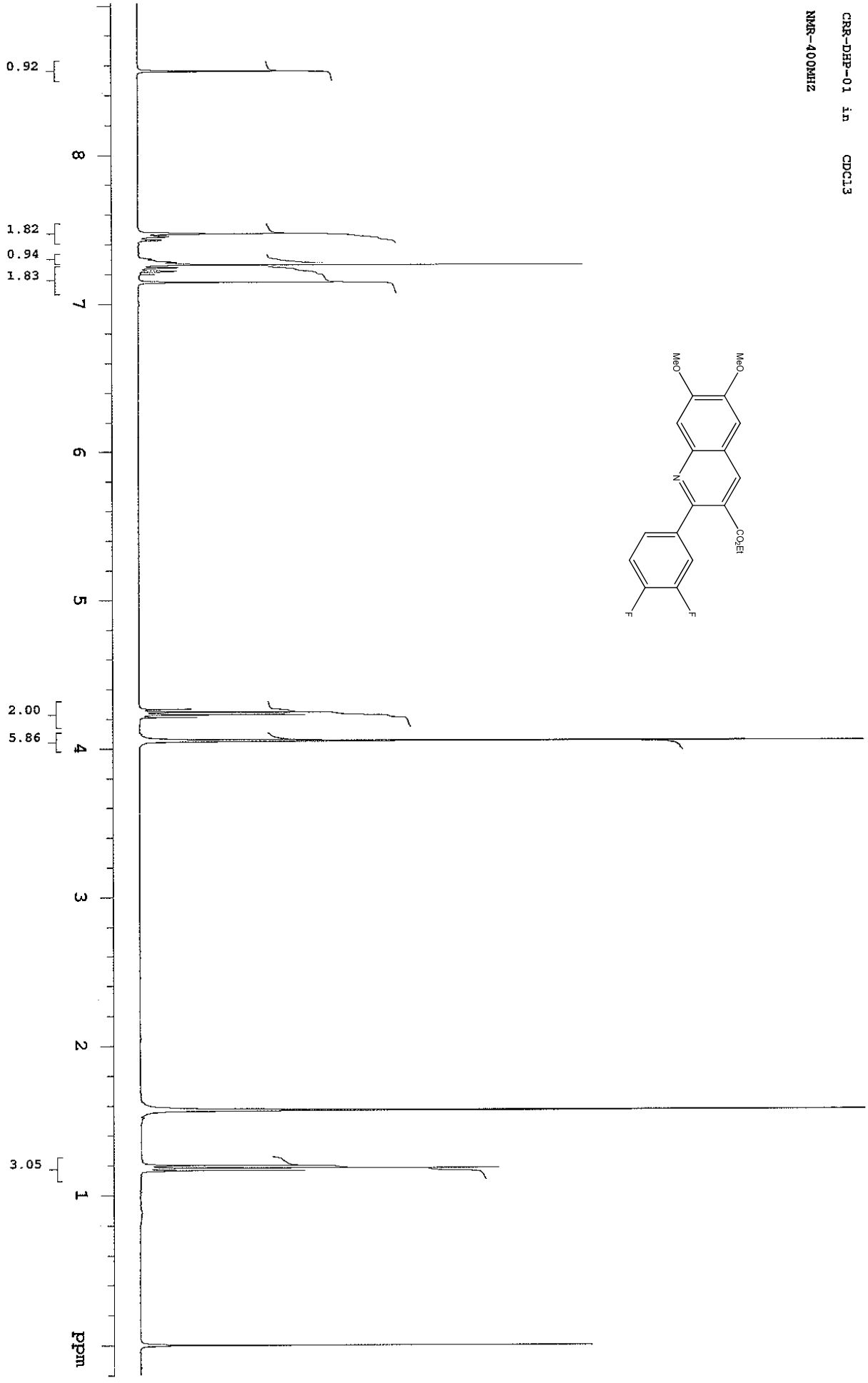
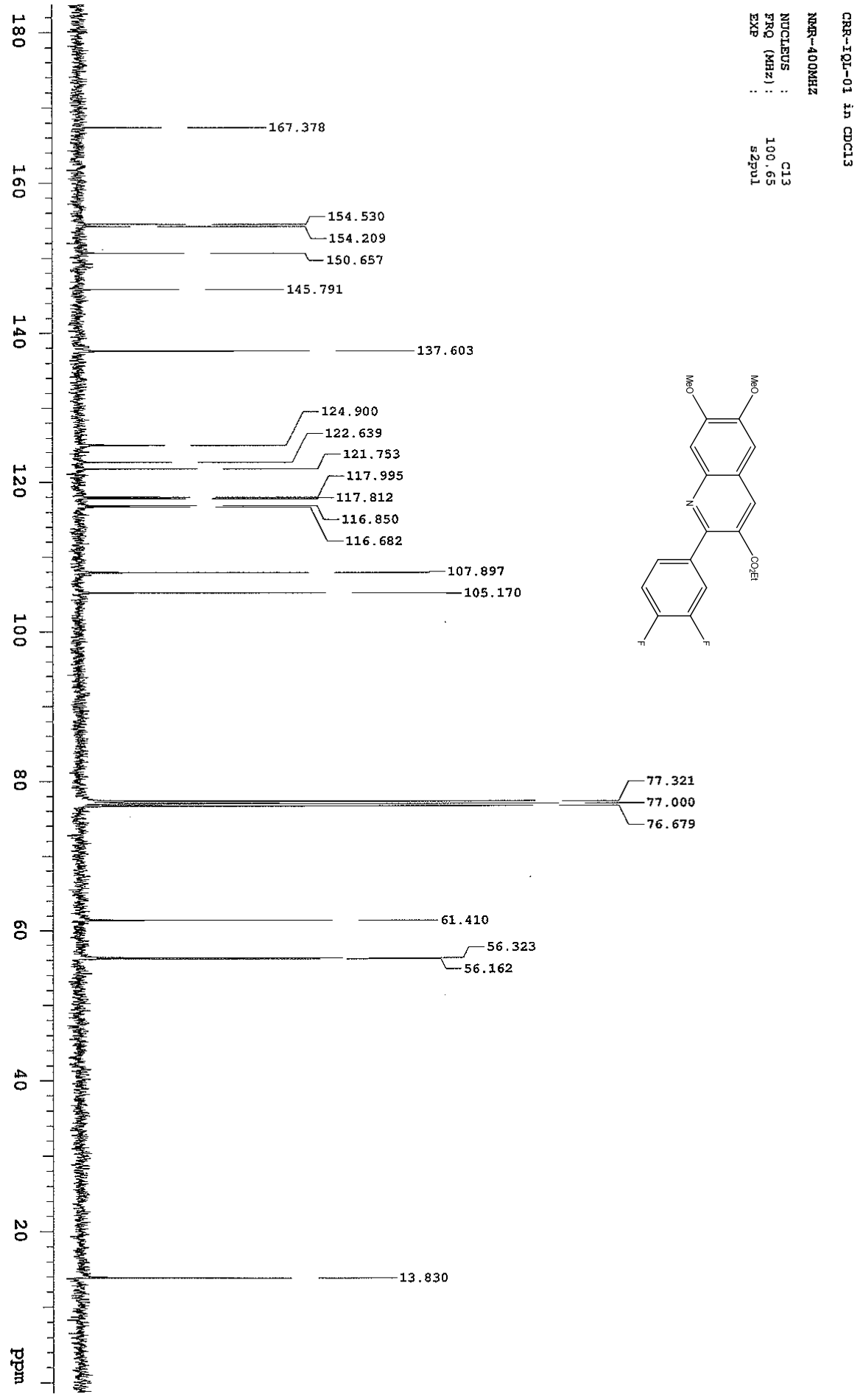
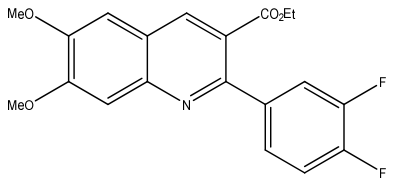




Elemental Composition Report

Single Mass Analysis

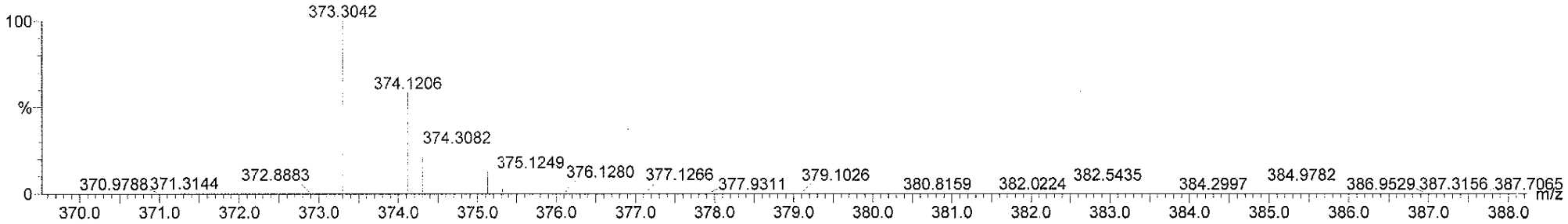
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4



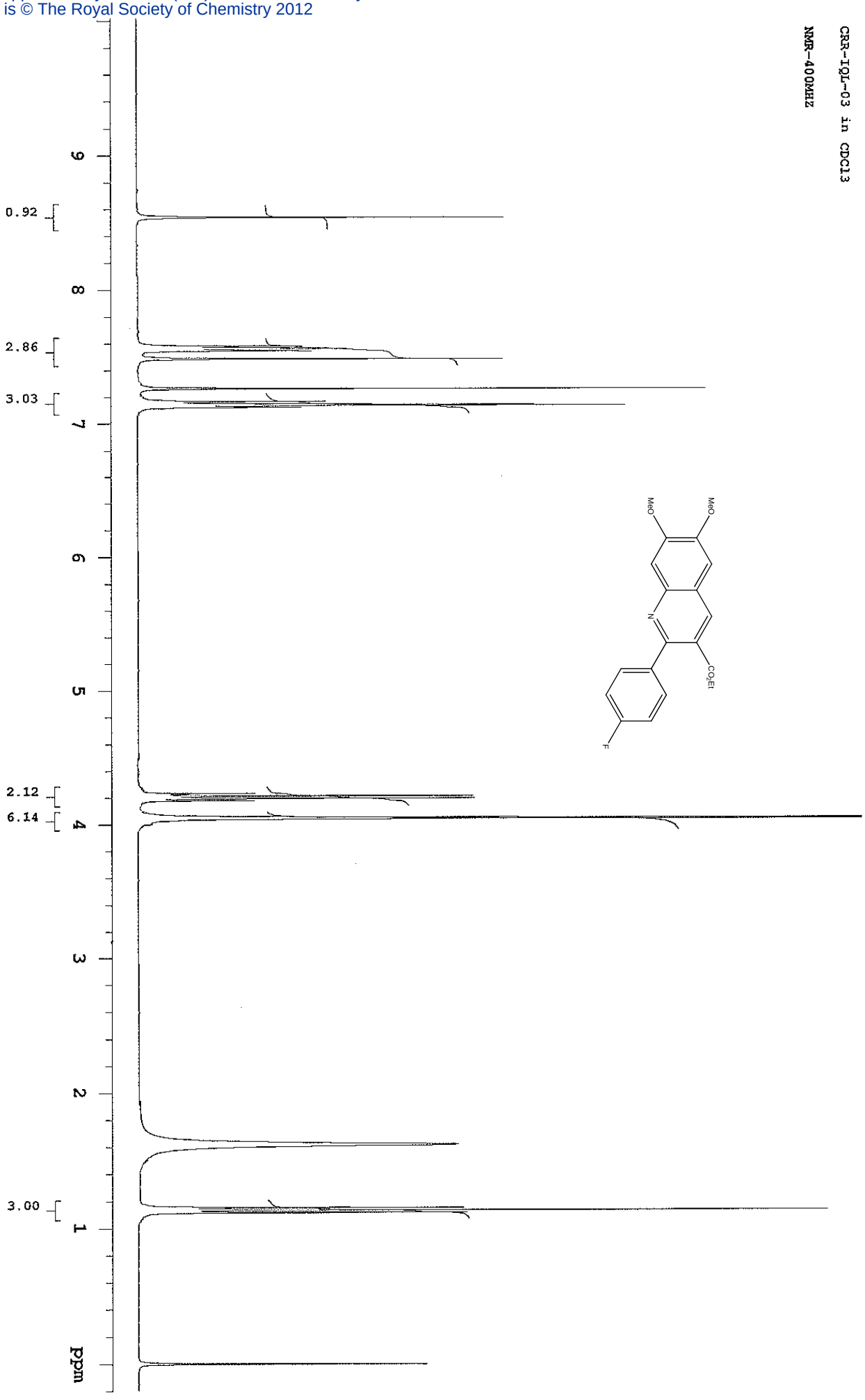
Monoisotopic Mass, Even Electron Ions
137 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-2 O: 0-4 F: 0-2
CRR-IQL/01

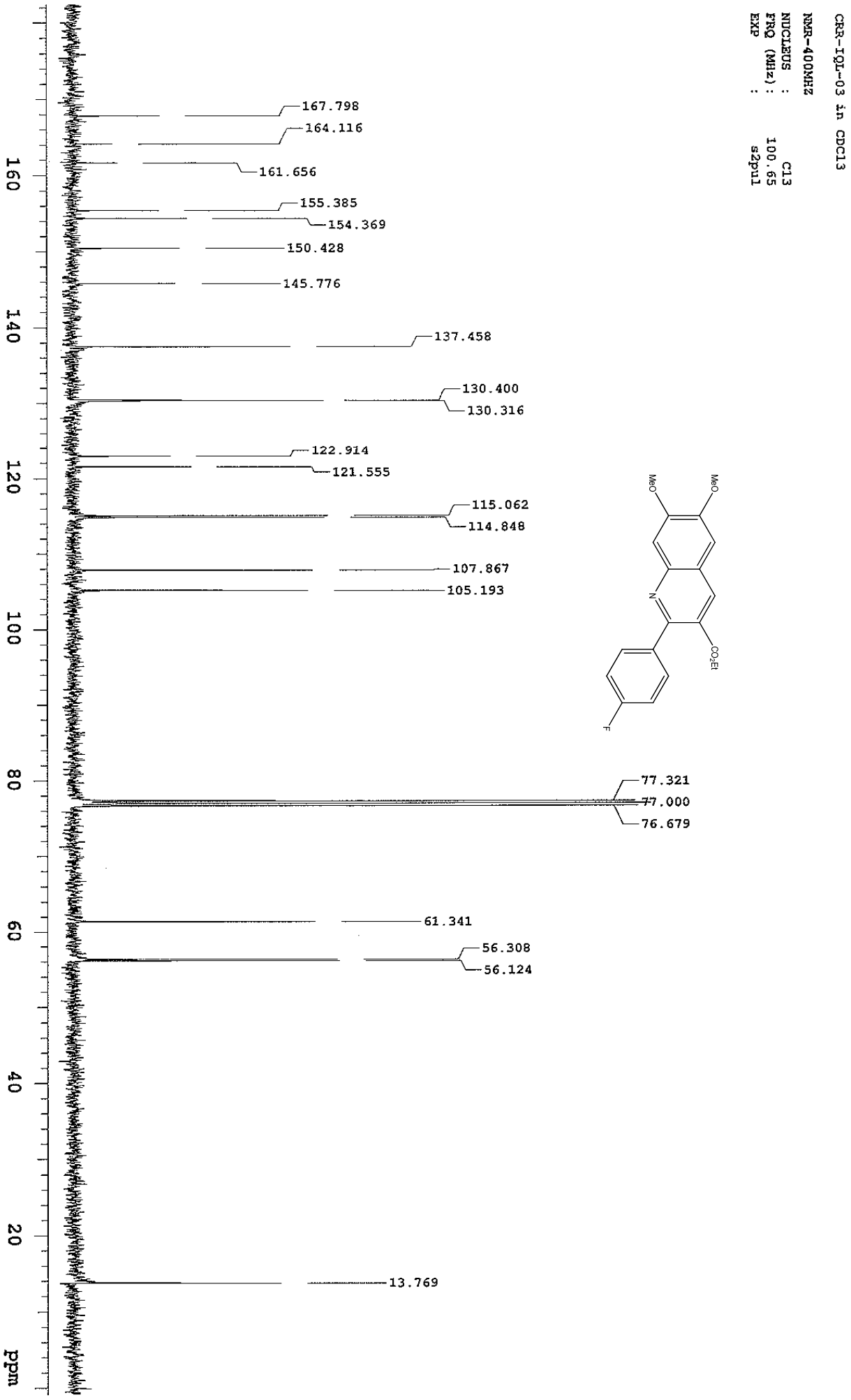
UT1011_53 27 (0.615) Cm (27:29-71:84x0.010)

1: TOF MS ES+
1.55e+004



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
374.1206	374.1204	0.2	0.5	11.5	3.9	C20 H18 N O4 F2
	374.1192	1.4	3.7	15.5	41.0	C23 H17 N O3 F



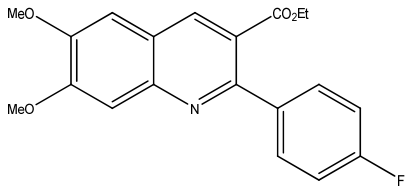


Elemental Composition Report

Single Mass Analysis

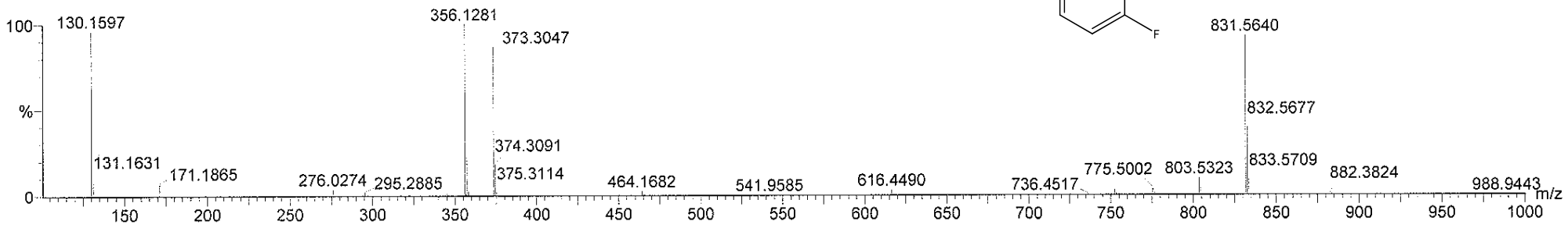
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
137 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-2 O: 0-4 F: 0-2
CRR-IQL/03

