Electronic Supplementary Material (ESI) for MedChemComm.

SUPPORTING INFORMATION

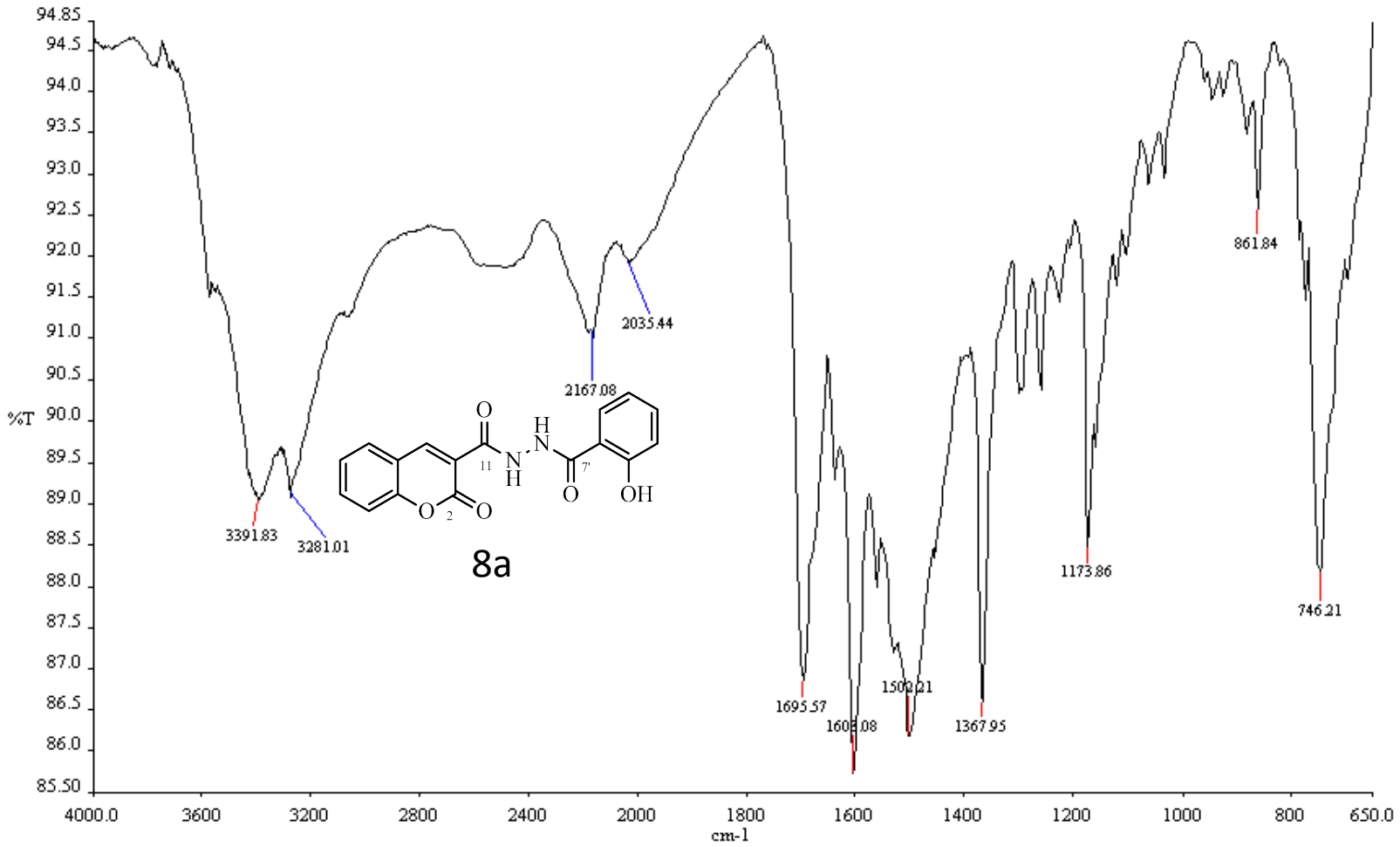
DOCKING STUDIES AND BIOLOGICAL EVALUATION OF NOVEL *N*'-(3-HYDROXYBENZOYL)-2-OXO-2*H*-CHROMENE-3-CARBOHYDRAZIDE DERIVATIVES AS POTENTIAL HIV-1 INTEGRASE INHIBITOR.

Omobolanle J. Jesumoroti,[a] Faridoon,[a] Dumisani Mnkadhla,[b,c] Heinrich C. Hoppe[b,c] and Rosalyn Klein*[a,c]

[a] Department of Chemistry, [b] Department of Biochemistry and Microbiology and [c]Center for Chemico – and Biomedical Research, Rhodes University, Grahamstown, 6140, South Africa.

General procedure for synthesis of coumarin hydrazides 8a-8t.[21] To a stirred solution of the appropriate 2-hydroxybenzohydrazide (1.25 mmol) in 4 mL of water, was added the appropriate solution of 2-oxo-*2H*-chromene-3-carbonyl chlorides **4a** (1.25 mmol) in 6 mL of toluene. Thereafter, 6 mL of a saturated aqueous solution of Na_2CO_3 was added to maintain pH ~8, and the mixture was stirred for 4 h and left overnight. After the completion of the reaction as monitored by TLC, the precipitate was filtered off, washed with water and air-dried. The resultant crude material was recrystallized from ethanol to afford the corresponding coumarin hydrazides derivatives **8a-8t**.

The spectroscopic data which follows is in the order of the compounds in the main paper. EXCEPT the full 2D nmr data set for compound 8i has been included at the end as an example of the data used for assignment of the spectra.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92.0
91.5
91.0
90.5
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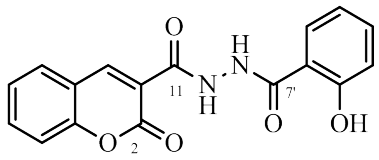
89.5
89.0
88.5
88.0
87.5
87.0
86.5
86.0
85.50
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3391.83
3281.01
2167.08
2035.44
1695.57
1608.08
1502.21
1367.95
1173.86
861.84
746.21
O
H
N
N
11
H
7'
O
O
O
2
O
OH

8a

8a



11.91
8.88
8.01
8.01
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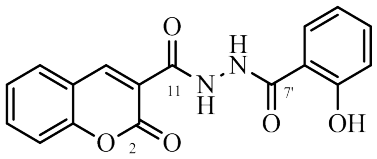
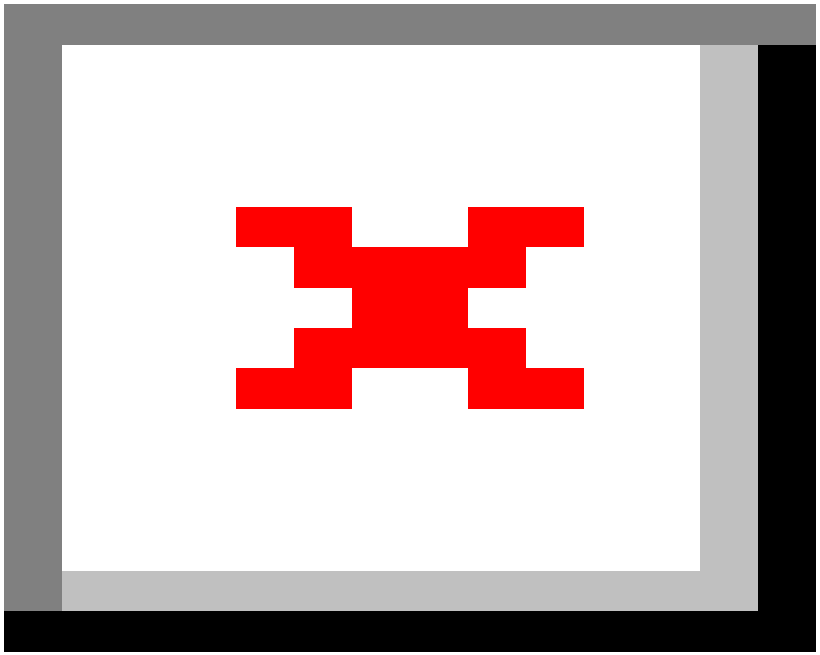
7.98
7.79
7.77
7.76
7.73
7.53
7.50
7.44
7.11
7.10
6.67
6.65
6.64
3.42
2.50

0.93
0.98
1.02
2.03
0.96
1.00
0.86
1.90

f1 (ppm)


O
H
N
11
N
H
7'
O
OH
O
2
O



Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

670 formula(e) evaluated with 65 results within limits (all results (up to 1000) for each mass)

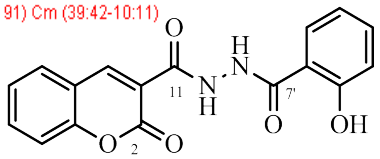
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	P
325.0819	325.0817	0.2	0.6	4.5	C13 H19 O6 Na P	127.9	9.295	0.01	13	19		6	1	1
	325.0824	-0.5	-1.5	12.5	C17 H13 N2 O5	122.0	3.422	3.26	17	13	2	5		
	325.0830	-1.1	-3.4	9.5	C14 H15 N4 O2 Na P	125.5	6.950	0.10	14	15	4	2	1	1
	325.0800	1.9	5.8	9.5	C15 H14 N2 O5 Na	125.0	6.403	0.17	15	14	2	5	1	
	325.0841	-2.2	-6.8	13.5	C20 H14 O3 Na	120.9	2.291	10.11	20	14		3	1	
	325.0841	-2.2	-6.8	7.5	C15 H18 O6 P	126.3	7.726	0.04	15	18		6		1
	325.0784	3.5	10.8	8.5	C12 H13 N4 O7	125.8	7.264	0.07	12	13	4	7		
	325.0854	-3.5	-10.8	12.5	C16 H14 N4 O2 P	123.4	4.801	0.82	16	14	4	2		1
	325.0782	3.7	11.4	16.5	C22 H14 O P	125.7	7.120	0.08	22	14		1		1

OJ 105a

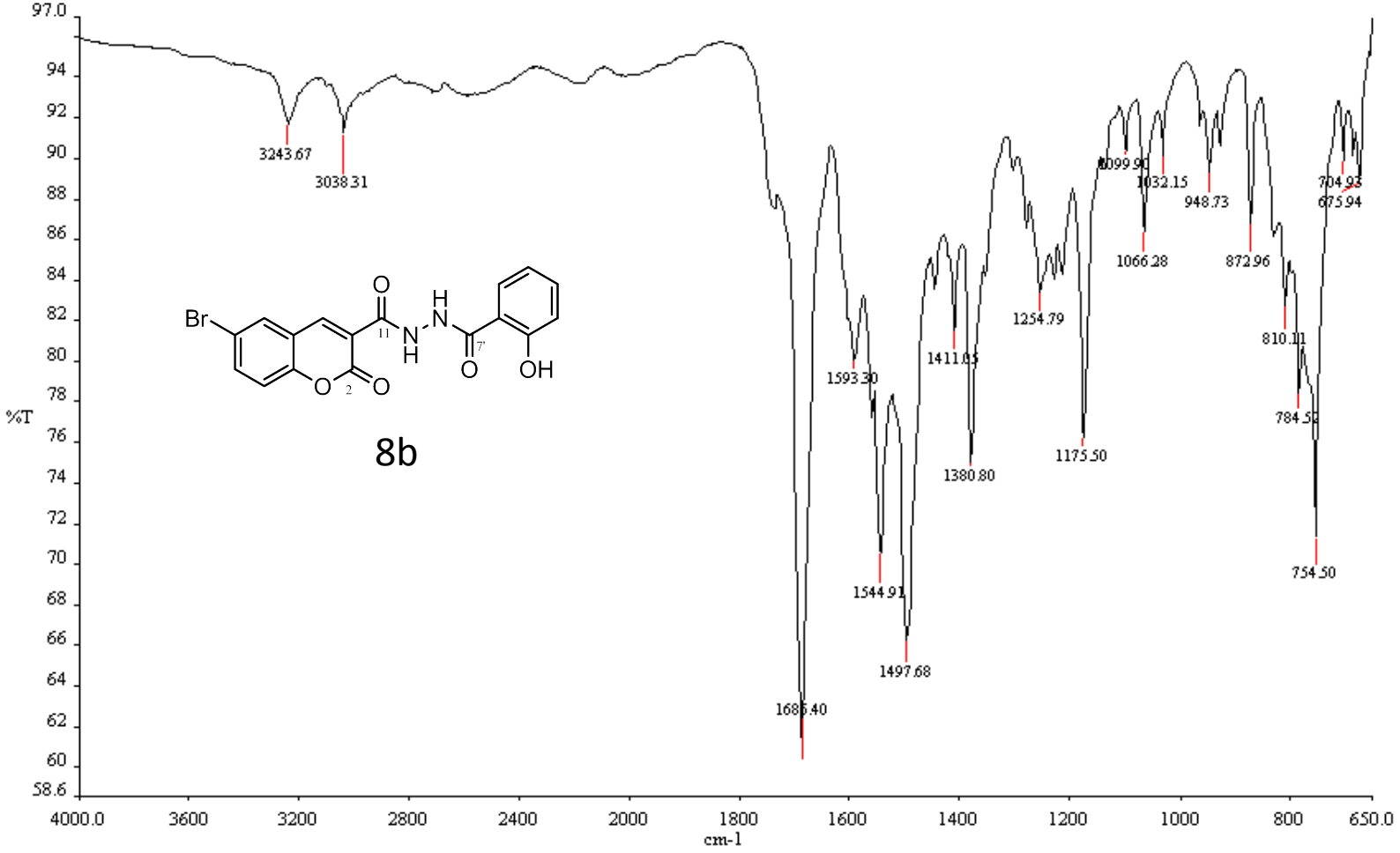
MS_Direct_151019_73 42 (0.191) Cm (39:42-10:11)

1: TOF MS ES+
1.77e+004



8a

For Help, press F1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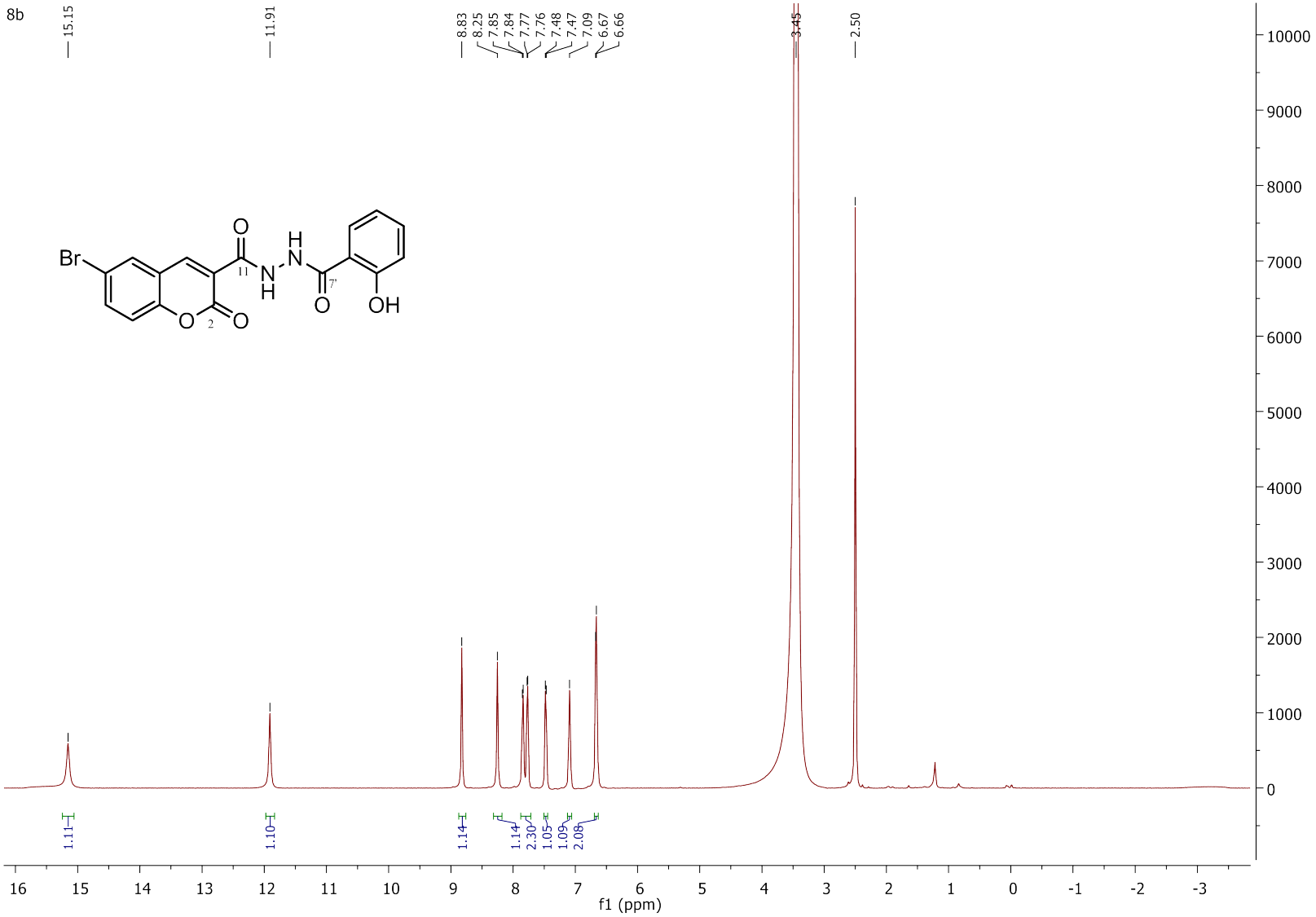
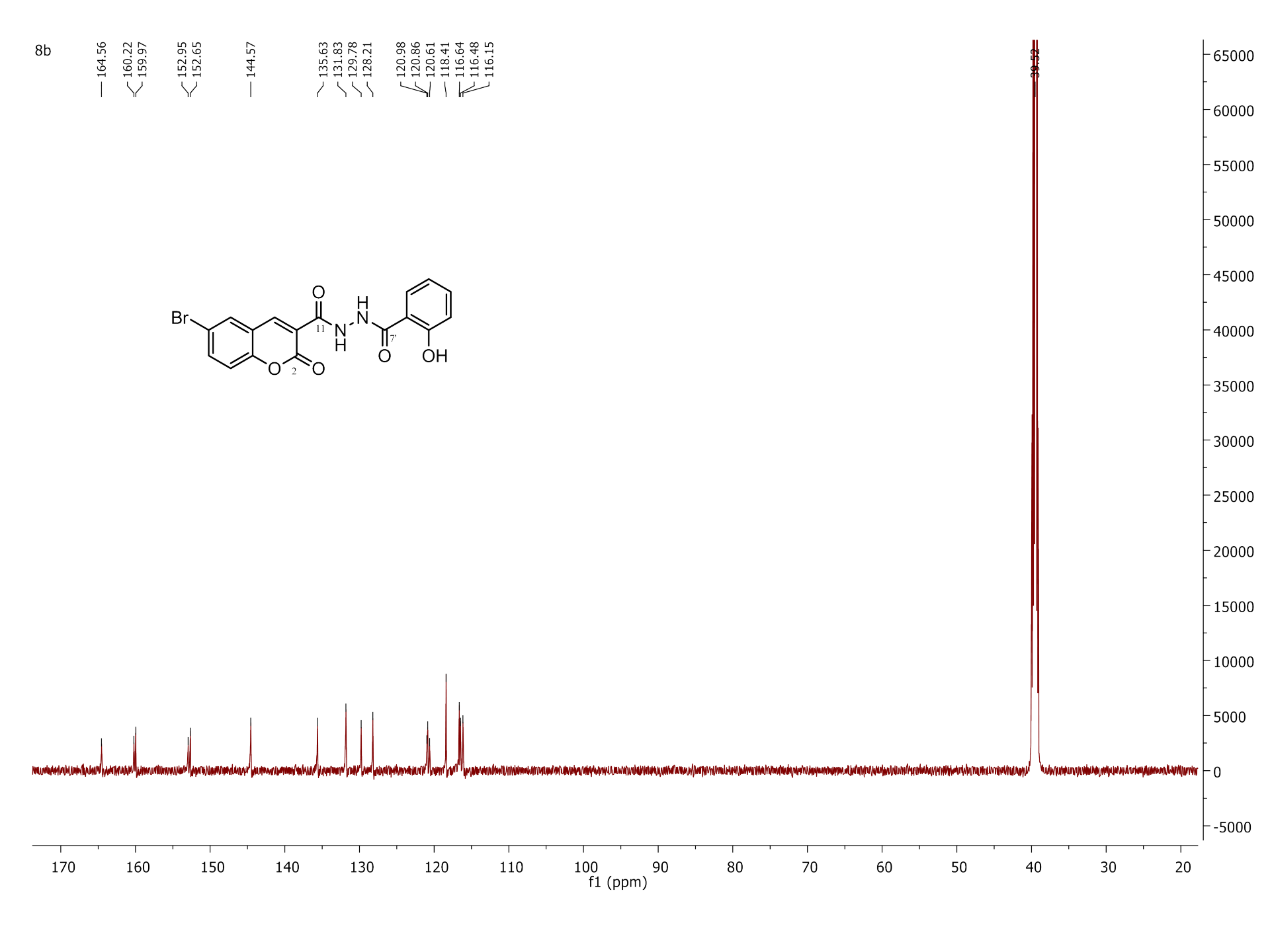
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58.6
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3243.67
3038.31
1686.40
1593.30
1544.91
1497.68
1411.05
1380.80
1254.79
1175.50
1099.90
1066.28
1032.15
948.73
872.96
810.11
784.52
754.50
704.93
675.94
Br
O
N
H
N
H
O
OH
O
O
2
11
7'
8b


8b
15.15
11.91
8.83
8.25
7.85
7.84
7.77
7.76
7.48
7.47
7.09
6.67
6.66
3.45
2.50
Br
O
N
H
N
H
O
OH
O
O
2
11
7'
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
1.11
1.10
1.14
1.14
2.30
1.05
1.09
2.08
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


8b
164.56
160.22
159.97
152.95
152.65
144.57
135.63
131.83
129.78
128.21
120.98
120.86
120.61
118.41
116.64
116.48
116.15
39.52
Br
O
N
H
N
H
O
OH
O
O
2
11
7'
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1495 formula(e) evaluated with 132 results within limits (all results (up to 1000) for each mass)

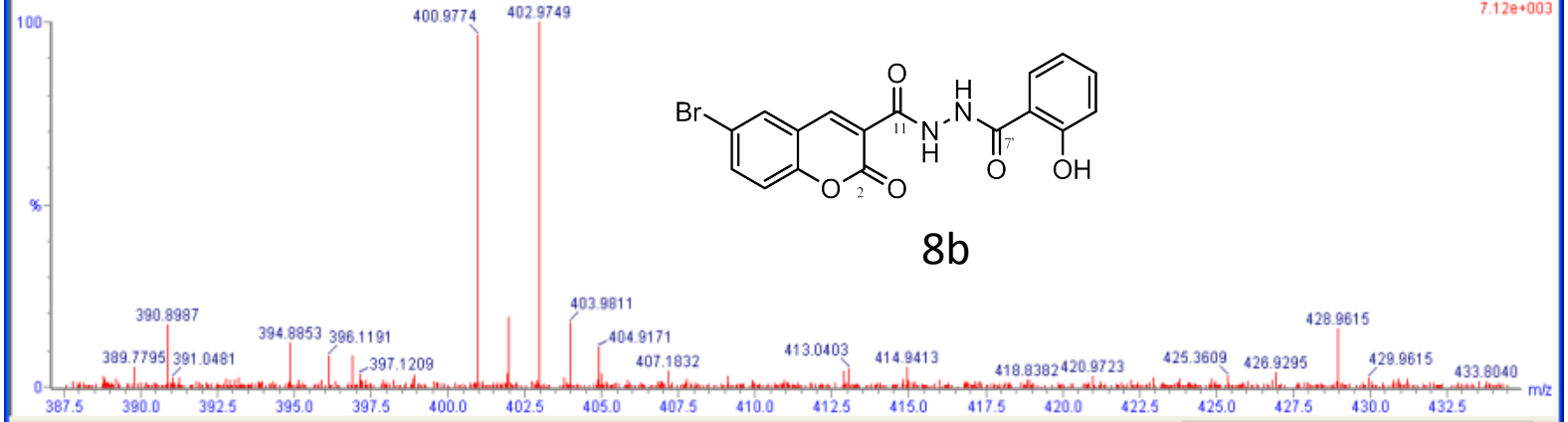
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	P	Br
400.9774	400.9773	0.1	0.2	13.5	C17 H10 N2 O5 Br	257.4	1.825	16.13	17	10	2	5			1
	400.9779	-0.5	-1.2	10.5	C14 H12 N4 O2 Na P Br	260.2	4.567	1.04	14	12	4	2	1	1	1
	400.9768	0.6	1.5	25.5	C26 H3 O2 Na P	281.5	25.859	0.00	26	3		2	1	1	
	400.9766	0.8	2.0	5.5	C13 H16 O6 Na P Br	263.3	7.655	0.05	13	16		6	1	1	1
	400.9789	-1.5	-3.7	14.5	C20 H11 O3 Na Br	260.9	5.292	0.50	20	11		3	1		1
	400.9790	-1.6	-4.0	8.5	C15 H15 O6 P Br	261.1	5.524	0.40	15	15		6		1	1
	400.9792	-1.8	-4.5	28.5	C28 H2 O2 P	281.5	25.880	0.00	28	2		2		1	
	400.9752	2.2	5.5	24.5	C23 H2 N2 O4 P	281.2	25.603	0.00	23	2	2	4		1	
	400.9749	2.5	6.2	10.5	C15 H11 N2 O5 Na Br	259.9	4.256	1.42	15	11	2	5	1		1

OJ 105b

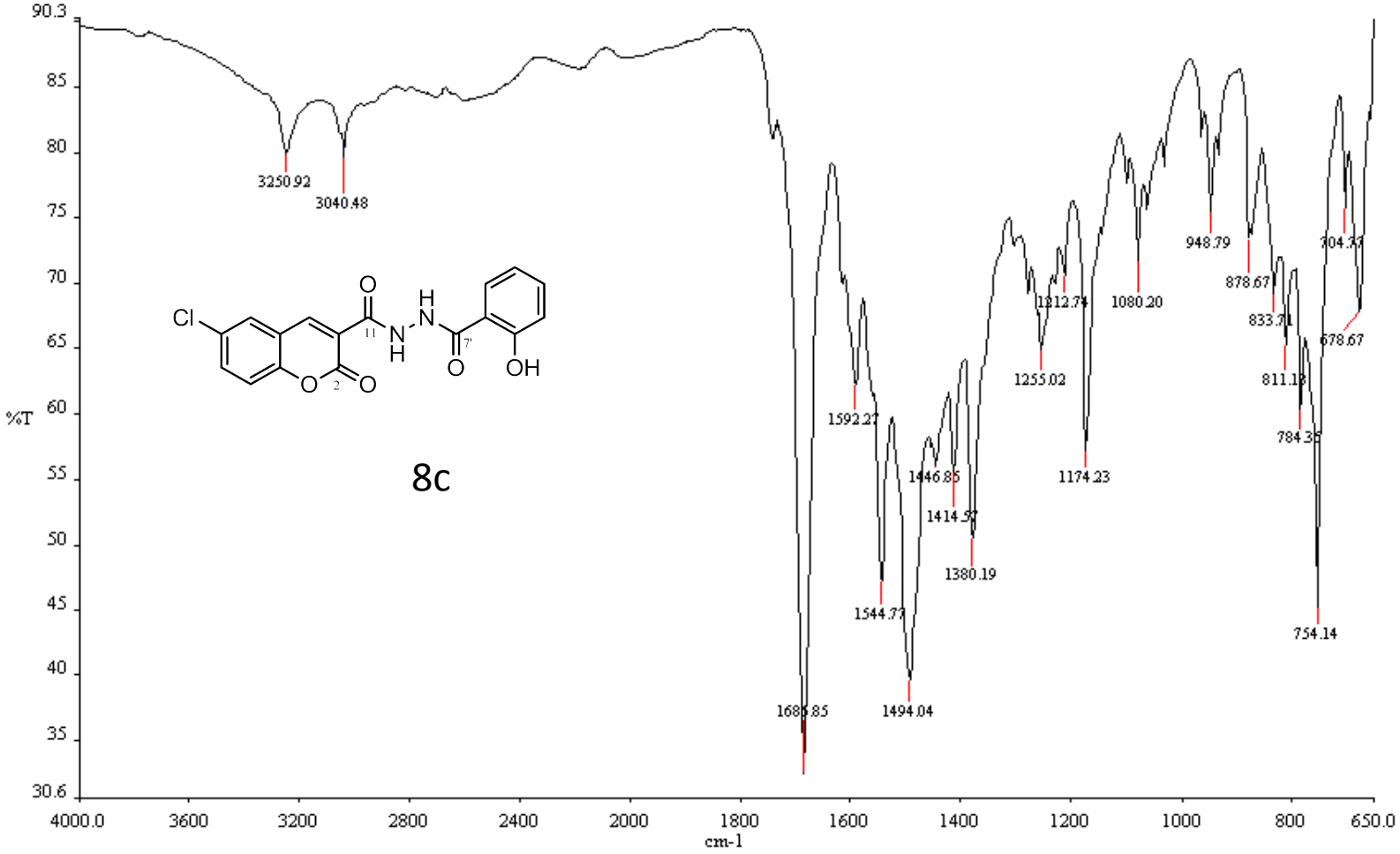
MS_Direct_151019_74n 72 (0.322) Cm (15:81-5:9)

1: TOF MS ES-
7.12e+003

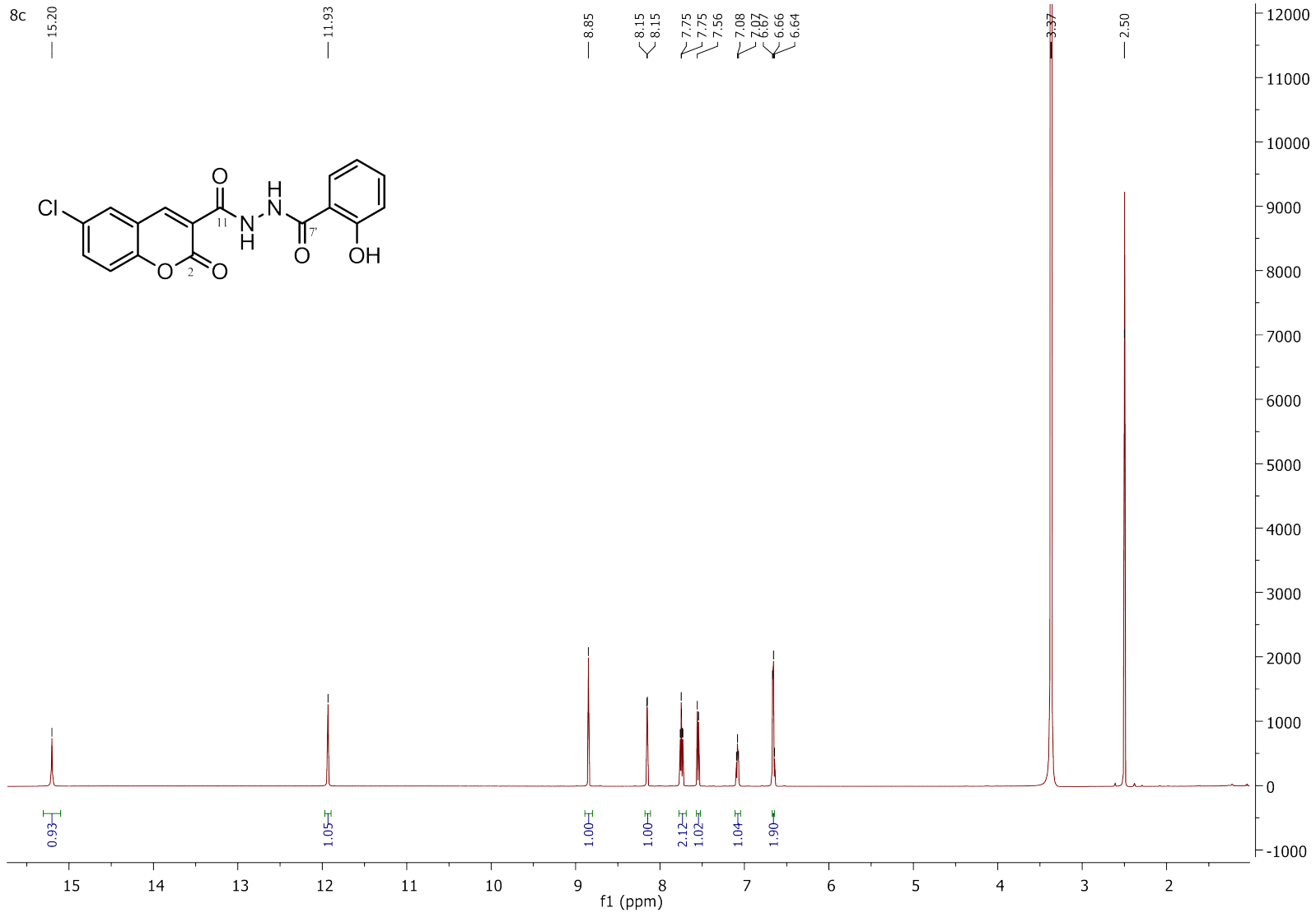


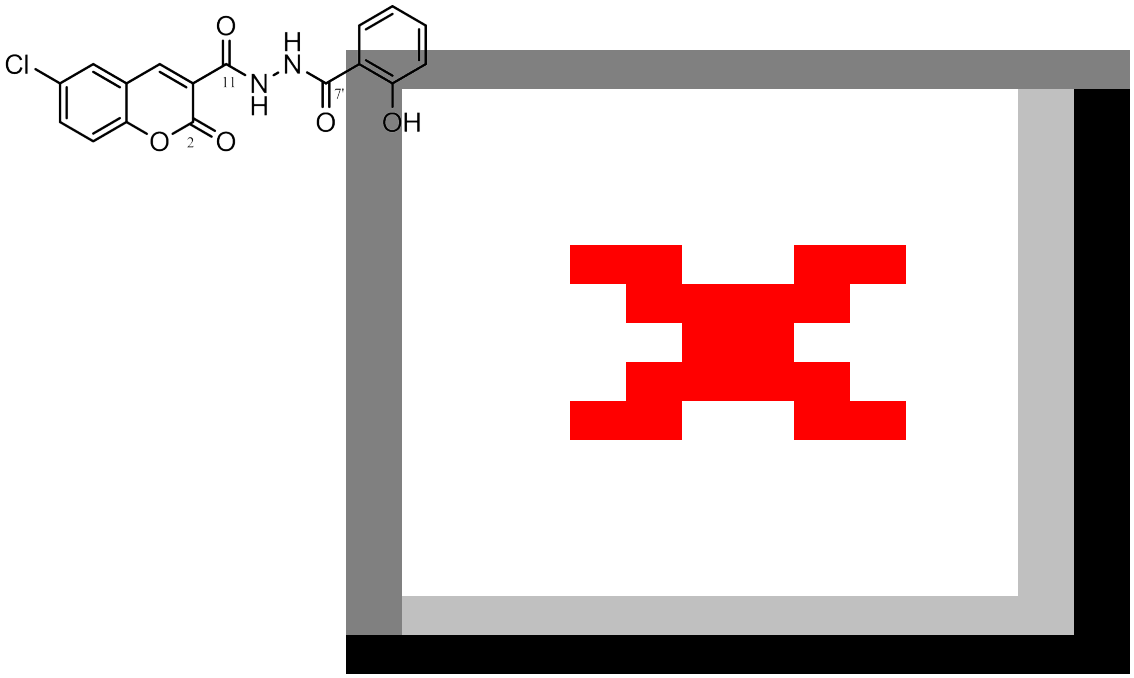
8b

For Help, press F1


90.3
85
80
75
70
65
60
55
50
45
40
35
30.6
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3250.92
3040.48
1592.27
1544.77
1494.04
1446.85
1414.57
1380.19
1255.02
1212.74
1174.23
1080.20
948.79
878.67
833.71
811.13
784.35
754.14
678.67
Cl
O
N
H
N
H
O
OH
O
O
11
7'
2

8c


8c
15.20
11.93
8.85
8.15
8.15
7.75
7.75
7.56
7.08
7.07
6.67
6.66
6.64
3.37
2.50
Cl
O
N
H
N
H
O
OH
O
O
11
7'
2
0.93
1.05
1.00
1.00
2.12
1.02
1.04
1.90
f1 (ppm)


Cl
O
11
N
H
H
N
7'
O
OH
O
2
O

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2409 formula(e) evaluated with 268 results within limits (all results (up to 1000) for each mass)

