Electronic Supplementary Material (ESI) for RSC Advances

Copies of spectra

Iodine catalyzed four-component reaction: A straightforward one-pot synthesis of functionalized pyrroles under metal-free conditions

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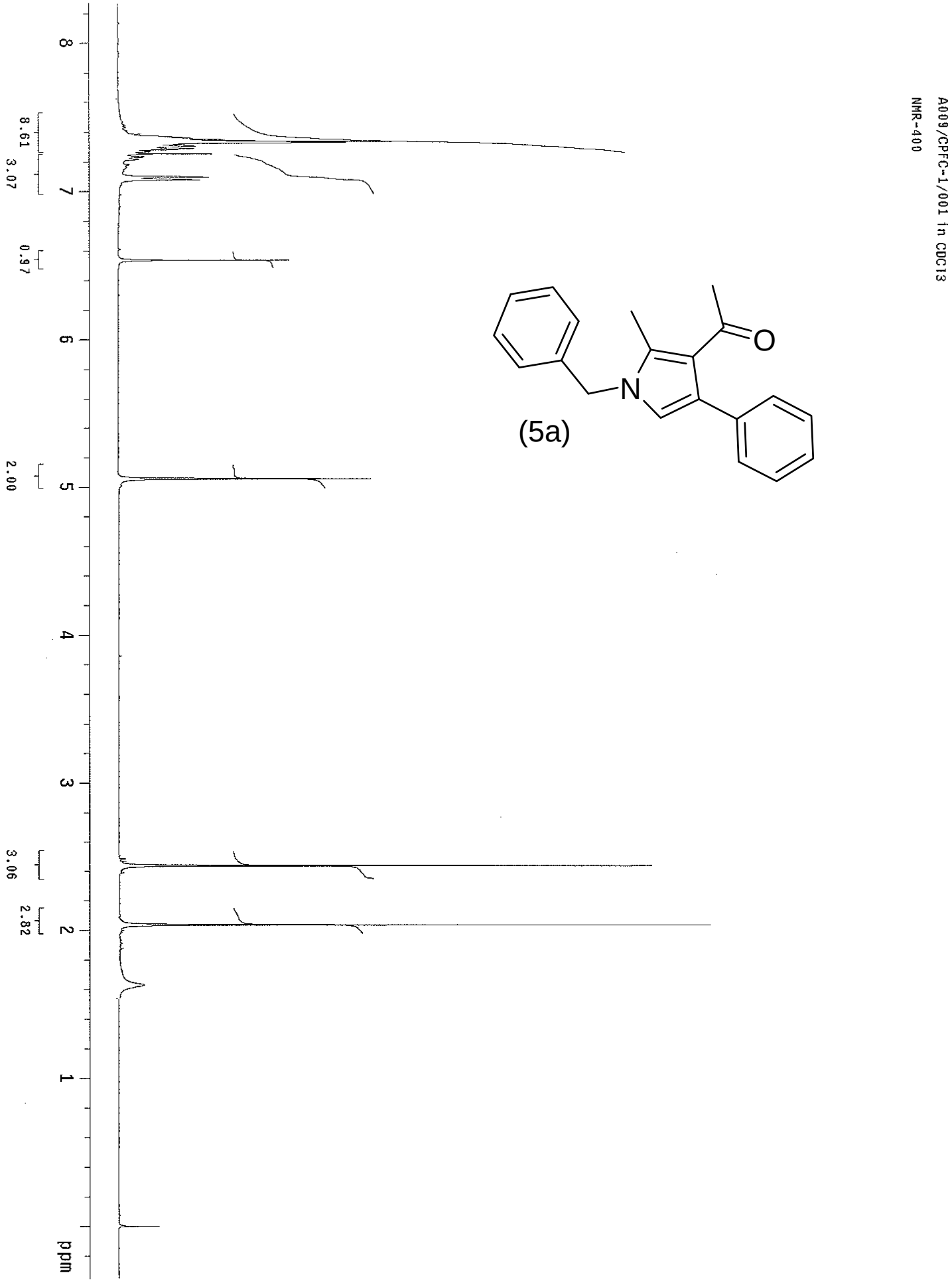
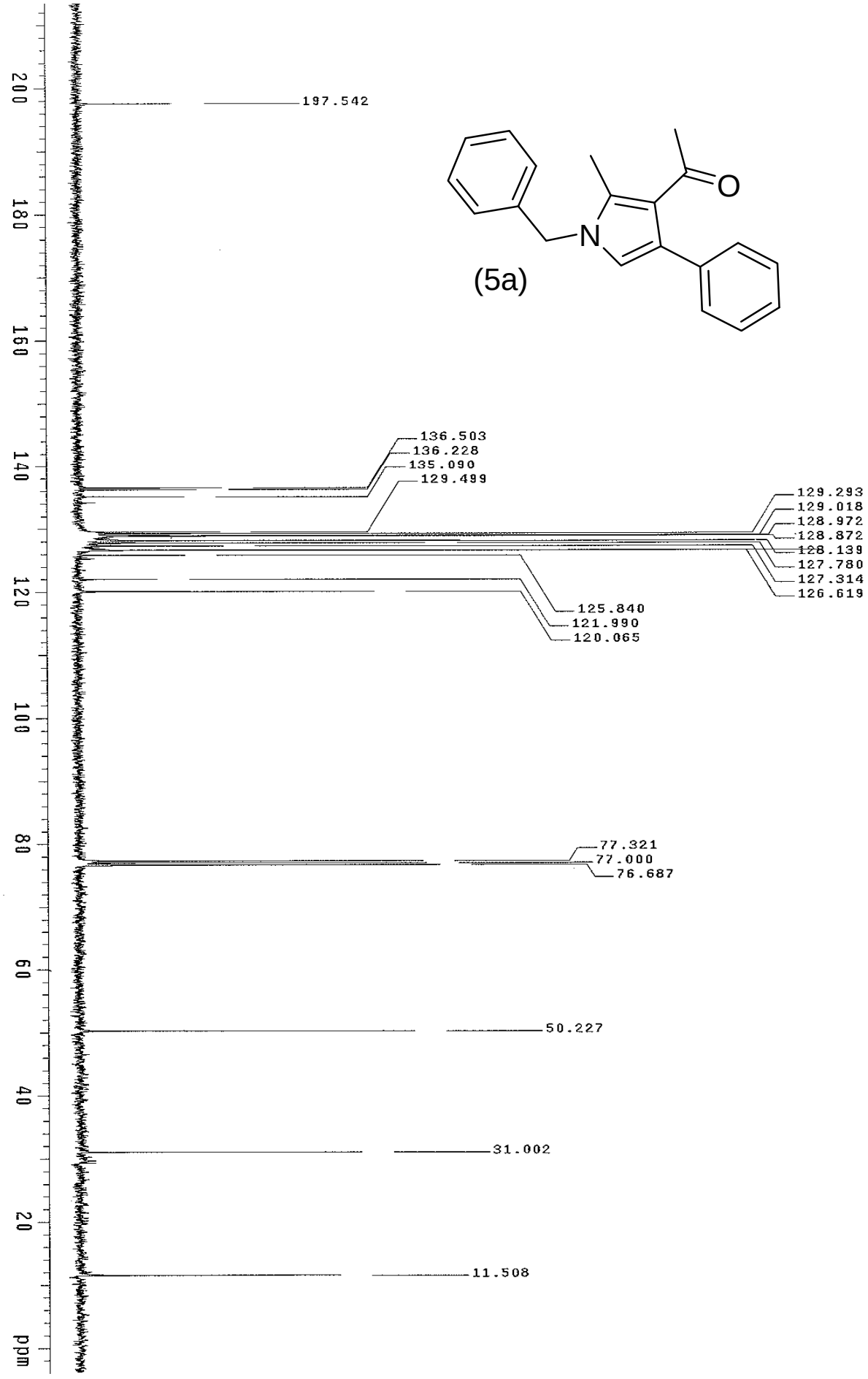
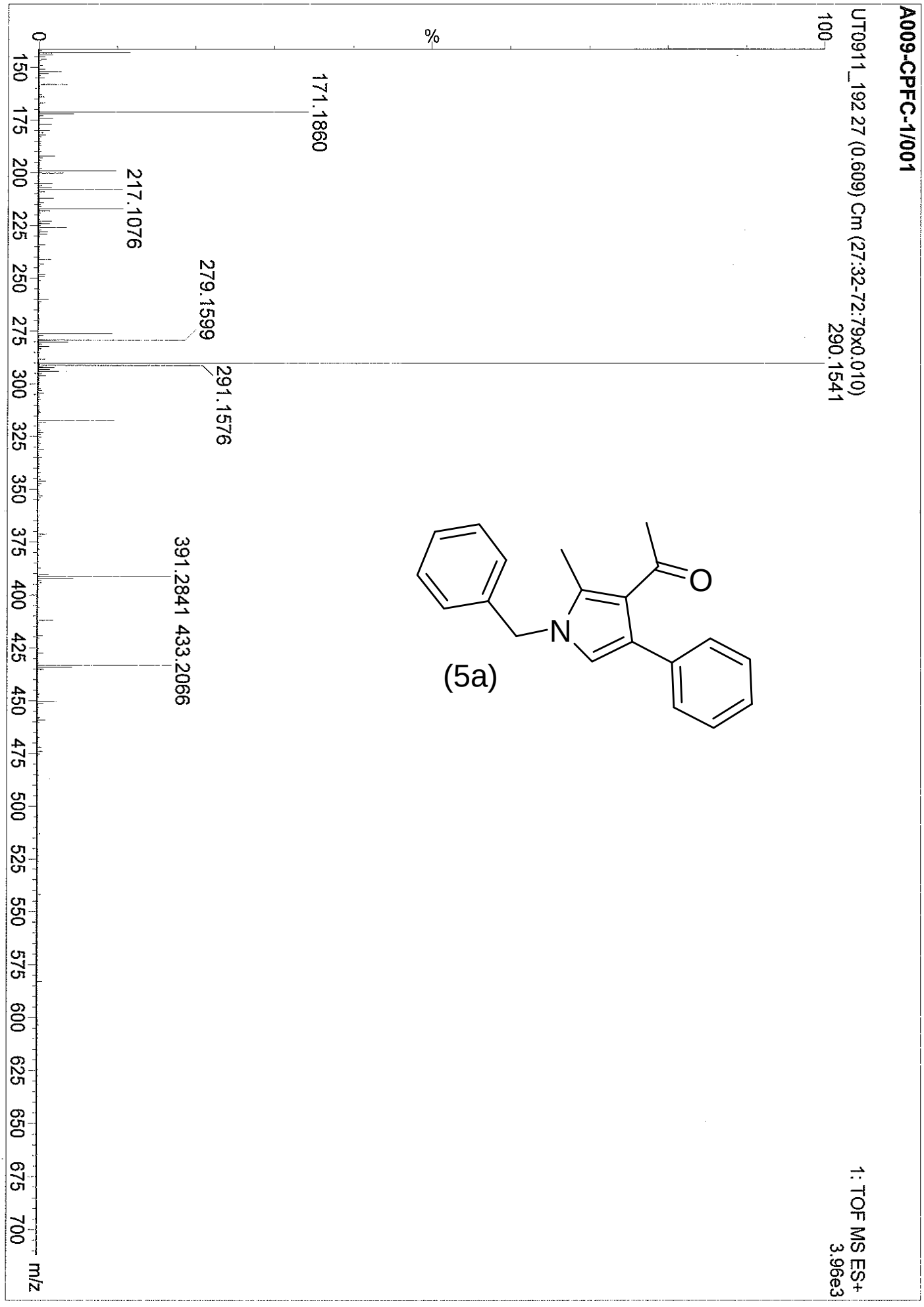




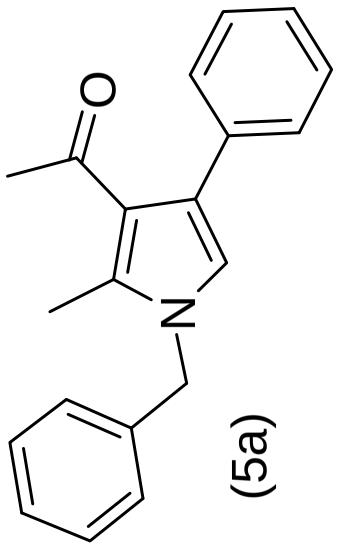


Elemental Composition Report

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

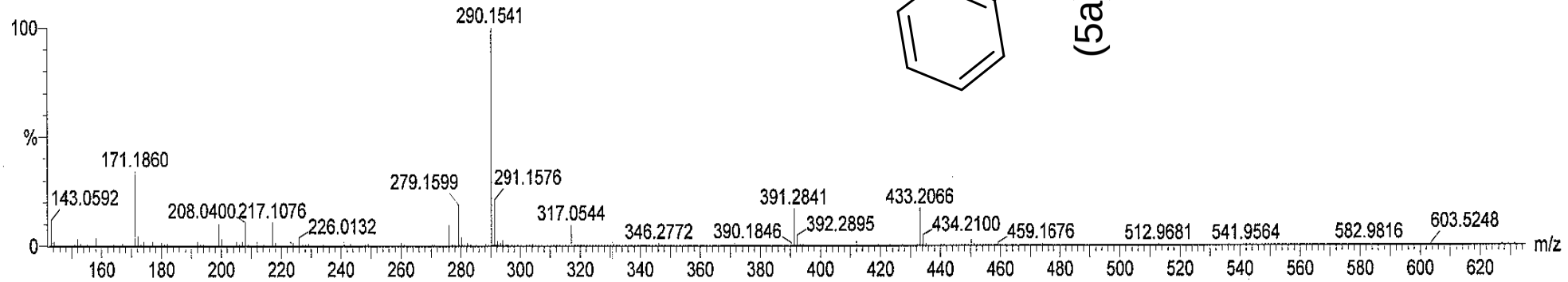
Monoisotopic Mass, Even Electron Ions
202 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-70 H: 0-80 N: 0-5 O: 0-10
A009-CPFC-1/001



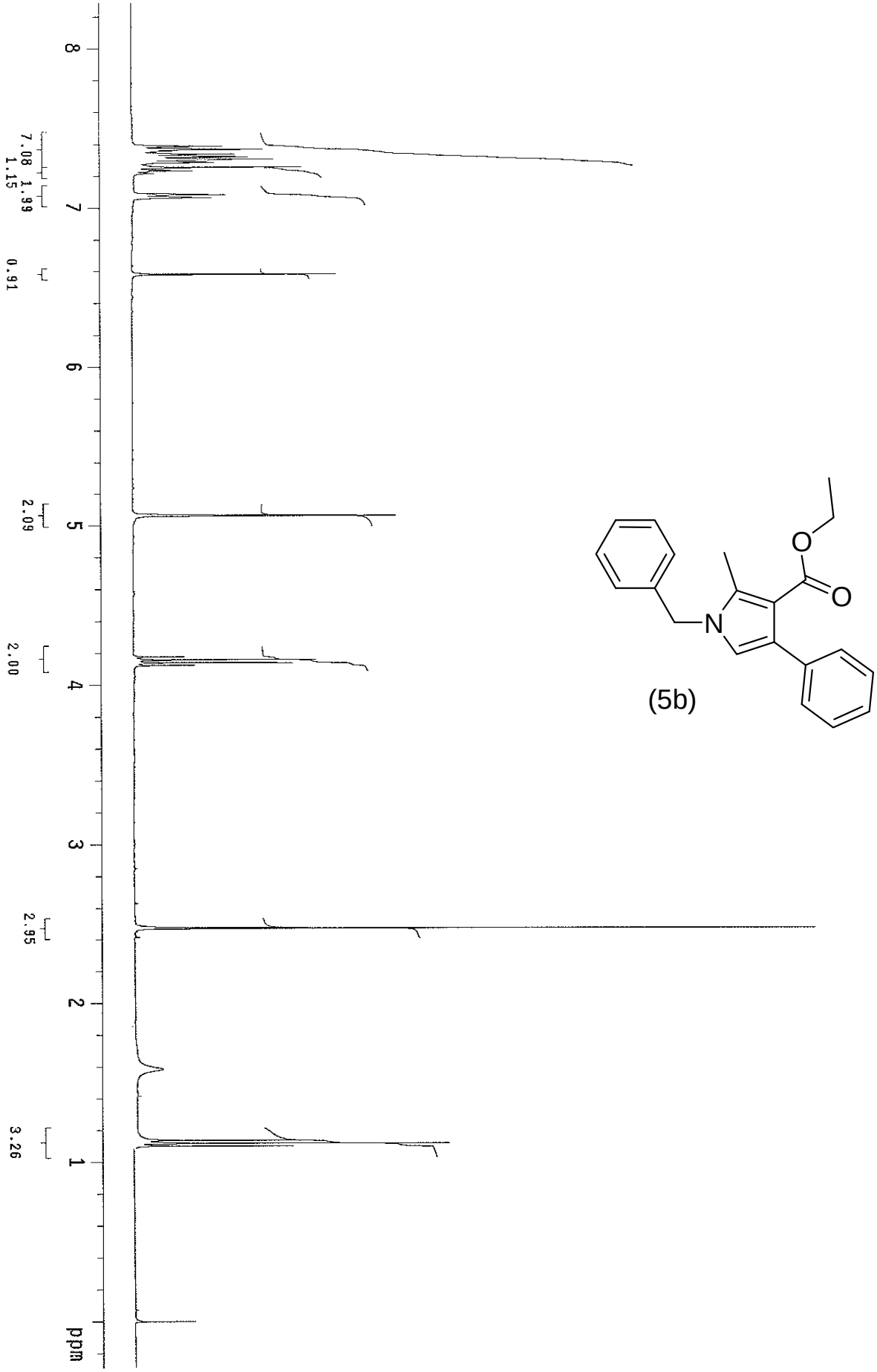
(5a)

UT0911_192 27 (0.609) Cm (27:32-72:79x0.010)

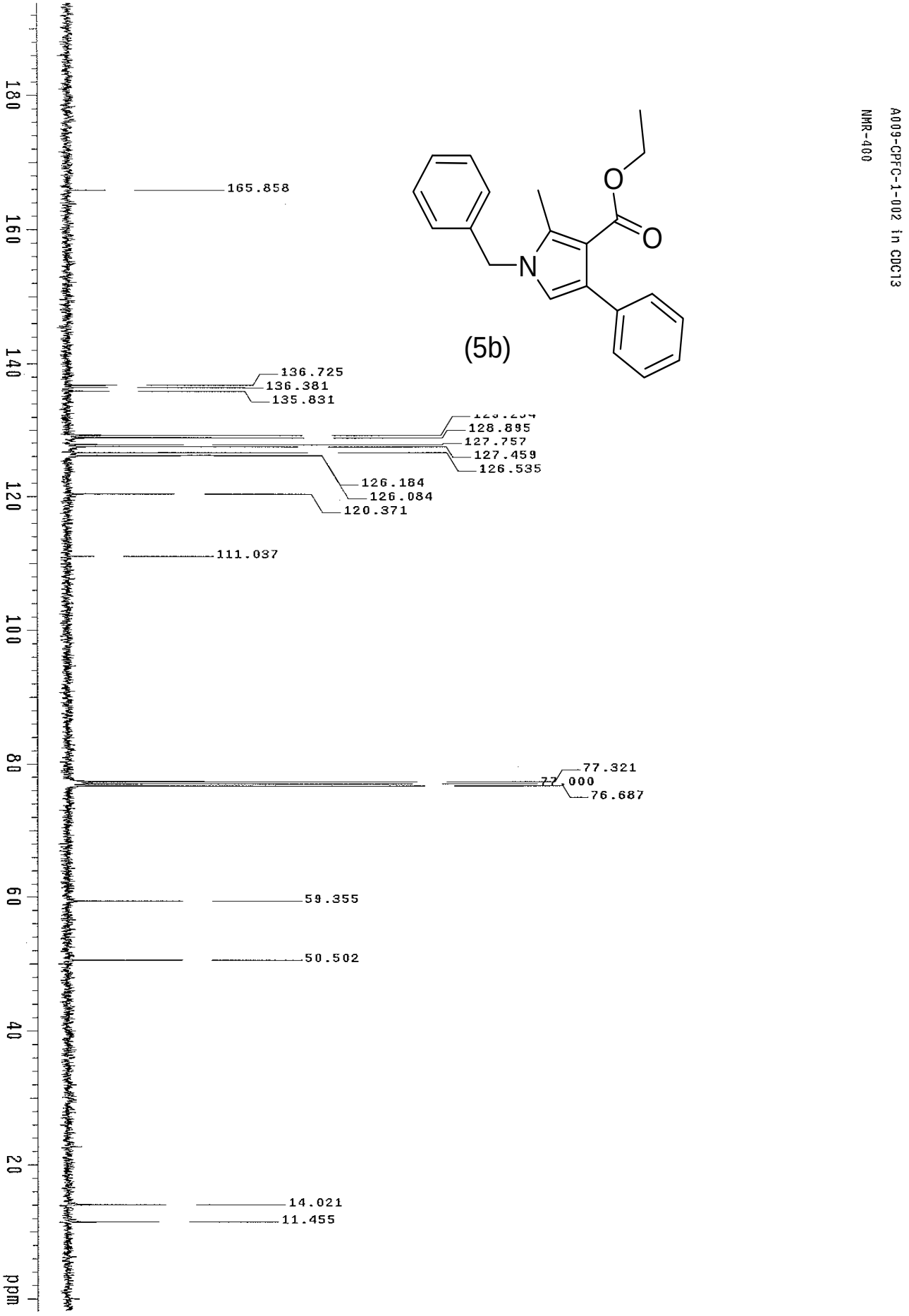
1: TOF MS ES+
3.96e+003

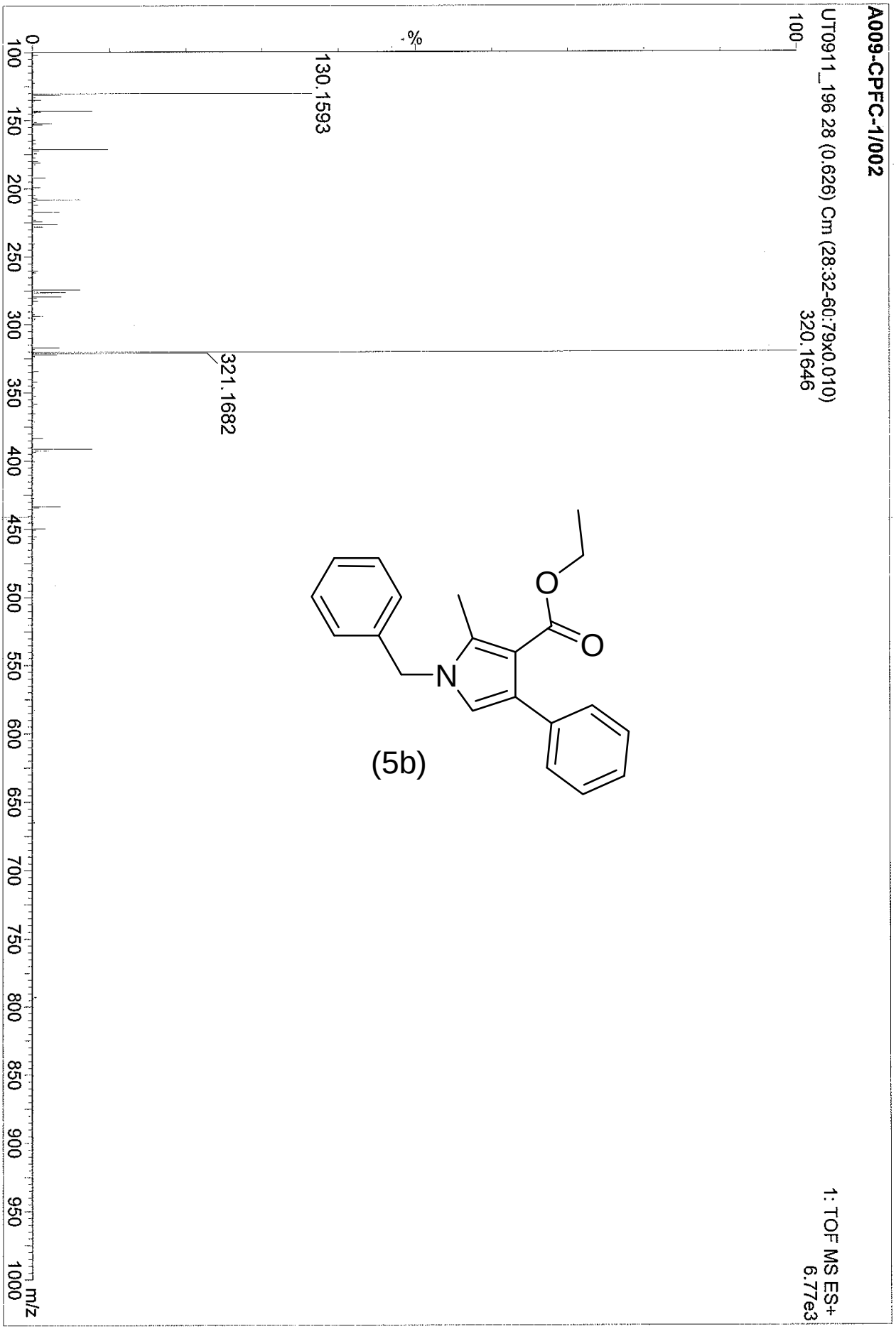


Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.1541	290.1545	-0.4	-1.4	11.5	28.2	C20 H20 N O



(5b)





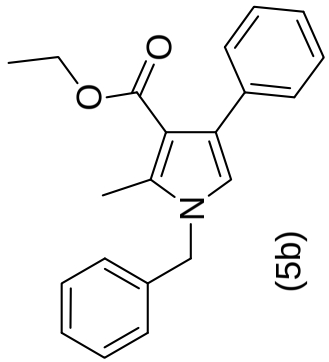
(5b)

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

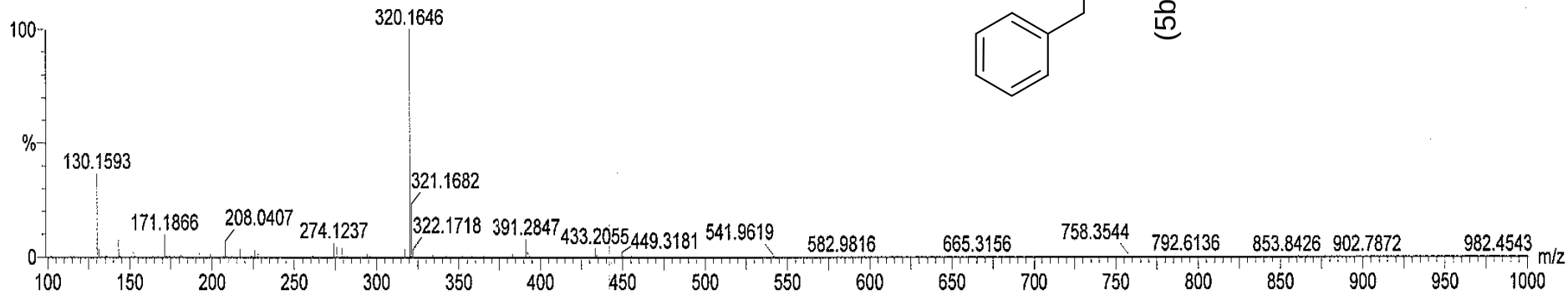
Monoisotopic Mass, Even Electron Ions
380 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-70 H: 0-80 N: 0-5 O: 0-10 Br: 0-1
A009-CPFC-1/002



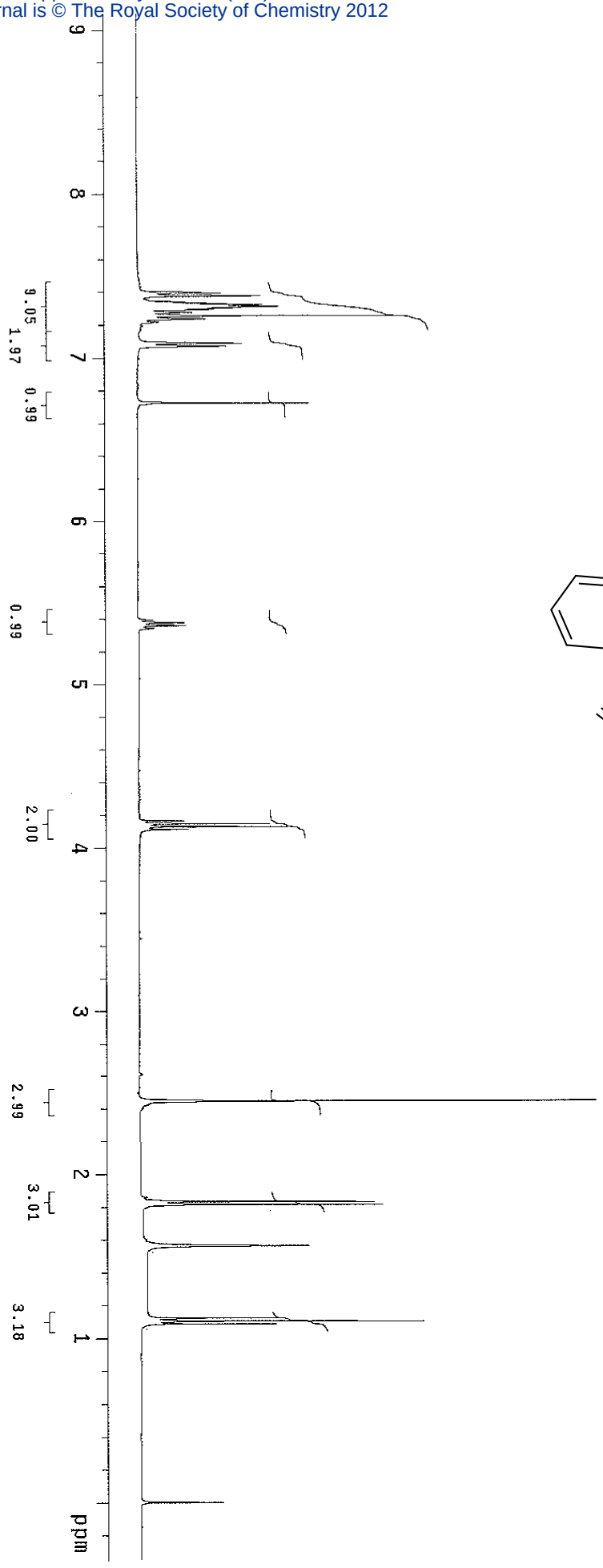
(5b)

UT0911_196 28 (0.626) Cm (28:32-60:79x0.010)

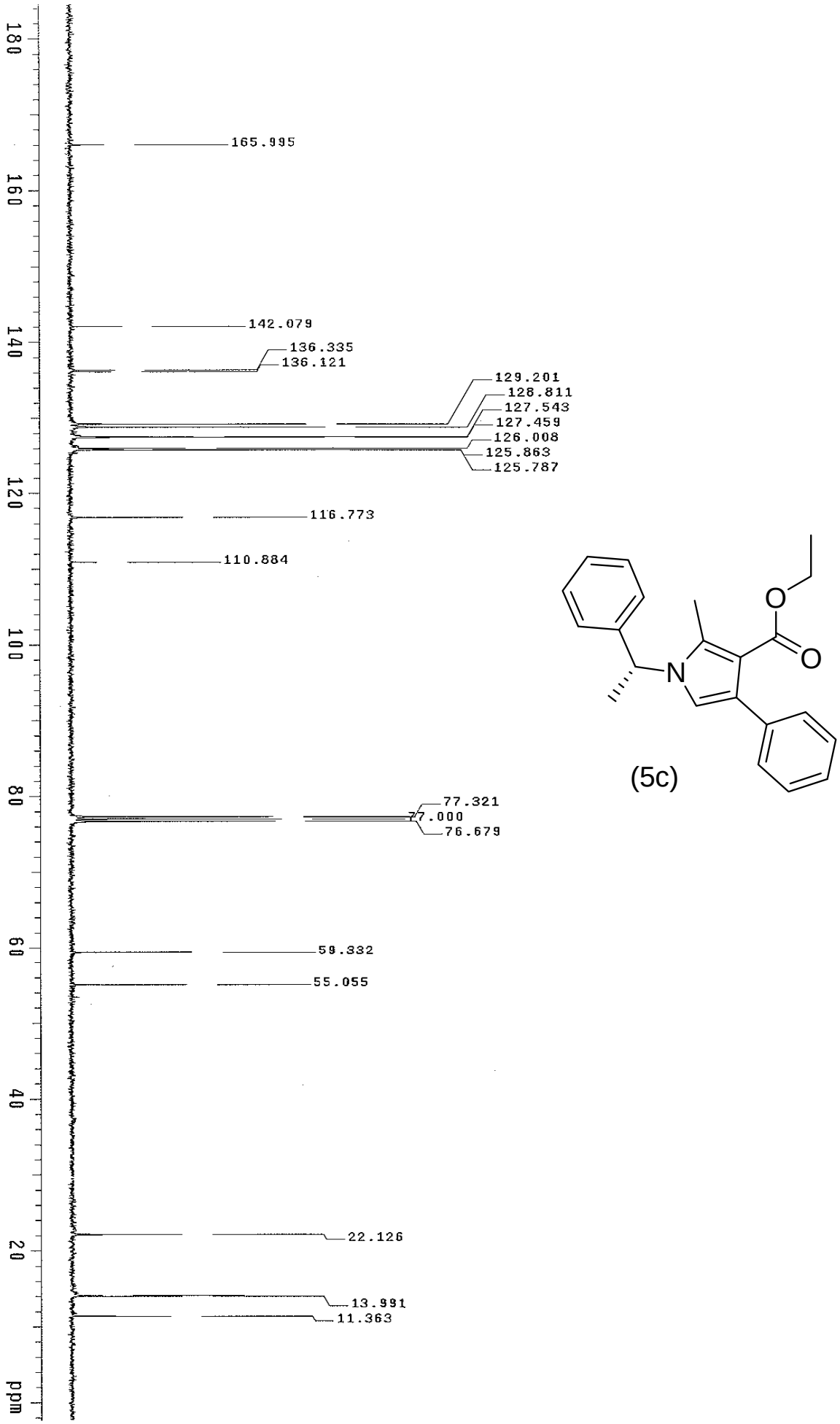
1: TOF MS ES+
6.77e+003

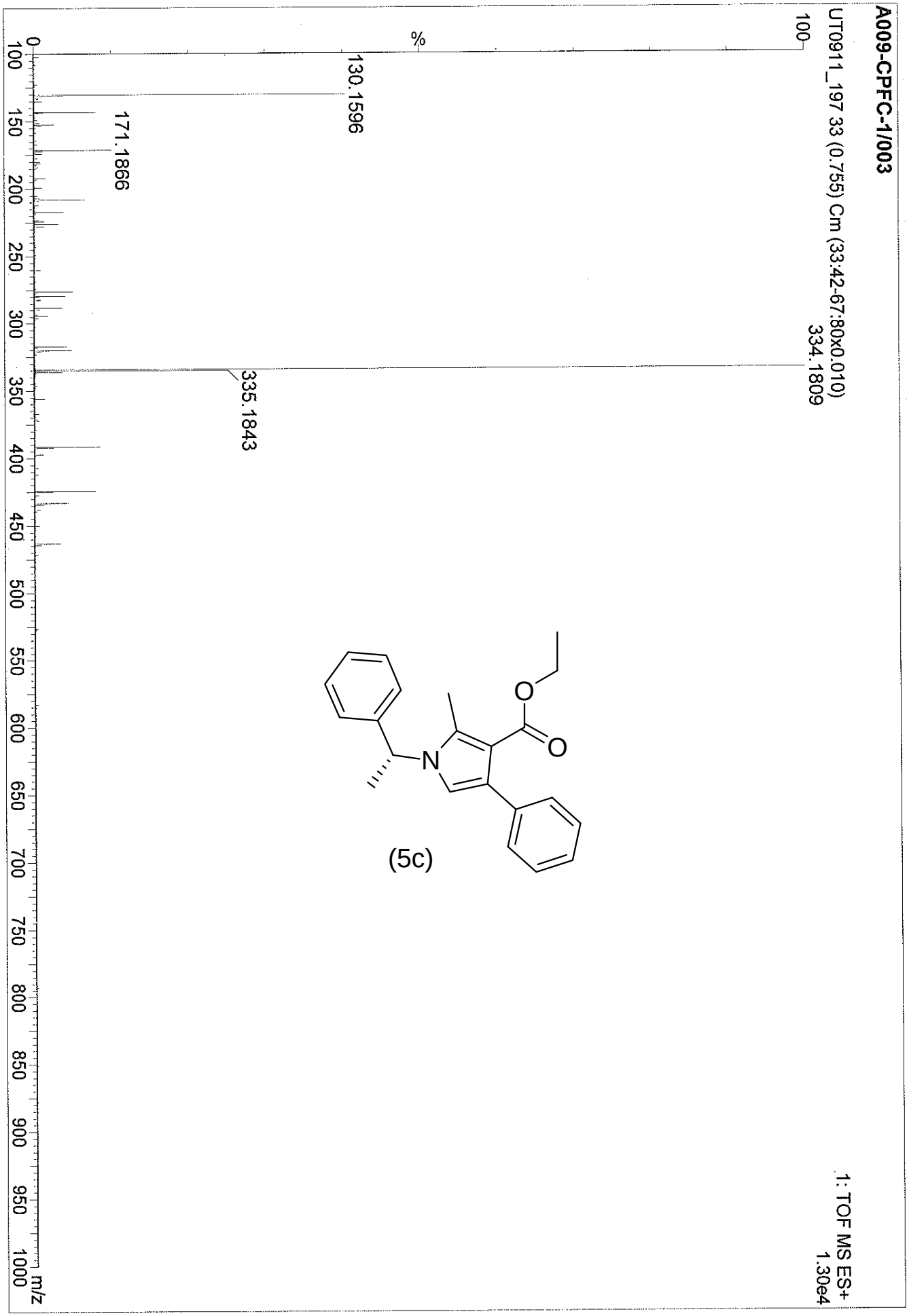


Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
320.1646	320.1651	-0.5	-1.6	11.5	2.6	C21 H22 N O2