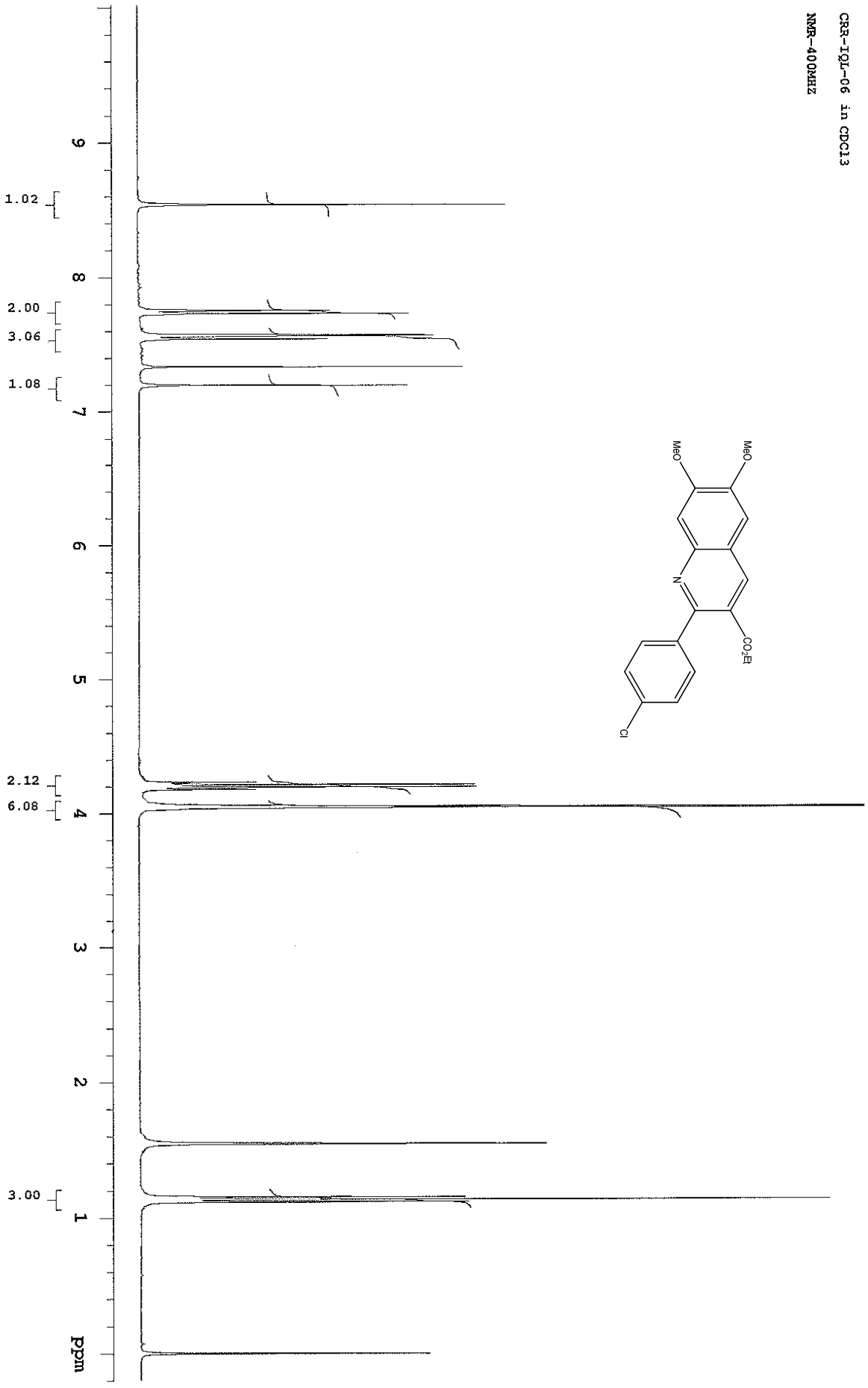


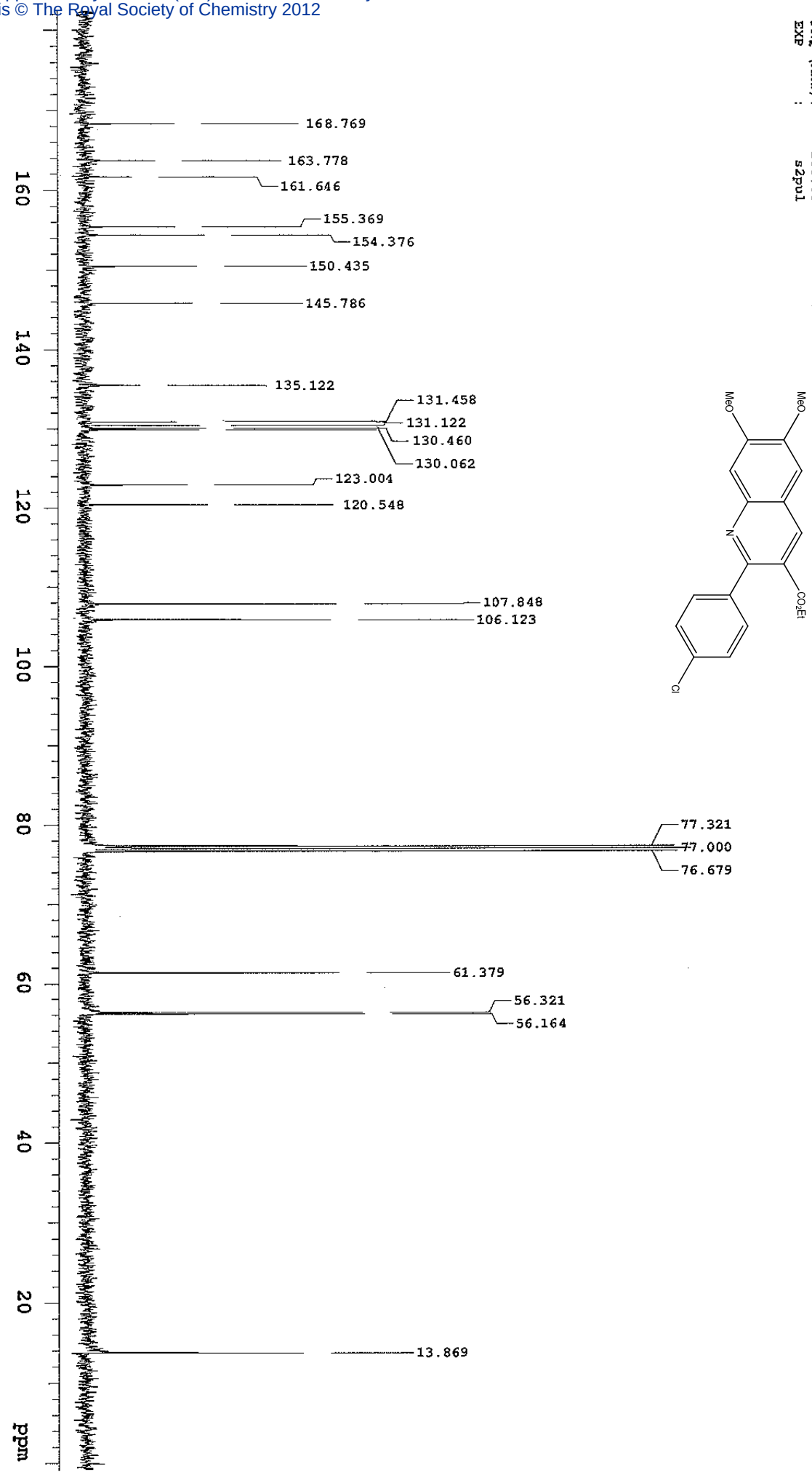
UT1011_54 27 (0.615) Cm (27:30-73:80x0.010)

1: TOF MS ES+
2.49e+004



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
356.1281	356.1298	-1.7	-4.8	11.5	23.5	C20 H19 N O4 F
	356.1287	-0.6	-1.7	15.5	110.2	C23 H18 N O3



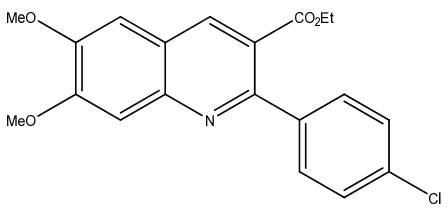


Elemental Composition Report

Single Mass Analysis

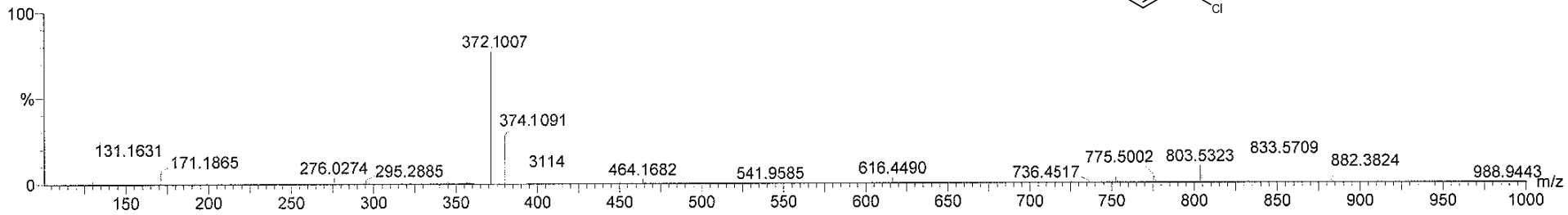
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
137 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-2 O: 0-4 Cl: 0-1
CRR-IQL/06

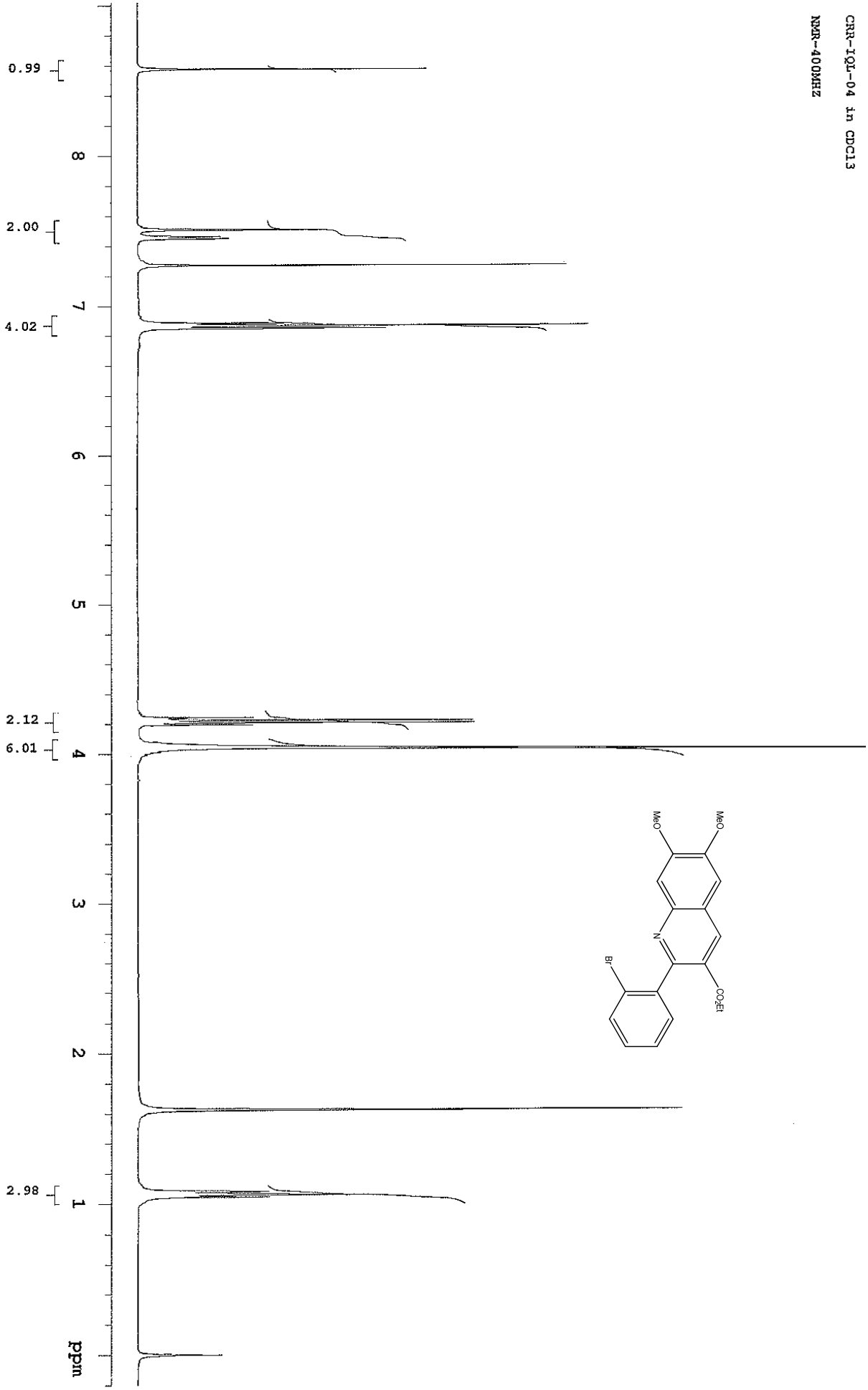


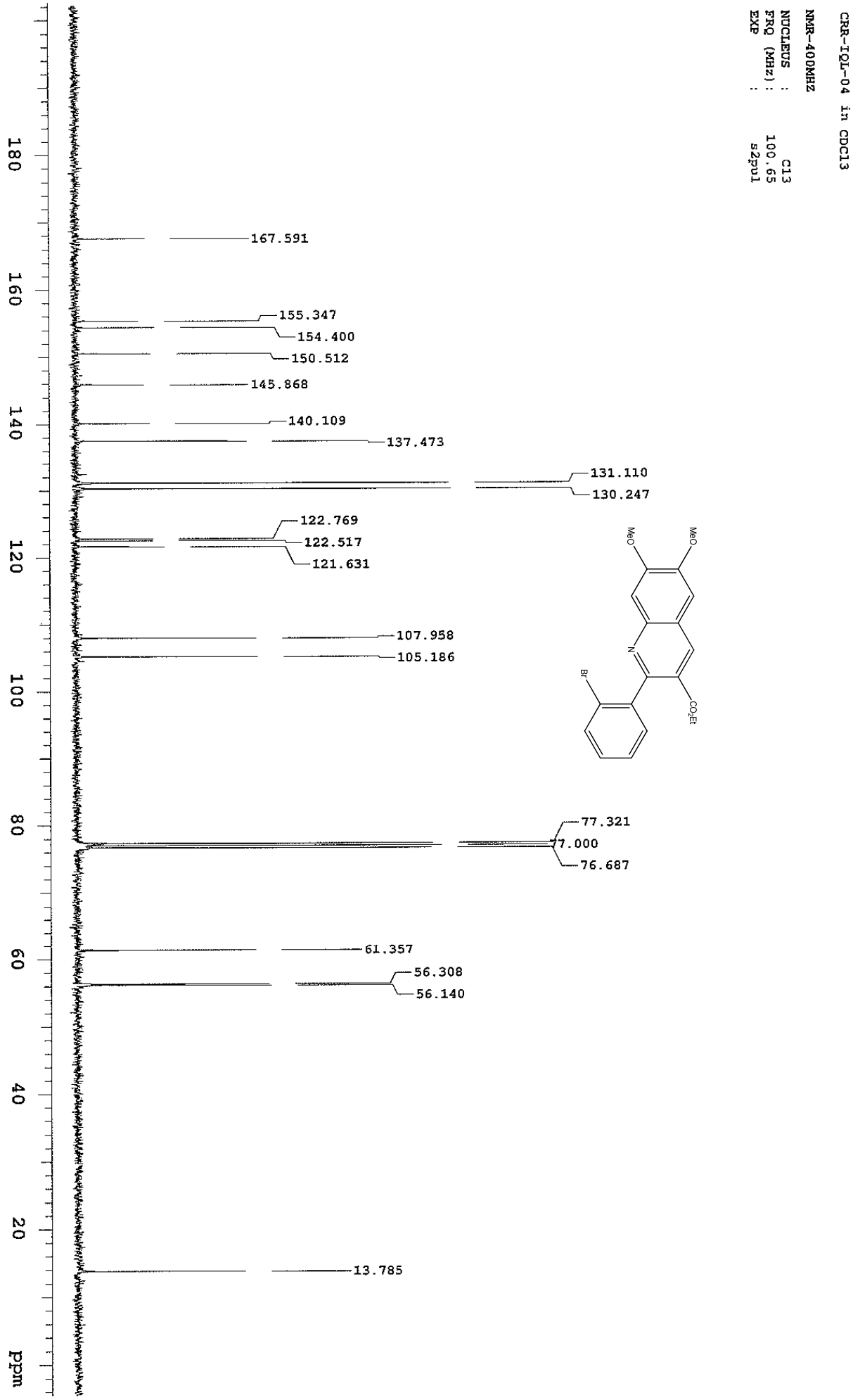
UT1011_54 27 (0.615) Cm (27:30-73:80x0.010)

1: TOF MS ES+
5.39e+002



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
372.1007	372.1003	-1.7	-3.6	12.5	23.5	C20 H19 N O4 Cl





Elemental Composition Report

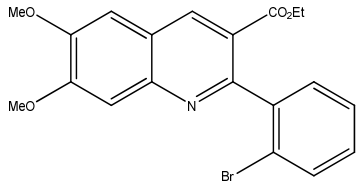
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -2.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

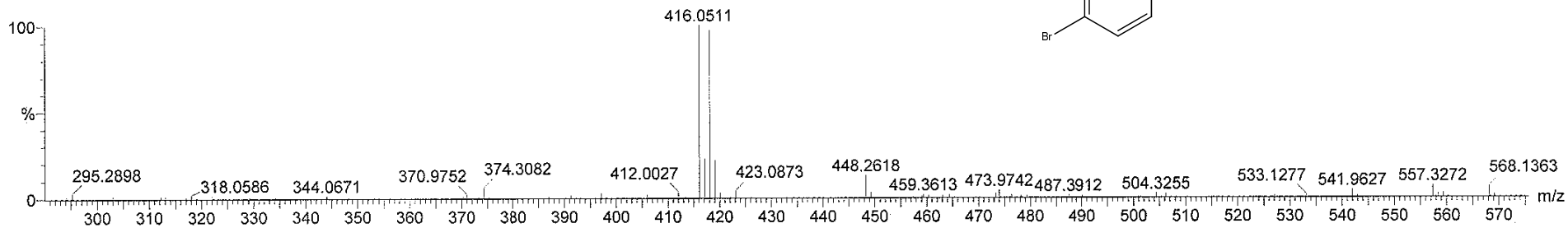
Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-1 O: 0-4 Br: 0-1