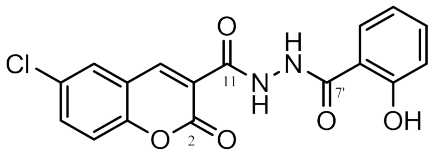
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	P	Cl
	357.0272	-0.4	-1.1	5.5	C14 H16 O5 Na Cl2	54.1	7.365	0.06	14	16		5	1		2
	357.0264	0.4	1.1	1.5	C9 H17 N4 O3 Na Cl3	56.1	9.393	0.01	9	17	4	3	1		3
	357.0262	0.6	1.7	1.5	C8 H17 N4 O4 Na P Cl2	54.9	8.198	0.03	8	17	4	4	1	1	2
	357.0275	-0.7	-2.0	-0.5	C10 H20 O7 Cl3	55.9	9.134	0.01	10	20		7			3
	357.0260	0.8	2.2	18.5	C18 H5 N4 O5	55.8	9.089	0.01	18	5	4	5			
	357.0276	-0.8	-2.2	13.5	C16 H10 N2 O6 P	55.9	9.144	0.01	16	10	2	6		1	
	357.0276	-0.8	-2.2	19.5	C21 H6 N2 O3 Na	55.8	9.106	0.01	21	6	2	3	1		
	357.0278	-1.0	-2.8	13.5	C17 H10 N2 O5 Cl	51.6	4.809	0.82	17	10	2	5			1
	357.0256	1.2	3.4	4.5	C11 H15 N2 O7 Cl2	54.5	7.749	0.04	11	15	2	7			2
	357.0254	1.4	3.9	10.5	C15 H11 N2 O5 Na Cl	52.2	5.451	0.43	15	11	2	5	1		1
	357.0252	1.6	4.5	10.5	C14 H11 N2 O6 Na P	56.0	9.242	0.01	14	11	2	6	1	1	
	357.0284	-1.6	-4.5	10.5	C14 H12 N4 O2 Na P Cl	52.5	5.770	0.31	14	12	4	2	1	1	1
	357.0286	-1.8	-5.0	4.5	C10 H16 N4 O4 P Cl2	54.7	7.916	0.04	10	16	4	4		1	2
	357.0286	-1.8	-5.0	10.5	C15 H12 N4 O Na Cl2	54.0	7.266	0.07	15	12	4	1	1		2

OJ 105c

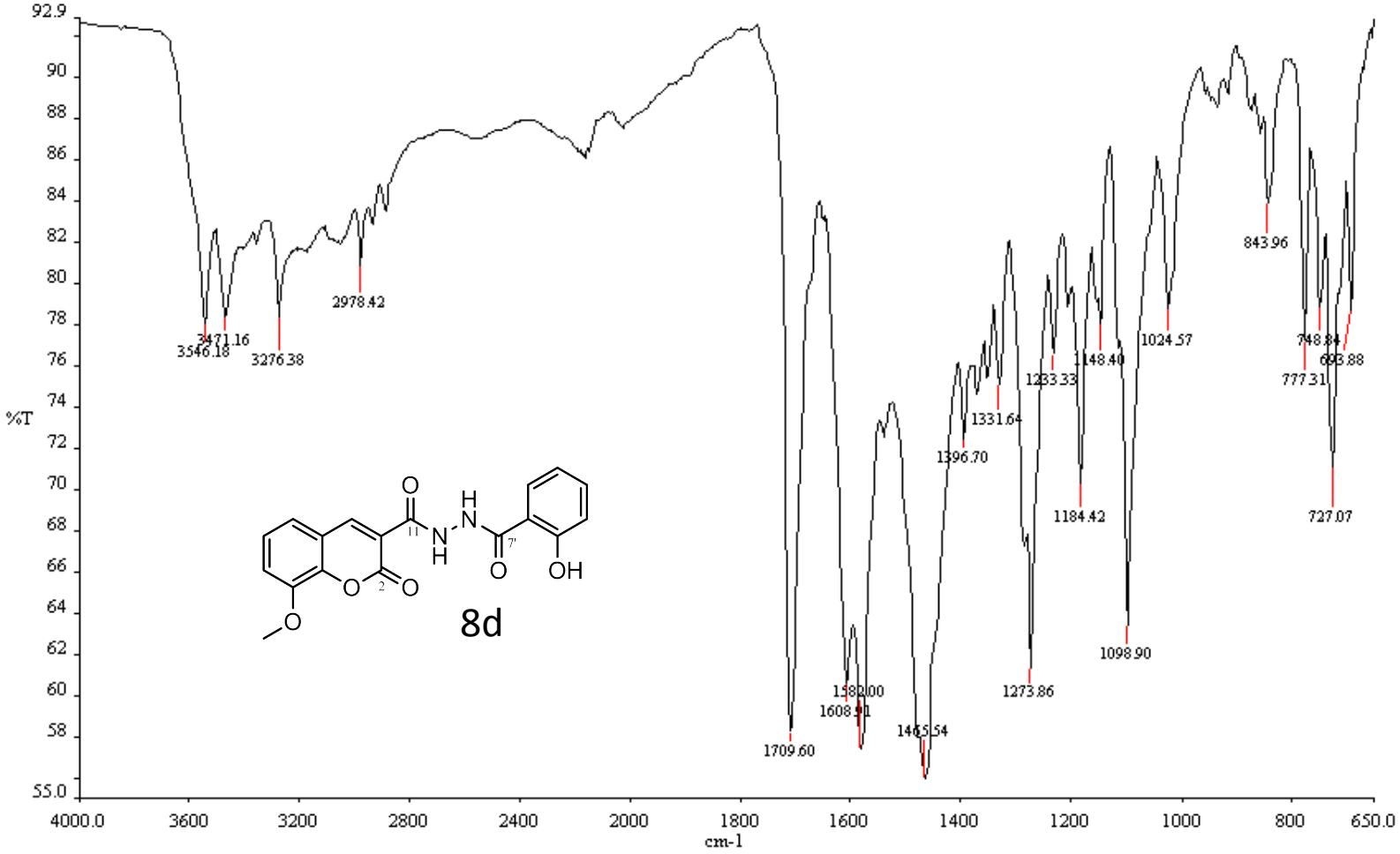
MS_Direct_151019_75n 21 (0.106) Cm (21:27)

1: TOF MS ES-
7.92e+002



8c

For Help, press F1


92.9
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86
84
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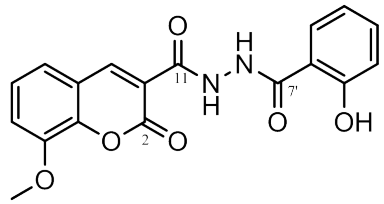
80
78
76
74
72
70
68
66
64
62
60
58
55.0
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3546.18
3471.16
3276.38
2978.42
1709.60
1608.91
1582.00
1465.54
1396.70
1331.64
1273.86
1233.33
1184.42
1148.40
1098.90
1024.57
843.96
777.31
748.84
693.88
727.07
O
H
N
N
O
O
O
OH
11
7'
2
8d

8d


O
H
N
N
H
11
7'
O
O
2
O
OH
O

11.94
8.81
7.80
7.79
7.49
7.48
7.37
7.36
7.34
7.13
7.12
7.11
6.70
6.69
6.68
6.67
3.93
3.62
2.50
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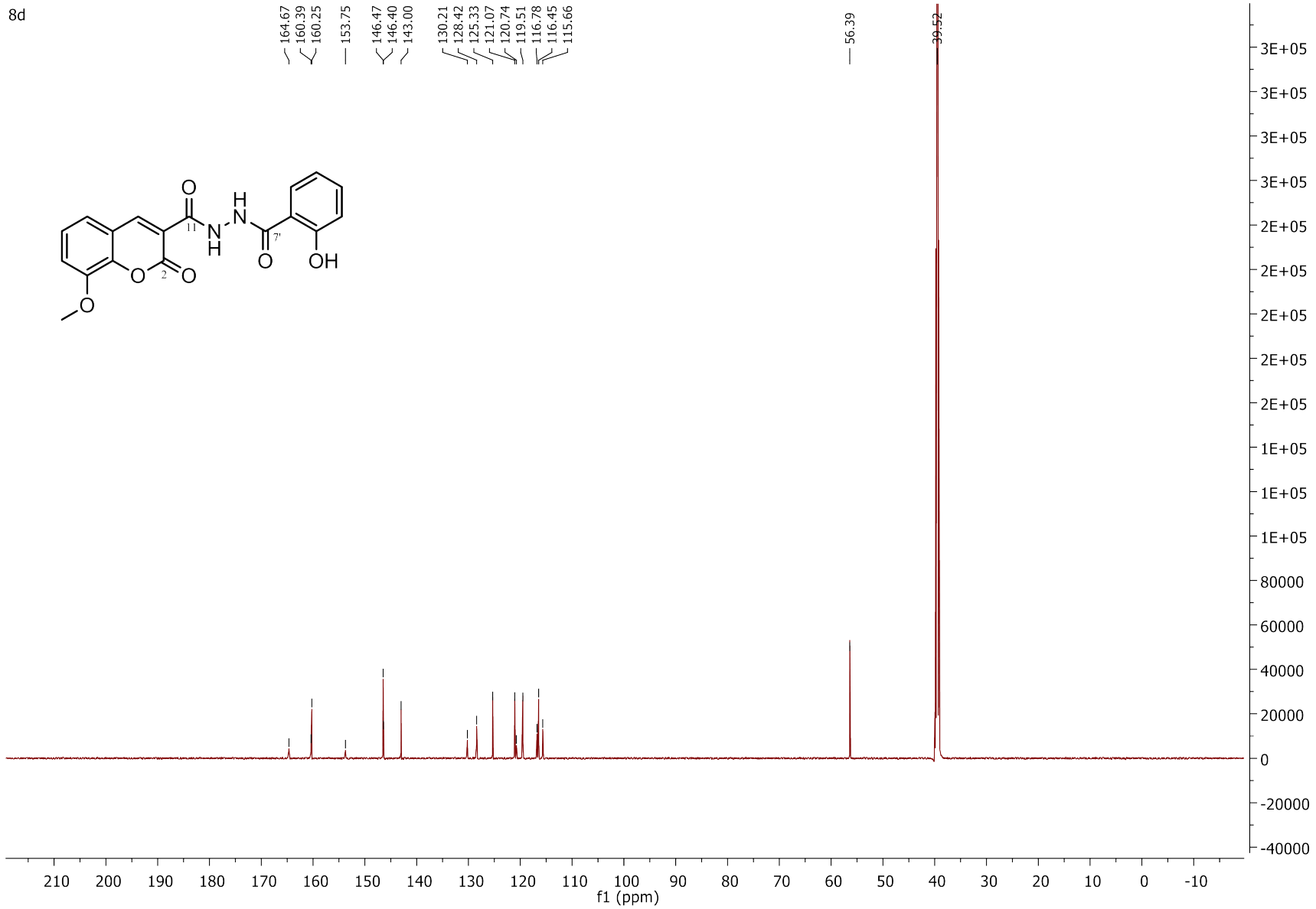
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
0.61
0.75
0.75
0.80
1.59
0.75
1.62
3.00
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)


8d
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160.39
160.25
153.75
146.47
146.40
143.00
130.21
128.42
125.33
121.07
120.74
119.51
116.78
116.45
115.66
56.39
39.52
O
H
N
N
H
11
7'
O
OH
O
2
O
O
3E+05
3E+05
3E+05
3E+05
2E+05
2E+05
2E+05
2E+05
2E+05
1E+05
1E+05
1E+05
80000
60000
40000
20000
0
-20000
-40000
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)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1009 formula(e) evaluated with 107 results within limits (all results (up to 1000) for each mass)

Elements Used:

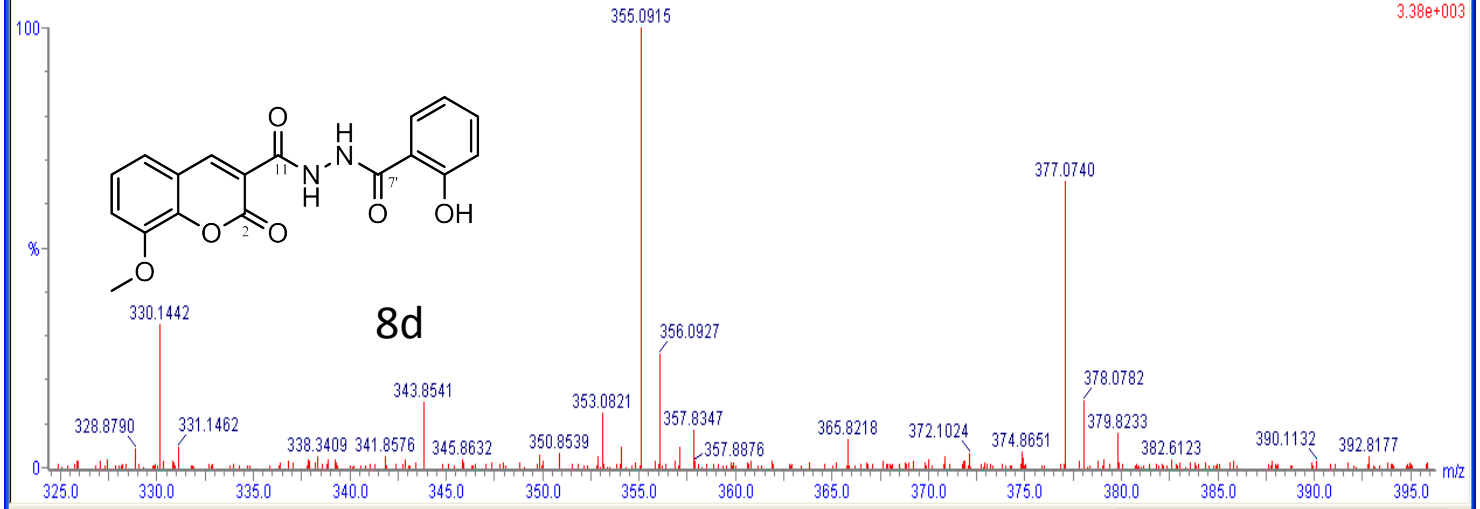
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	Cl
355.0915	355.0916	-0.1	-0.3	0.5	C10 H22 N4 O4 Na Cl2	65.3	17.746	0.00	10	22	4	4	1	2
	355.0924	-0.9	-2.5	4.5	C15 H21 O6 Na Cl	64.4	16.786	0.00	15	21		6	1	1
	355.0906	0.9	2.5	9.5	C16 H16 N2 O6 Na	53.9	6.313	0.18	16	16	2	6	1	
	355.0930	-1.5	-4.2	12.5	C18 H15 N2 O6	52.6	4.979	0.69	18	15	2	6		
	355.0938	-2.3	-6.5	9.5	C16 H17 N4 O2 Na Cl	64.1	16.491	0.00	16	17	4	2	1	1
	355.0890	2.5	7.0	16.5	C24 H16 O Cl	64.1	16.491	0.00	24	16		1		1
	355.0940	-2.5	-7.0	3.5	C12 H21 N4 O4 Cl2	65.3	17.759	0.00	12	21	4	4		2
	355.0946	-3.1	-8.7	13.5	C21 H16 O4 Na	51.6	4.004	1.82	21	16		4	1	
	355.0948	-3.3	-9.3	7.5	C17 H20 O6 Cl	64.3	16.708	0.00	17	20		6		1

OJ 105d

MS_Direct_151019_76 28 (0.133) Cm (22:28-8:15)

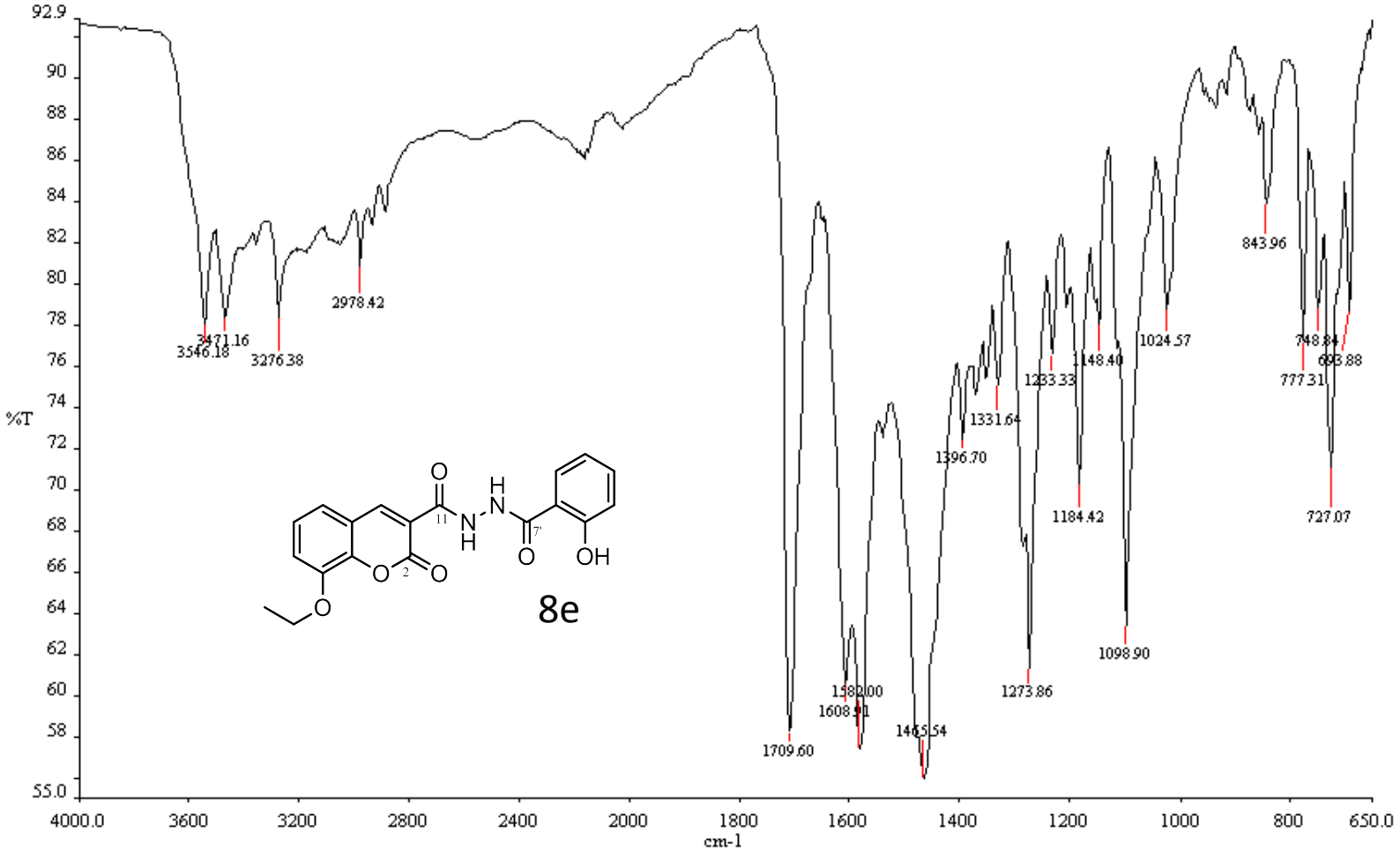
1: TOF MS ES+

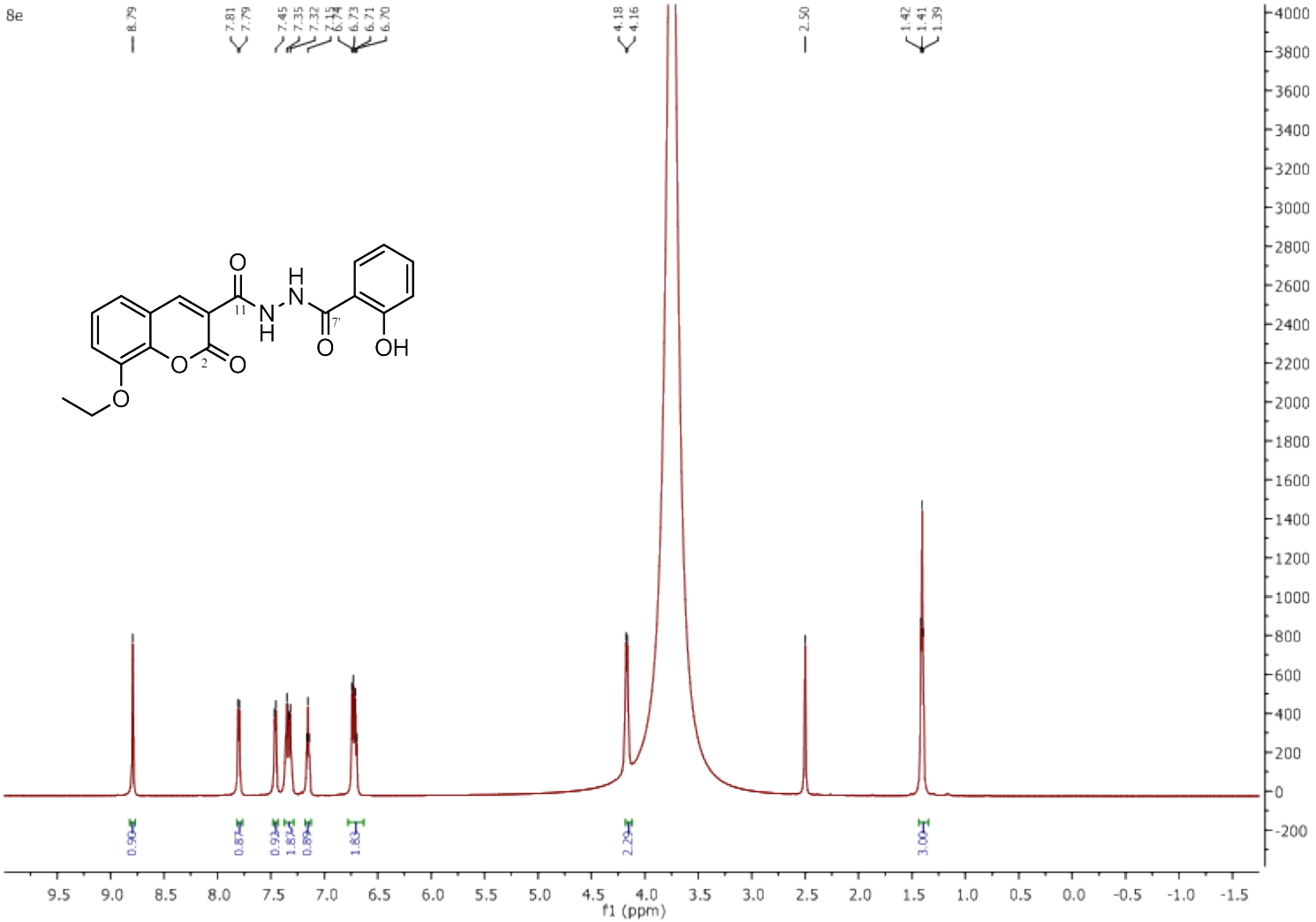
3.38e+003

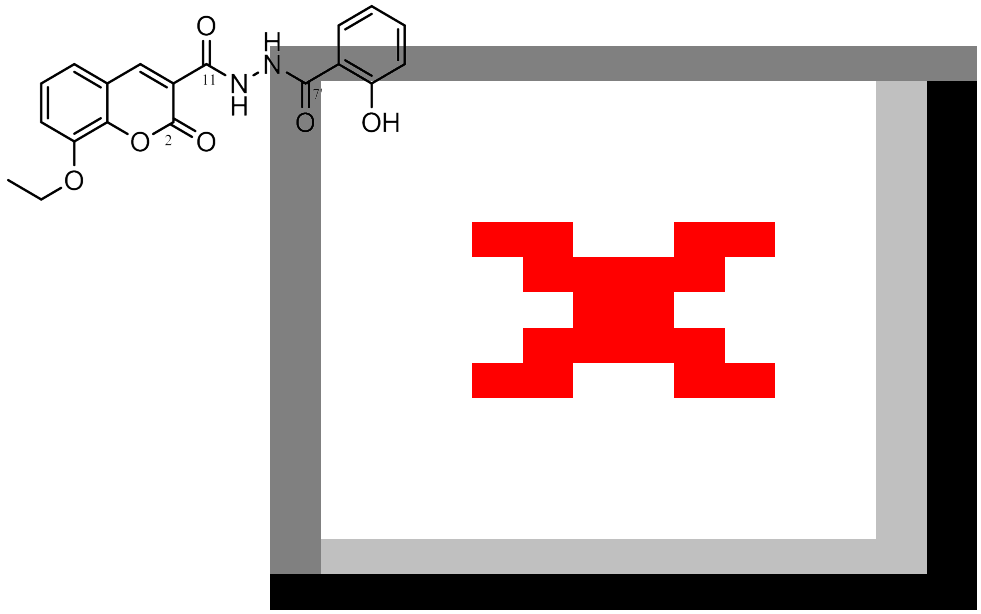


8d

For Help, press F1


92.9
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
55.0
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3546.18
3471.16
3276.38
2978.42
1709.60
1608.91
1582.00
1465.54
1396.70
1331.64
1273.86
1233.33
1184.42
1148.40
1098.90
1024.57
843.96
777.31
748.84
727.07
693.88
O
H
N
N
H
O
O
O
O
OH
11
7'
2
8e


8e
8.79
7.81
7.79
7.45
7.35
7.32
6.73
6.71
6.70
4.18
4.16
2.50
1.42
1.41
1.39
O
H
N
N
H
O
O
O
O
OH
11
2
7
0.90
0.87
0.92
1.84
0.89
1.83
2.29
3.00
f1 (ppm)


O
11
N
H
N
H
O
7
OH
O
2
O
O

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1057 formula(e) evaluated with 111 results within limits (all results (up to 1000) for each mass)

Elements Used:

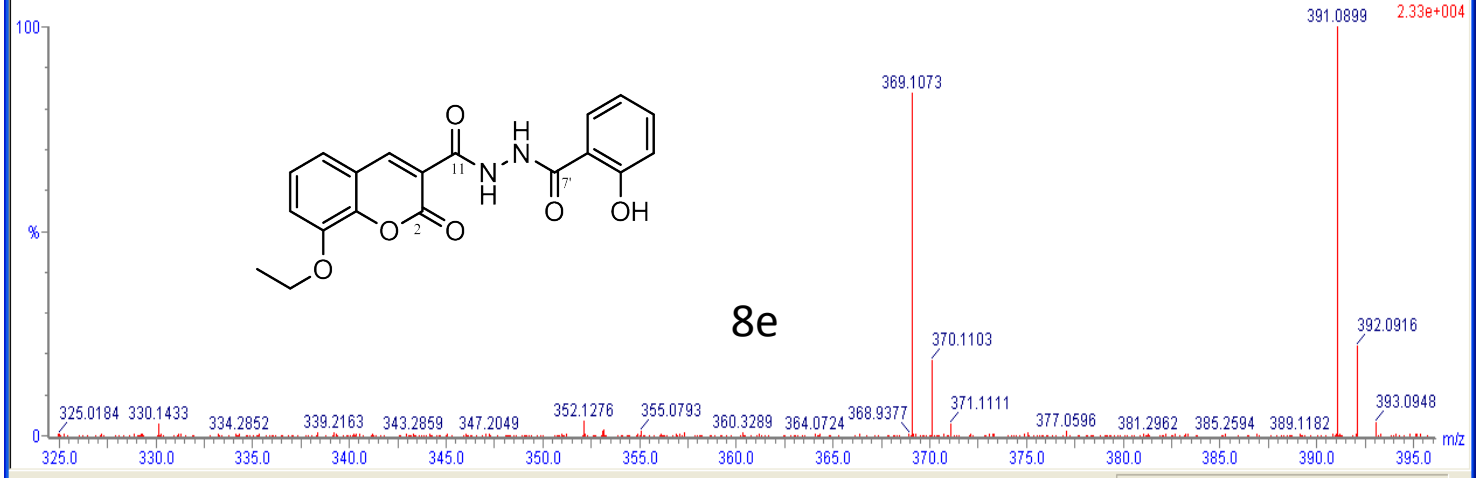
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	Cl
369.1073	369.1072	0.1	0.3	0.5	C11 H24 N4 O4 Na Cl2	146.8	24.031	0.00	11	24	4	4	1	2
	369.1081	-0.8	-2.2	4.5	C16 H23 O6 Na Cl	145.7	22.967	0.00	16	23		6	1	1
	369.1063	1.0	2.7	9.5	C17 H18 N2 O6 Na	128.5	5.746	0.32	17	18	2	6	1	
	369.1087	-1.4	-3.8	12.5	C19 H17 N2 O6	123.4	0.666	51.40	19	17	2	6		
	369.1094	-2.1	-5.7	9.5	C17 H19 N4 O2 Na Cl	145.6	22.823	0.00	17	19	4	2	1	1
	369.1096	-2.3	-6.2	3.5	C13 H23 N4 O4 Cl2	146.8	24.018	0.00	13	23	4	4		2
	369.1046	2.7	7.3	16.5	C25 H18 O Cl	145.4	22.629	0.00	25	18		1		1
	369.1103	-3.0	-8.1	13.5	C22 H18 O4 Na	128.8	6.053	0.24	22	18		4	1	
	369.1105	-3.2	-8.7	7.5	C18 H22 O6 Cl	145.7	22.900	0.00	18	22		6		1

OJ 105e

MS_Direct_151019_77 47 (0.210) Cm (42:47-7:12)

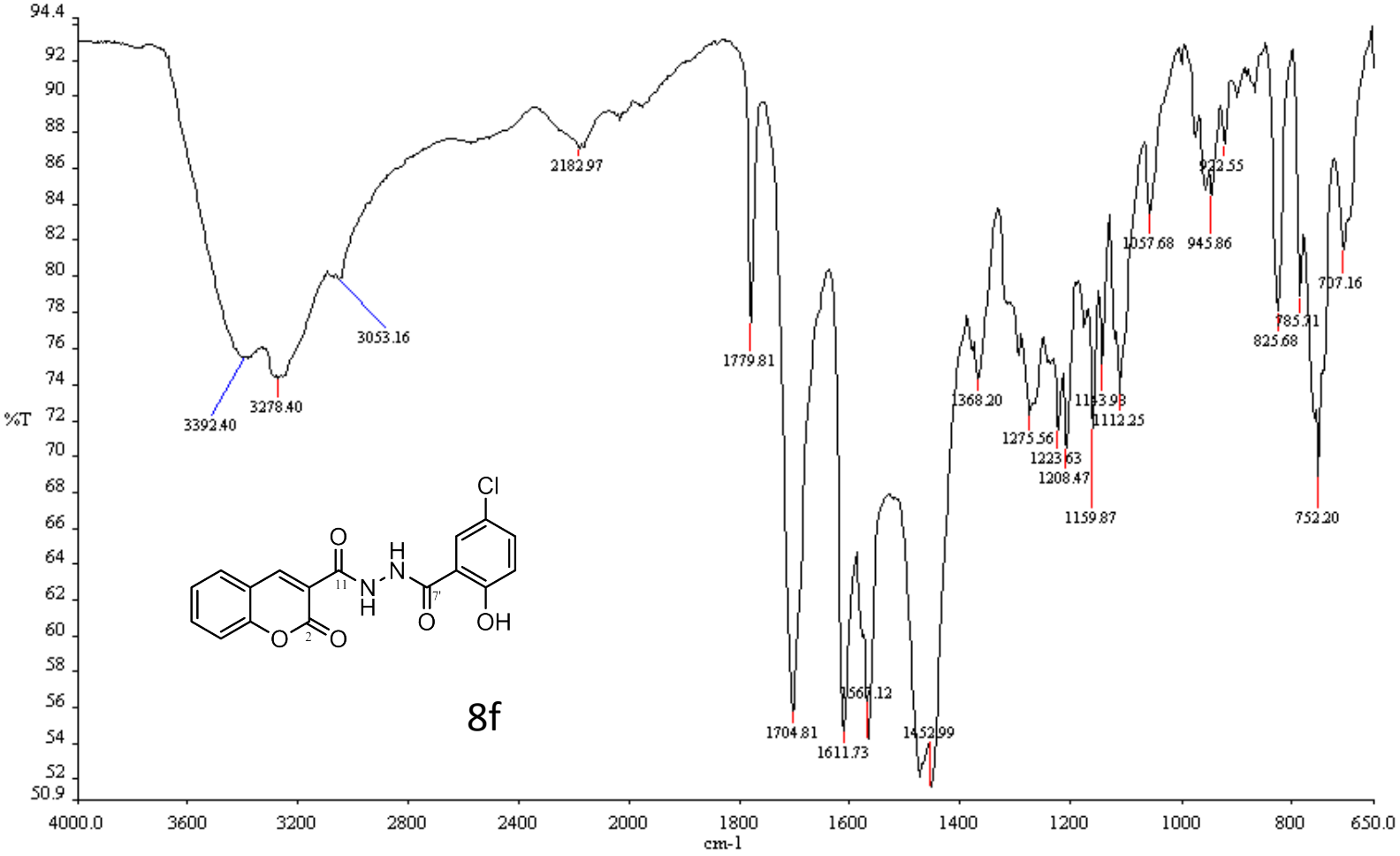
1: TOF MS ES+

2.33e+004

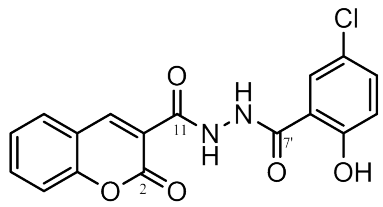


8e

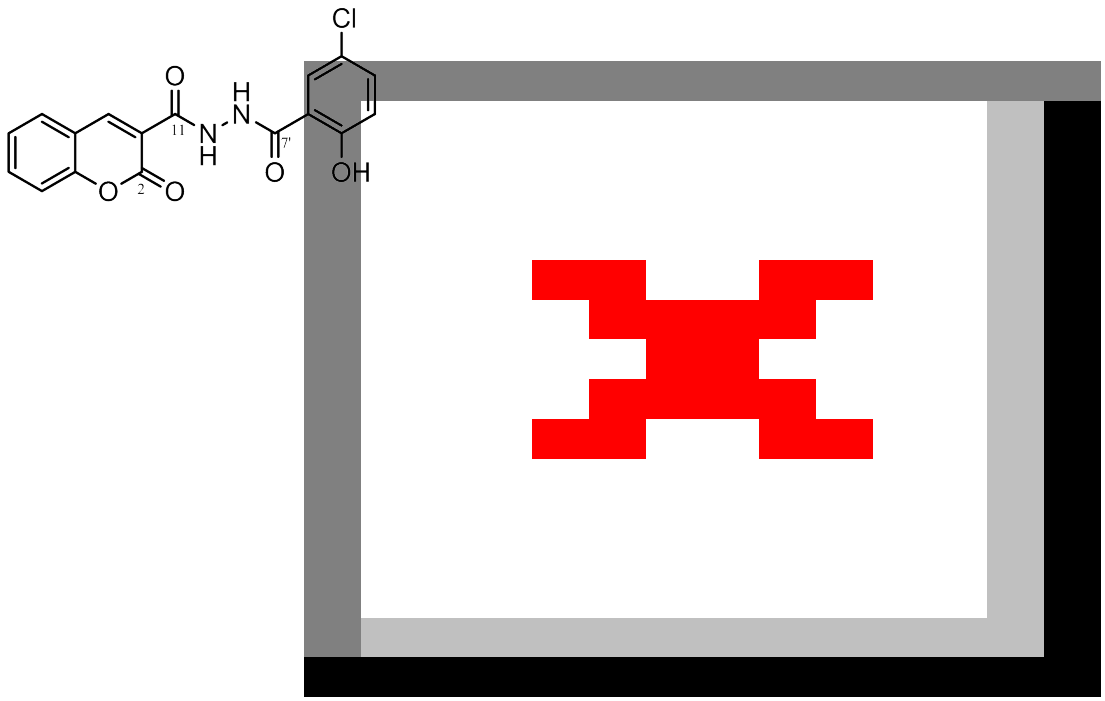
For Help, press F1


94.4
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
56
54
52
50.9
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3392.40
3278.40
3053.16
2182.97
1779.81
1704.81
1611.73
1566.12
1452.99
1368.20
1275.56
1223.63
1208.47
1159.87
1153.93
1112.25
1057.68
945.86
922.55
825.68
785.31
752.20
707.16
Cl
O
H
N
N
H
O
O
O
OH
11
7'
2
8f

8f


Cl
O
H
N
N
H
11
7'
O
OH
O
2
O

11.82
8.00
7.98
7.74
7.73
7.72
7.52
7.51
7.45
7.44
7.43
7.13
7.11
6.72
6.71
3.51
2.50
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
0.92
1.00
1.18
2.39
1.24
1.22
1.03
1.02
12.5
11.5
10.5
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
f1 (ppm)