(5c)





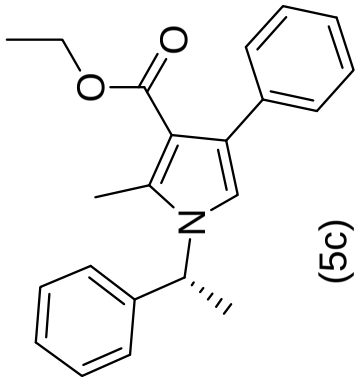
(5c)

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

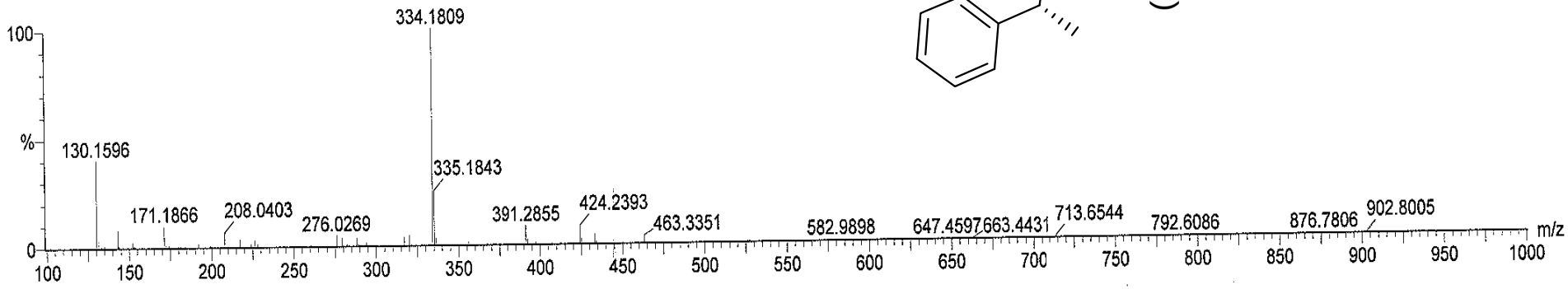
Monoisotopic Mass, Even Electron Ions
402 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-70 H: 0-80 N: 0-5 O: 0-10 Br: 0-1
A009-CPFC-1/003



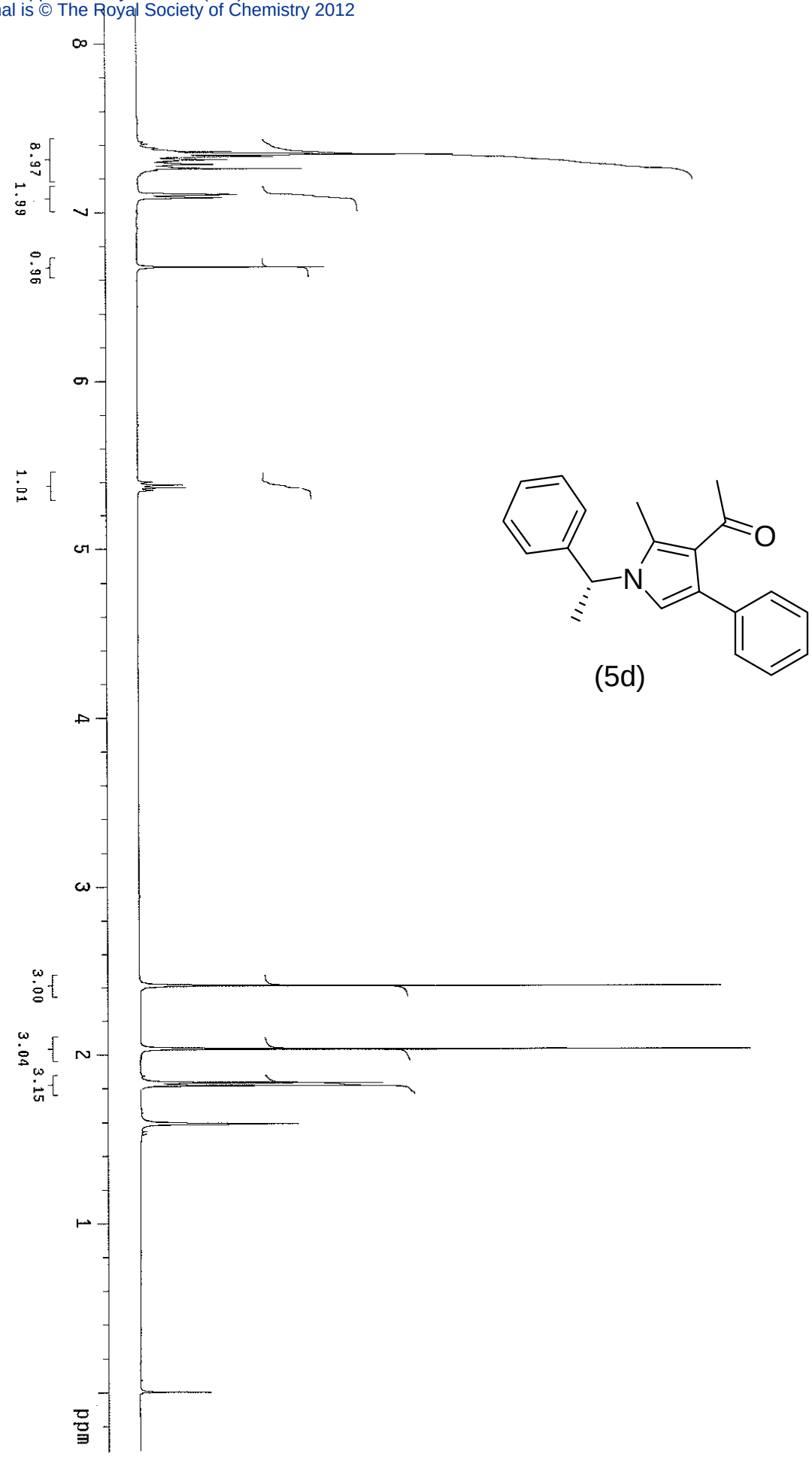
(5c)

UT0911_197 33 (0.755) Cm (33:42-67:80x0.010)

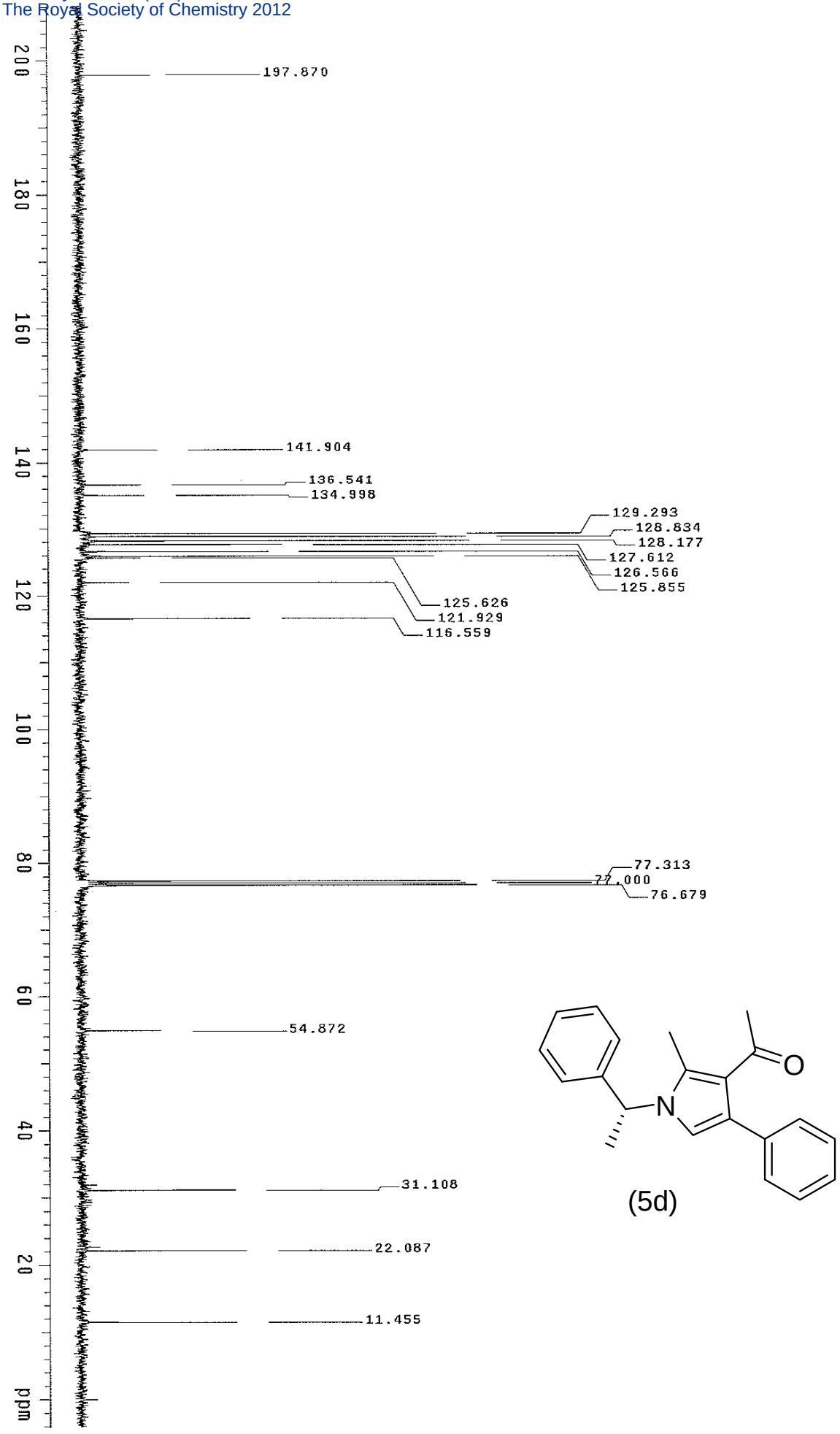
1: TOF MS ES+
1.30e+004



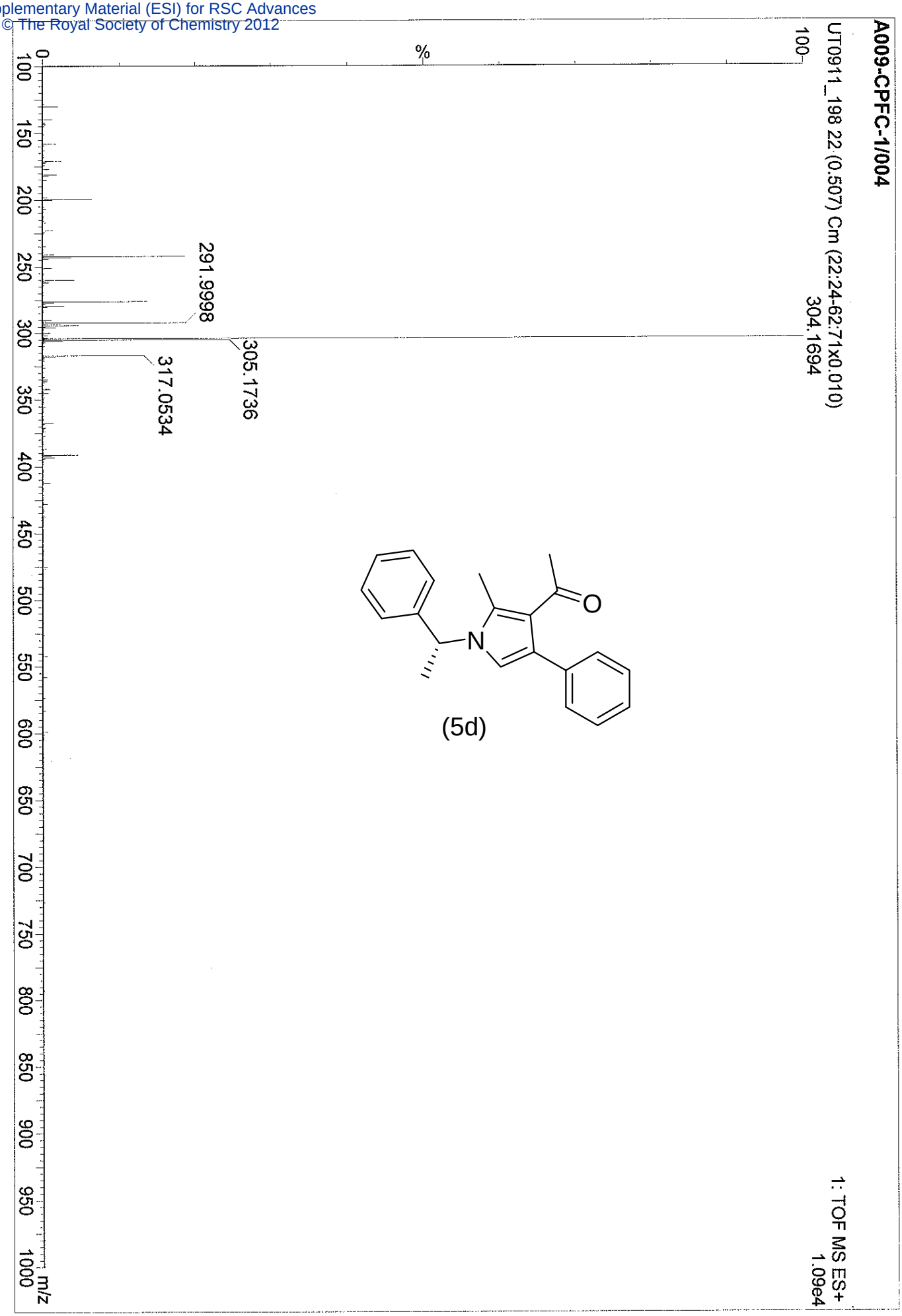
Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
334.1809	334.1807	0.2	0.6	11.5	2.4	C22 H24 N O2



(5d)



(5d)



(5d)

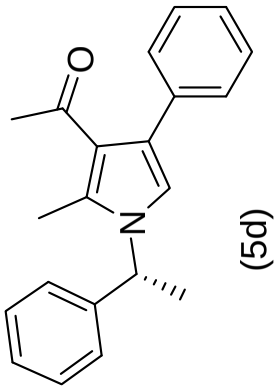
Elemental Composition Report

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

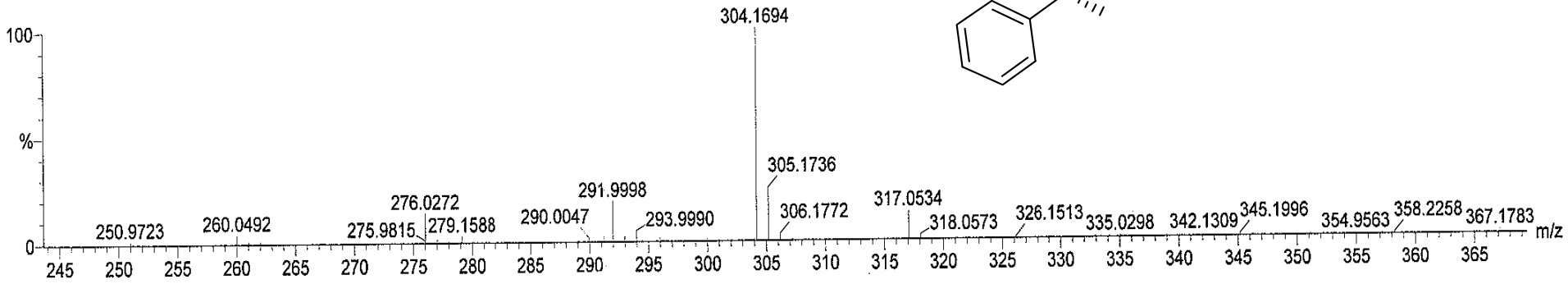
Monoisotopic Mass, Even Electron Ions
127 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-55 N: 0-4 O: 0-6
A009-CPFC-1/004

UT0911_198 22 (0.507) Cm (22:24-62:71x0.010)

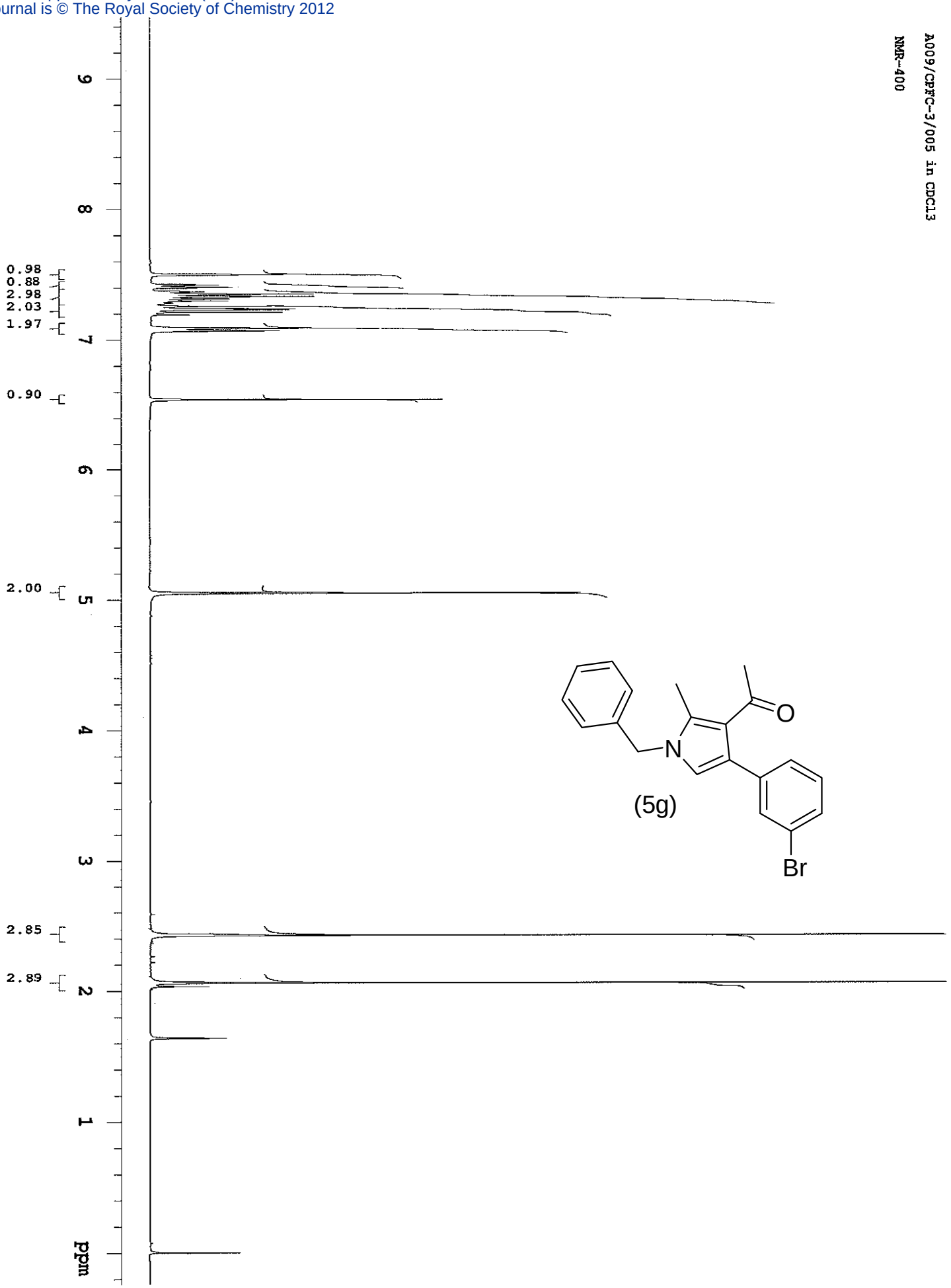


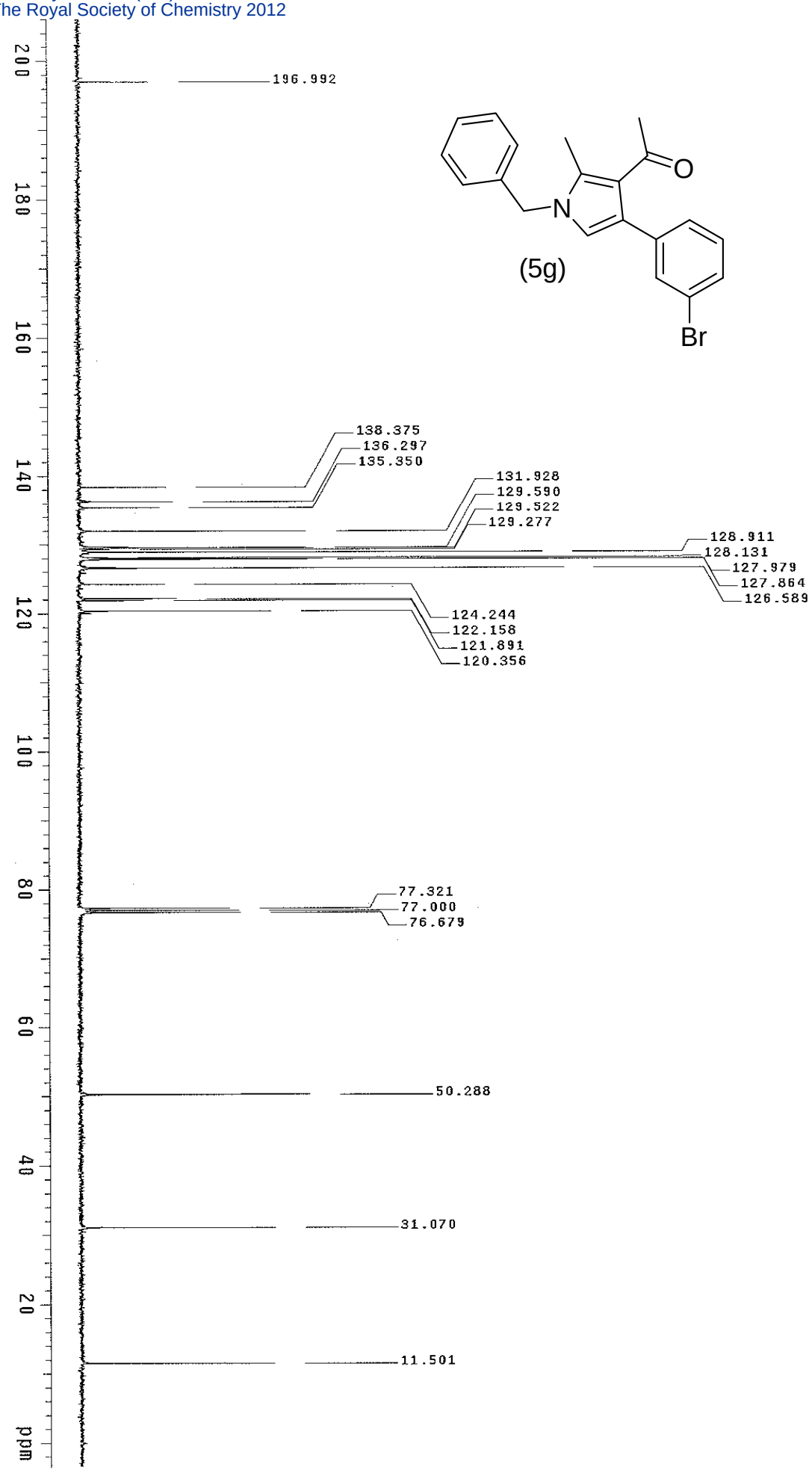
(5d)

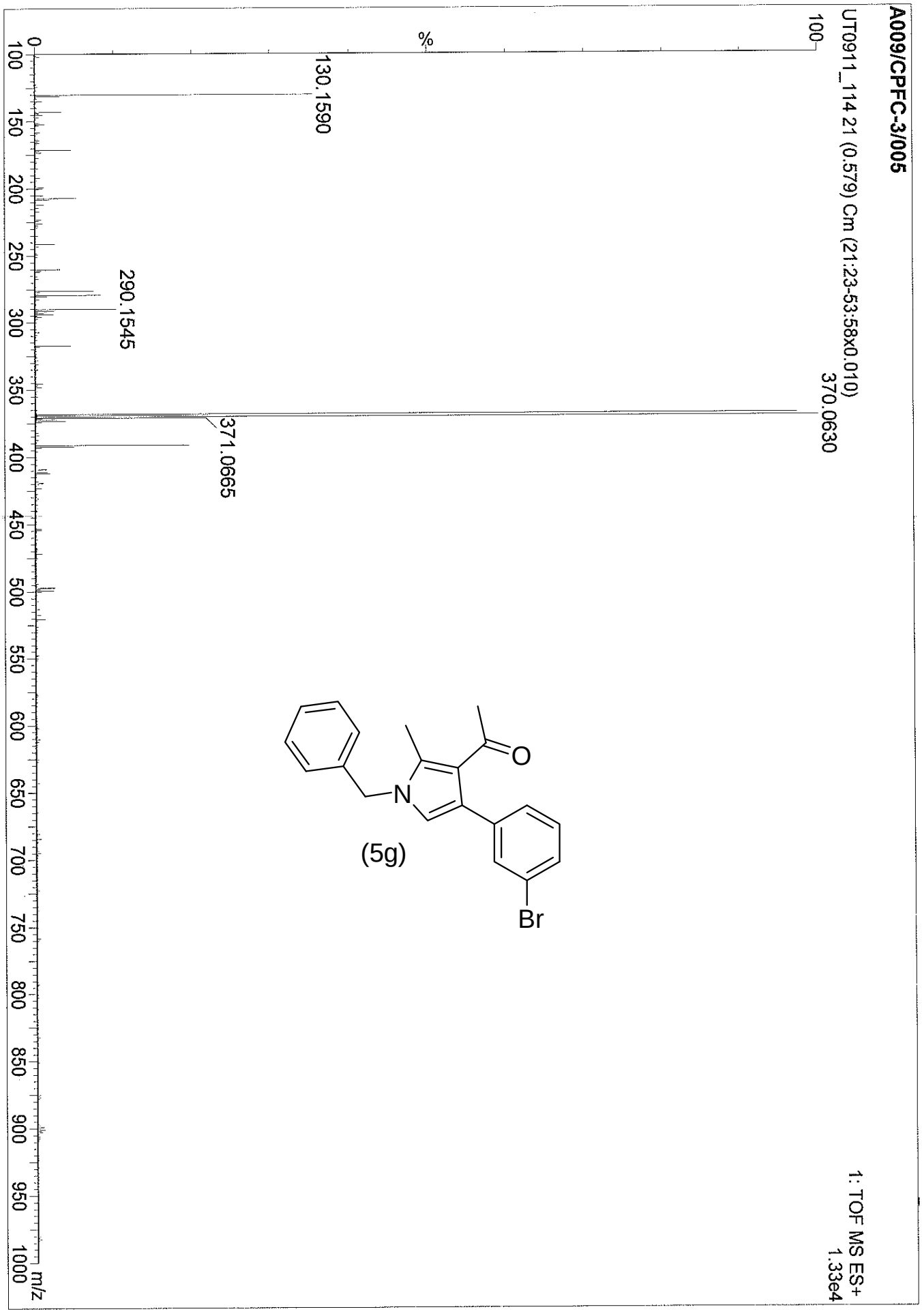
1: TOF MS ES+
1.09e+004



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
304.1694	304.1701	-0.7	-2.3	11.5	5.5	C21 H22 N O





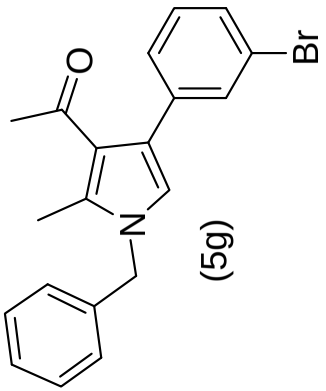


Elemental Composition Report

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 = 3

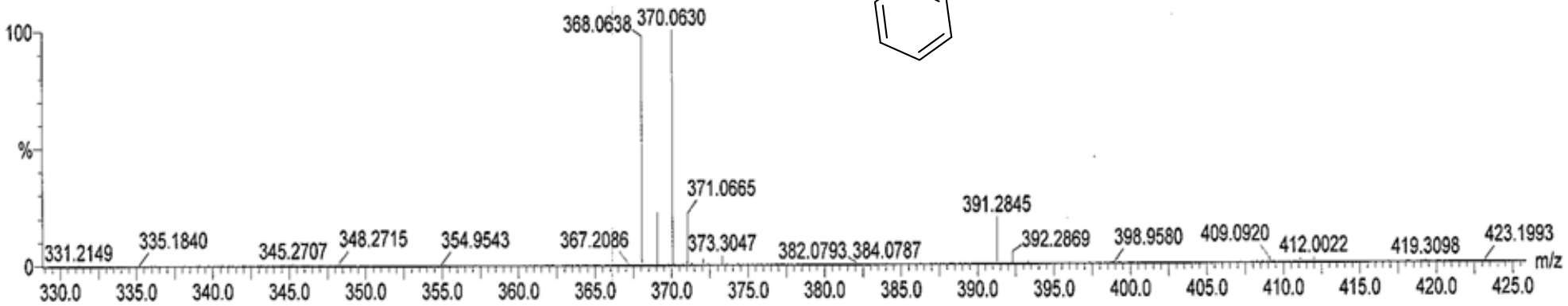
Monoisotopic Mass, Even Electron Ions
315 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-65 N: 0-5 O: 0-4 Br: 0-2
A009/CPFC-3/005



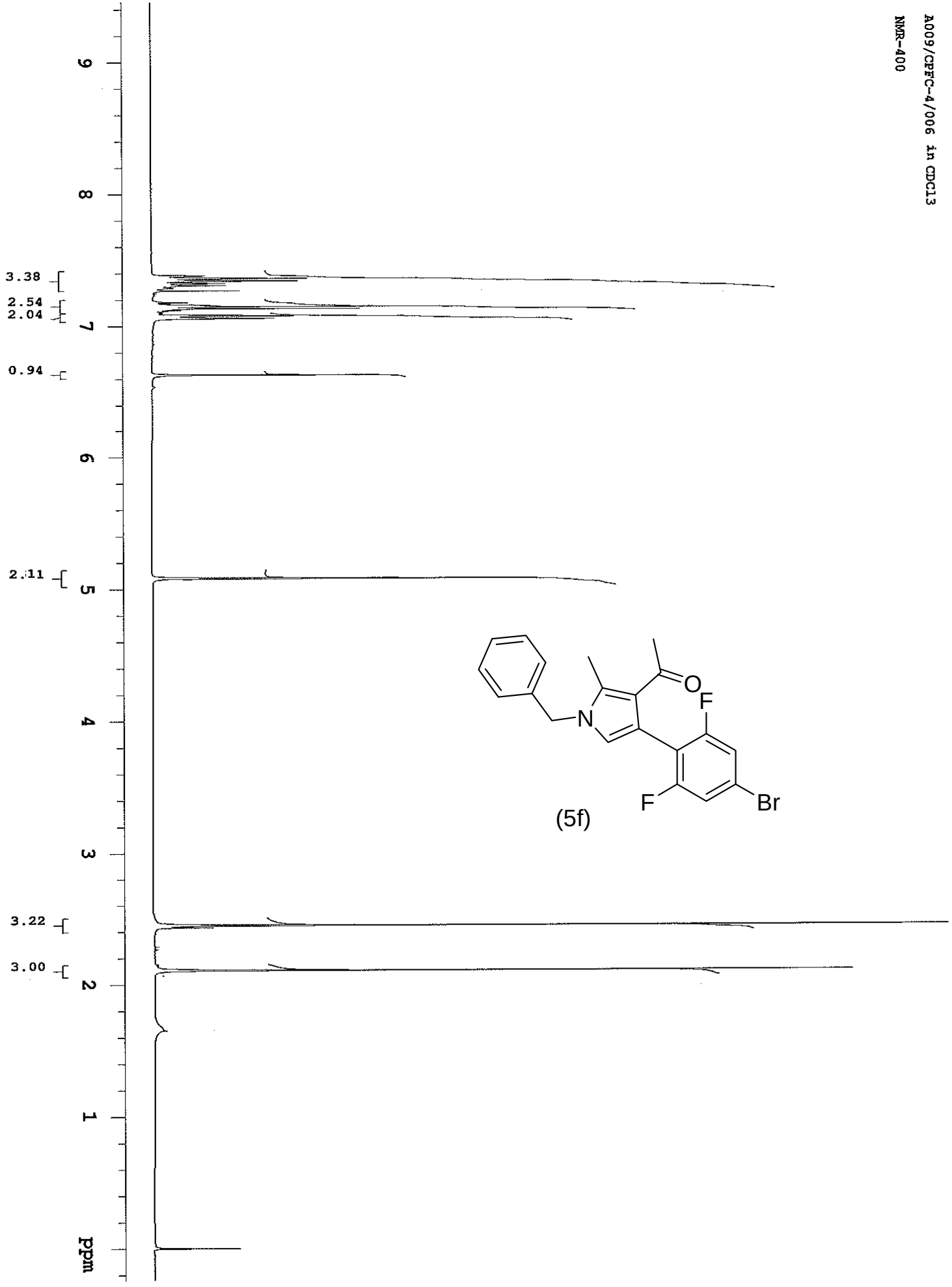
(5g)

UT0911_114 21 (0.579) Cm (21:23-53:58x0.010)

