2.6	8.0	3.5	399.3	3.7	C9 H16 N4 S2 Br
	323.0065	-3.9	-12.1	3.5	399.8	4.1	C10 H16 N2 O3 S Br
	323.0033	-0.7	-2.2	-1.5	400.0	4.3	C6 H20 N4 S3 Br
	322.9991	3.5	10.8	4.5	400.1	4.4	C8 H12 N4 O5 Br



Chemical Formula: $C_{13}H_{11}BrN_2O_2S$
Exact Mass: 337.97

Thioxo MeEst, ESI - no column MeOH (TQD), RT 0.1193 mins, Scan# 7, NL 1.207E8, 25/09/2015 07:05, mz [100.7-1997.8]

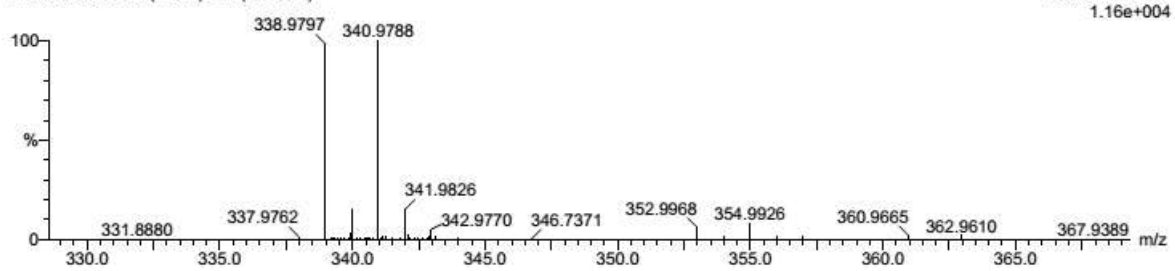


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

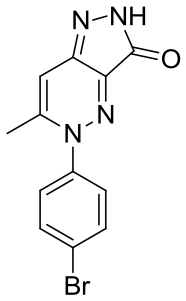
Monoisotopic Mass, Even Electron Ions
11162 formula(e) evaluated with 147 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 S: 0-6 Cl: 0-8 Br: 0-8

Paolo Filipponi
Thioxo MeEst 427 (3.514) Cm (427:430)

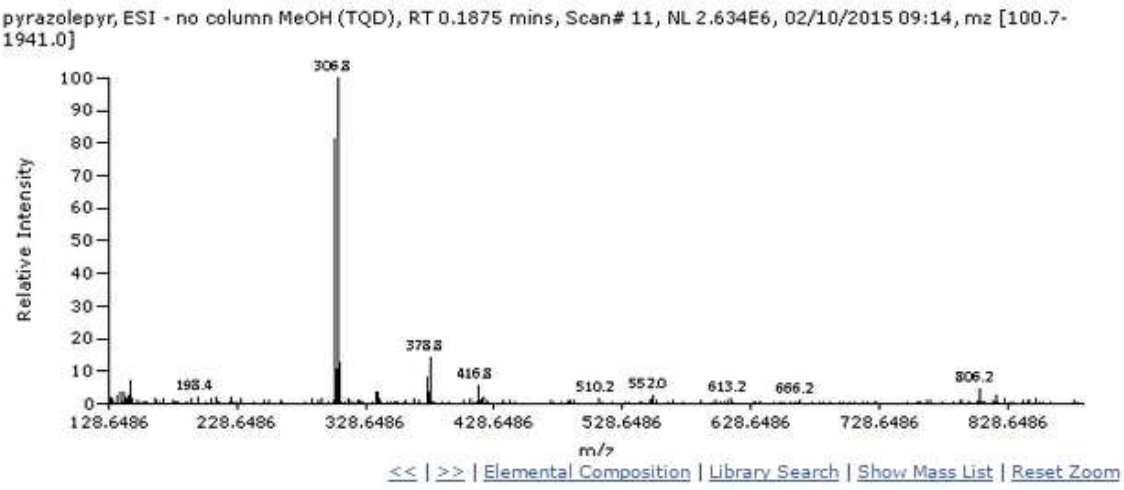
1: TOF MS ES+
1.16e+004



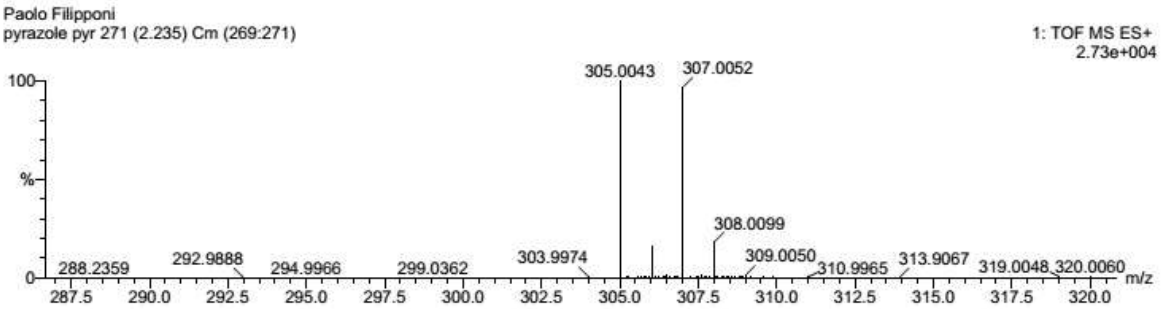
Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
338.9797	338.9780	1.7	5.0	5.5	245.9	0.4	C13 H14 O2 S Cl
	338.9803	-0.6	-1.8	8.5	246.6	1.1	C13 H12 N2 O2 S Br
	338.9776	2.1	6.2	9.5	251.1	5.6	C9 H8 N8 S Br
	338.9841	-4.4	-13.0	9.5	251.2	5.7	C10 H8 N6 O3 Br
	338.9837	-4.0	-11.8	3.5	252.0	6.6	C10 H16 N2 O2 S2 Br



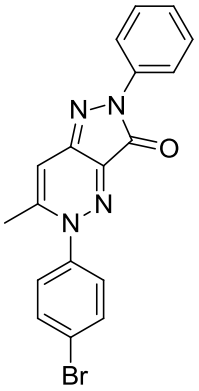
Chemical Formula: $C_{12}H_9BrN_4O$
Exact Mass: 304.00



Monoisotopic Mass, Even Electron Ions
728 formula(e) evaluated with 24 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-10 Br: 0-2

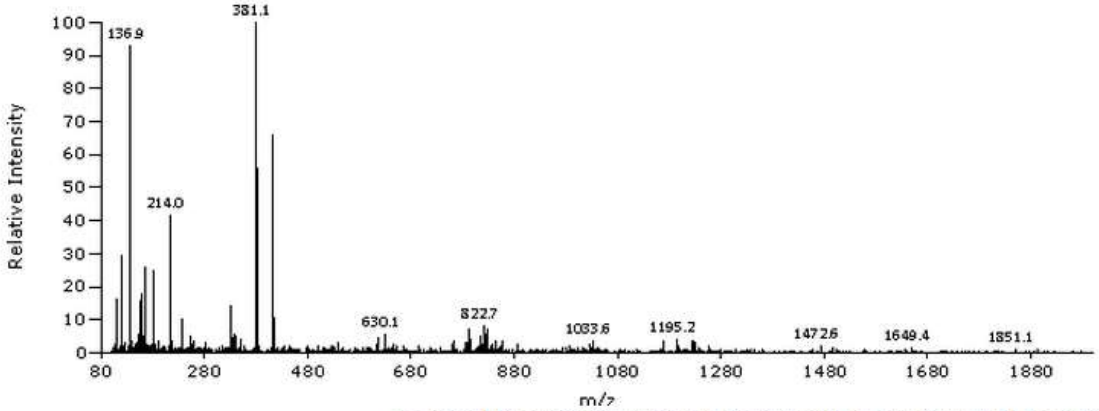


Minimum:				-1.5			
Maximum:		10.0	100.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
305.0043	305.0038	0.5	1.6	9.5	324.5	0.1	C12 H10 N4 O Br
	304.9966	7.7	25.2	13.5	328.1	3.7	C18 H10 Br
	305.0025	1.8	5.9	4.5	328.4	4.0	C11 H14 O5 Br
	305.0137	-9.4	-30.8	4.5	328.9	4.5	C10 H14 N2 O4 Br
	304.9998	4.5	14.8	5.5	330.1	5.7	C7 H10 N6 O3 Br
	305.0110	-6.7	-22.0	5.5	330.5	6.1	C6 H10 N8 O2 Br
	304.9984	5.9	19.3	0.5	331.5	7.1	C6 H14 N2 O7 Br



Chemical Formula: $C_{18}H_{13}BrN_4O$
Exact Mass: 380.03

Ph CSerie, ESI - no column MeOH (TQD), RT 0.2898 mins, Scan# 17, NL 4.480E6, 24/09/2015 14:38, mz [101.1-1977.3]

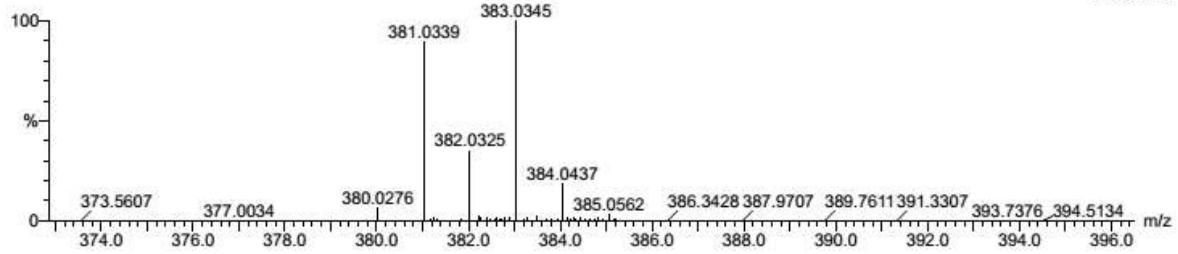


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

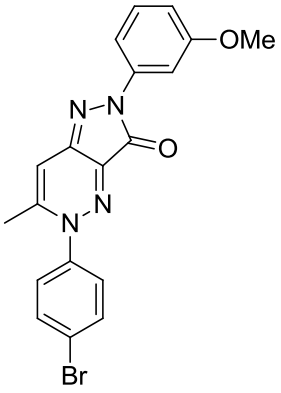
Monoisotopic Mass, Even Electron Ions
2078 formula(e) evaluated with 14 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 Br: 0-8

Paolo Filipponi
Ph C Serie 427 (3.513) Cm (427:428)