Cl
O
H
N
11
N
H
7'
O
OH
O
2
O

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2409 formula(e) evaluated with 269 results within limits (all results (up to 1000) for each mass)

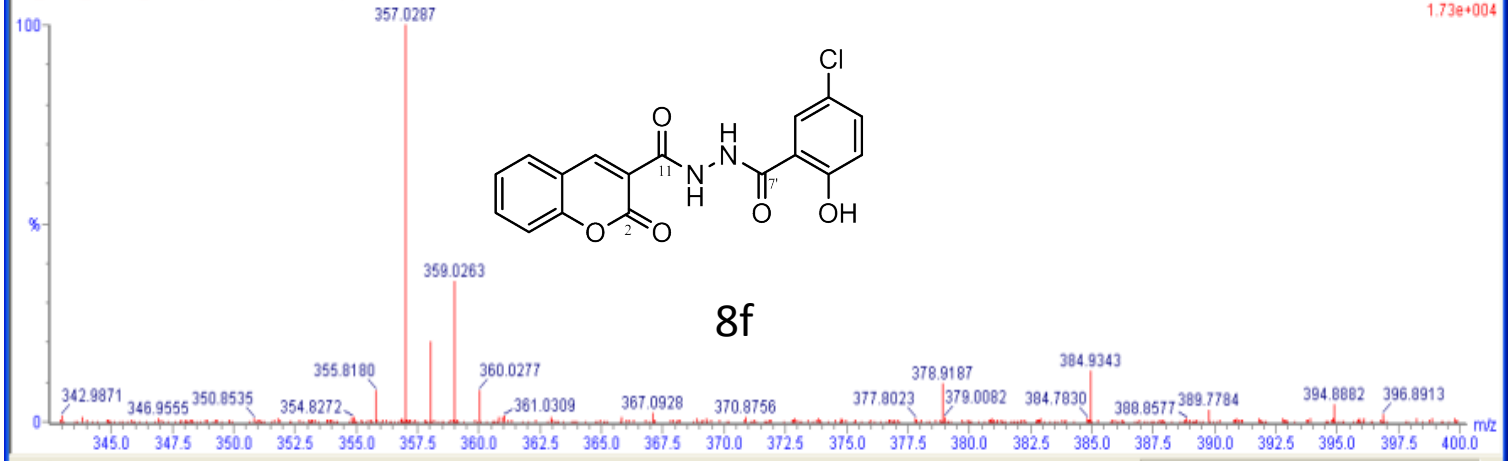
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	P	Cl
357.0287	357.0288	-0.1	-0.3	4.5	C11 H16 N4 O3 Cl3	185.6	16.644	0.00	11	16	4	3			3
	357.0286	0.1	0.3	4.5	C10 H16 N4 O4 P Cl2	184.0	15.035	0.00	10	16	4	4		1	2
	357.0286	0.1	0.3	10.5	C15 H12 N4 O Na Cl2	183.2	14.189	0.00	15	12	4	1	1		2
	357.0284	0.3	0.8	10.5	C14 H12 N4 O2 Na P Cl	176.6	7.623	0.05	14	12	4	2	1	1	1
	357.0293	-0.6	-1.7	14.5	C19 H11 O4 Na P	195.0	26.044	0.00	19	11		4	1	1	
	357.0294	-0.7	-2.0	14.5	C20 H11 O3 Na Cl	173.2	4.163	1.56	20	11		3	1		1
	357.0295	-0.8	-2.2	8.5	C15 H15 O6 P Cl	176.0	6.970	0.09	15	15		6		1	1
	357.0278	0.9	2.5	13.5	C17 H10 N2 O5 Cl	170.9	1.888	15.13	17	10	2	5			1
	357.0297	-1.0	-2.8	8.5	C16 H15 O5 Cl2	182.6	13.636	0.00	16	15		5			2

OJ 108a

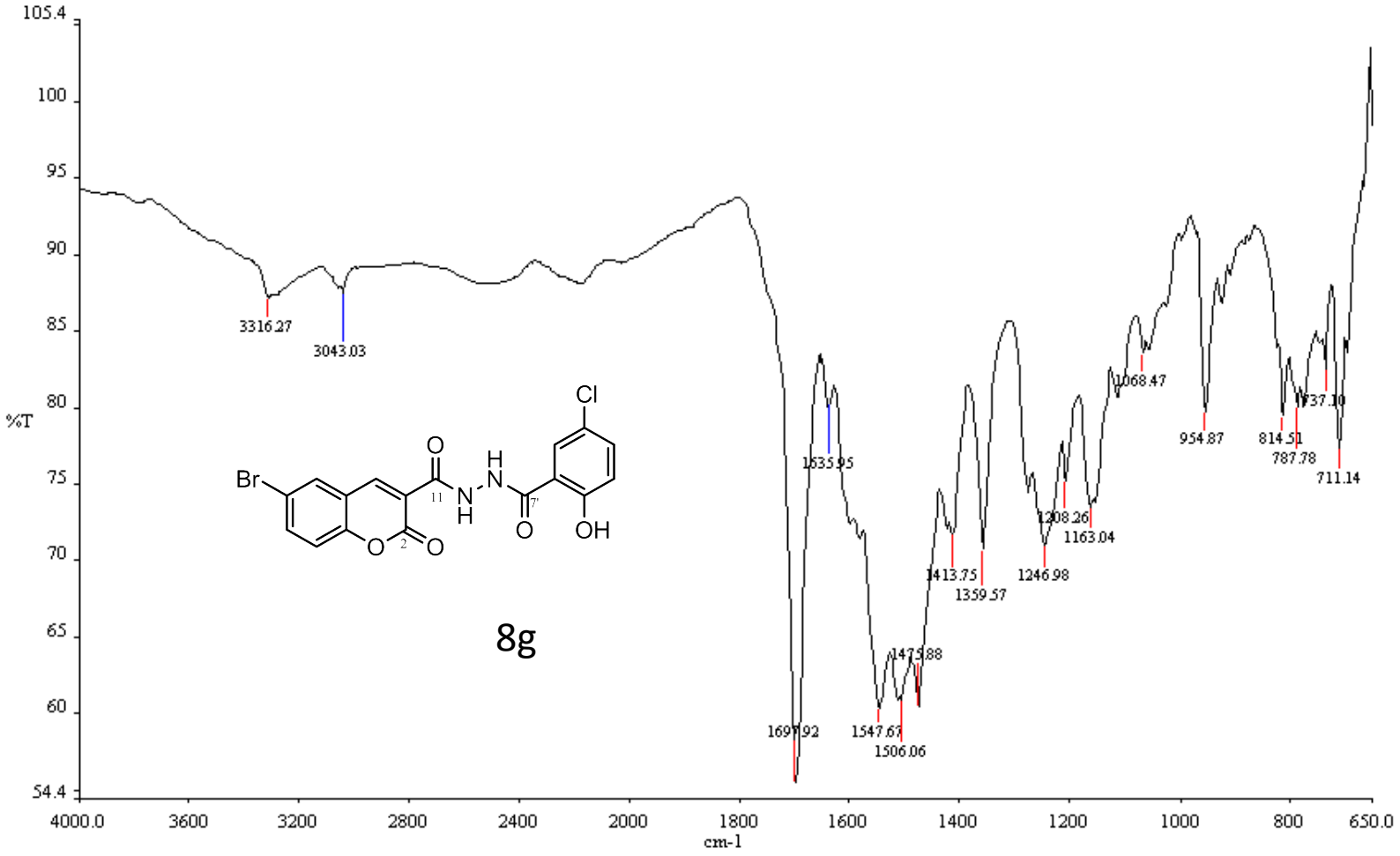
MS_Direct_151019_78n 15 (0.084) Cm (15:39-5:8)

1: TOF MS ES-
1.73e+004

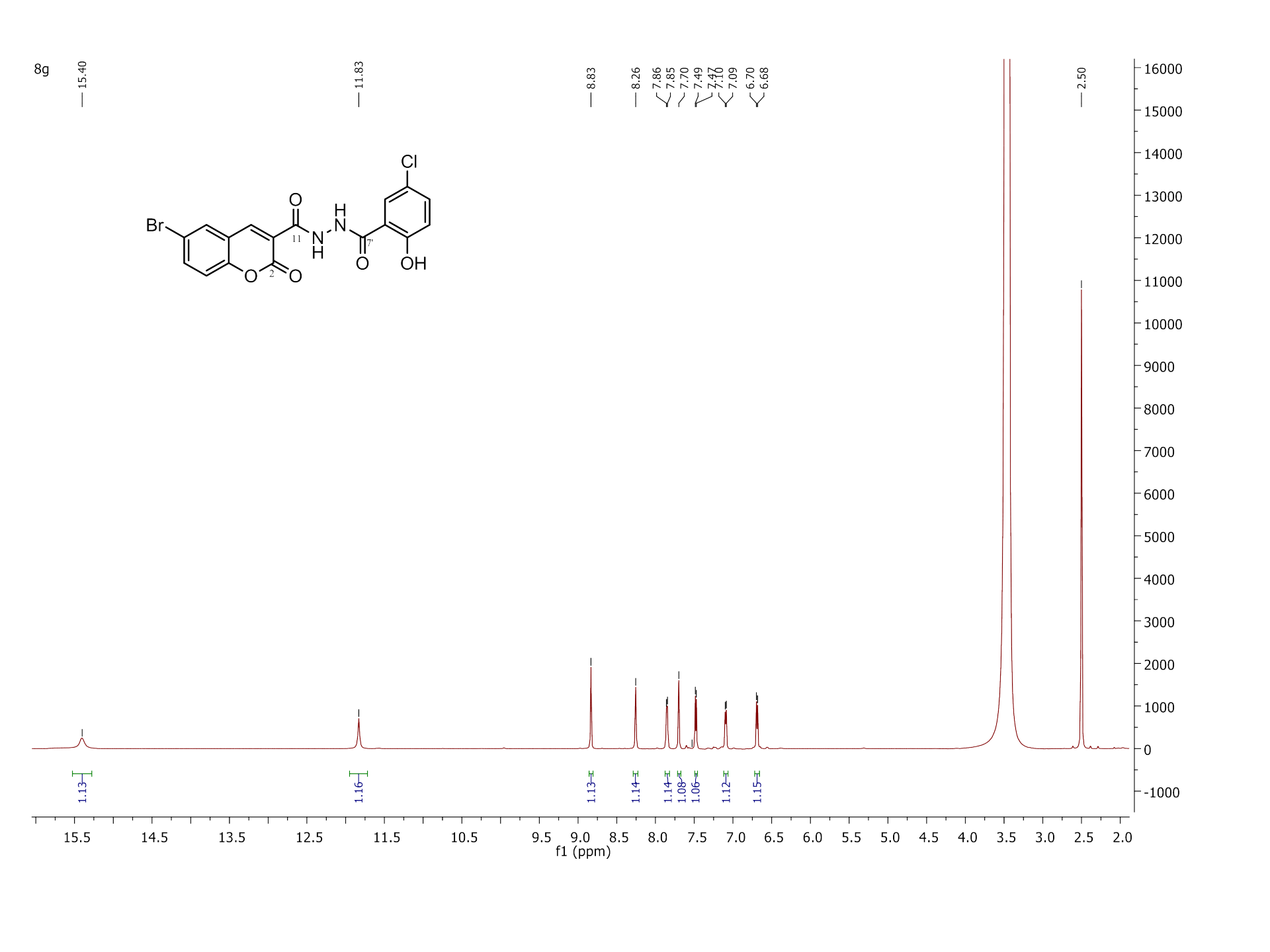


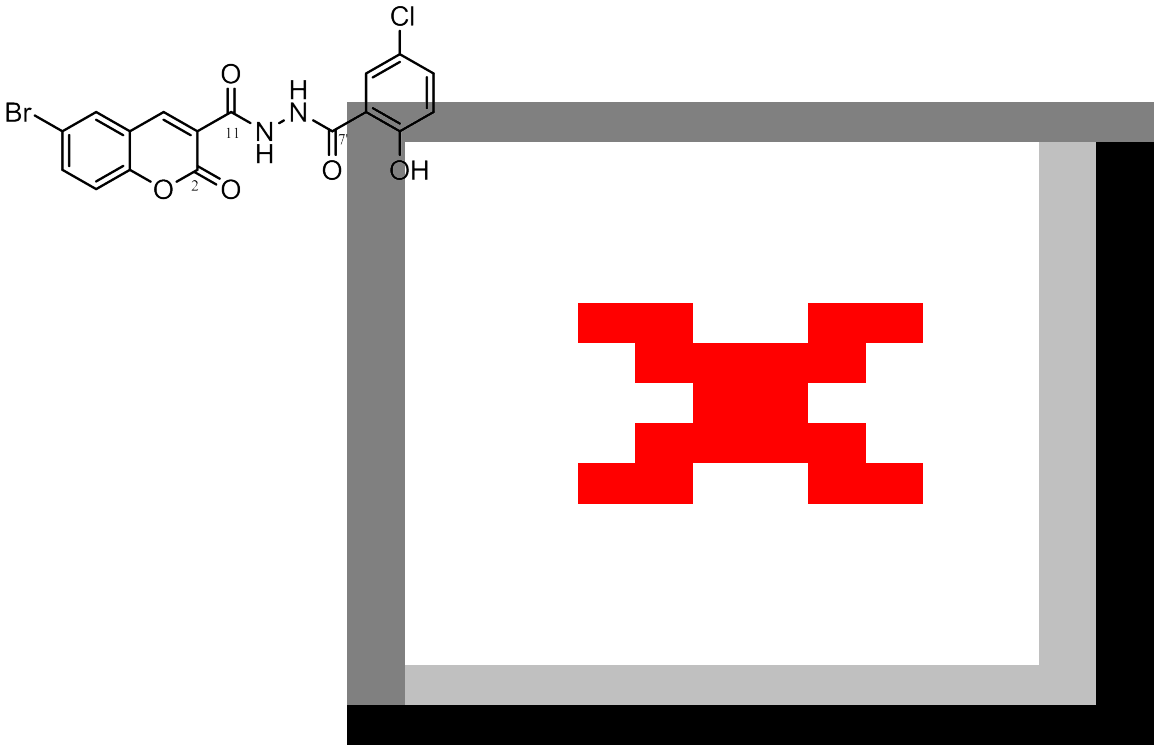
8f

For Help, press F1


105.4
100
95
90
85
80
75
70
65
60
54.4
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3316.27
3043.03
1635.95
1697.92
1547.67
1506.06
1475.88
1413.75
1359.57
1246.98
1208.26
1163.04
1068.47
954.87
814.51
787.78
737.10
711.14
Br
O
N
H
N
H
O
Cl
OH
O
O
11
2
7'

8g


8g
15.40
11.83
8.83
8.26
7.86
7.85
7.70
7.49
7.47
7.10
7.09
6.70
6.68
2.50
Br
O
N
H
N
H
Cl
O
OH
O
O
11
2
7'
1.13
1.16
1.13
1.14
1.14
1.08
1.06
1.12
1.15
f1 (ppm)


Cl
Br
O
H
N
N
H
11
7'
O
O
O
2
OH

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1491 formula(e) evaluated with 121 results within limits (all results (up to 1000) for each mass)

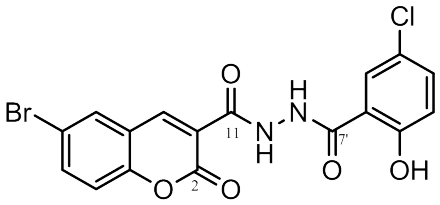
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Cl	Br
434.9381	434.9380	0.1	0.2	-0.5	C10 H19 O7 Cl3 Br	206.9	8.102	0.03	10	19		7	3	1
	434.9383	-0.2	-0.5	19.5	C23 H6 O3 Cl3	208.2	9.364	0.01	23	6		3	3	
	434.9383	-0.2	-0.5	13.5	C17 H9 N2 O5 Cl Br	201.0	2.203	11.05	17	9	2	5	1	1
	434.9393	-1.2	-2.8	4.5	C11 H15 N4 O3 Cl3 Br	206.8	7.974	0.03	11	15	4	3	3	1
	434.9365	1.6	3.7	18.5	C18 H4 N4 O5 Br	206.0	7.217	0.07	18	4	4	5		1
	434.9364	1.7	3.9	24.5	C24 H N2 O3 Cl2	209.9	11.076	0.00	24	1	2	3	2	
	434.9361	2.0	4.6	4.5	C11 H14 N2 O7 Cl2 Br	204.4	5.566	0.38	11	14	2	7	2	1
	434.9402	-2.1	-4.8	8.5	C16 H14 O5 Cl2 Br	202.2	3.378	3.41	16	14		5	2	1
	434.9404	-2.3	-5.3	28.5	C29 H O Cl2	209.9	11.099	0.00	29	1		1	2	

OJ 108b

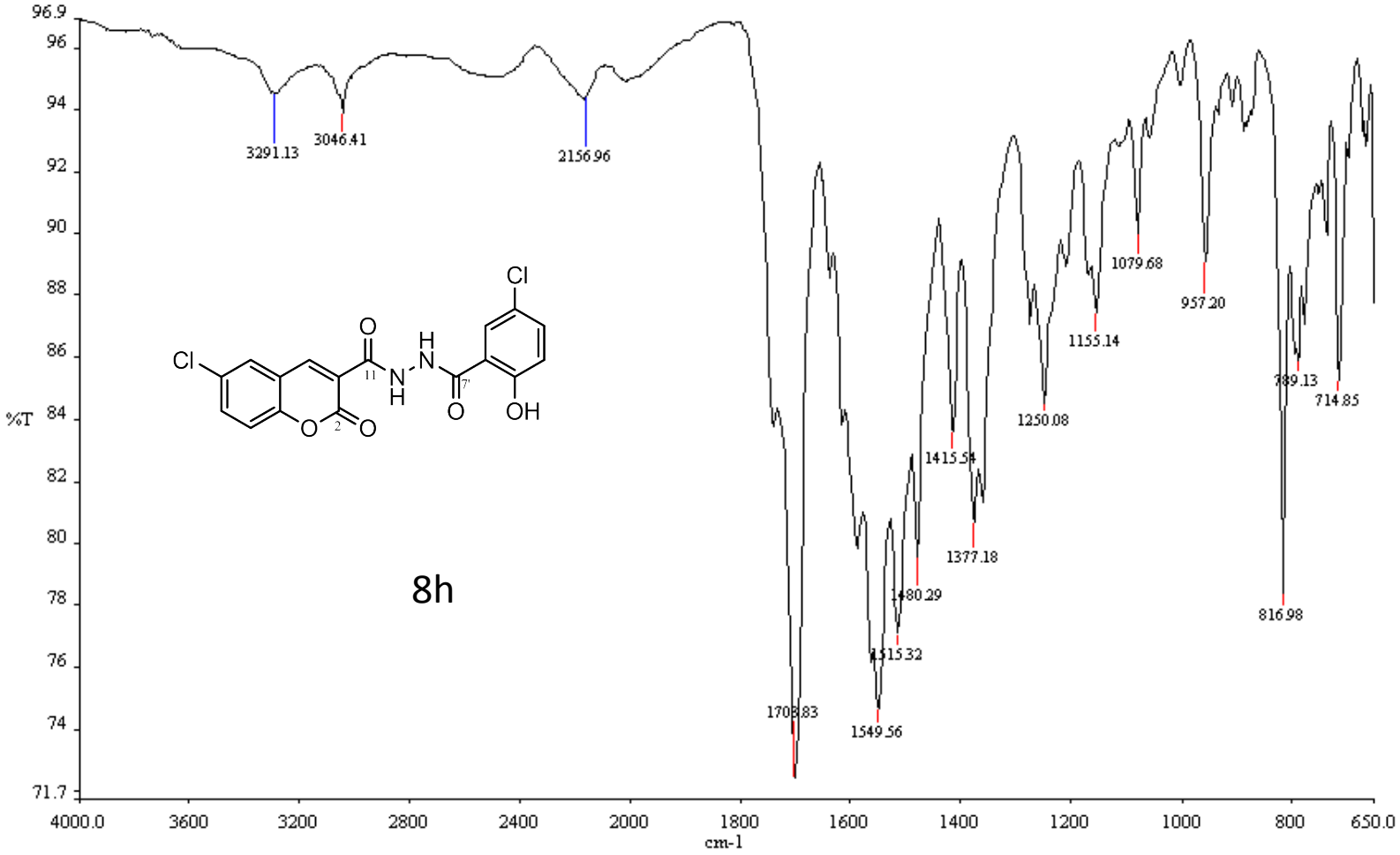
MS_Direct_151019_79n 65 (0.296) Cm (20:66-5:10)

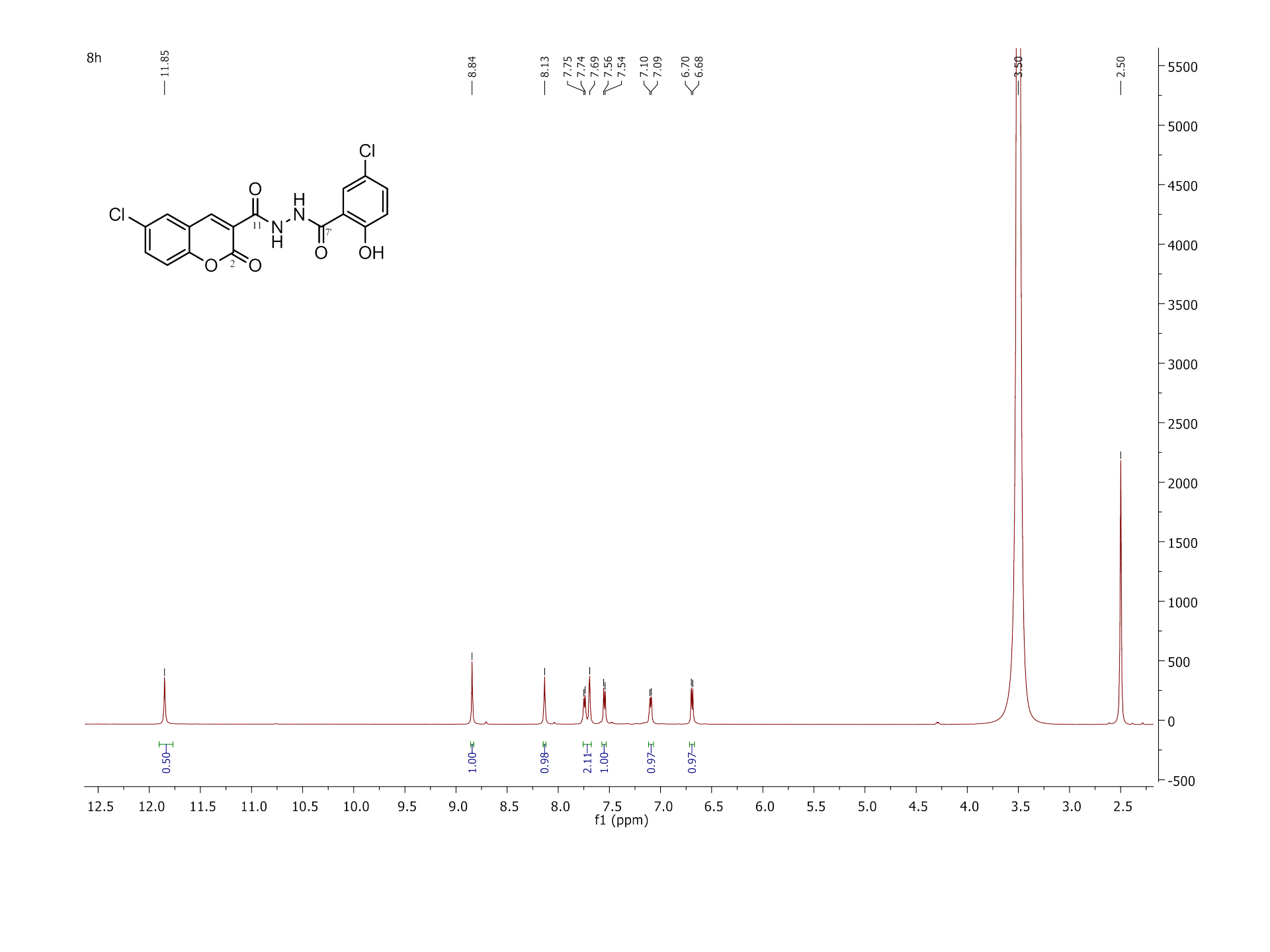
1: TOF MS ES-
2.30e+004

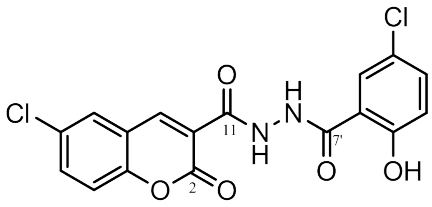


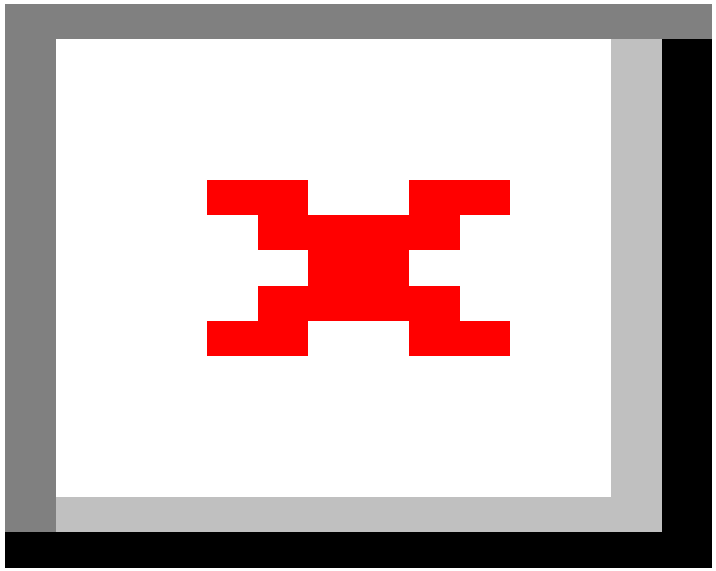
8g

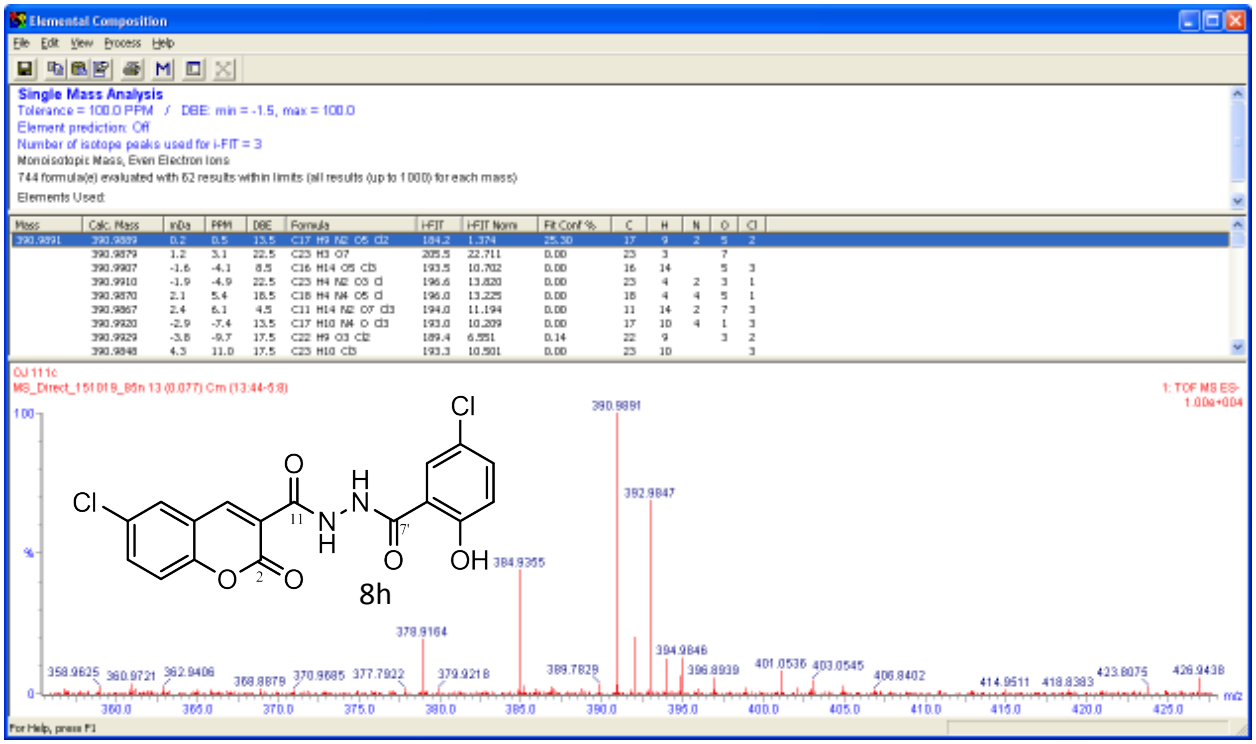
For Help, press F1

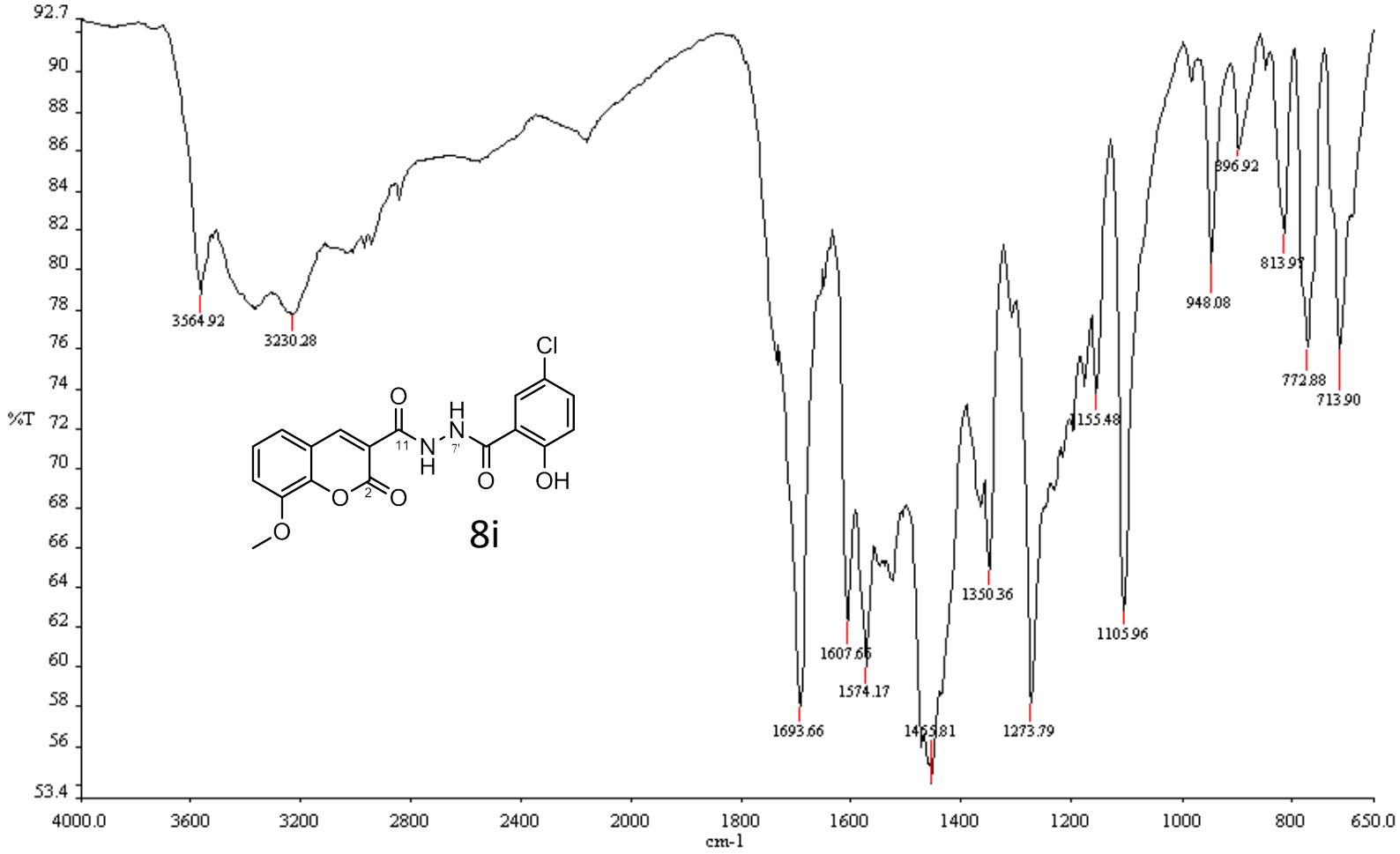

96.9
96
94
92
90
88
86
84
82
80
78
76
74
71.7
%T
3291.13
3046.41
2156.96
1708.83
1549.56
1515.32
1480.29
1415.58
1377.18
1250.08
1155.14
1079.68
957.20
816.98
789.13
714.85
Cl
O
H
N
N
H
O
11
7'
Cl
O
O
2
OH
8h
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1

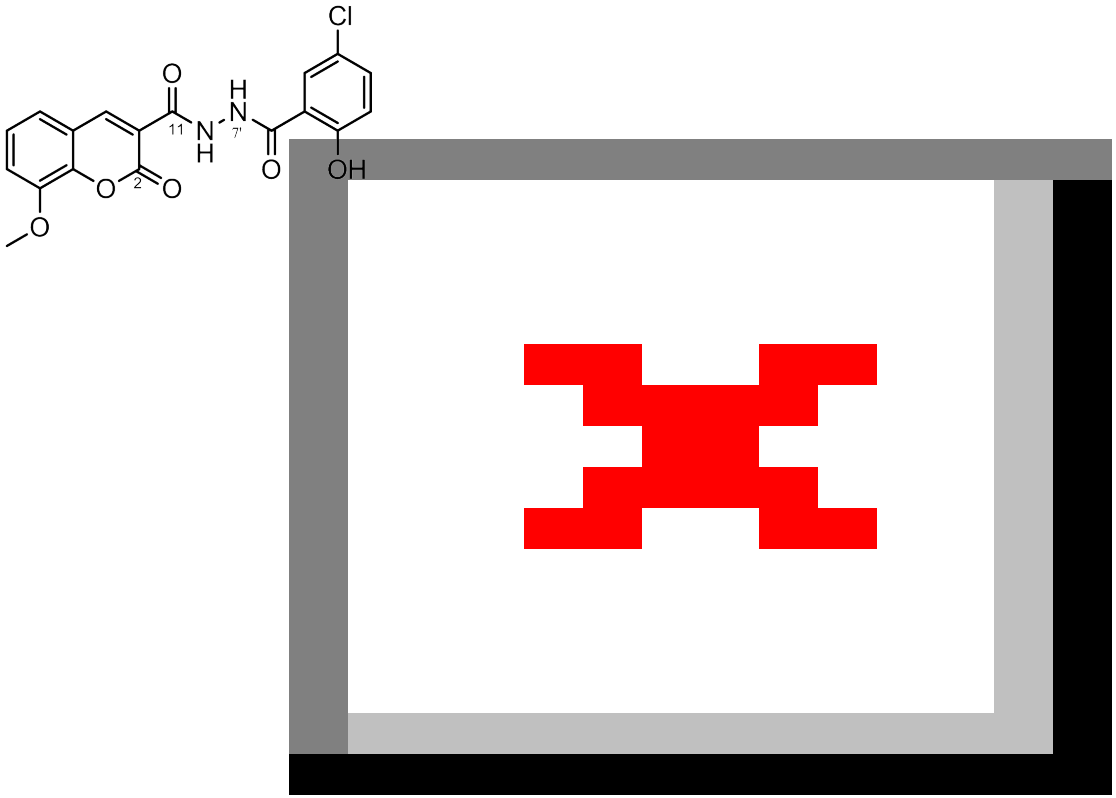

8h
11.85
8.84
8.13
7.75
7.74
7.69
7.56
7.54
7.10
7.09
6.70
6.68
3.50
2.50
Cl
O
H
N
N
H
O
11
7'
Cl
Cl
O
2
O
O
OH
0.50
1.00
0.98
2.11
1.00
0.97
0.97
f1 (ppm)