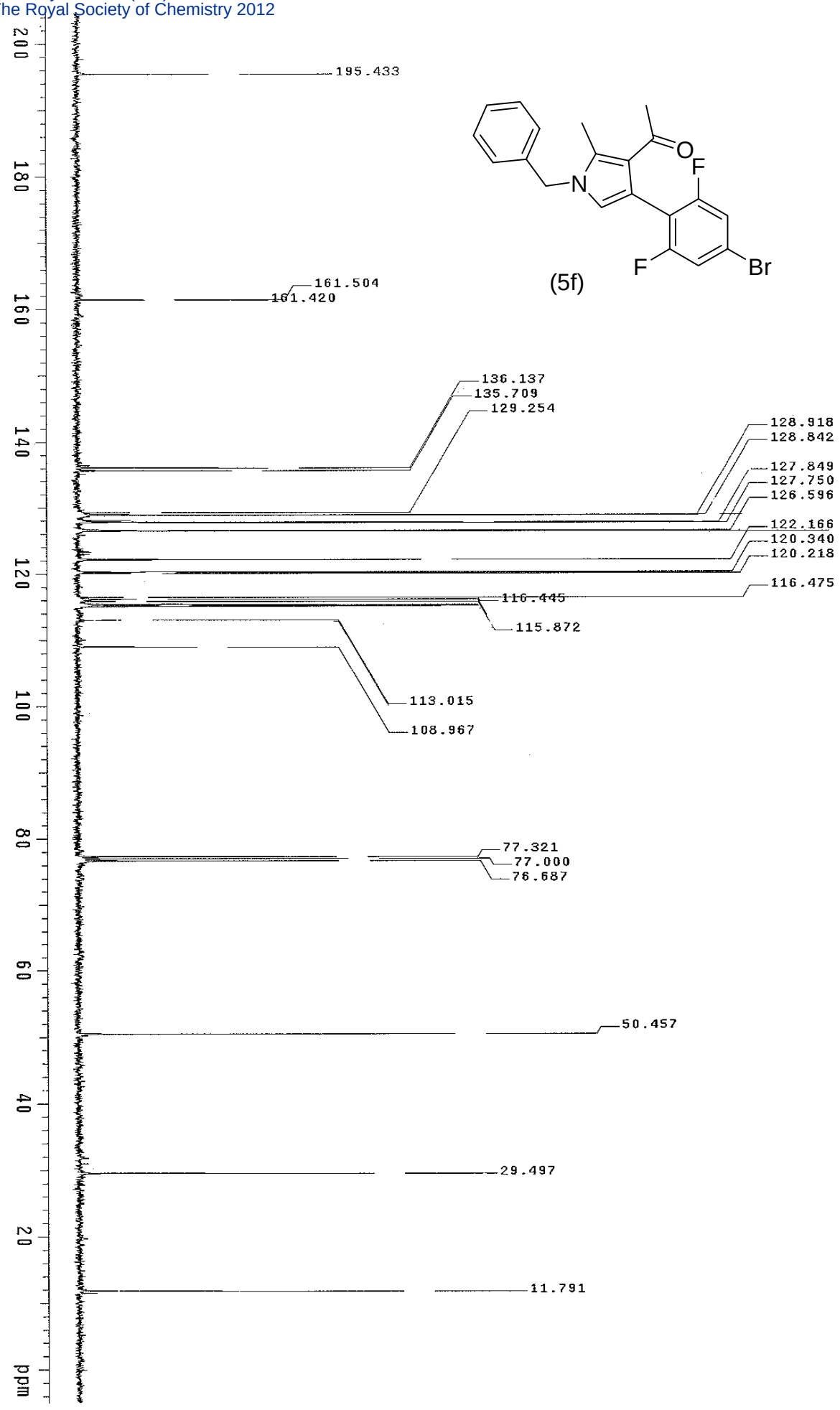
1: TOF MS ES+
1.33e+004

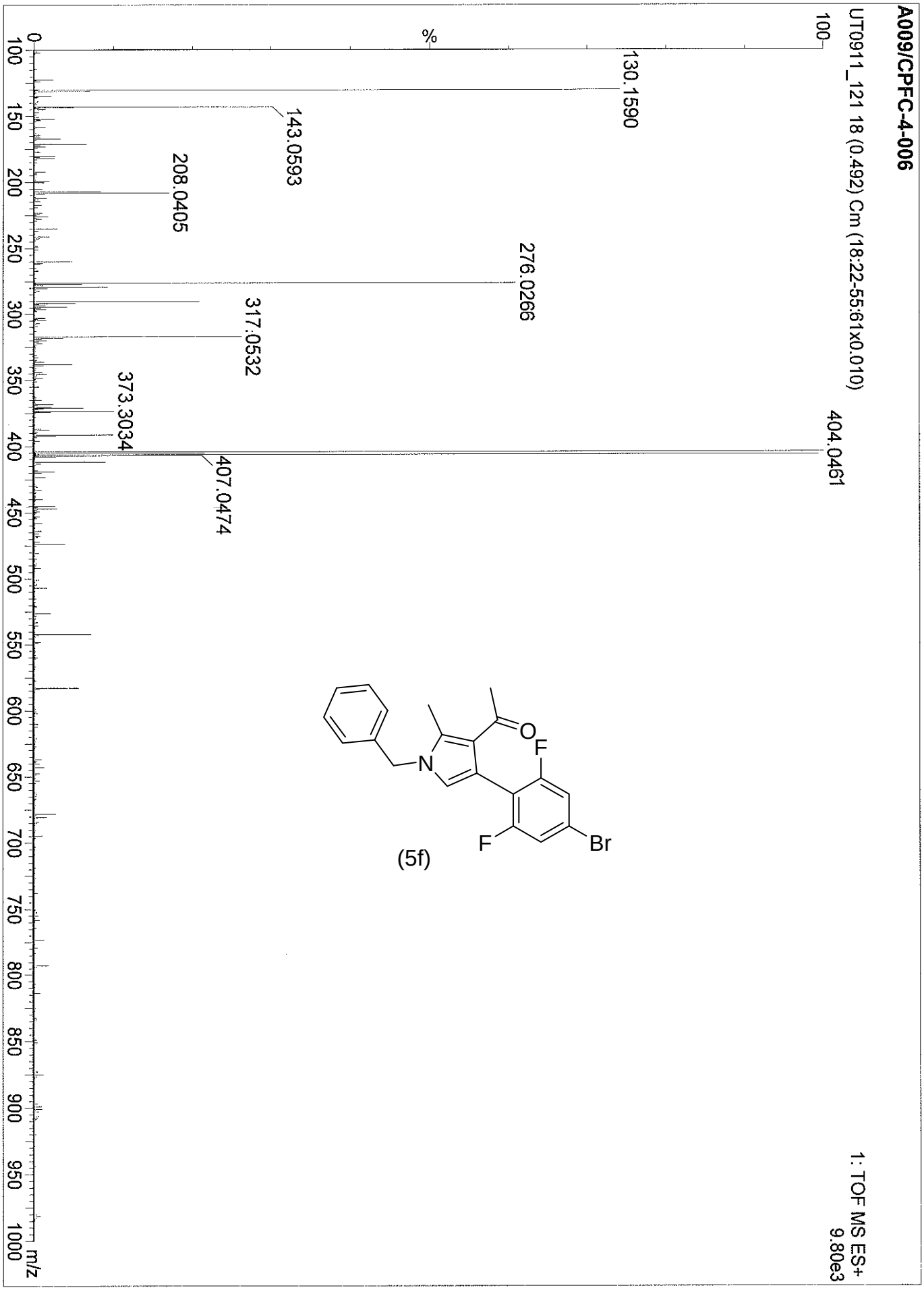


Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
368.0638	368.0650	-1.2	-3.3	11.5	3.4	C20 H19 N O Br



(5f)





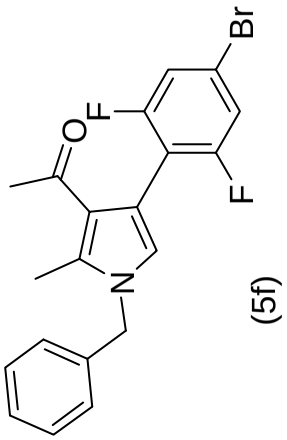
(5f)

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 = 3

Monoisotopic Mass, Even Electron Ions
390 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-65 N: 0-2 O: 0-4 F: 0-2 Br: 0-1

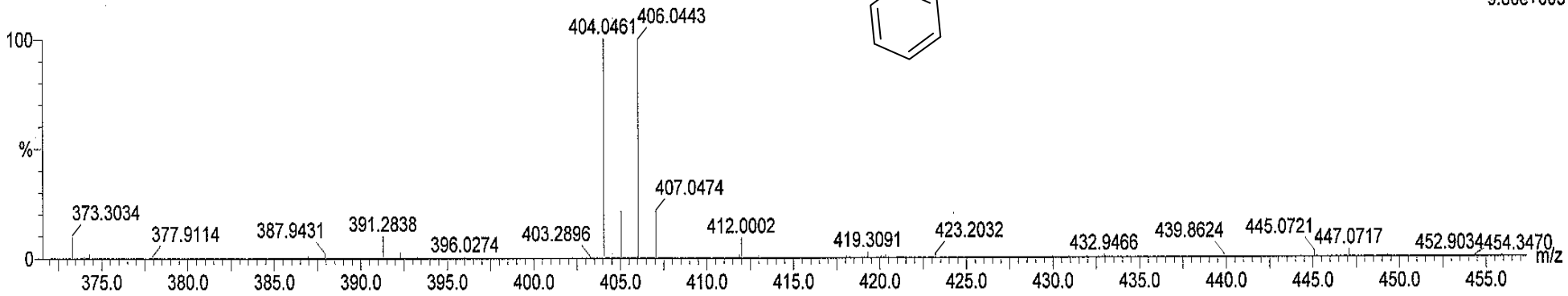


(5f)

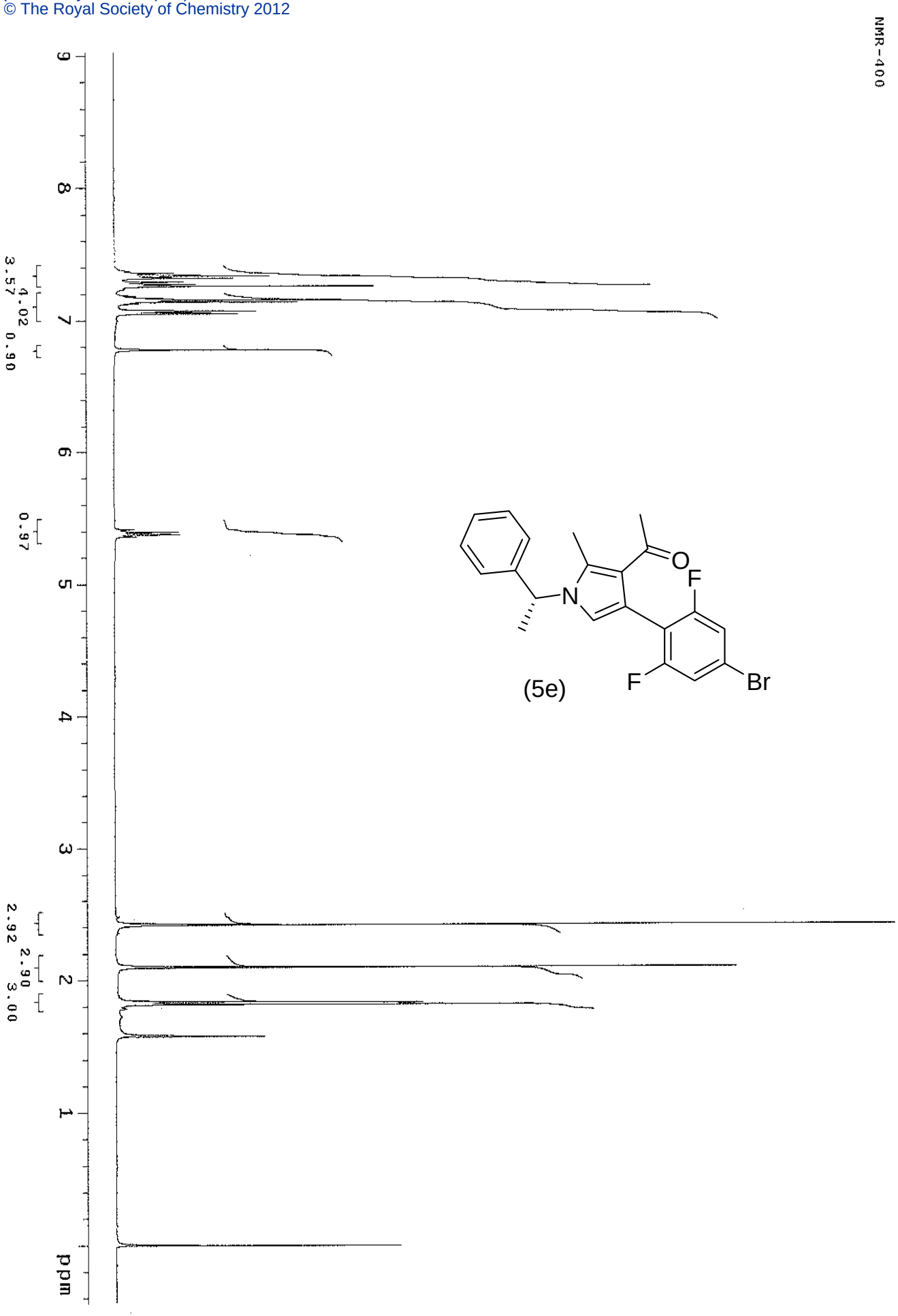
A009/CPFC-4-006

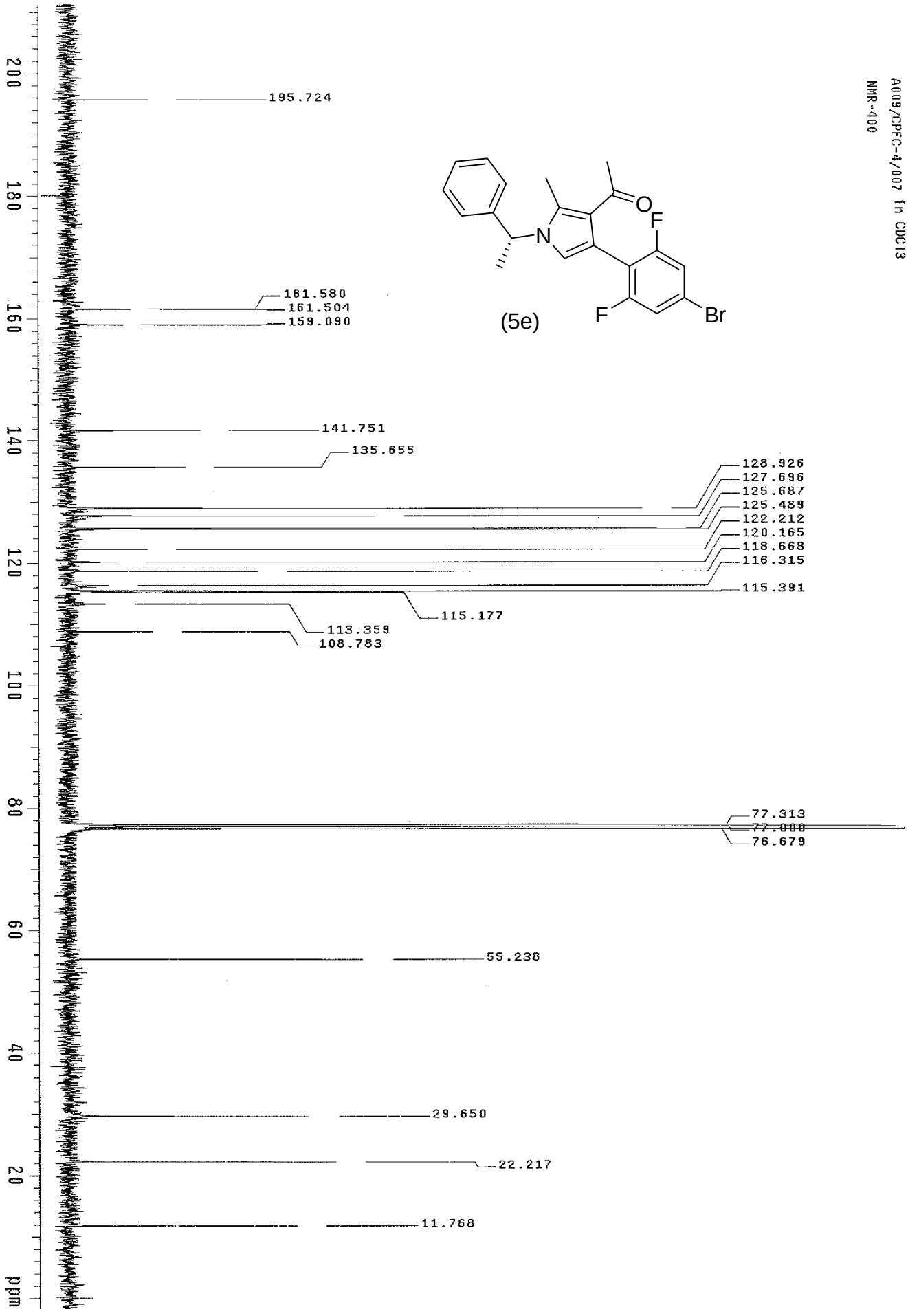
UT0911_121 18 (0.492) Cm (18:22-55:61x0.010)

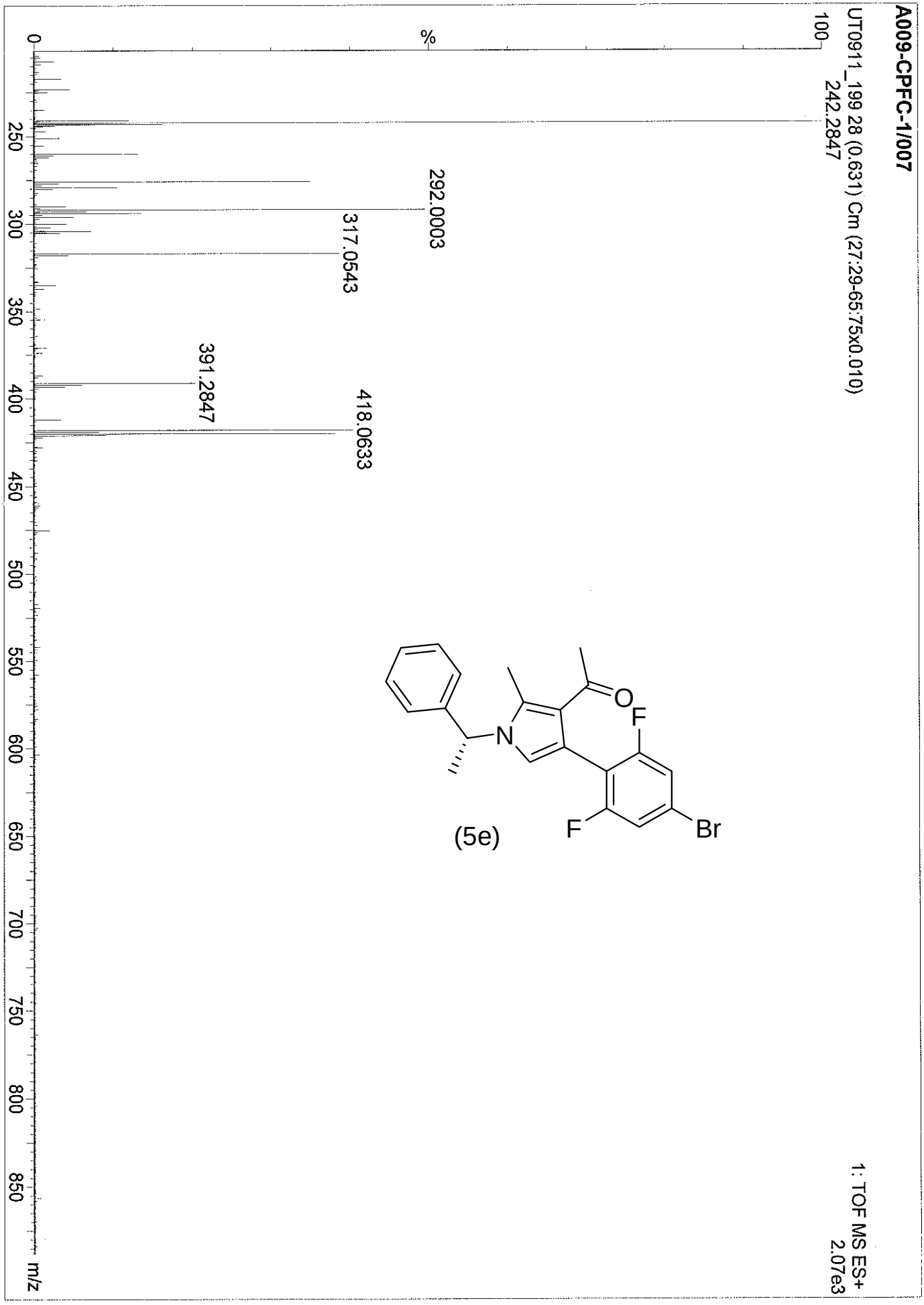
1: TOF MS ES+
9.80e+003



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
404.0461	404.0462	-0.1	-0.2	11.5	3.2	C20 H17 N O F2 Br







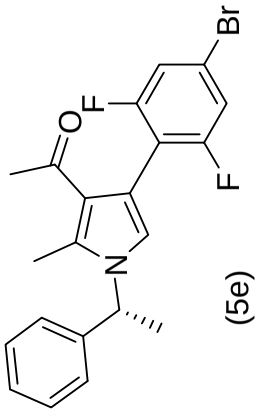
(5e)

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
274 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-55 N: 0-4 O: 0-6 Br: 0-1 F: 2-2

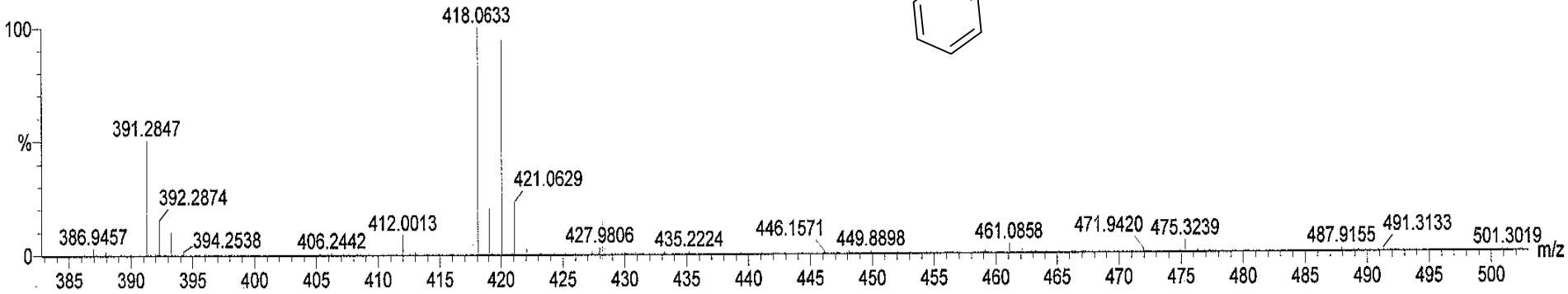


(5e)

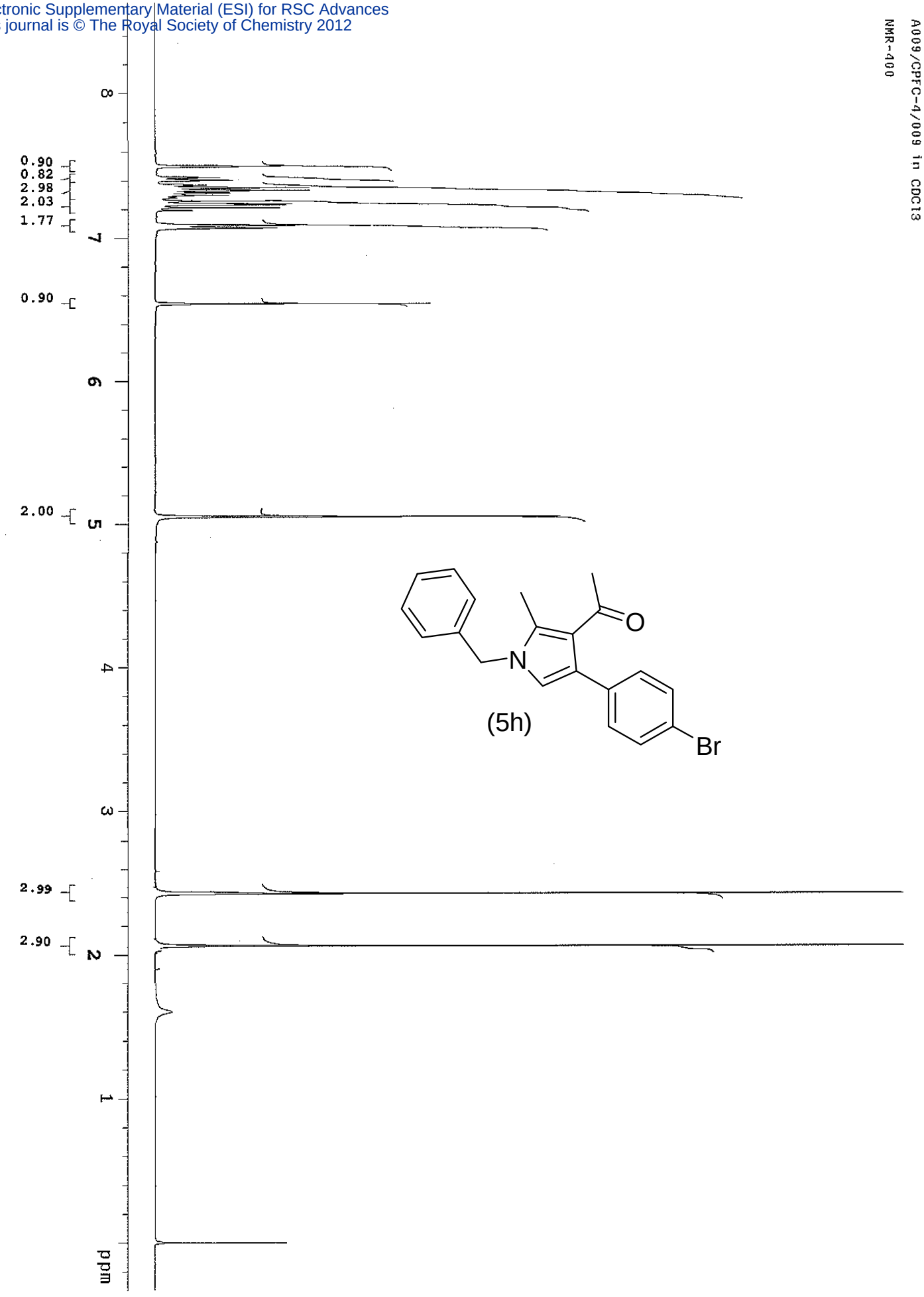
A009-CPFC-1/007

UT0911_199 28 (0.631) Cm (27:29-65:75x0.010)

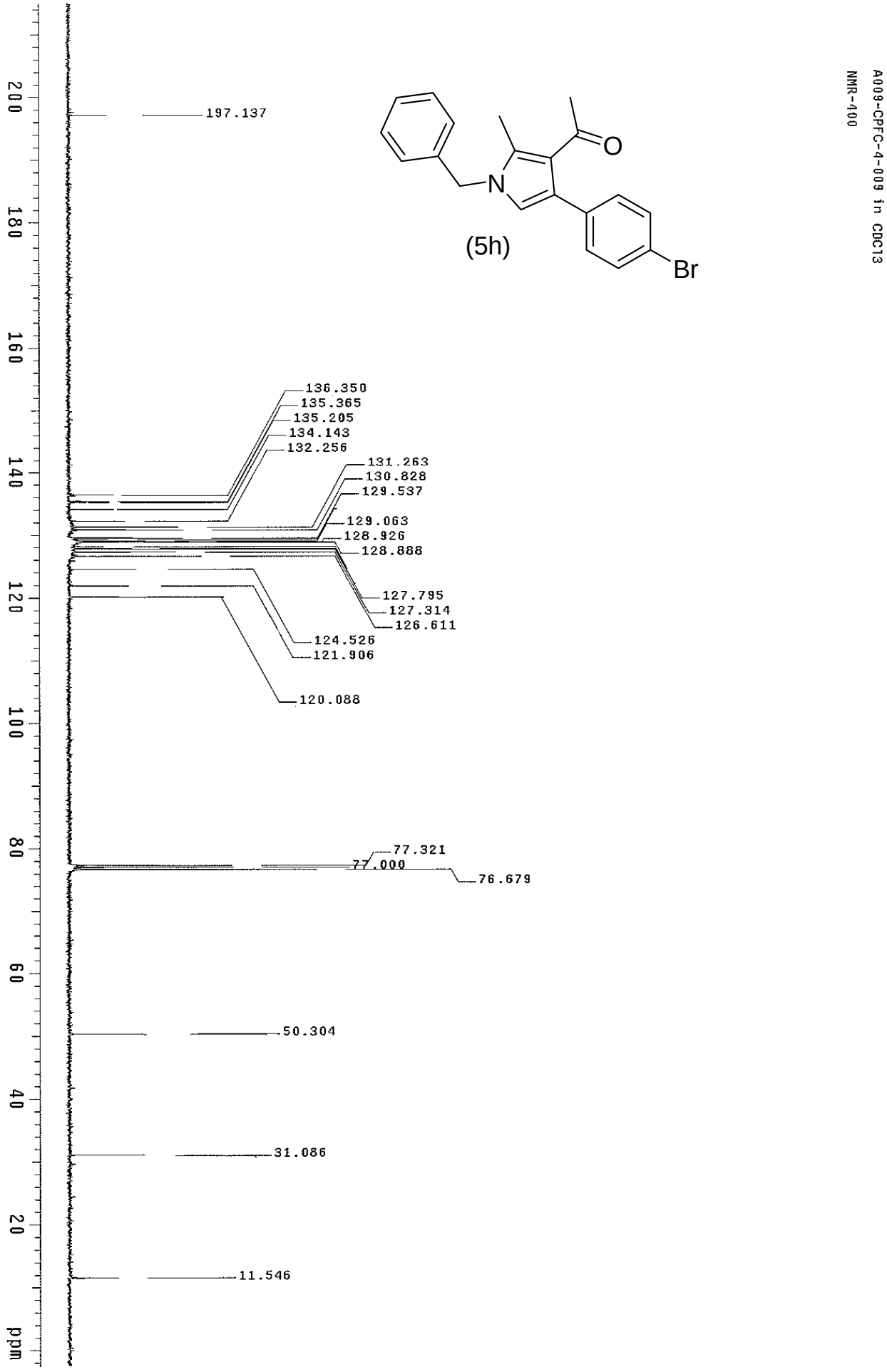
1: TOF MS ES+
8.36e+002

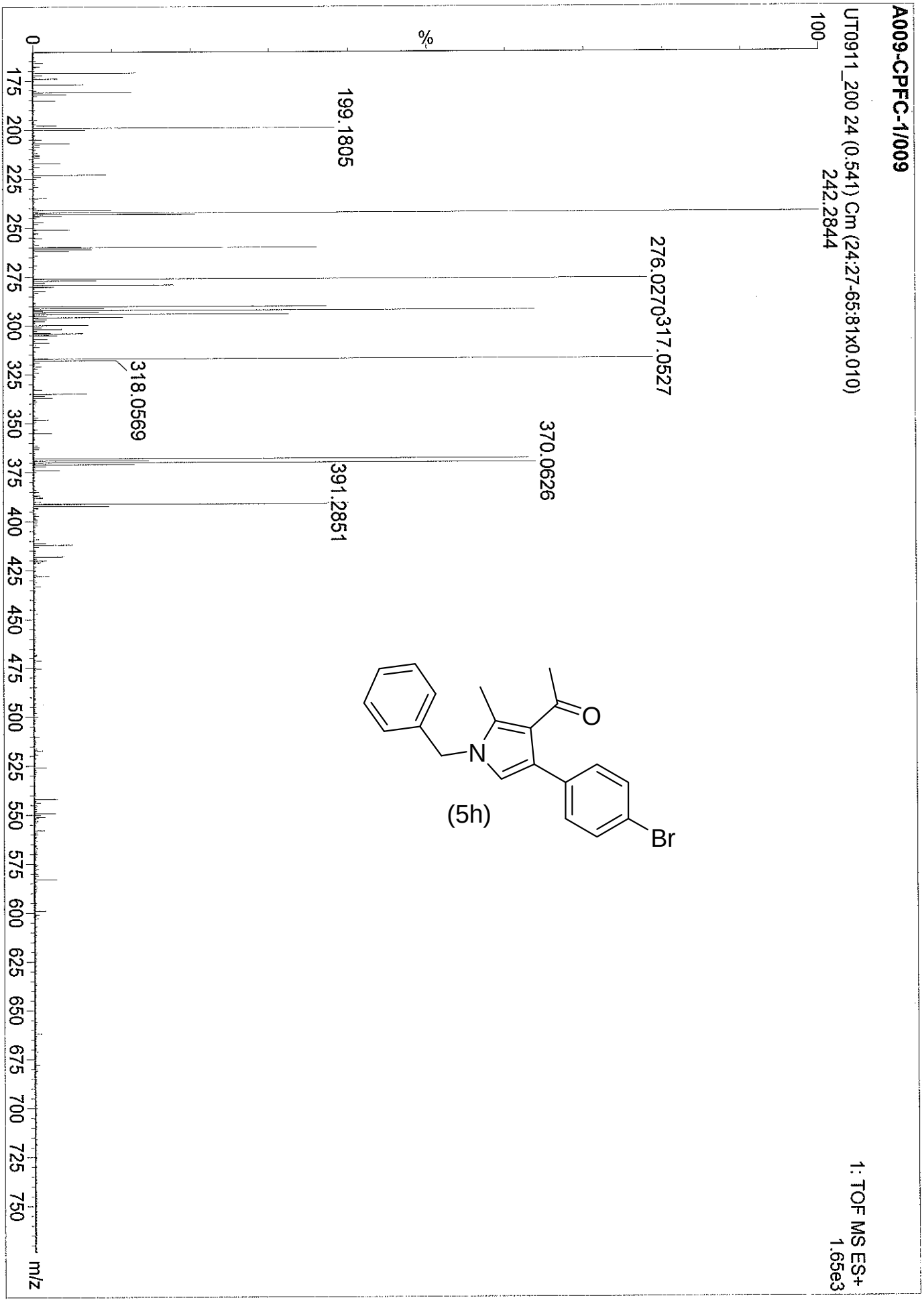


Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
418.0633	418.0618	1.5	3.6	11.5	2.3	C21 H19 N O Br F2



(5h)



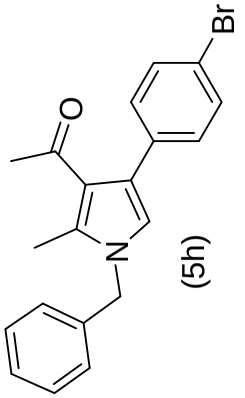


Elemental Composition Report

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

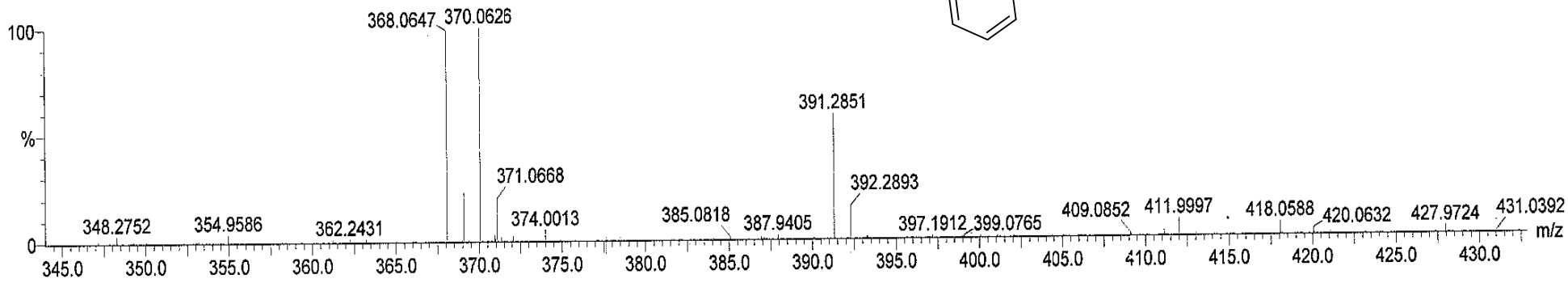
Monoisotopic Mass, Even Electron Ions
273 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-55 N: 0-4 O: 0-6 Br: 0-1
A009-CPFC-1/009