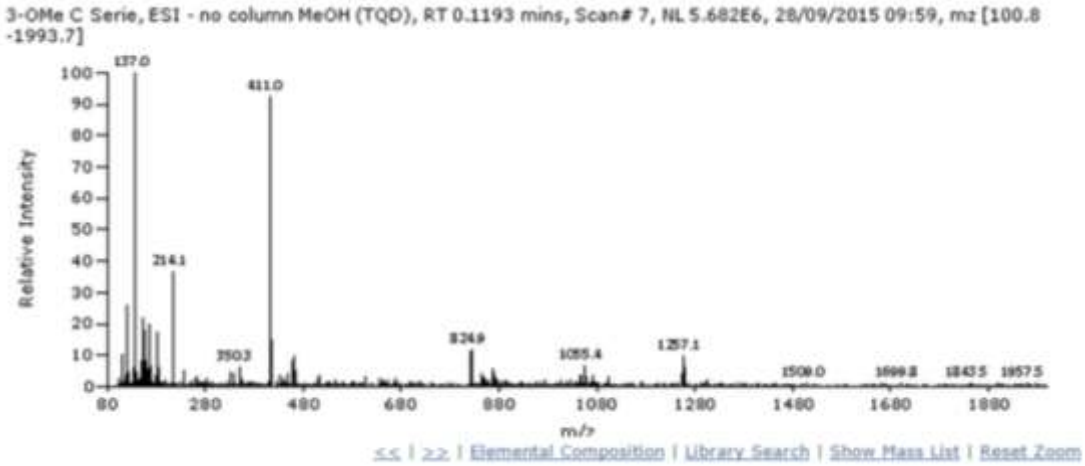
1: TOF MS ES+
8.05e+003



Minimum:				-1.5			
Maximum:		3.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
381.0339	381.0351	-1.2	-3.1	13.5	177.7	1.3	C18 H14 N4 O Br
	381.0356	-1.7	-4.5	6.5	177.8	1.4	C3 H10 N16 O2 Br
	381.0343	-0.4	-1.0	1.5	178.1	1.6	C2 H14 N12 O6 Br
	381.0338	0.1	0.3	8.5	178.5	2.1	C17 H18 O5 Br
	381.0311	2.8	7.3	9.5	178.7	2.2	C13 H14 N6 O3 Br
	381.0362	-2.3	-6.0	-1.5	180.7	4.2	C6 H23 N8 O Br2



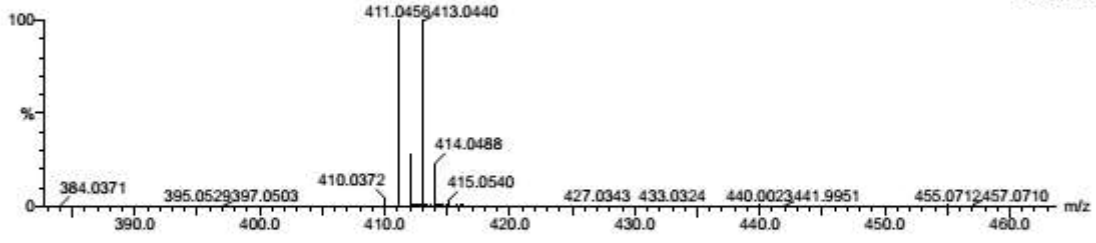
Chemical Formula: $C_{19}H_{15}BrN_4O_2$
Exact Mass: 410.04



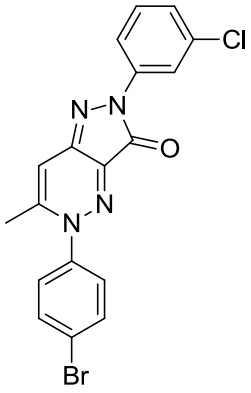
Monoisotopic Mass, Even Electron Ions
2611 formula(e) evaluated with 27 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 Br: 0-3

Paolo Filipponi
3OMe 441 (3.632) Cm (431:459)

1: TOF MS ES+
2.13e+005

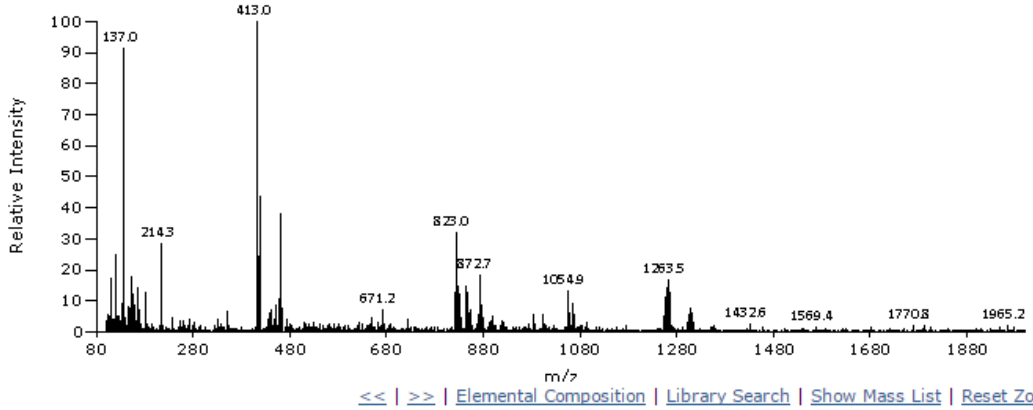


Minimum:				-1.5			
Maximum:		3.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
411.0456	411.0497	-4.1	-10.0	17.5	620.7	0.0	C24 H16 N2 Br
	411.0457	-0.1	-0.2	13.5	625.9	5.2	C19 H16 N4 O2 Br
	411.0430	2.6	6.3	14.5	628.9	8.2	C15 H12 N10 Br
	411.0443	1.3	3.2	8.5	629.0	8.3	C18 H20 O6 Br
	411.0416	4.0	9.7	9.5	631.3	10.6	C14 H16 N6 O4 Br



Chemical Formula: $C_{18}H_{12}BrClN_4O$
Exact Mass: 413.99

3-Cl C Serie, ESI - no column MeOH (TQD), RT 0.0852 mins, Scan# 5, NL 4.249E6, 28/09/2015 10:00, mz [100.2-1999.3]

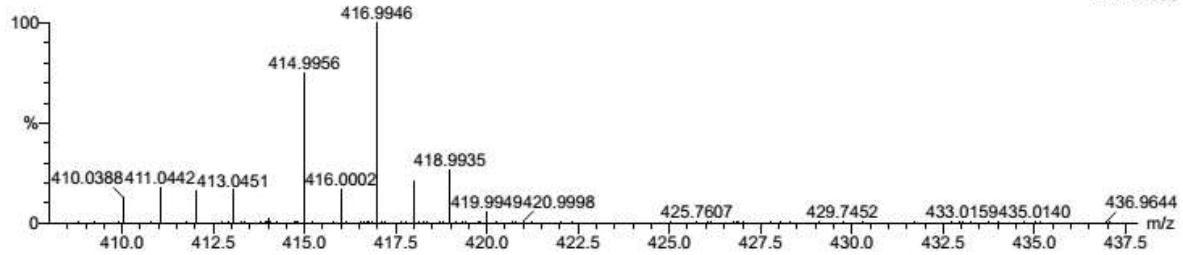


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

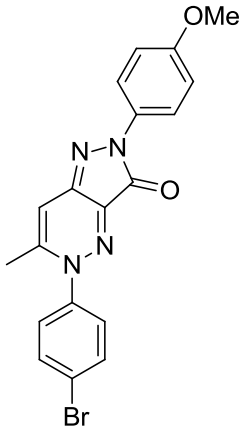
Monoisotopic Mass, Even Electron Ions
8640 formula(e) evaluated with 80 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 Cl: 0-8 Br: 0-3

Paolo Filipponi
3Cl 329 (2.709) Cm (311:343)

1: TOF MS ES+
4.47e+003

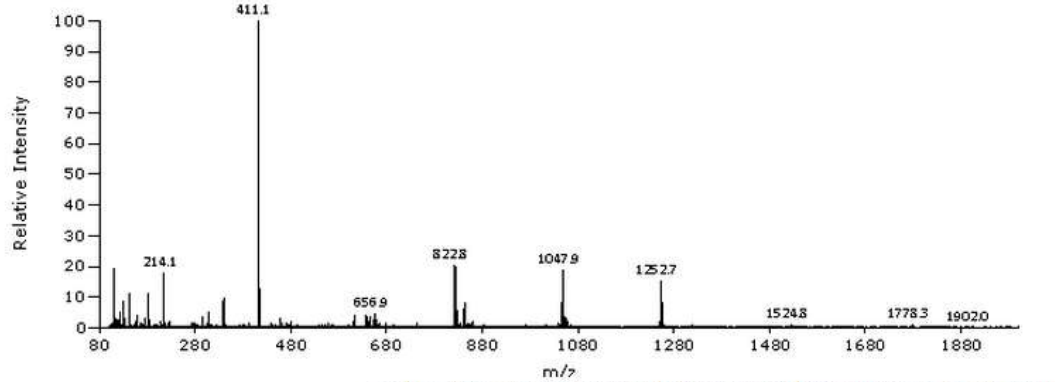


Minimum:				-1.5			
Maximum:		3.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
414.9956	414.9961	-0.5	-1.2	13.5	260.5	0.1	C18 H13 N4 O Cl Br
	414.9938	1.8	4.3	10.5	263.2	2.9	C18 H15 N2 O Cl4
	414.9948	0.8	1.9	8.5	263.5	3.2	C17 H17 O5 Cl Br
	414.9980	-2.4	-5.8	8.5	267.8	7.4	C17 H18 N2 O Cl2 Br
	414.9970	-1.4	-3.4	17.5	267.8	7.5	C23 H12 O3 Br
	414.9921	3.5	8.4	9.5	268.0	7.7	C13 H13 N6 O3 Cl Br



Chemical Formula: $C_{19}H_{15}BrN_4O_2$
Exact Mass: 410.04

4OMe C Serie, ESI - no column MeOH (TQD), RT 0.1534 mins, Scan# 9, NL 2.290E7, 24/09/2015 14:37, mz [99.9-1998.4]

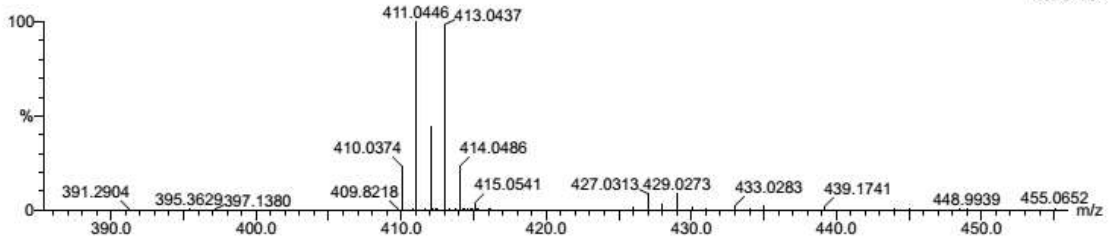


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

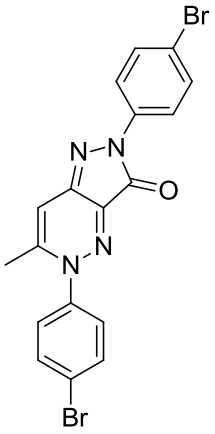
Monoisotopic Mass, Even Electron Ions
2653 formula(e) evaluated with 20 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 Br: 0-8

Paolo Filipponi
4-OMe C serie 436 (3.619) Cm (436:455)