CRR/IQL/04

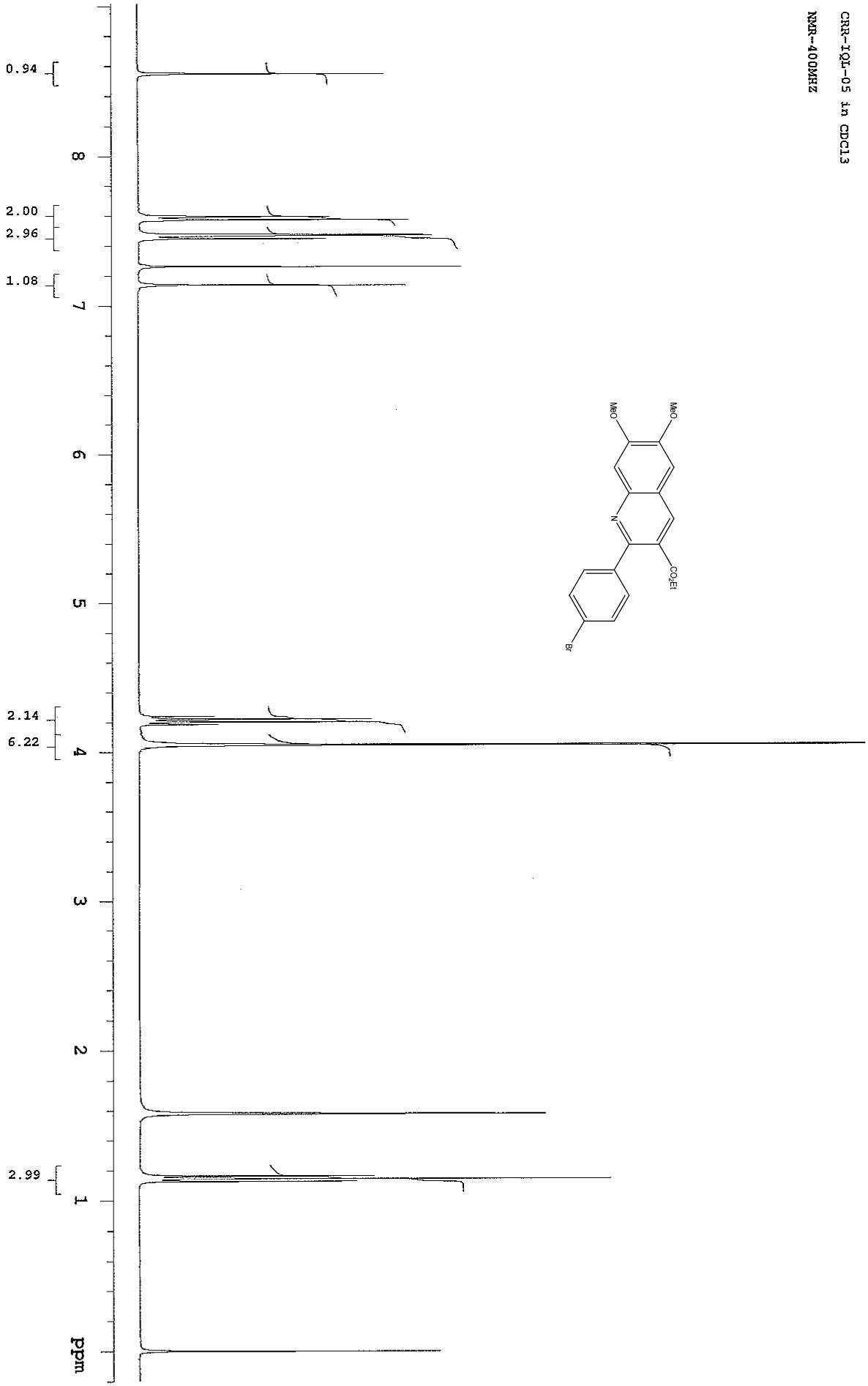
UT1111_91 25 (0.580) Cm (25-1:3x0.010)

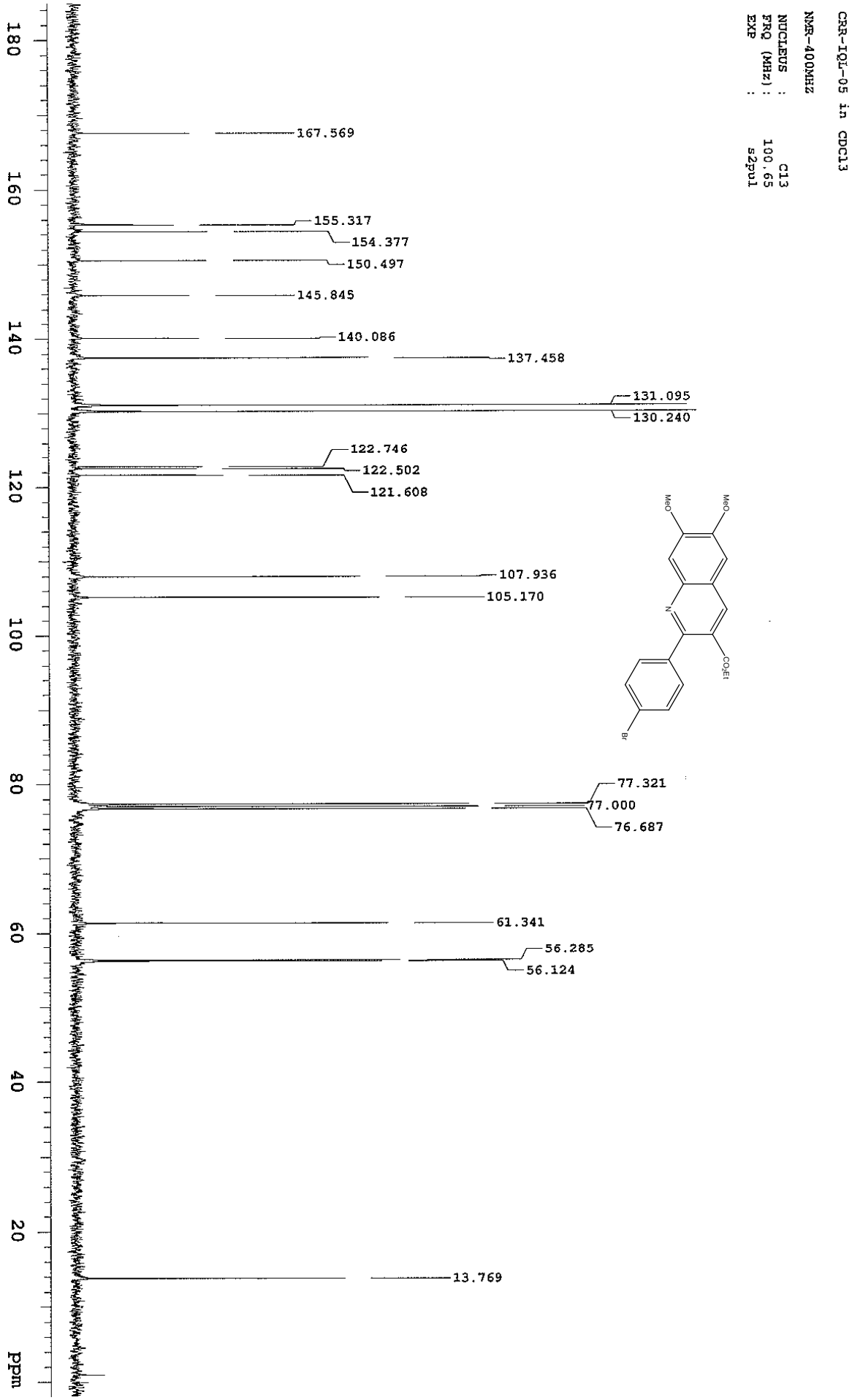


1: TOF MS ES+
4.57e+004



Minimum:				-2.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
416.0511	416.0497	1.4	2.6	11.5	1.6	C20 H19 N O4 Br


CRR-IQL-05 in CDCl3
NMR-400MHZ
0.94
2.00
2.96
1.08
2.14
6.22
2.99
MeO
MeO
N
CO2Et
Br
8
7
6
5
4
3
2
1
ppm

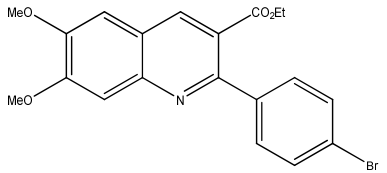


Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -2.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

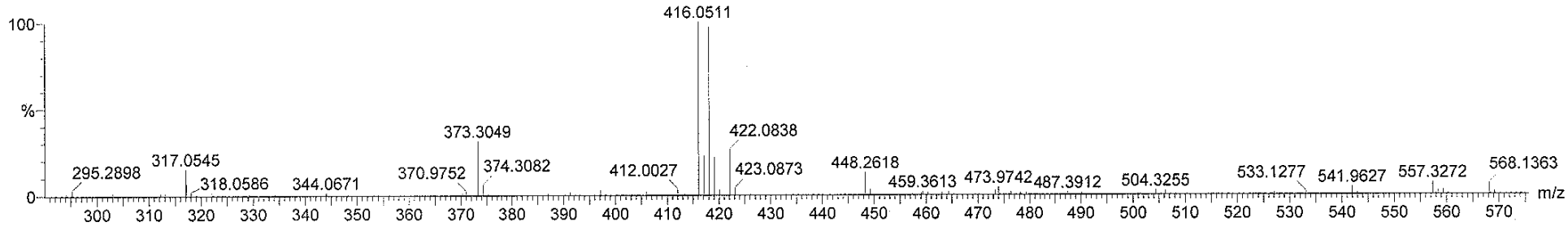
Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-1 O: 0-4 Br: 0-1



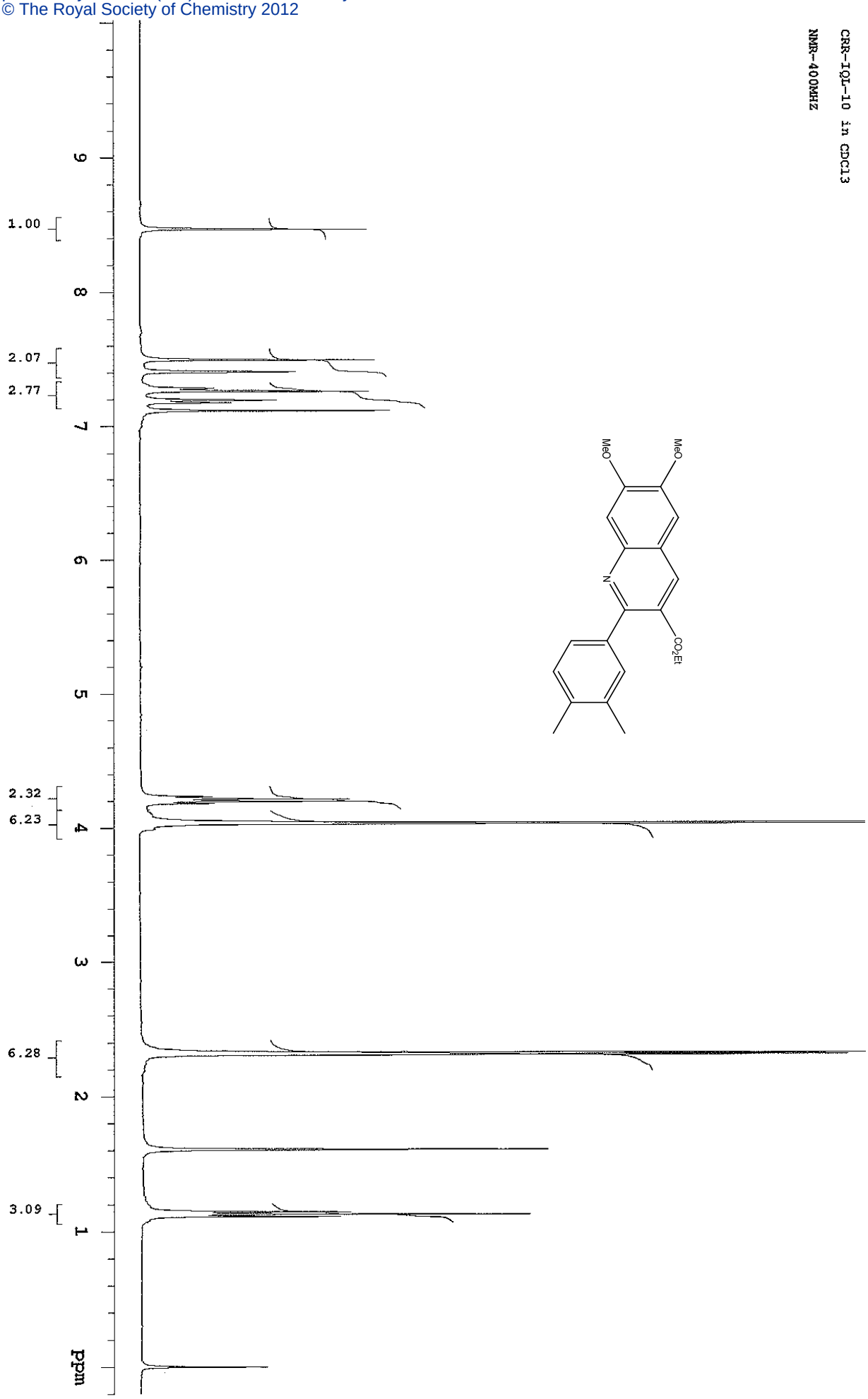
CRR/IQL/05

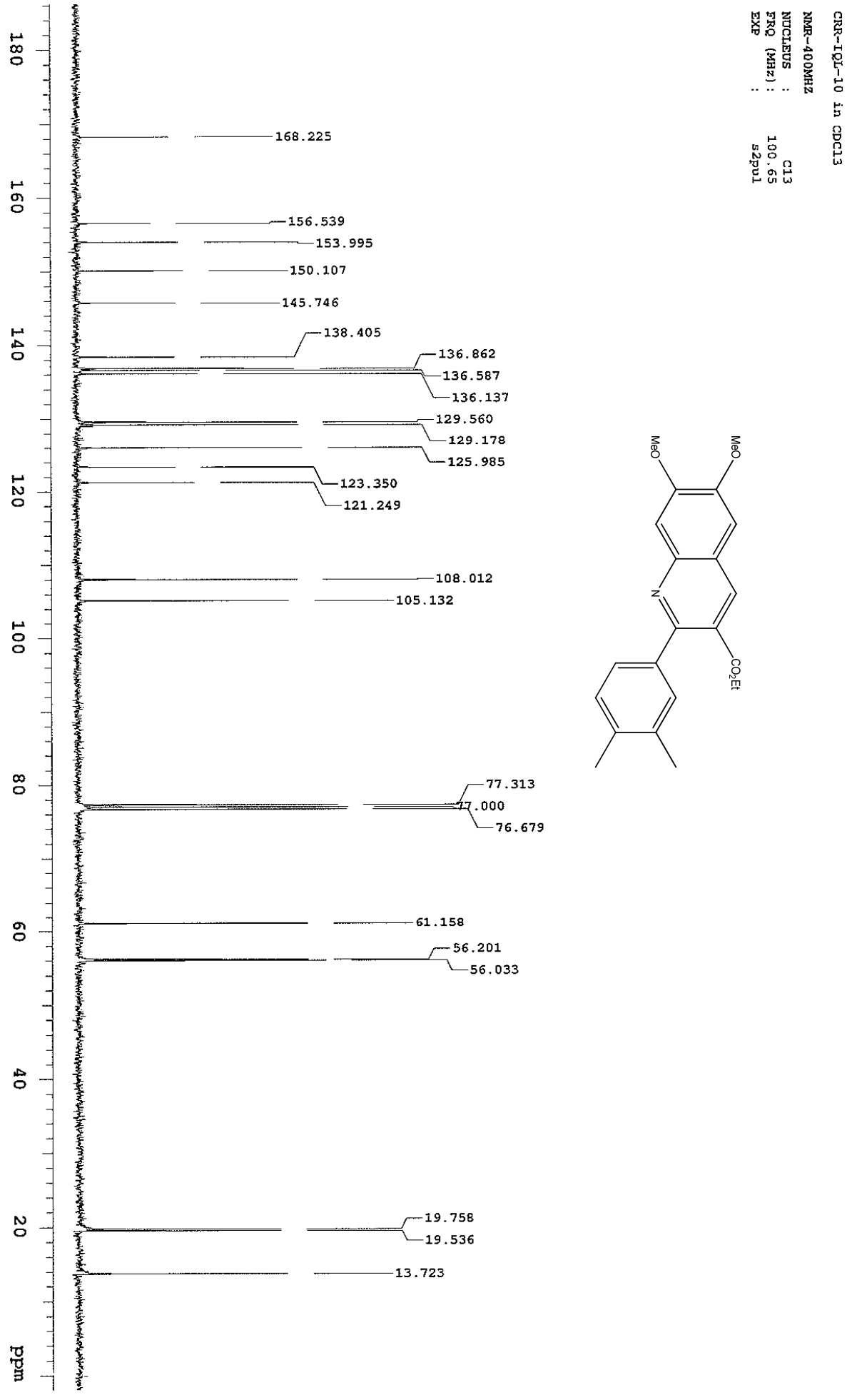
UT1111_91 25 (0.580) Cm (25-1:3x0.010)

1: TOF MS ES+
3.25e+003

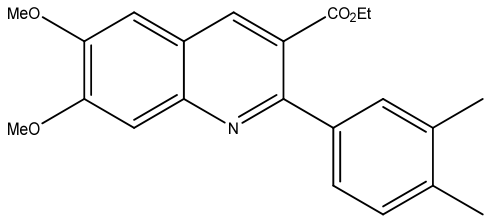


Minimum:				-2.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
416.0511	416.0497	1.4	3.4	11.5	1.6	C20 H19 N O4 Br





Elemental Composition Report



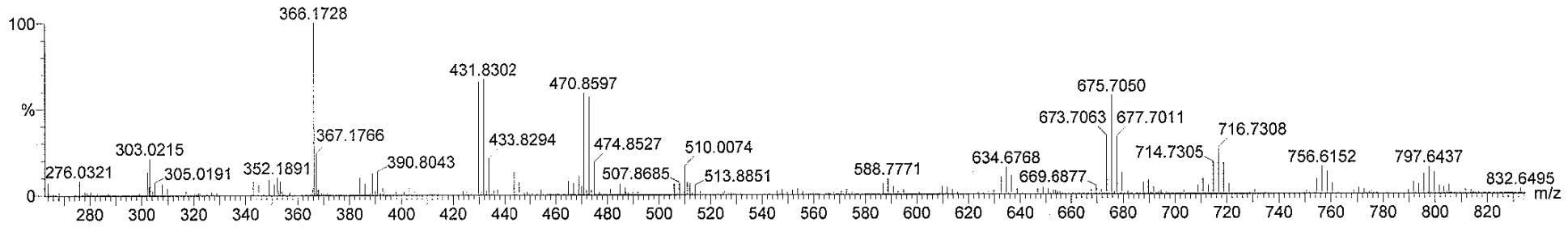
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -2.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