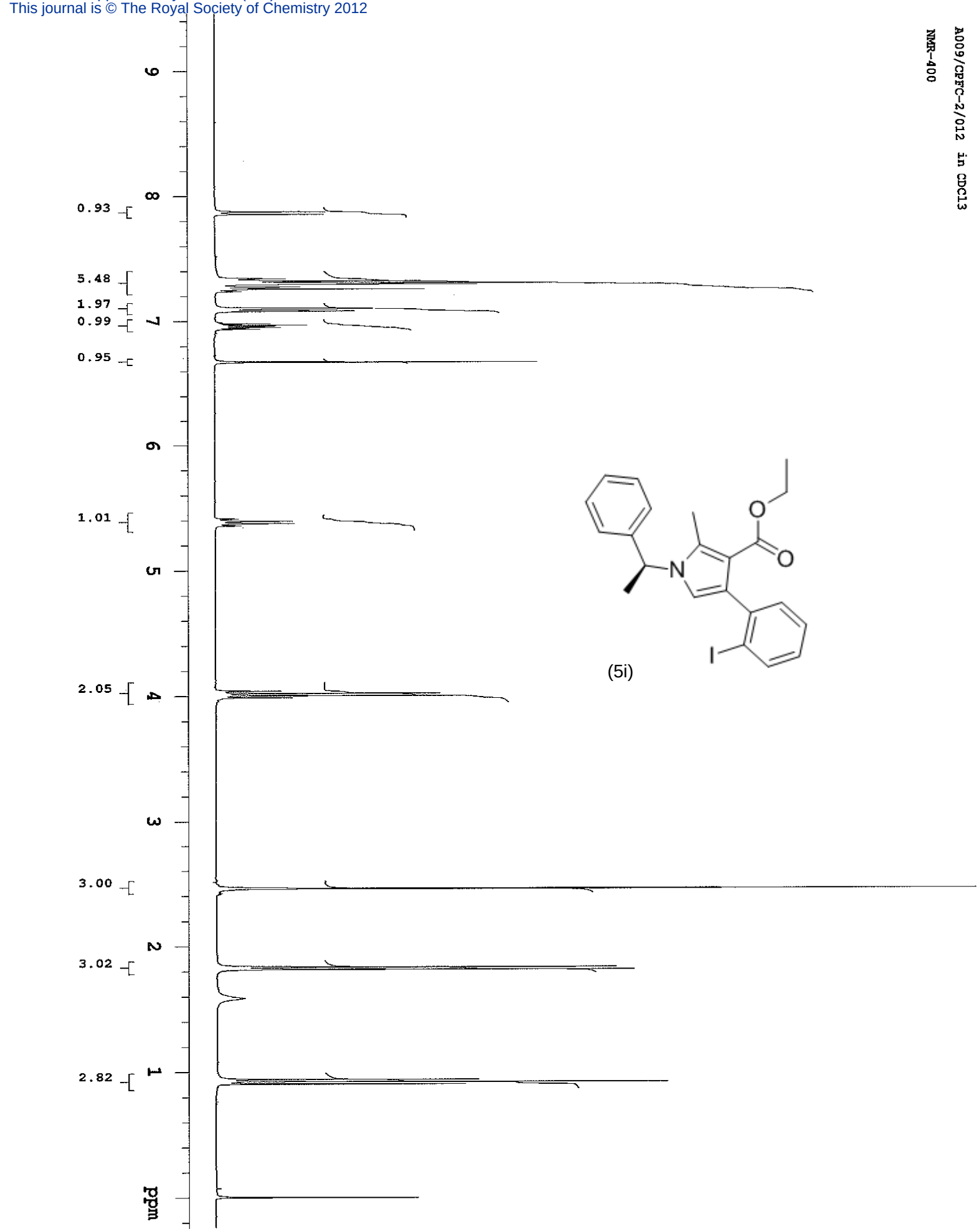
(5h)

UT0911_200 24 (0.541) Cm (24:27-65:81x0.010)

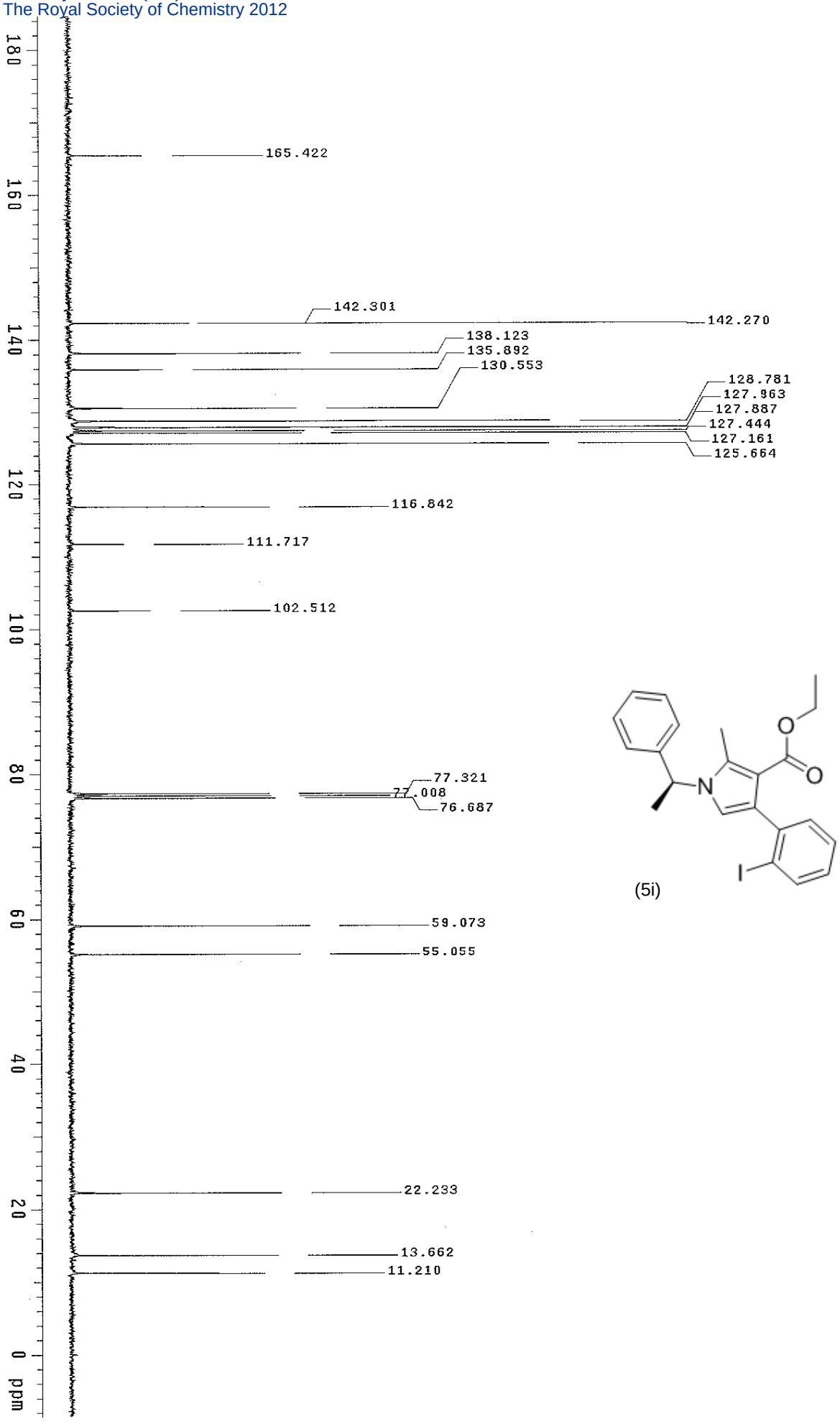
1: TOF MS ES+
1.05e+003



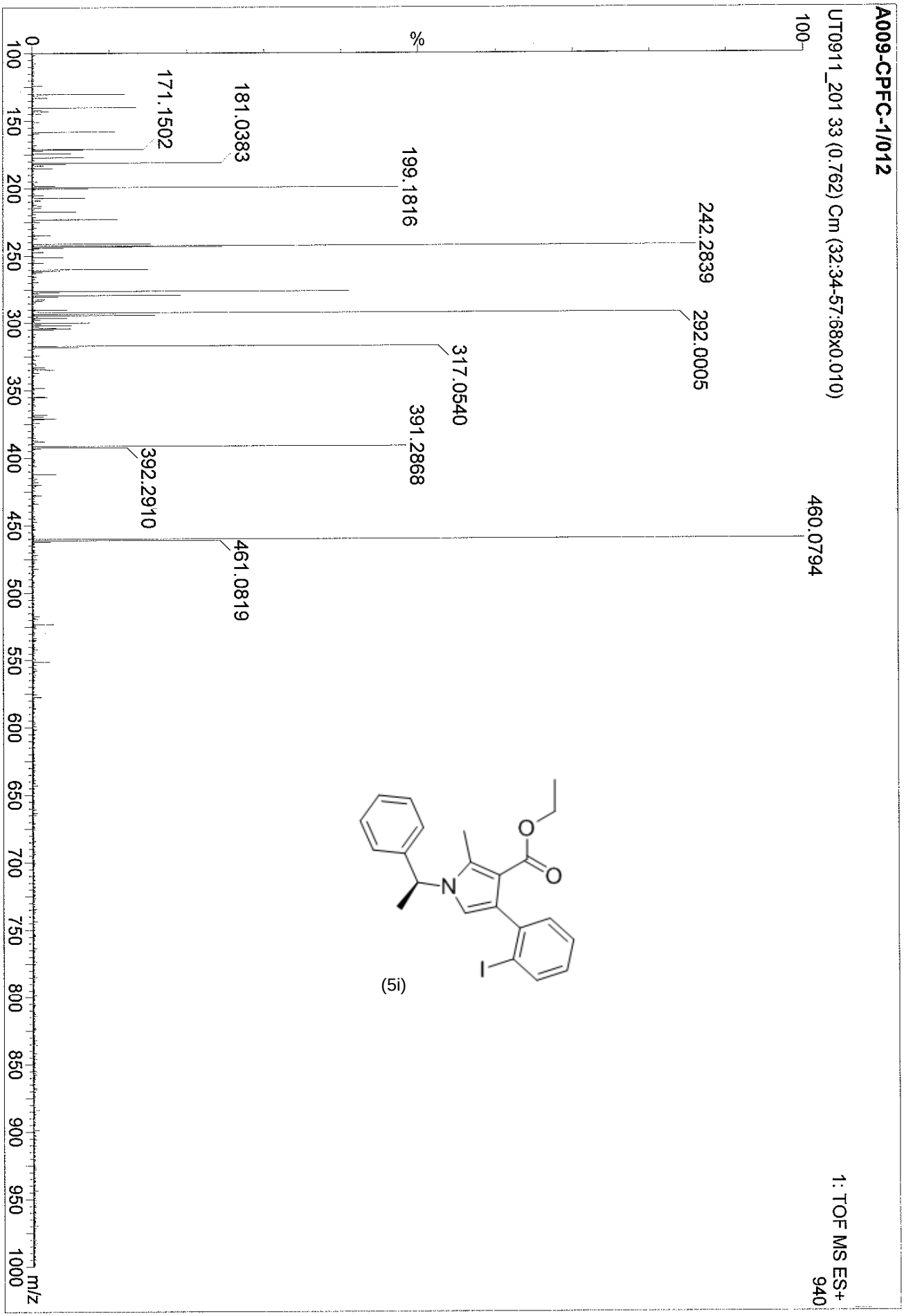
Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
370.0626	370.0650	-0.3	-0.8	11.5	1.4	C20 H19 N O Br



(5i)



(5i)



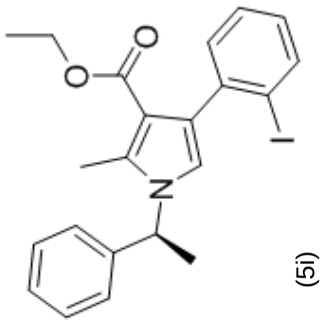
(5i)

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

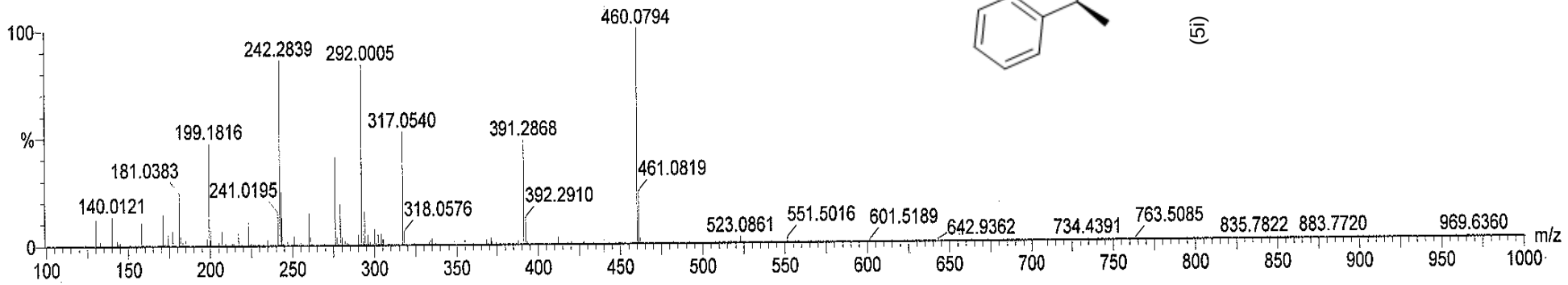
Monoisotopic Mass, Even Electron Ions
670 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-55 N: 0-4 O: 0-6 Br: 0-1 I: 0-2
A009-CPFC-1/012



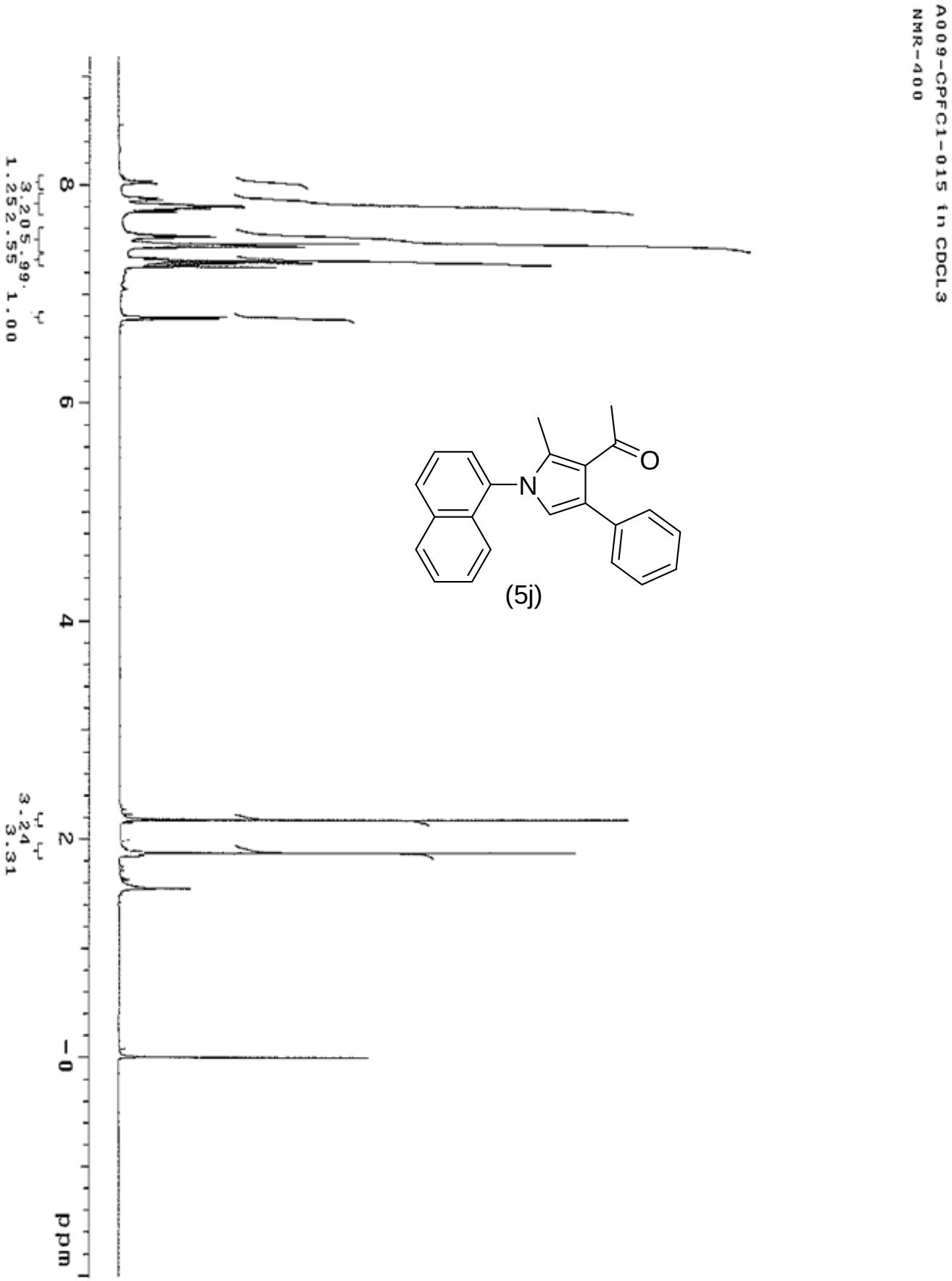
(5i)

UT0911_201 33 (0.762) Cm (32:34-57:68x0.010)

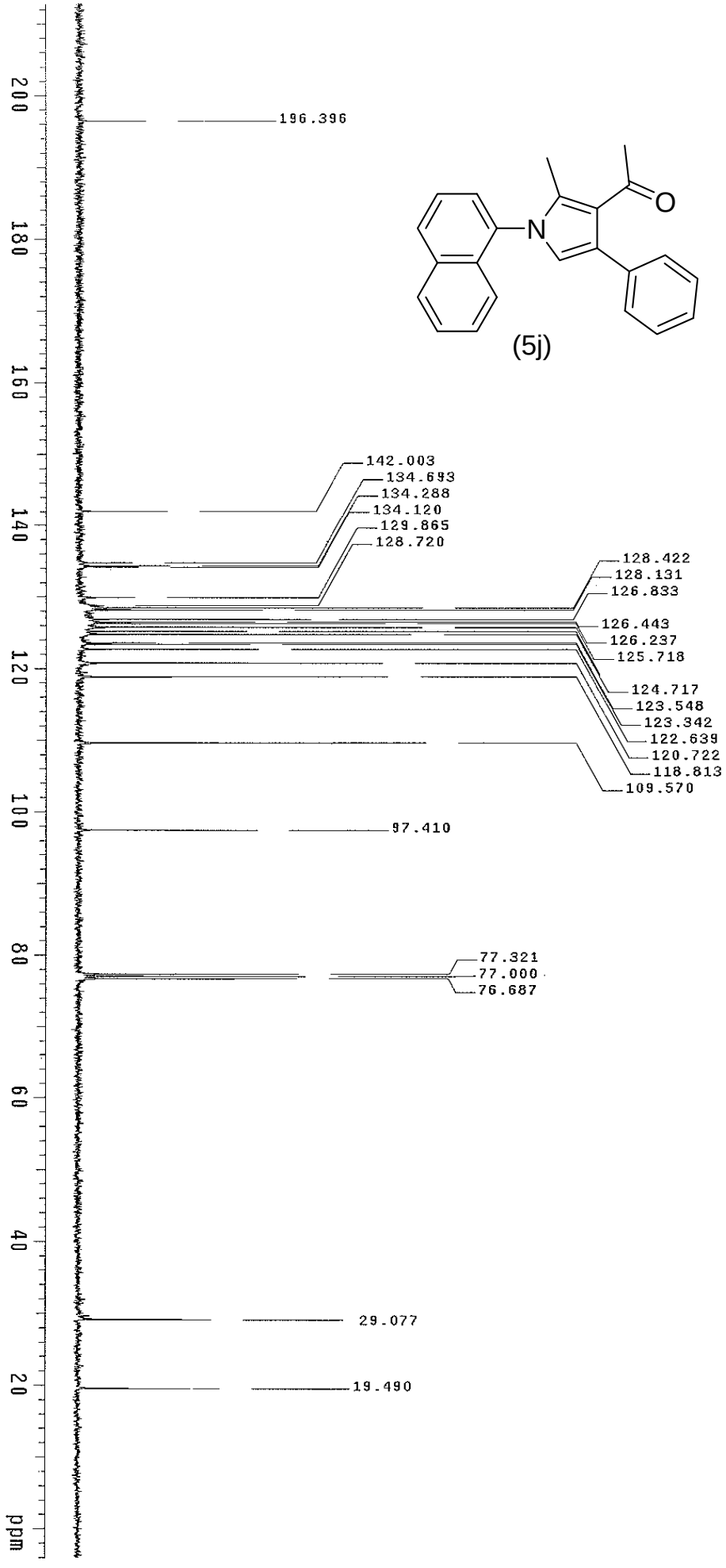
1: TOF MS ES+
9.40e+002

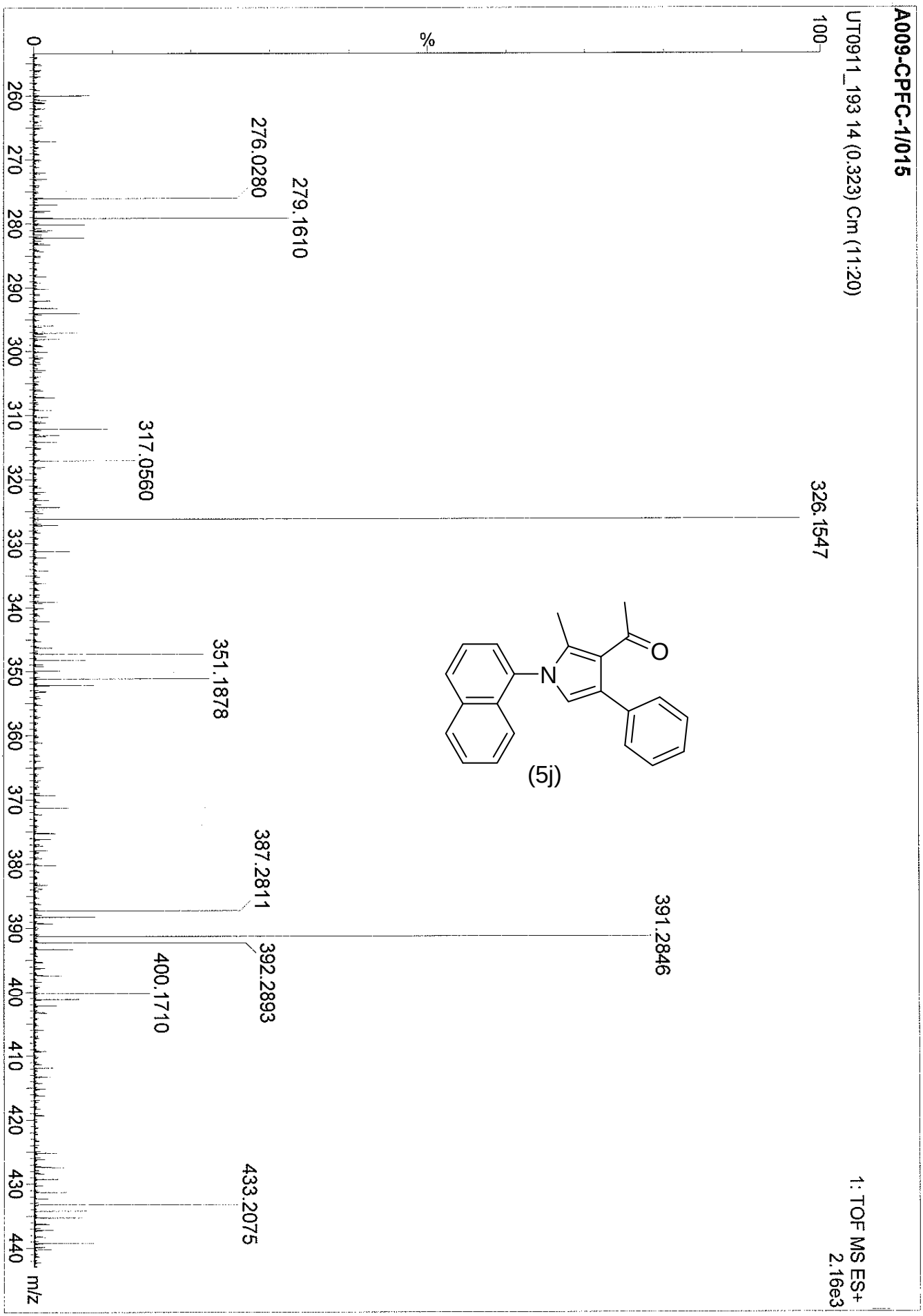


Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
460.0794	460.0774	2.0	4.3	11.5	2.4	C22 H23 N O2 I



(5j)



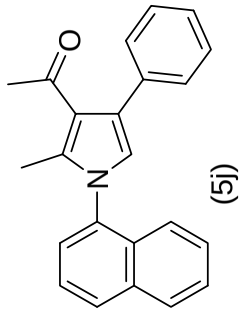


Elemental Composition Report

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

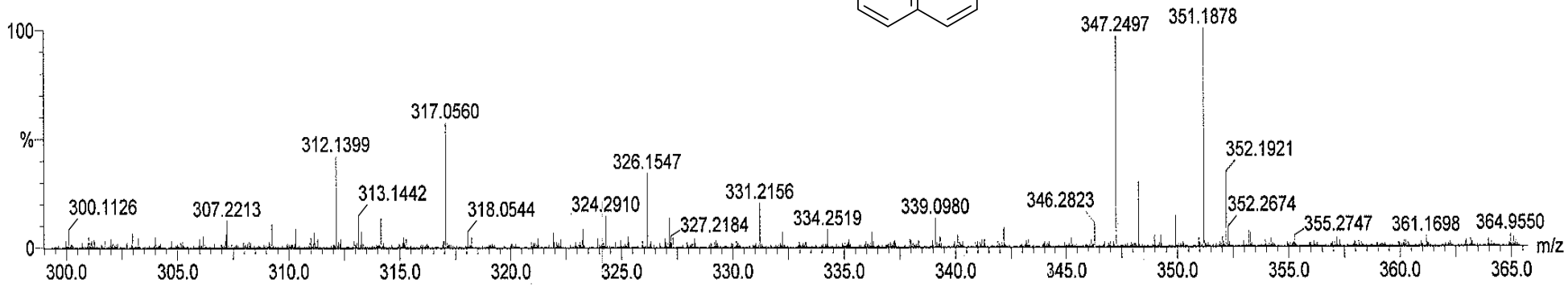
Monoisotopic Mass, Even Electron Ions
223 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-70 H: 0-80 N: 0-5 O: 0-10
A009-CPFC-1/015



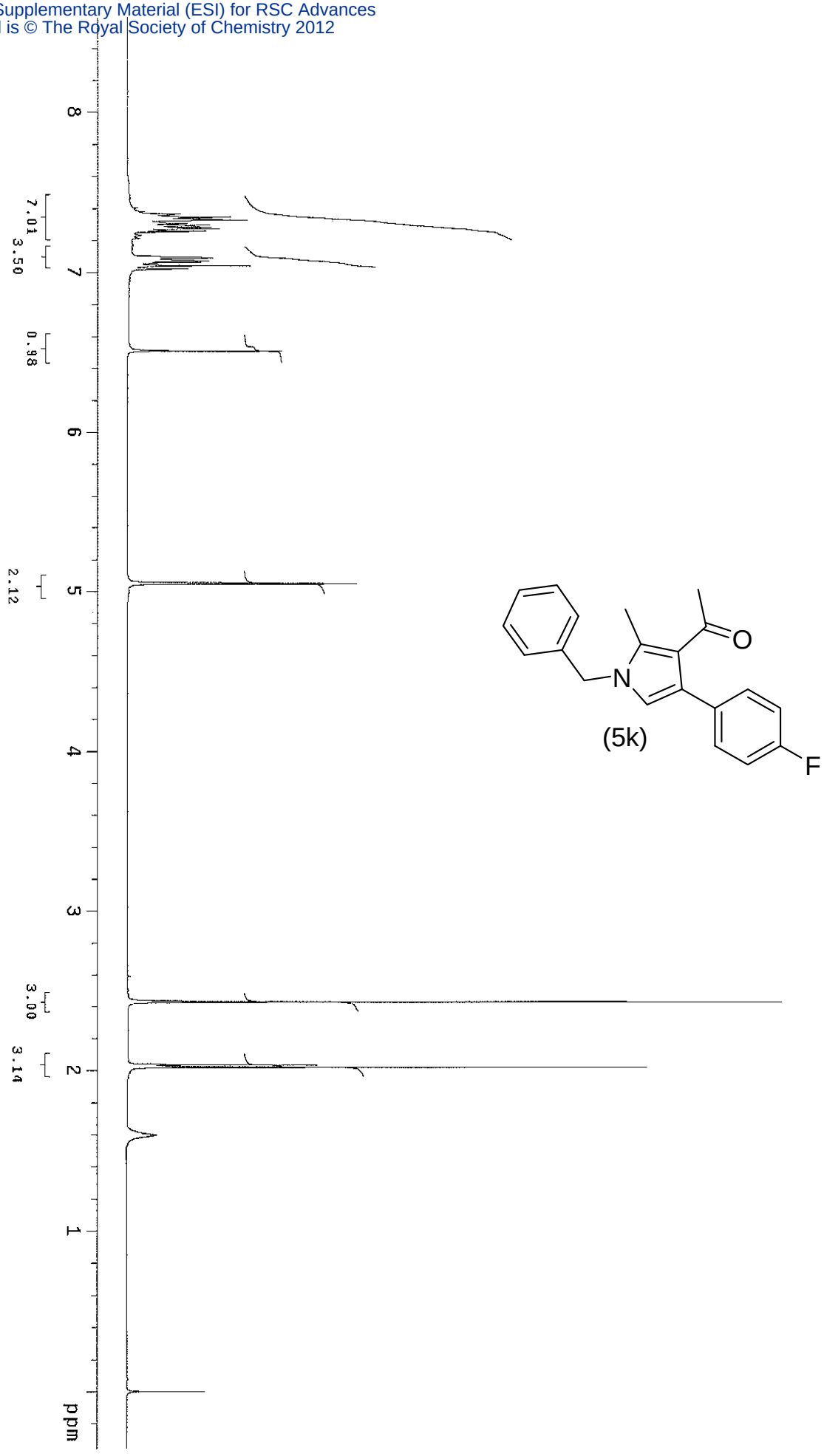
(5j)

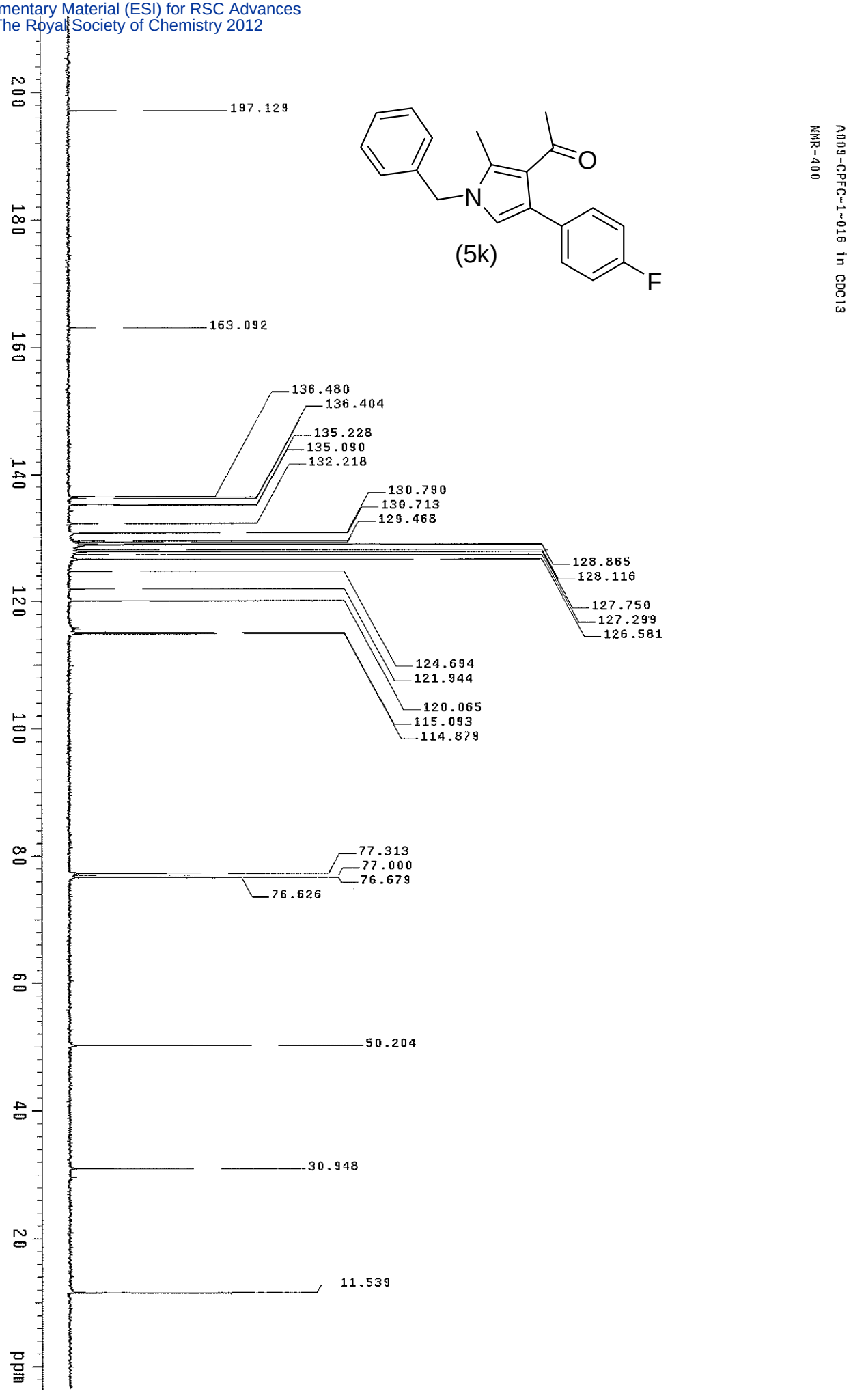
UT0911_193 14 (0.323) Cm (11:20)

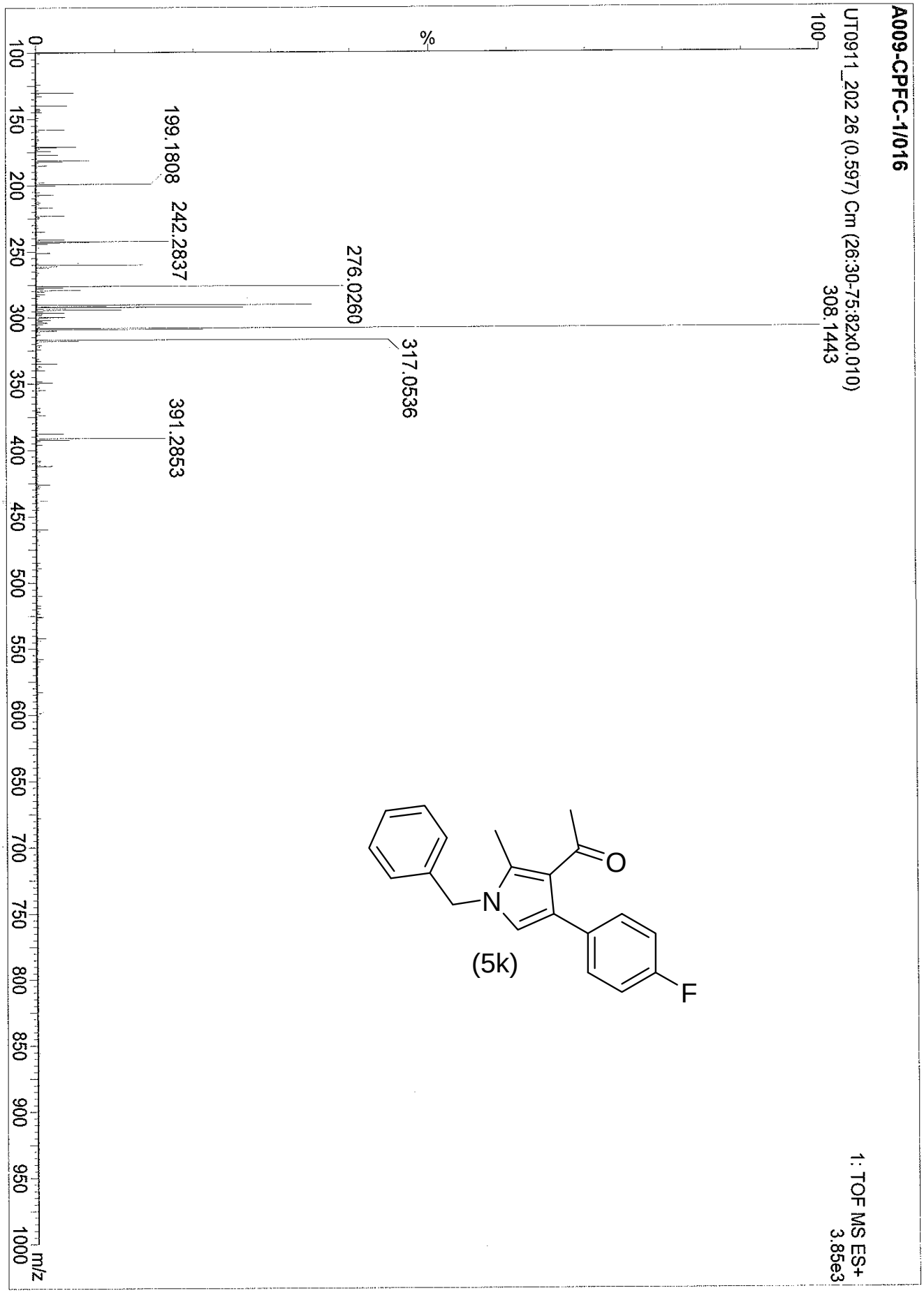
1: TOF MS ES+
4.83e+002



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
326.1547	326.1545	0.2	0.6	14.5	9.1	C23 H20 N O