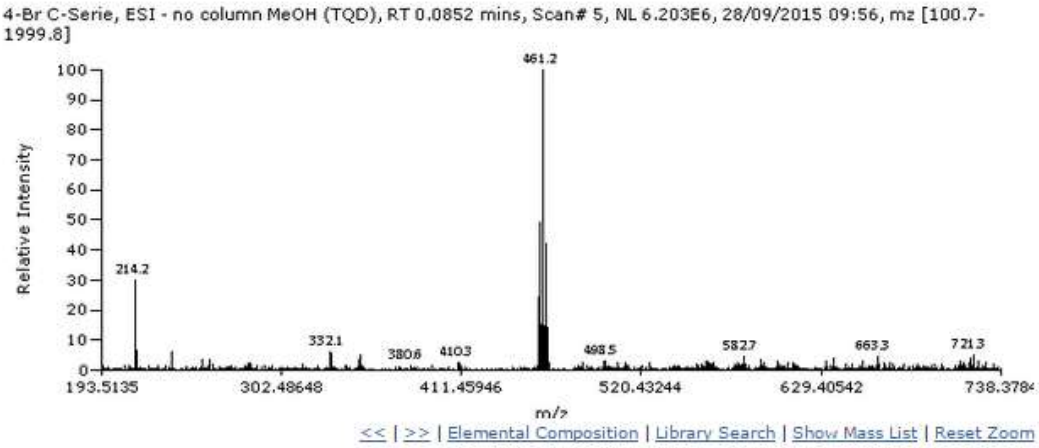
1: TOF MS ES+
1.92e+004



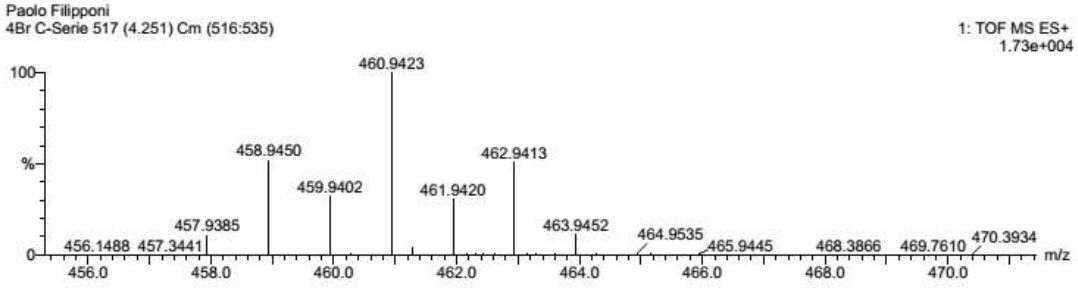
Minimum:				-1.5			
Maximum:		3.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
411.0446	411.0424	2.2	5.4	11.5	366.9	8.5	C14 H11 N4 O11
	411.0416	3.0	7.3	9.5	361.9	3.5	C14 H16 N6 O4 Br
	411.0430	1.6	3.9	14.5	361.0	2.6	C15 H12 N10 Br
	411.0438	0.8	1.9	16.5	366.7	8.3	C15 H7 N8 O7
	411.0451	-0.5	-1.2	21.5	366.5	8.1	C16 H3 N12 O3
	411.0443	0.3	0.7	8.5	361.9	3.5	C18 H20 O6 Br
	411.0465	-1.9	-4.6	15.5	367.5	9.1	C19 H11 N2 O9
	411.0457	-1.1	-2.7	13.5	361.2	2.8	C19 H16 N4 O2 Br
	411.0443	0.3	0.7	-1.5	366.8	8.4	C2 H15 N6 O18



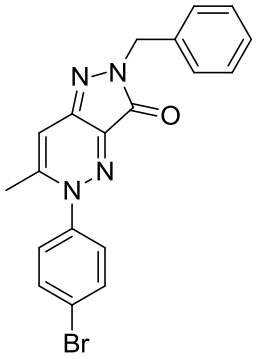
Chemical Formula: $C_{18}H_{12}Br_2N_4O$
Exact Mass: 457.94



Monoisotopic Mass, Even Electron Ions
3714 formula(e) evaluated with 28 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 Br: 0-3

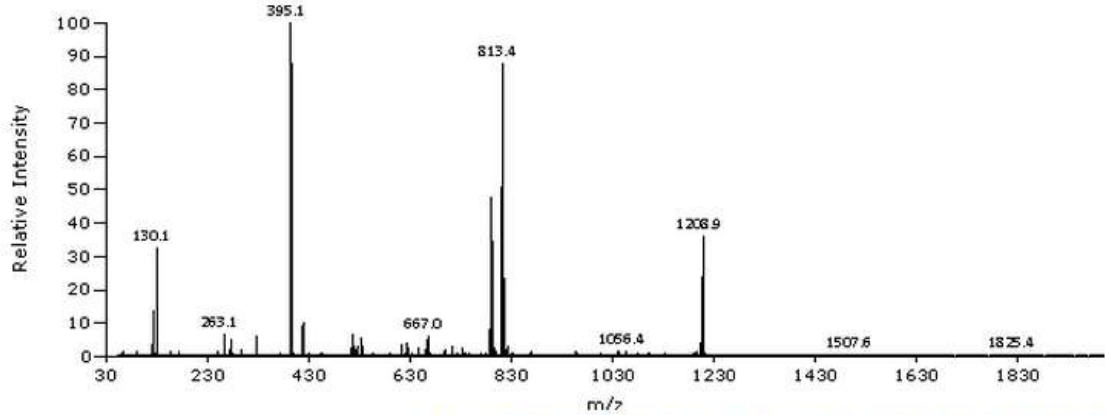


Minimum:				-1.5			
Maximum:		3.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
458.9450	458.9461	-1.1	-2.4	6.5	307.0	1.6	C3 H9 N16 O2 Br2
	458.9448	0.2	0.4	1.5	307.1	1.8	C2 H13 N12 O6 Br2
	458.9482	-3.2	-7.0	13.5	308.2	2.9	C4 N18 O5 Br
	458.9469	-1.9	-4.1	8.5	308.2	2.9	C3 H4 N14 O9 Br
	458.9456	-0.6	-1.3	13.5	308.3	3.0	C18 H13 N4 O Br2
	458.9456	-0.6	-1.3	3.5	308.4	3.0	C2 H8 N10 O13 Br
	458.9416	3.4	7.4	9.5	308.5	3.2	C13 H13 N6 O3 Br2
	458.9488	-3.8	-8.3	5.5	308.5	3.2	C7 H13 N10 O4 Br2
	458.9443	0.7	1.5	8.5	308.7	3.4	C17 H17 O5 Br2
	458.9442	0.8	1.7	-1.5	308.7	3.4	C H12 N6 O17 Br



Chemical Formula: $C_{19}H_{15}BrN_4O$
Exact Mass: 394.04

Bz C serie, ESI - no column MeOH (TQD), RT 0.2216 mins, Scan# 13, NL 6.167E7, 06/10/2015 09:21, mz [54.7-1999.1]

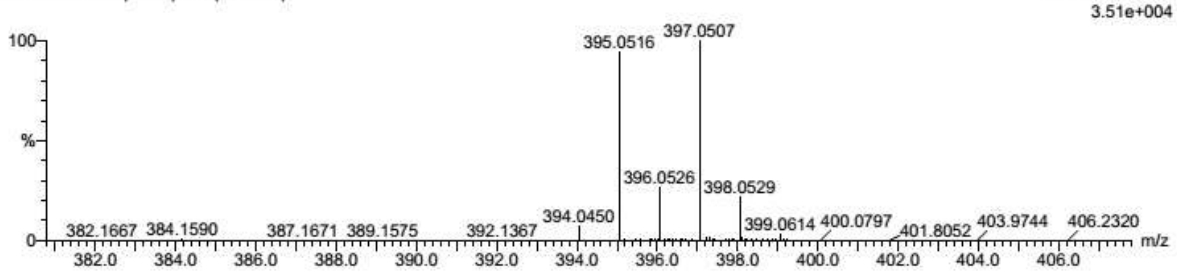


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

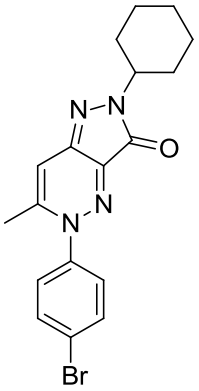
Monoisotopic Mass, Even Electron Ions
1174 formula(e) evaluated with 10 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-10 Br: 0-2

Paolo Filipponi
Bz C serie 408 (3.362) Cm (398:409)

1: TOF MS ES+
3.51e+004

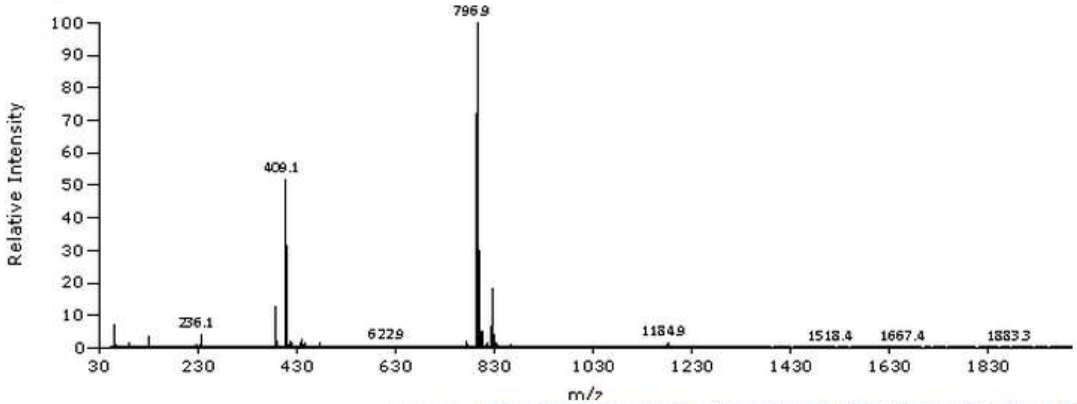


Minimum:				-1.5			
Maximum:		3.0	100.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
395.0516	395.0507	0.9	2.3	13.5	493.7	0.2	C19 H16 N4 O Br
	395.0494	2.2	5.6	8.5	495.9	2.3	C18 H20 O5 Br
	395.0539	-2.3	-5.8	5.5	496.7	3.2	C8 H16 N10 O4 Br
	395.0526	-1.0	-2.5	0.5	497.5	4.0	C7 H20 N6 O8 Br
	395.0518	-0.2	-0.5	-1.5	499.3	5.7	C7 H25 N8 O Br2
	395.0489	2.7	6.8	16.5	506.4	12.9	C15 H7 N8 O6
	395.0542	-2.6	-6.6	25.5	506.9	13.4	C21 H3 N10



Chemical Formula: $C_{18}H_{19}BrN_4O$
Exact Mass: 386.07

CHEX C Serie, ESI - no column MeOH (TQD), RT 0.3239 mins, Scan# 19, NL 6.609E7, 06/10/2015 09:25, mz [54.8-1999.4]

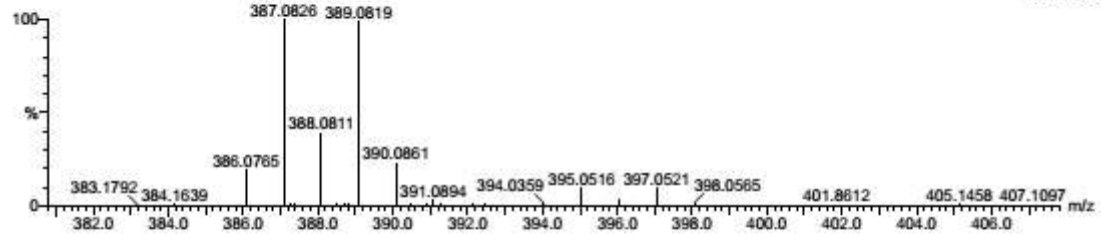


<< | >> | Elemental Composition | Library Search | Show Mass List | Reset Zoom

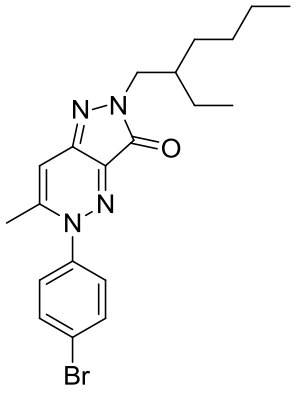
Monoisotopic Mass, Even Electron Ions
1128 formula(e) evaluated with 8 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-10 Br: 0-2

Paolo Filipponi
CHEX C serie 392 (3.227) Cm (390:397)