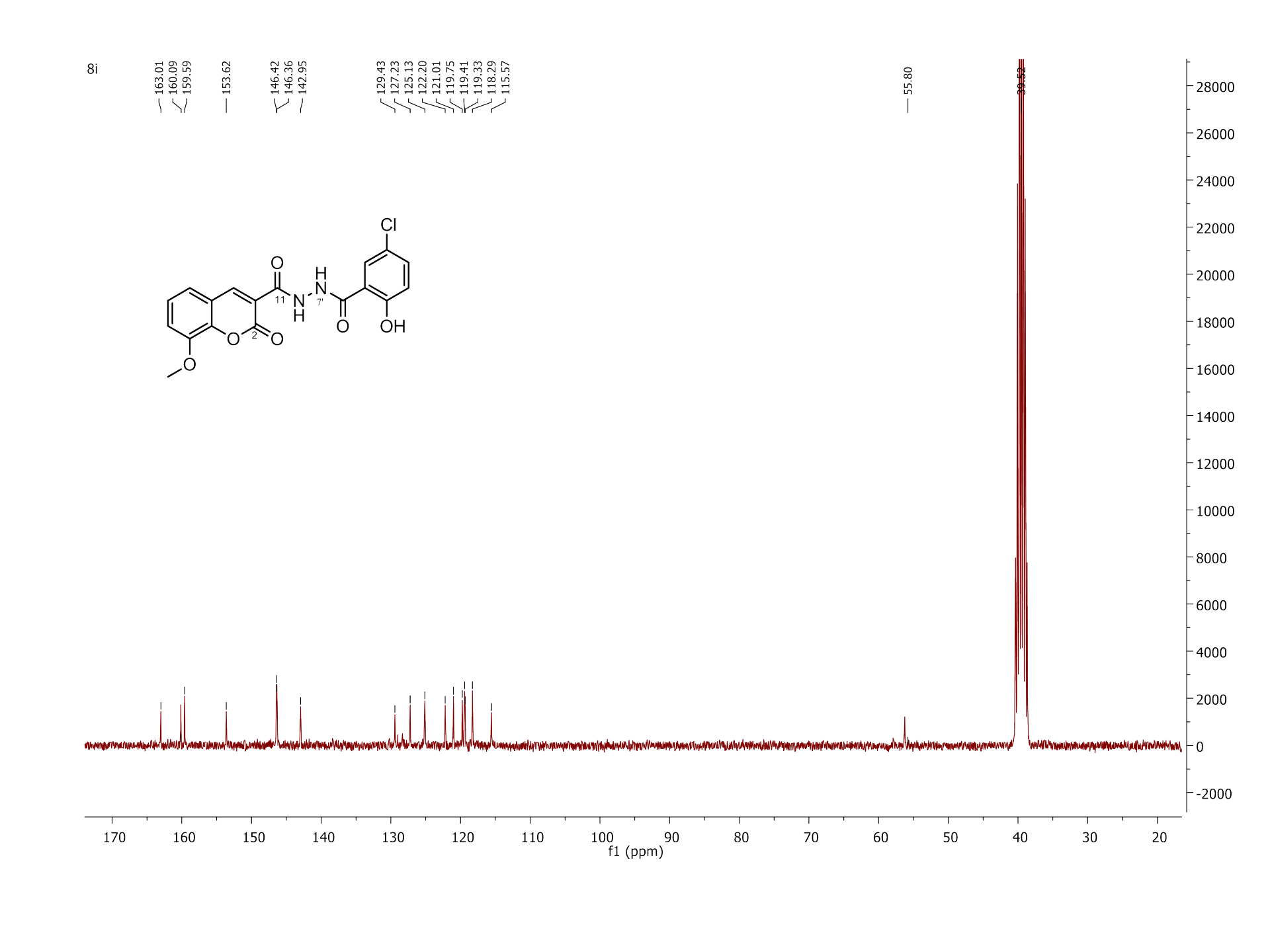

Cl
O
H
N
N
H
Cl
11
7'
O
OH
O
2
O




Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
744 formula(e) evaluated with 62 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O Cl
390.9891 390.9889 0.2 0.5 13.5 C17 H9 N2 O5 Cl2 184.2 1.374 25.30 17 9 2 5 2
390.9879 1.2 3.1 22.5 C23 H3 O7 205.5 22.711 0.00 23 3 7
390.9907 -1.6 -4.1 8.5 C16 H14 O5 Cl3 193.5 10.702 0.00 16 14 5 3
390.9910 -1.9 -4.9 22.5 C23 H4 N2 O3 Cl 196.6 13.820 0.00 23 4 2 3 1
390.9870 2.1 5.4 18.5 C18 H4 N4 O5 Cl 196.0 13.225 0.00 18 4 4 5 1
390.9867 2.4 6.1 4.5 C11 H14 N2 O7 Cl3 194.0 11.194 0.00 11 14 2 7 3
390.9920 -2.9 -7.4 13.5 C17 H10 N4 O Cl3 193.0 10.209 0.00 17 10 4 1 3
390.9929 -3.8 -9.7 17.5 C22 H9 O3 Cl2 189.4 6.551 0.14 22 9 3 2
390.9848 4.3 11.0 17.5 C23 H10 Cl3 193.3 10.501 0.00 23 10 3
OJ 111c
MS_Direct_151018_85n 13 (0.077) Cm (13:44-58)
1: TOF MS ES-
1.00e+004
100
%
0
Cl
O
H
N
N
H
O
OH
Cl
O
O
11
2
7'
8h
390.9891
392.9847
384.9355
378.9164
394.9846
396.8939
401.0536
403.0545
406.8402
414.9511
418.8383
423.8075
426.9438
358.9625
360.9721
362.9406
368.8878
370.9685
377.7922
379.9218
389.7829
360.0
365.0
370.0
375.0
380.0
385.0
390.0
395.0
400.0
405.0
410.0
415.0
420.0
425.0
m/z
For Help, press F1


92.7
90
88
86
84
82
80
78
76
74
%T
72
70
68
66
64
62
60
58
56
53.4
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3564.92
3230.28
1693.66
1607.66
1574.17
1463.81
1350.36
1273.79
1155.48
1105.96
948.08
896.92
813.97
772.88
713.90
Cl
OH
O
N
H
11
7'
2
8i


Cl
O
H
N
11
N
7'
H
O
OH
O
2
O
O


8i
163.01
160.09
159.59
153.62
146.42
146.36
142.95
129.43
127.23
125.13
122.20
121.01
119.75
119.41
119.33
118.29
115.57
55.80
39.52
Cl
O
H
N
11
N
7'
H
O
OH
O
2
O
O
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1269 formula(e) evaluated with 130 results within limits (all results (up to 1000) for each mass)

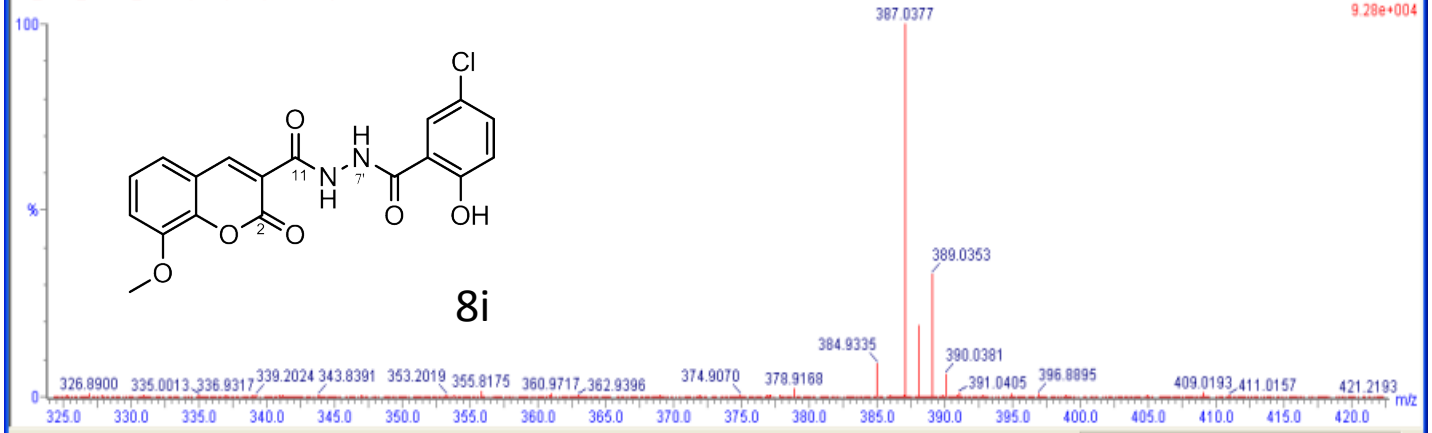
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Cl	Br
387.0377	387.0384	-0.7	-1.8	13.5	C18 H12 N2 O6 Cl	279.6	1.103	33.19	18	12	2	6	1	
	387.0385	-0.8	-2.1	15.5	C23 H16 O Br	291.0	12.470	0.00	23	16		1		1
	387.0366	1.1	2.8	18.5	C19 H7 N4 O6	300.0	21.425	0.00	19	7	4	6		
	387.0363	1.4	3.6	6.5	C17 H21 O3 Cl Br	291.0	12.456	0.00	17	21		3	1	1
	387.0394	-1.7	-4.4	4.5	C12 H18 N4 O4 Cl3	291.0	12.496	0.00	12	18	4	4	3	
	387.0354	2.3	5.9	2.5	C12 H22 N4 O Cl2 Br	292.5	13.997	0.00	12	22	4	1	2	1
	387.0402	-2.5	-6.5	8.5	C17 H17 O6 Cl2	288.3	9.769	0.01	17	17		6	2	
	387.0406	-2.9	-7.5	22.5	C24 H7 N2 O4	300.3	21.750	0.00	24	7	2	4		
	387.0344	3.3	8.5	11.5	C18 H16 N2 O3 Br	291.4	12.891	0.00	18	16	2	3		1

OJ 108d

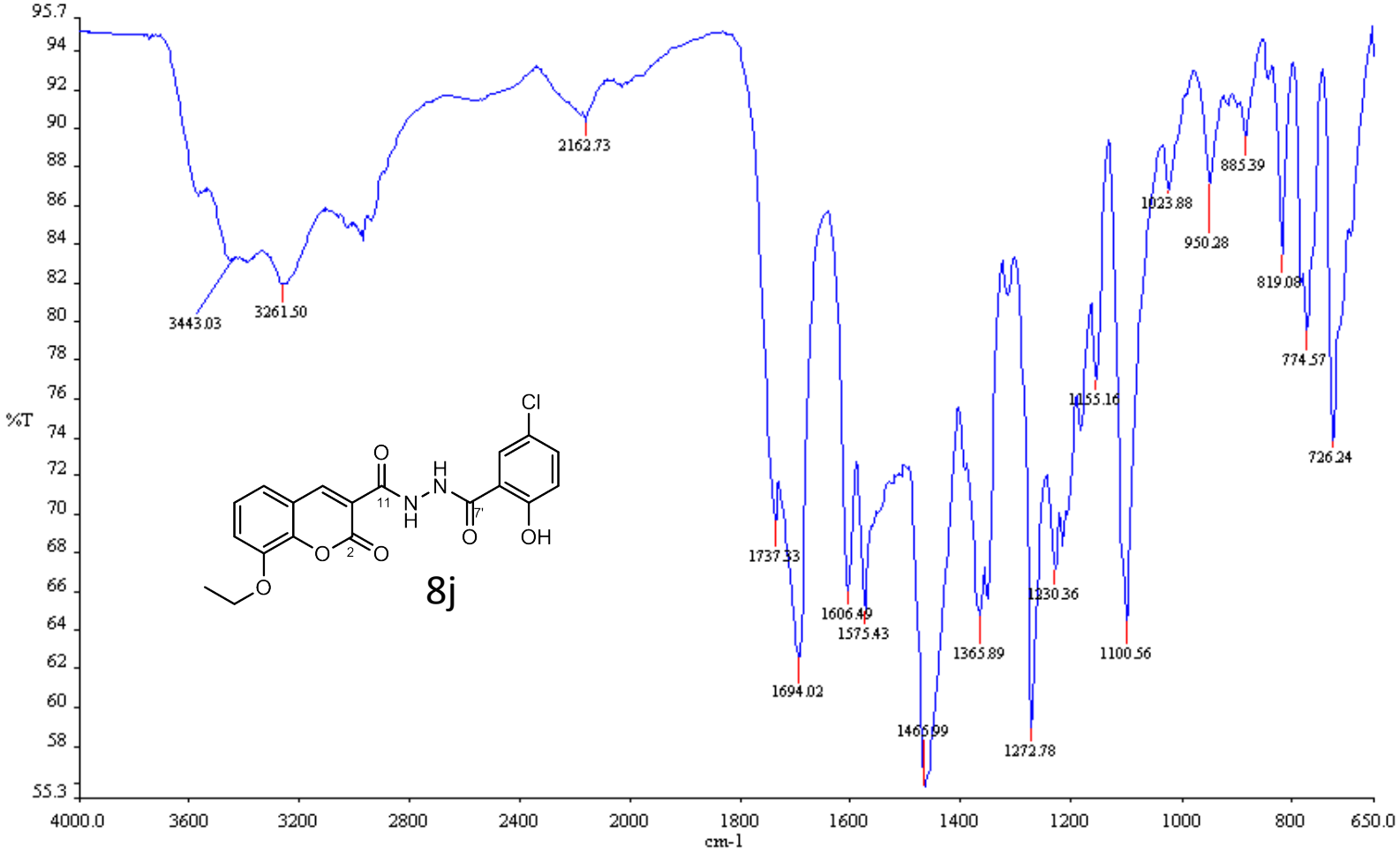
MS_Direct_151019_81n 59 (0.267) Cm (14:60-5:11)

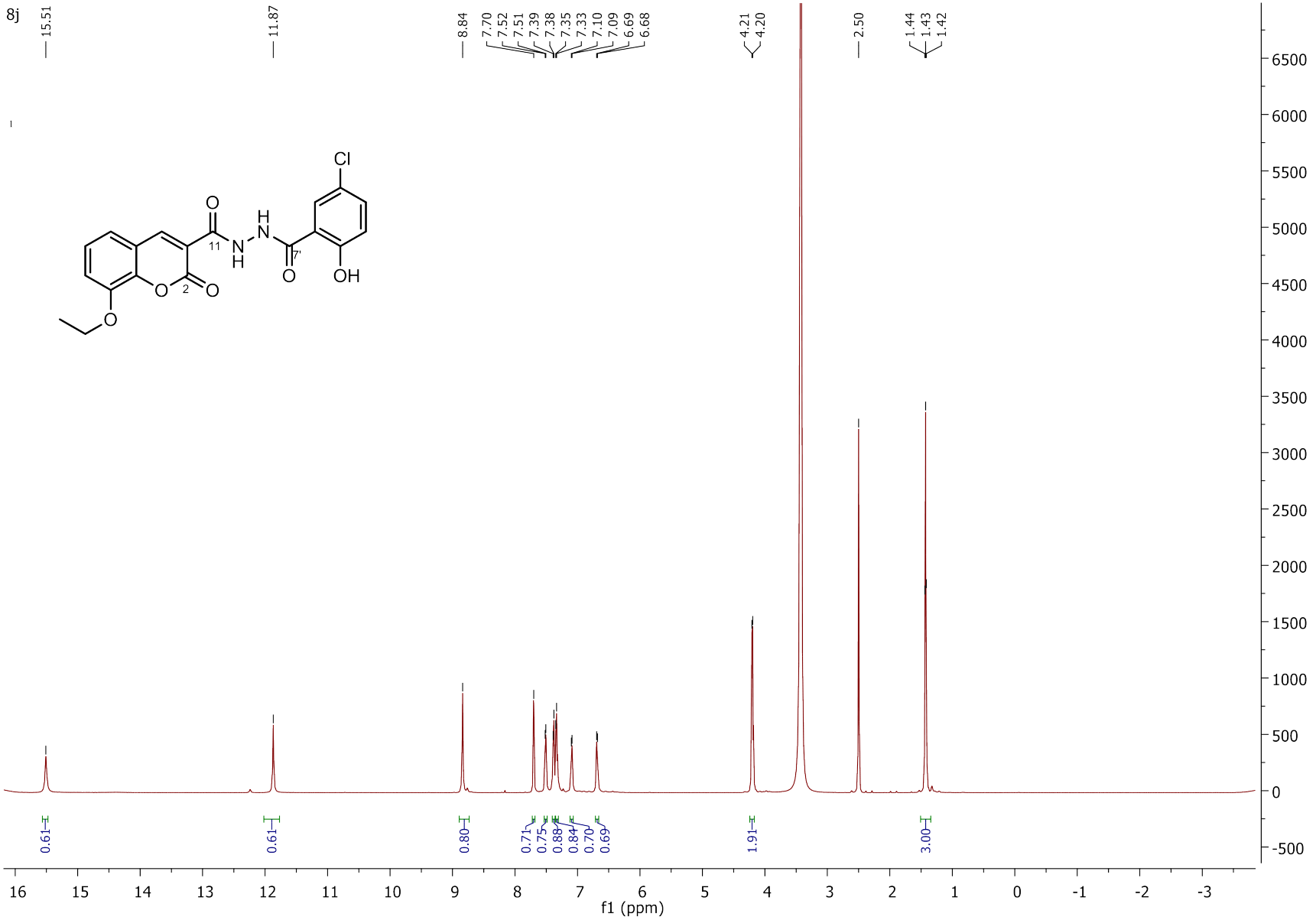
1: TOF MS ES-
9.28e+004



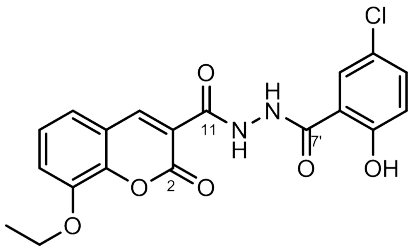
8i

For Help, press F1


95.7
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
55.3
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3443.03
3261.50
2162.73
1737.33
1694.02
1606.49
1575.43
1466.99
1365.89
1330.36
1272.78
1155.16
1100.56
1023.88
950.28
885.39
819.08
774.57
726.24
Cl
OH
O
N
H
O
O
O
O
11
7'
2
8j


8j
15.51
11.87
8.84
7.70
7.52
7.51
7.39
7.38
7.35
7.33
7.10
7.09
6.69
6.68
4.21
4.20
2.50
1.44
1.43
1.42
Cl
O
H
N
N
H
11
7'
O
OH
O
2
O
O
0.61
0.61
0.80
0.71
0.75
0.88
0.84
0.70
0.69
1.91
3.00
f1 (ppm)

8j


Cl
O
H
N
N
H
11
7'
O
O
2
O
O
OH

162.93
160.19
159.56
153.53
146.42
145.58
143.00
129.33
127.19
125.08
122.29
120.93
119.68
119.52
119.31
118.24
116.33
64.56
40.06
39.94
39.80
39.66
39.52
39.38
39.24
39.10
14.70
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
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)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1176 formula(e) evaluated with 125 results within limits (all results (up to 1000) for each mass)

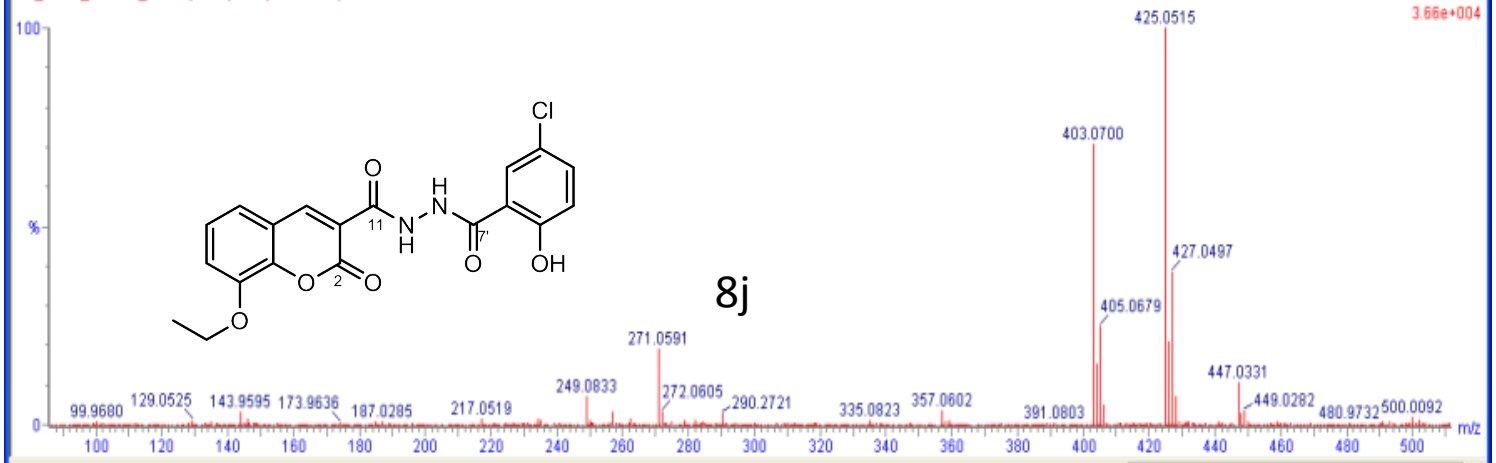
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	Cl
403.0700	403.0697	0.3	0.7	12.5	C19 H16 N2 O6 Cl	84.7	0.871	41.86	19	16	2	6		1
	403.0705	-0.5	-1.2	9.5	C17 H18 N4 O2 Na Cl2	99.2	15.363	0.00	17	18	4	2	1	2
	403.0695	0.5	1.2	18.5	C23 H12 N2 O4 Na	110.4	26.599	0.00	23	12	2	4	1	
	403.0691	0.9	2.2	4.5	C16 H22 O6 Na Cl2	99.9	16.079	0.00	16	22		6	1	2
	403.0713	-1.3	-3.2	13.5	C22 H17 O4 Na Cl	90.6	6.785	0.11	22	17		4	1	1
	403.0715	-1.5	-3.7	7.5	C18 H21 O6 Cl2	99.7	15.906	0.00	18	21		6		2
	403.0719	-1.9	-4.7	21.5	C25 H11 N2 O4	110.4	26.625	0.00	25	11	2	4		
	403.0679	2.1	5.2	17.5	C20 H11 N4 O6	110.1	26.341	0.00	20	11	4	6		
	403.0726	-2.6	-6.5	18.5	C23 H13 N4 Na Cl	93.0	9.166	0.01	23	13	4		1	1

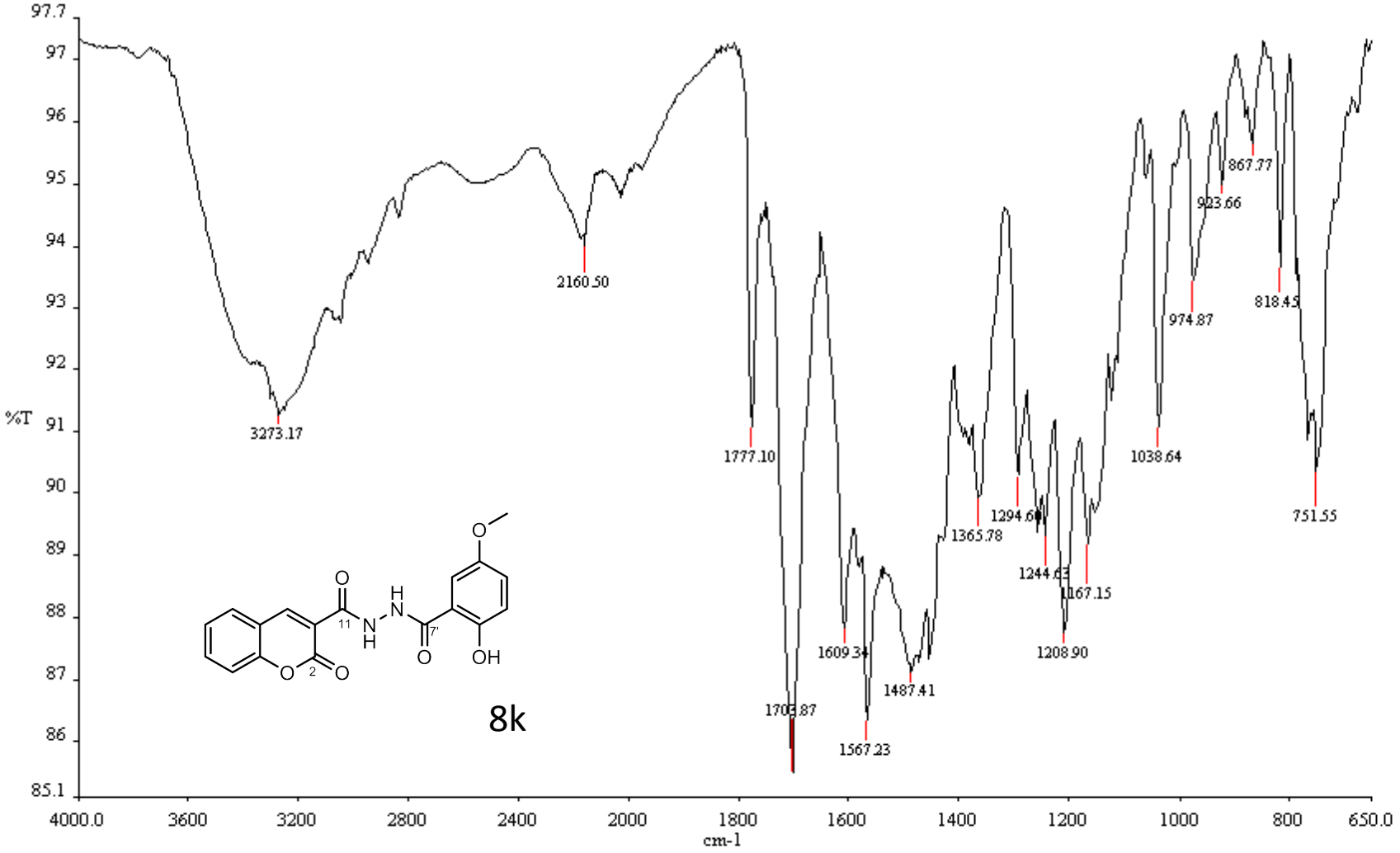
OJ 108e

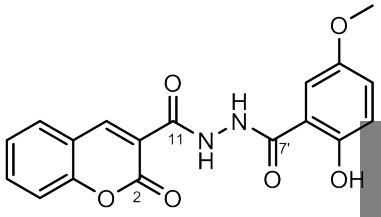
MS_Direct_151019_82 36 (0.169) Cm (34:36-7:11)

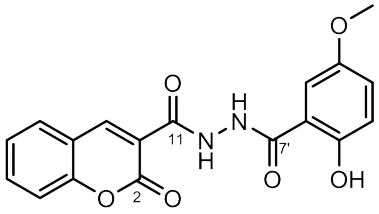
1: TOF MS ES+
3.66e+004

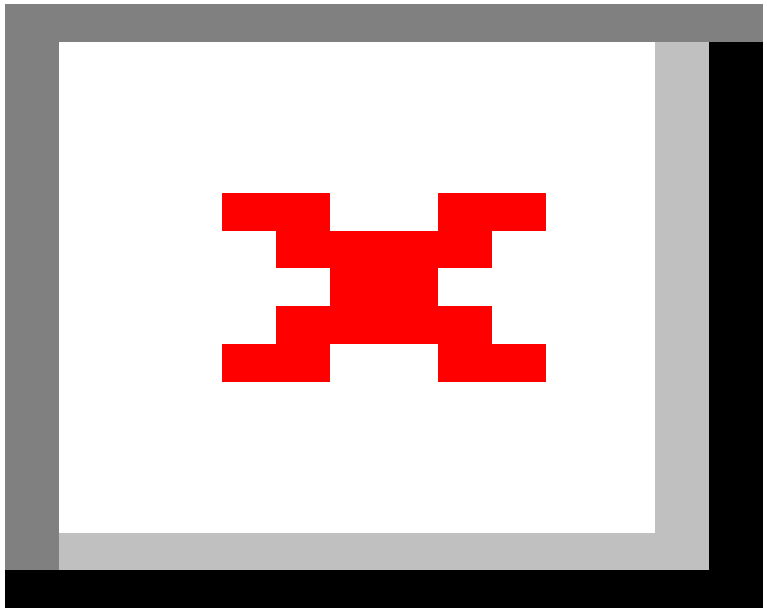


For Help, press F1


97.7
97
96
95
94
93
92
91
90
89
88
87
86
85.1
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3273.17
2160.50
1777.10
1705.87
1609.34
1567.23
1487.41
1365.78
1294.66
1244.63
1208.90
1167.15
1038.64
974.87
923.66
867.77
818.45
751.55
O
O
11
N
H
N
H
7'
O
O
O
2
O
OH
8k


O
O
11
N
H
H
N
7'
O
O
OH
O
2
O


O
O
11
N
H
H
N
7'
O
O
OH
O
2
O



Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

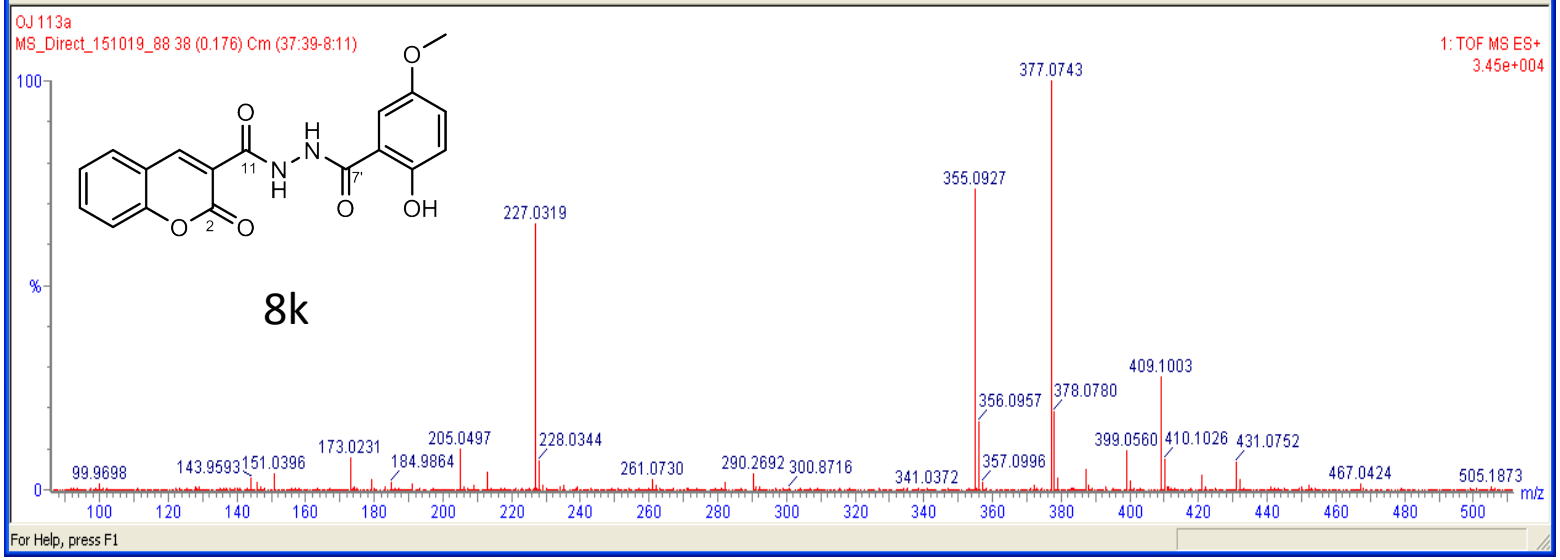
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

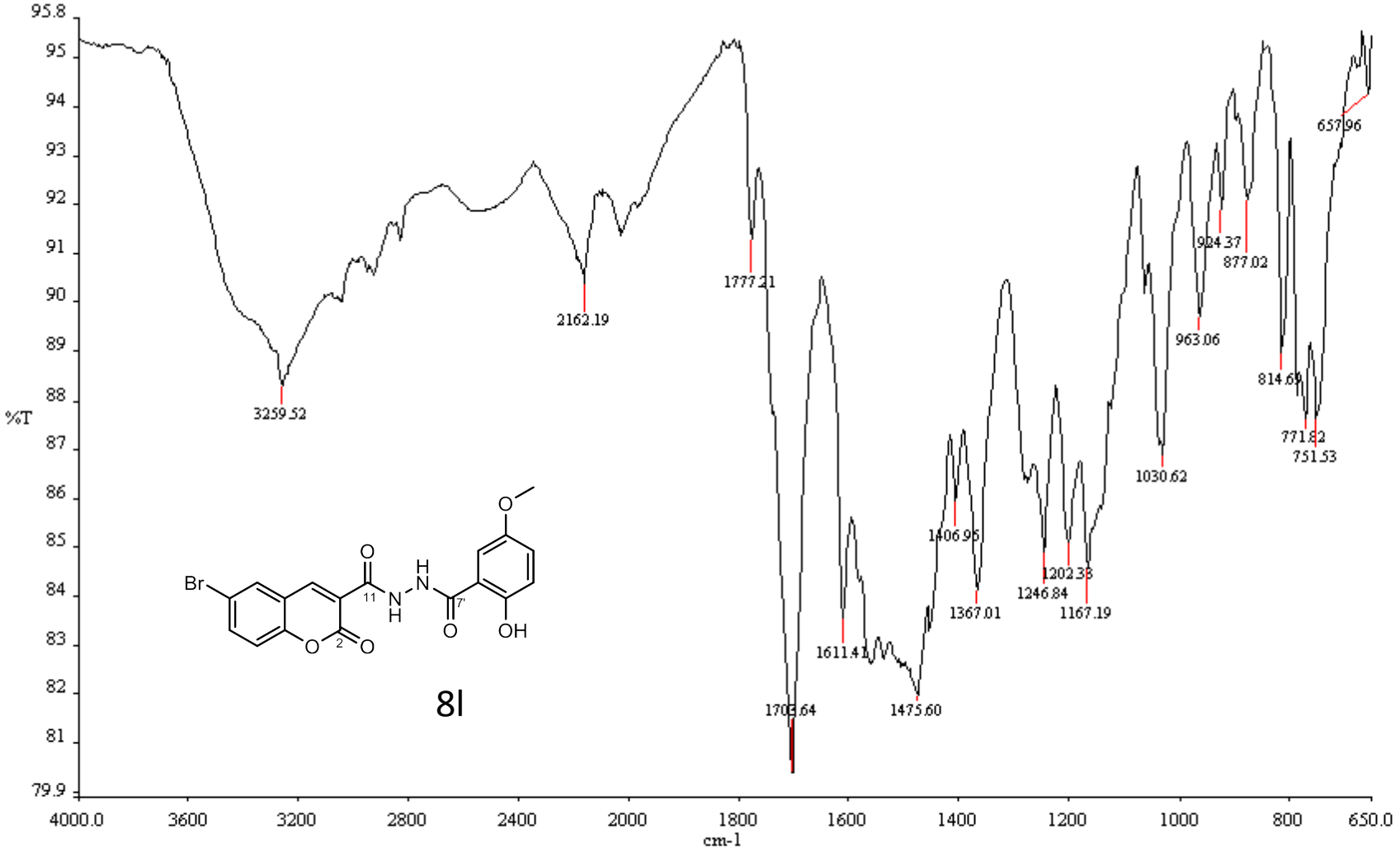
1009 formula(e) evaluated with 107 results within limits (all results (up to 1000) for each mass)

Elements Used:

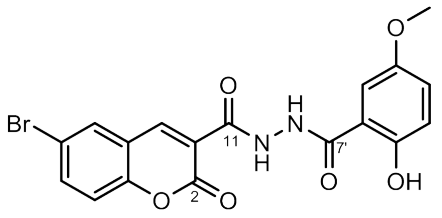
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	Cl
355.0927	355.0924	0.3	0.8	4.5	C15 H21 O6 Na Cl	75.7	23.461	0.00	15	21		6	1	1
	355.0930	-0.3	-0.8	12.5	C18 H15 N2 O6	57.0	4.754	0.86	18	15	2	6		
	355.0938	-1.1	-3.1	9.5	C16 H17 N4 O2 Na Cl	75.6	23.352	0.00	16	17	4	2	1	1
	355.0916	1.1	3.1	0.5	C10 H22 N4 O4 Na Cl2	76.6	24.352	0.00	10	22	4	4	1	2
	355.0940	-1.3	-3.7	3.5	C12 H21 N4 O4 Cl2	76.6	24.345	0.00	12	21	4	4		2
	355.0946	-1.9	-5.4	13.5	C21 H16 O4 Na	55.2	2.924	5.37	21	16		4	1	
	355.0906	2.1	5.9	9.5	C16 H16 N2 O6 Na	58.6	6.306	0.18	16	16	2	6	1	
	355.0948	-2.1	-5.9	7.5	C17 H20 O6 Cl	75.7	23.405	0.00	17	20		6		1
	355.0956	-2.9	-8.2	4.5	C15 H22 N2 O2 Na Cl2	76.7	24.377	0.00	15	22	2	2	1	2