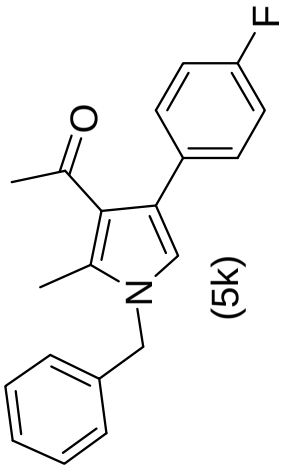


Elemental Composition Report

Single Mass Analysis

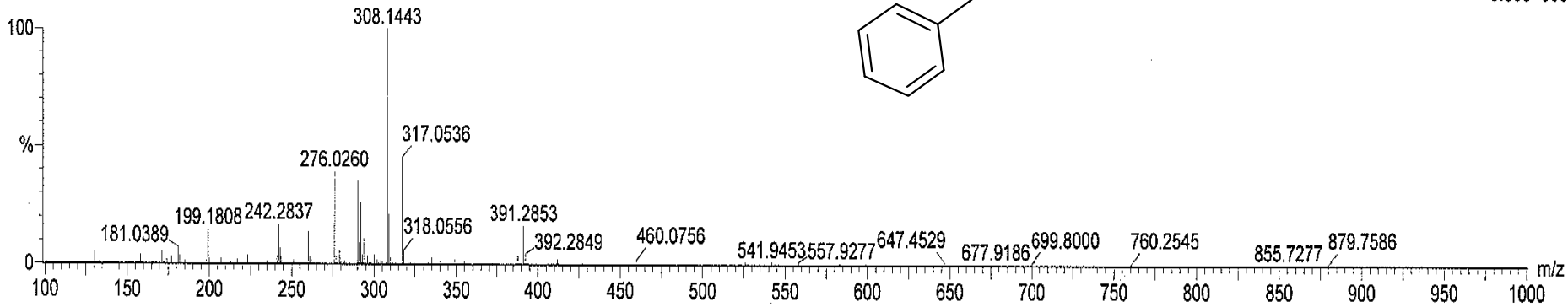
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
249 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-55 N: 0-4 O: 0-6 F: 0-1
A009-CPFC-1/016

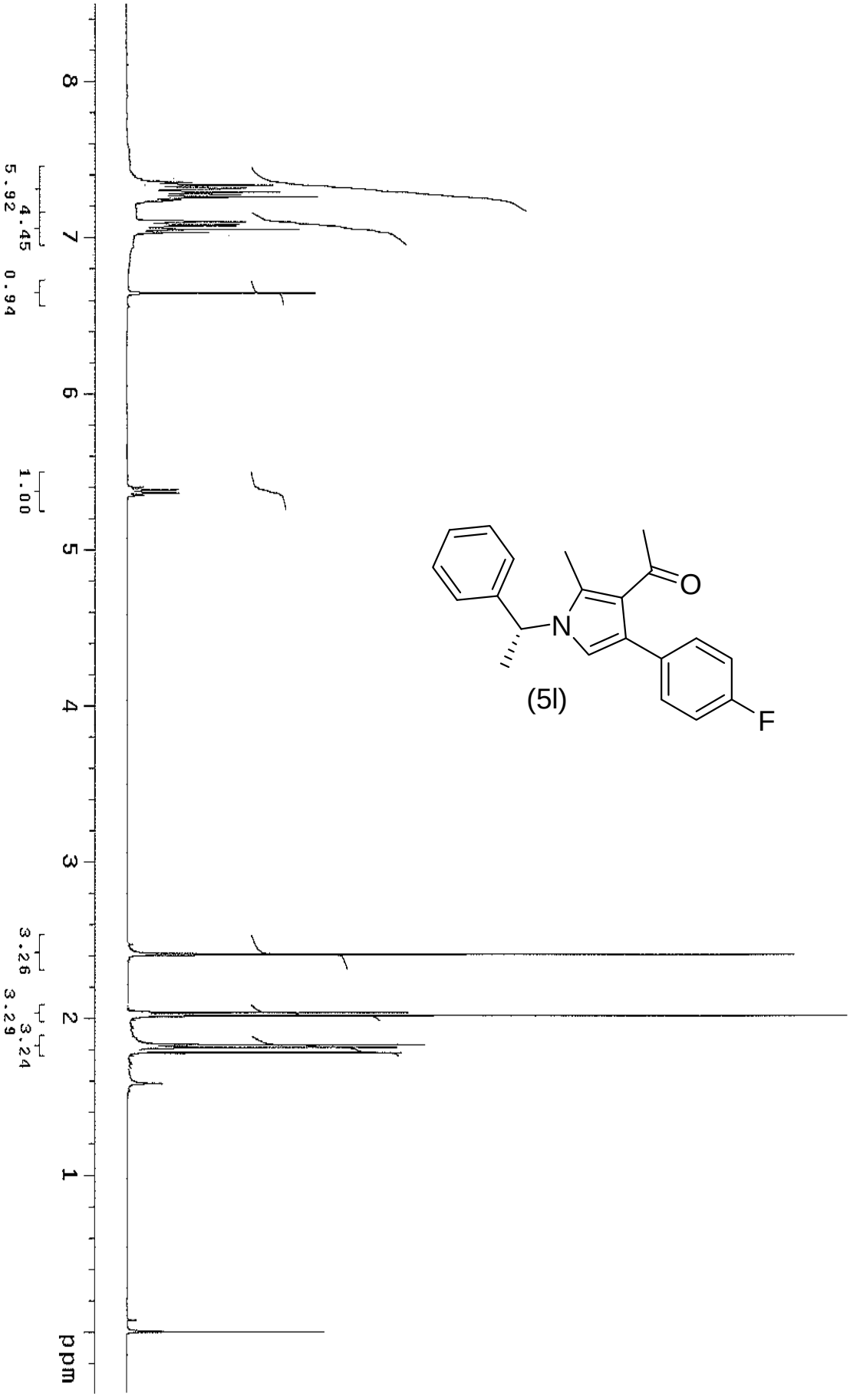


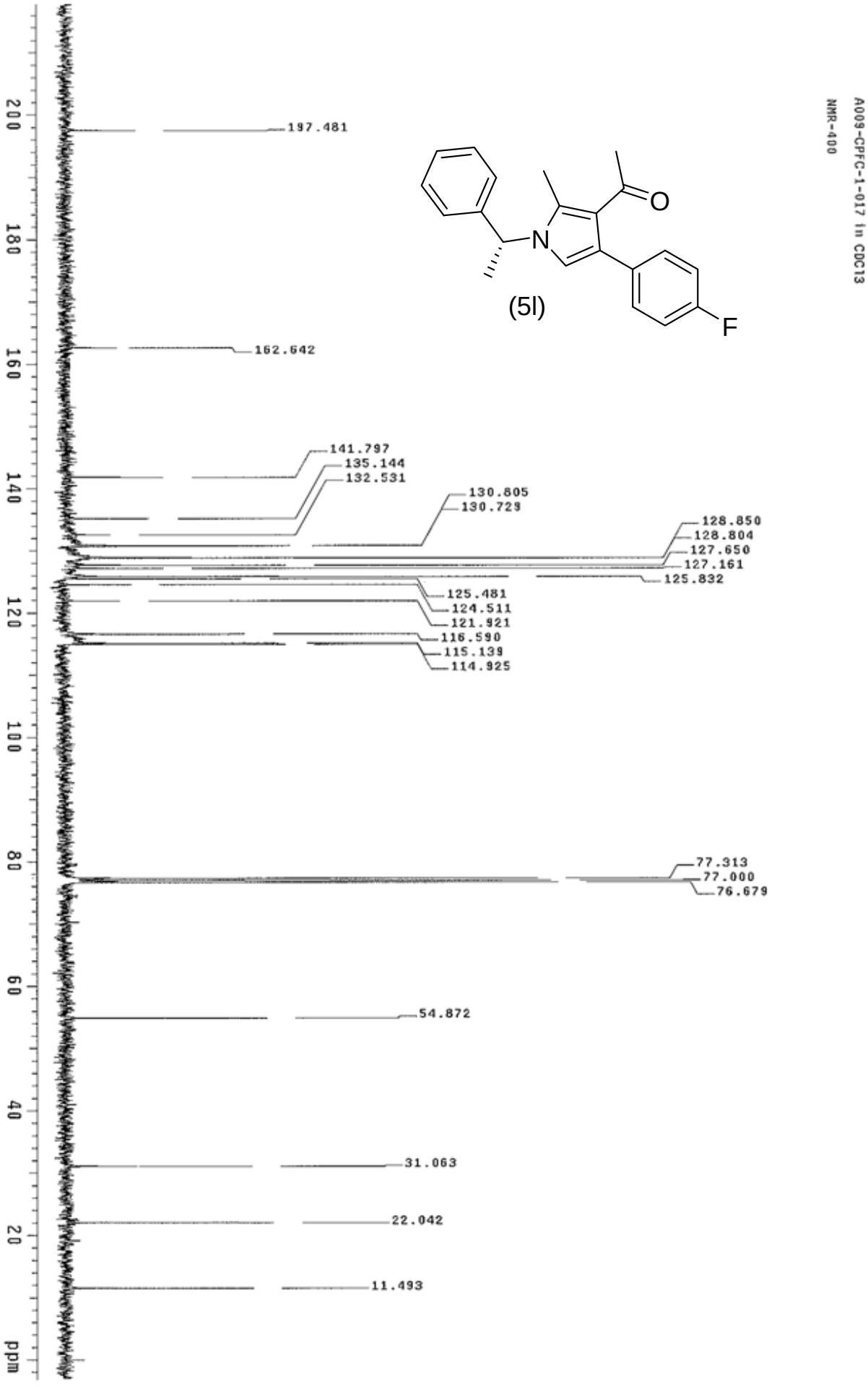
UT0911_202 26 (0.597) Cm (26:30-75:82x0.010)

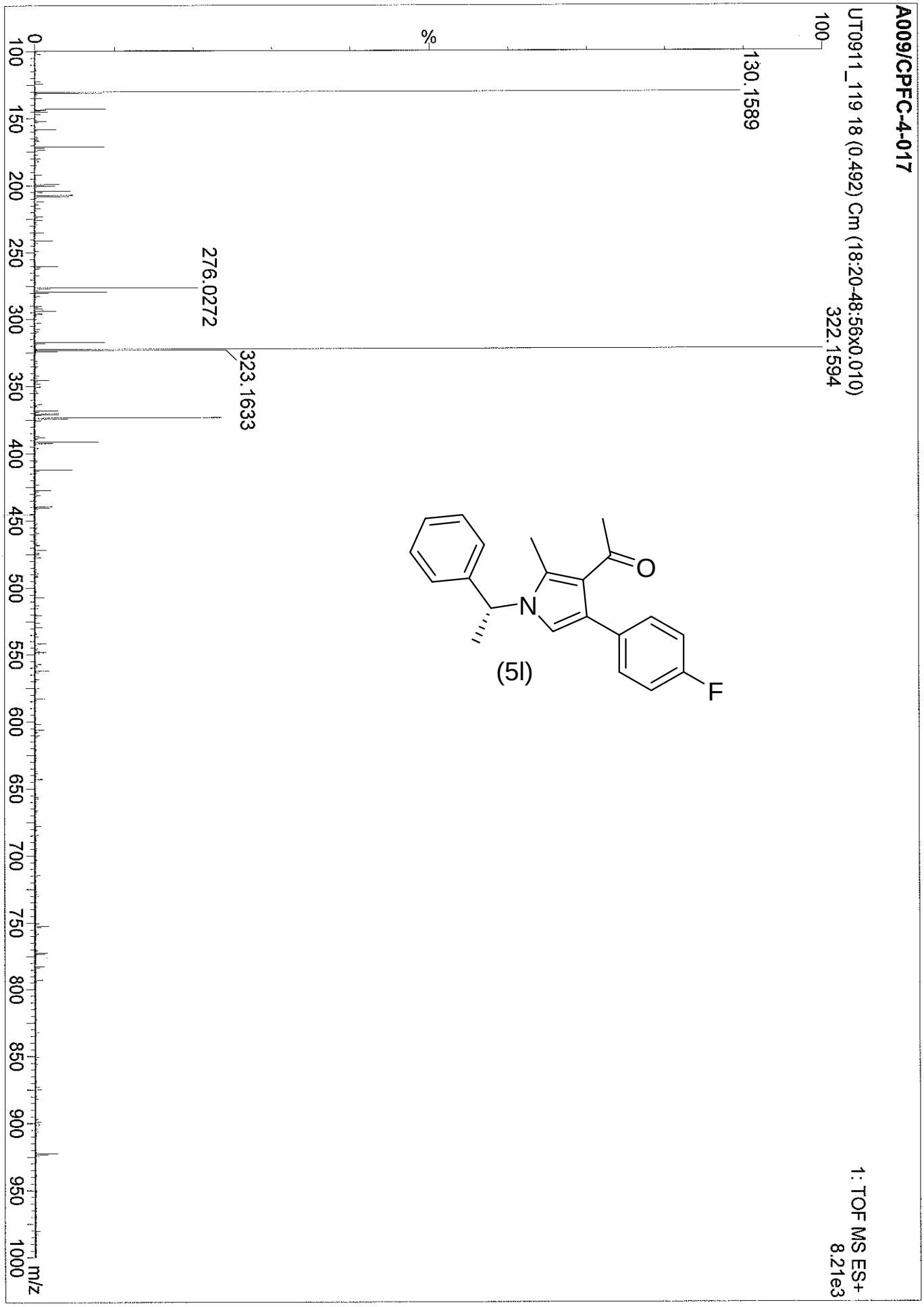
1: TOF MS ES+
3.85e+003



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
308.1443	308.1451	-0.8	-2.6	11.5	5.6	C20 H19 N O F





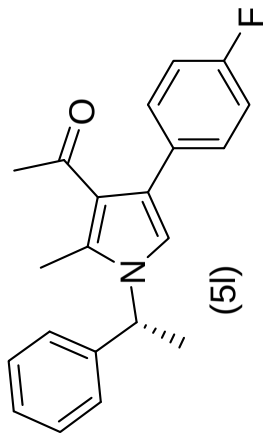


Elemental Composition Report

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 = 3

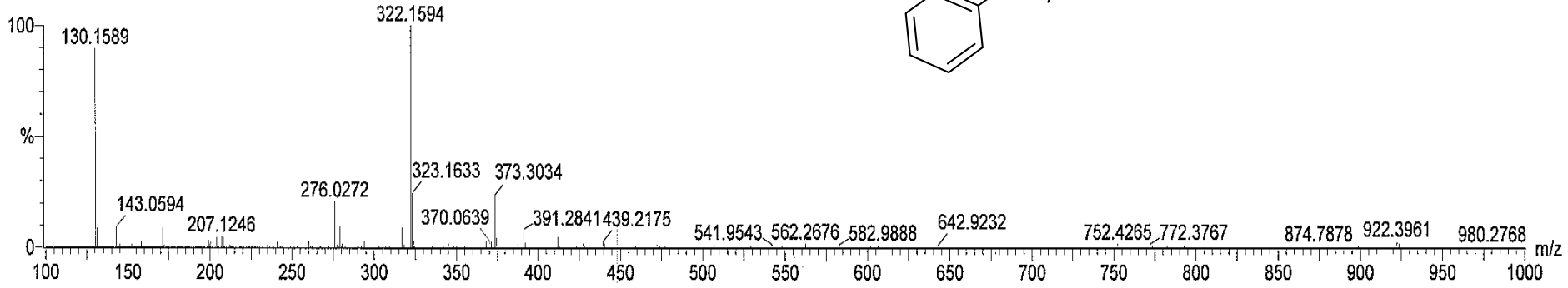
Monoisotopic Mass, Even Electron Ions
235 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-65 N: 0-5 O: 0-4 F: 0-1
A009/CPFC-4-017



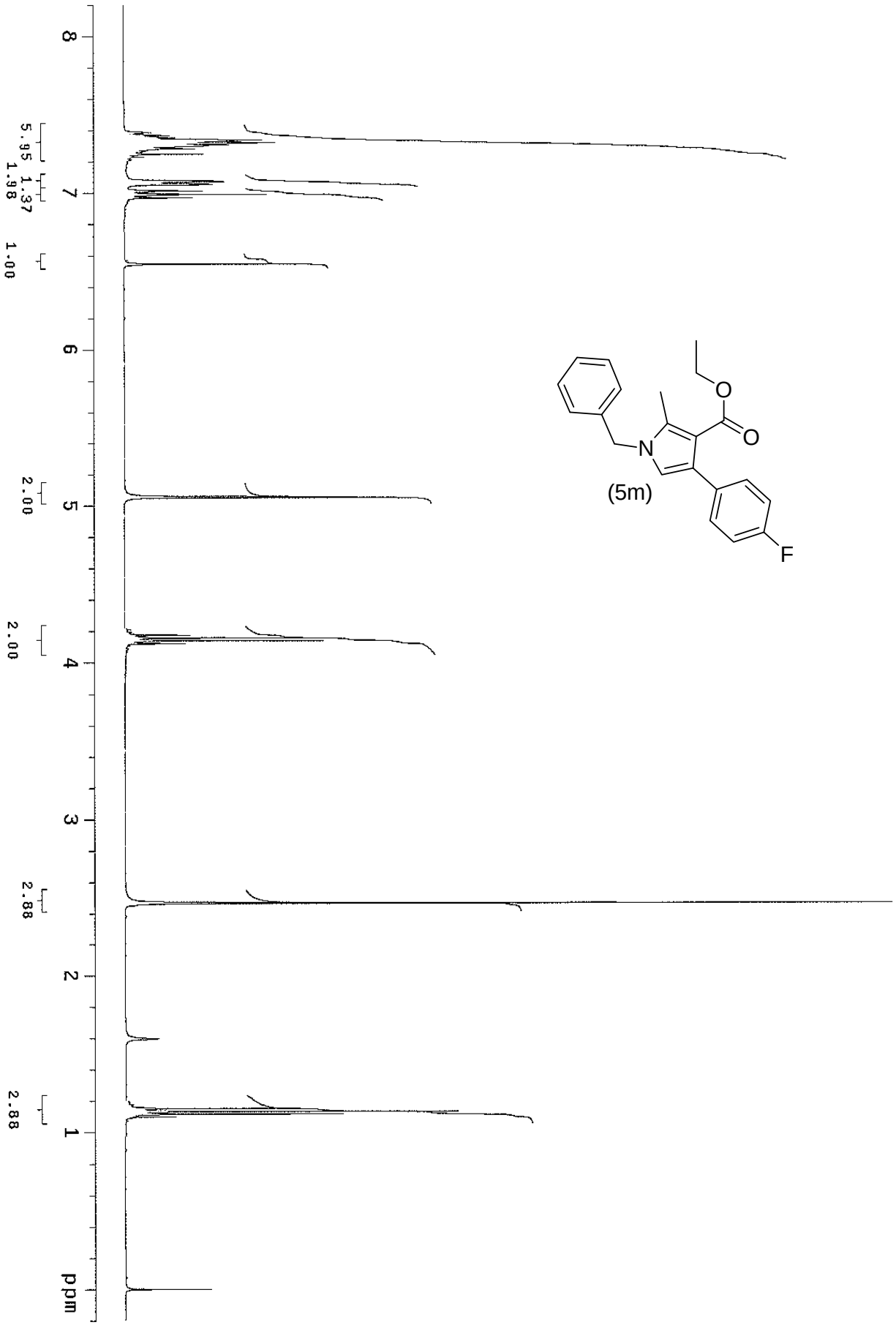
(5l)

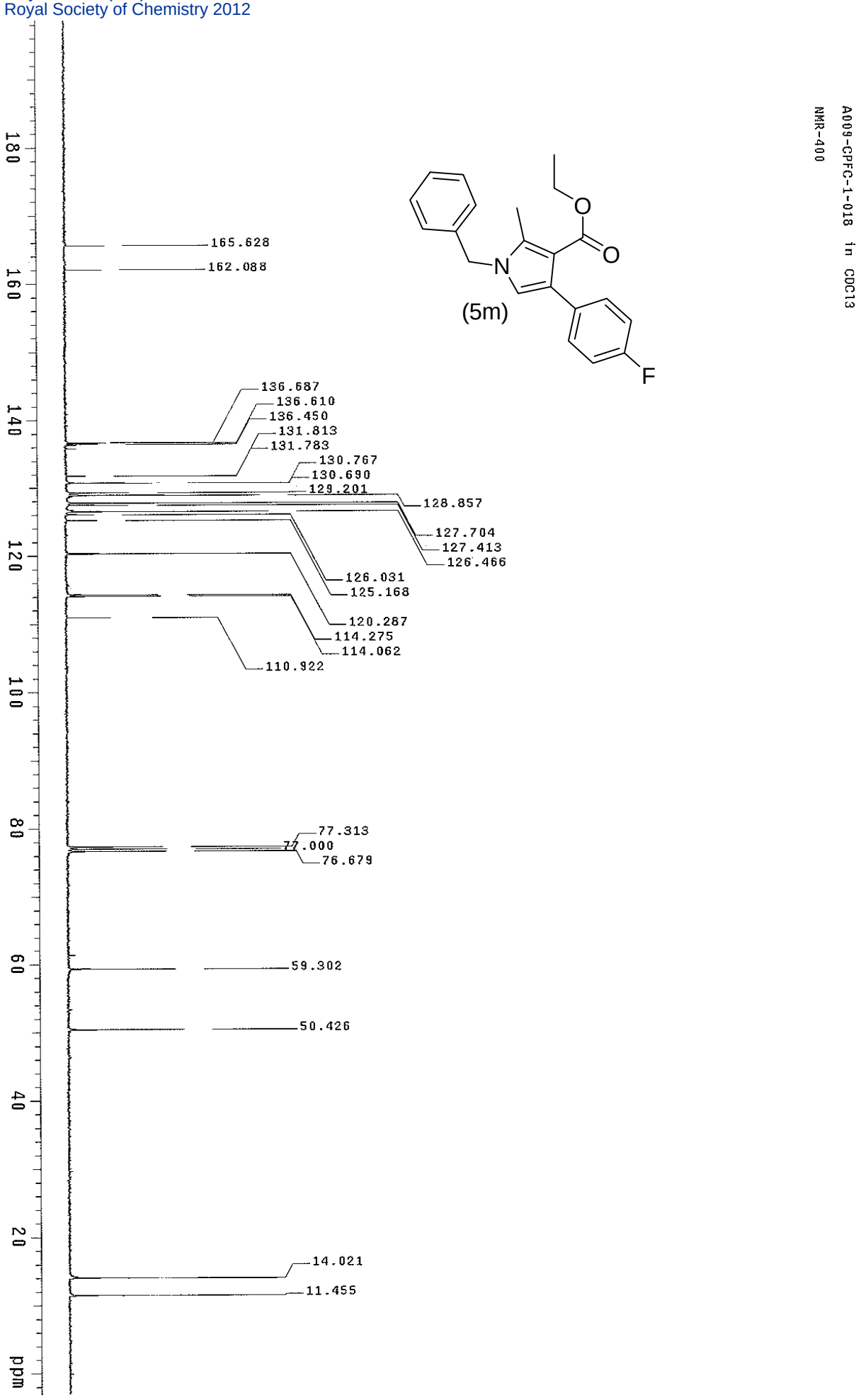
UT0911_119 18 (0.492) Cm (18:20-48:56x0.010)

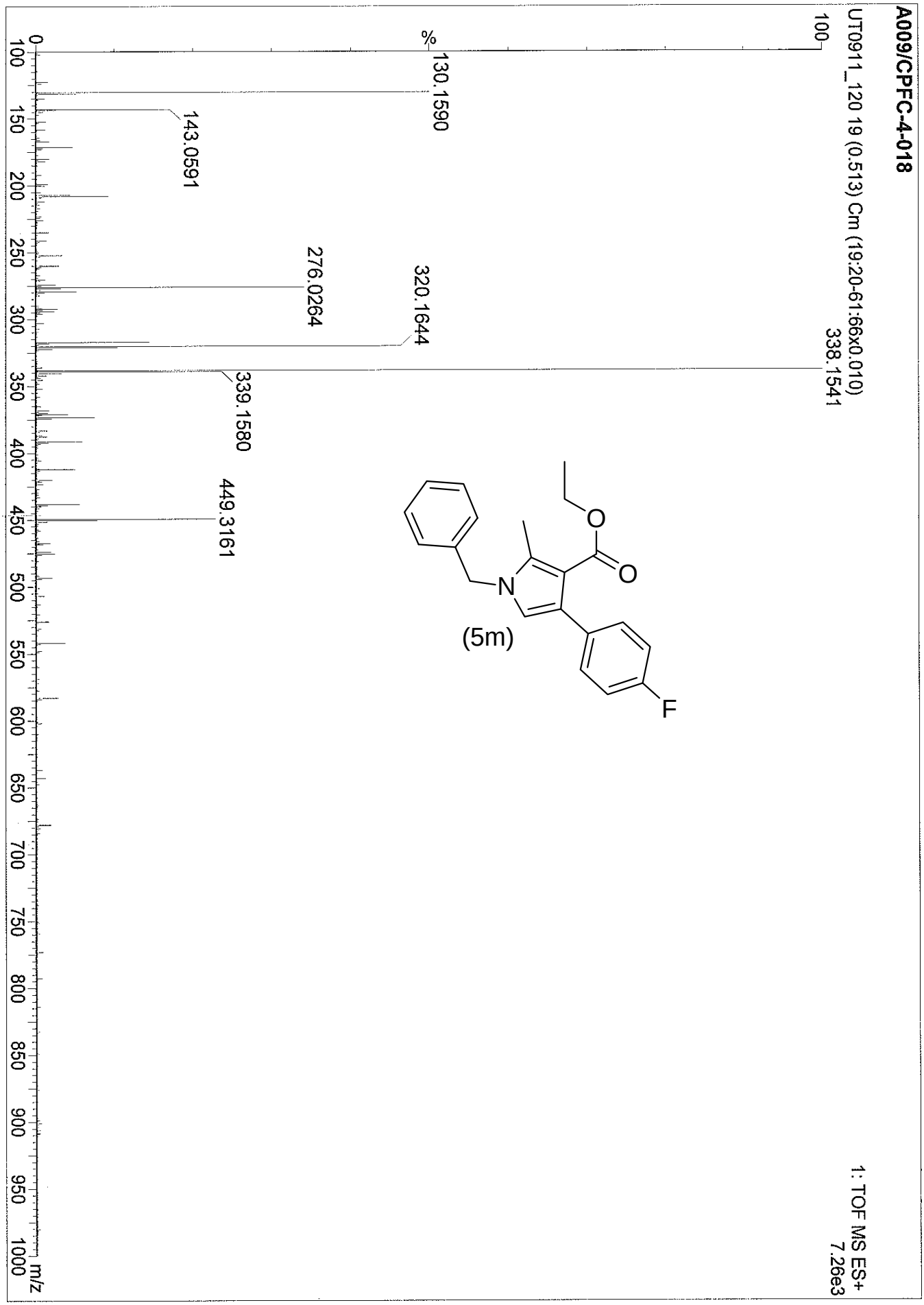
1: TOF MS ES+
8.21e+003



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
322.1594	322.1607	-1.3	-4.0	11.5	0.6	C21 H21 N O F





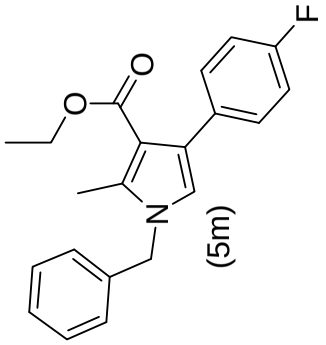


Elemental Composition Report

Single Mass Analysis

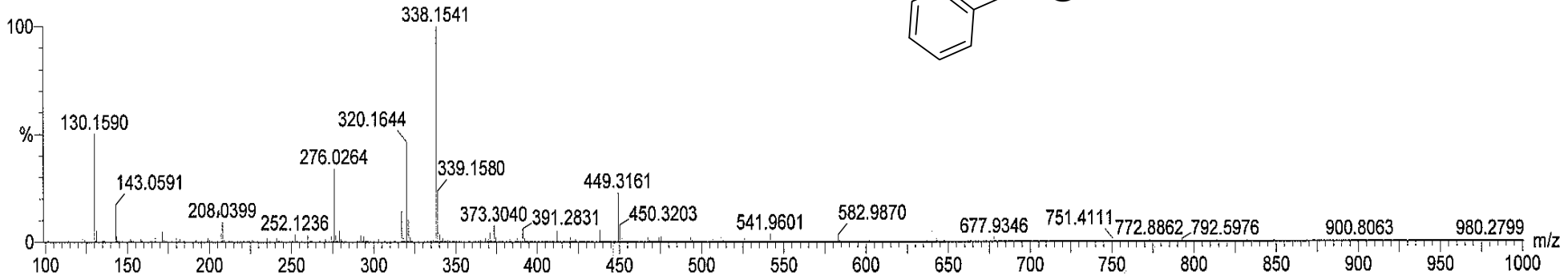
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
246 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-65 N: 0-5 O: 0-4 F: 0-1
A009/CPFC-4-018

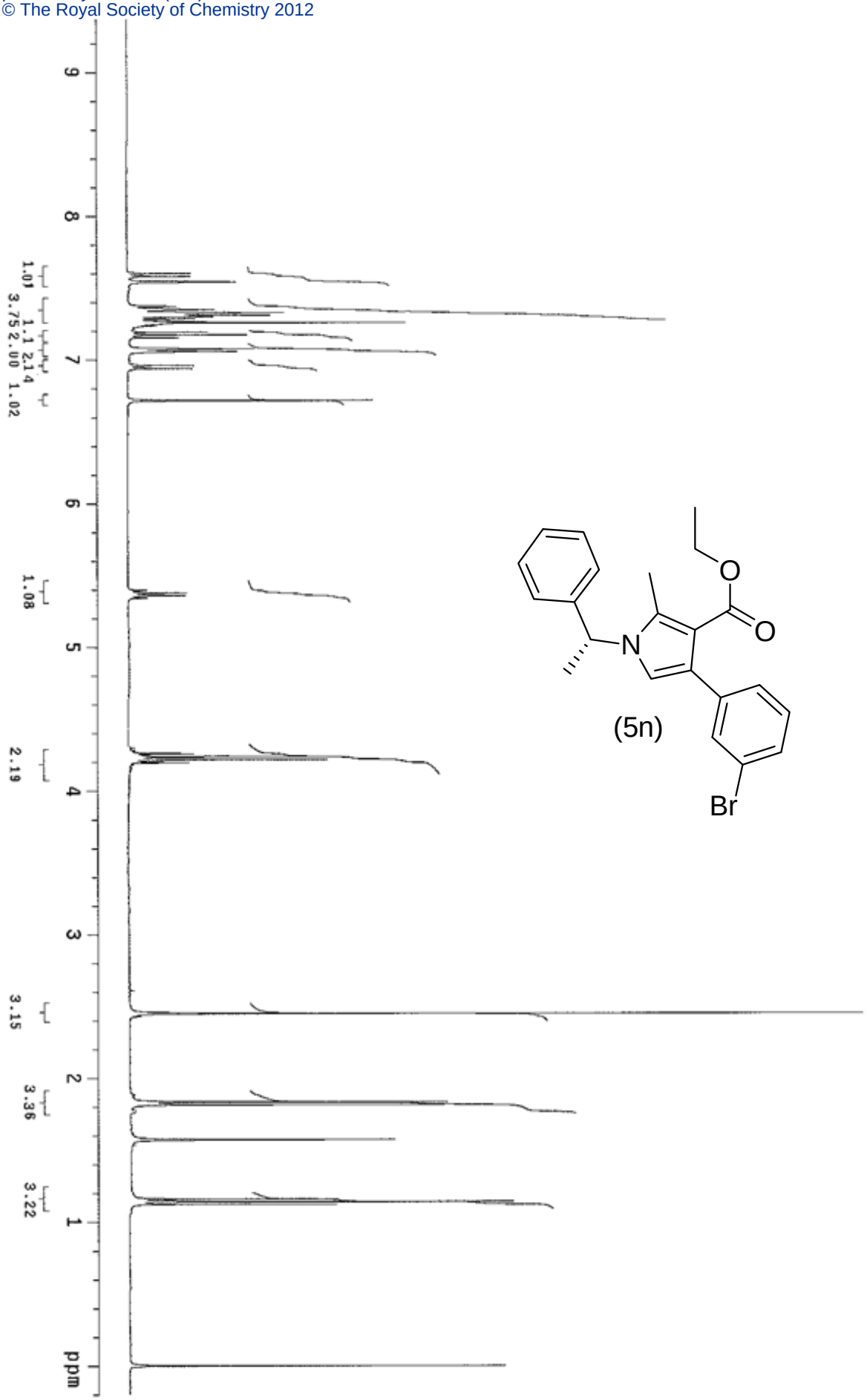


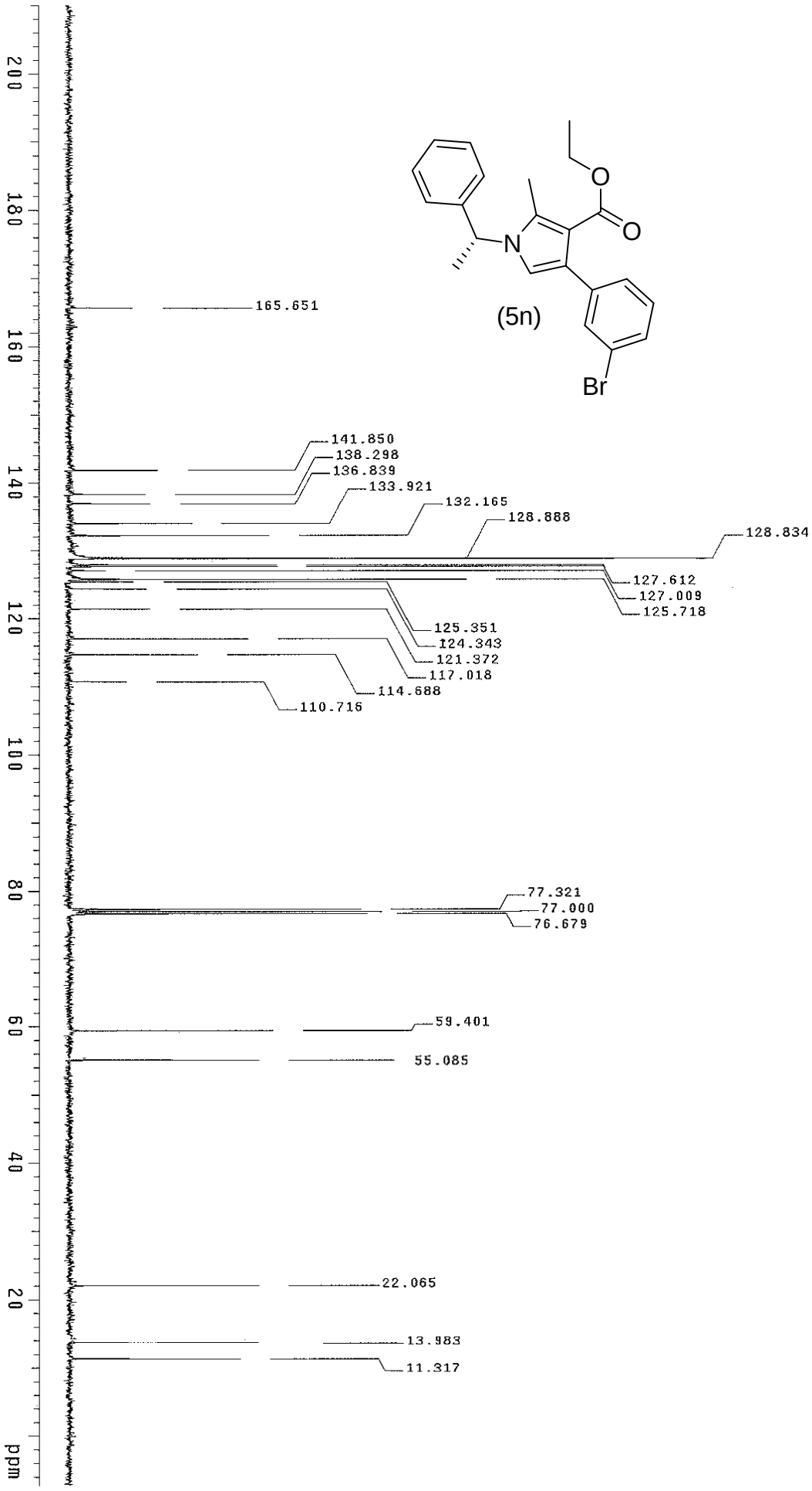
UT0911_120 19 (0.513) Cm (19:20-61:66x0.010)