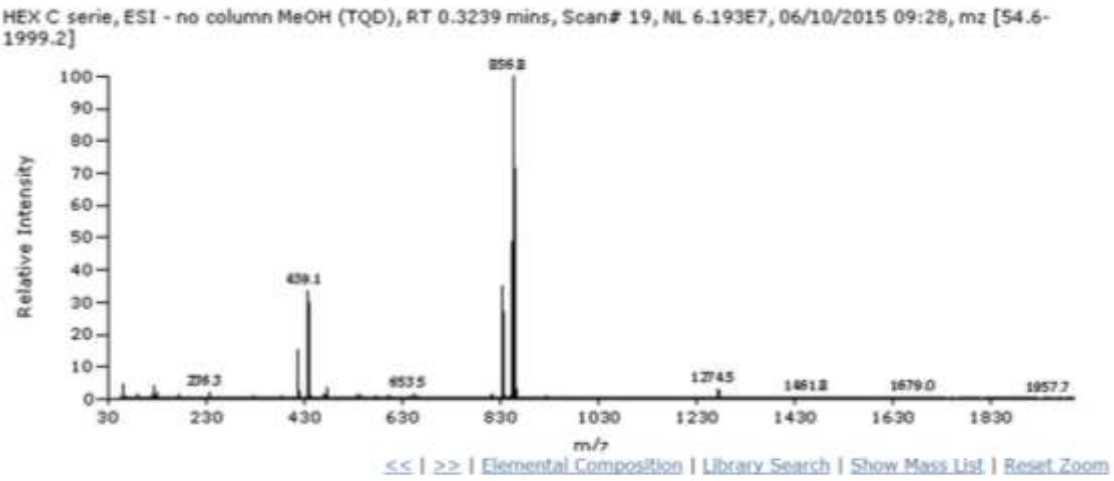
1: TOF MS ES+
2.81e+003



Minimum:				-1.5			
Maximum:		3.0	100.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
387.0826	387.0820	0.6	1.6	10.5	209.5	0.5	C18 H20 N4 O Br
	387.0807	1.9	4.9	5.5	210.4	1.4	C17 H24 O5 Br
	387.0852	-2.6	-6.7	2.5	210.8	1.9	C7 H20 N10 O4 Br
	387.0802	2.4	6.2	13.5	215.6	6.6	C14 H11 N8 O6
	387.0828	-0.2	-0.5	12.5	216.5	7.5	C18 H15 N2 O8
	387.0842	-1.6	-4.1	17.5	216.6	7.6	C19 H11 N6 O4
	387.0810	1.6	4.1	25.5	216.7	7.7	C30 H11 O
	387.0855	-2.9	-7.5	22.5	216.7	7.7	C20 H7 N10



Chemical Formula: $C_{20}H_{25}BrN_4O$
Exact Mass: 416.12



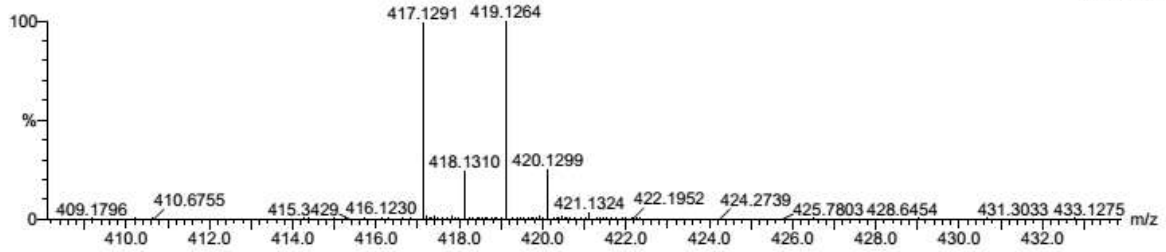
Monoisotopic Mass, Even Electron Ions
602 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-80 N: 0-6 O: 0-6 Br: 0-2

Paolo Filipponi
1: TOF MS ES+

LCT Premier

HEX C Series 176 (3.982)

2.86e+004



Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
417.1291	417.1290	0.1	0.2	9.5	284.7	0.0	C20 H26 N4 O Br
	417.1277	1.4	3.4	4.5	291.0	6.3	C19 H30 O5 Br
	417.1311	-2.0	-4.8	16.5	311.1	26.4	C21 H17 N6 O4
	417.1279	1.2	2.9	24.5	311.3	26.7	C32 H17 O

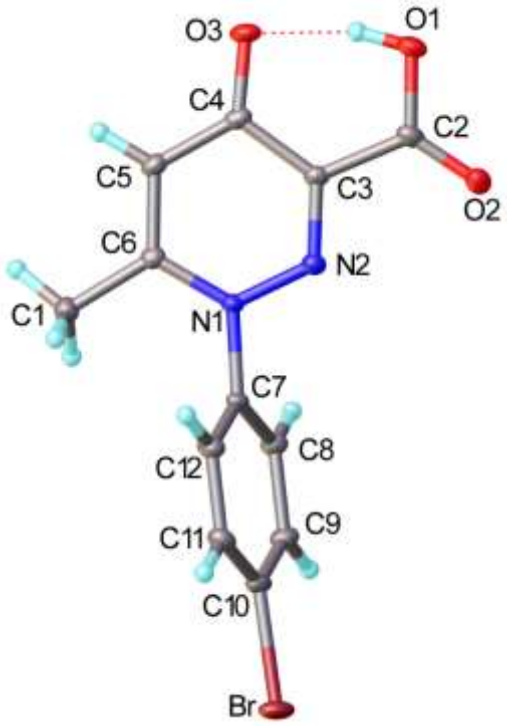
C. Single crystal X-Ray diffraction analysis

C1. 1-(4-bromophenyl)-6-methyl-4-oxo-1,4-dihydropyridazine-3-carboxylic acid, 2.

Cambridge Crystallographic Data Centre deposition reference CCDC 1424303

Formula: $C_{12}H_9BrN_2O_3$
Unit Cell Parameters: a 13.1231(11) b 6.7122(6) c 13.6238(12) P21/c

Single crystals of **2** were grown by slow evaporation of its methanol solution. The experiment was carried out on a Bruker D8 Venture 3-circle diffractometer with a CCD detector PHOTON 100 CMOS, using Mo-*K*α radiation from a ImuS microsource with focusing mirrors. The structure was solved by direct methods using SHELXS 2013/1 software[1] and refined by full-matrix least squares using SHELXL 2014/7[2] and OLEX2[3] software.



Molecular structure of **2**, showing thermal ellipsoids at 50% probability level. The dihedral angle between the phenyl and pyridazine rings equals 69.5°. The carboxylic group is coplanar with the latter within experimental error.

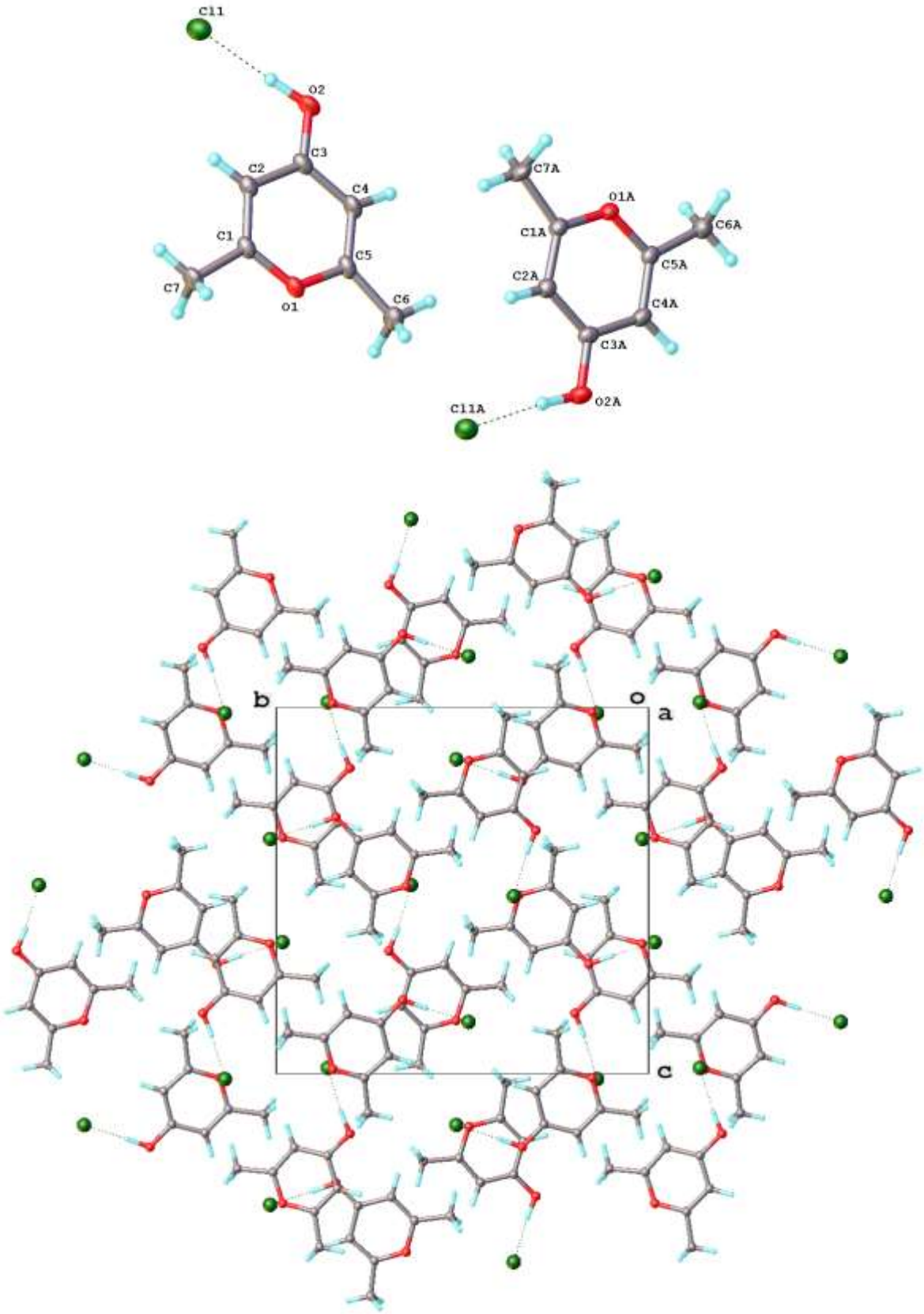
References

1. G. M. Sheldrick, Acta Crystallogr. **2008**, *A64*, 112-122.

2. G. M. Sheldrick, Acta Crystallogr. **2015**, *C71*, 3-8.

3. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, *42*, 339-341.

C2. X-Ray data for intermediates 6.