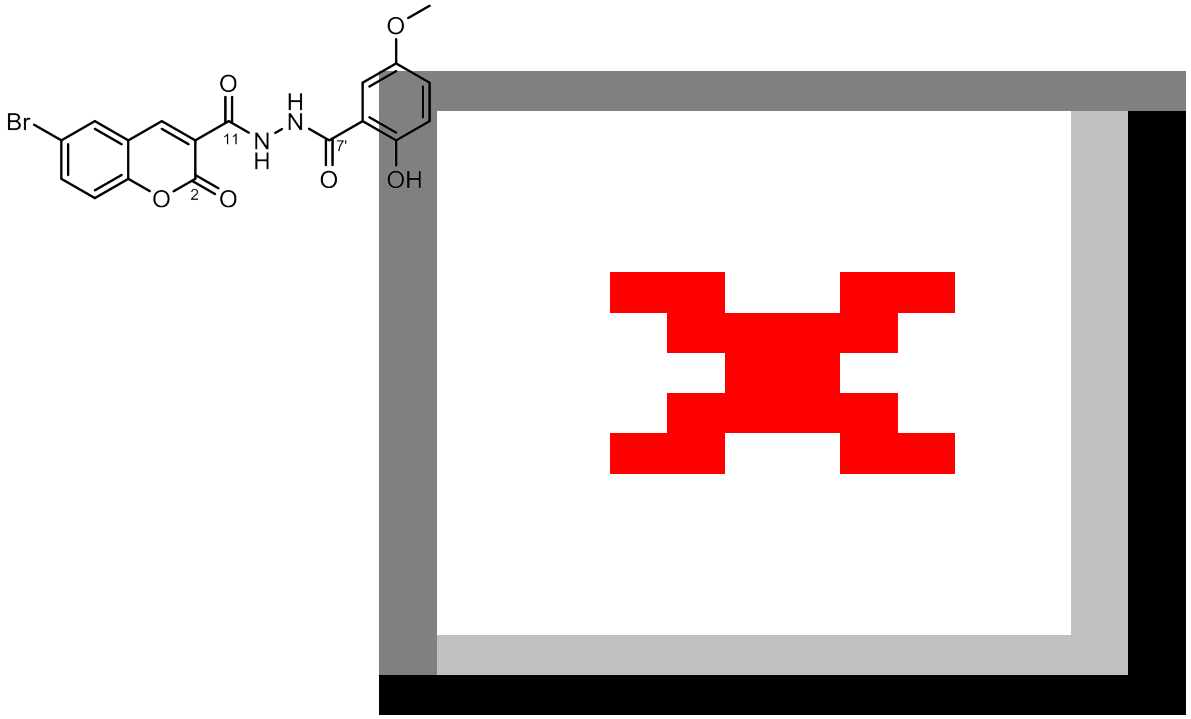
For Help, press F1

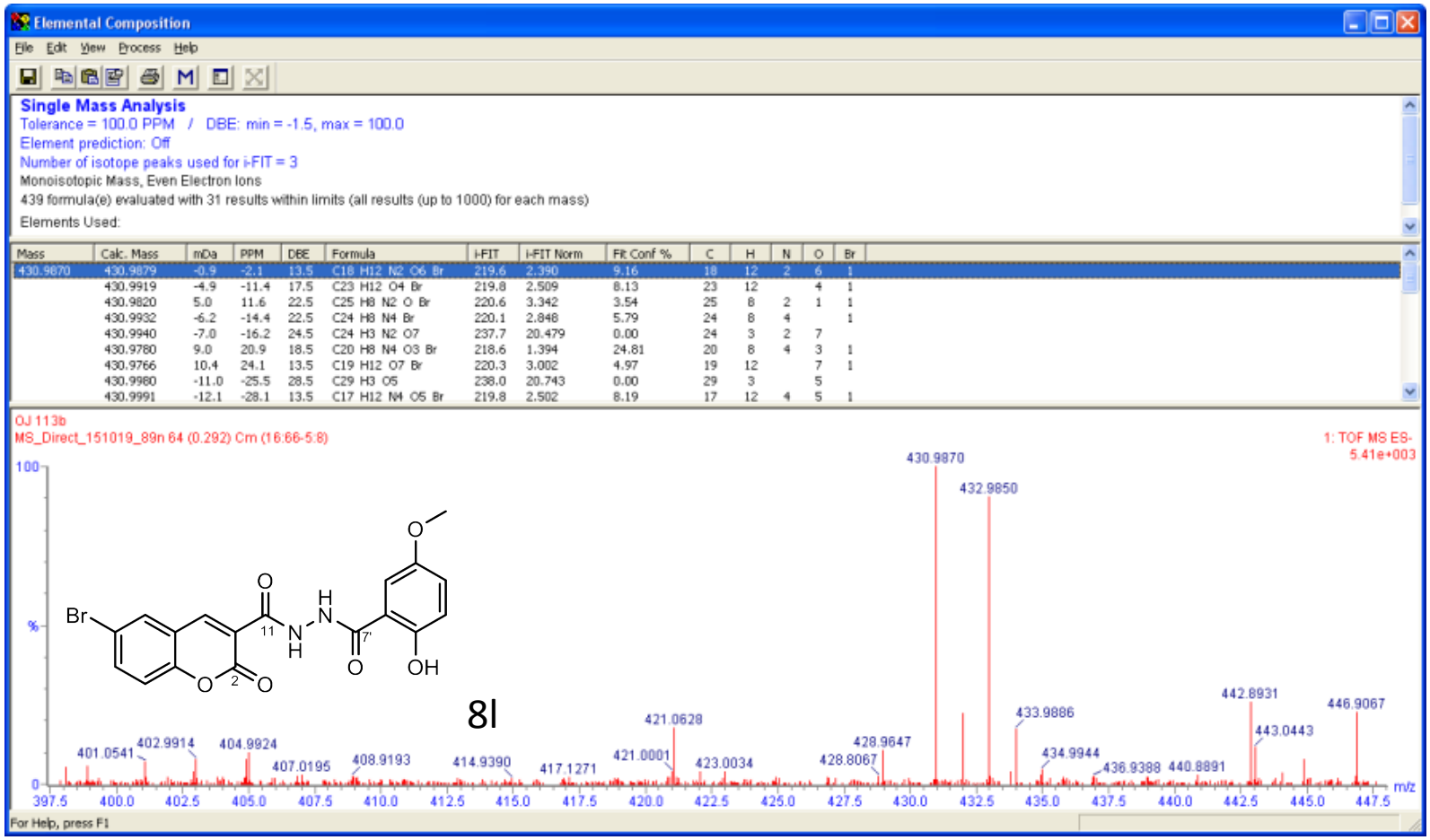

95.8
95
94
93
92
91
90
89
88
87
86
85
84
83
82
81
79.9
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3259.52
2162.19
1777.21
1705.64
1611.41
1475.60
1406.96
1367.01
1246.84
1202.33
1167.19
1030.62
963.06
924.37
877.02
814.69
771.82
751.53
657.96
Br
O
11
N
H
N
H
O
7'
O
OH
O
2
O
8l

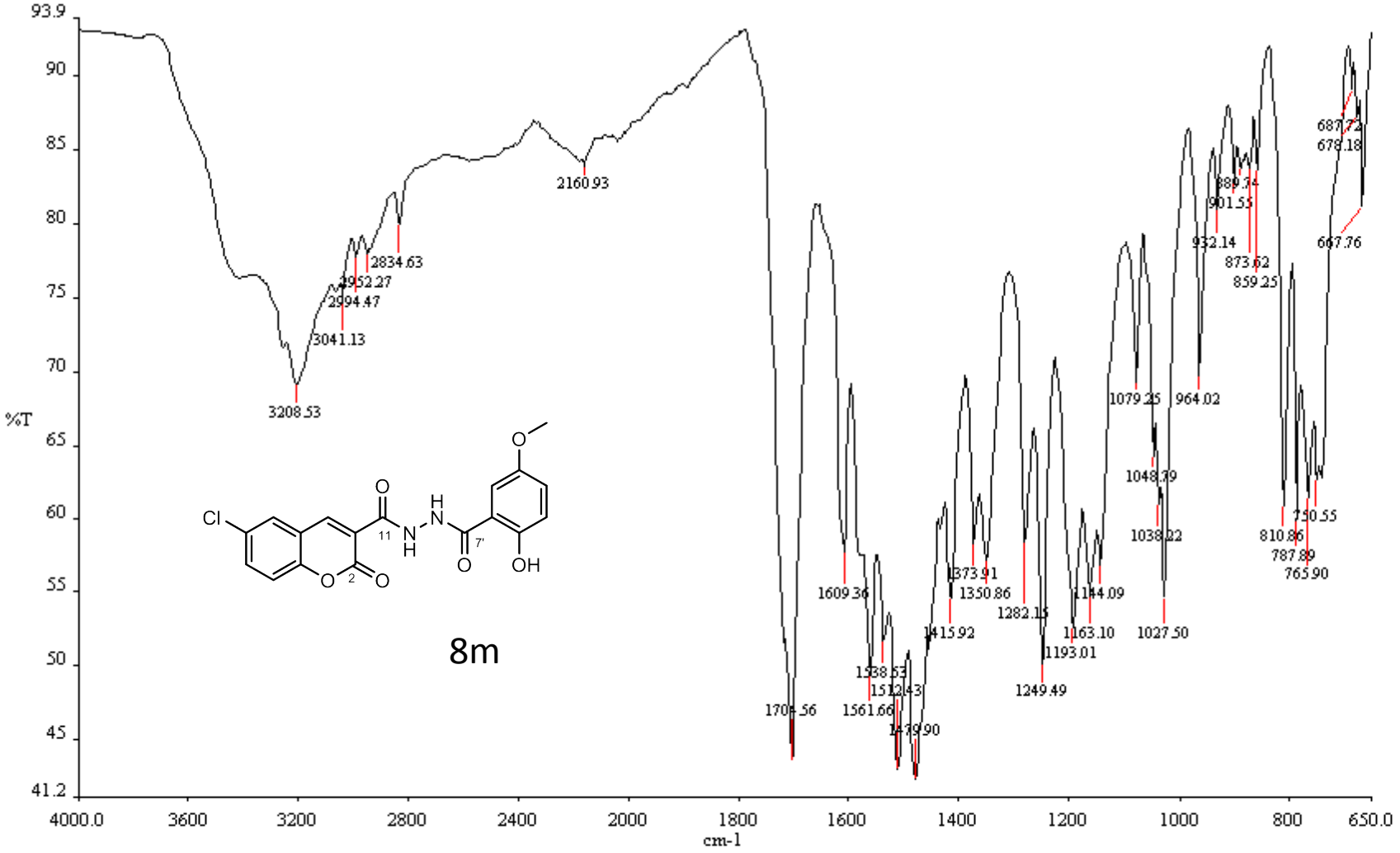
8l


Br
O
11
N
H
N
H
O
7'
O
OH
O
2
O

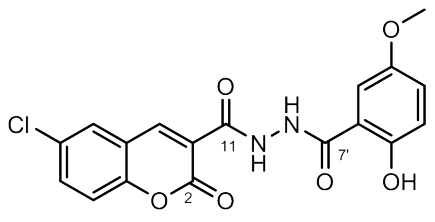
11.87
8.82
8.26
7.85
7.48
7.36
6.74
6.65
3.68
3.49
2.50
0.63
0.92
0.97
1.14
1.30
1.30
1.26
1.22
2.88
f1 (ppm)


Br
O
11
N
H
H
N
7'
O
O
OH
O
2
O


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
439 formula(e) evaluated with 31 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | N | O | Br
430.9870 | 430.9879 | -0.9 | -2.1 | 13.5 | C18 H12 N2 O6 Br | 219.6 | 2.390 | 9.16 | 18 | 12 | 2 | 6 | 1
430.9919 | -4.9 | -11.4 | 17.5 | C23 H12 O4 Br | 219.8 | 2.509 | 8.13 | 23 | 12 | | 4 | 1
430.9820 | 5.0 | 11.6 | 22.5 | C25 H8 N2 O Br | 220.6 | 3.342 | 3.54 | 25 | 8 | 2 | 1 | 1
430.9932 | -6.2 | -14.4 | 22.5 | C24 H8 N4 Br | 220.1 | 2.848 | 5.79 | 24 | 8 | 4 | | 1
430.9940 | -7.0 | -16.2 | 24.5 | C24 H3 N2 O7 | 237.7 | 20.479 | 0.00 | 24 | 3 | 2 | 7 |
430.9780 | 9.0 | 20.9 | 18.5 | C20 H8 N4 O3 Br | 218.6 | 1.394 | 24.81 | 20 | 8 | 4 | 3 | 1
430.9766 | 10.4 | 24.1 | 13.5 | C19 H12 O7 Br | 220.3 | 3.002 | 4.97 | 19 | 12 | | 7 | 1
430.9980 | -11.0 | -25.5 | 28.5 | C29 H3 O5 | 238.0 | 20.743 | 0.00 | 29 | 3 | | 5 |
430.9991 | -12.1 | -28.1 | 13.5 | C17 H12 N4 O5 Br | 219.8 | 2.502 | 8.19 | 17 | 12 | 4 | 5 | 1
OJ 113b
MS_Direct_151019_89n 64 (0.292) Cm (16:66-5:8)
1: TOF MS ES-
5.41e+003
100
%
0
Br
O
O
H
N
11
N
H
7'
O
O
2
O
OH
8l
430.9870
432.9850
442.8931
446.9067
433.9886
443.0443
421.0628
428.9647
434.9944
401.0541
402.9914
404.9824
407.0195
408.9193
414.9390
417.1271
421.0001
423.0034
428.8067
436.9388
440.8891
m/z
397.5
400.0
402.5
405.0
407.5
410.0
412.5
415.0
417.5
420.0
422.5
425.0
427.5
430.0
432.5
435.0
437.5
440.0
442.5
445.0
447.5
For Help, press F1


93.9
90
85
80
75
70
65
60
55
50
45
41.2
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3208.53
3041.13
2994.47
2952.27
2834.63
2160.93
1706.56
1609.36
1561.66
1538.53
1512.43
1479.90
1415.92
1373.91
1350.86
1282.15
1249.49
1193.01
1163.10
1144.09
1079.25
1048.79
1038.22
1027.50
964.02
932.14
901.55
889.34
873.62
859.25
810.86
787.89
765.90
750.55
687.72
678.18
667.76
Cl
O
H
N
N
H
O
O
O
O
OH
11
7'
2
8m

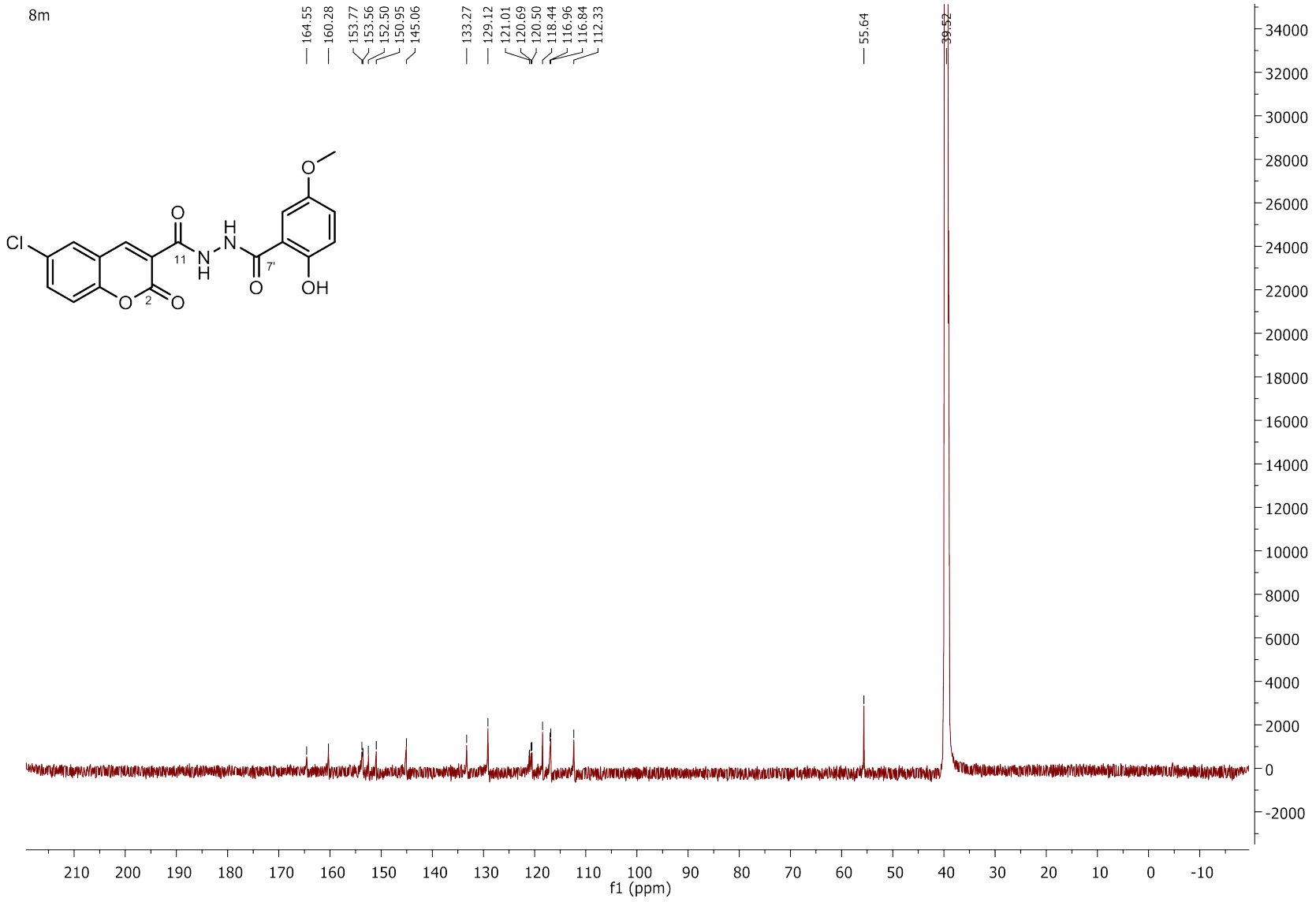
8m



11.91
8.81
8.10
7.73
7.53
7.37
6.73
6.64
3.66
2.50

2.30
2.11
2.16
1.78
1.76
1.67
1.74
1.57
3.60

f1 (ppm)


8m
164.55
160.28
153.77
153.56
152.50
150.95
145.06
133.27
129.12
121.01
120.69
120.50
118.44
116.96
116.84
112.33
55.64
39.52
Cl
O
H
N
N
H
O
11
7'
O
OH
O
2
O
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
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)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1128 formula(e) evaluated with 122 results within limits (all results (up to 1000) for each mass)

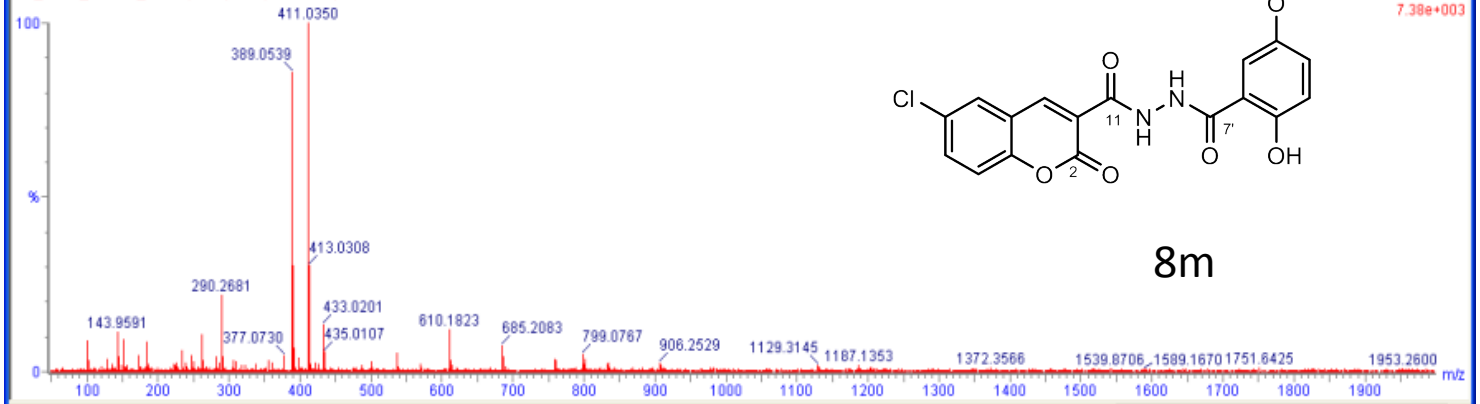
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	Cl
389.0539	389.0540	-0.1	-0.3	12.5	C18 H14 N2 O6 Cl	39.3	4.748	0.87	18	14	2	6		1
	389.0538	0.1	0.3	18.5	C22 H10 N2 O4 Na	55.7	21.170	0.00	22	10	2	4	1	
	389.0535	0.4	1.0	4.5	C15 H20 O6 Na Cl2	47.2	12.621	0.00	15	20		6	1	2
	389.0548	-0.9	-2.3	9.5	C16 H16 N4 O2 Na Cl2	46.1	11.572	0.00	16	16	4	2	1	2
	389.0522	1.7	4.4	17.5	C19 H9 N4 O6	55.4	20.889	0.00	19	9	4	6		
	389.0557	-1.8	-4.6	13.5	C21 H15 O4 Na Cl	42.4	7.857	0.04	21	15		4	1	1
	389.0559	-2.0	-5.1	7.5	C17 H19 O6 Cl2	47.0	12.499	0.00	17	19		6		2
	389.0562	-2.3	-5.9	21.5	C24 H9 N2 O4	55.8	21.237	0.00	24	9	2	4		
	389.0516	2.3	5.9	9.5	C16 H15 N2 O6 Na Cl	35.9	1.375	25.29	16	15	2	6	1	1

OJ 113c

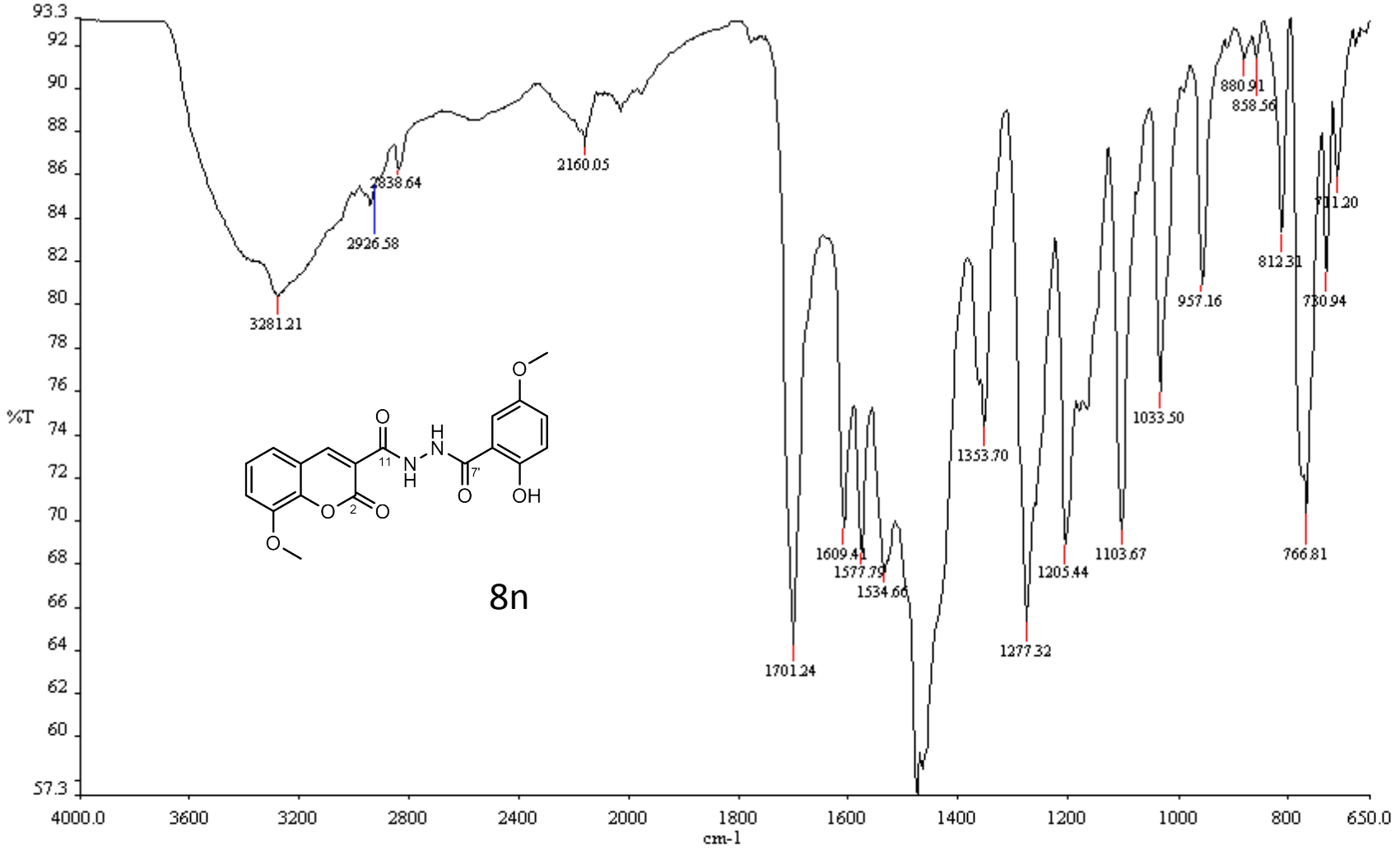
MS_Direct_151019_90 39 (0.180) Cm (37:39-8:12)

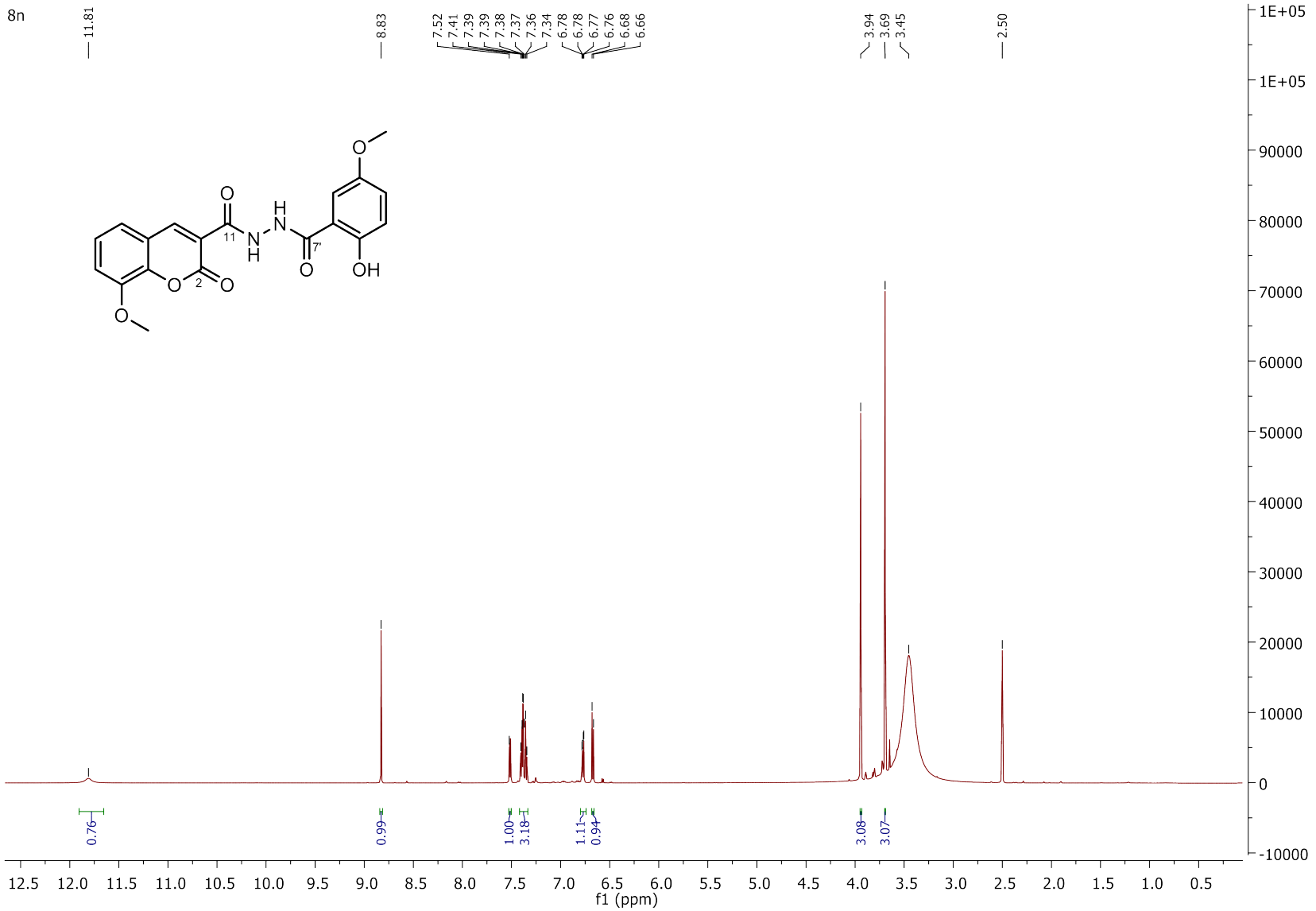
1: TOF MS ES+
7.38e+003

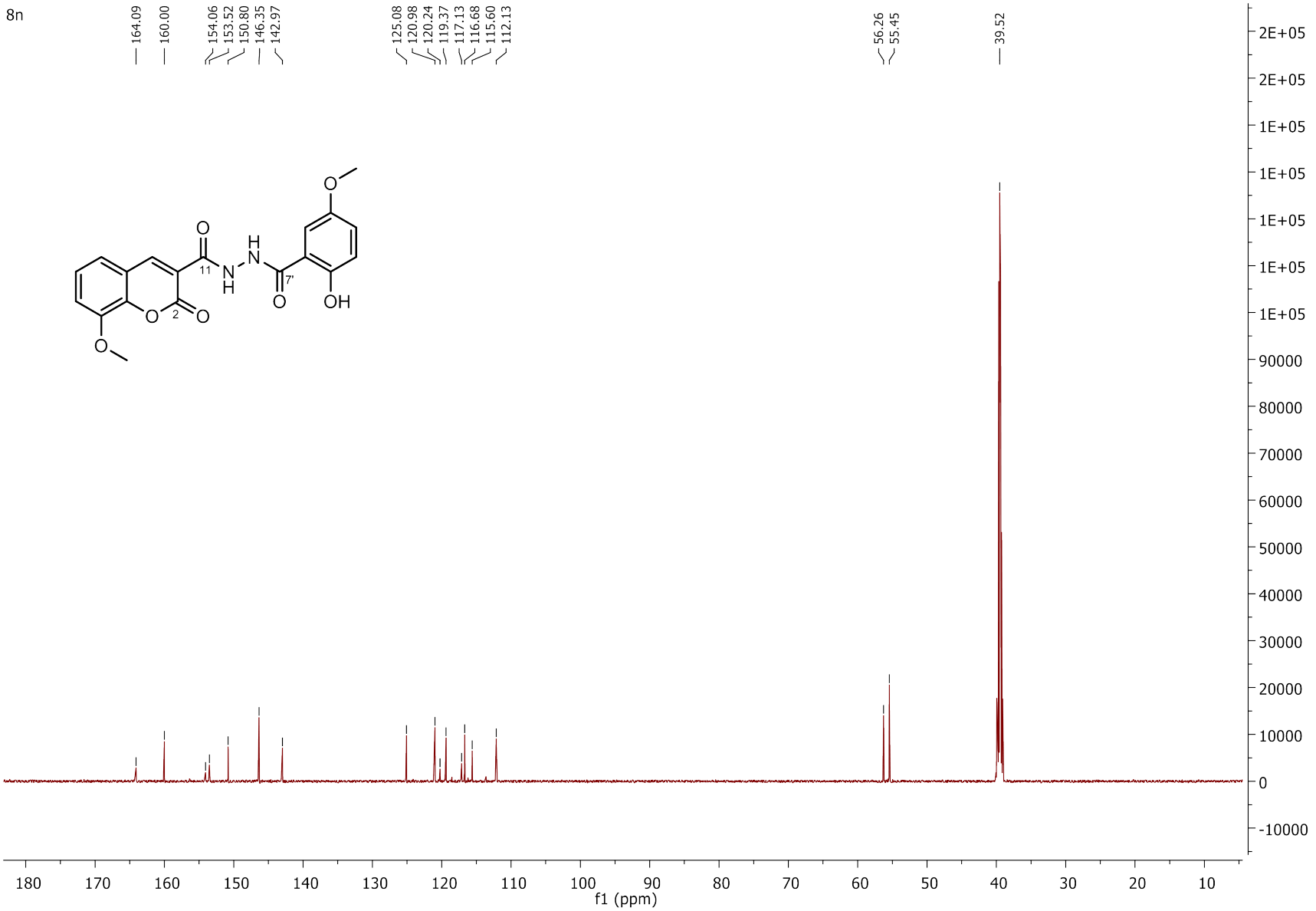


8m

For Help, press F1


93.3
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
57.3
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3281.21
2926.58
2838.64
2160.05
1701.24
1609.41
1577.79
1534.66
1353.70
1277.32
1205.44
1103.67
1033.50
957.16
880.91
858.56
812.31
766.81
730.94
711.20
O
O
O
O
O
O
H
N
N
H
OH
11
7'
2
8n


8n
11.81
8.83
7.52
7.41
7.39
7.39
7.38
7.37
7.36
7.34
6.78
6.78
6.77
6.76
6.68
6.66
3.94
3.69
3.45
2.50
O
O
H
N
N
H
O
11
7'
O
2
O
O
OH
O
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
0.76
0.99
1.00
3.18
1.11
0.94
3.08
3.07
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
f1 (ppm)


8n
164.09
160.00
154.06
153.52
150.80
146.35
142.97
125.08
120.98
120.24
119.37
117.13
116.68
115.60
112.13
56.26
55.45
39.52
O
O
H
N
N
H
O
11
7'
O
2
O
O
OH
2E+05
2E+05
1E+05
1E+05
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1113 formula(e) evaluated with 115 results within limits (all results (up to 1000) for each mass)

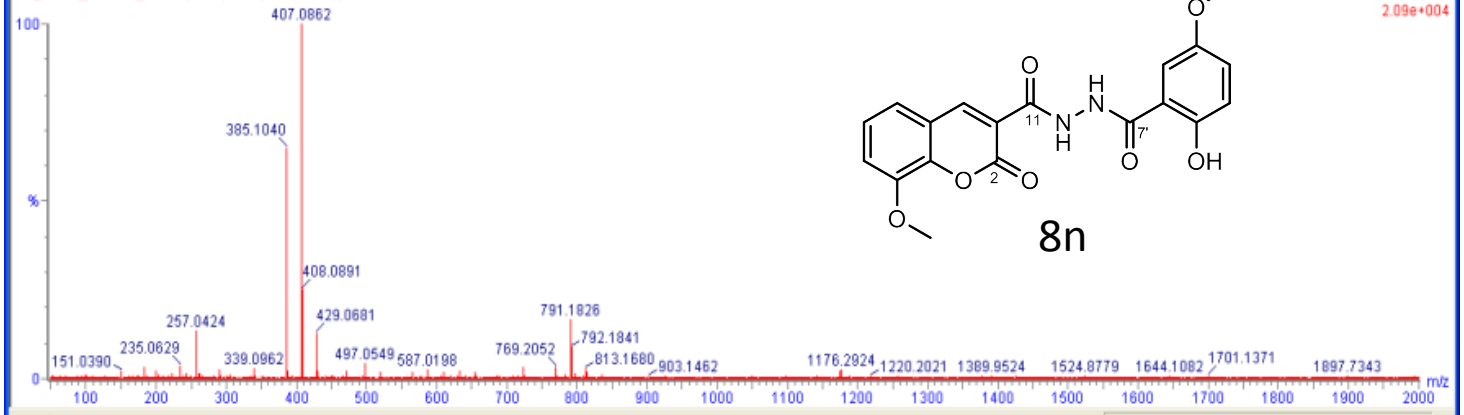
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	Cl
385.1040	385.1043	-0.3	-0.8	9.5	C17 H19 N4 O3 Na Cl	76.6	22.470	0.00	17	19	4	3	1	1
	385.1036	0.4	1.0	12.5	C19 H17 N2 O7	60.6	6.524	0.15	19	17	2	7		
	385.1046	-0.6	-1.6	3.5	C13 H23 N4 O5 Cl2	77.8	23.628	0.00	13	23	4	5		2
	385.1030	1.0	2.6	4.5	C16 H23 O7 Na Cl	76.8	22.684	0.00	16	23		7	1	1
	385.1052	-1.2	-3.1	13.5	C22 H18 O5 Na	63.9	9.740	0.01	22	18		5	1	
	385.1054	-1.4	-3.6	7.5	C18 H22 O7 Cl	76.7	22.610	0.00	18	22		7		1
	385.1021	1.9	4.9	0.5	C11 H24 N4 O5 Na Cl2	77.7	23.623	0.00	11	24	4	5	1	2
	385.1062	-2.2	-5.7	4.5	C16 H24 N2 O3 Na Cl2	77.8	23.709	0.00	16	24	2	3	1	2
	385.1017	2.3	6.0	25.5	C31 H13	68.5	14.340	0.00	31	13				