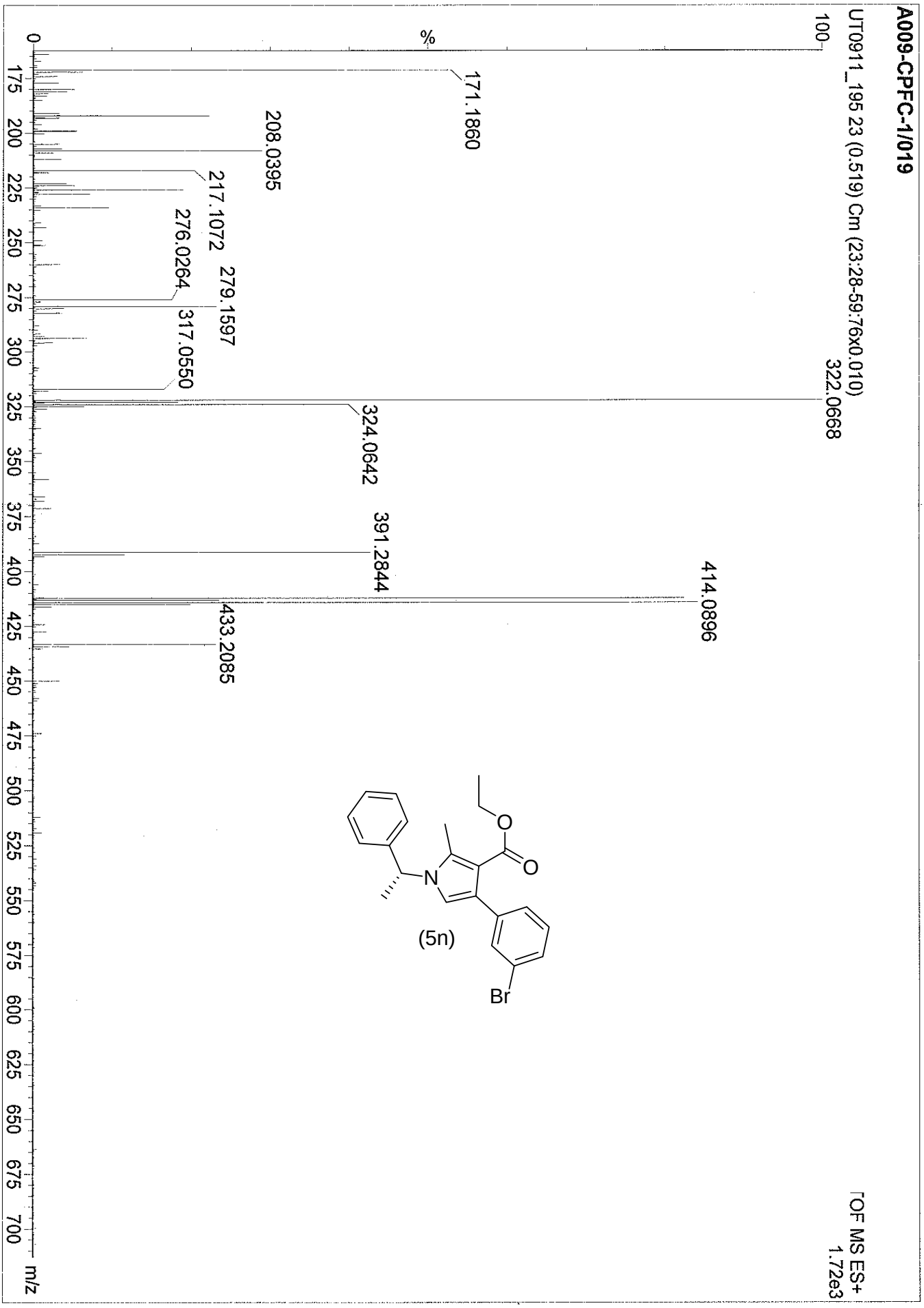
1: TOF MS ES+
7.27e+003



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
338.1541	338.1556	-1.5	-4.4	11.5	0.9	C21 H21 N O2 F





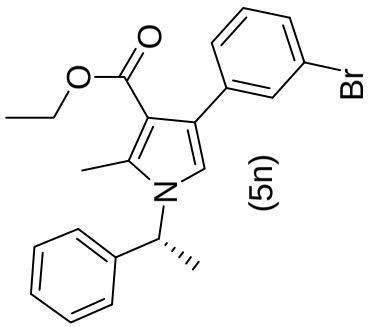


Elemental Composition Report

Single Mass Analysis

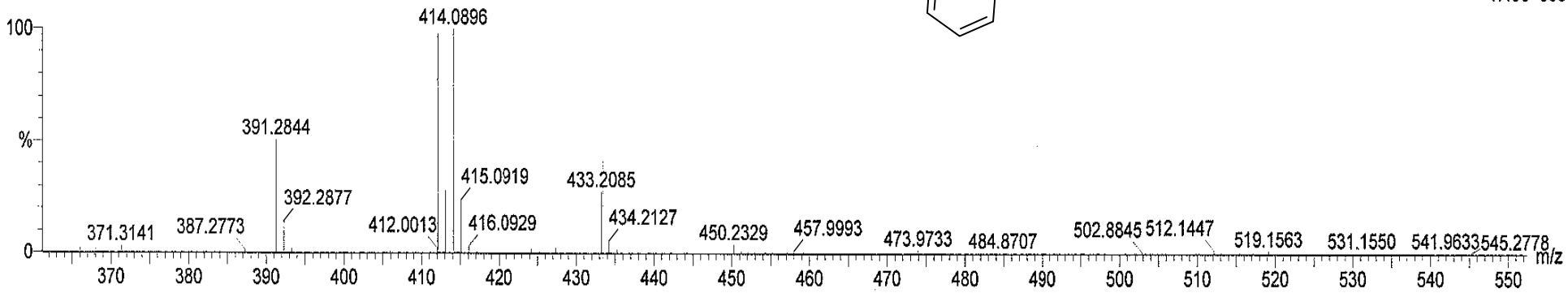
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
530 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-70 H: 0-80 N: 0-5 O: 0-10 Br: 0-1
A009-CPFC-1/019

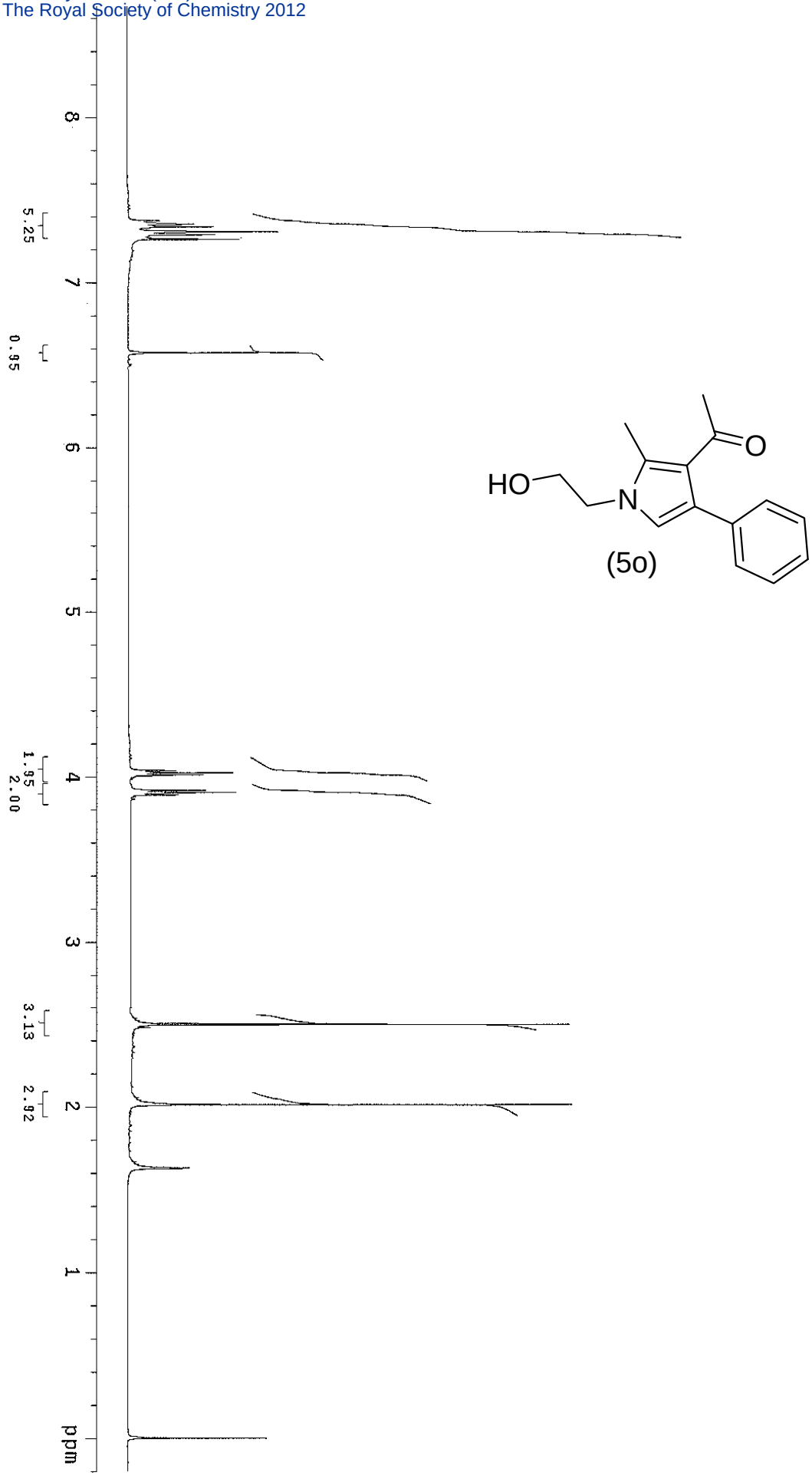


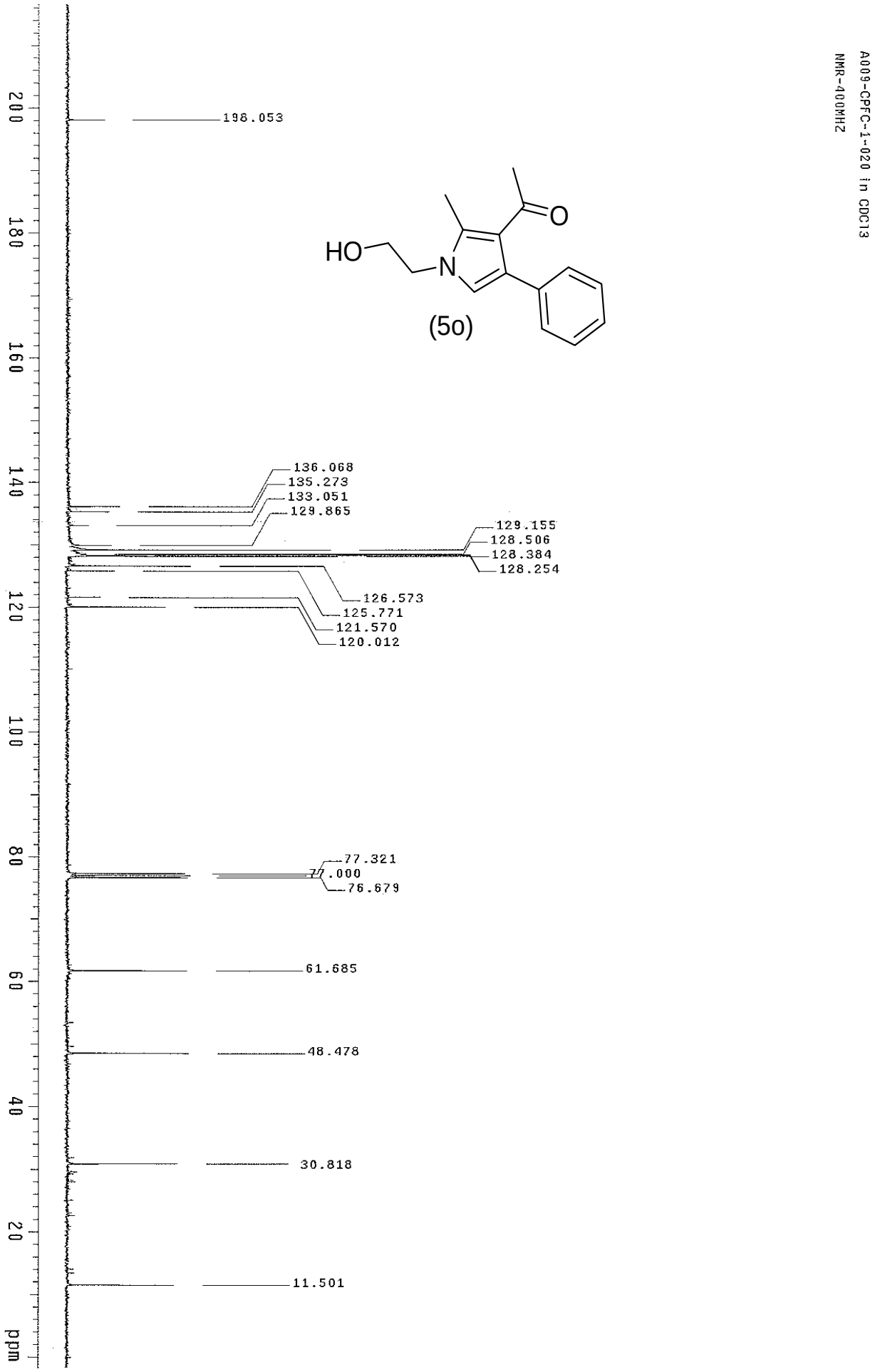
UT0911_195 23 (0.519) Cm (23:28-59:76x0.010)

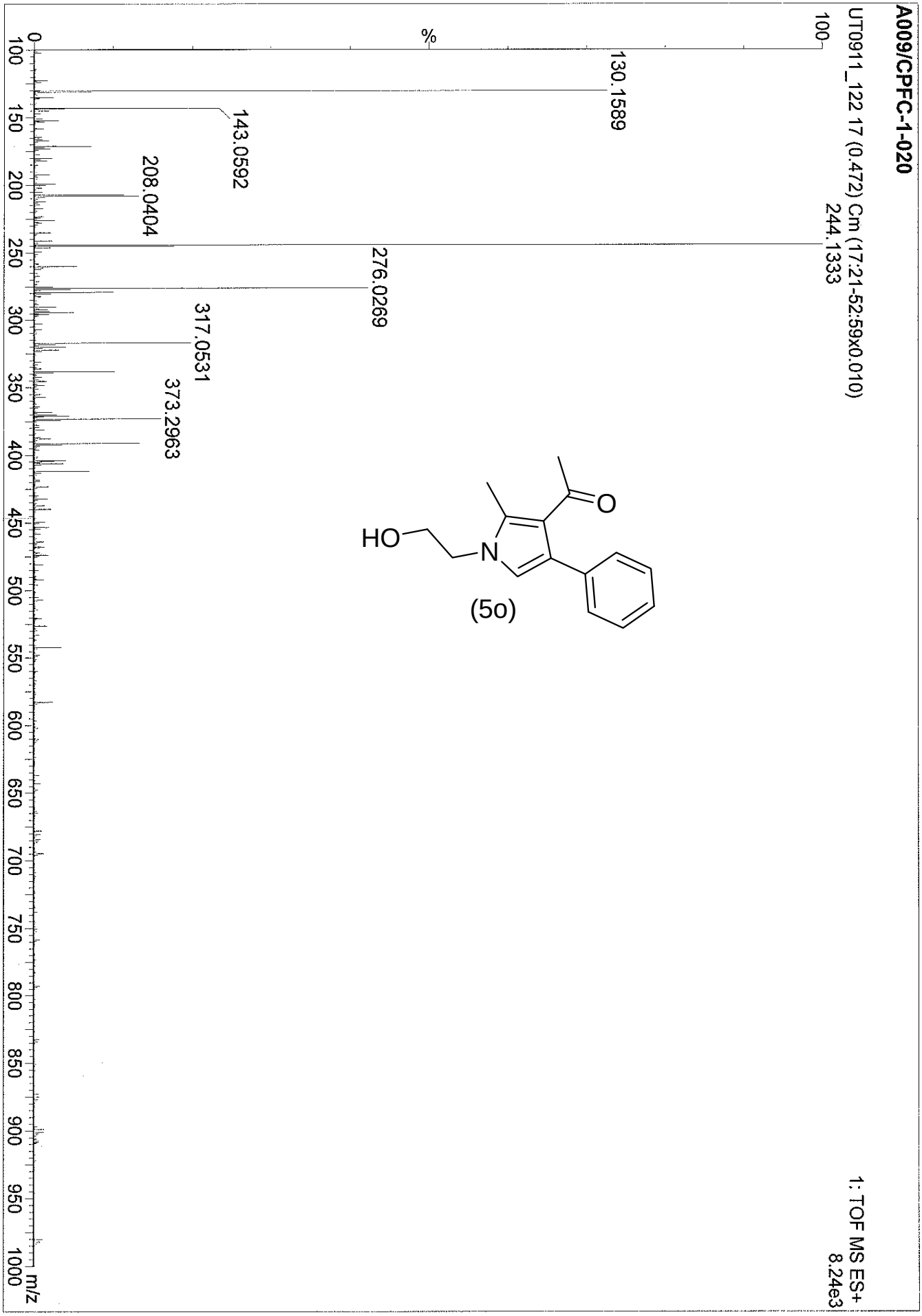
1: TOF MS ES+
1.45e+003



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
412.0915	412.0912	0.3	0.7	11.5	2.7	C22 H23 N O2 Br





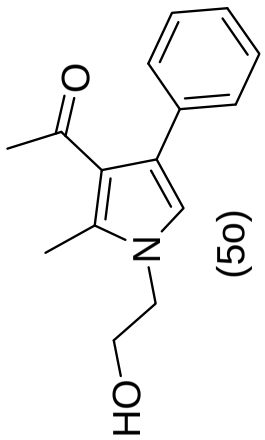


Elemental Composition Report

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 = 3

Monoisotopic Mass, Even Electron Ions
213 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-65 N: 0-2 O: 0-4 F: 0-2 Br: 0-1

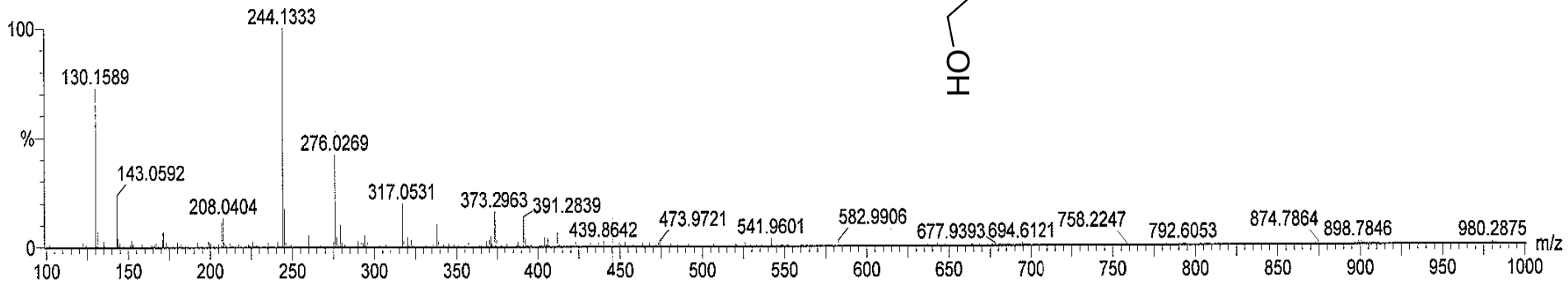


(5o)

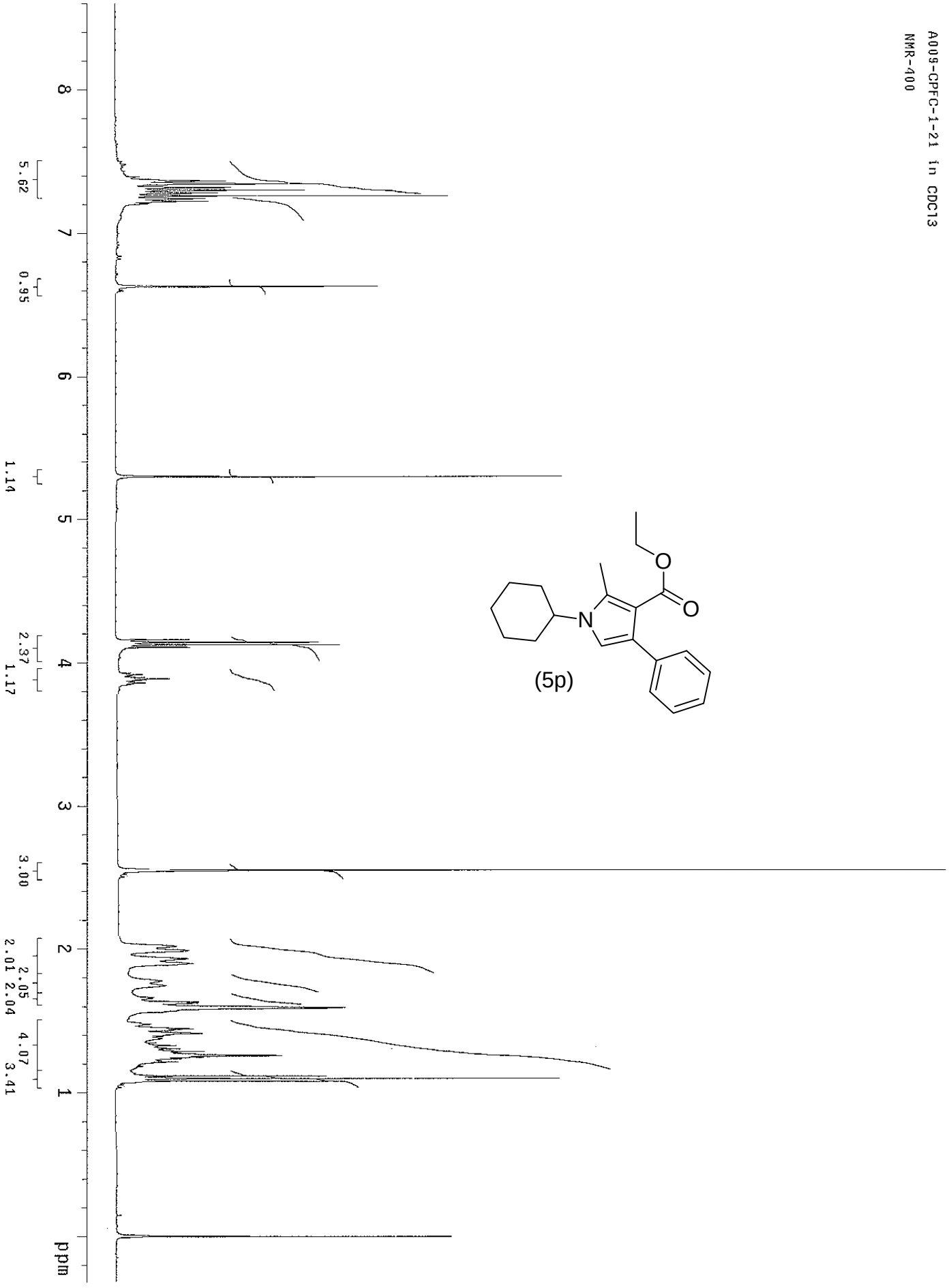
A009/CPFC-1-020

UT0911_122 17 (0.472) Cm (17:21-52:59x0.010)

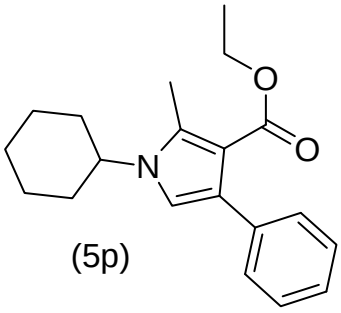
1: TOF MS ES+
8.24e+003



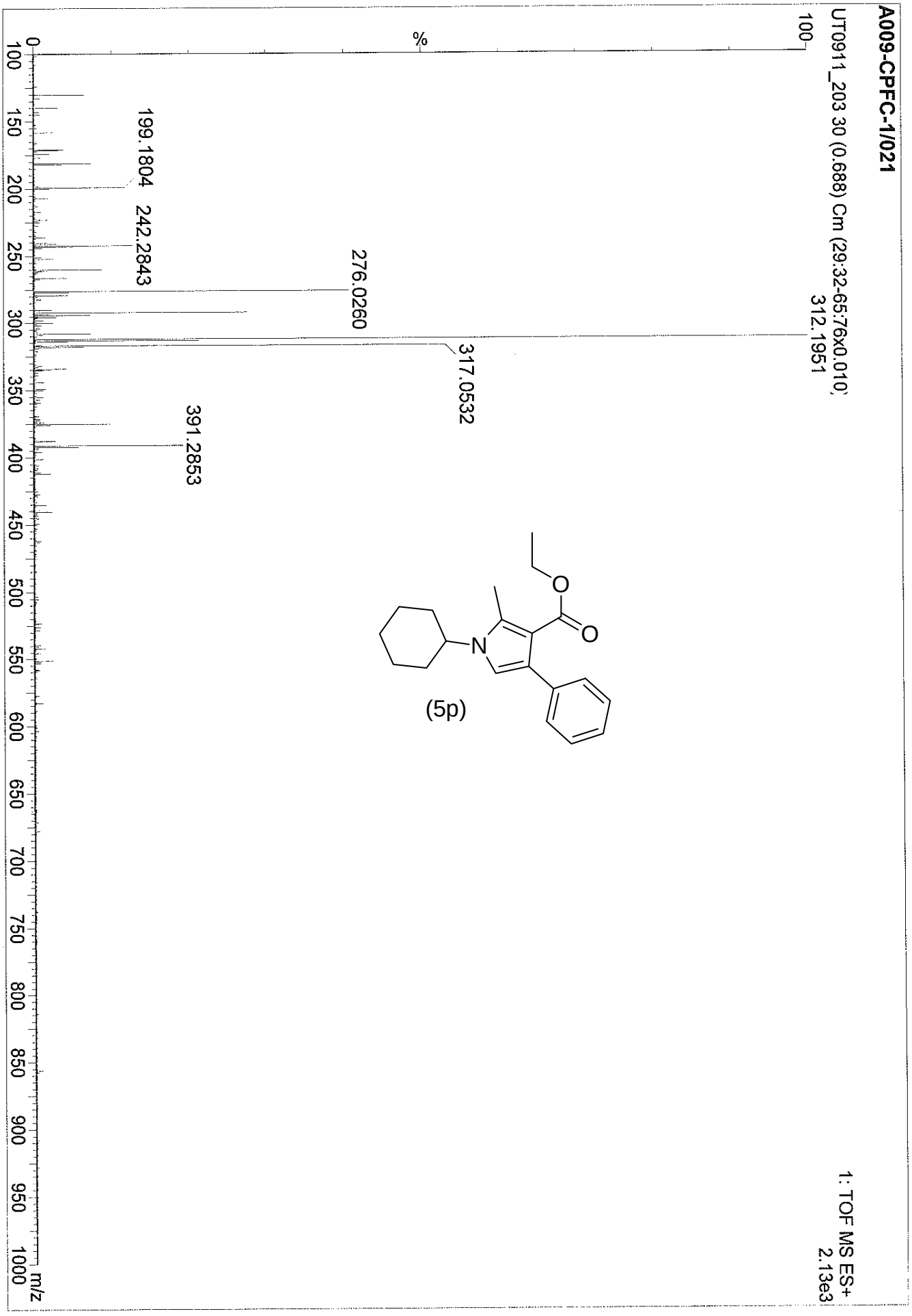
Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
244.1333	244.1338	-0.5	-2.0	7.5	1.4	C15 H18 N O2



A009-CPFC-1-021 in CDCl3
NMR-400MHZ



(5p)

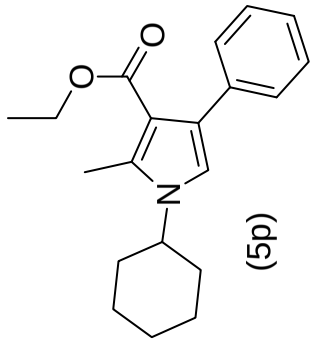


Elemental Composition Report

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

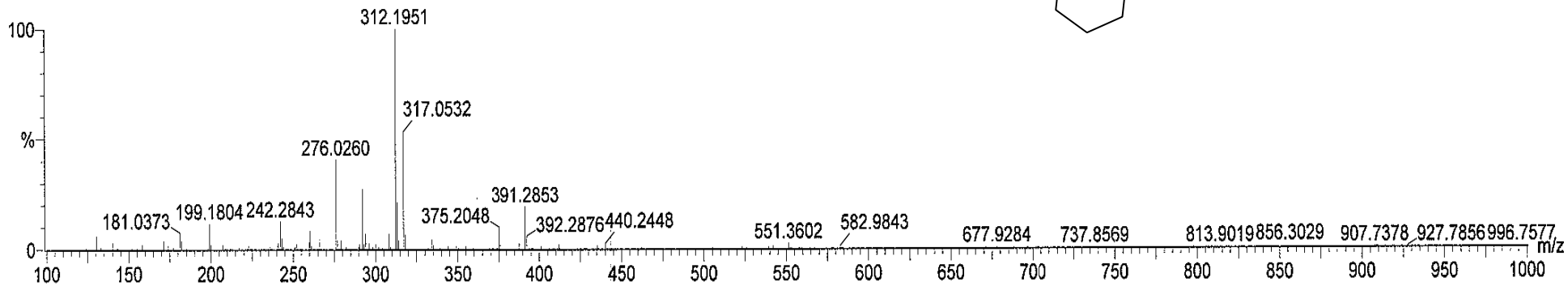
Monoisotopic Mass, Even Electron Ions
252 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-55 N: 0-4 O: 0-6 F: 0-1
A009-CPFC-1/021



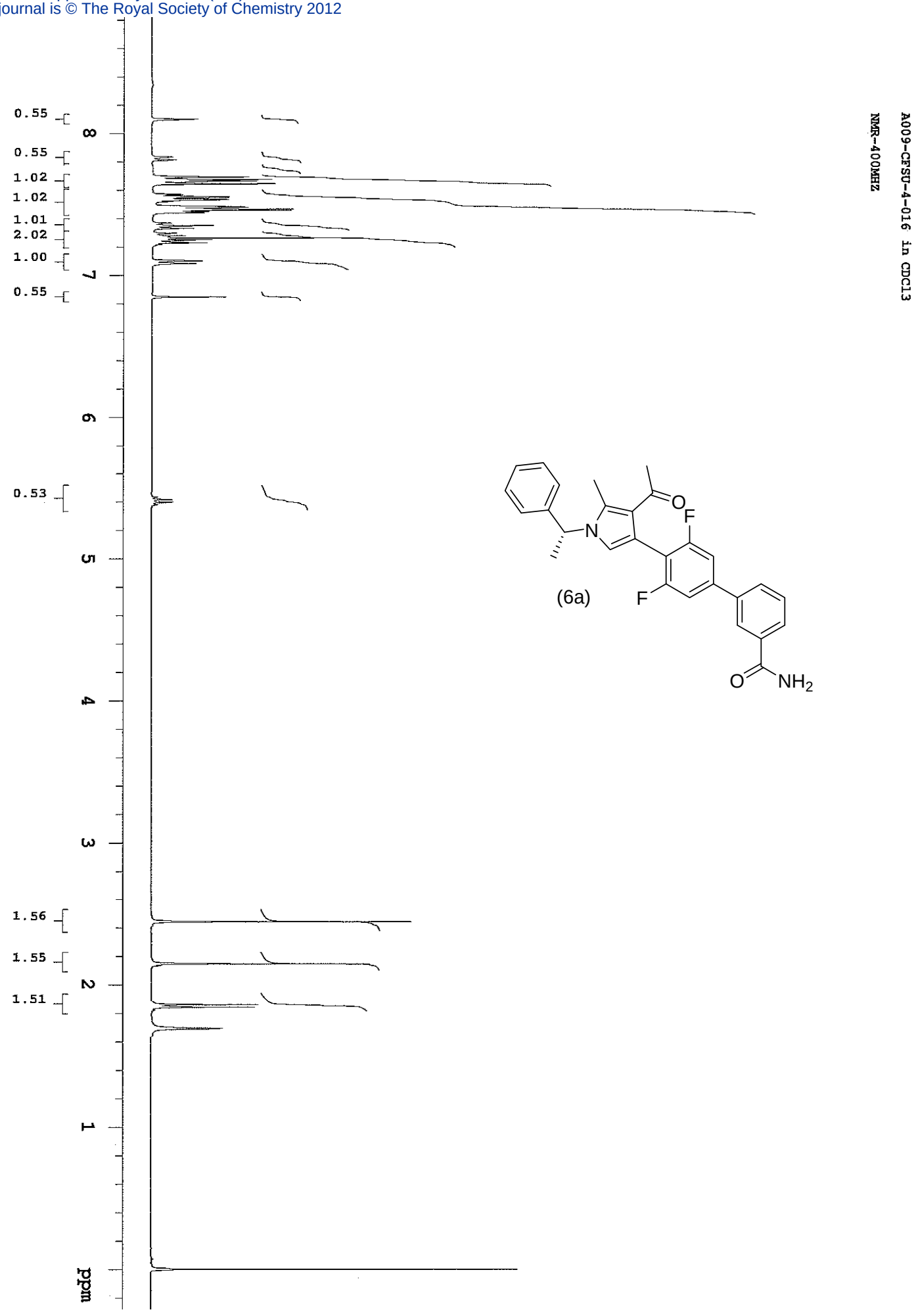
(5p)