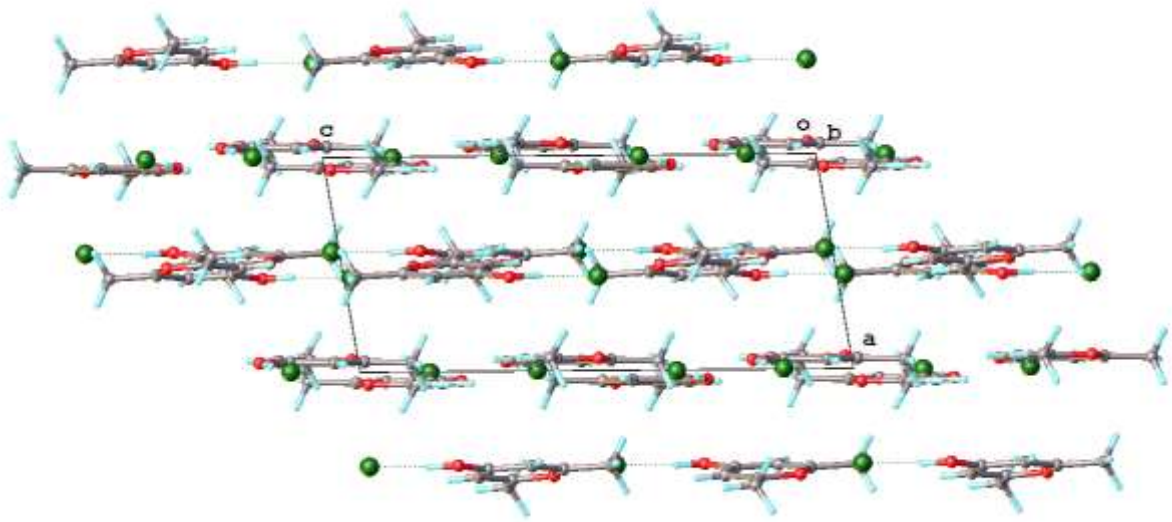


Table 1 Crystal data and structure refinement for CCDC 1448078.	
Identification code	CCDC 1448078
Empirical formula	$C_7H_9ClO_2$
Formula weight	160.59
Temperature/K	120.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.7201(3)
b/Å	15.2471(7)
c/Å	15.1879(7)
α/°	90.00
β/°	99.5435(17)
γ/°	90.00
Volume/Å^3	1534.65(12)
Z	8
ρ_{calc}g/cm^3	1.390
μ/mm^{-1}	0.432
F(000)	672.0
Crystal size/mm^3	0.58 × 0.43 × 0.18
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.34 to 59

Index ranges	$-9 \leq h \leq 9, -21 \leq k \leq 21, -21 \leq l \leq 21$
Reflections collected	23986
Independent reflections	4271 [R_{int} = 0.0302, R_{sigma} = 0.0245]
Data/restraints/parameters	4271/0/253
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0317, wR_2 = 0.0753
Final R indexes [all data]	R_1 = 0.0404, wR_2 = 0.0792
Largest diff. peak/hole / e $Å^{-3}$	0.37/-0.25

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 15srv255. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cl1	42.7(5)	10165.3(2)	3590.0(2)	26.23(9)
O1	572.8(13)	6514.5(6)	4878.7(5)	19.49(18)
O2	452.9(15)	8396.5(7)	2990.6(6)	25.6(2)
C1	491.5(18)	7361.5(8)	5118.0(8)	19.0(2)
C2	449.0(18)	8020.9(9)	4516.3(8)	19.5(2)
C3	487.2(18)	7804.3(9)	3615.0(8)	20.0(2)
C4	537(2)	6912.0(9)	3381.4(8)	22.1(2)
C5	579.1(19)	6288.7(9)	4020.4(8)	20.6(2)
C6	586(2)	5327.6(9)	3893.3(9)	27.1(3)
C7	430(2)	7468.3(10)	6081.5(8)	24.6(3)
Cl1A	4400.8(5)	3619.2(2)	5151.7(2)	23.79(8)
O1A	4890.6(13)	4826.3(5)	1450.6(6)	18.74(17)
O2A	4377.1(15)	3024.6(6)	3353.0(6)	25.4(2)
C1A	5055.8(19)	5089.8(8)	2305.7(8)	19.4(2)
C2A	4919.1(19)	4513.0(8)	2973.5(8)	19.1(2)
C3A	4566.3(18)	3622.8(8)	2757.6(8)	18.7(2)
C4A	4422.3(19)	3364.1(8)	1856.3(8)	19.5(2)
C5A	4575.3(18)	3976.6(8)	1225.7(8)	17.7(2)
C6A	4430(2)	3831.6(9)	253.2(9)	23.6(3)
C7A	5387(3)	6047.3(9)	2399(1)	29.5(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 15srv255. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cl1	29.93(17)	26.54(16)	21.26(15)	0.64(11)	1.45(12)	-4.69(12)
O1	20.2(4)	26.2(4)	12.2(4)	-0.1(3)	3.1(3)	1.1(3)
O2	33.4(5)	29.4(5)	14.8(4)	4.5(4)	6.6(4)	1.3(4)
C1	15.9(5)	27.7(6)	13.3(5)	-2.2(4)	2.0(4)	-0.5(5)
C2	17.5(6)	25.9(6)	15.0(5)	-1.3(4)	2.7(4)	-0.2(5)
C3	16.6(6)	29.4(6)	14.2(5)	1.9(4)	2.9(4)	0.2(5)
C4	23.8(6)	30.4(7)	12.3(5)	-1.4(5)	4.0(4)	2.3(5)
C5	18.9(6)	29.2(6)	13.6(5)	-2.2(4)	2.8(4)	1.8(5)
C6	36.6(8)	26.6(7)	18.3(6)	-1.5(5)	4.9(6)	3.9(6)
C7	30.5(7)	31.4(7)	12.4(5)	-0.8(5)	4.6(5)	0.1(6)
Cl1A	25.88(16)	23.56(15)	20.99(15)	2.03(11)	1.12(11)	-1.04(11)
O1A	21.9(4)	15.2(4)	19.6(4)	0.2(3)	4.7(3)	-1.7(3)
O2A	37.1(5)	17.5(4)	21.7(4)	4.5(3)	5.1(4)	-0.3(4)
C1A	20.9(6)	15.9(5)	21.5(6)	-1.4(4)	3.7(5)	-1.0(4)
C2A	19.9(6)	18.2(5)	19.1(6)	-0.8(4)	2.8(4)	-0.1(4)
C3A	17.3(6)	16.7(5)	21.5(6)	2.8(4)	1.6(4)	1.3(4)
C4A	20.9(6)	14.5(5)	22.6(6)	0.0(4)	2.0(5)	0.6(4)
C5A	15.5(5)	16.1(5)	21.2(6)	-1.6(4)	2.5(4)	1.2(4)
C6A	29.2(7)	20.9(6)	20.8(6)	-0.6(5)	4.8(5)	0.6(5)
C7A	46.6(9)	15.3(6)	27.0(7)	-1.6(5)	7.6(6)	-5.7(6)

Table 4 Bond Lengths for 15srv255.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
O1	C1	1.3452(15)		O1A	C1A	1.3464(15)
O1	C5	1.3490(14)		O1A	C5A	1.3476(14)
O2	C3	1.3068(15)		O2A	C3A	1.3055(15)
C1	C2	1.3558(17)		C1A	C2A	1.3571(17)
C1	C7	1.4797(17)		C1A	C7A	1.4800(18)
C2	C3	1.4125(16)		C2A	C3A	1.4072(17)
C3	C4	1.4077(19)		C3A	C4A	1.4124(17)
C4	C5	1.3552(18)		C4A	C5A	1.3537(17)
C5	C6	1.4782(19)		C5A	C6A	1.4806(17)

Table 5 Bond Angles for 15srv255.								
Atom	**Atom**	**Atom**	**Angle/°**		**Atom**	**Atom**	**Atom**	**Angle/°**
C1	O1	C5	120.85(10)		C1A	O1A	C5A	121.05(10)
O1	C1	C2	121.81(11)		O1A	C1A	C2A	121.51(11)
O1	C1	C7	112.45(11)		O1A	C1A	C7A	111.95(11)
C2	C1	C7	125.73(12)		C2A	C1A	C7A	126.54(12)
C1	C2	C3	118.56(12)		C1A	C2A	C3A	118.72(12)
O2	C3	C2	122.73(12)		O2A	C3A	C2A	122.99(11)
O2	C3	C4	118.89(11)		O2A	C3A	C4A	118.51(11)
C4	C3	C2	118.37(11)		C2A	C3A	C4A	118.49(11)
C5	C4	C3	119.72(11)		C5A	C4A	C3A	119.47(11)
O1	C5	C4	120.67(12)		O1A	C5A	C4A	120.74(11)
O1	C5	C6	112.31(11)		O1A	C5A	C6A	112.21(10)
C4	C5	C6	127.01(12)		C4A	C5A	C6A	127.06(11)

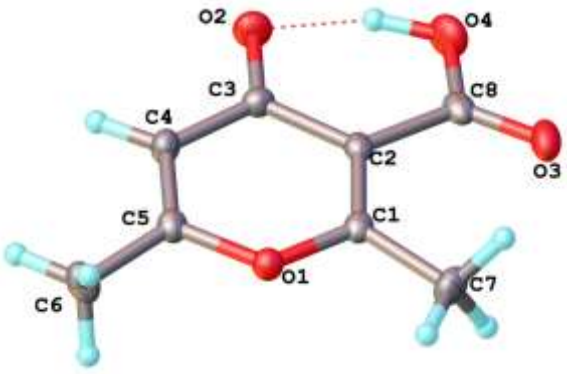
Table 6 Hydrogen Bonds for 15srv255.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
O2	H2	Cl1	0.99(2)	1.89(2)	2.8742(11)	178.3(19)
O2A	H2AA	Cl1A	0.95(2)	1.92(2)	2.8759(10)	174(2)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 15srv255.				
Atom	***x***	***y***	***z***	**U(eq)**
H2	320(30)	9001(15)	3209(14)	62(6)
H2A	380(20)	8601(11)	4689(11)	24(4)
H4	560(20)	6738(11)	2790(11)	26(4)
H6A	1750(30)	5076(12)	4274(12)	37(5)
H6B	590(30)	5207(12)	3273(12)	37(5)
H6C	-640(30)	5083(12)	4063(12)	35(5)
H7A	330(30)	8064(13)	6213(12)	42(5)
H7B	1620(30)	7231(13)	6416(13)	48(5)
H7C	-730(30)	7185(14)	6229(13)	51(6)
H2AA	4440(30)	3257(15)	3940(16)	69(7)
H2AB	5050(20)	4719(10)	3560(10)	22(4)
H4A	4210(20)	2766(11)	1690(10)	25(4)
H6AA	4310(20)	3235(12)	140(11)	30(4)
H6AB	3260(30)	4151(12)	-72(11)	33(4)
H6AC	5600(30)	4051(11)	45(11)	29(4)
H7AA	5510(30)	6200(12)	3019(13)	42(5)
H7AB	6600(30)	6213(13)	2153(13)	47(5)
H7AC	4260(30)	6349(12)	2045(13)	44(5)

Refinement model description

Number of restraints - 0, number of constraints -0.

C3. X-Ray data for intermediates 7.