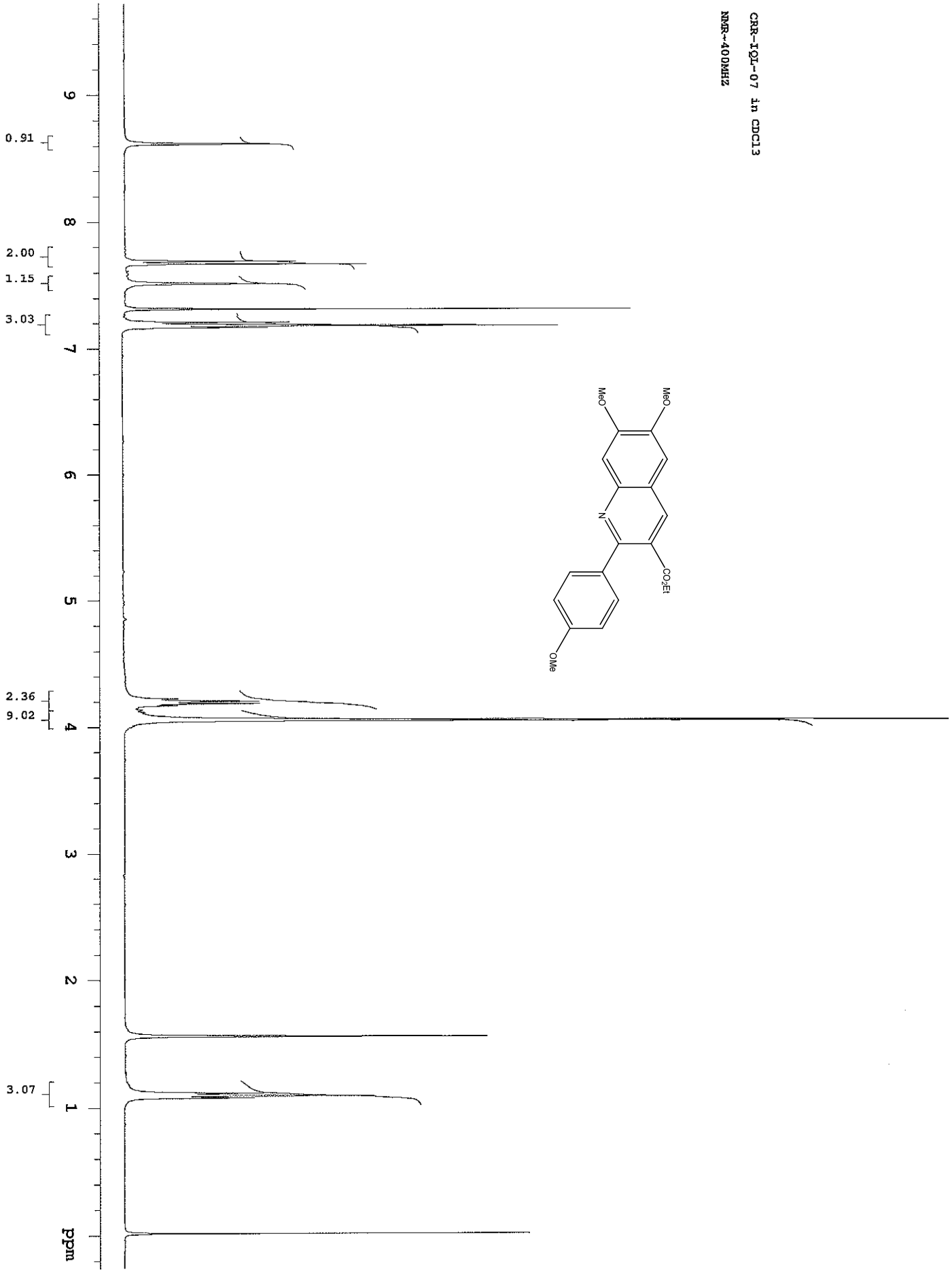
Monoisotopic Mass, Even Electron Ions
112 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-23 H: 0-25 N: 0-2 O: 0-5 S: 0-3
CRR-IQ1-10

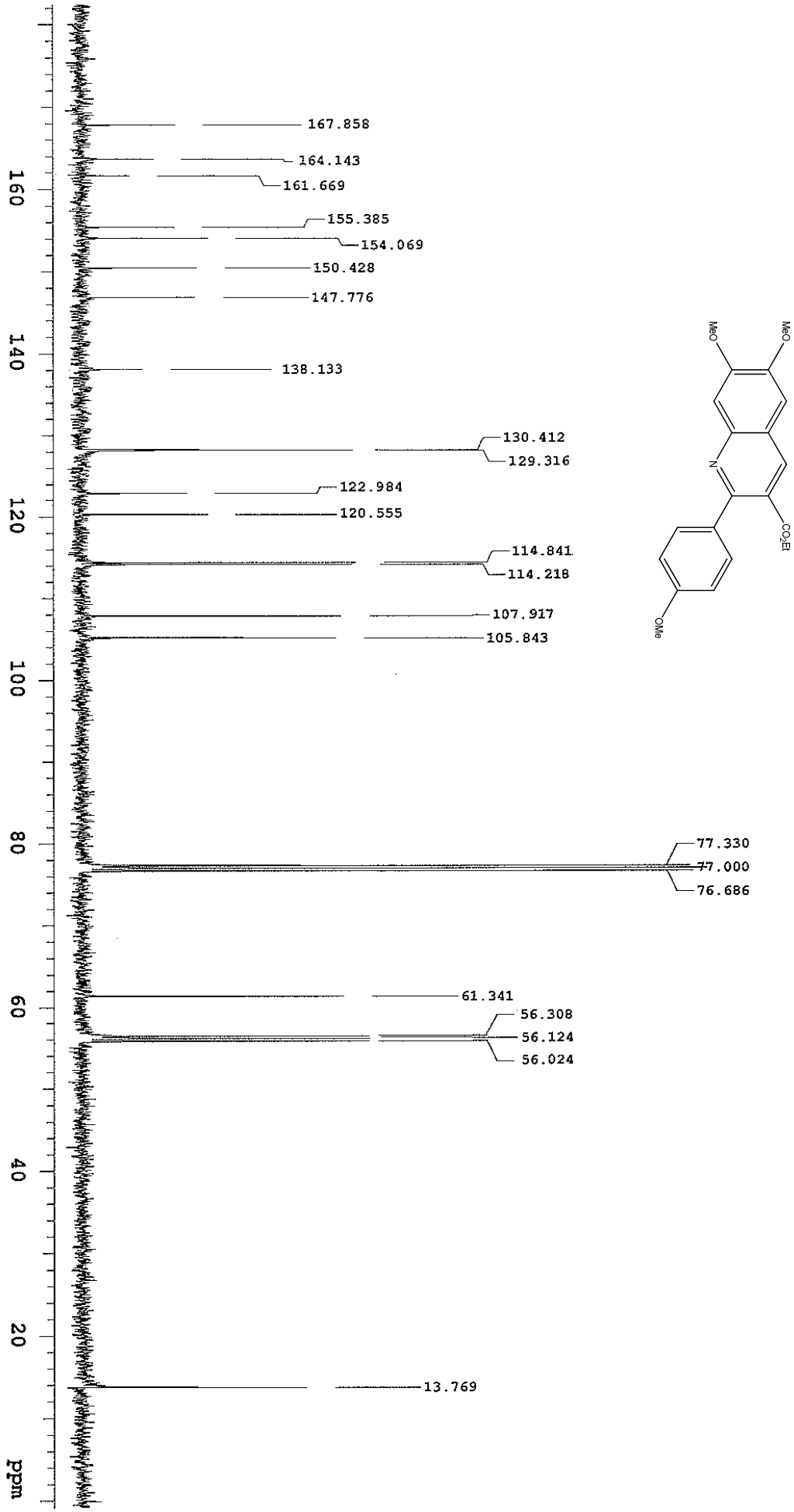
UT1112_35 33 (0.621) Cm (33:35-57:81x0.010)

1: TOF MS ES+
3.13e+003



Minimum:				-2.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
366.1728	366.1705	2.3	6.3	11.5	1.3	C22 H24 N O4



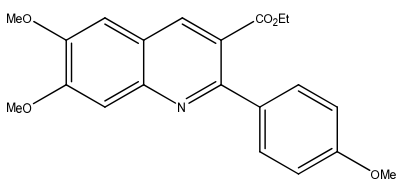


Elemental Composition Report

Single Mass Analysis

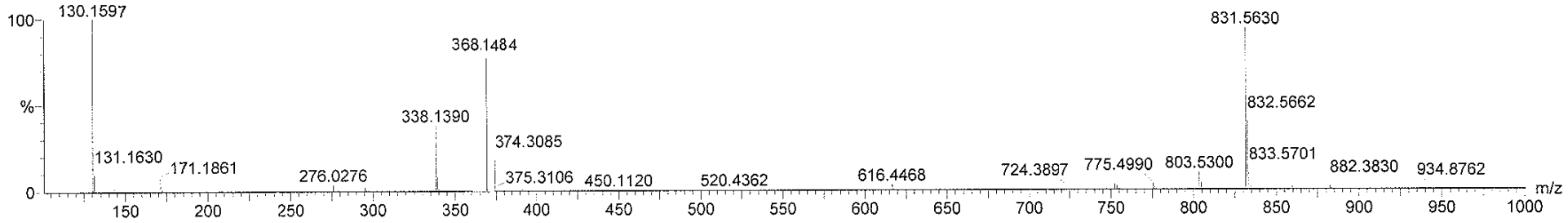
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
166 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-2 O: 0-5
CRR-IQL/07

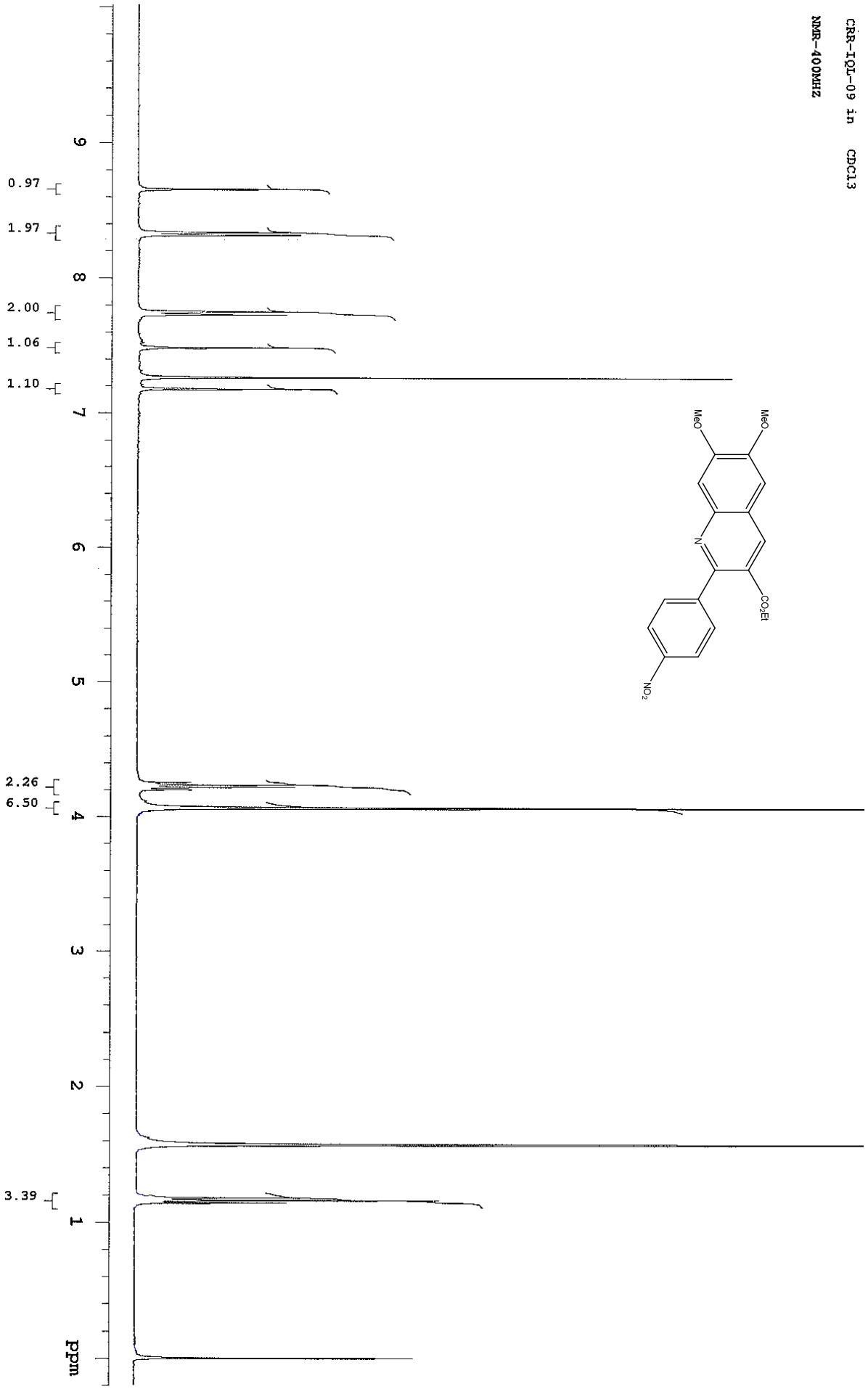


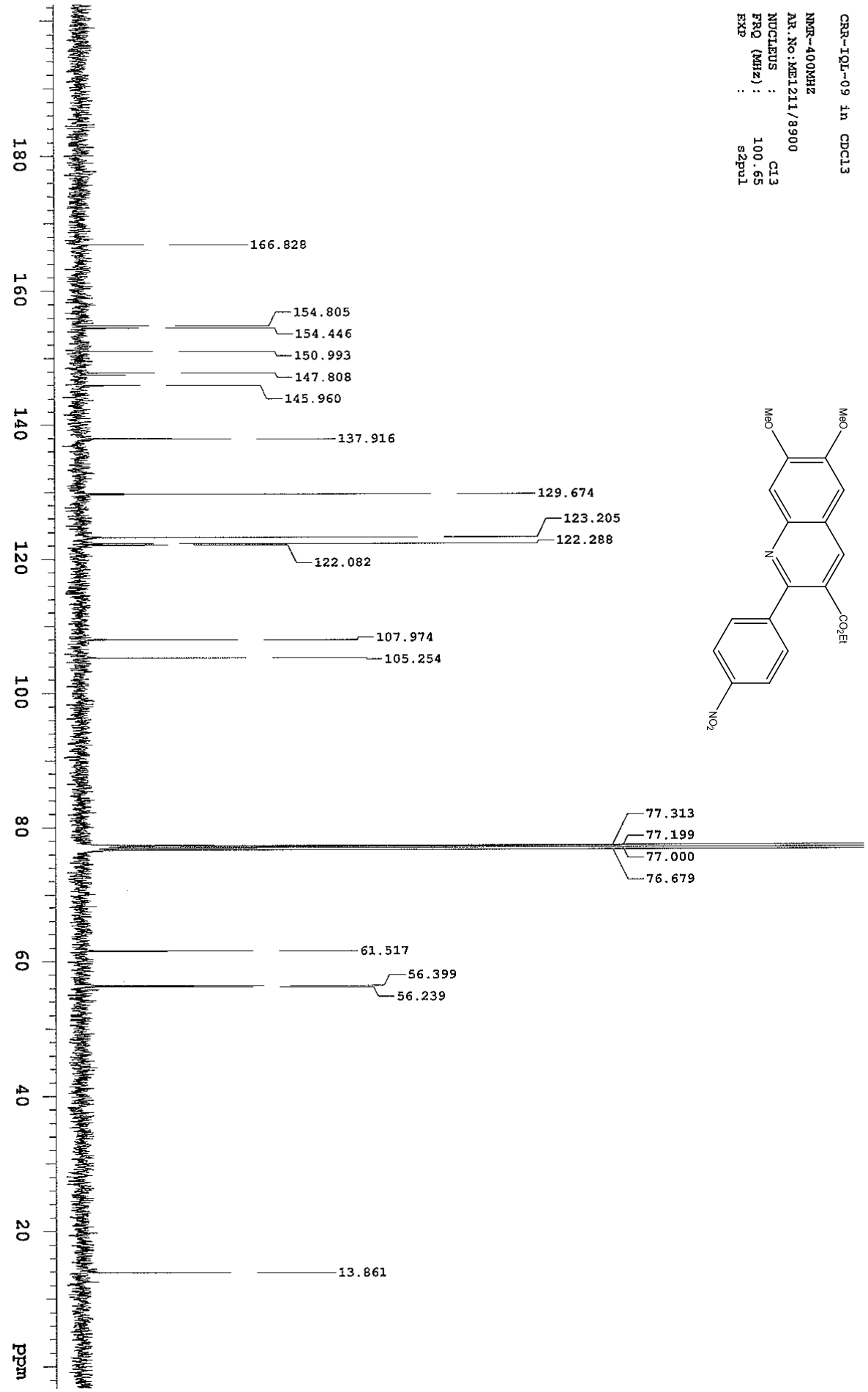
UT1011_59 23 (0.523) Cm (29:36-68:80x0.010)

1: TOF MS ES+
5.39e+004



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
368.1484	368.1486	-1.4	-0.6	11.5	3.7	C21 H22 N O5



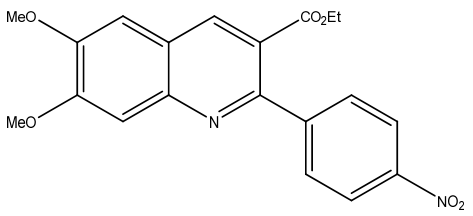


Elemental Composition Report

Single Mass Analysis

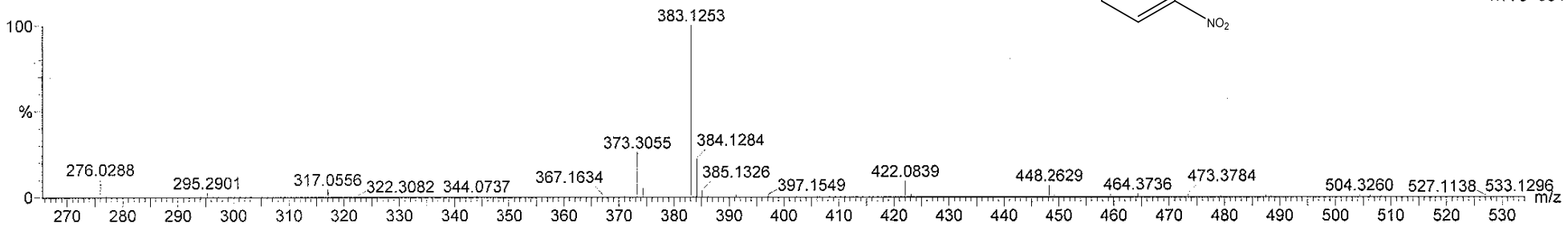
Tolerance = 5.0 PPM / DBE: min = -2.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
27 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-2 O: 0-6
CRR/IQL/09