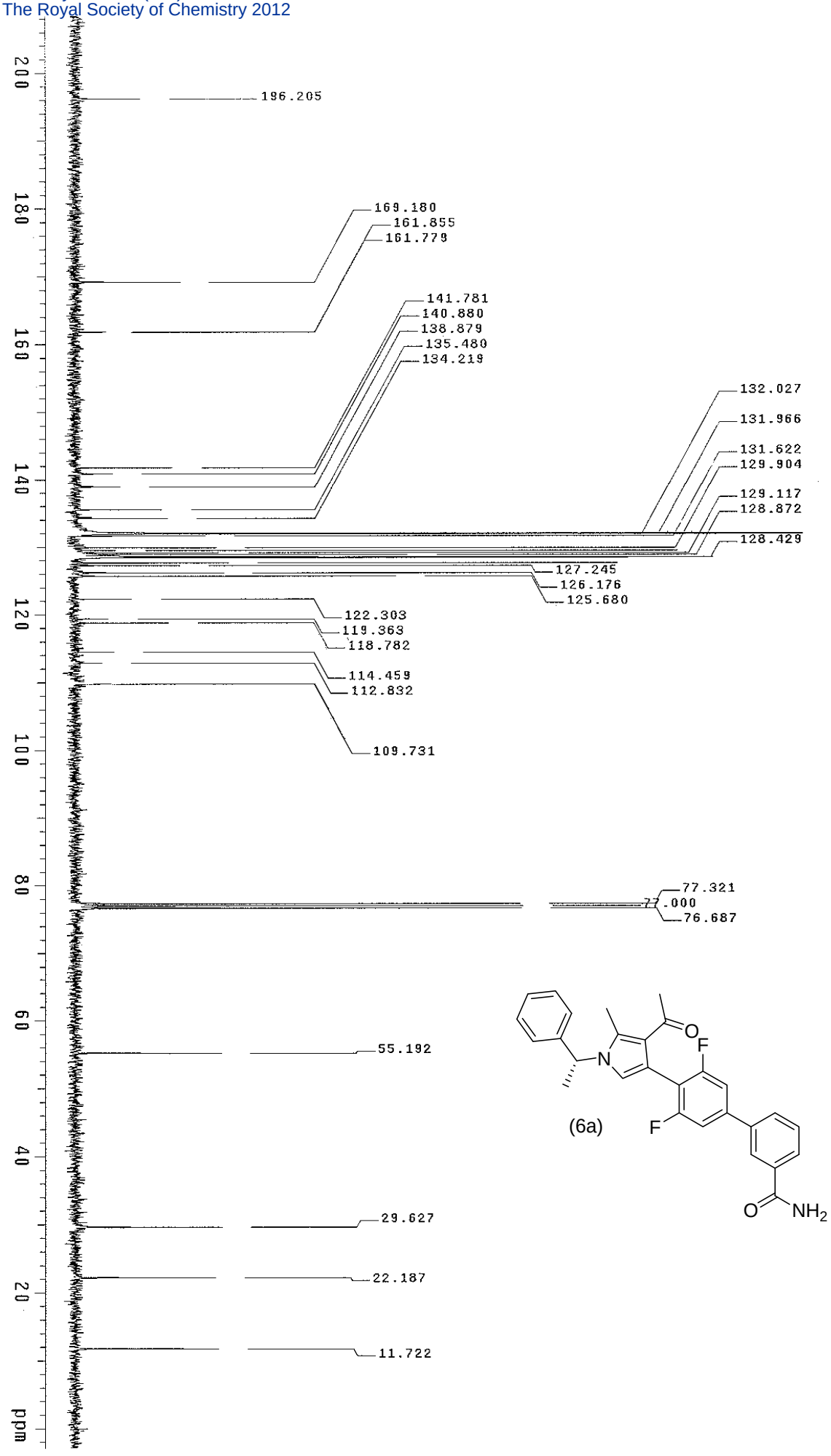
UT0911_203 30 (0.688) Cm (29:32-65:76x0.010)

1: TOF MS ES+
2.13e+003

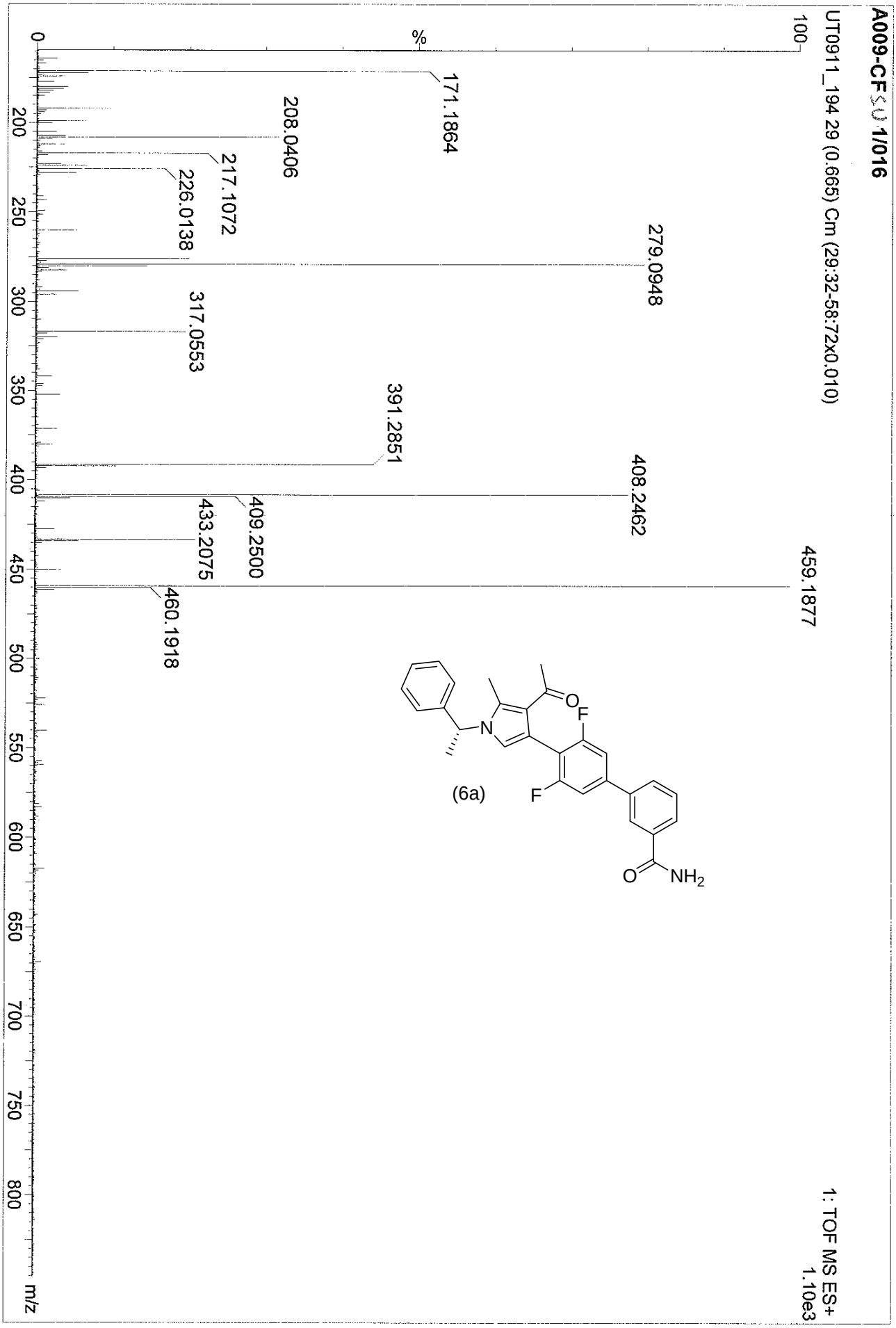


Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
312.1951	312.1964	-1.3	-4.2	8.5	7.7	C20 H26 N O2





(6a)



Elemental Composition Report

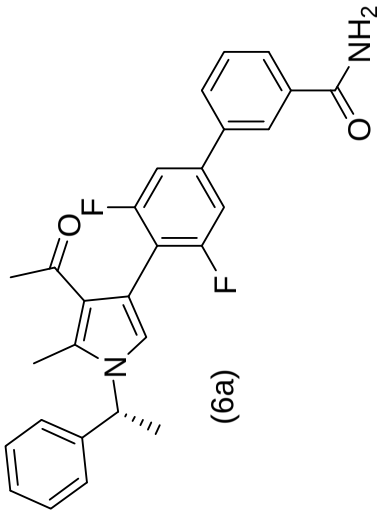
Single Mass Analysis

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
296 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-70 H: 0-80 N: 0-5 O: 0-10 F: 2-2

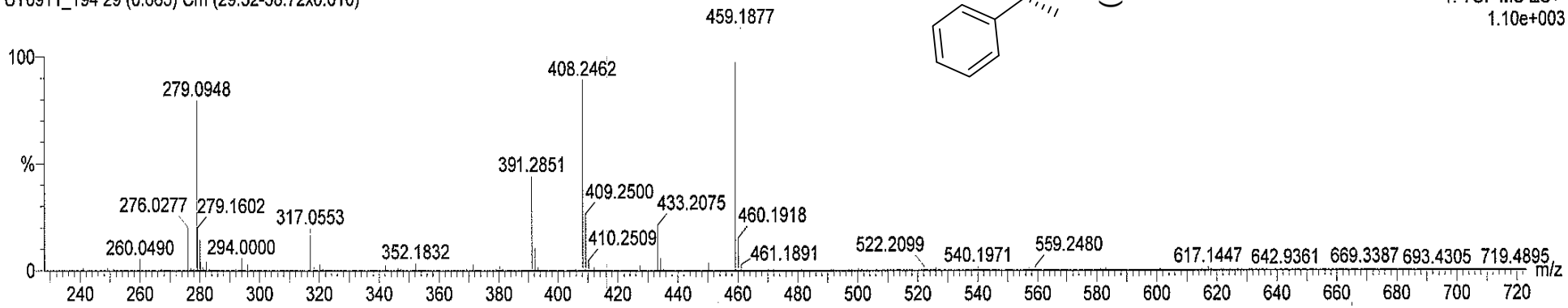
A009-CFSU-1/016

UT0911_194 29 (0.665) Cm (29:32-58:72x0.010)

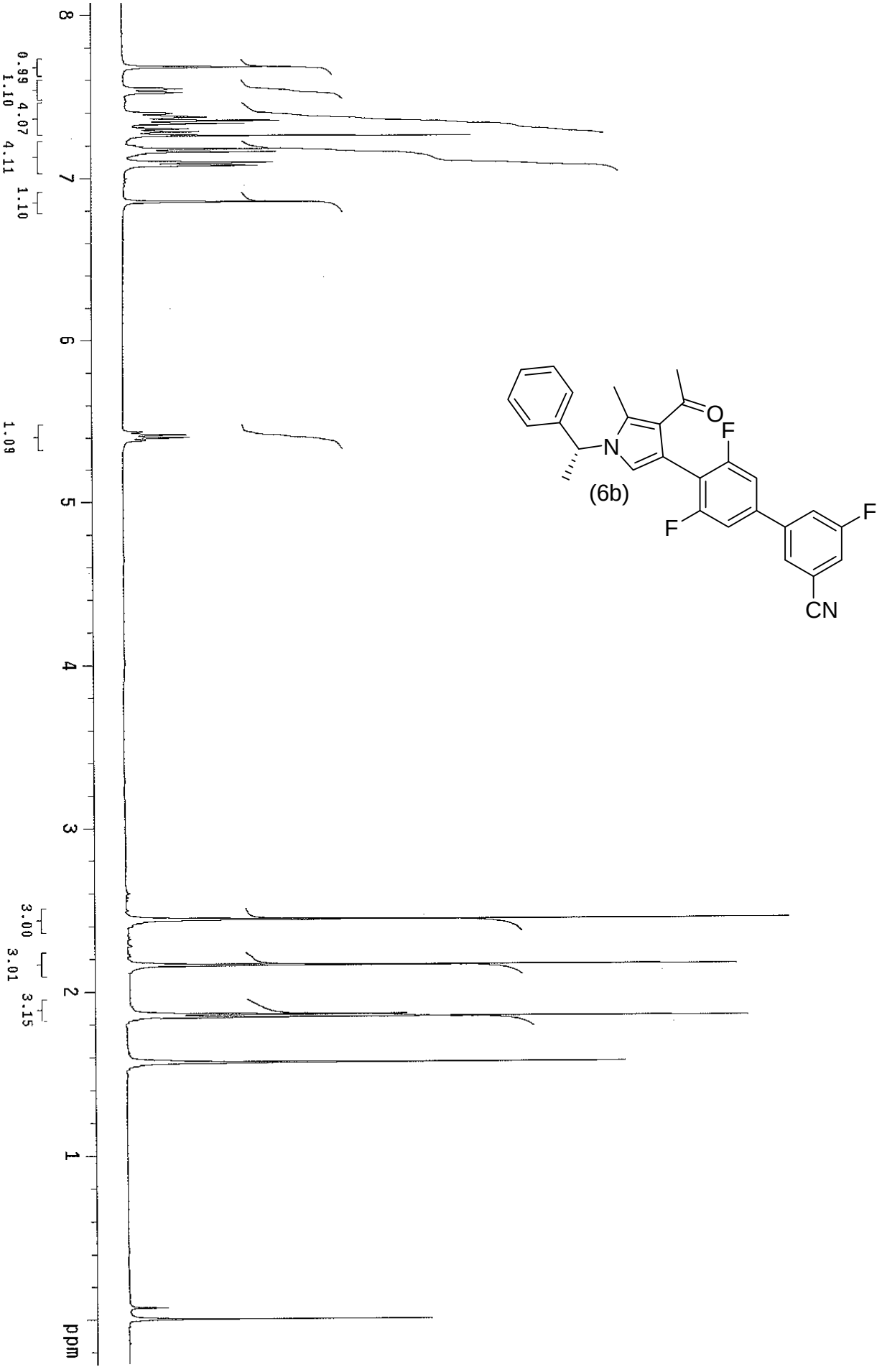


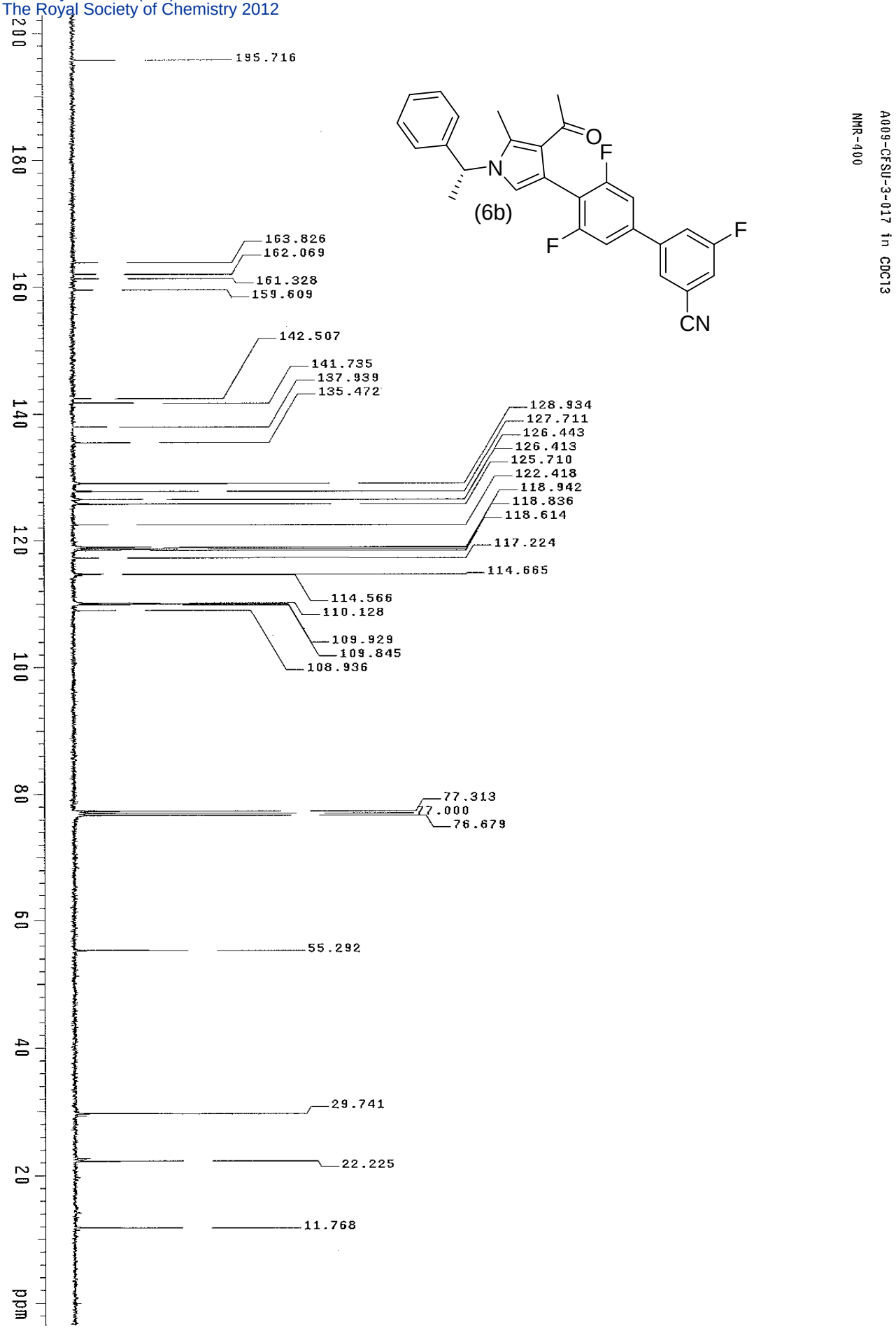
(6a)

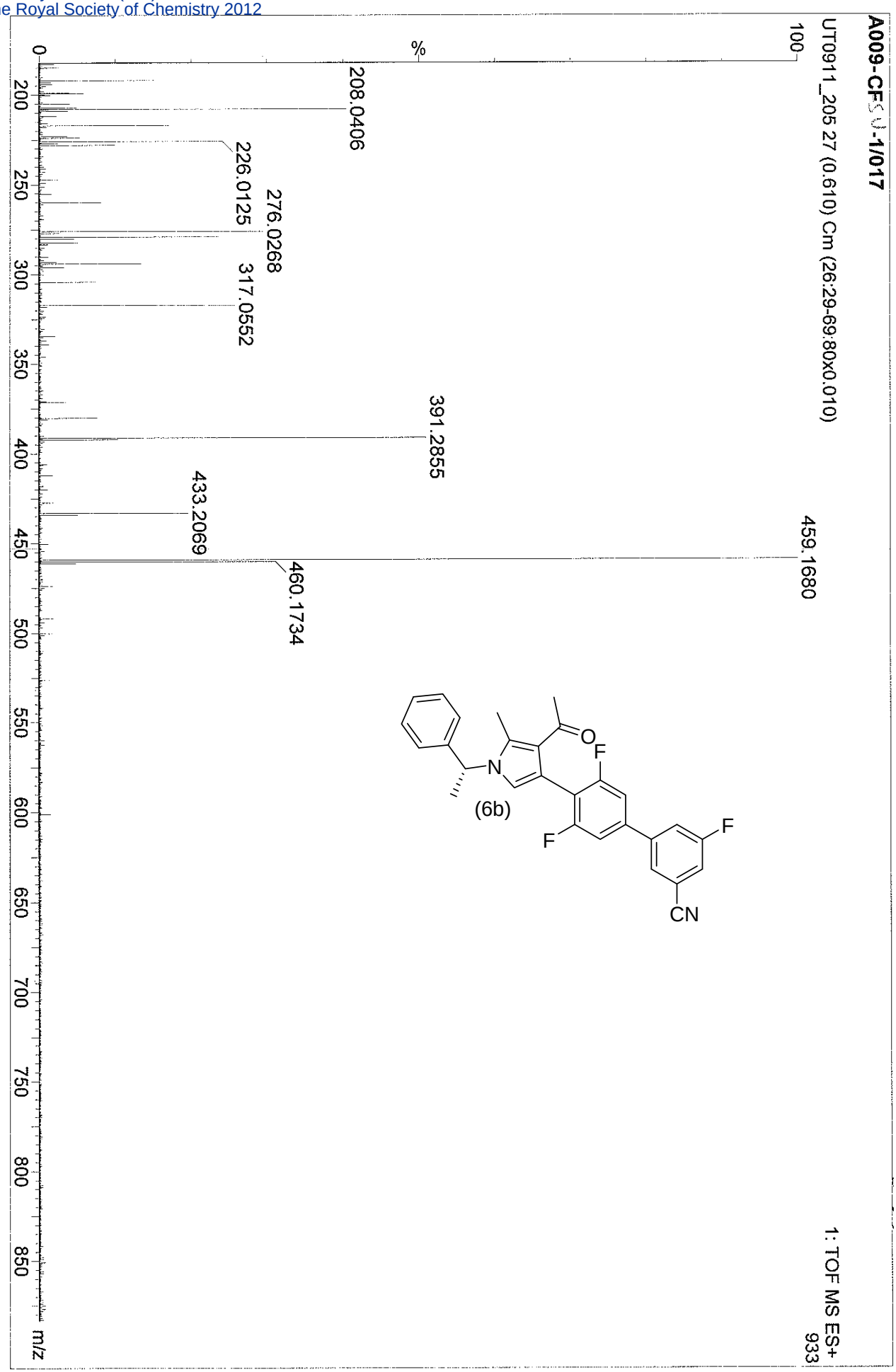
1: TOF MS ES+
1.10e+003



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
459.1877	459.1884	-0.7	-1.5	16.5	1.8	C28 H25 N2 O2 F2





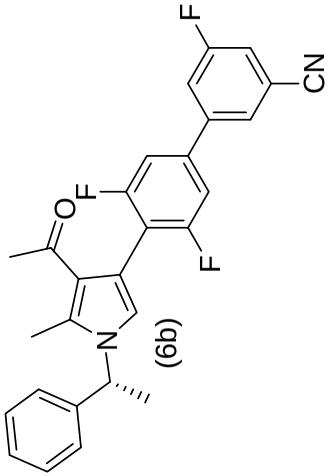


Elemental Composition Report

Single Mass Analysis

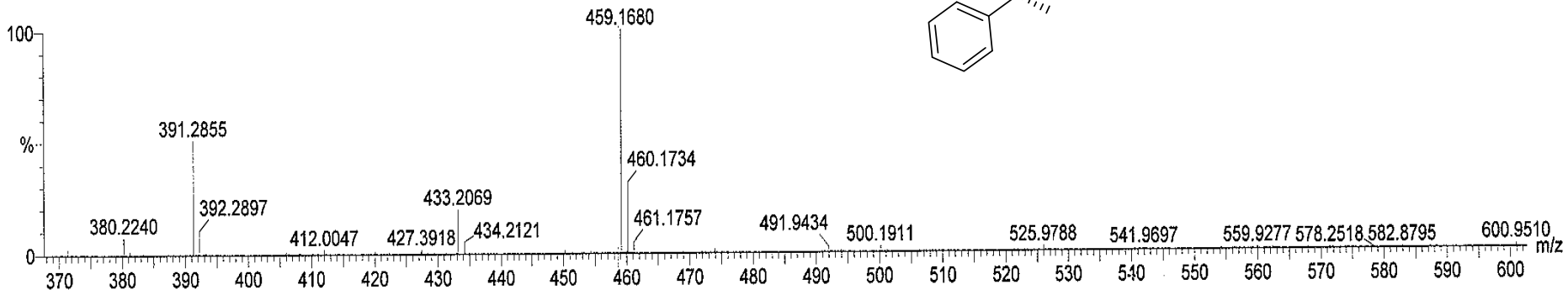
Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
276 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-55 N: 0-4 O: 0-2 F: 0-3
A009-CFSu-1/017

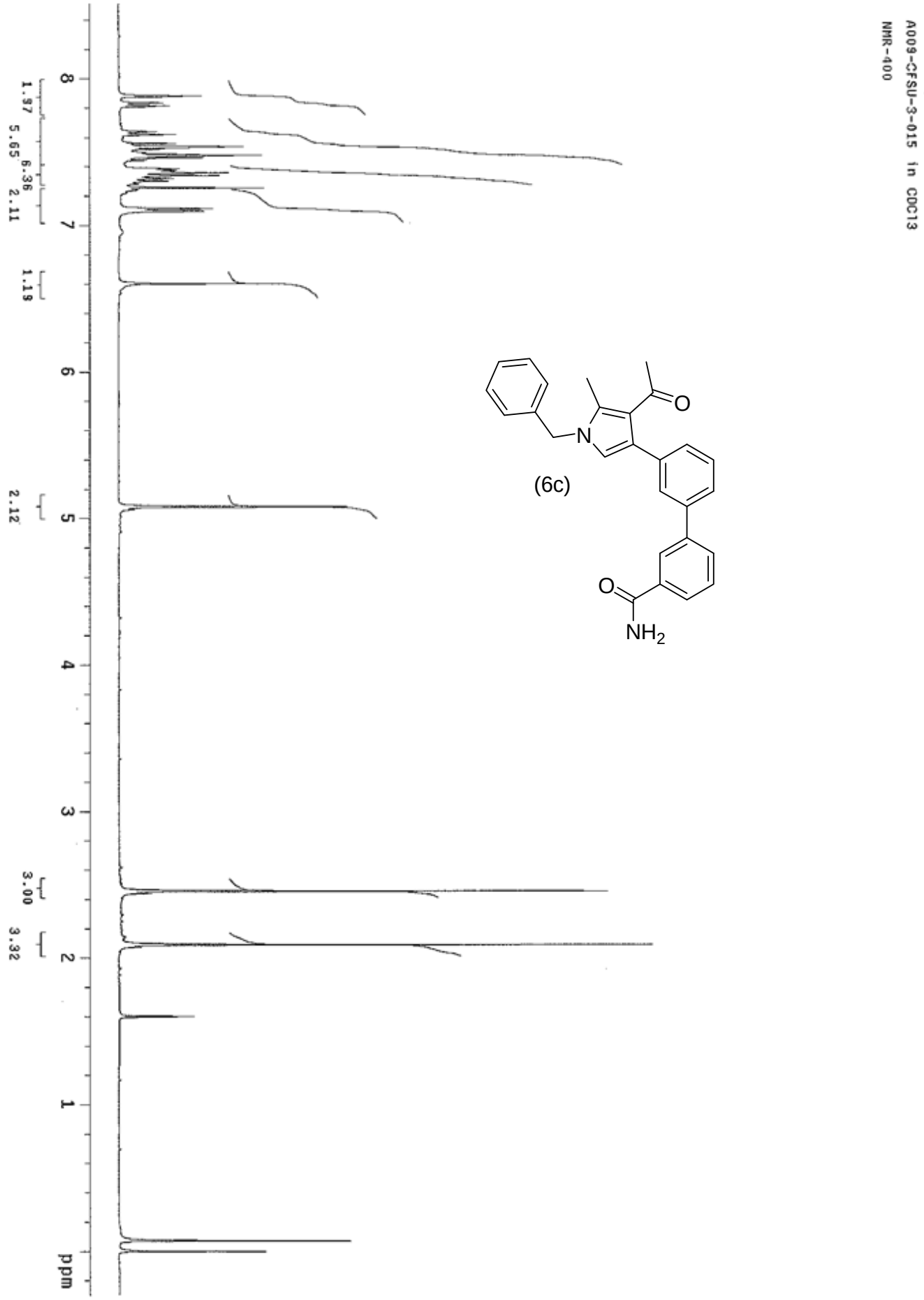


UT0911_205 27 (0.610) Cm (26:29-69:80x0.010)

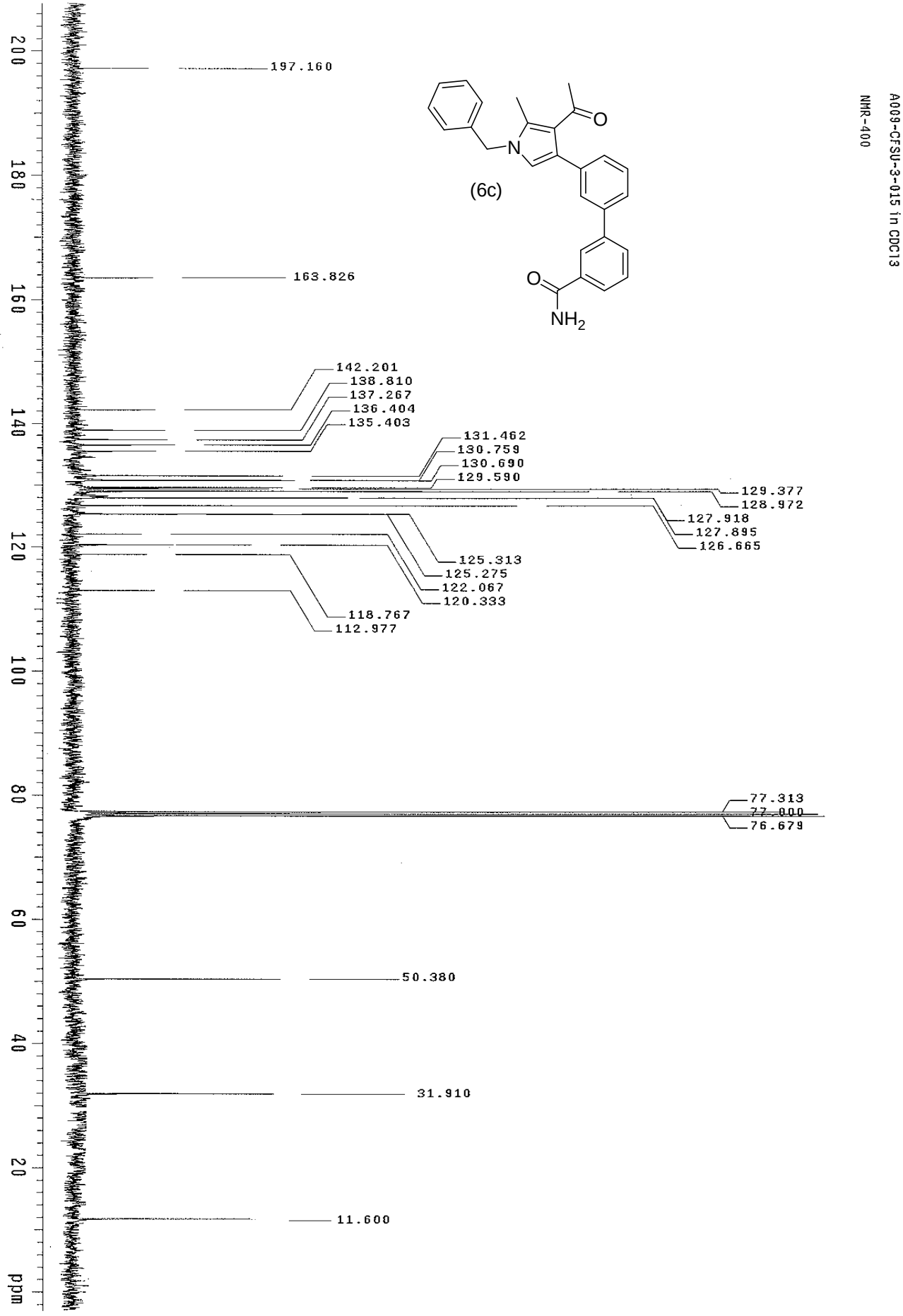
1: TOF MS ES+
9.33e+002

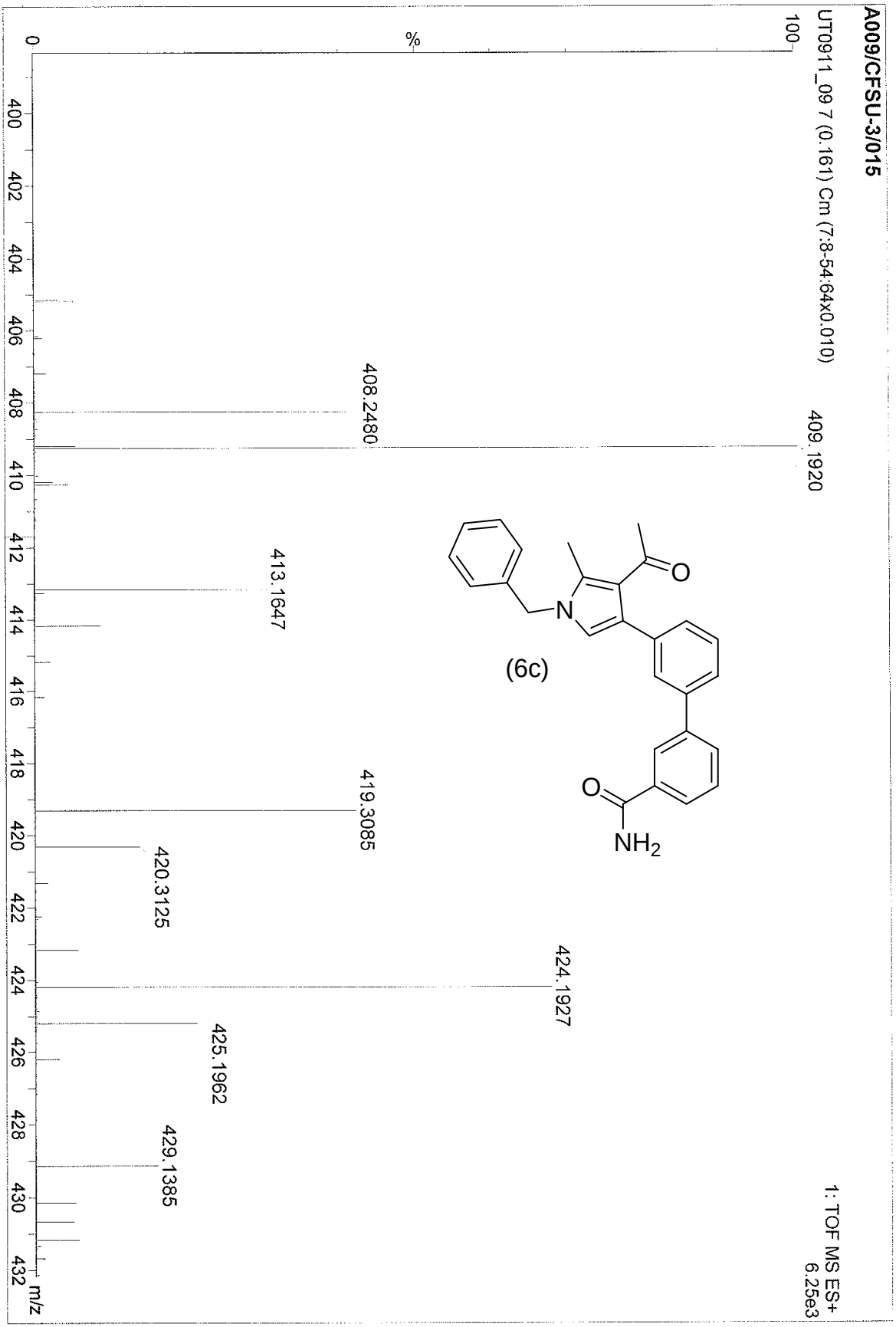


Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
459.1680	459.1684	-0.4	-0.9	17.5	8.6	C28 H22 N2 O F3

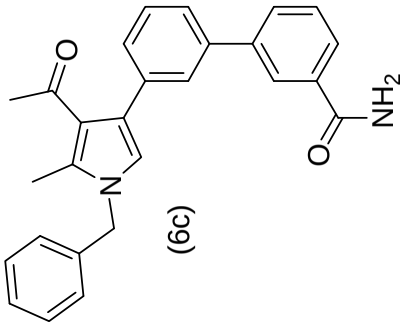


(6c)





Elemental Composition Report



(6c)