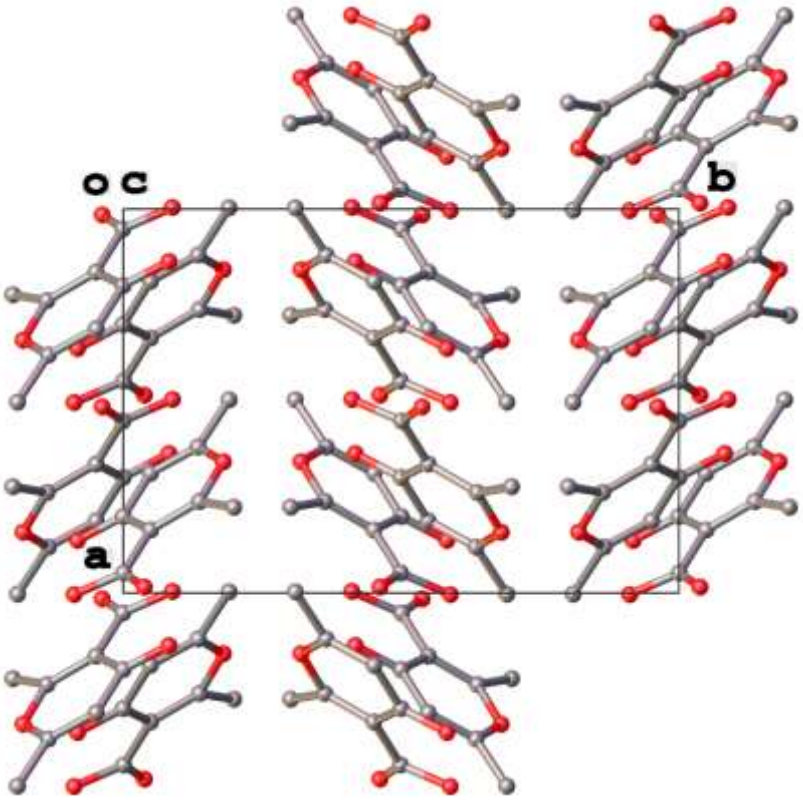


Table 1 Crystal data and structure refinement for CCDC 1448079.	
Identification code	CCDC 1448079
Empirical formula	$C_8H_8O_4$
Formula weight	168.14
Temperature/K	120.0
Crystal system	orthorhombic
Space group	Pbca
a/Å	8.9431(6)
b/Å	12.9158(9)
c/Å	13.2871(9)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	1534.76(18)
Z	8
ρ_{calc}g/cm^3	1.455
μ/mm^{-1}	0.118

F(000)	704.0
Crystal size/mm^3	0.31 × 0.18 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.14 to 59
Index ranges	$-12 \leq h \leq 12$, $-17 \leq k \leq 17$, $-18 \leq l \leq 18$
Reflections collected	22648
Independent reflections	2140 [R_{int} = 0.0384, R_{sigma} = 0.0195]
Data/restraints/parameters	2140/0/141
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0371, wR_2 = 0.0935
Final R indexes [all data]	R_1 = 0.0464, wR_2 = 0.0991
Largest diff. peak/hole / e $Å^{-3}$	0.37/-0.29

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 15srv256. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	3418.1(8)	6802.6(5)	4010.8(5)	17.06(17)
O2	1367.7(9)	4176.0(6)	4906.6(6)	24.56(19)
O3	152.7(9)	5379.8(7)	2179.8(6)	26.4(2)
O4	-41.2(10)	4114.4(7)	3286.8(7)	29.2(2)
C1	2383.1(11)	6372.1(8)	3400.8(7)	16.0(2)
C2	1642.7(10)	5491.6(8)	3669.1(7)	15.3(2)
C3	1990.9(11)	4998.4(8)	4623.3(8)	17.0(2)
C4	3117.2(12)	5487.6(8)	5222.1(8)	18.7(2)
C5	3803.0(11)	6347.2(8)	4899.8(7)	17.2(2)
C6	5031.4(13)	6904.1(9)	5416.4(9)	23.6(2)
C7	2232.6(14)	6988.1(9)	2457.5(9)	24.3(2)
C8	521.3(11)	5008.0(8)	2978.7(8)	19.1(2)

Table 3 Anisotropic Displacement Parameters ($Å^2$×10^3) for 15srv256. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	18.8(3)	14.8(3)	17.6(3)	0.4(3)	-0.6(3)	0.0(3)
O2	26.9(4)	19.2(4)	27.5(4)	4.9(3)	-0.3(3)	-5.0(3)
O3	22.6(4)	36.1(5)	20.4(4)	-4.4(3)	-5.4(3)	5.1(3)
O4	29.3(4)	26.8(4)	31.4(5)	-5.1(4)	-5.9(4)	-8.7(3)
C1	16.4(4)	16.5(4)	15.3(4)	-1.8(4)	0.4(3)	4.5(4)
C2	13.6(4)	17.0(4)	15.3(4)	-2.2(3)	0.3(3)	2.9(3)
C3	17.3(4)	15.6(4)	18.1(5)	1.1(4)	1.6(4)	1.3(4)
C4	20.6(5)	19.0(5)	16.6(5)	1.8(4)	-3.0(4)	1.0(4)
C5	17.2(4)	16.6(4)	17.9(5)	-2.1(4)	-1.4(4)	3.9(4)
C6	22.6(5)	19.1(5)	29.1(6)	-2.7(4)	-7.1(5)	-0.3(4)
C7	30.6(6)	24.0(5)	18.2(5)	5.6(4)	-0.9(4)	2.4(5)
C8	14.8(4)	22.7(5)	19.8(5)	-6.7(4)	0.4(4)	3.7(4)

Table 4 Bond Lengths for 15srv256.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
O1	C1	1.3501(12)		C1	C7	1.4905(14)
O1	C5	1.3638(12)		C2	C3	1.4526(14)
O2	C3	1.2573(12)		C2	C8	1.4958(14)
O3	C8	1.2107(14)		C3	C4	1.4307(14)
O4	C8	1.3239(14)		C4	C5	1.3388(14)
C1	C2	1.3634(14)		C5	C6	1.4817(14)

Table 5 Bond Angles for 15srv256.								
Atom	**Atom**	**Atom**	**Angle/°**		**Atom**	**Atom**	**Atom**	**Angle/°**
C1	O1	C5	121.02(8)		C4	C3	C2	116.28(9)
O1	C1	C2	121.30(9)		C5	C4	C3	120.72(10)
O1	C1	C7	110.30(9)		O1	C5	C6	112.27(9)
C2	C1	C7	128.40(9)		C4	C5	O1	121.28(9)
C1	C2	C3	119.33(9)		C4	C5	C6	126.45(10)
C1	C2	C8	120.90(9)		O3	C8	O4	120.89(10)
C3	C2	C8	119.73(9)		O3	C8	C2	123.68(10)
O2	C3	C2	122.47(9)		O4	C8	C2	115.41(9)
O2	C3	C4	121.24(10)					

Table 6 Hydrogen Bonds for 15srv256.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
O4	H4	O2	0.96(2)	1.58(2)	2.4953(12)	157.2(18)

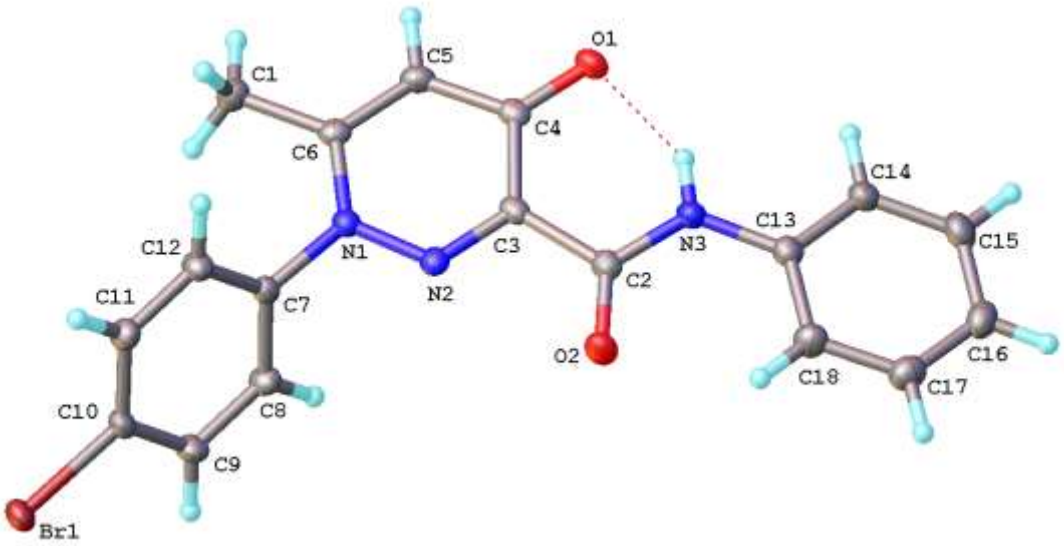
Table 7 Selected Torsion Angles for 15srv256.										
A	**B**	**C**	**D**	**Angle/°**		**A**	**B**	**C**	**D**	**Angle/°**
C1	C2	C8	O3	-3.54(15)		C3	C2	C8	O3	178.72(9)
C1	C2	C8	O4	175.09(9)		C3	C2	C8	O4	-2.66(13)

Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 15srv256.				
Atom	***x***	***y***	***z***	**U(eq)**
H4	370(20)	3983(15)	3943(16)	61(6)
H4A	3426(15)	5178(12)	5850(11)	30(4)
H6A	5296(18)	6566(13)	6045(13)	38(4)
H6B	5874(18)	6905(12)	4982(12)	37(4)
H6C	4723(17)	7602(13)	5547(12)	34(4)
H7A	2560(18)	6581(11)	1874(11)	33(4)
H7B	2850(20)	7608(14)	2509(12)	45(4)
H7C	1200(20)	7176(13)	2331(13)	47(5)

Refinement model description

Number of restraints - 0, number of constraints - 0.

C4. *N*-phenyl-1-(4-bromophenyl)-6-methyl-4-oxo-1,4-dihydropyridazine-3-carboxamide, 16a



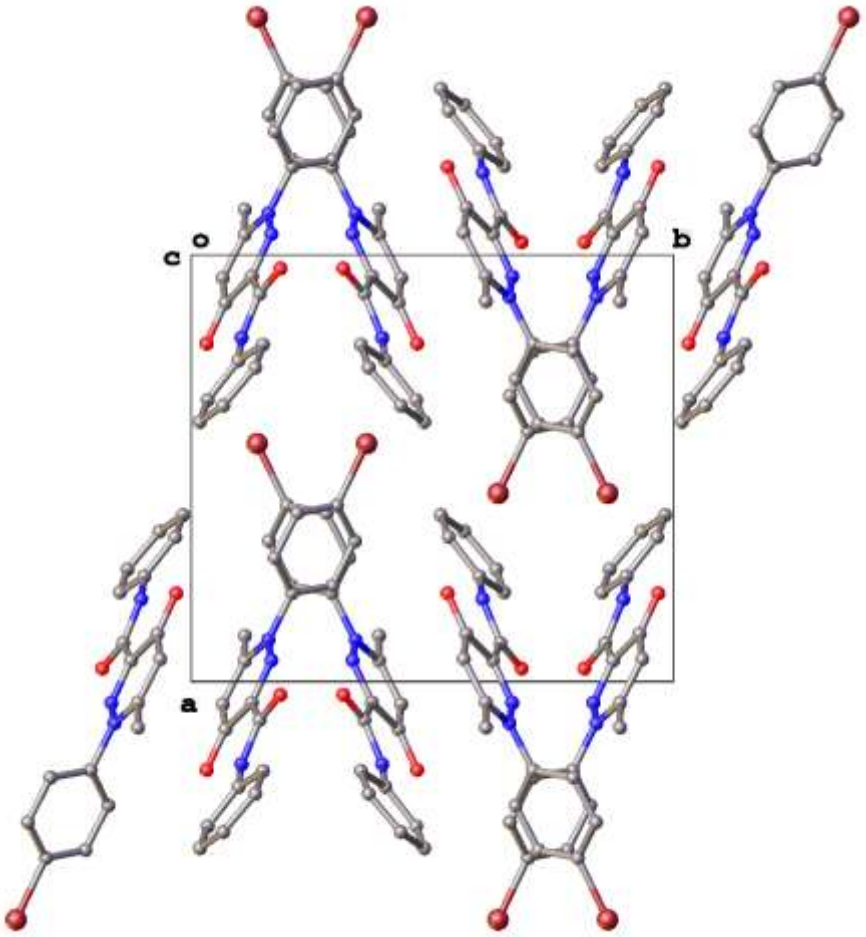

c
o
b
a

Table 1 Crystal data and structure refinement for CCDC 1448080.	
Identification code	CCDC 1448080
Empirical formula	$C_{18}H_{14}BrN_3O_2$
Formula weight	384.23
Temperature/K	120.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.7446(3)
b/Å	13.3908(3)
c/Å	10.0901(3)
α/°	90.00
β/°	111.706(3)
γ/°	90.00
Volume/Å^3	1599.88(6)
Z	4
ρ_{calc}g/cm^3	1.595
μ/mm^{-1}	2.585
F(000)	776.0
Crystal size/mm^3	0.39 × 0.18 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.6 to 58
Index ranges	$-17 \leq h \leq 17$, $-18 \leq k \leq 18$, $-13 \leq l \leq 13$
Reflections collected	25926
Independent reflections	4257 [R_{int} = 0.0524, R_{sigma} = 0.0361]
Data/restraints/parameters	4257/0/222
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0314, wR_2 = 0.0700
Final R indexes [all data]	R_1 = 0.0455, wR_2 = 0.0756
Largest diff. peak/hole / e Å^{-3}	0.45/-0.32