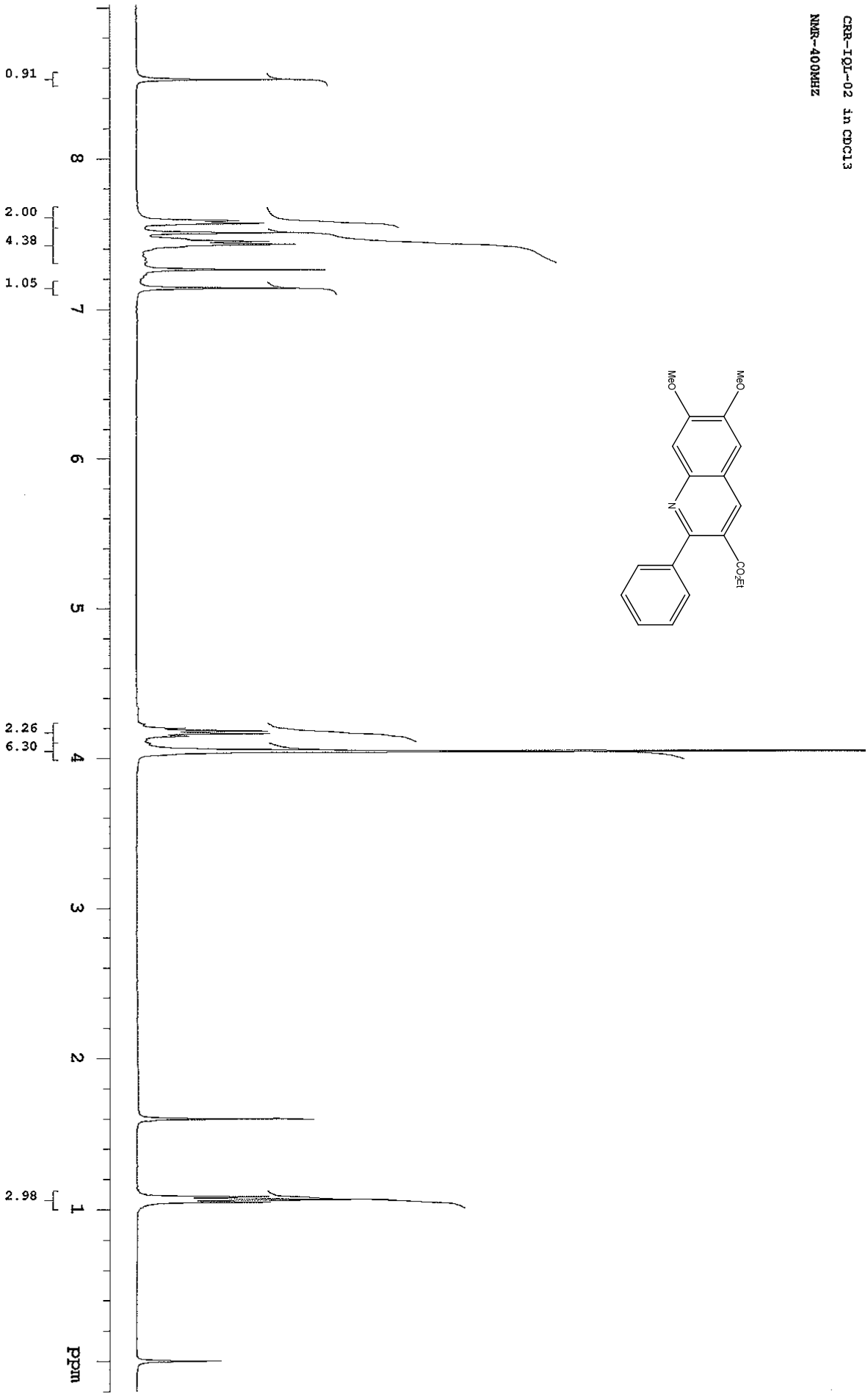


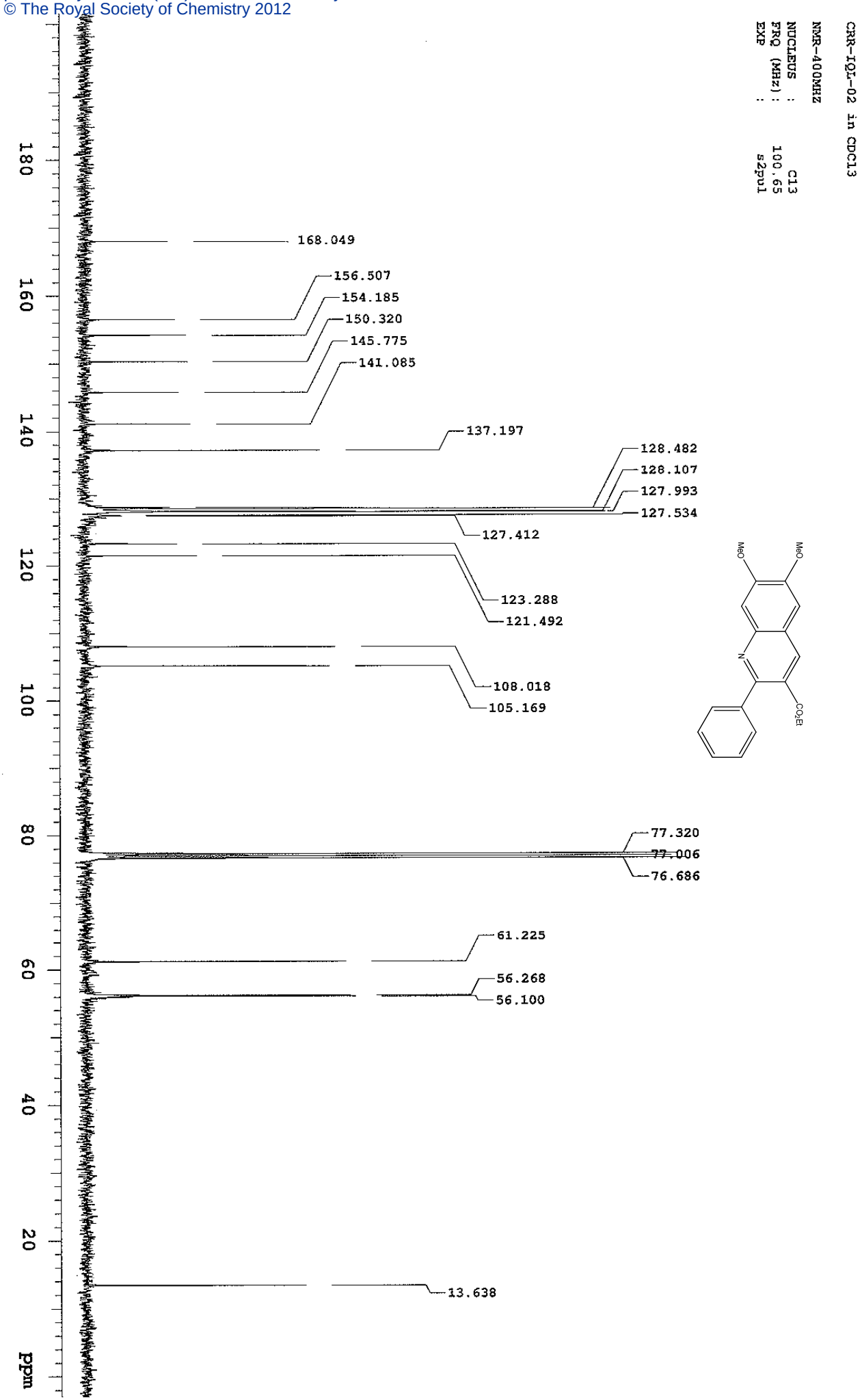
UT1111_93 18 (0.416) Cm (18:20-(5+1:4)x0.010)

1: TOF MS ES+
1.77e+004



Minimum:				-2.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
383.1253	383.1243	1.0	2.6	12.5	3.9	C20 H19 N2 O6



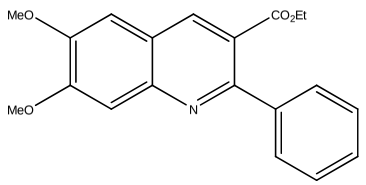


Elemental Composition Report

Single Mass Analysis

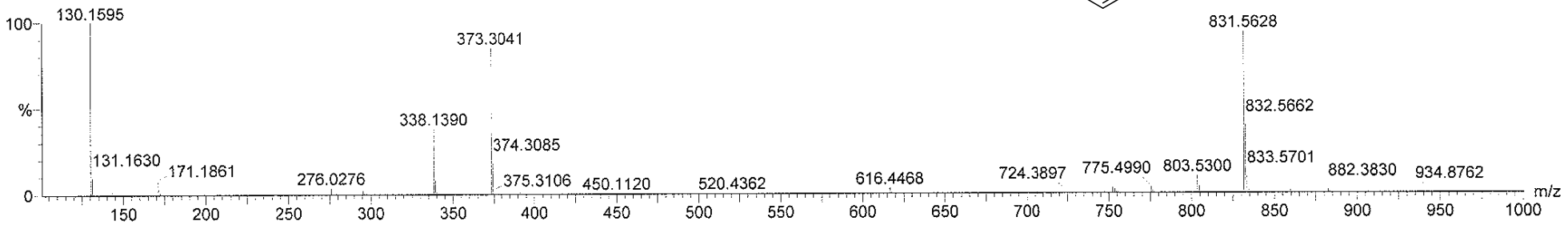
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
166 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-2 O: 0-5 F: 0-2
CRR-IQL/02

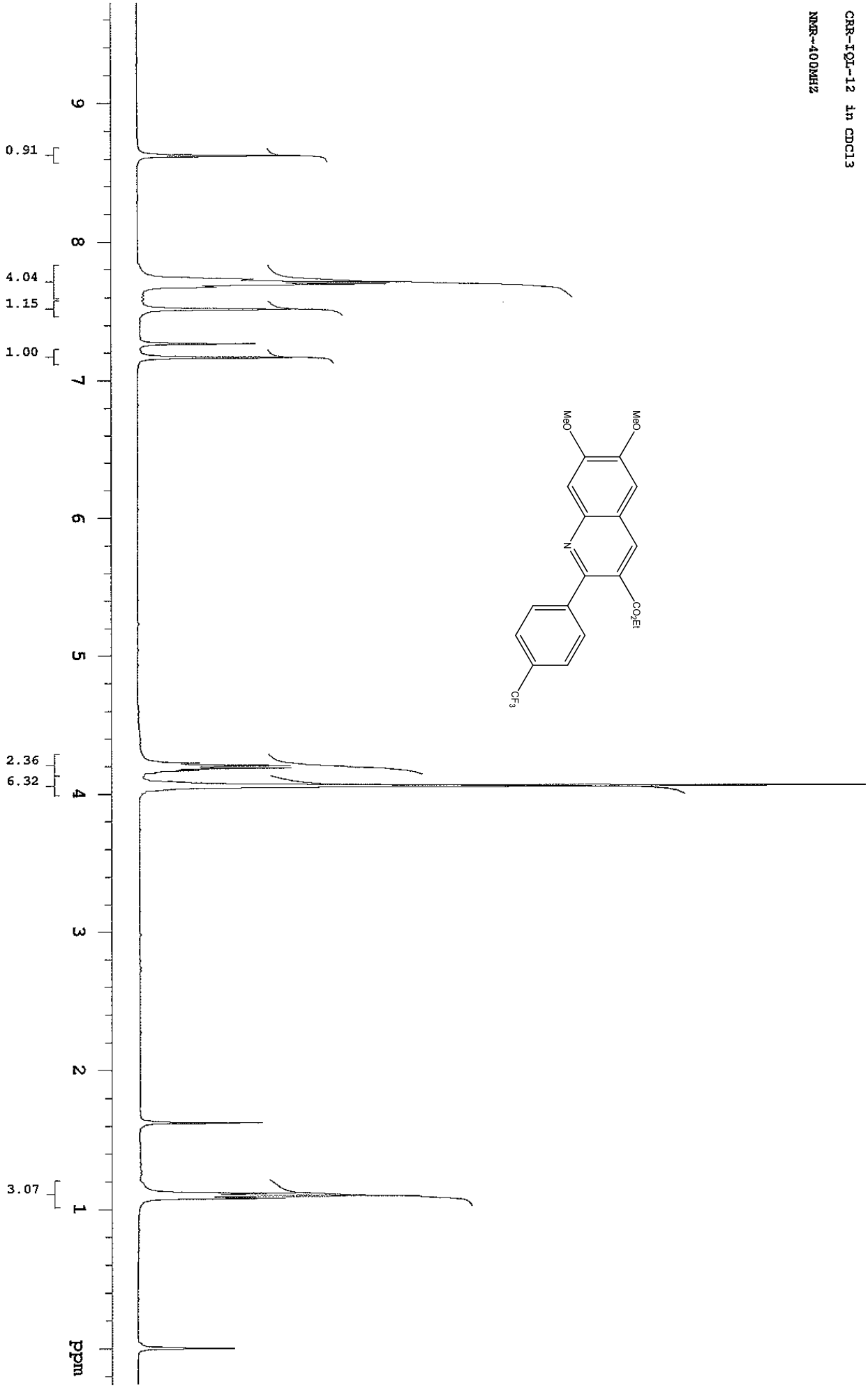


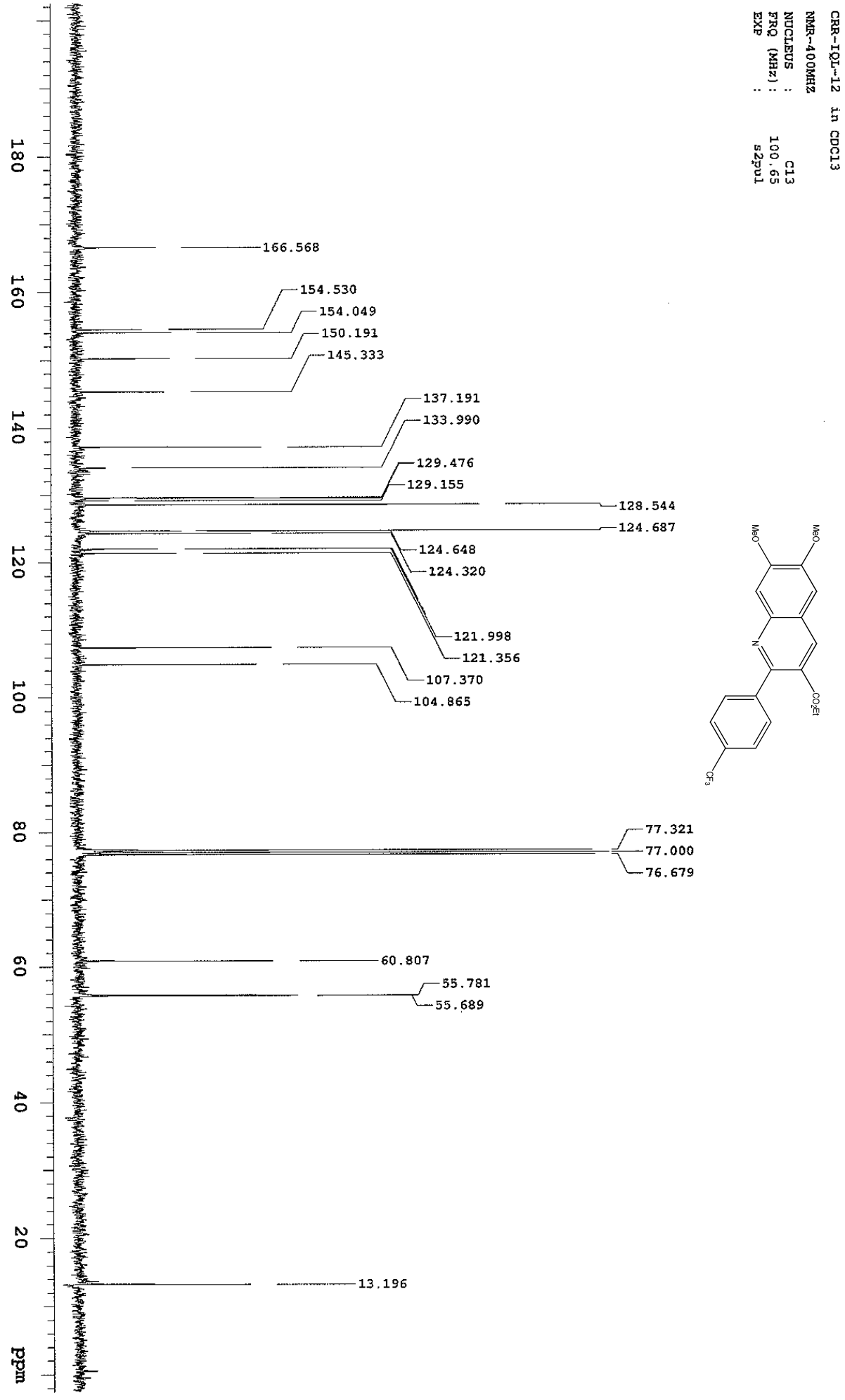
UT1011_57 29 (0.670) Cm (29:36-68:80x0.010)

1: TOF MS ES+
4.76e+004



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
338.1390	338.1392	-0.2	-0.6	11.5	3.7	C20 H20 N O4
	338.1404	-1.4	-4.1	7.5	37.7	C17 H21 N O5 F



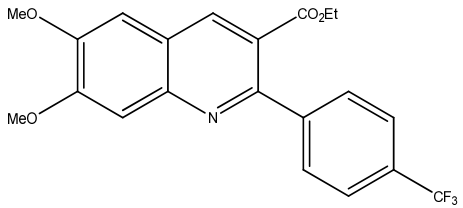


Elemental Composition Report

Single Mass Analysis

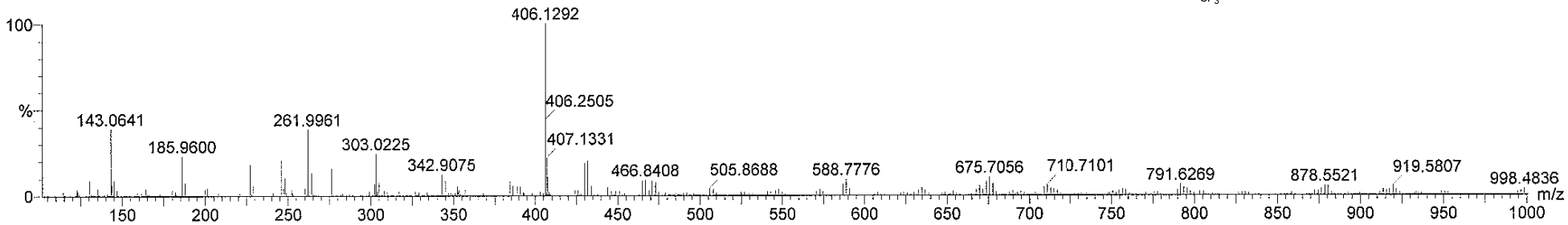
Tolerance = 8.0 PPM / DBE: min = -2.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
65 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-2 O: 0-5 F: 0-3
CRR-IQ1-12