OJ 113d

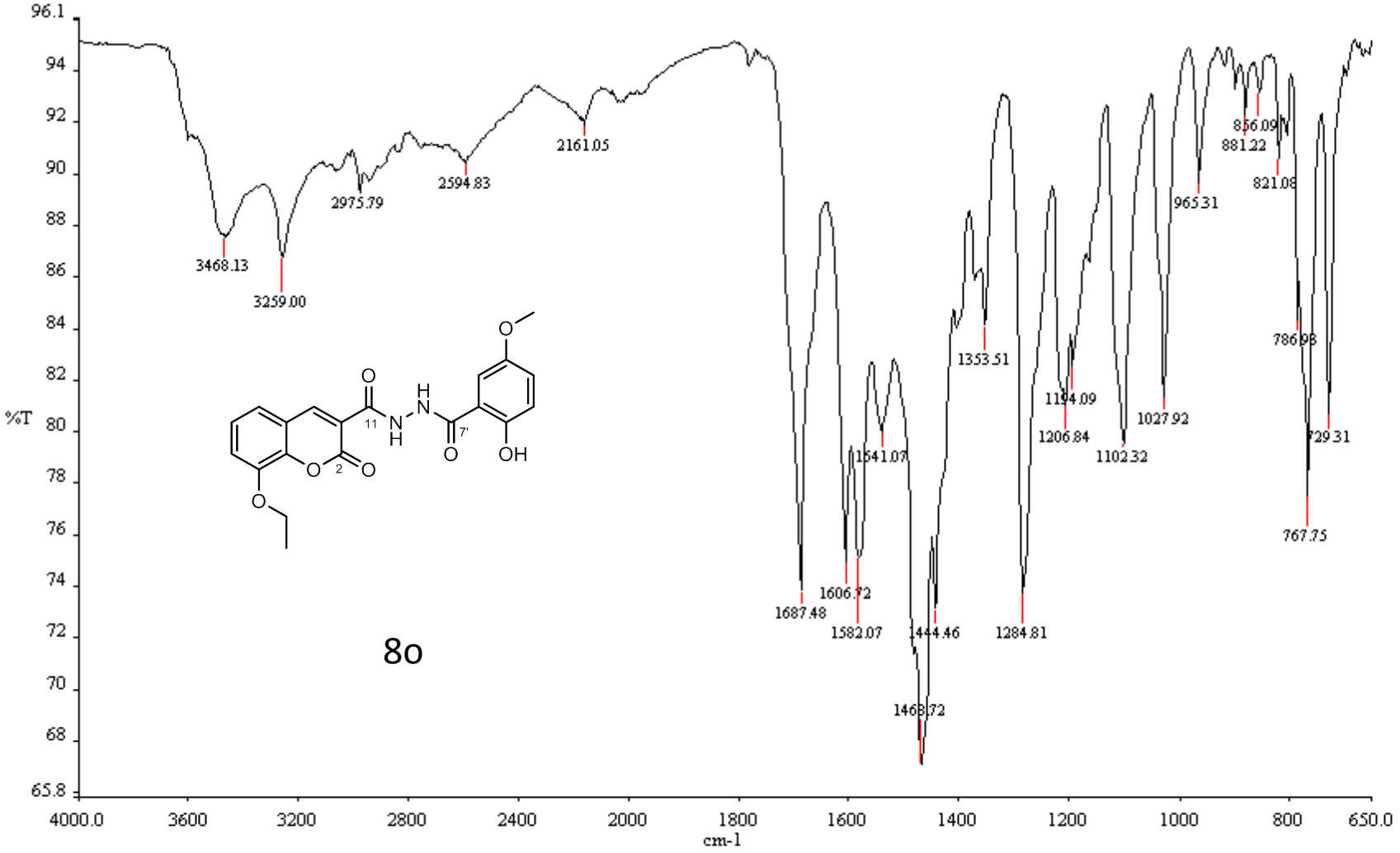
MS_Direct_151019_91 54 (0.242) Cm (53:56-12:15)

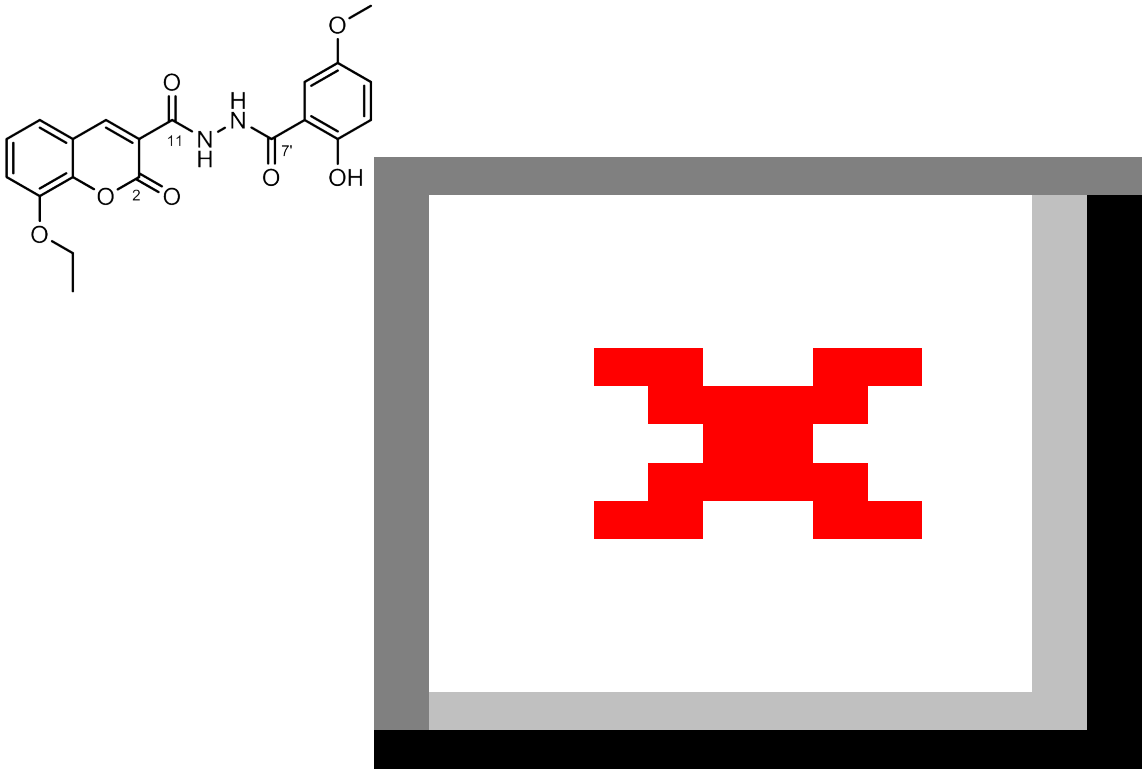
1: TOF MS ES+
2.09e+004



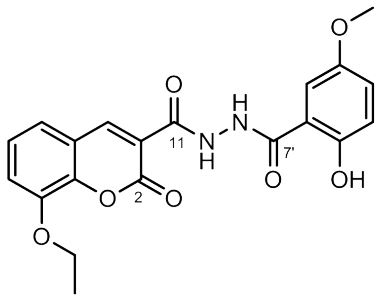
8n

For Help, press F1

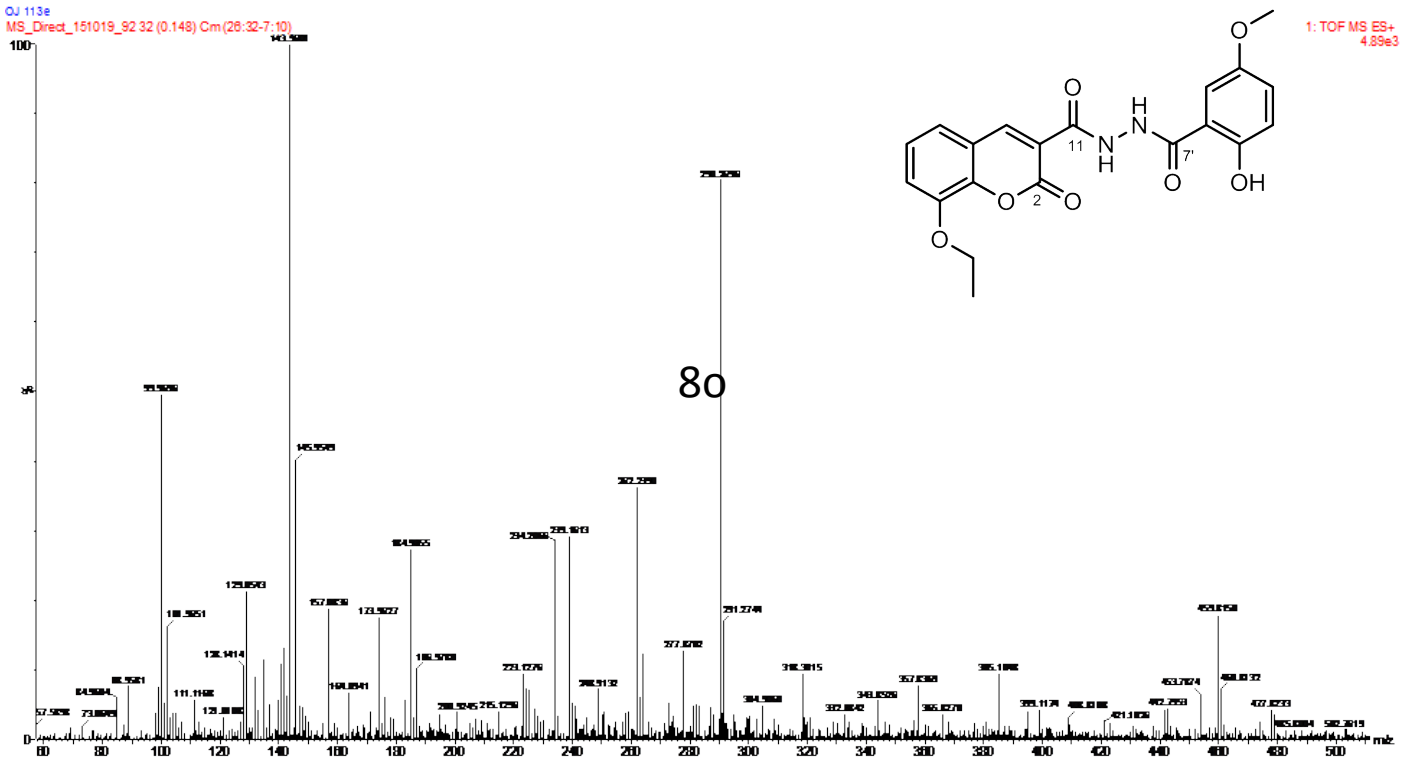

96.1
94
92
90
88
86
84
82
80
78
76
74
72
70
68
65.8
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3468.13
3259.00
2975.79
2594.83
2161.05
1687.48
1606.72
1582.07
1541.07
1468.72
1444.46
1353.51
1284.81
1206.84
1184.09
1102.32
1027.92
965.31
881.22
856.09
821.08
786.98
767.75
729.31
O
O
N
H
N
H
O
O
O
O
O
OH
11
7'
2
8o

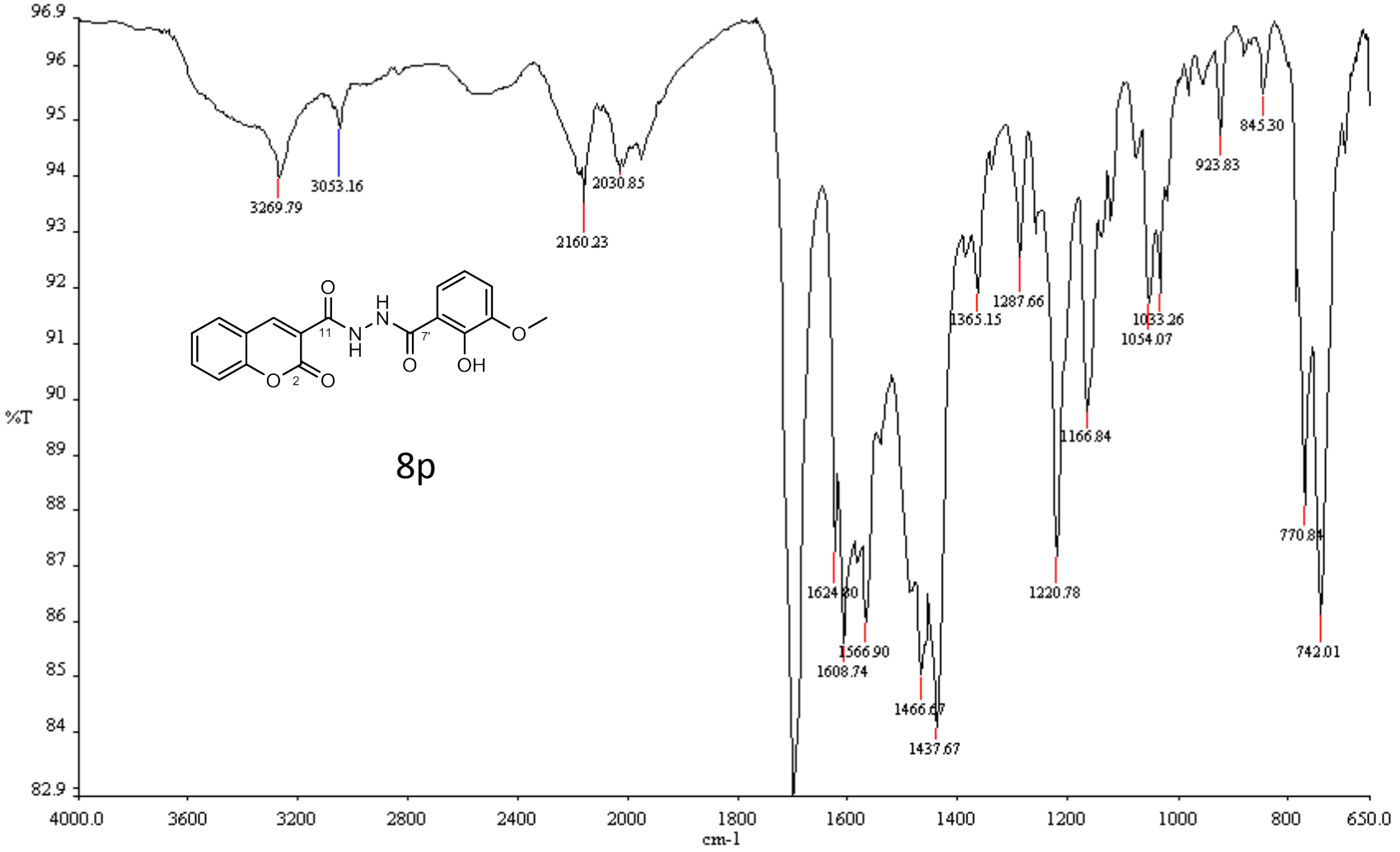

O
H
N
N
H
11
7'
O
O
O
2
O
O
OH

8o

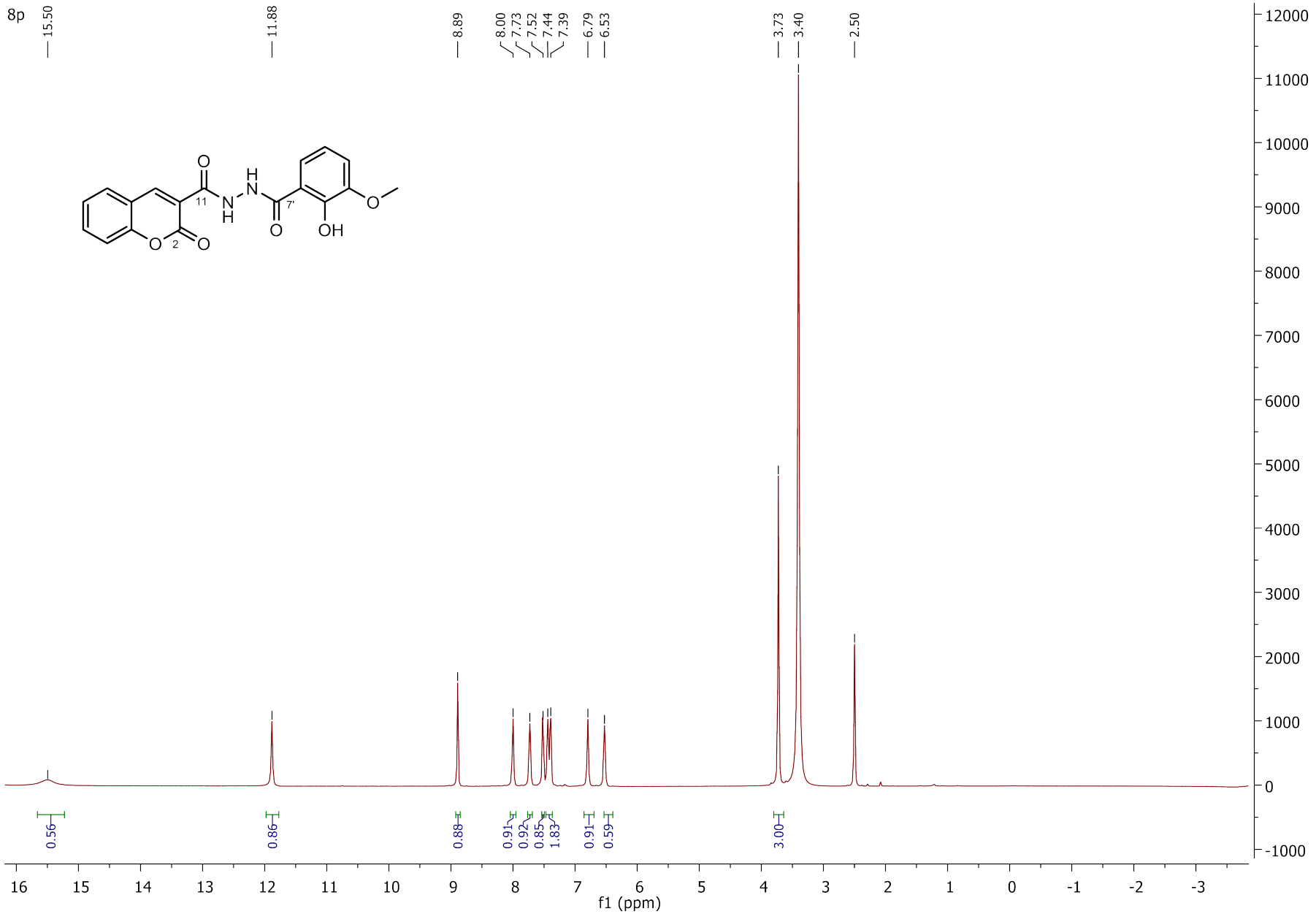

O
H
N
O
11
N
H
7'
O
OH
O
2
O
O

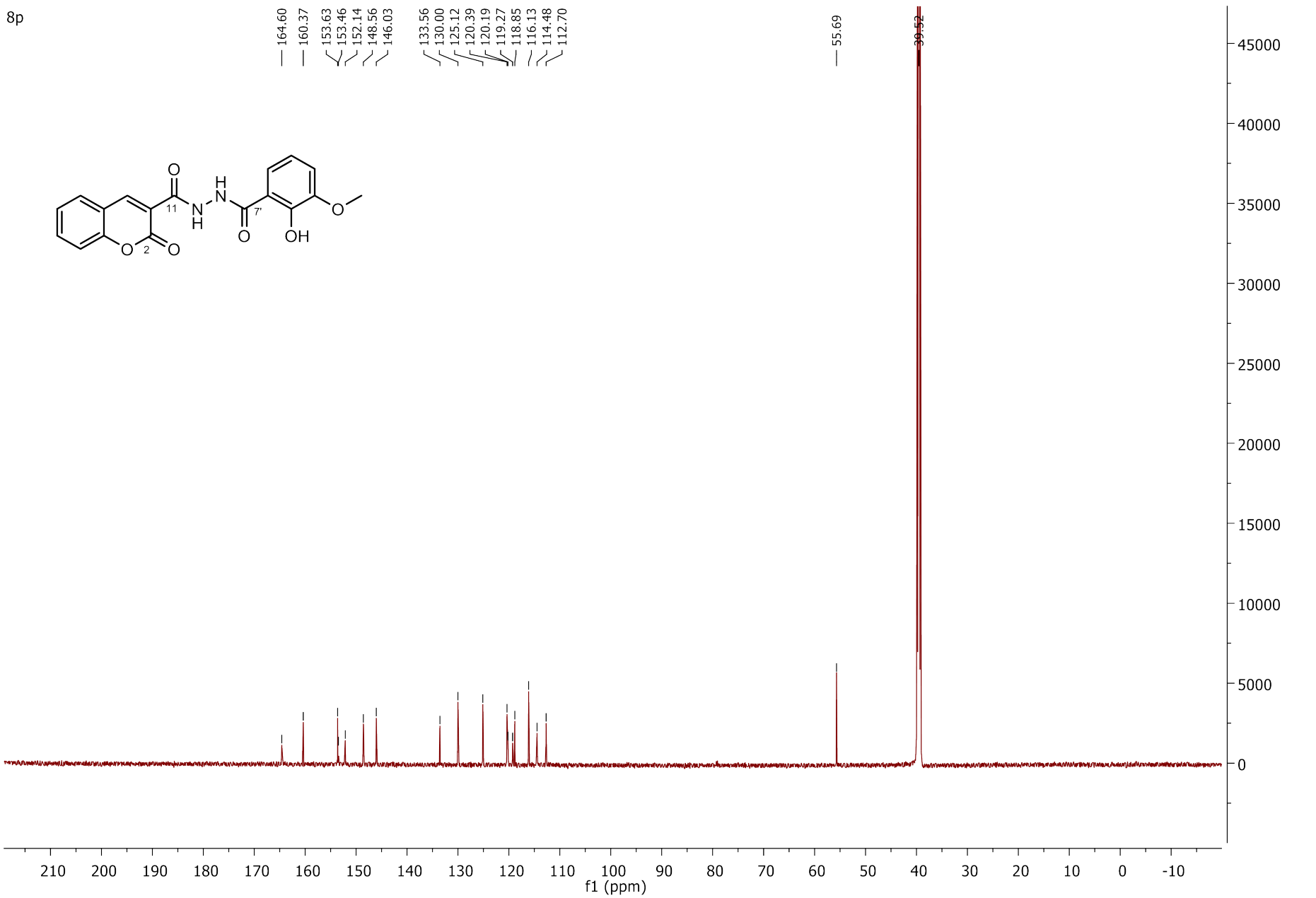
164.09
160.08
153.91
153.56
150.74
146.31
145.57
143.01
125.07
120.89
120.47
119.46
119.39
116.94
116.61
116.38
112.13
64.61
64.43
55.44
55.30
39.52
14.67
2E+05
2E+05
2E+05
2E+05
2E+05
2E+05
2E+05
1E+05
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OJ 113e
MS_Direct_151019_92 32 (0.148) Cm (26:32-7:10)
1: TOF MS ES+
4.89e3
8o
m/z


96.9
96
95
94
93
92
91
90
89
88
87
86
85
84
82.9
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3269.79
3053.16
2160.23
2030.85
1624.80
1608.74
1566.90
1466.67
1437.67
1365.15
1287.66
1220.78
1166.84
1054.07
1033.26
923.83
845.30
770.84
742.01
O
H
N
N
H
O
11
7'
O
2
O
OH
O

8p


8p
15.50
11.88
8.89
8.00
7.73
7.52
7.44
7.39
6.79
6.53
3.73
3.40
2.50
O
H
N
N
H
O
11
7'
O
OH
O
2
O
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
0.56
0.86
0.88
0.91
0.92
0.85
1.83
0.91
0.59
3.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


8p
164.60
160.37
153.63
153.46
152.14
148.56
146.03
133.56
130.00
125.12
120.39
120.19
119.27
118.85
116.13
114.48
112.70
55.69
39.52
O
H
N
N
H
O
11
7'
O
OH
O
O
2
45000
40000
35000
30000
25000
20000
15000
10000
5000
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)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

390 formula(e) evaluated with 18 results within limits (all results (up to 1000) for each mass)

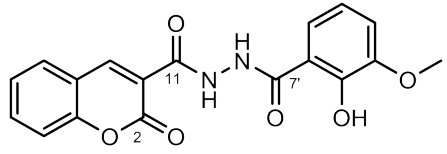
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
355.0931	355.0930	0.1	0.3	12.5	C18 H15 N2 O6	208.1	0.035	96.52	18	15	2	6
	355.0949	-1.8	-5.1	-0.5	C6 H19 N4 O13	221.0	12.975	0.00	6	19	4	13
	355.0970	-3.9	-11.0	16.5	C23 H15 O4	221.5	13.417	0.00	23	15		4
	355.0890	4.1	11.5	8.5	C13 H15 N4 O8	217.6	9.536	0.01	13	15	4	8
	355.0984	-5.3	-14.9	21.5	C24 H11 N4	222.7	14.647	0.00	24	11	4	
	355.0877	5.4	15.2	3.5	C12 H19 O12	220.1	12.058	0.00	12	19		12
	355.0989	-5.8	-16.3	3.5	C11 H19 N2 O11	219.4	11.408	0.00	11	19	2	11
	355.0871	6.0	16.9	21.5	C25 H11 N2 O	223.4	15.354	0.00	25	11	2	1
	355.0836	9.5	26.8	-0.5	C7 H19 N2 O14	221.8	13.767	0.00	7	19	2	14

OJ 151a

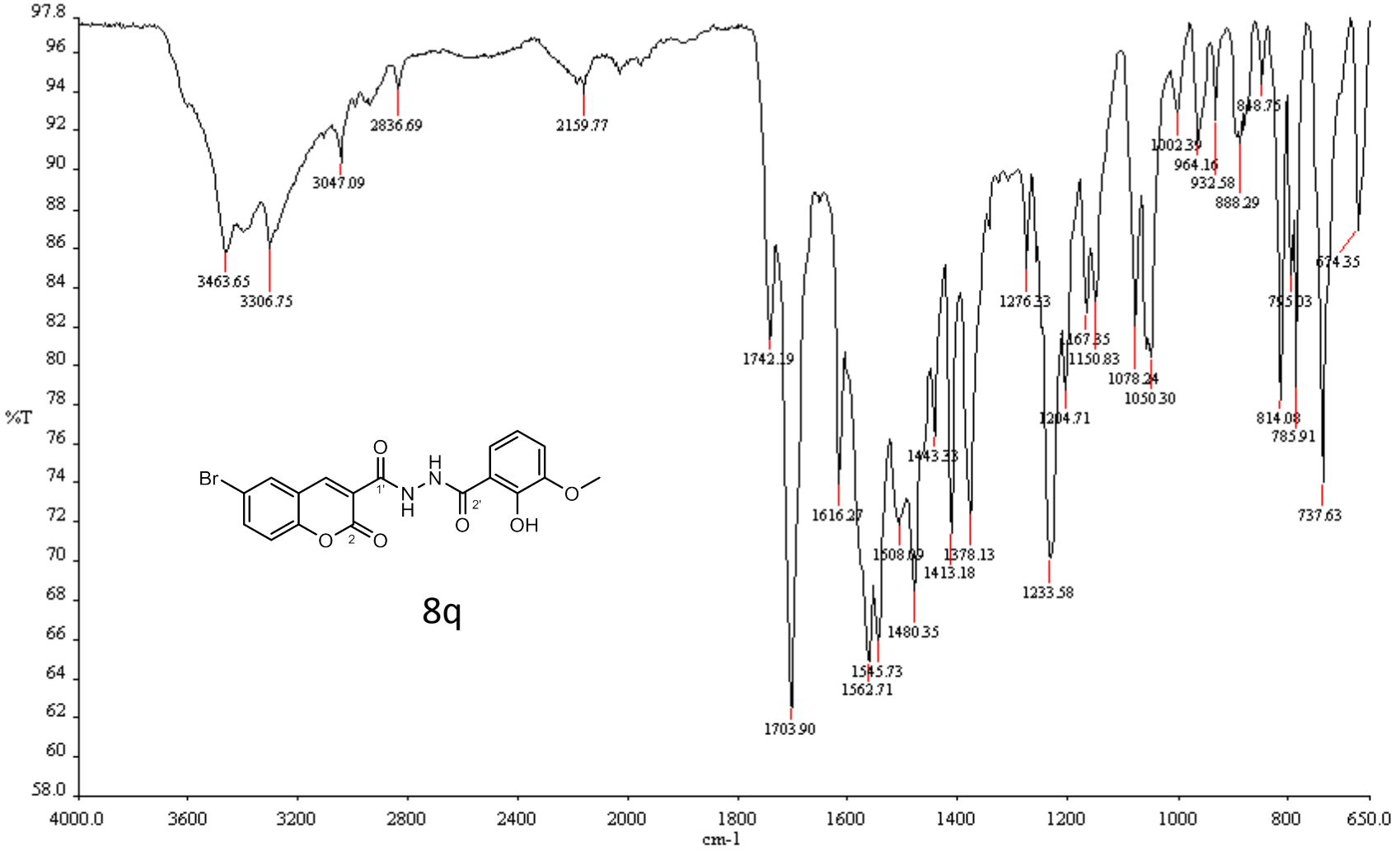
MS_Direct_160325_6 22 (0.137) Cm (13:27-(4:8+50:60))

1: TOF MS ES+
3.63e+005

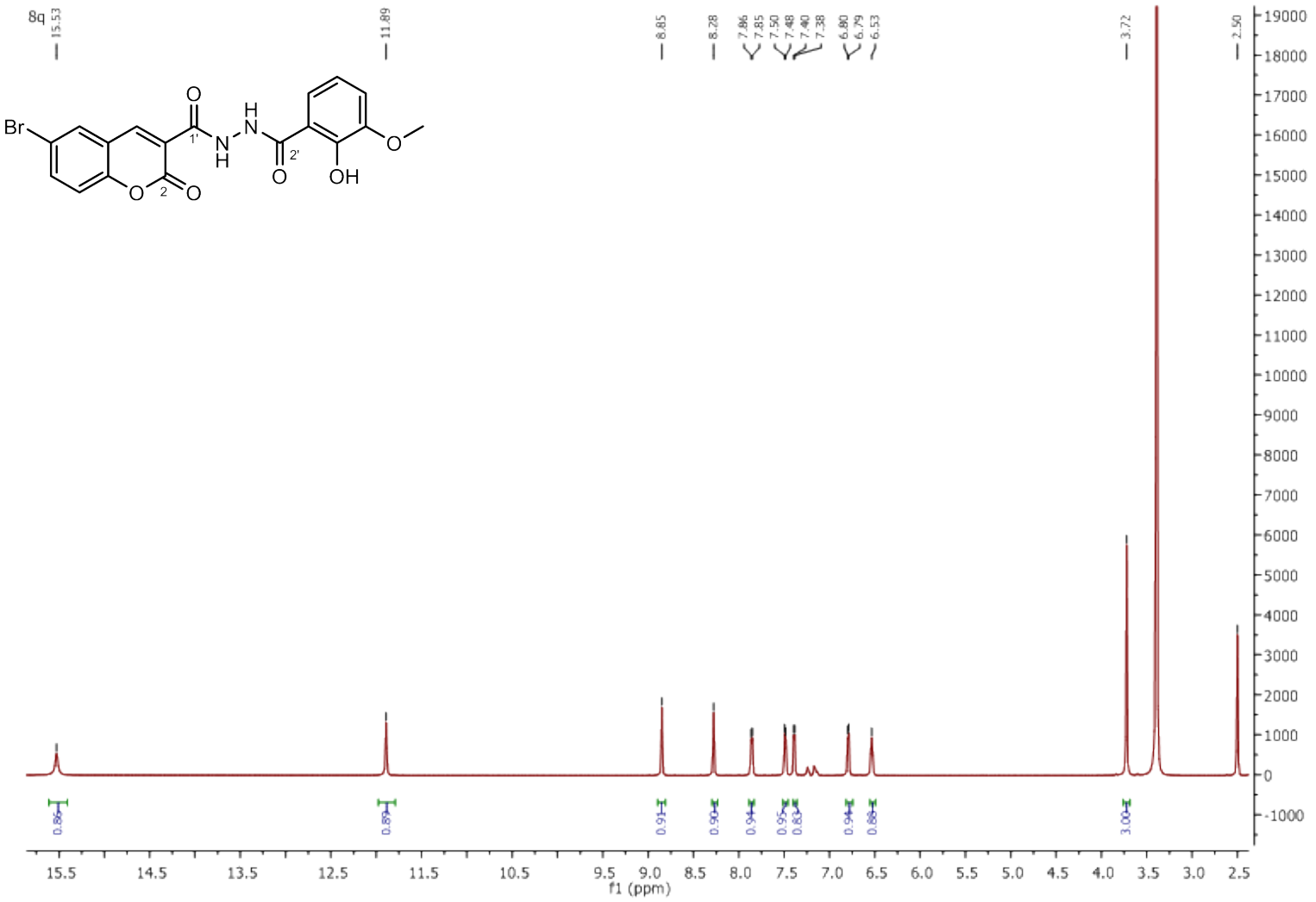


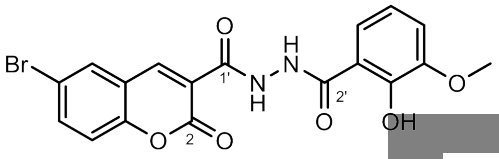
8p

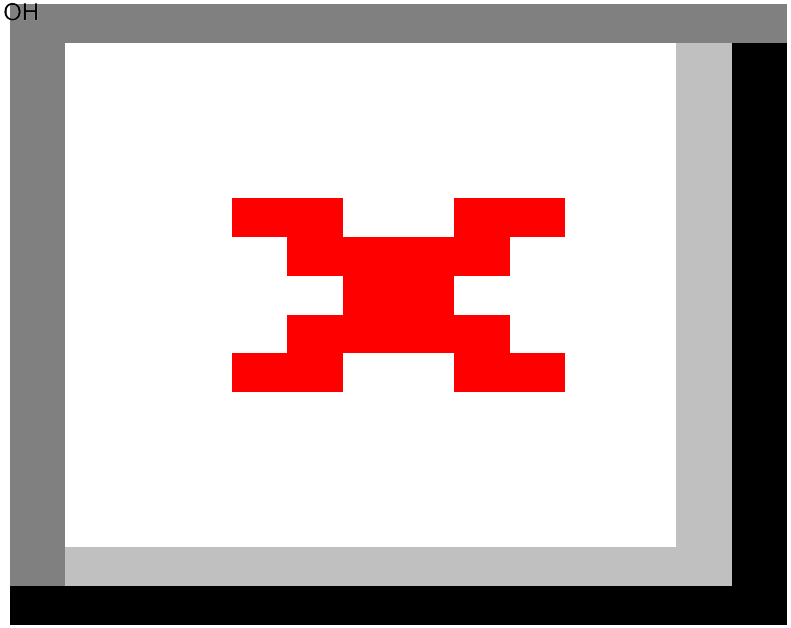
For Help, press F1

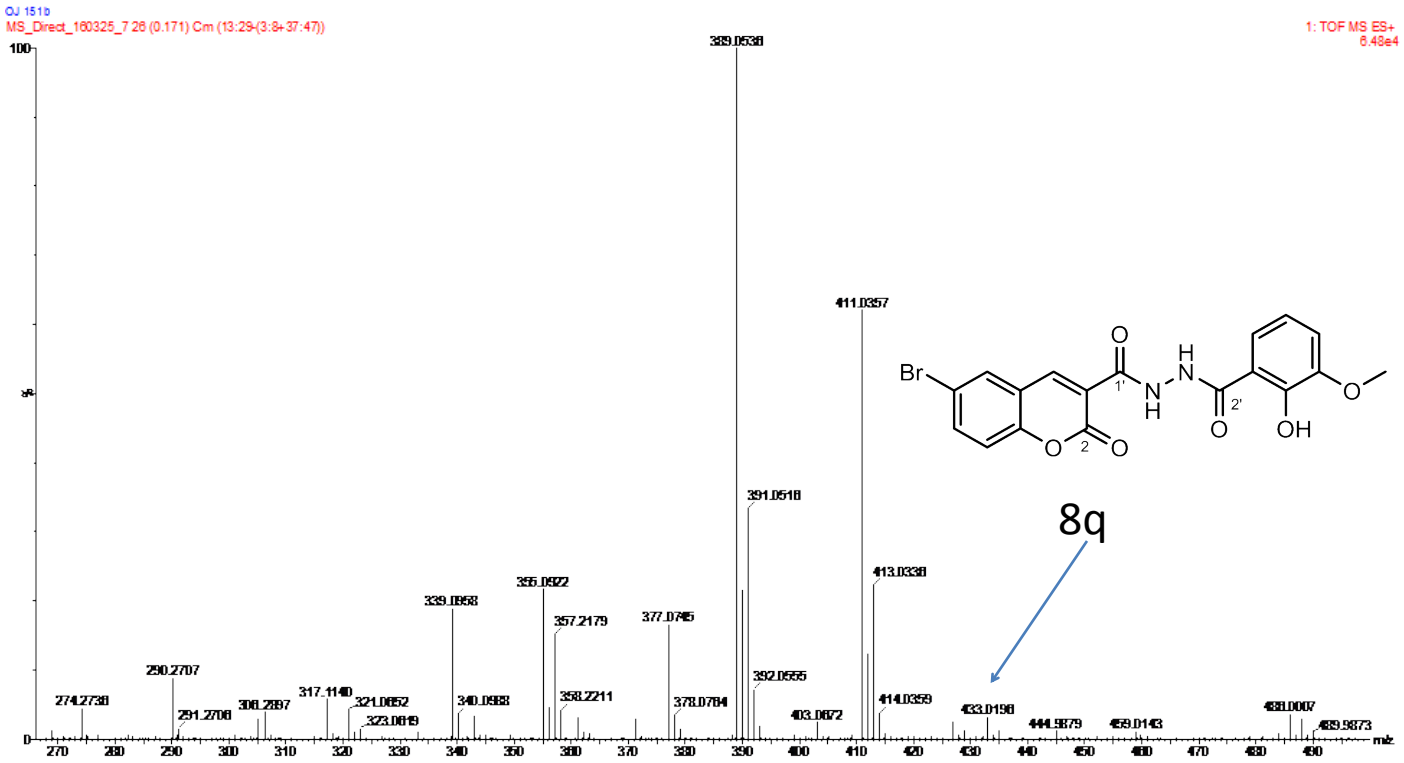

97.8
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58.0
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3463.65
3306.75
3047.09
2836.69
2159.77
1742.19
1703.90
1616.27
1562.71
1545.73
1508.09
1480.35
1443.33
1413.18
1378.13
1276.33
1233.58
1204.71
1167.35
1150.83
1078.24
1050.30
1002.39
964.16
932.58
888.29
848.75
814.08
795.03
785.91
737.63
674.35
Br
O
N
H
O
O
O
2
1'
2'
OH