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 15srv244. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.				
Atom	***x***	***y***	***z***	**U(eq)**
Br1	4416.08(16)	3635.93(15)	5885.8(2)	23.06(7)
O1	12070.4(11)	315.1(10)	9996.8(15)	21.9(3)
O2	10308.2(12)	1847.4(11)	12209.4(15)	26.4(3)
N1	9022.1(13)	1596.7(11)	7989.4(17)	16.5(3)
N2	9500.5(14)	1658.2(11)	9411.5(17)	16.4(3)
N3	11935.9(14)	1040.8(13)	12415.3(18)	19.2(3)
C1	8923.8(19)	1108.2(15)	5589(2)	22.1(4)
C2	10900.9(16)	1413.0(13)	11675(2)	17.8(4)
C3	10495.6(16)	1253.4(13)	10079(2)	16.4(4)
C4	11118.4(16)	704.7(13)	9350(2)	17.4(4)
C5	10531.1(17)	647.9(14)	7848(2)	19.3(4)
C6	9510.9(17)	1107.3(14)	7171(2)	17.5(4)
C7	7925.9(16)	2087.3(14)	7436(2)	16.7(4)
C8	7095.2(17)	1727.0(15)	7890(2)	19.8(4)
C9	6049.1(17)	2198.4(15)	7437(2)	21.1(4)
C10	5862.3(16)	3019.2(15)	6547(2)	19.0(4)
C11	6701.6(18)	3391.6(15)	6126(2)	21.6(4)
C12	7749.1(17)	2923.5(15)	6574(2)	20.7(4)
C13	12469.0(16)	977.0(15)	13910(2)	19.2(4)
C14	13392.8(17)	337.9(15)	14444(2)	22.7(4)
C15	13907.4(18)	173.2(17)	15894(2)	27.5(5)
C16	13524.3(18)	659.9(16)	16839(2)	26.4(5)
C17	12634.6(19)	1323.0(16)	16325(2)	26.5(5)
C18	12095.6(19)	1484.3(15)	14872(2)	24.1(4)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 15srv244. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Br1	14.73(10)	29.44(12)	23.08(11)	2.82(8)	4.71(8)	3.33(8)
O1	17.5(7)	23.1(7)	25.7(7)	0.8(6)	8.7(6)	5.3(6)
O2	23.0(8)	32.0(8)	23.4(8)	-2.7(6)	7.8(6)	9.2(6)
N1	15.3(8)	16.6(8)	18.1(8)	1.0(6)	6.7(7)	-0.4(6)
N2	17.2(8)	14.8(7)	17.9(8)	1.4(6)	7.5(7)	-1.6(6)
N3	16.4(8)	22.4(8)	19.7(8)	0.3(7)	7.9(7)	3.0(7)
C1	24.5(11)	22.5(10)	19.6(10)	-1.5(8)	8.6(8)	-0.9(8)
C2	17.9(9)	14.5(9)	21.1(10)	1.6(7)	7.2(8)	-1.0(7)
C3	14.4(9)	12.8(9)	22.6(10)	2.3(7)	7.6(8)	-0.6(7)
C4	16.5(9)	13.3(8)	23.8(10)	1.5(7)	9.2(8)	-2.0(7)
C5	20.8(10)	17.0(9)	23.3(10)	-2.1(7)	12.0(8)	-0.6(8)
C6	19(1)	15.4(9)	20.9(10)	-0.5(7)	10.7(8)	-2.7(7)
C7	15.2(9)	18.4(9)	16.1(9)	-0.8(7)	5.3(7)	1.1(7)
C8	21.1(10)	18.4(9)	22(1)	4.1(8)	10.3(8)	0.2(8)
C9	16.7(9)	24(1)	24.7(10)	1.7(8)	10.0(8)	-1.6(8)
C10	13.5(9)	23.4(10)	18.6(9)	0.0(7)	4.0(8)	1.8(7)
C11	22(1)	22.1(10)	21(1)	5.6(8)	8.2(8)	2.7(8)
C12	17.8(9)	22.4(10)	22.9(10)	4.4(8)	8.6(8)	-0.6(8)
C13	17.4(10)	19.1(9)	20.6(10)	-0.1(7)	6.5(8)	-1.5(8)
C14	16.8(9)	29.0(11)	22.4(10)	0.0(8)	7.4(8)	1.7(8)
C15	18(1)	32.8(12)	27.6(11)	2.5(9)	3.5(9)	2.1(9)
C16	25.3(11)	31.5(11)	19.6(10)	1.9(8)	4.9(9)	-4.5(9)
C17	29.3(12)	27.8(11)	23.7(11)	-4.5(9)	11.3(9)	-3.6(9)
C18	26.3(11)	22.5(10)	23.9(11)	-1.5(8)	9.8(9)	3.1(8)

Table 4 Bond Lengths for 15srv244.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
Br1	C10	1.9013(19)		C5	C6	1.371(3)
O1	C4	1.259(2)		C7	C8	1.387(3)
O2	C2	1.225(2)		C7	C12	1.384(3)
N1	N2	1.338(2)		C8	C9	1.391(3)
N1	C6	1.371(2)		C9	C10	1.383(3)
N1	C7	1.455(2)		C10	C11	1.382(3)
N2	C3	1.313(2)		C11	C12	1.390(3)
N3	C2	1.348(3)		C13	C14	1.393(3)
N3	C13	1.410(3)		C13	C18	1.404(3)
C1	C6	1.492(3)		C14	C15	1.382(3)
C2	C3	1.513(3)		C15	C16	1.384(3)
C3	C4	1.464(3)		C16	C17	1.381(3)
C4	C5	1.422(3)		C17	C18	1.386(3)

Table 5 Bond Angles for 15srv244.								
Atom	**Atom**	**Atom**	**Angle/°**		**Atom**	**Atom**	**Atom**	**Angle/°**
N2	N1	C6	123.16(16)		C8	C7	N1	117.25(17)
N2	N1	C7	112.07(15)		C12	C7	N1	121.10(17)
C6	N1	C7	124.75(16)		C12	C7	C8	121.49(18)
C3	N2	N1	119.68(16)		C7	C8	C9	119.33(18)
C2	N3	C13	126.95(18)		C10	C9	C8	119.20(18)
O2	C2	N3	124.58(19)		C9	C10	Br1	118.98(15)
O2	C2	C3	120.81(18)		C11	C10	Br1	119.72(15)
N3	C2	C3	114.62(17)		C11	C10	C9	121.30(18)
N2	C3	C2	111.85(16)		C10	C11	C12	119.77(18)
N2	C3	C4	123.36(18)		C7	C12	C11	118.88(18)
C4	C3	C2	124.78(17)		C14	C13	N3	117.05(18)
O1	C4	C3	123.04(18)		C14	C13	C18	118.98(19)
O1	C4	C5	123.85(18)		C18	C13	N3	123.92(18)
C5	C4	C3	113.11(17)		C15	C14	C13	120.62(19)
C6	C5	C4	122.40(18)		C14	C15	C16	120.3(2)
N1	C6	C1	118.98(18)		C17	C16	C15	119.6(2)
C5	C6	N1	118.20(18)		C16	C17	C18	121.0(2)
C5	C6	C1	122.82(18)		C17	C18	C13	119.6(2)

Table 6 Hydrogen Bonds for 15srv244.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N3	H3	O1	0.83(2)	1.95(2)	2.690(2)	147(2)

Table 7 Selected Torsion Angles for 15srv244.										
A	**B**	**C**	**D**	**Angle/°**		**A**	**B**	**C**	**D**	**Angle/°**
N2	C3	C2	O2	2.2(3)		C8	C7	N1	C6	118.1(2)
N2	C3	C2	N3	-178.00(16)		C12	C7	N1	N2	114.84(19)
C3	C2	N3	C13	-172.12(17)		C12	C7	N1	C6	-66.4(3)
C4	C3	C2	O2	-177.03(18)		C13	N3	C2	O2	7.7(3)
C4	C3	C2	N3	2.8(3)		C14	C13	N3	C2	163.38(19)
C8	C7	N1	N2	-60.6(2)		C18	C13	N3	C2	-14.0(3)

Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 15srv244.				
Atom	***x***	***y***	***z***	**U(eq)**
H1A	8115	989	5345	33
H1B	9239	580	5175	33
H1C	9032	1757	5207	33
H5	10858	278	7295	23
H8	7239	1164	8504	24
H9	5470	1960	7736	25
H11	6563	3965	5532	26
H12	8334	3173	6294	25
H14	13672	12	13805	27
H15	14526	-276	16244	33
H16	13871	539	17835	32
H17	12388	1674	16976	32
H18	11478	1935	14530	29
H3	12233(18)	754(16)	11910(20)	17(6)