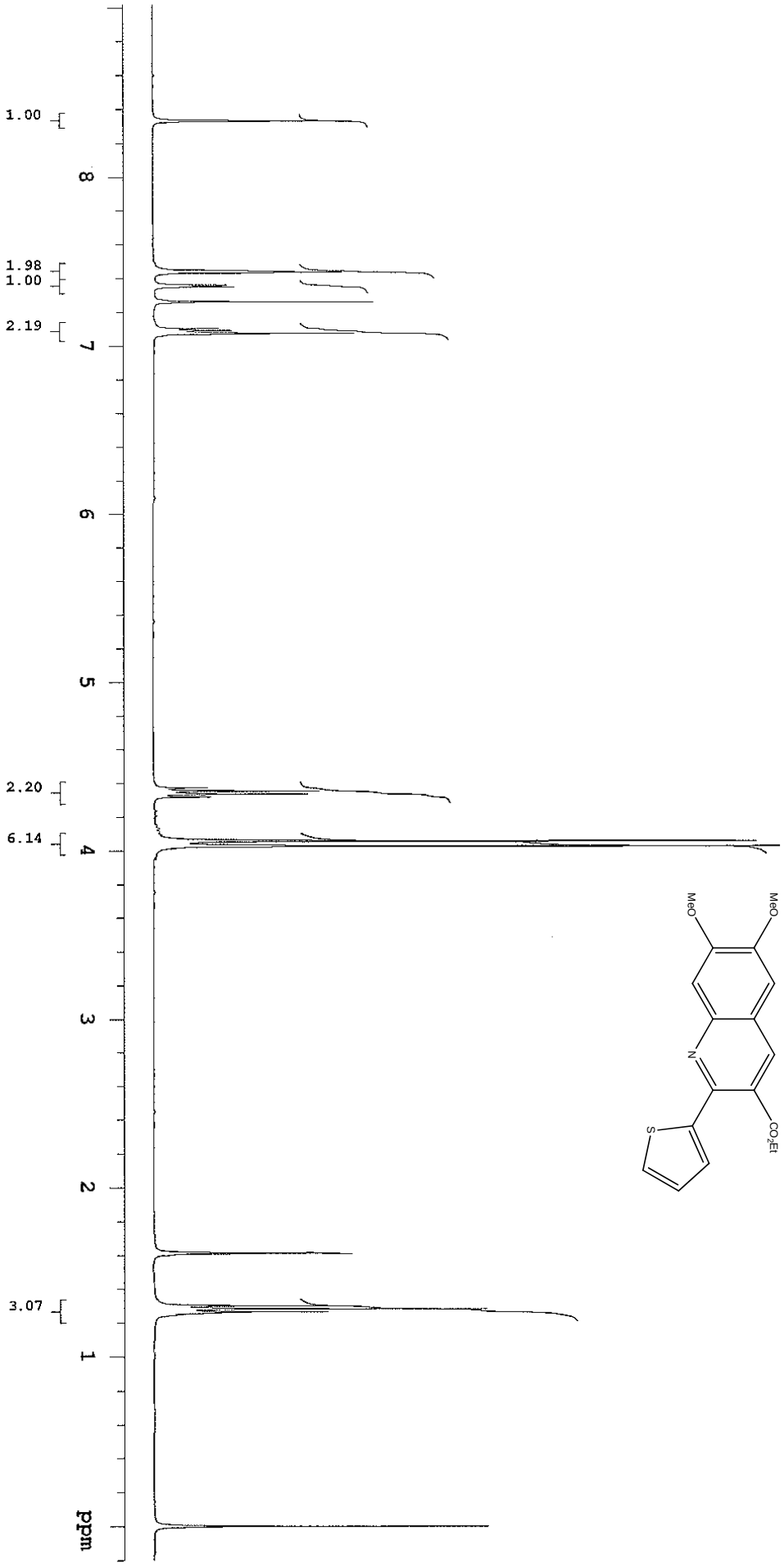


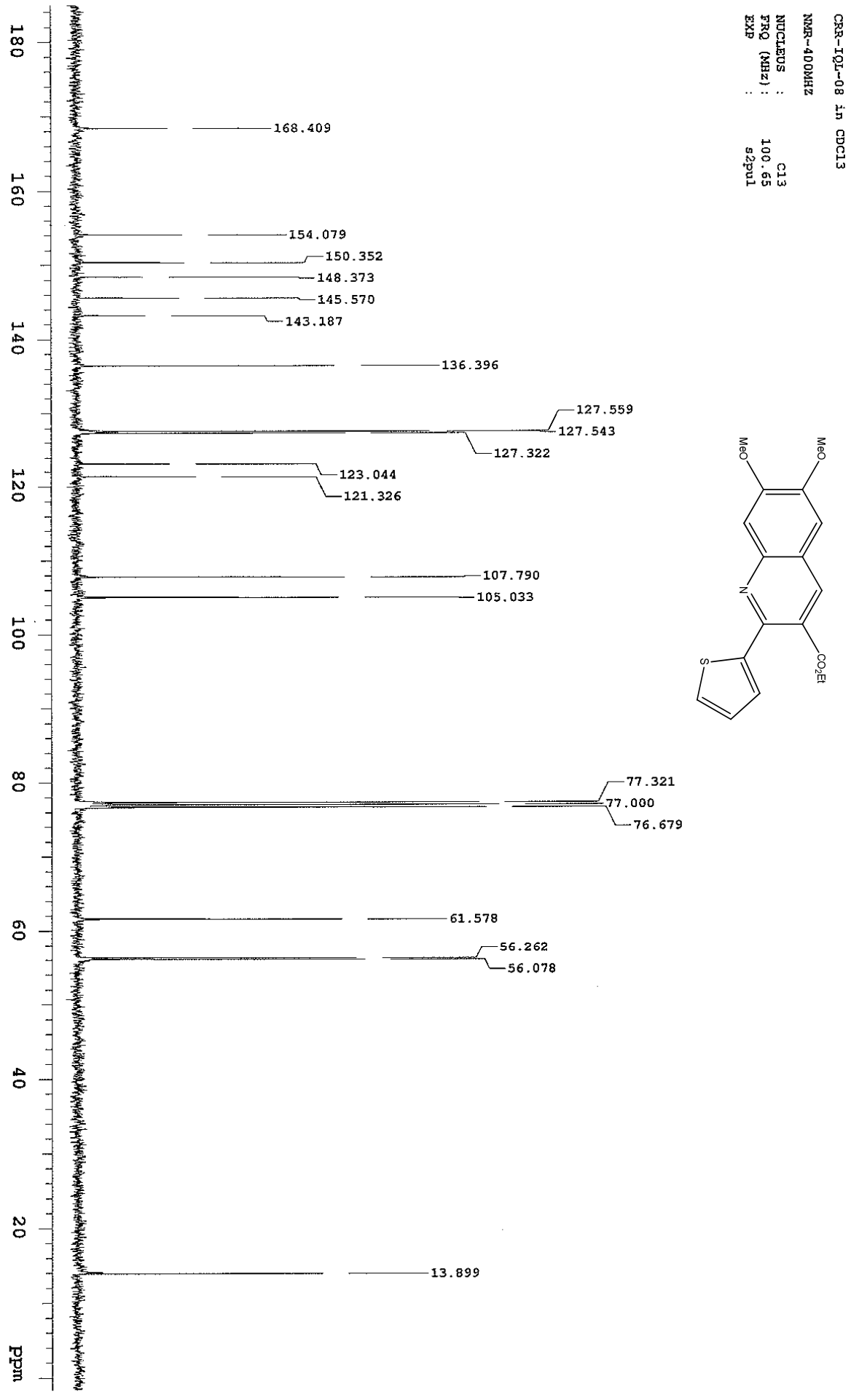
UT1112_34 23 (0.426) Cm (21:23-35:68x0.010)

1: TOF MS ES+
5.74e+003



Minimum:				-2.0		
Maximum:		5.0	8.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
406.1292	406.1266	2.6	6.4	11.5	5.1	C21 H19 N O4 F3



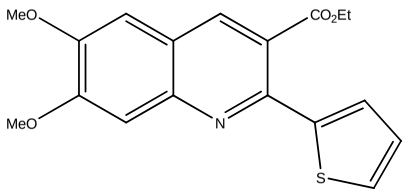


Elemental Composition Report

Single Mass Analysis

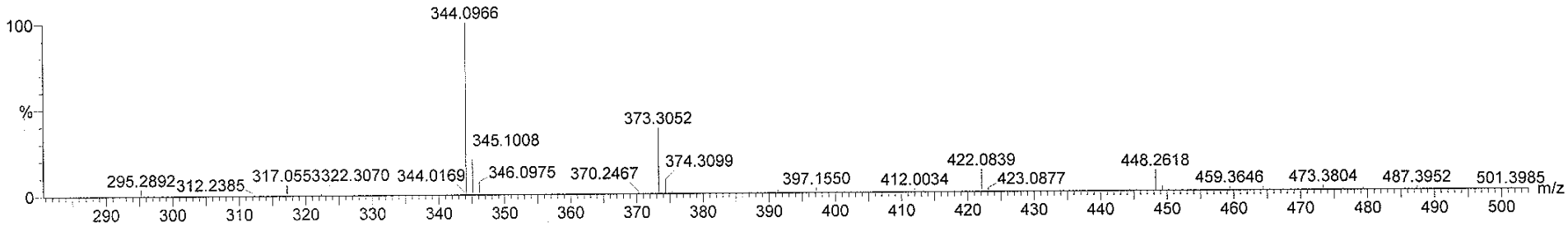
Tolerance = 5.0 PPM / DBE: min = -2.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
34 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-1 O: 0-4 S: 0-1
CRR/IQL/08

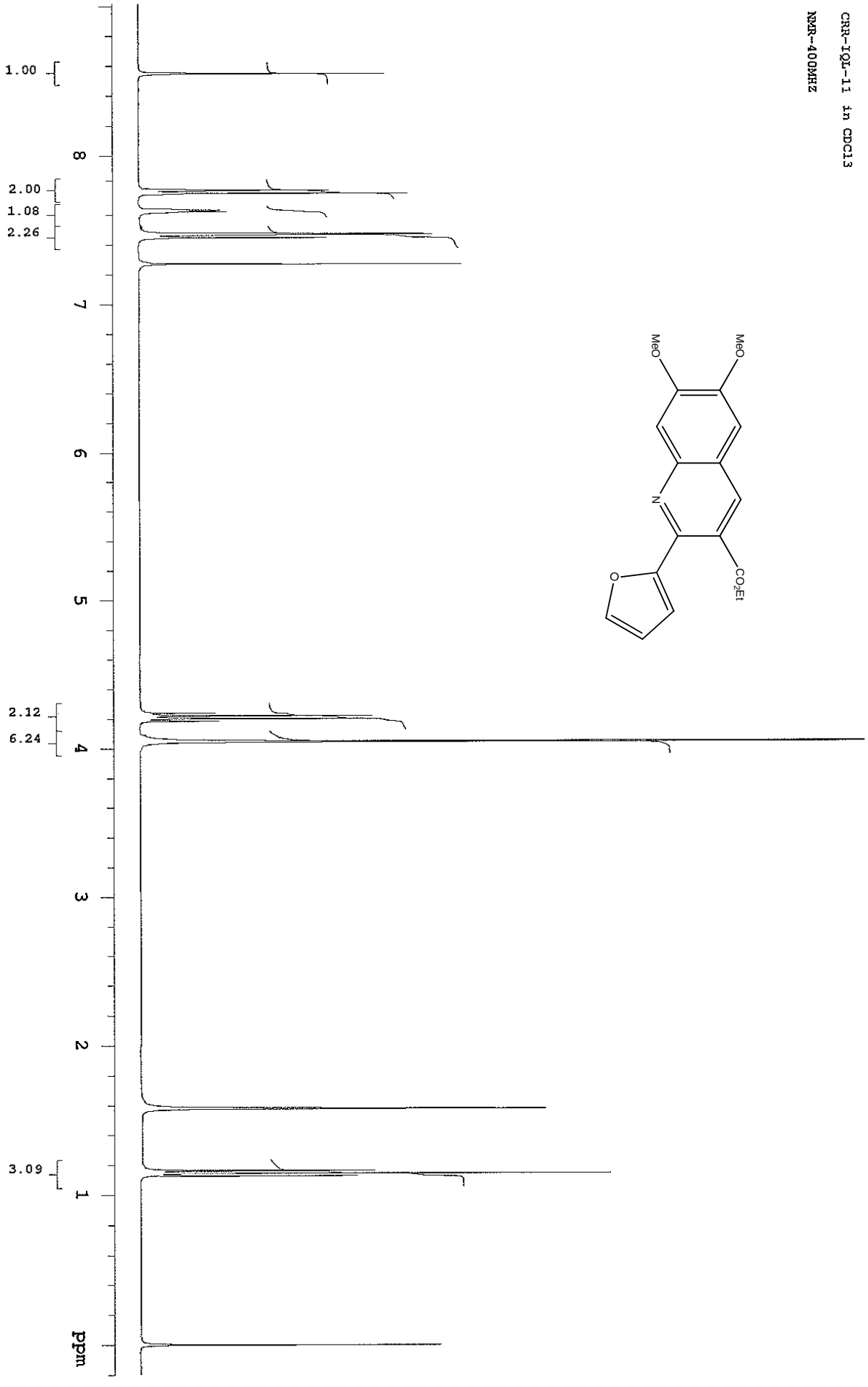


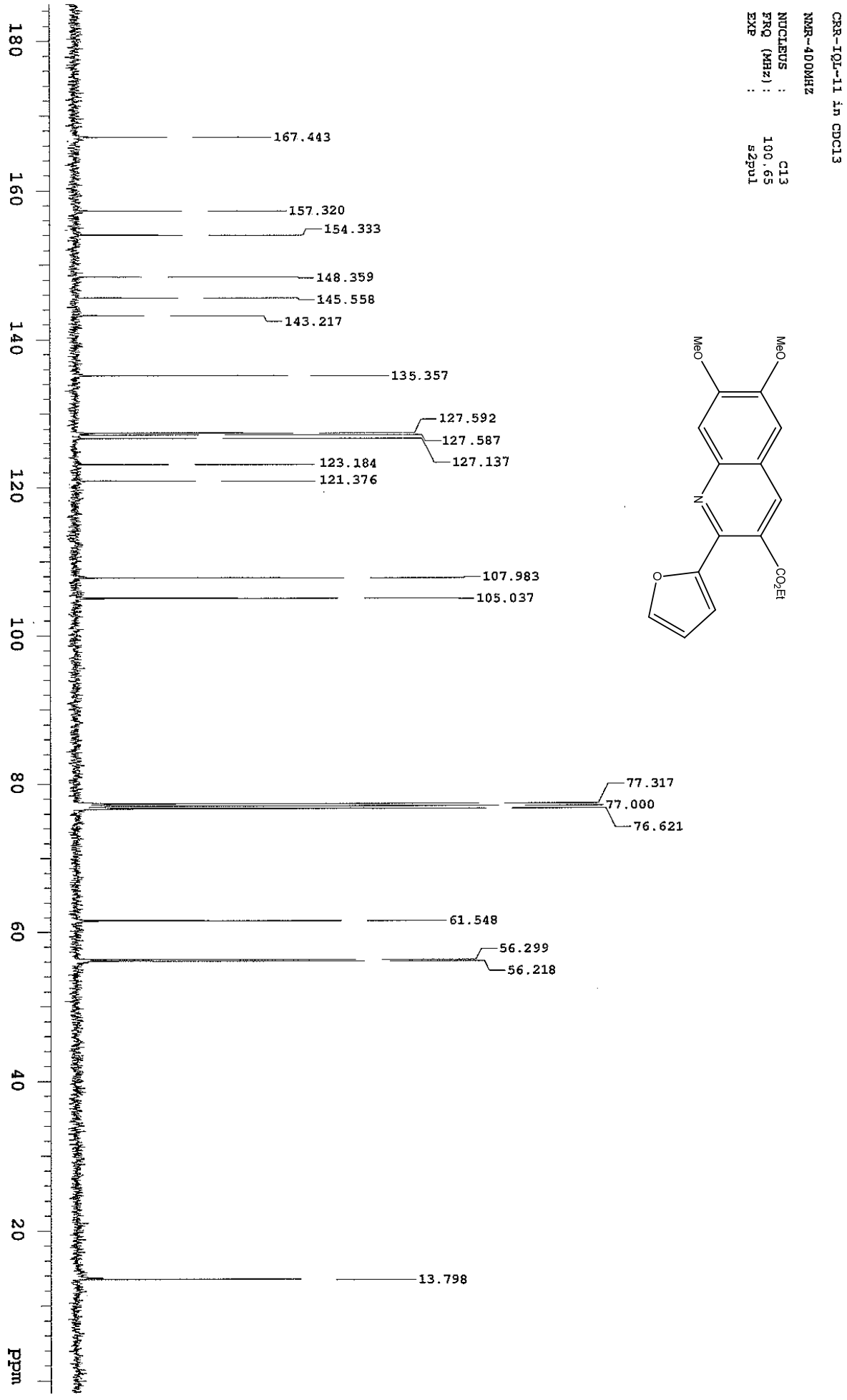
UT1111_92 22 (0.506) Cm (22:25-1:2x0.010)

1: TOF MS ES+
1.62e+004



Minimum:				-2.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
344.0966	344.0957	0.9	2.6	10.5	3.4	C18 H18 N O4 S



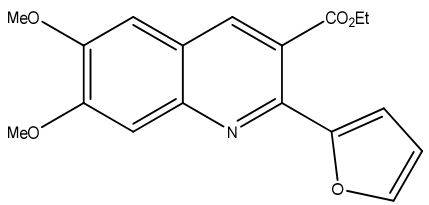


Elemental Composition Report

Single Mass Analysis

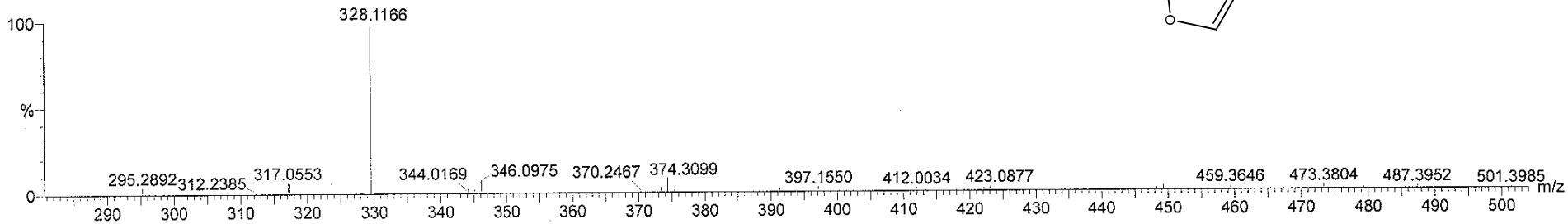
Tolerance = 5.0 PPM / DBE: min = -2.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
34 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-1 O: 0-5
CRR/IQL/11