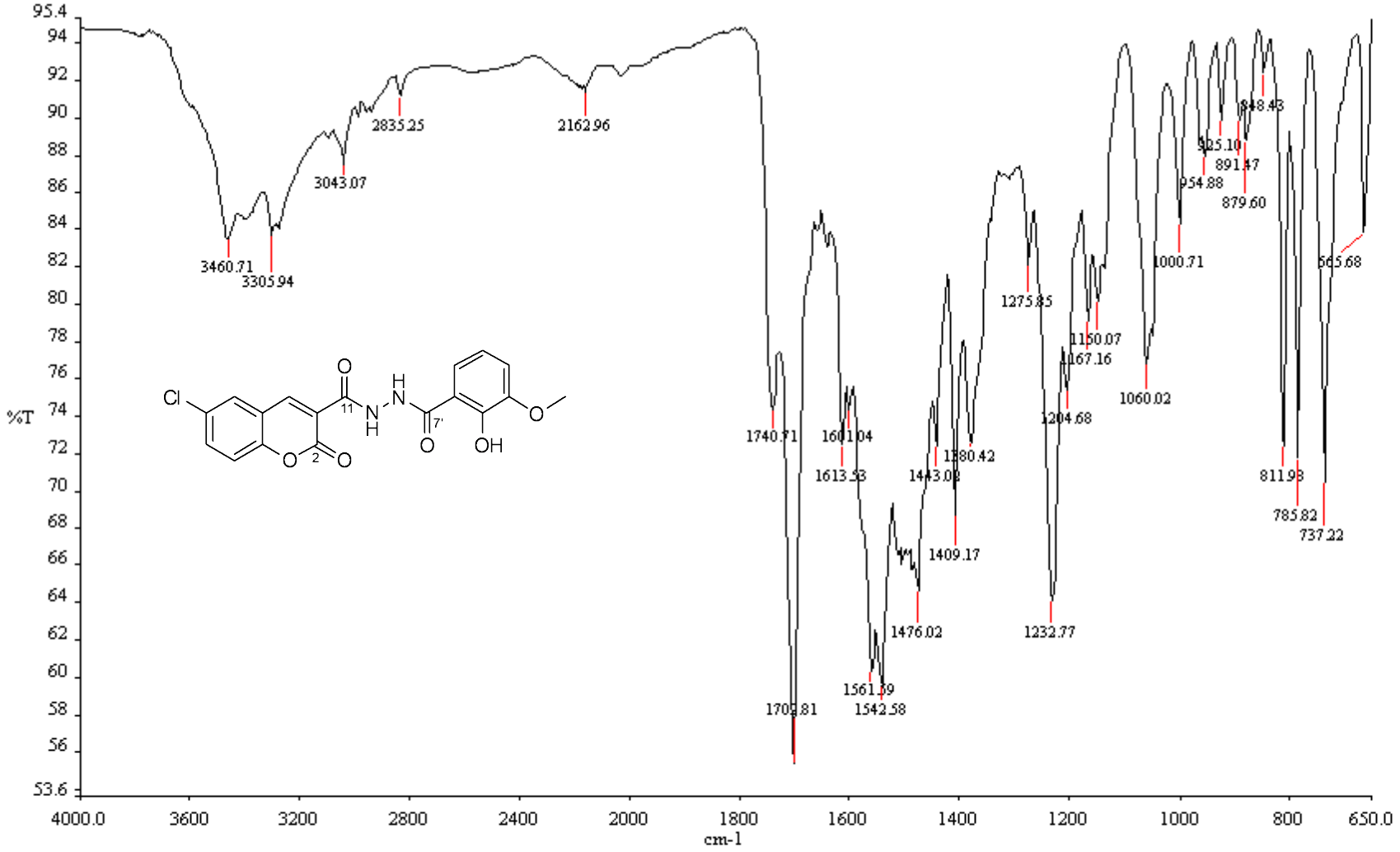
8q

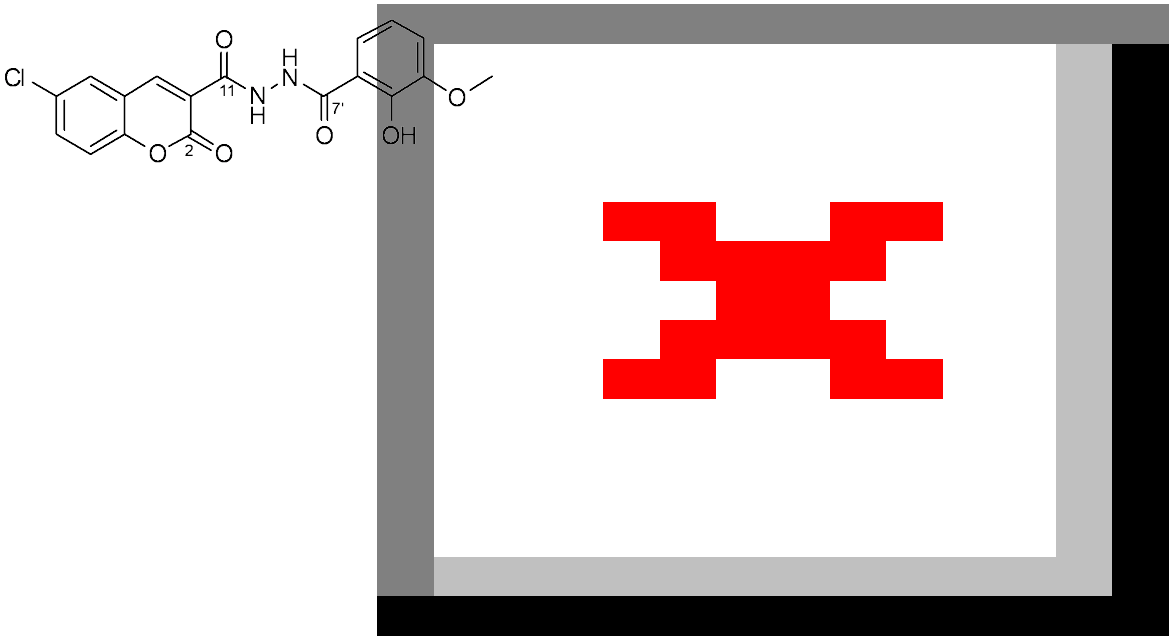

8q
15.53
11.89
8.85
8.28
7.86
7.85
7.50
7.48
7.40
7.38
6.80
6.79
6.53
3.72
2.50
Br
O
N
H
N
H
O
O
O
O
OH
1'
2'
2
f1 (ppm)


Br
O
1'
N
H
H
N
O
2'
O
OH
O
O
2
O




OJ 151b
MS_Direct_160325_7 26 (0.171) Cm (13:29-(3:8+37:47))
1: TOF MS ES+
6.48e4
100
%
0
389.0536
411.0357
391.0518
413.0338
355.0922
339.0958
357.2179
377.0745
290.2707
392.0555
414.0359
403.0672
433.0198
444.9879
459.0143
488.0007
489.9873
274.2738
291.2706
306.2697
317.1140
321.0652
323.0619
340.0988
358.2211
378.0784
270
280
290
300
310
320
330
340
350
360
370
380
390
400
410
420
430
440
450
460
470
480
490
m/z
Br
O
H
N
N
H
O
1'
2'
O
OH
O
2
O
8q


95.4
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
56
53.6
%T
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1
3460.71
3305.94
3043.07
2835.25
2162.96
1740.71
1709.81
1661.04
1613.53
1561.39
1542.58
1476.02
1443.08
1409.17
1380.42
1275.85
1232.77
1204.68
1167.16
1150.07
1060.02
1000.71
954.88
925.10
891.47
879.60
848.43
811.93
785.82
737.22
665.68
Cl
O
N
H
O
O
O
11
2
7'
OH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N
H
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N
7'
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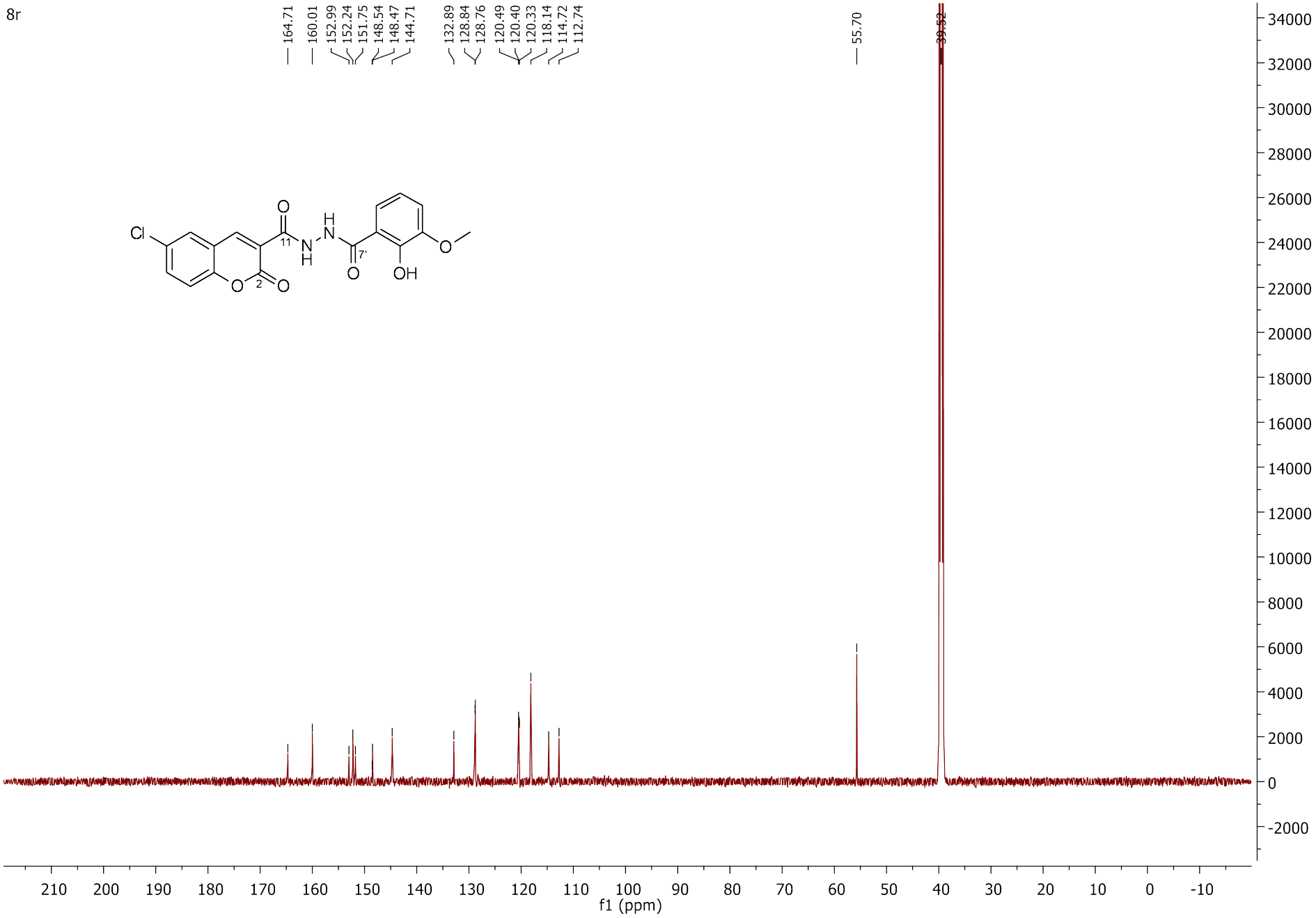
O
2
O


8r
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152.24
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120.49
120.40
120.33
118.14
114.72
112.74
55.70
39.52
Cl
O
11
N
H
N
H
7'
O
O
OH
O
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O
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32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
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200
190
180
170
160
150
140
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100
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80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1372 formula(e) evaluated with 71 results within limits (all results (up to 1000) for each mass)

Elements Used:

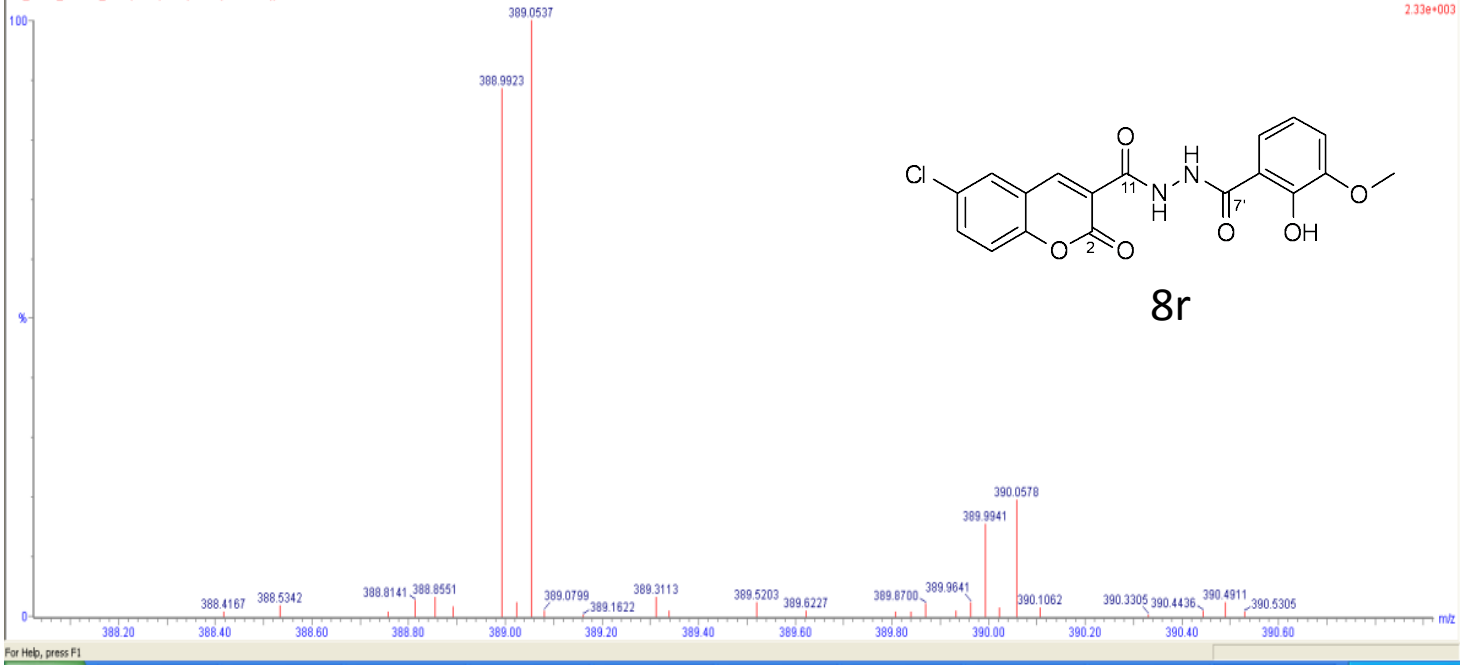
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Cl
	389.0540	-0.3	-0.8	12.5	C18 H14 N2 O6 Cl	144.5	4.929	0.72	18	14	2	6	1
	389.0527	1.0	2.6	-0.5	C6 H17 N2 O17	142.6	2.997	4.99	6	17	2	17	
	389.0550	-1.3	-3.3	3.5	C12 H20 N4 O4 Cl3	145.8	6.210	0.20	12	20	4	4	3
	389.0522	1.5	3.9	17.5	C19 H9 N4 O6	142.2	2.601	7.42	19	9	4	6	
	389.0518	1.9	4.9	3.5	C12 H19 N2 O8 Cl2	145.2	5.549	0.39	12	19	2	8	2
	389.0559	-2.2	-5.7	-0.5	C6 H18 N4 O13 Cl	145.8	6.170	0.21	6	18	4	13	1
	389.0559	-2.2	-5.7	7.5	C17 H19 O6 Cl2	144.8	5.148	0.58	17	19		6	2
	389.0562	-2.5	-6.4	21.5	C24 H9 N2 O4	142.2	2.588	7.52	24	9	2	4	
	389.0509	2.8	7.2	12.5	C18 H13 O10	141.9	2.300	10.02	18	13		10	

OJ 151c

MS_Direct_160325_8 25 (0.168) Cm (13:28-(4:9+37:45))

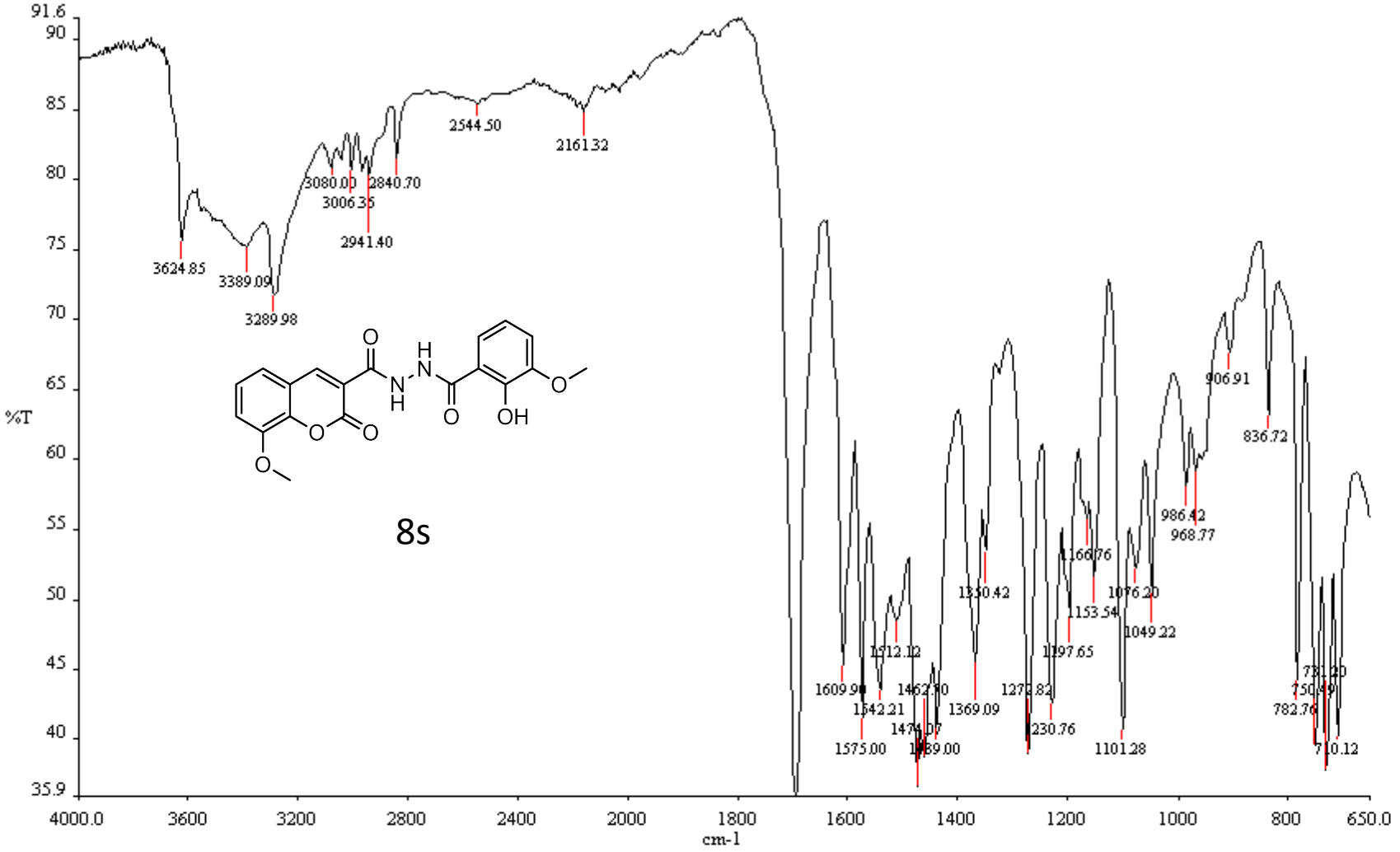
1: TOF MS ES+

2.33e+003



8r

For Help, press F1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60
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50
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40
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2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
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3389.09
3289.98
3080.00
3006.35
2941.40
2840.70
2544.50
2161.32
1609.90
1575.00
1542.21
1512.12
1474.07
1462.80
1439.00
1369.09
1350.42
1297.65
1272.82
1230.76
1166.76
1153.54
1101.28
1076.20
1049.22
986.42
968.77
906.91
836.72
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710.12
O
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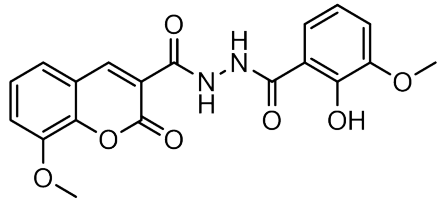
N
N
O
O
O
O
OH
O

8s

8s



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3.72
3.42
2.50

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0.98
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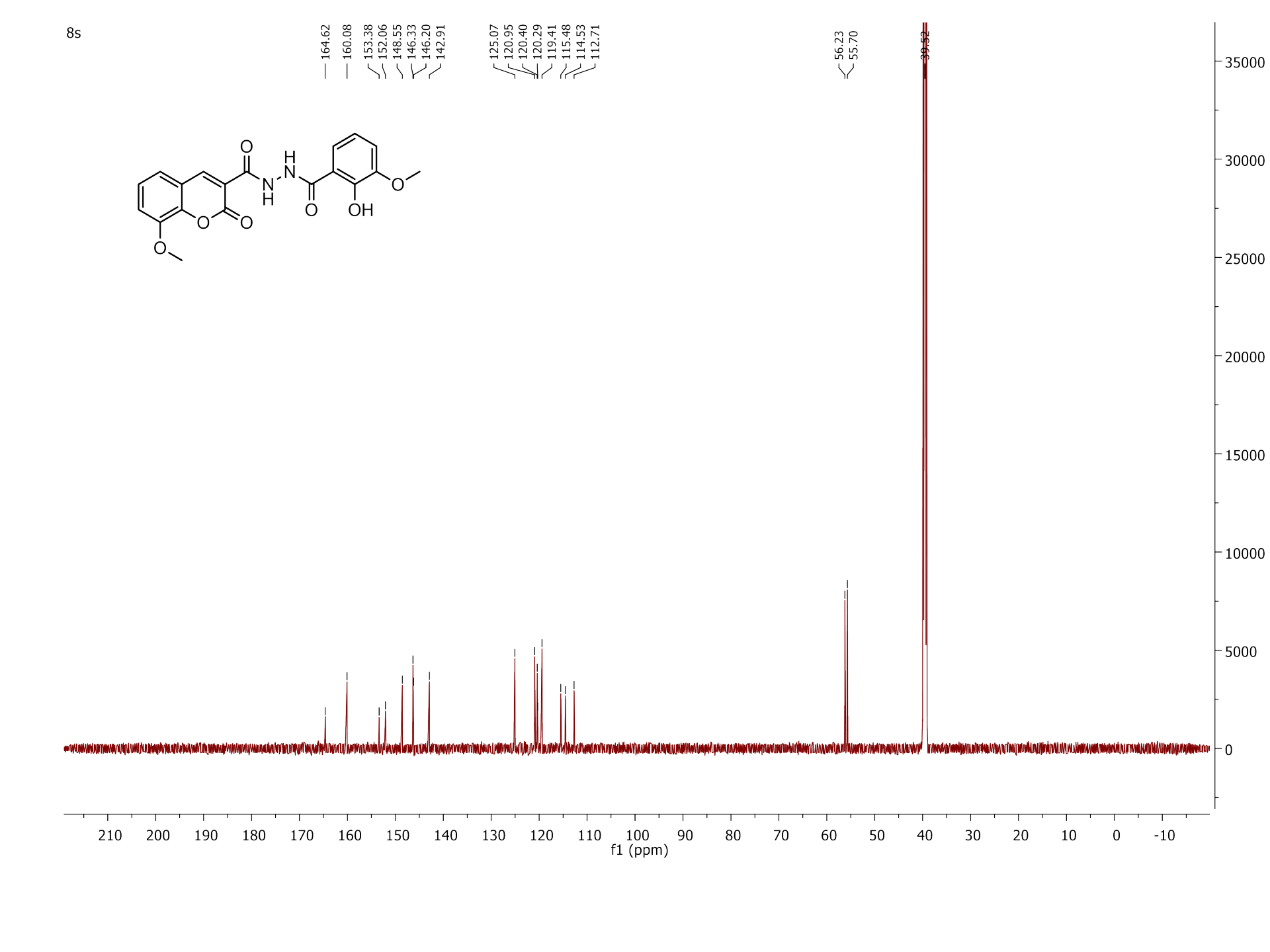
0.89
3.07
3.00

f1 (ppm)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146.20
142.91
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120.29
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115.48
114.53
112.71
56.23
55.70
39.52
O
H
N
N
H
O
O
O
O
O
OH
35000
30000
25000
20000
15000
10000
5000
0
210
200
190
180
170
160
150
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130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1337 formula(e) evaluated with 58 results within limits (all results (up to 1000) for each mass)

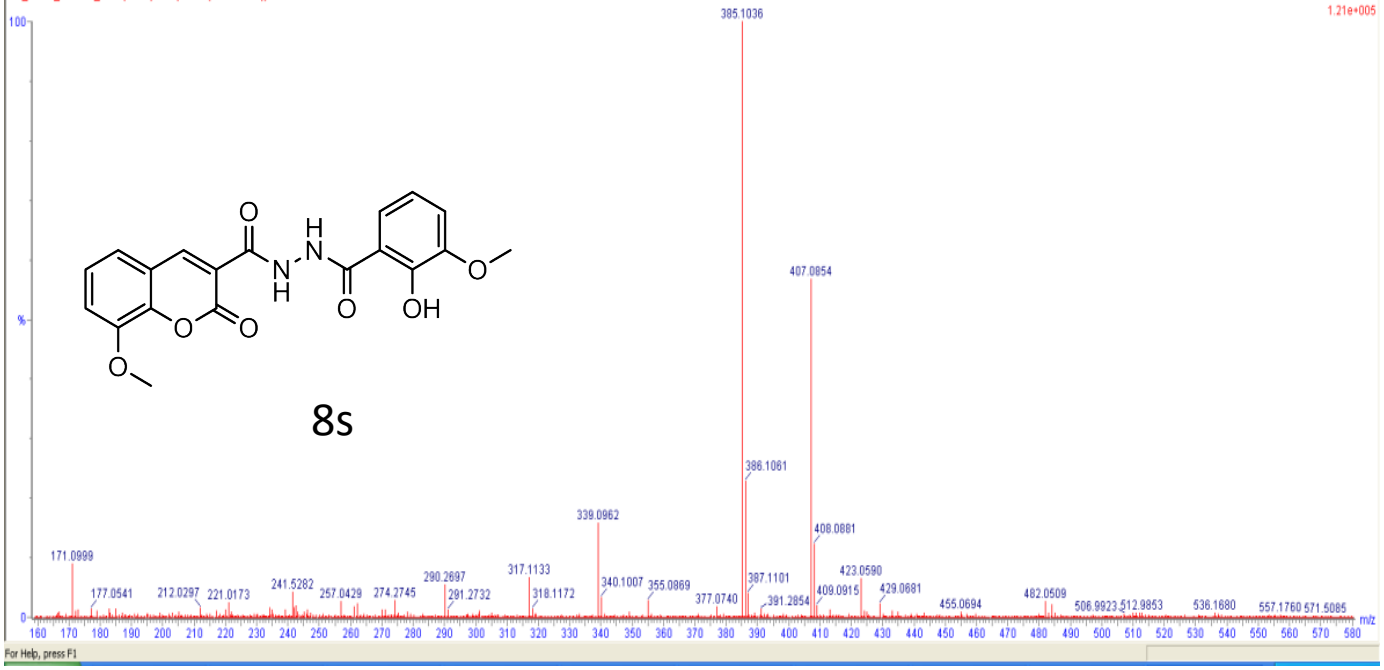
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Cl
385.1036	385.1036	0.0	0.0	12.5	C19 H17 N2 O7	328.2	2.325	9.78	19	17	2	7	
	385.1032	0.4	1.0	-1.5	C12 H27 O9 Cl2	351.1	25.214	0.00	12	27		9	2
	385.1046	-1.0	-2.6	3.5	C13 H23 N4 O5 Cl2	350.9	25.067	0.00	13	23	4	5	2
	385.1054	-1.8	-4.7	-0.5	C7 H21 N4 O14	339.1	13.287	0.00	7	21	4	14	
	385.1054	-1.8	-4.7	7.5	C18 H22 O7 Cl	349.8	23.916	0.00	18	22		7	1
	385.1017	1.9	4.9	25.5	C31 H13	334.2	8.315	0.02	31	13			
	385.1014	2.2	5.7	3.5	C13 H22 N2 O9 Cl	349.8	23.978	0.00	13	22	2	9	1
	385.1064	-2.8	-7.3	-1.5	C12 H28 N2 O6 Cl3	351.4	25.569	0.00	12	28	2	5	3
	385.1005	3.1	8.0	7.5	C19 H24 N2 Cl3	351.4	25.507	0.00	19	24	2		3

OJ 151d

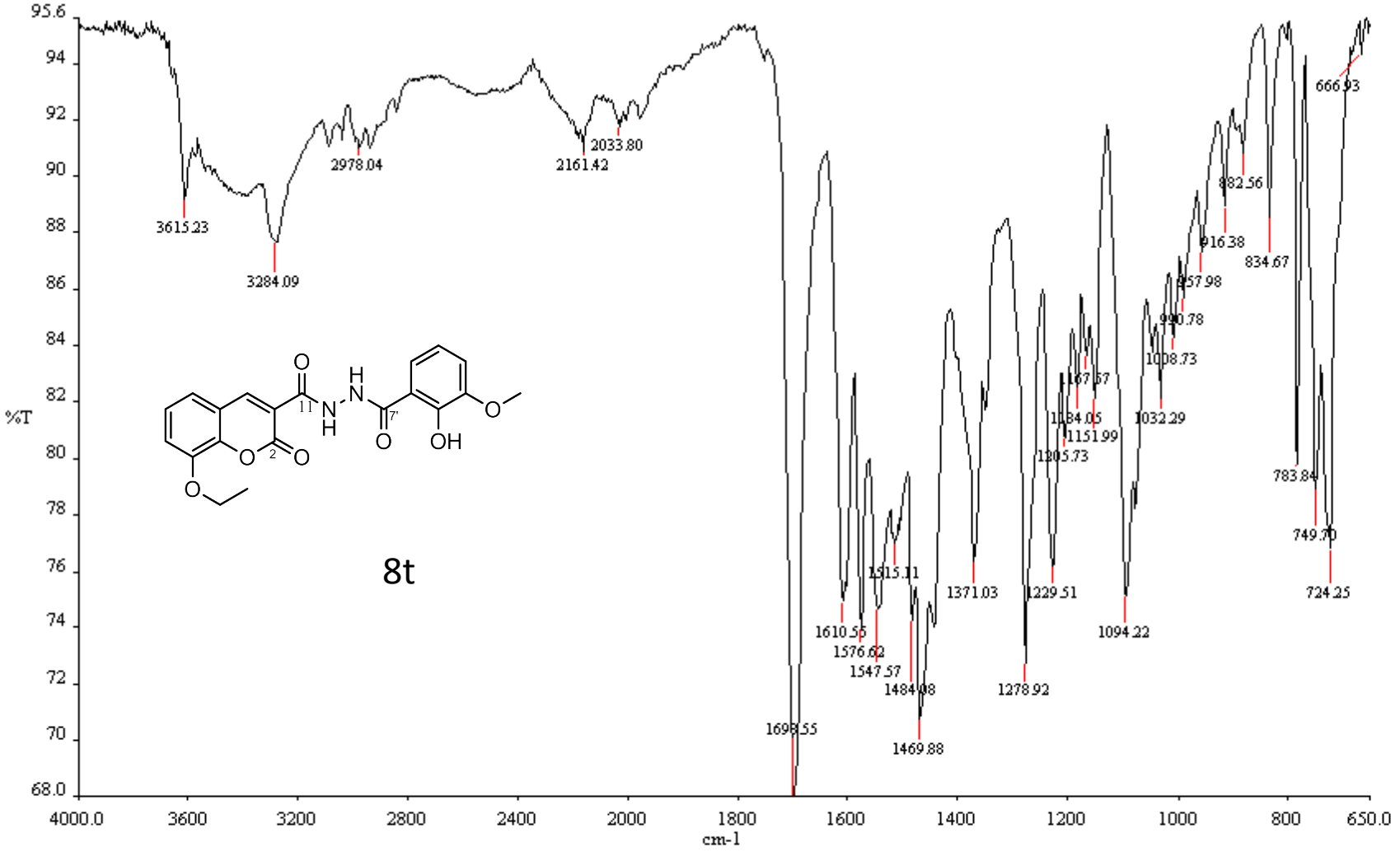
MS_Direct_160325_9 25 (0.168) Cm (13:31-(4:10+47:48))