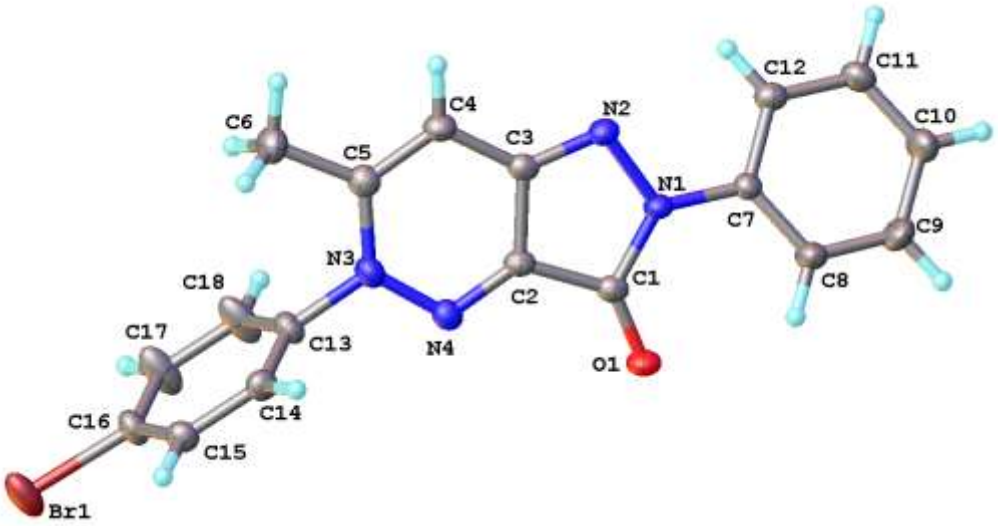
Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C5(H5), C8(H8), C9(H9), C11(H11), C12(H12), C14(H14), C15(H15), C16(H16),
 C17(H17), C18(H18)
2.b Idealised Me refined as rotating group:
 C1(H1A,H1B,H1C)
```

C5. 5-(4-bromophenyl)-2-phenyl-6-methyl-2*H*-pyrazolo[4,3-*c*]pyridazin-3(5*H*)-one, 27a



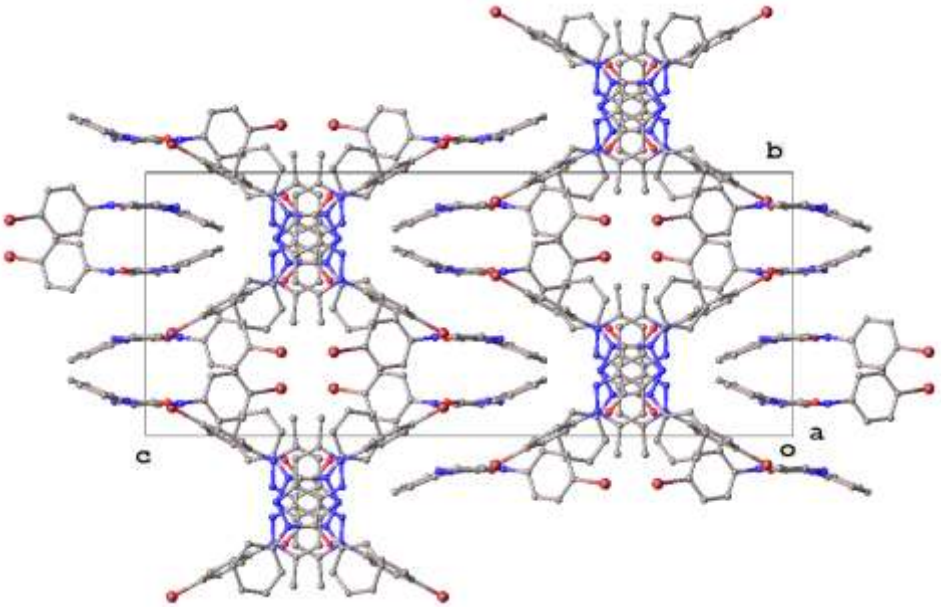


Table 1 Crystal data and structure refinement for CCDC 1448081.	
Identification code	CCDC 1448081
Empirical formula	$C_{18}H_{13}BrN_4O$
Formula weight	381.23
Temperature/K	120.0
Crystal system	tetragonal
Space group	$I4_1/a$
a/Å	13.79563(17)
b/Å	13.79563(17)
c/Å	33.9608(6)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	6463.40(16)
Z	16
ρ_{calc}g/cm^3	1.567
μ/mm^{-1}	2.556
F(000)	3072.0
Crystal size/mm^3	0.37 × 0.18 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.66 to 58
Index ranges	$-18 \leq h \leq 18$, $-18 \leq k \leq 18$, $-46 \leq l \leq 46$
Reflections collected	63894
Independent reflections	4308 [R_{int} = 0.0927, R_{sigma} = 0.0391]
Data/restraints/parameters	4308/0/218
Goodness-of-fit on F^2	1.020
Final R indexes [I>=2σ (I)]	R_1 = 0.0392, wR_2 = 0.0864
Final R indexes [all data]	R_1 = 0.0637, wR_2 = 0.0945
Largest diff. peak/hole / e Å^{-3}	0.60/-0.36

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 15srv243. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Br1	4308.71(18)	6093.9(2)	406.46(7)	37.29(10)
O1	3788.6(12)	913.9(11)	2154.3(4)	25.7(3)
N1	3839.3(13)	1578.4(13)	2790.5(5)	18.8(4)
N2	3812.0(13)	2504.9(13)	2977.1(5)	20.6(4)
N3	3740.8(13)	4056.5(14)	1978.1(5)	22.7(4)
N4	3744.1(13)	3081.0(13)	1962.8(5)	21.6(4)
C1	3781.8(15)	1604.9(16)	2383.4(6)	19.9(4)
C2	3735.7(14)	2653.3(16)	2305.0(6)	18.9(4)
C3	3747.5(15)	3119.0(16)	2685.9(6)	19.0(4)
C4	3713.9(16)	4144.4(16)	2681.8(7)	22.8(5)
C5	3727.3(16)	4597.1(16)	2324.0(7)	23.5(5)
C6	3728.1(19)	5678.0(17)	2284.3(8)	31.6(6)
C7	4036.7(15)	763.5(15)	3033.5(6)	19.2(4)
C8	3848.3(18)	-166.7(17)	2895.9(7)	27.9(5)
C9	4054(2)	-954.3(18)	3138.5(8)	37.1(6)
C10	4437(2)	-822.2(18)	3511.7(7)	33.4(6)
C11	4618.3(17)	108.8(17)	3645.1(7)	26.4(5)
C12	4423.9(15)	905.1(17)	3408.1(6)	22.1(5)
C13	3862.6(16)	4518.3(17)	1597.3(6)	24.1(5)
C14	3070.1(17)	4694.8(17)	1361.9(6)	24.0(5)
C15	3196.0(16)	5161.1(16)	999.9(7)	23.9(5)
C16	4118.2(17)	5437.0(17)	891.0(7)	26.1(5)
C17	4916.0(18)	5259(2)	1124.5(8)	40.8(7)
C18	4785.7(18)	4794(2)	1483.5(8)	40.2(7)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 15srv243. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Br1	25.21(14)	59.5(2)	27.15(14)	19.05(12)	-4.39(10)	-4.30(11)
O1	32.5(9)	26.0(8)	18.7(8)	-6.0(6)	0.9(6)	-0.3(7)
N1	21.3(9)	18.8(9)	16.4(8)	-3.0(7)	0.1(7)	0.7(7)
N2	21.7(9)	20.3(9)	19.7(9)	-4.1(7)	1.3(7)	0.3(7)
N3	23(1)	25.5(10)	19.6(9)	3.3(7)	-1.6(7)	1.3(8)
N4	19.1(9)	25(1)	20.8(9)	1.4(7)	0.2(7)	-0.5(7)
C1	16.5(10)	24.6(11)	18.5(10)	-2.5(8)	0.5(8)	-0.5(8)
C2	15.7(10)	23.1(11)	18.1(10)	-3.2(8)	0.1(8)	1.2(8)
C3	14.5(10)	24.5(11)	18.2(10)	-2.0(8)	0.5(8)	0.0(8)
C4	23.4(11)	24.5(11)	20.5(10)	-3.5(9)	1.1(9)	1.4(9)
C5	20.2(11)	25.8(12)	24.5(11)	-0.2(9)	0.0(9)	2.7(9)
C6	37.8(14)	24.3(12)	32.7(13)	3.5(10)	-1.1(11)	2.1(10)
C7	20.4(11)	20(1)	17.1(10)	-0.1(8)	1.0(8)	-0.2(8)
C8	38.8(14)	24.6(12)	20.4(11)	-2.1(9)	-4.1(10)	-2(1)
C9	59.2(18)	20.0(12)	32.2(13)	-2.9(10)	-7.2(13)	-2.3(11)
C10	47.1(16)	25.9(13)	27.2(12)	4.1(10)	-9.4(11)	3.4(11)
C11	26.4(12)	31.9(13)	20.9(11)	0.6(9)	-5.1(9)	1.2(10)
C12	19.5(11)	25.6(11)	21.1(10)	-3.3(9)	-0.6(8)	-0.8(8)
C13	26.6(12)	27.7(12)	18.1(10)	4.6(9)	0.4(9)	2.2(9)
C14	21.9(11)	26.1(12)	23.9(11)	0.0(9)	0.2(9)	-4.6(9)
C15	20.8(11)	27.5(12)	23.2(11)	1.0(9)	-4.1(9)	0.2(9)
C16	26.3(12)	31.4(13)	20.6(11)	8.2(9)	-0.4(9)	0.4(10)
C17	18.5(12)	71(2)	32.5(14)	21.9(13)	-1.8(10)	-0.9(12)
C18	21.7(12)	68(2)	30.9(13)	20.7(13)	-5.7(10)	0.6(12)

Table 4 Bond Lengths for 15srv243.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
Br1	C16	1.897(2)		C5	C6	1.497(3)
O1	C1	1.231(3)		C7	C8	1.390(3)
N1	N2	1.427(2)		C7	C12	1.394(3)
N1	C1	1.385(3)		C8	C9	1.393(3)
N1	C7	1.421(3)		C9	C10	1.385(3)
N2	C3	1.305(3)		C10	C11	1.385(3)
N3	N4	1.347(3)		C11	C12	1.388(3)
N3	C5	1.392(3)		C13	C14	1.376(3)
N3	C13	1.452(3)		C13	C18	1.384(3)
N4	C2	1.303(3)		C14	C15	1.398(3)
C1	C2	1.472(3)		C15	C16	1.378(3)
C2	C3	1.445(3)		C16	C17	1.379(3)
C3	C4	1.415(3)		C17	C18	1.389(3)
C4	C5	1.366(3)				

Table 5 Bond Angles for 15srv243.								
Atom	**Atom**	**Atom**	**Angle/°**		**Atom**	**Atom**	**Atom**	**Angle/°**
C1	N1	N2	114.71(17)		C4	C5	C6	122.4(2)
C1	N1	C7	127.69(18)		C8	C7	N1	119.96(19)
C7	N1	N2	117.11(16)		C8	C7	C12	120.5(2)
C3	N2	N1	104.28(17)		C12	C7	N1	119.52(19)
N4	N3	C5	124.62(18)		C7	C8	C9	118.9(2)
N4	N3	C13	113.82(18)		C10	C9	C8	121.1(2)
C5	N3	C13	121.23(19)		C11	C10	C9	119.4(2)
C2	N4	N3	114.70(18)		C10	C11	C12	120.6(2)
O1	C1	N1	127.6(2)		C11	C12	C7	119.5(2)
O1	C1	C2	130.3(2)		C14	C13	N3	120.2(2)
N1	C1	C2	102.06(17)		C14	C13	C18	121.3(2)
N4	C2	C1	127.29(19)		C18	C13	N3	118.4(2)
N4	C2	C3	126.7(2)		C13	C14	C15	119.6(2)
C3	C2	C1	105.92(18)		C16	C15	C14	118.5(2)
N2	C3	C2	112.99(19)		C15	C16	Br1	119.50(17)
N2	C3	C4	131.2(2)		C17	C16	Br1	118.26(18)
C4	C3	C2	115.79(19)		C17	C16	C15	122.2(2)
C5	C4	C3	117.7(2)		C16	C17	C18	118.9(2)
N3	C5	C6	117.2(2)		C13	C18	C17	119.4(2)
C4	C5	N3	120.4(2)					

Table 6 Selected Torsion Angles for 15srv243.										
A	**B**	**C**	**D**	**Angle/°**		**A**	**B**	**C**	**D**	**Angle/°**
C8	C7	N1	N2	164.59(19)		C14	C13	N3	N4	86.6(3)
C8	C7	N1	C1	-23.8(3)		C14	C13	N3	C5	-99.7(3)
C12	C7	N1	N2	-15.8(3)		C18	C13	N3	N4	-94.9(3)
C12	C7	N1	C1	155.8(2)		C18	C13	N3	C5	78.8(3)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 15srv243.				
Atom	***x***	***y***	***z***	**U(eq)**
H4	3683	4506	2920	27
H6A	4345	5890	2170	47
H6B	3646	5974	2545	47
H6C	3194	5878	2112	47
H8	3584	-264	2641	34
H9	3930	-1593	3046	45
H10	4573	-1365	3675	40
H11	4878	203	3901	32
H12	4554	1542	3501	26
H14	2442	4501	1445	29
H15	2658	5285	833	29
H17	5545	5451	1041	49
H18	5325	4667	1649	48

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C4(H4), C8(H8), C9(H9), C10(H10), C11(H11), C12(H12), C14(H14), C15(H15),
 C17(H17), C18(H18)
2.b Idealised Me refined as rotating group:
 C6(H6A,H6B,H6C)
```