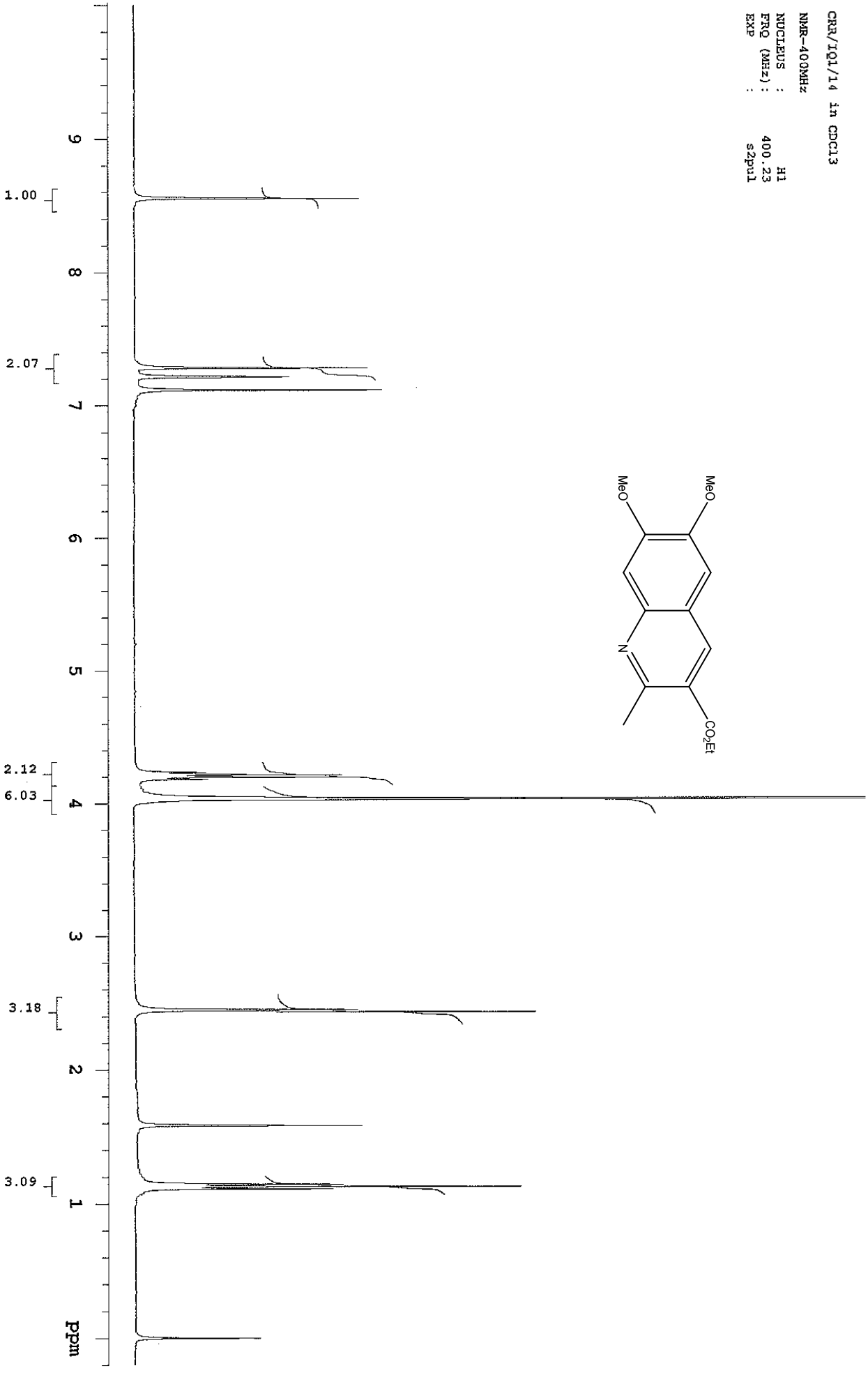


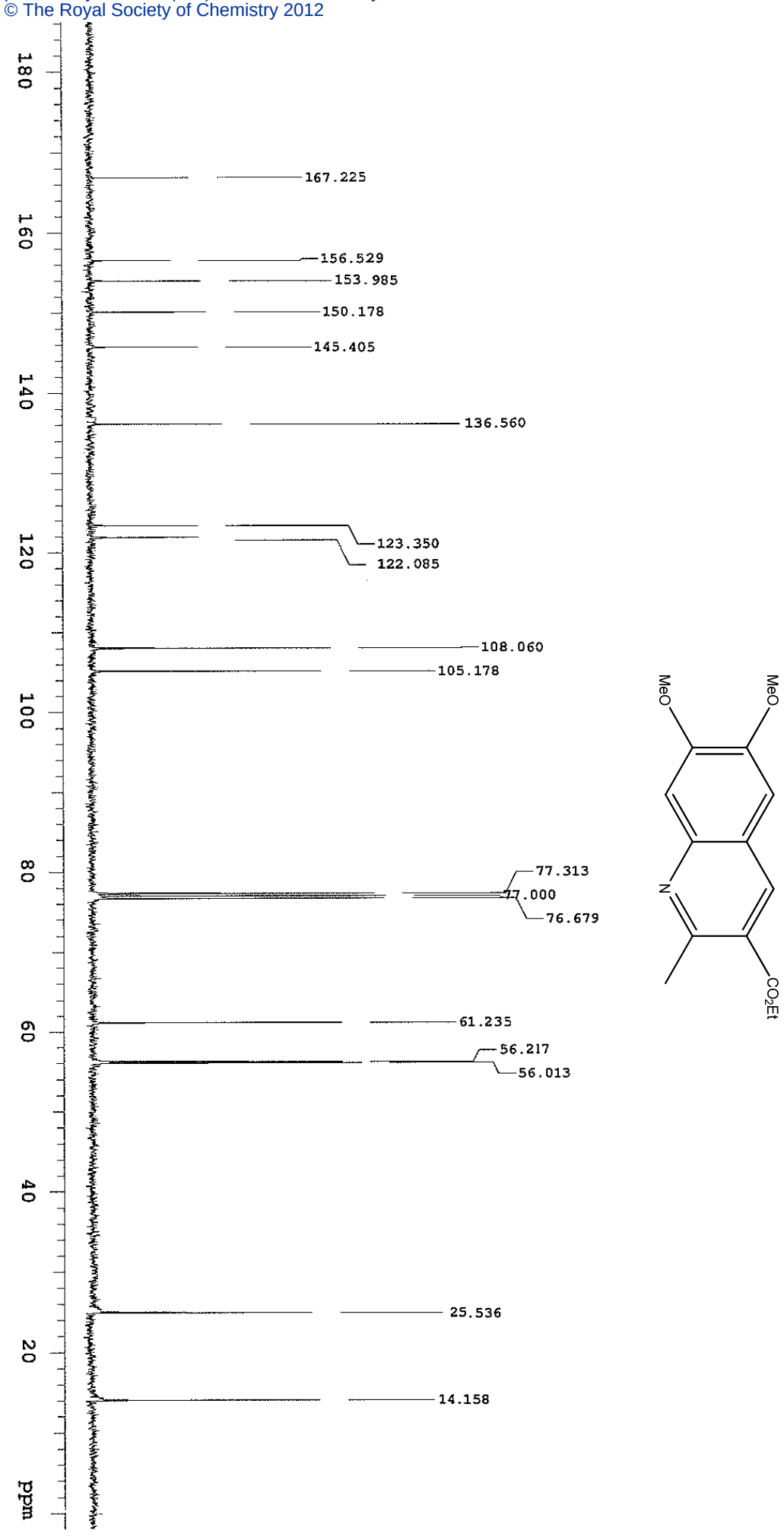
UT1111_92 25 (0.580) Cm (22:25-1:2x0.010)

1: TOF MS ES+
1.55e+004



Minimum:				-2.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
328.1166	328.1156	0.9	2.6	10.5	3.4	C18 H18 N O5

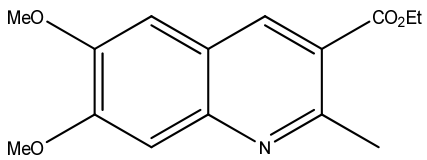




Elemental Composition Report

Single Mass Analysis

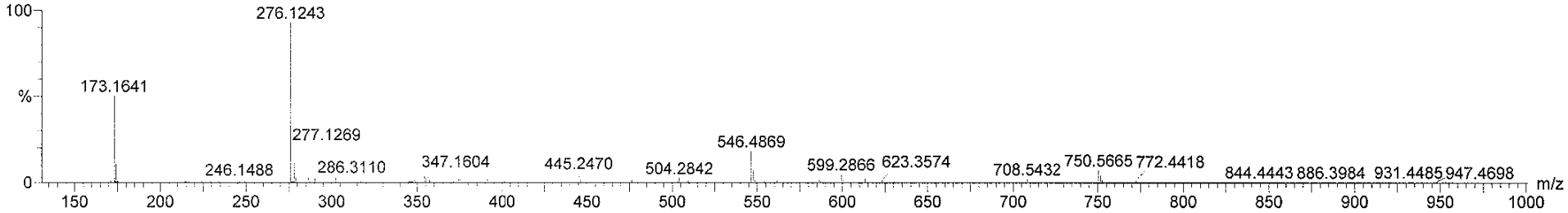
Tolerance = 50.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



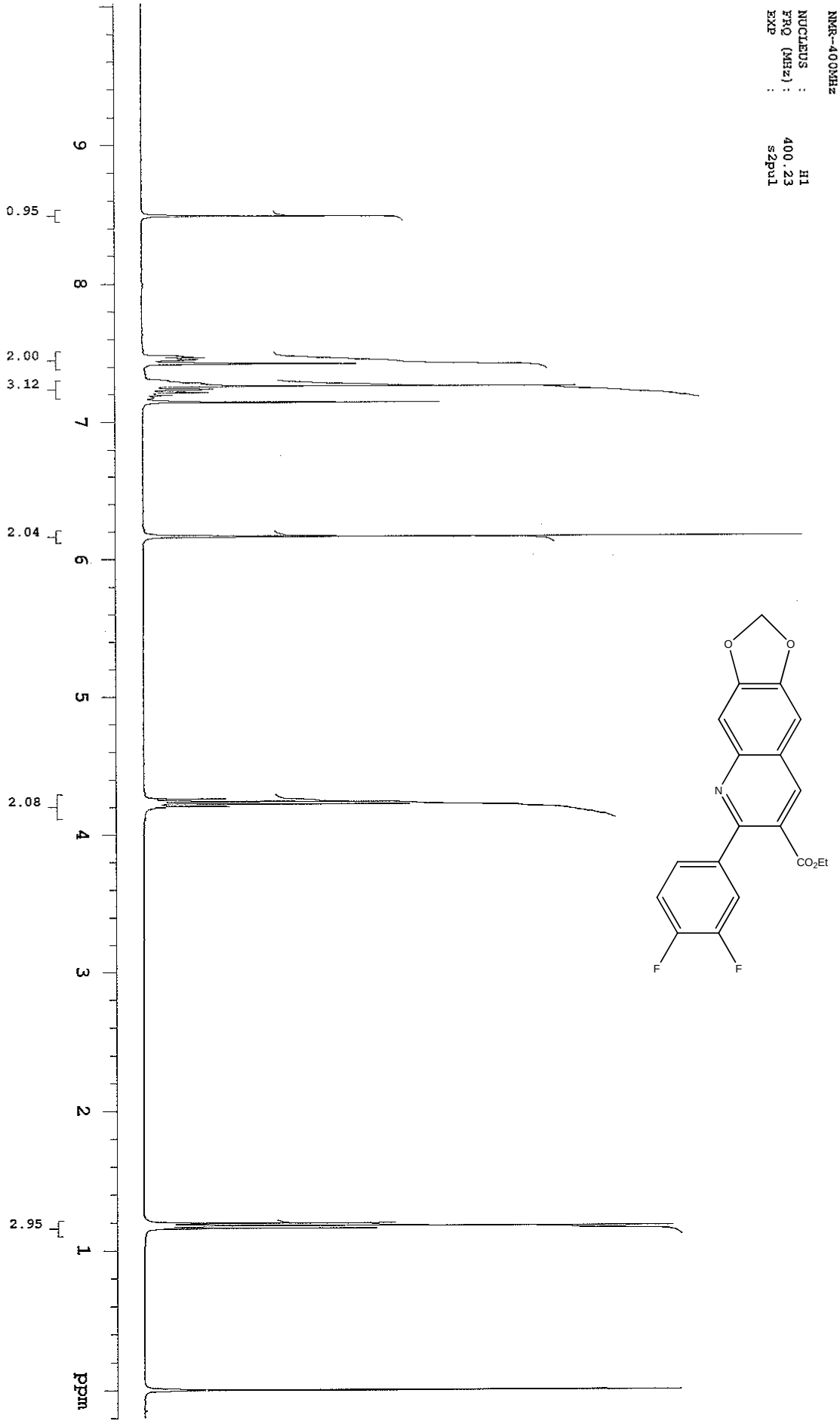
Monoisotopic Mass, Even Electron Ions
36 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-28 N: 0-2 O: 0-4
CRR/IQL/14

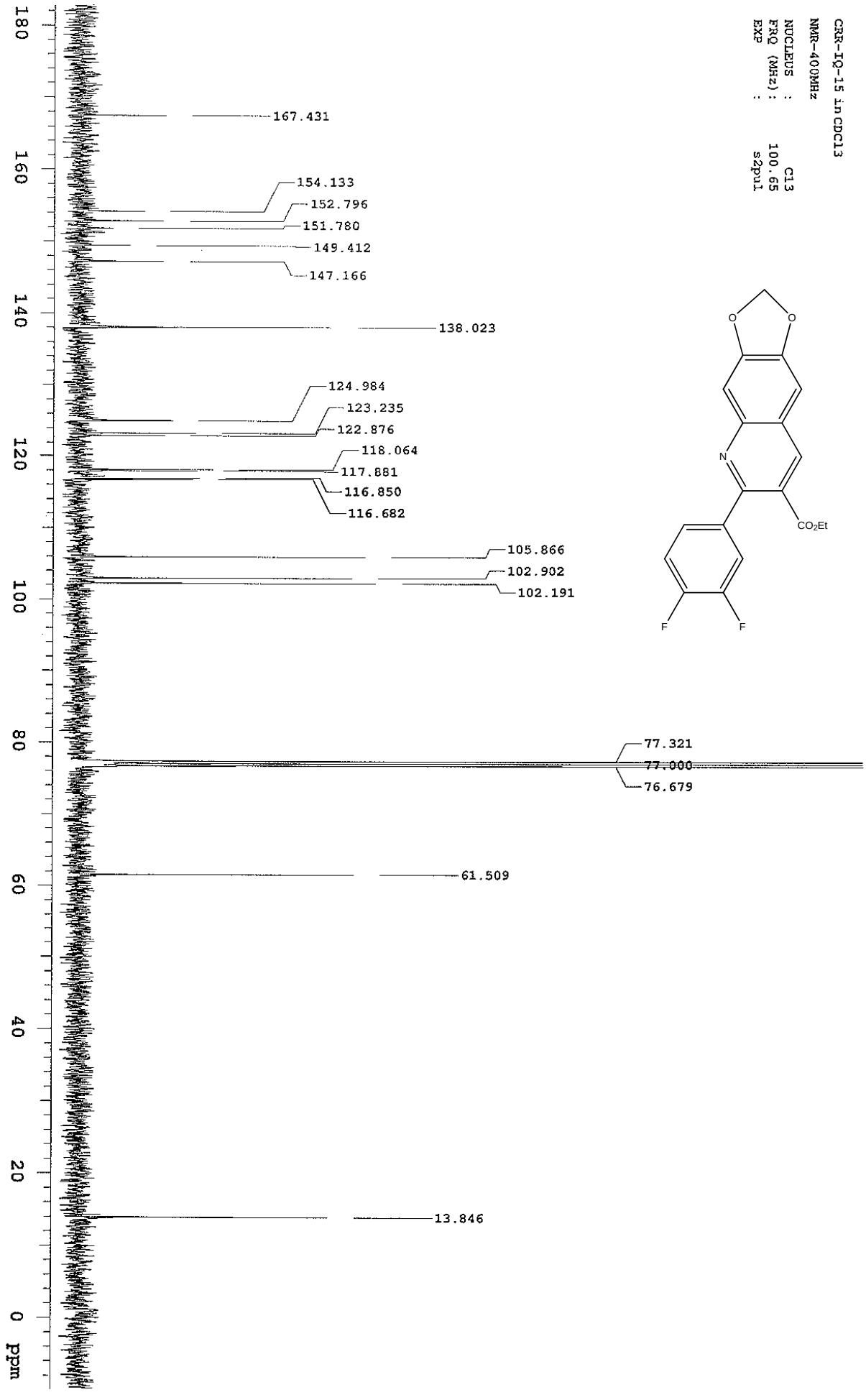
UT0215_82 176 (3.253) Cm (175:176-146:148x0.010)

1: TOF MS ES+
7.36e+003



Minimum:				-5.0		
Maximum:		5.0	50.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
276.1243	276.1236	0.7	2.5	7.5	293.6	C15 H18 N O4



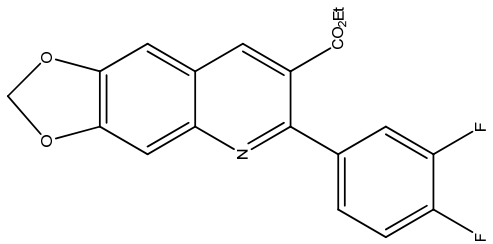


Elemental Composition Report

Single Mass Analysis

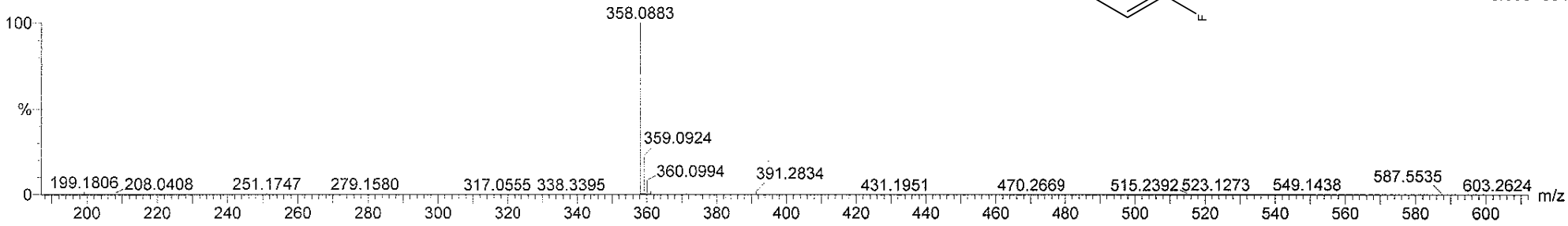
Tolerance = 5.0 PPM / DBE: min = 10.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 5-20 H: 10-15 N: 0-1 O: 0-4 F: 0-2
CRR-IQL/15