1: TOF MS ES+
1.21e+005



8s

For Help, press F1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2800
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1200
1000
800
650.0
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1610.55
1576.62
1547.57
1484.08
1469.88
1371.03
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1278.92
1229.51
1205.73
1184.05
1151.99
1094.22
1032.29
1008.73
990.78
957.98
916.38
882.56
834.67
783.84
749.70
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O
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N
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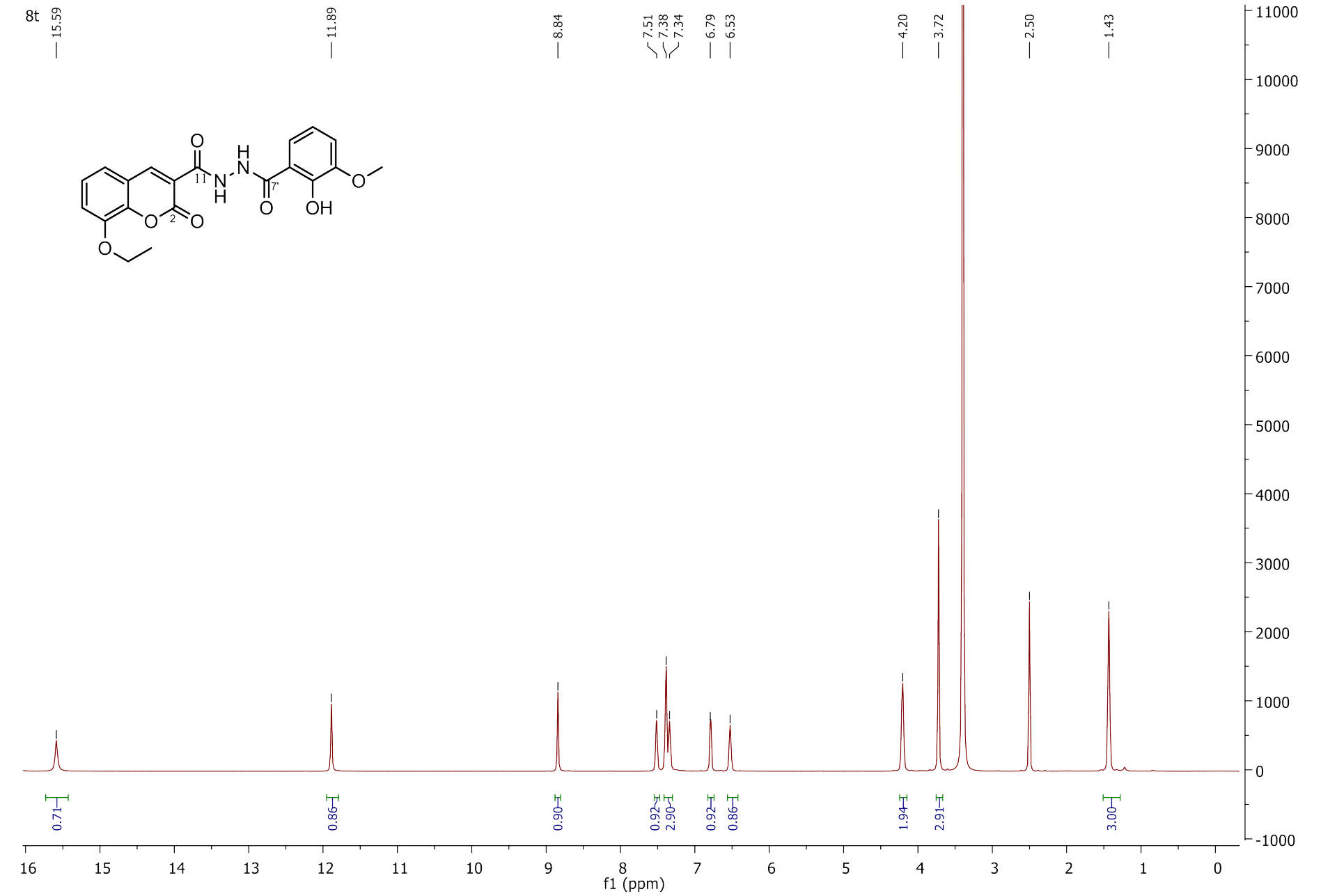
O
O
OH
11
7'
2
8t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7.38
7.34
6.79
6.53
4.20
3.72
2.50
1.43
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N
N
H
O
O
O
O
O
OH
11'
7'
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11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
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0.86
0.90
0.92
2.90
0.92
0.86
1.94
2.91
3.00
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12
11
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9
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6
5
4
3
2
1
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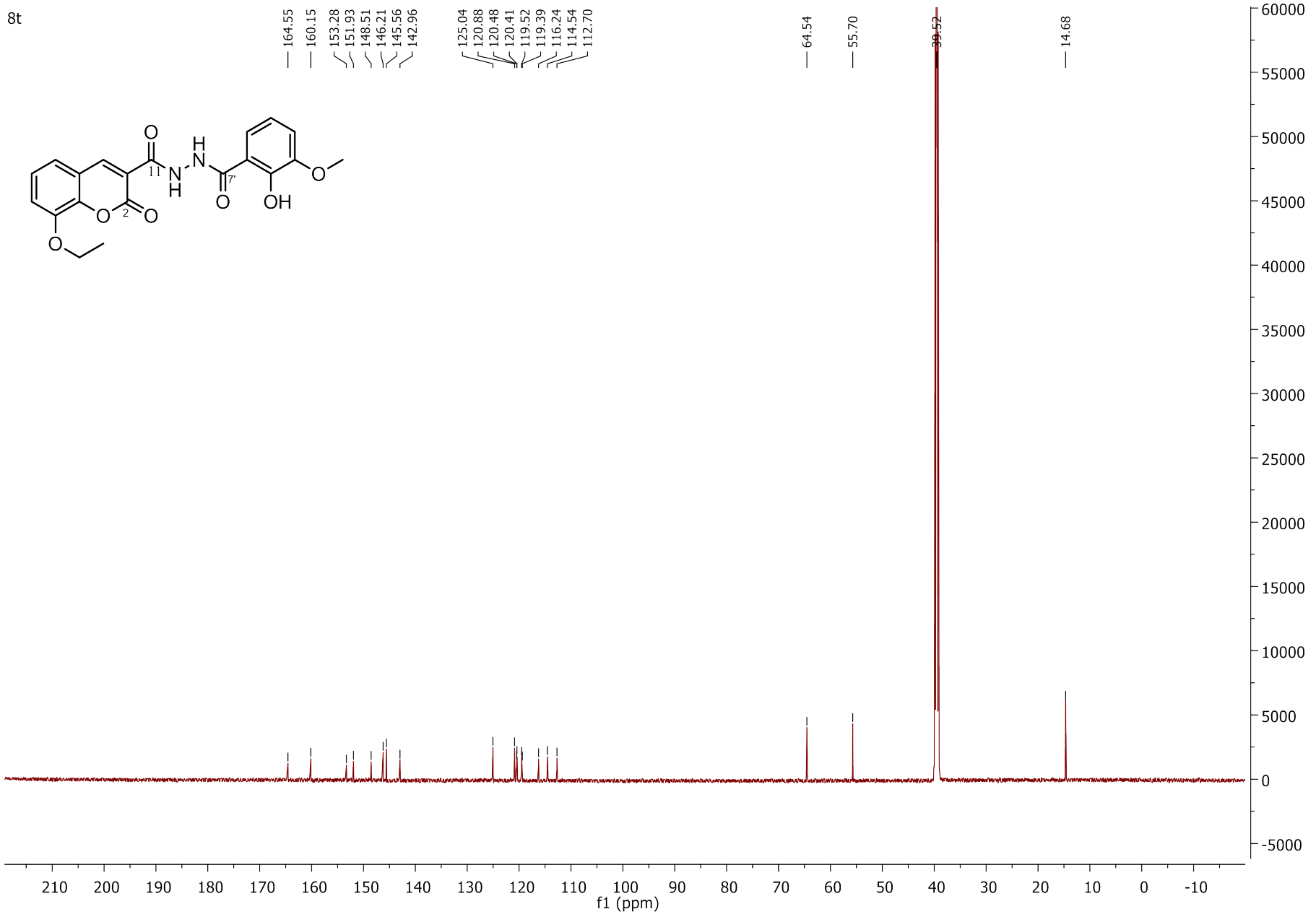
f1 (ppm)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120.48
120.41
119.52
119.39
116.24
114.54
112.70
64.54
55.70
39.52
14.68
O
H
N
N
H
O
11
7'
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2
O
O
O
OH
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1432 formula(e) evaluated with 81 results within limits (all results (up to 1000) for each mass)

Elements Used:

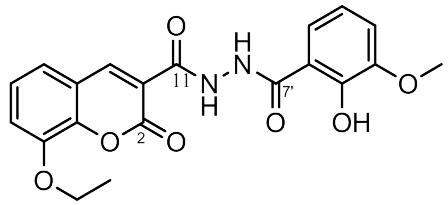
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Cl
	399.1192	-0.3	-0.8	12.5	C20 H19 N2 O7	258.5	0.086	91.72	20	19	2	7	
	399.1202	-1.3	-3.3	3.5	C14 H25 N4 O5 Cl2	287.2	28.801	0.00	14	25	4	5	2
	399.1174	1.5	3.8	25.5	C32 H15	272.5	14.111	0.00	32	15			
	399.1170	1.9	4.8	3.5	C14 H24 N2 O9 Cl	286.1	27.660	0.00	14	24	2	9	1
	399.1211	-2.2	-5.5	7.5	C19 H24 O7 Cl	286.0	27.591	0.00	19	24		7	1
	399.1211	-2.2	-5.5	-0.5	C8 H23 N4 O14	272.4	13.999	0.00	8	23	4	14	
	399.1162	2.7	6.8	7.5	C20 H26 N2 Cl3	287.7	29.261	0.00	20	26	2		3
	399.1220	-3.1	-7.8	-1.5	C13 H30 N2 O5 Cl3	287.7	29.325	0.00	13	30	2	5	3
	399.1224	-3.5	-8.8	12.5	C20 H20 N4 O3 Cl	285.9	27.474	0.00	20	20	4	3	1

OJ 151e

MS_Direct_160325_10 22 (0.137) Cm (13:28-(5:8+47:57))

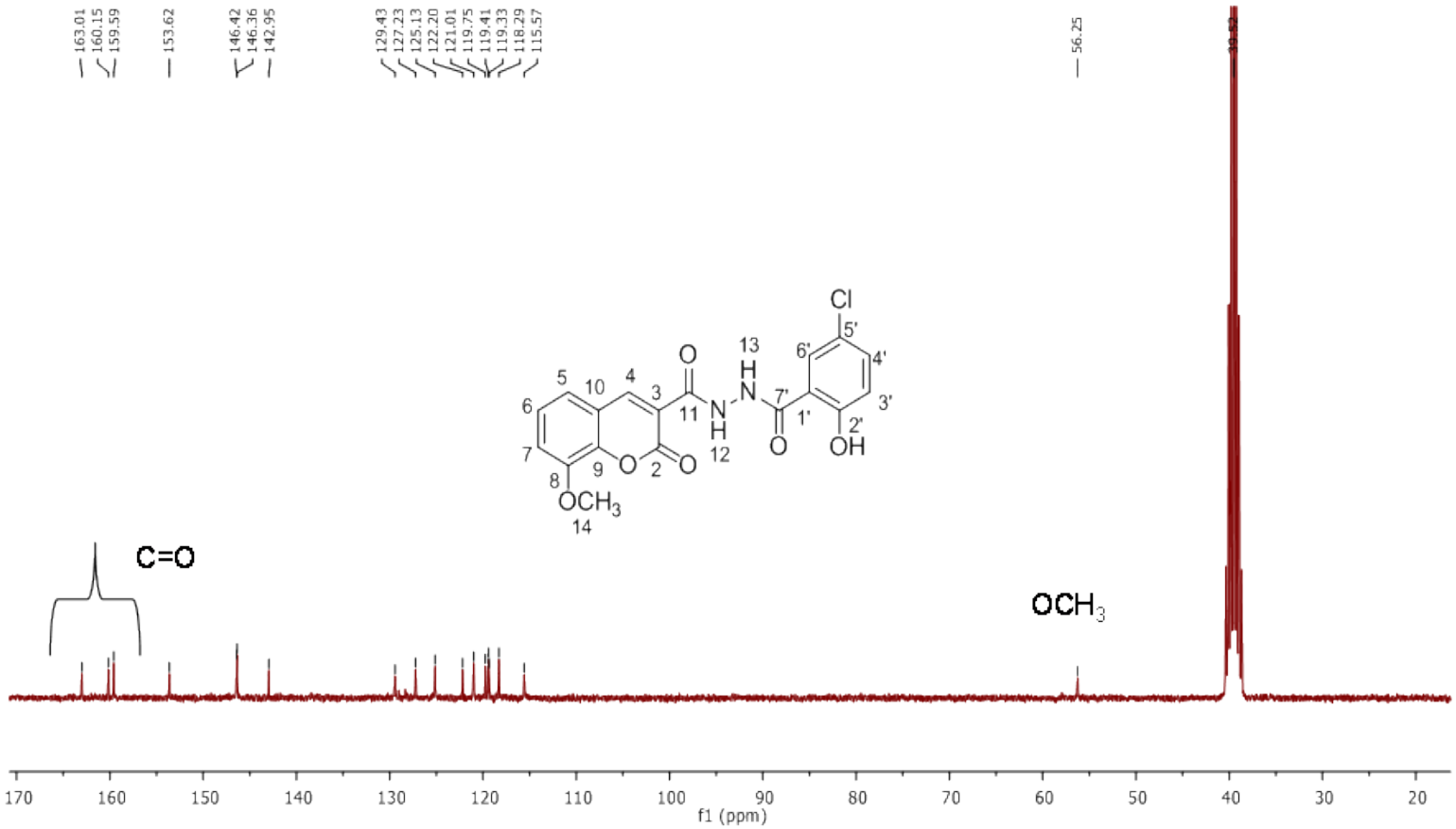
1: TOF MS ES+

4.84e+005

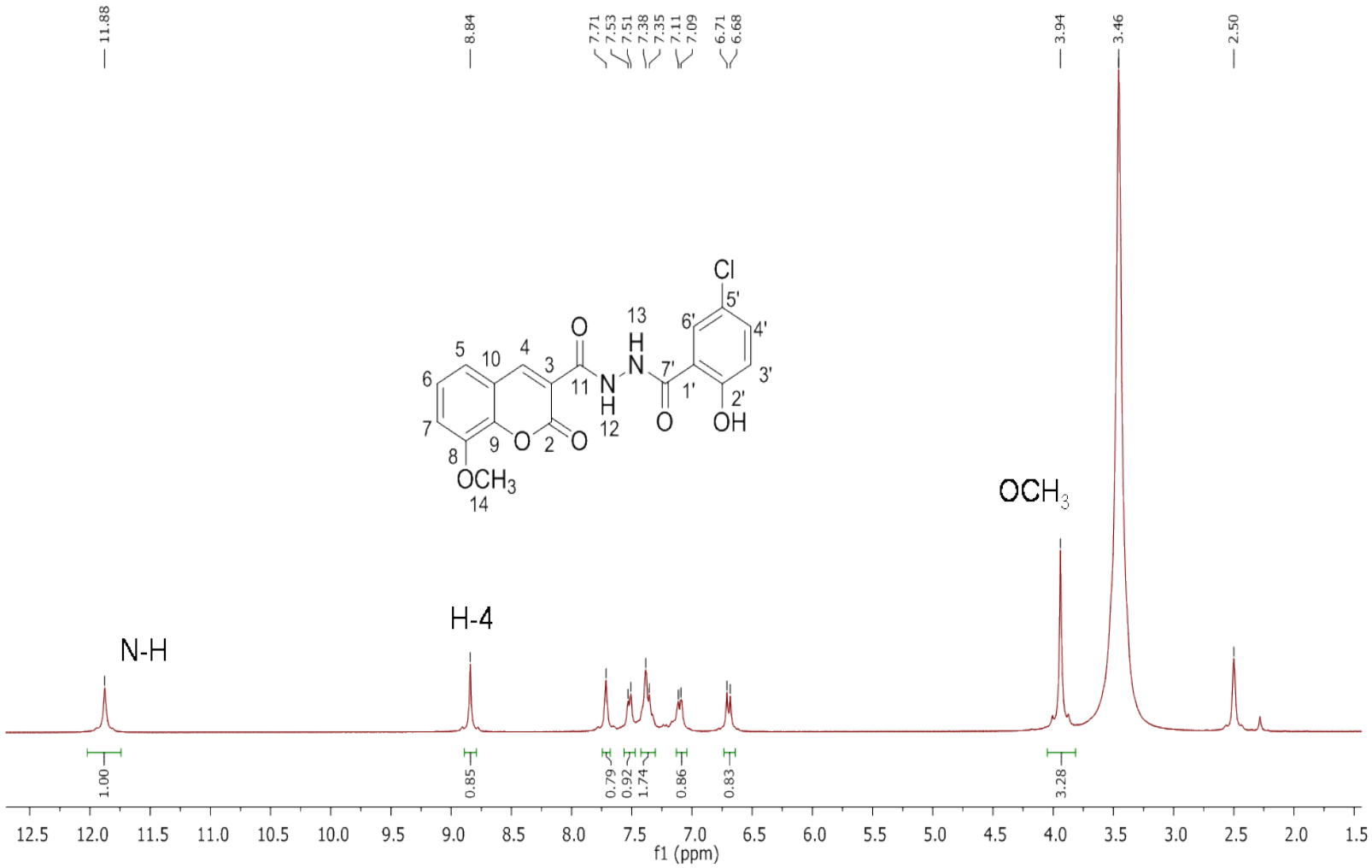


8t

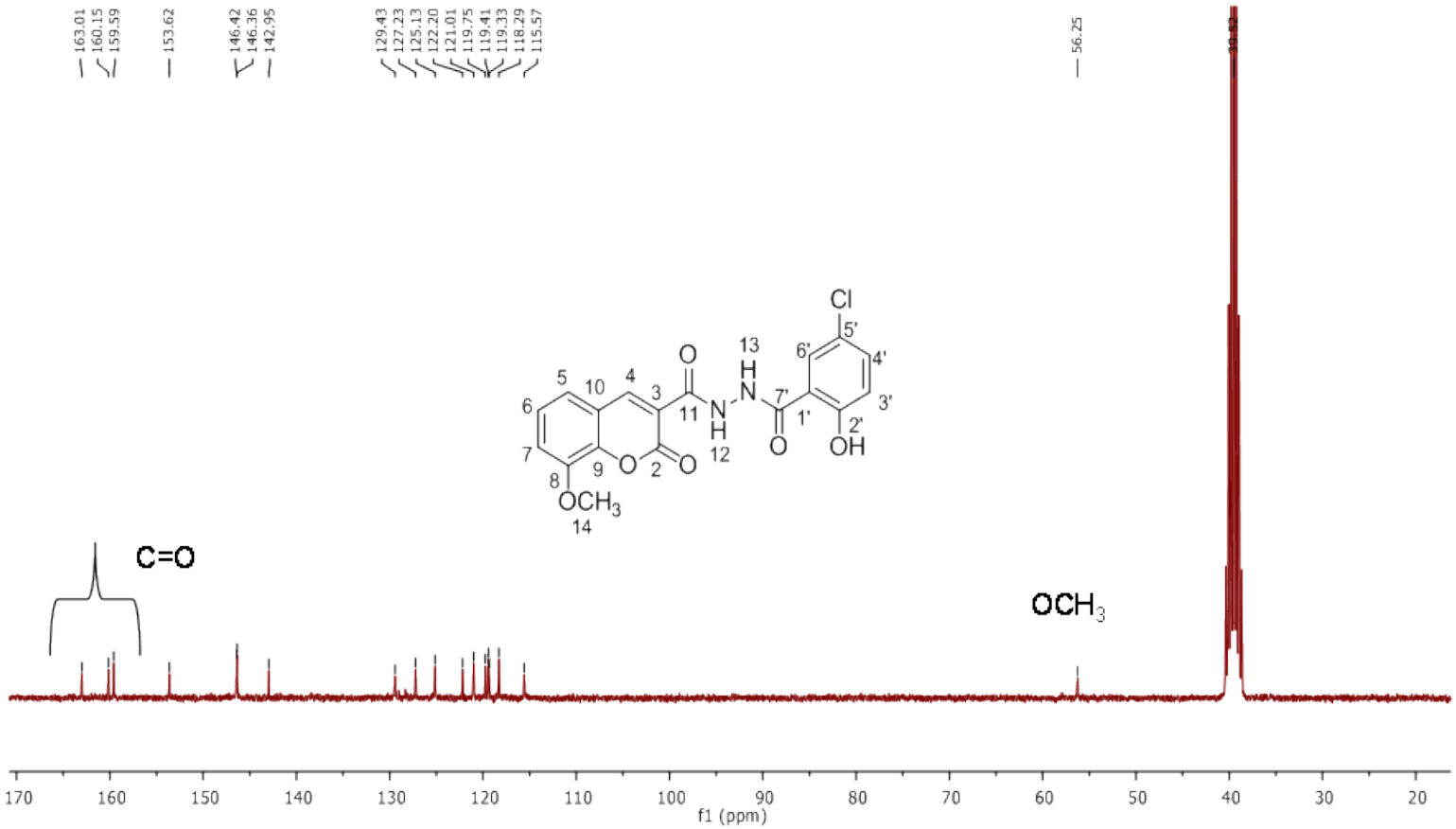
For Help, press F1



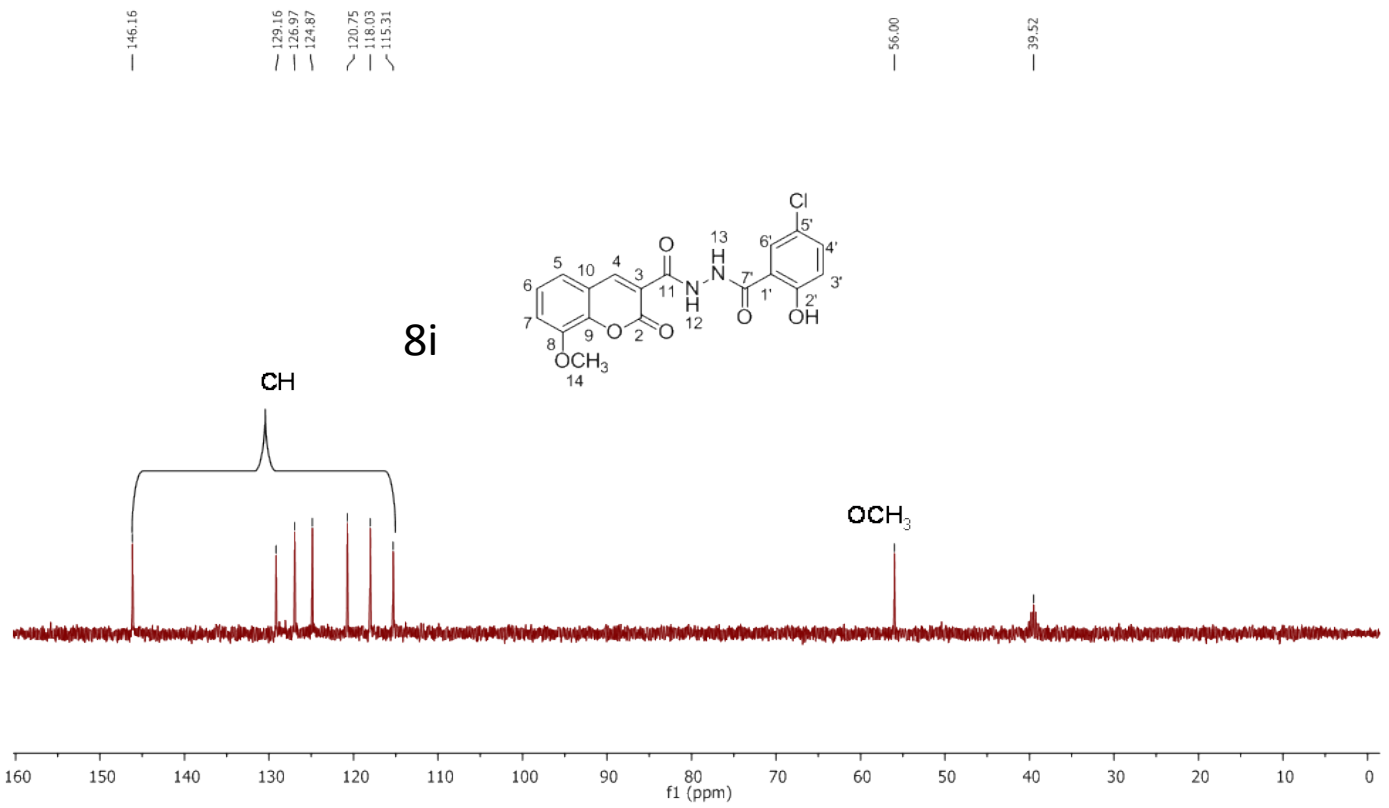
75 MH_Z ^{13}C NMR spectrum of compound **8i** in DMSO-d_6.



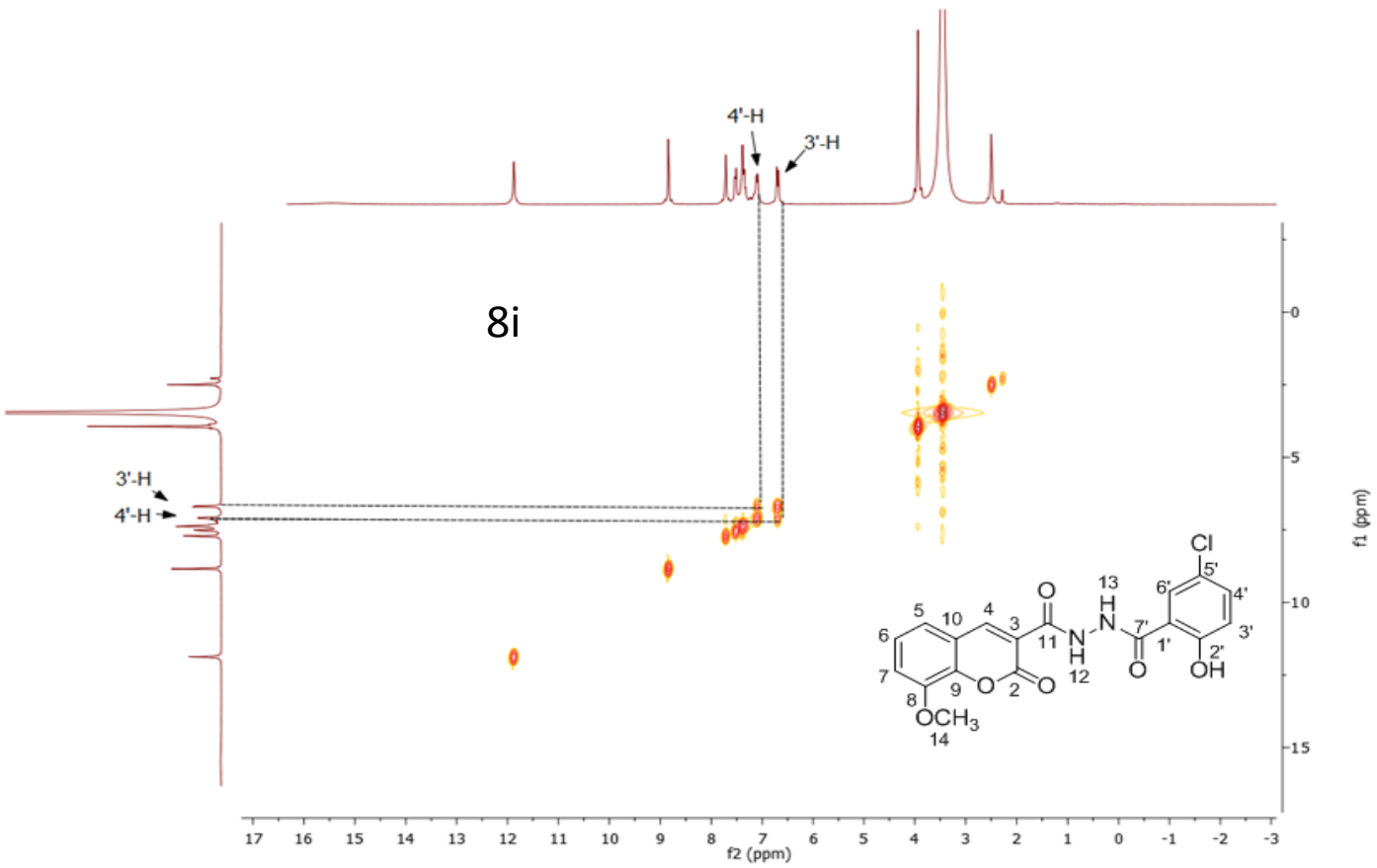
300 MH_Z ^1H NMR spectrum of compound **8i** in DMSO-d_6.



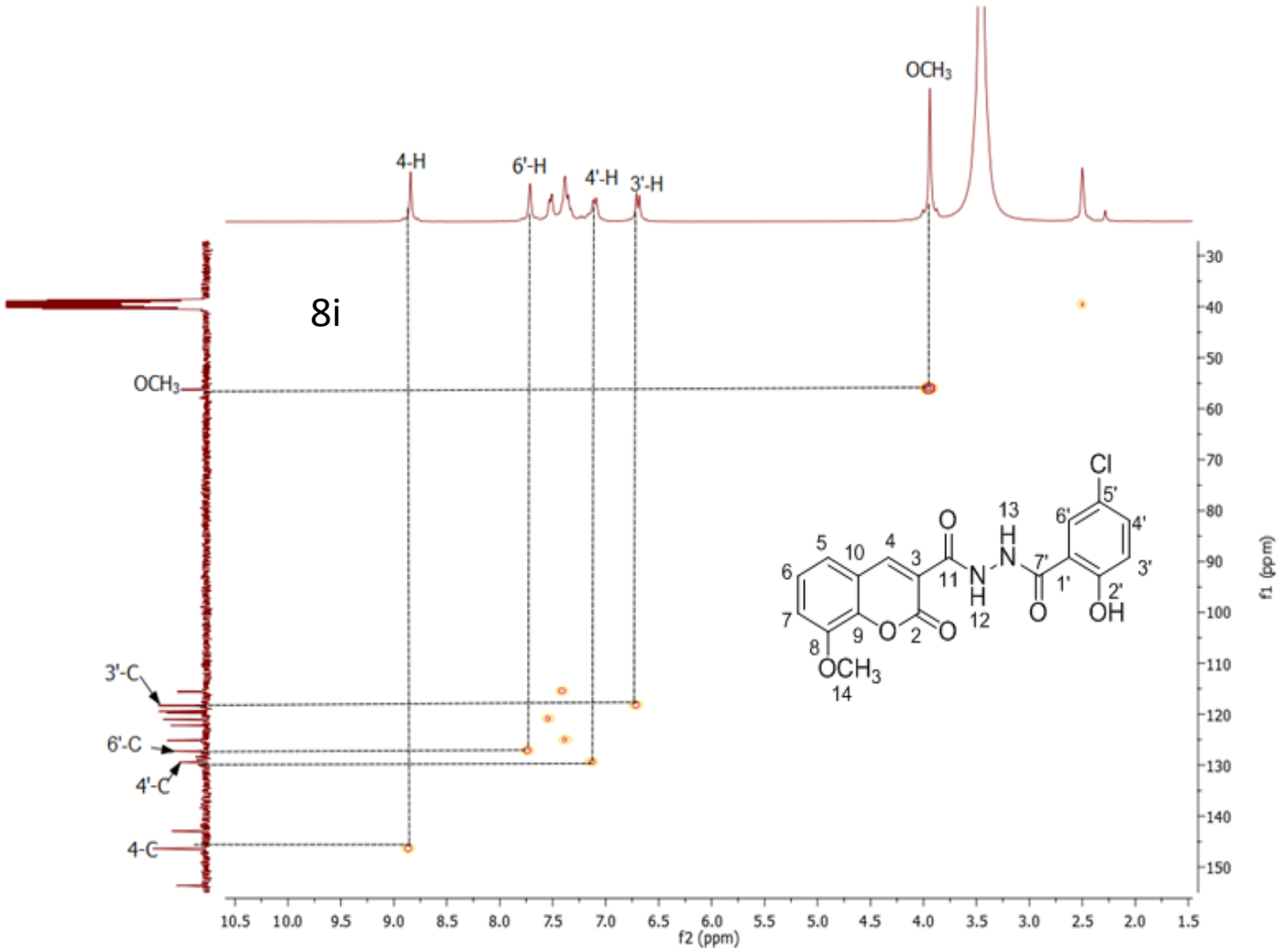
75 MH_Z ^{13}C NMR spectrum of compound **8i** in DMSO-d_6.



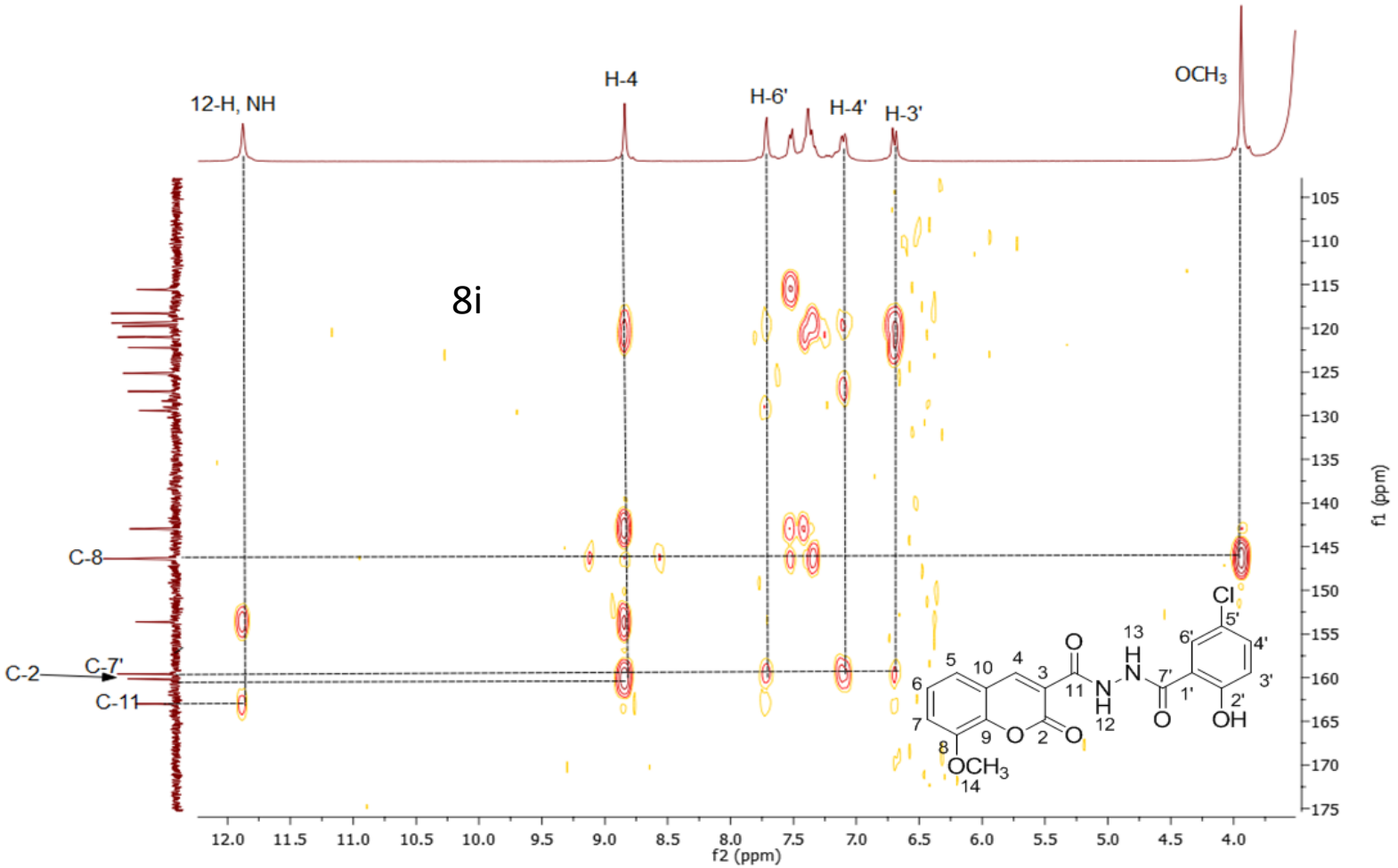
DEPT 135 spectrum of compound **8i** in DMSO-d_6.



^{1}H, ^{1}H-COSY NMR spectrum of compound **8i** in DMSO-d_6.



HSQC NMR spectrum of compound **8i** in DMSO-d_6



HMBC NMR spectrum of compound **8i** in DMSO-d_6.