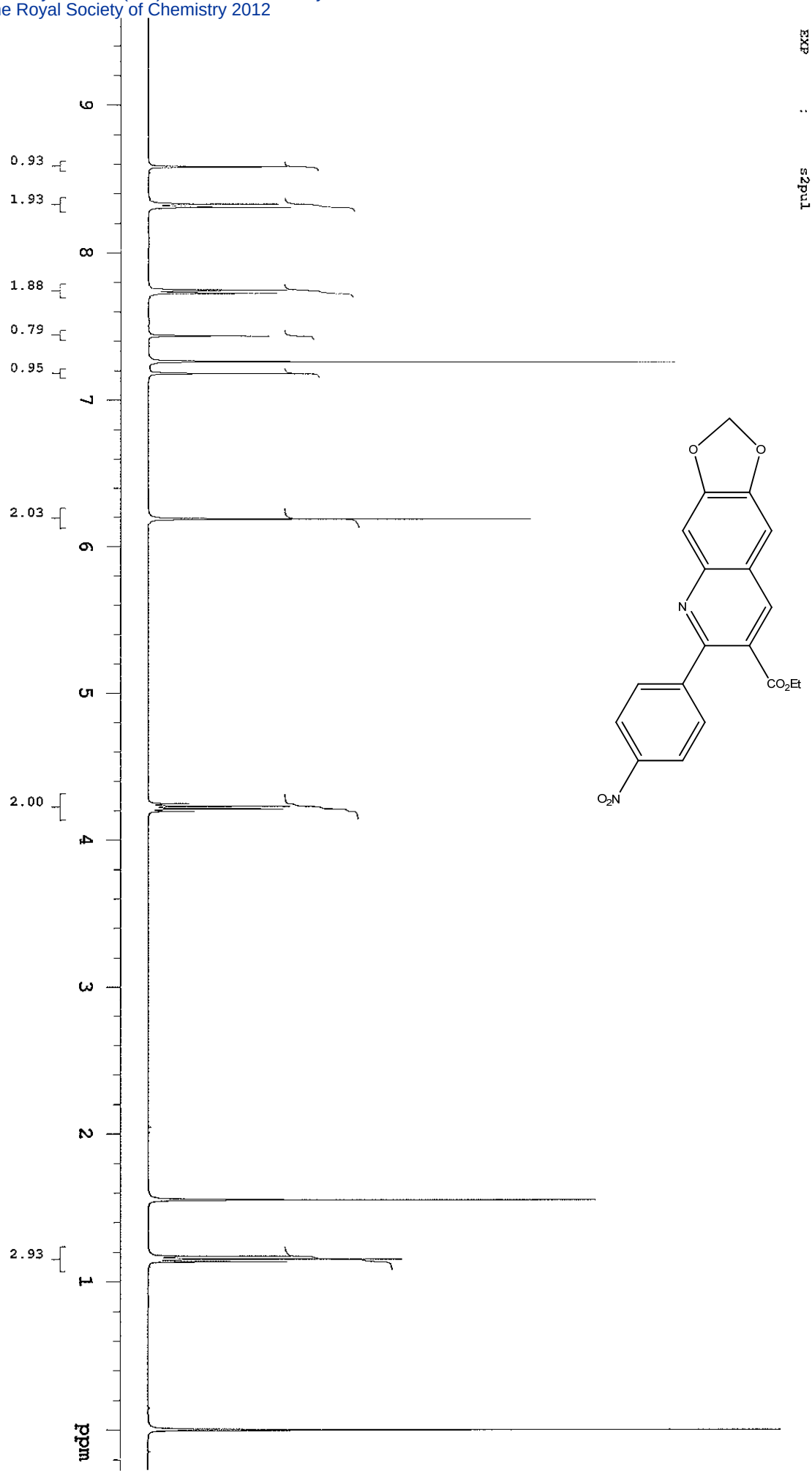


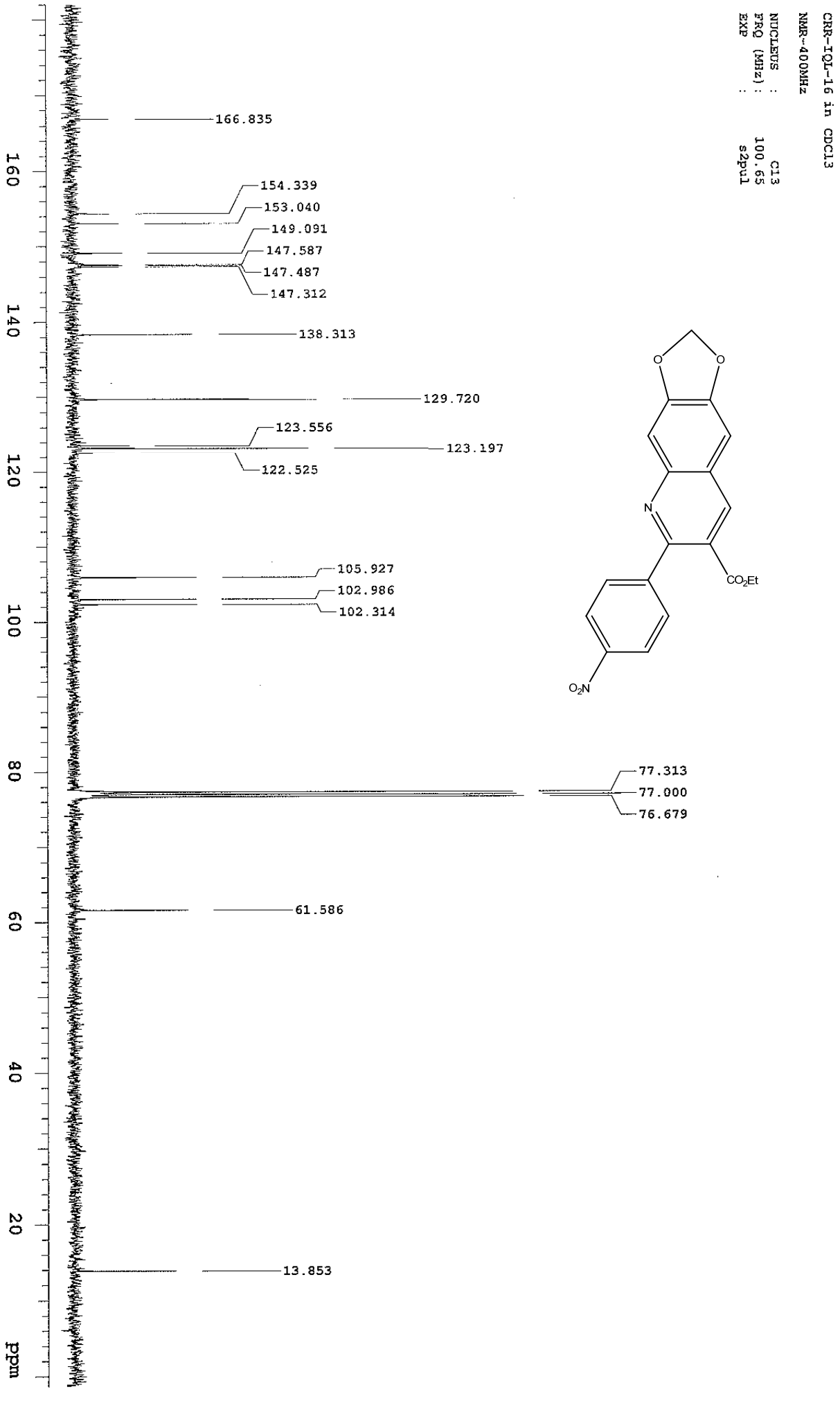
UT0215_127 28 (0.515) Cm (28:29-1:5x0.010)

1: TOF MS ES+
3.36e+004



Minimum:				10.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
358.0883	358.0891	-0.8	-2.2	12.5	518.6	C19 H14 N O4 F2



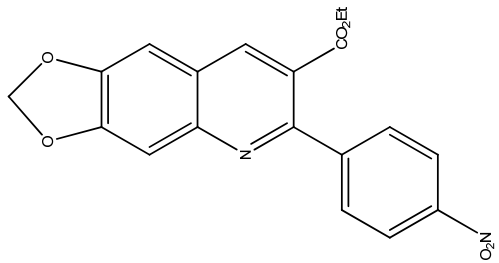


Elemental Composition Report

Single Mass Analysis

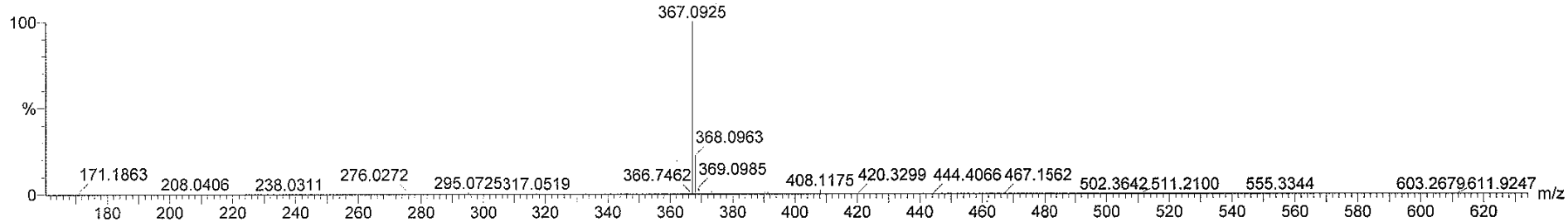
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-20 N: 0-2 O: 0-6
CRR/IQL/16

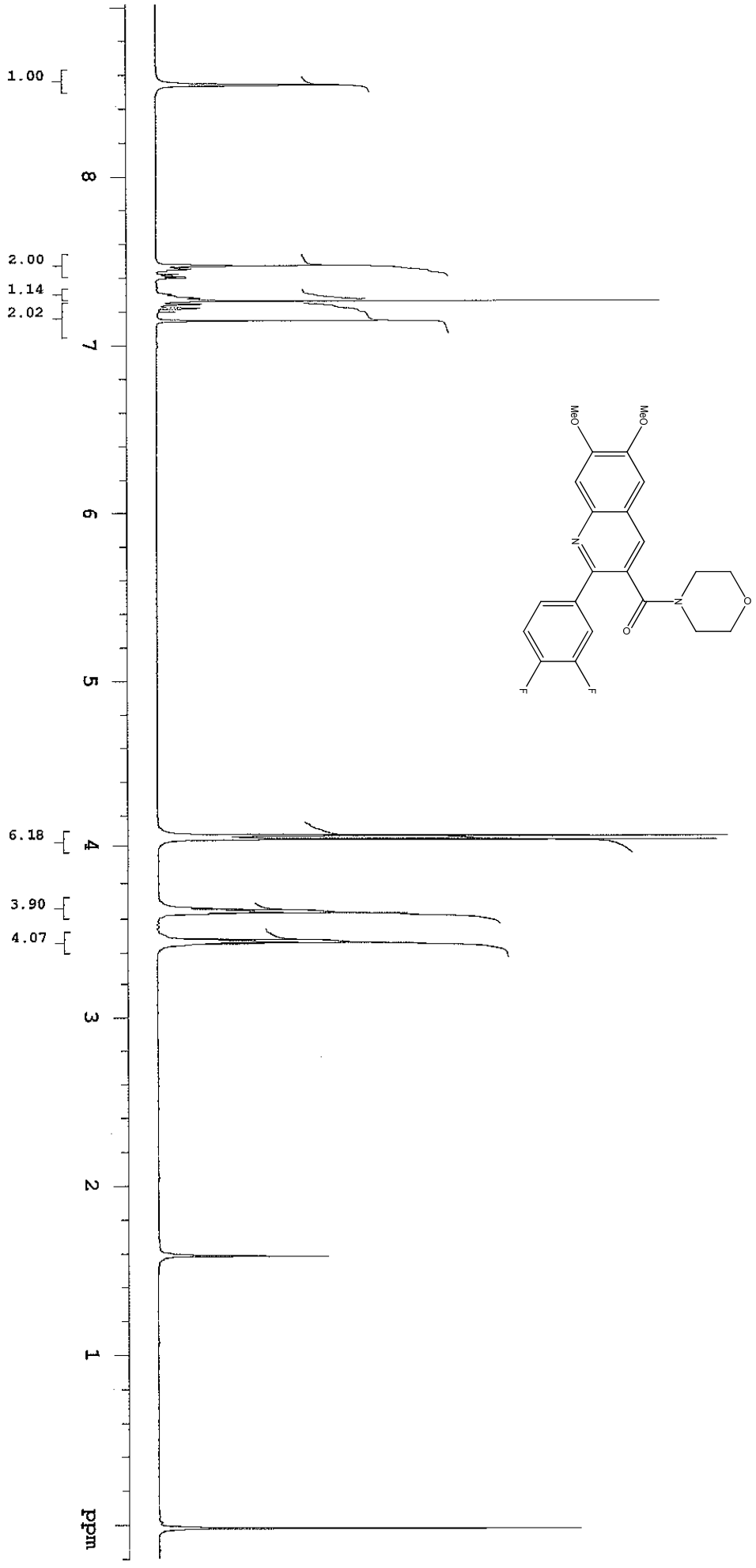


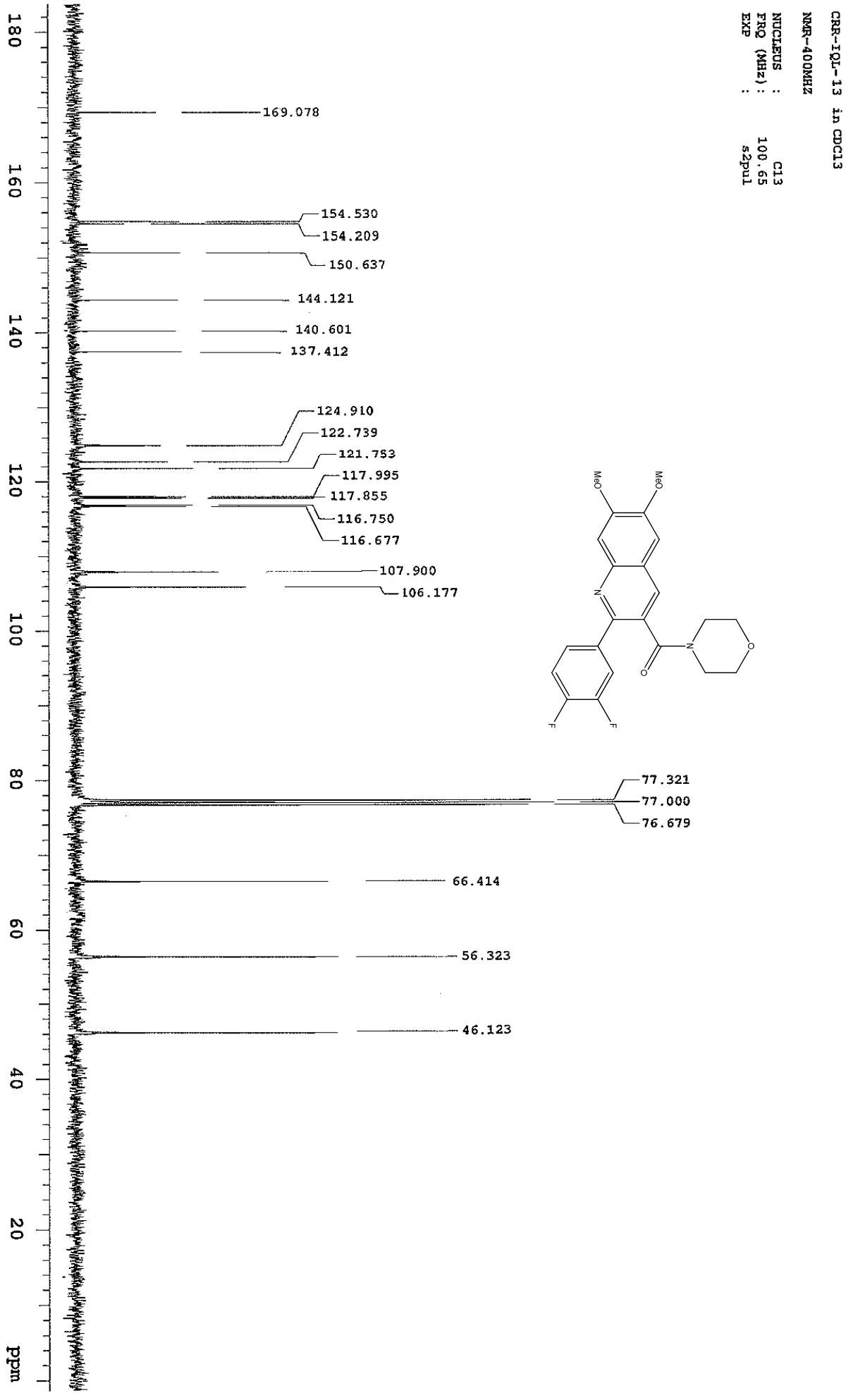
UT0215_139 11 (0.204) Cm (9:13)

1: TOF MS ES+
7.86e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
367.0925	367.0930	-0.5	-1.4	13.5	0.1	C19 H15 N2 O6



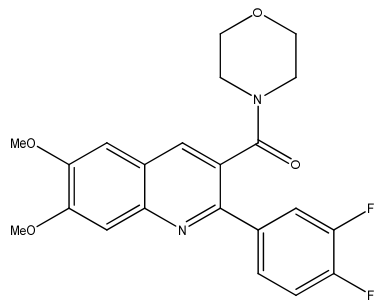


Elemental Composition Report

Single Mass Analysis

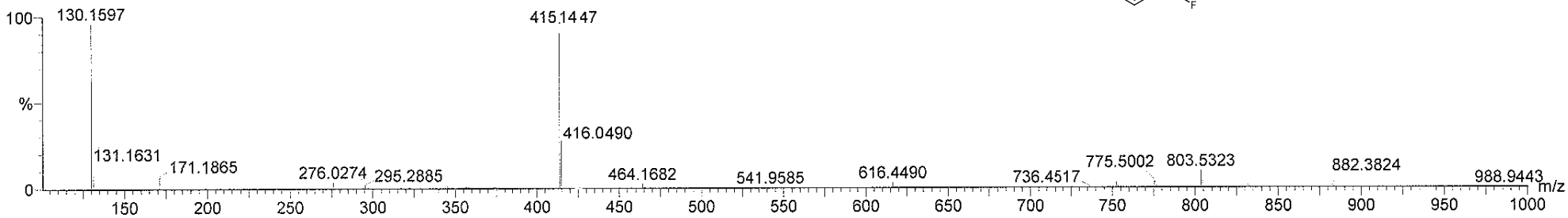
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
137 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-2 O: 0-4 F: 0-2
CRR-IQL/13



UT1112_54 27 (0.615) Cm (27:30-73:80x0.010)

1: TOF MS ES+
2.49e+004



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
415.1447	415.1443	1.0	2.6	11.5	3.9	C22 H21 N2 O4 F2