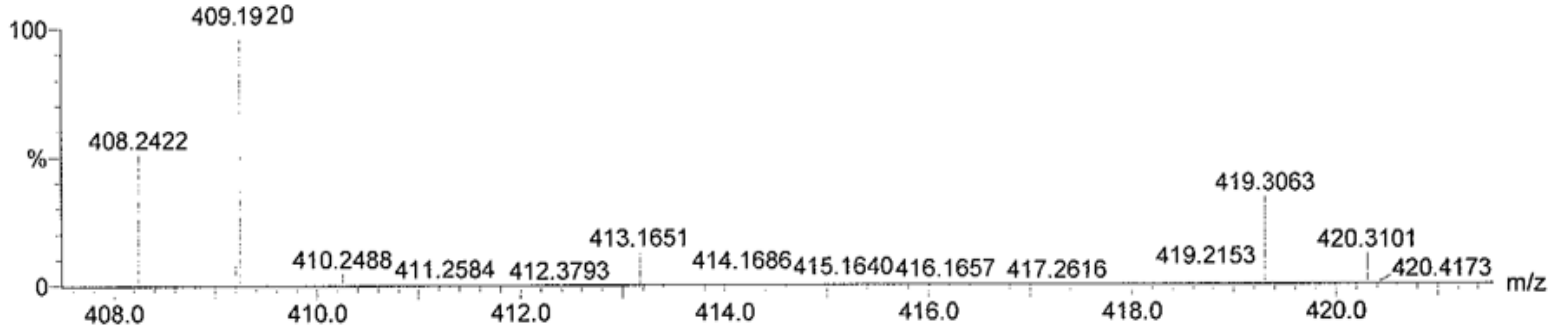
Single Mass Analysis

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

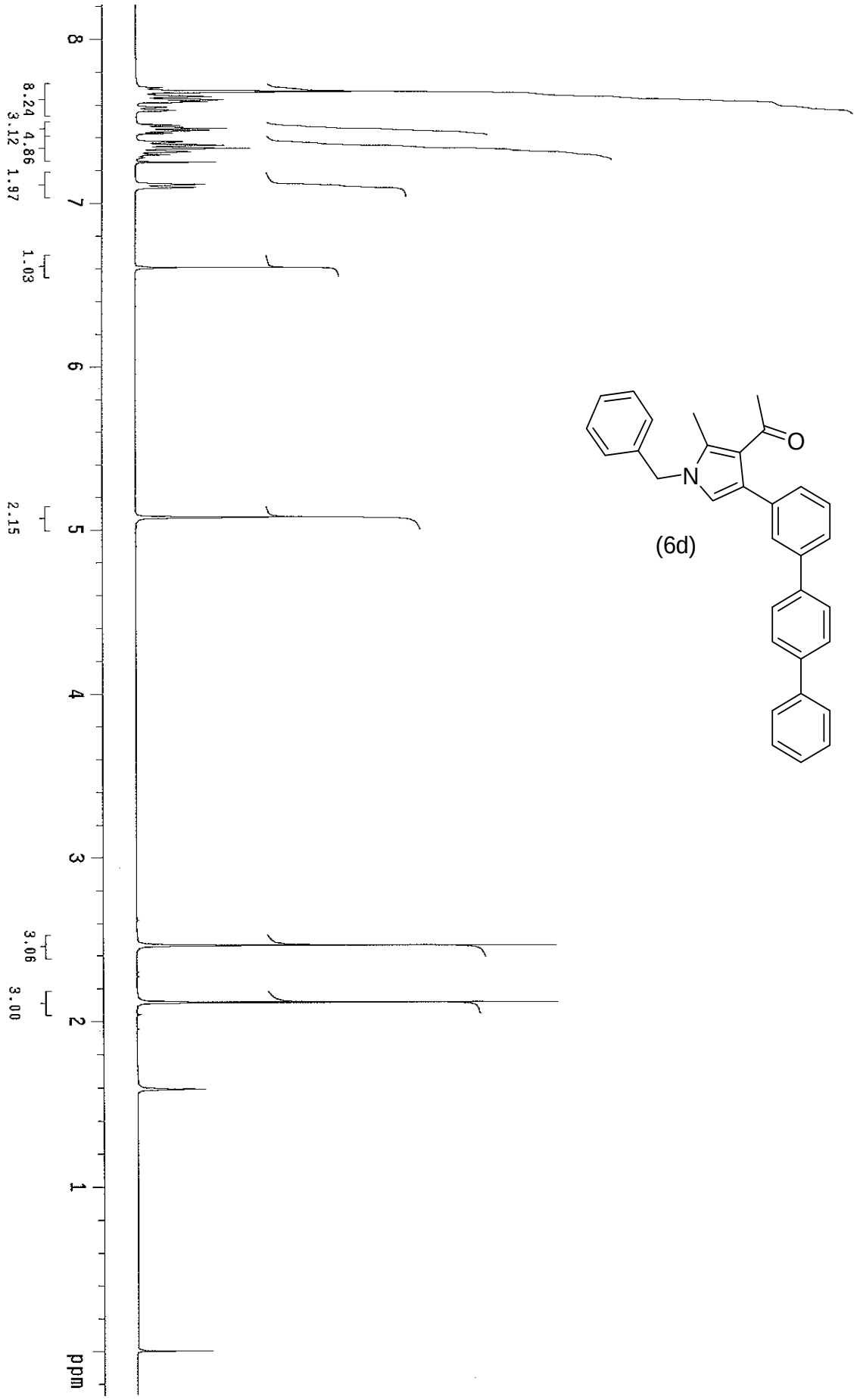
Monoisotopic Mass, Even Electron Ions
120 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-4 O: 0-5
A009/CFSU-3/015

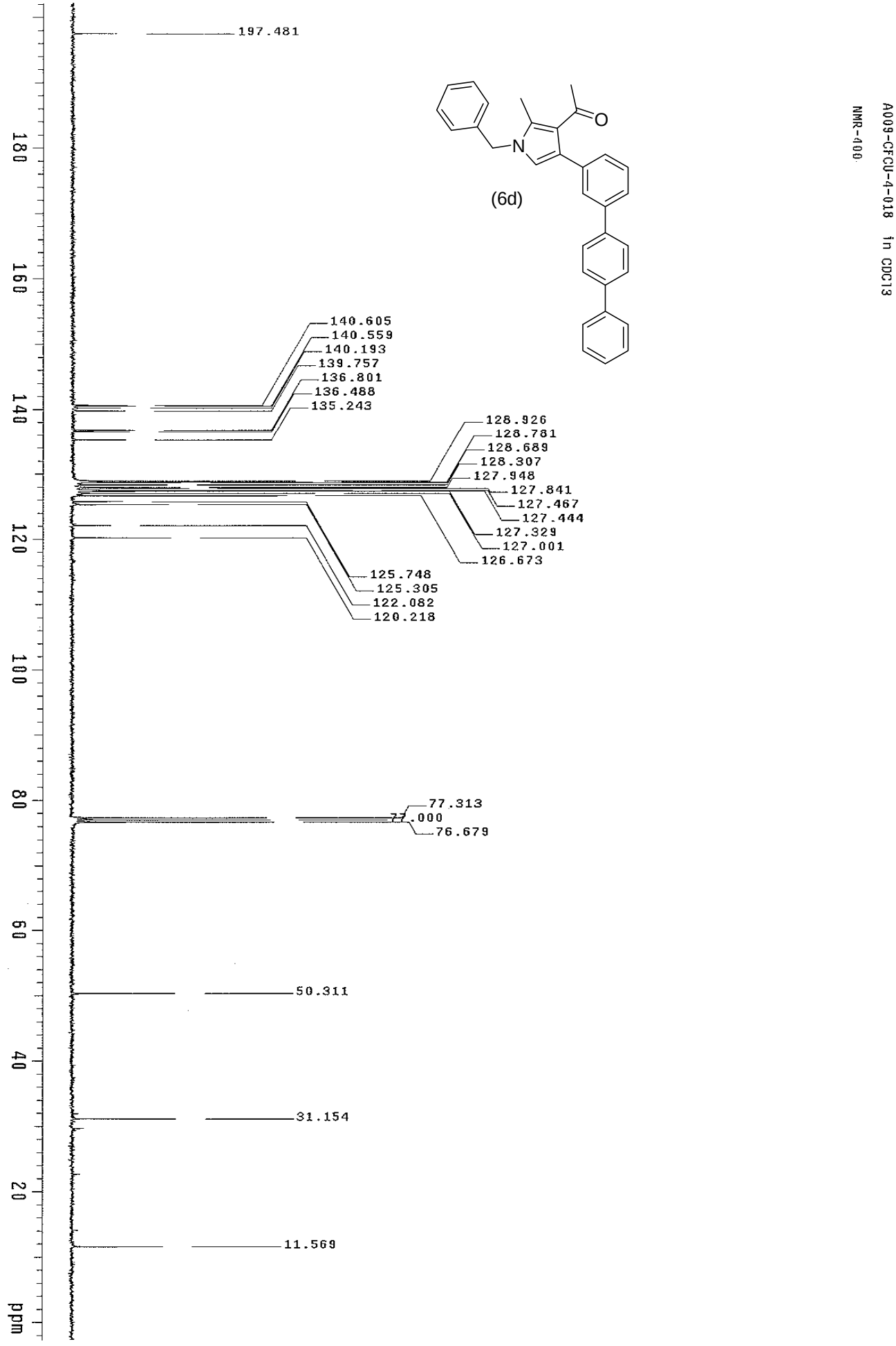
UT0911_09 5 (0.127) Cm (5:8-69:83x0.010)

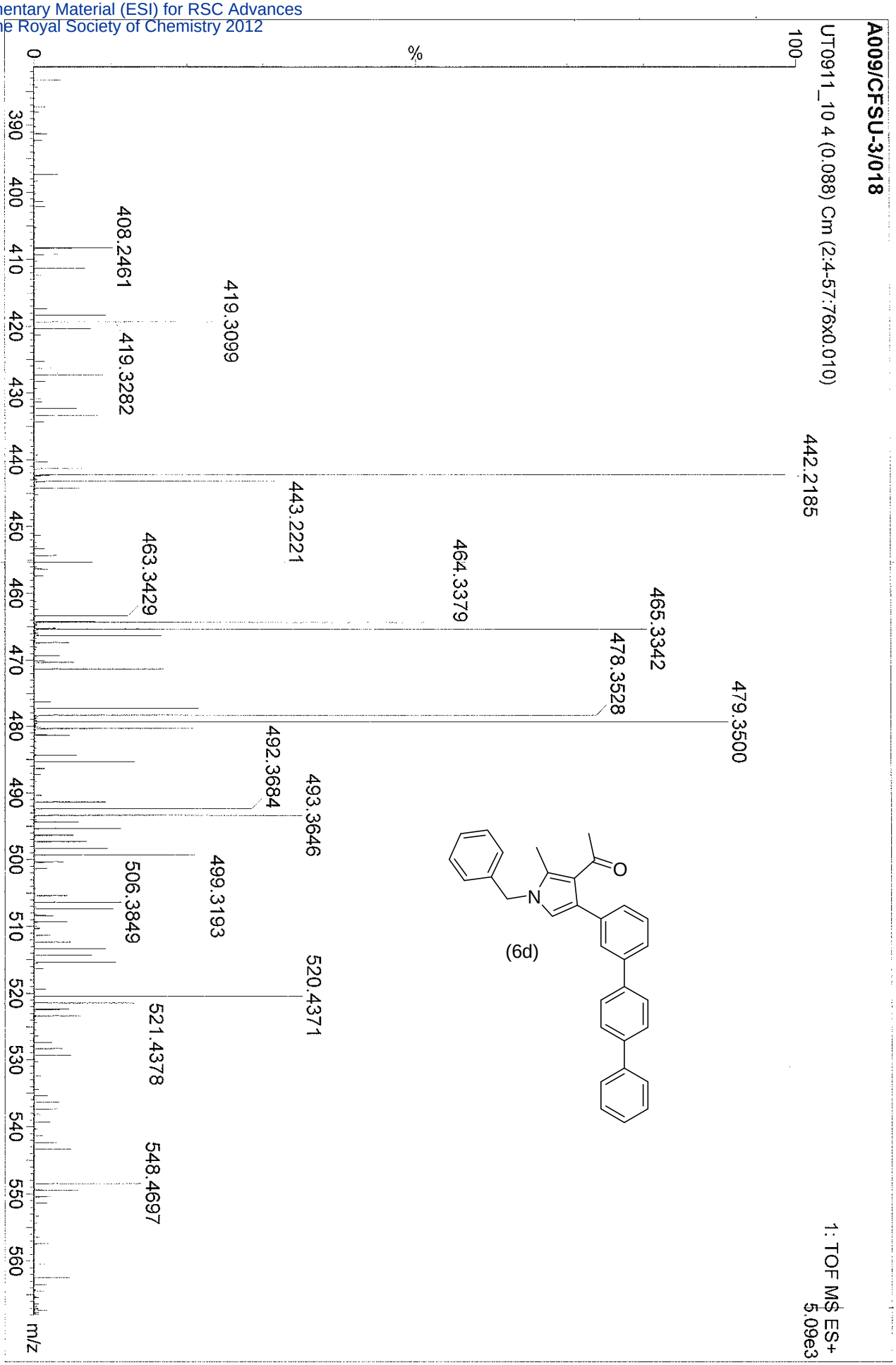
1: TOF MS ES+
3.52e+004



Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
409.1920	409.1991	-1.4	-3.4	10.5	391.0	C27 H25 N2 O2

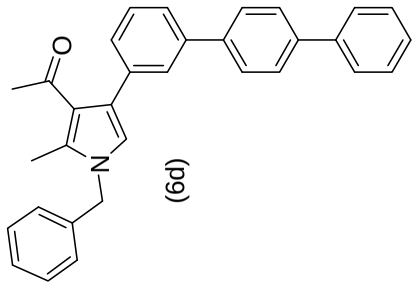






Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

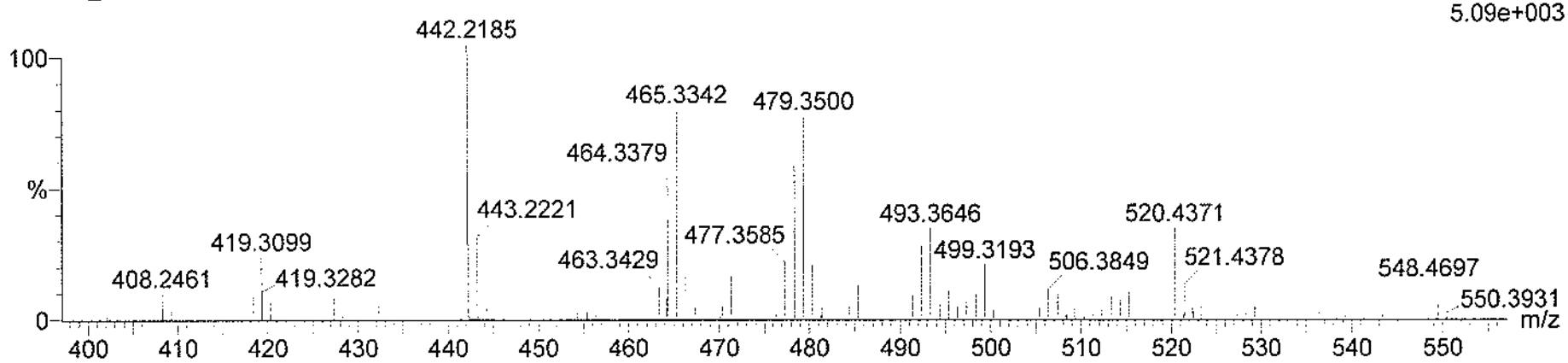


(6d)

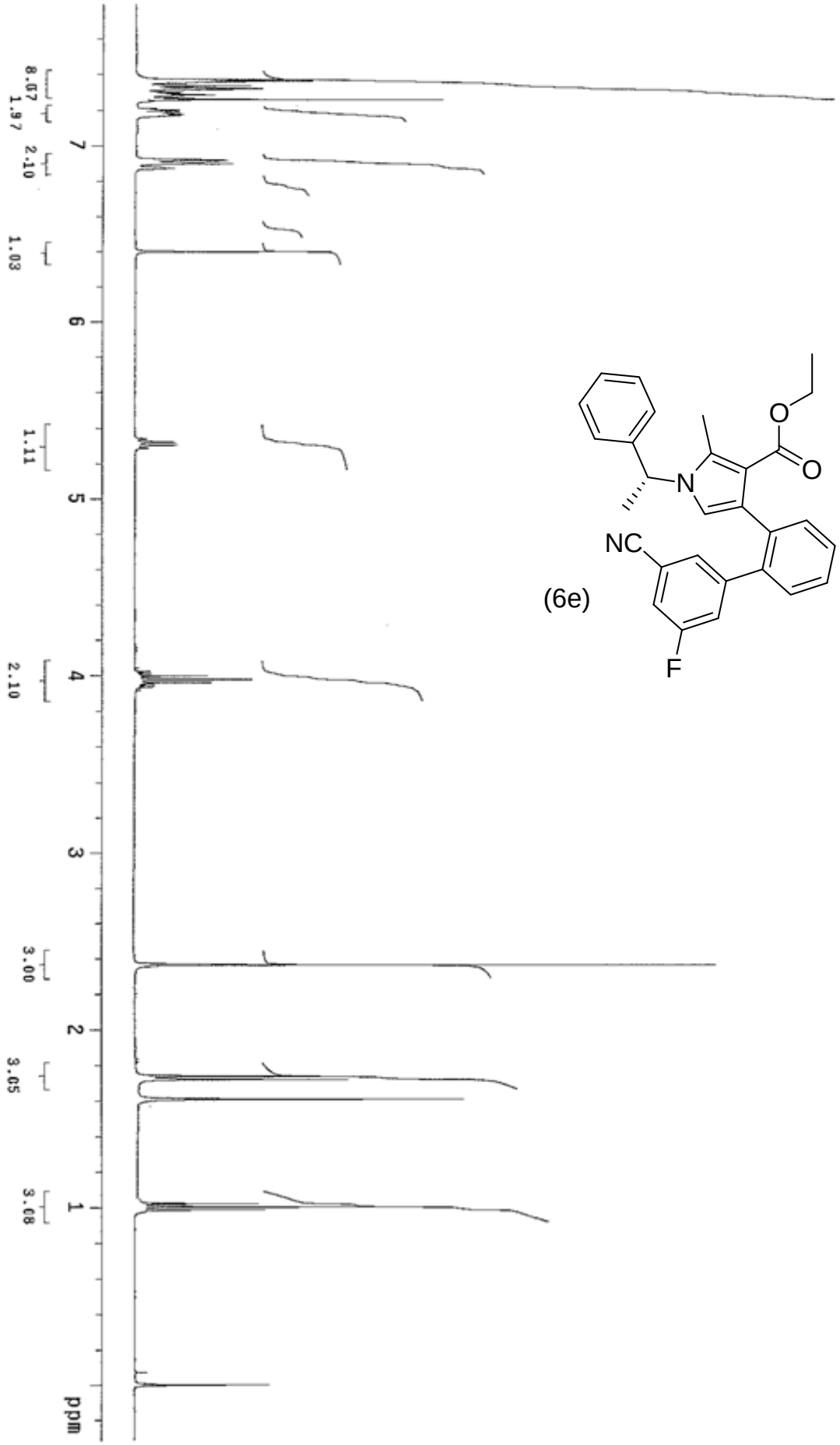
Monoisotopic Mass, Even Electron Ions
91 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-3 O: 0-5
A009/CFSU-3/018

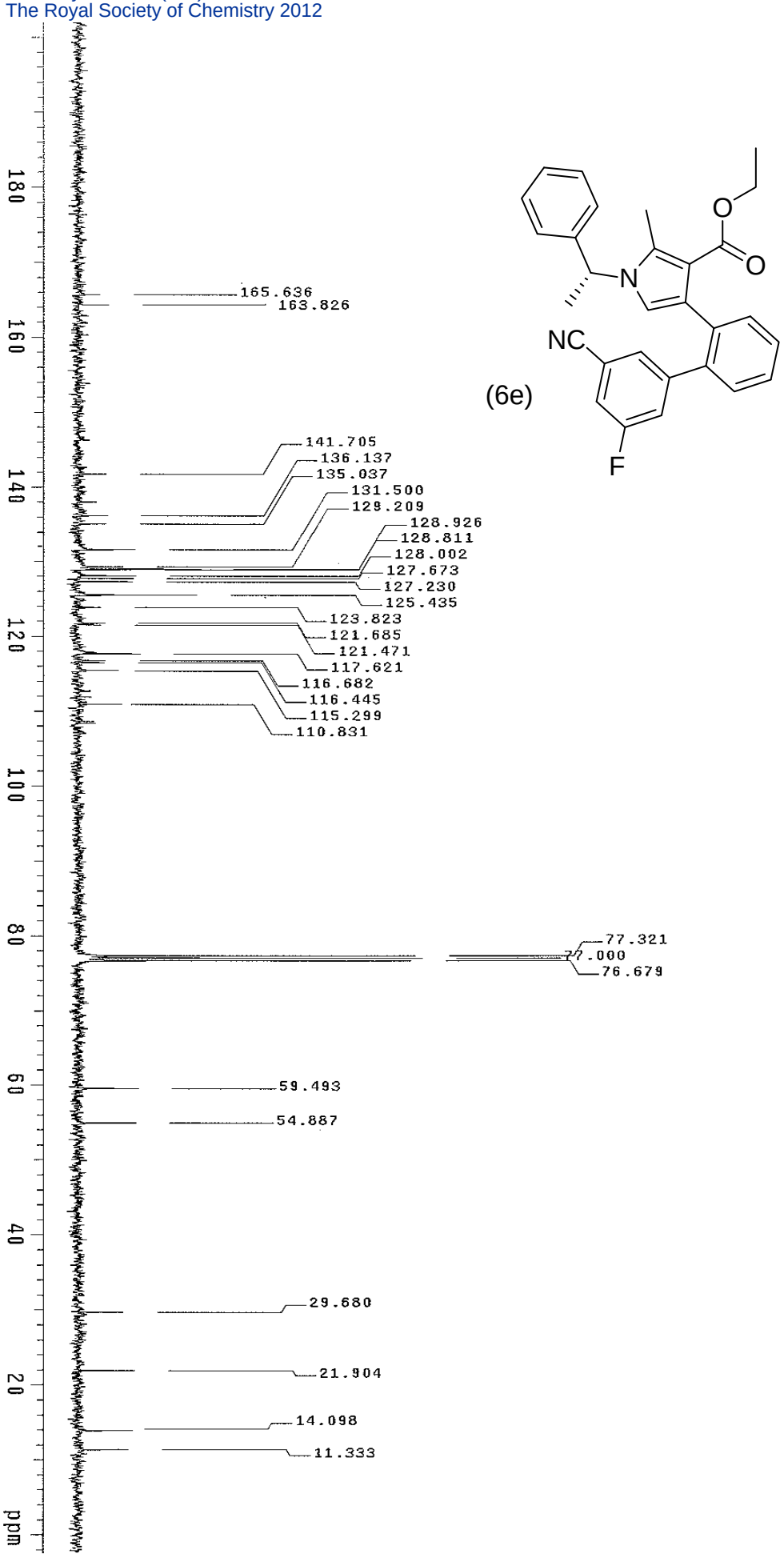
UT0911_10 4 (0.088) Cm (2:4-57:76x0.010)

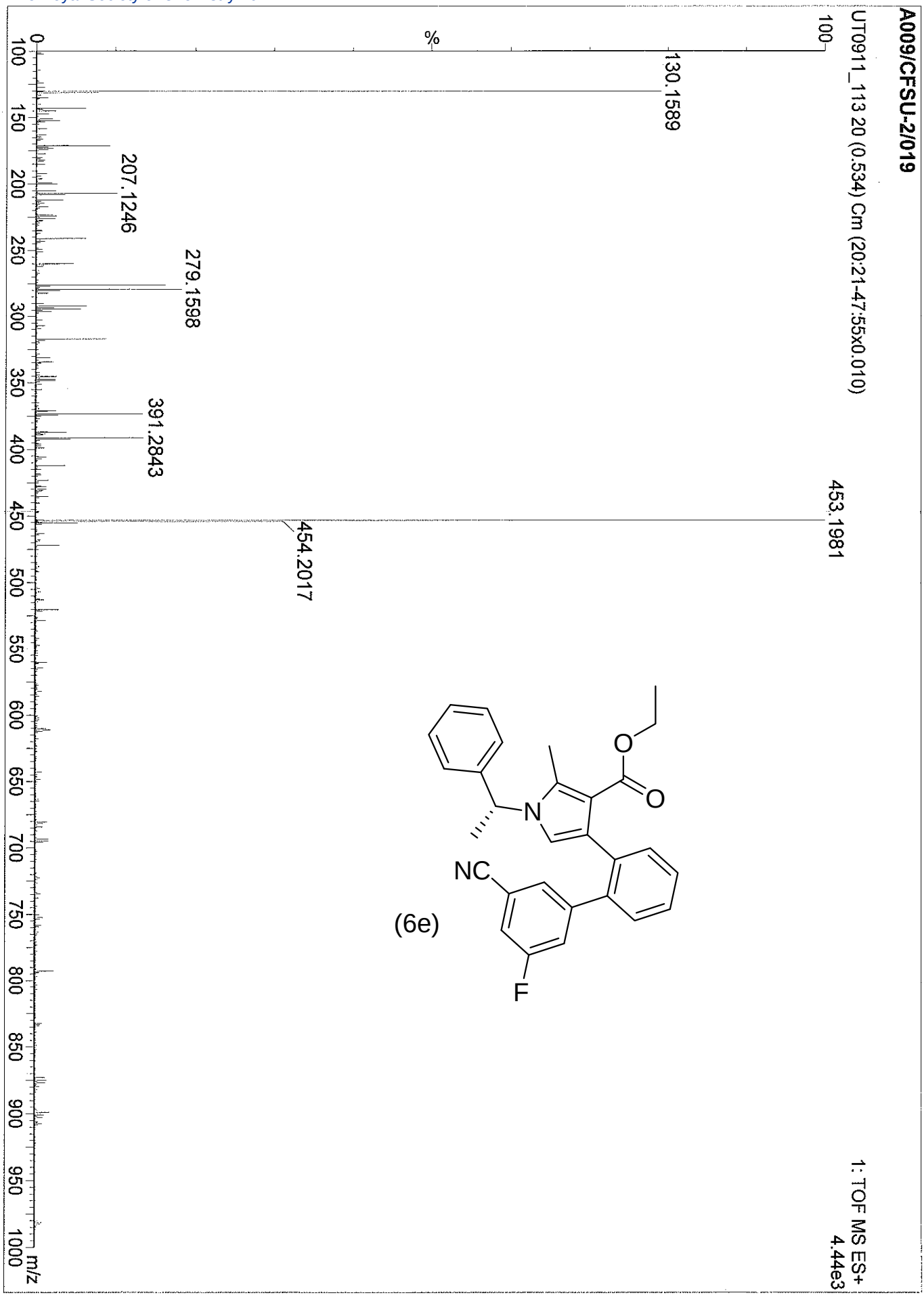
1: TOF MS ES+
5.09e+003



Minimum:				0.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
442.2185	442.2171	1.4	3.2	19.5	2.1	C32 H28 N O







Elemental Composition Report

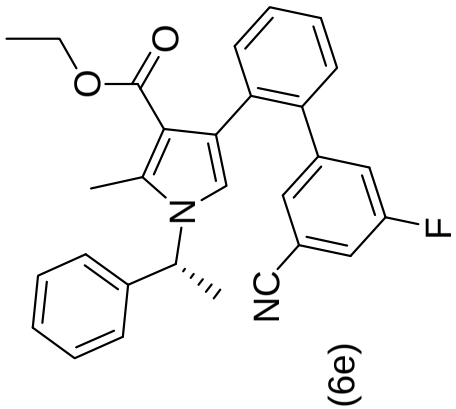
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
322 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-65 N: 0-5 O: 0-4 F: 0-1

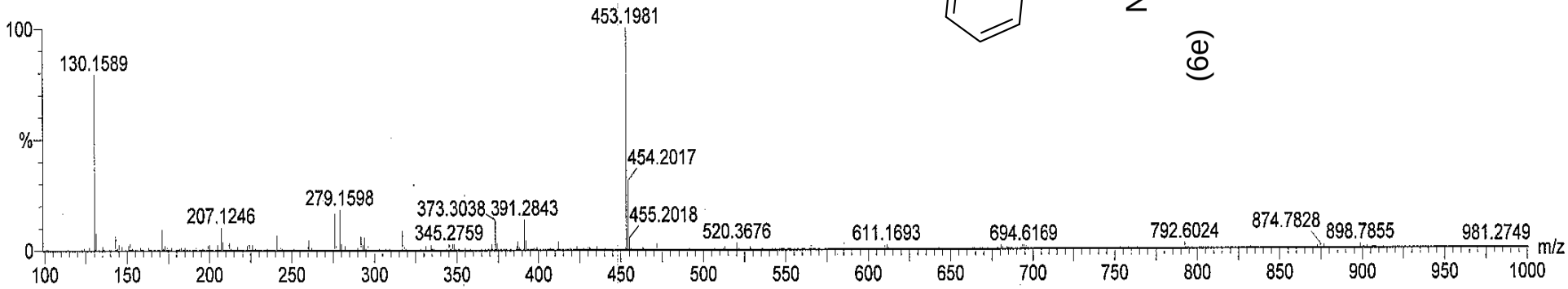
A009/CFSU-2/019

UT0911_113 20 (0.534) Cm (20:21-47:55x0.010)

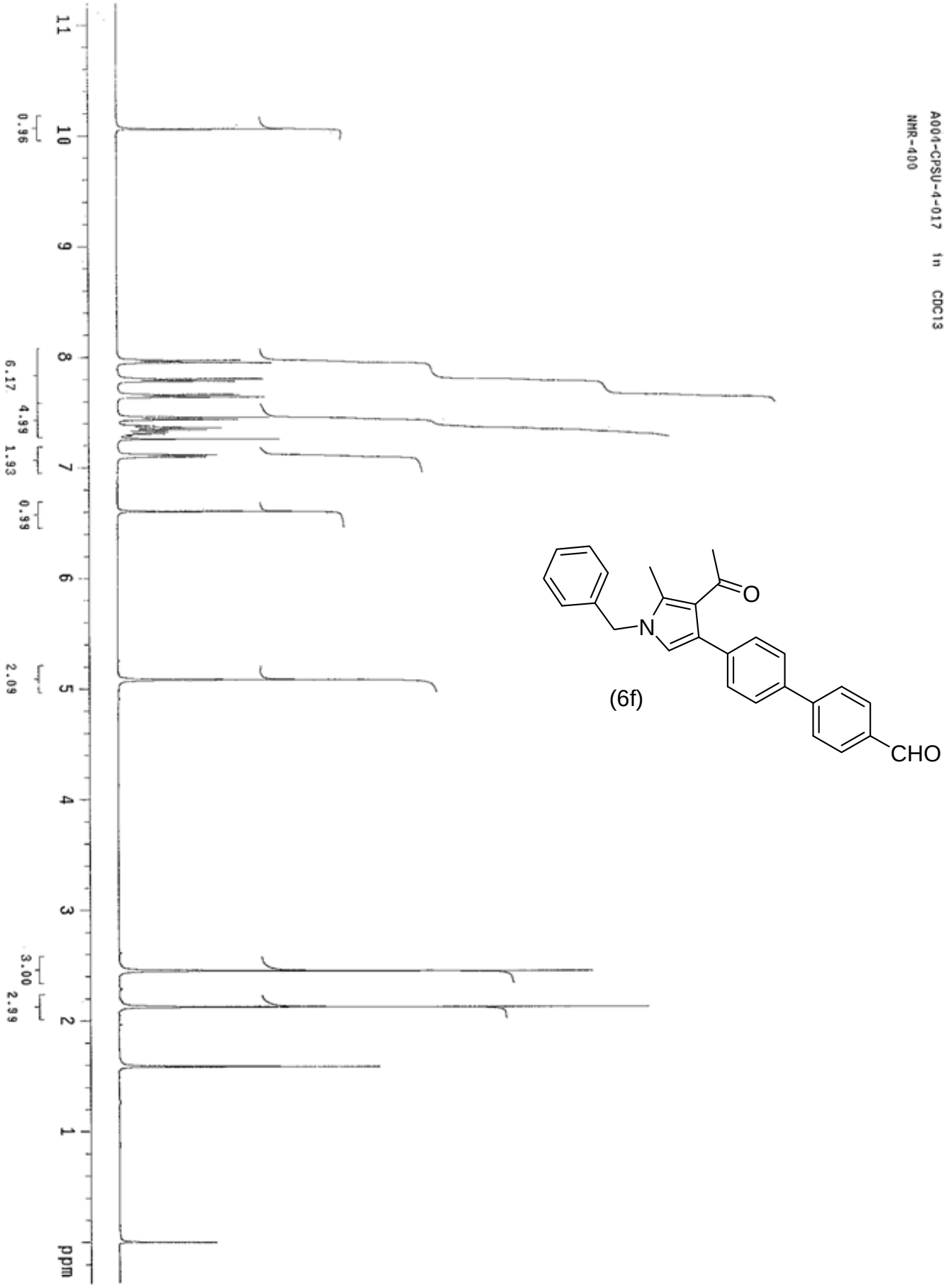


(6e)

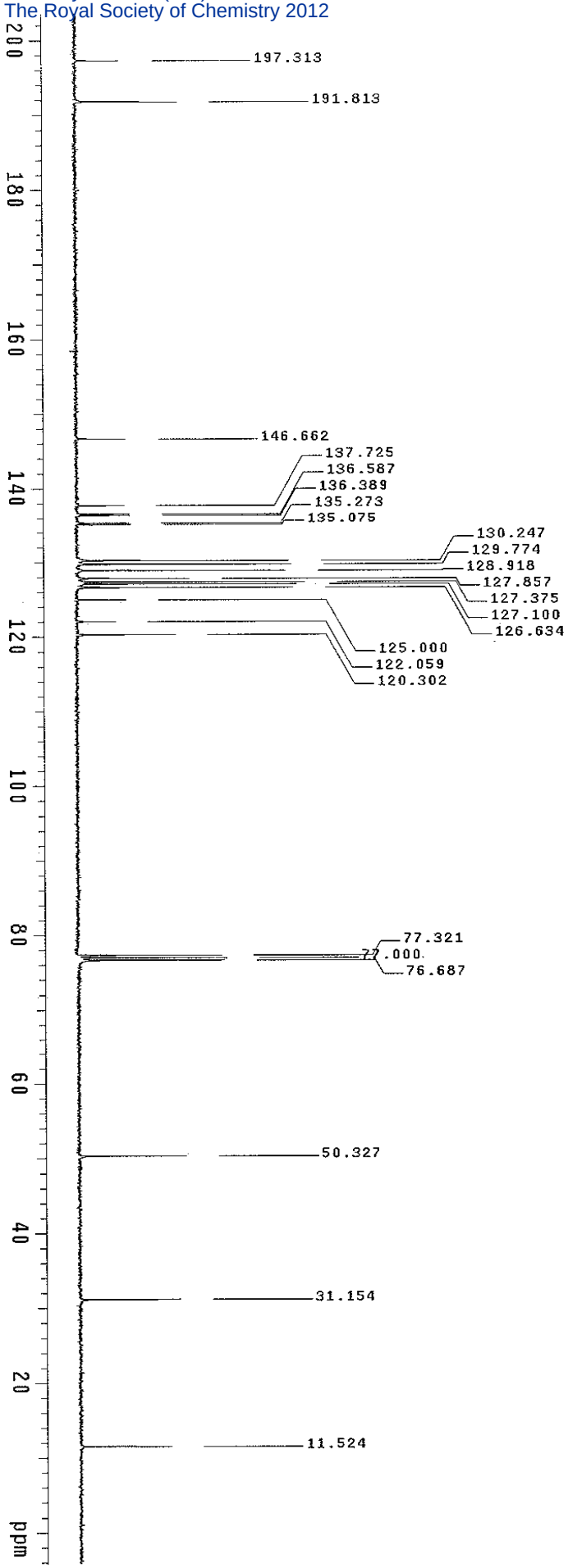
1: TOF MS ES+
4.44e+003

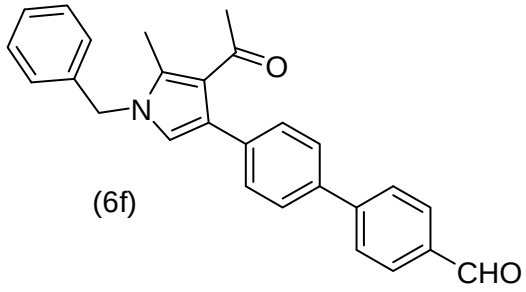


Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
453.1981	453.1978	0.3	0.7	17.5	3.3	C29 H26 N2 O2 F

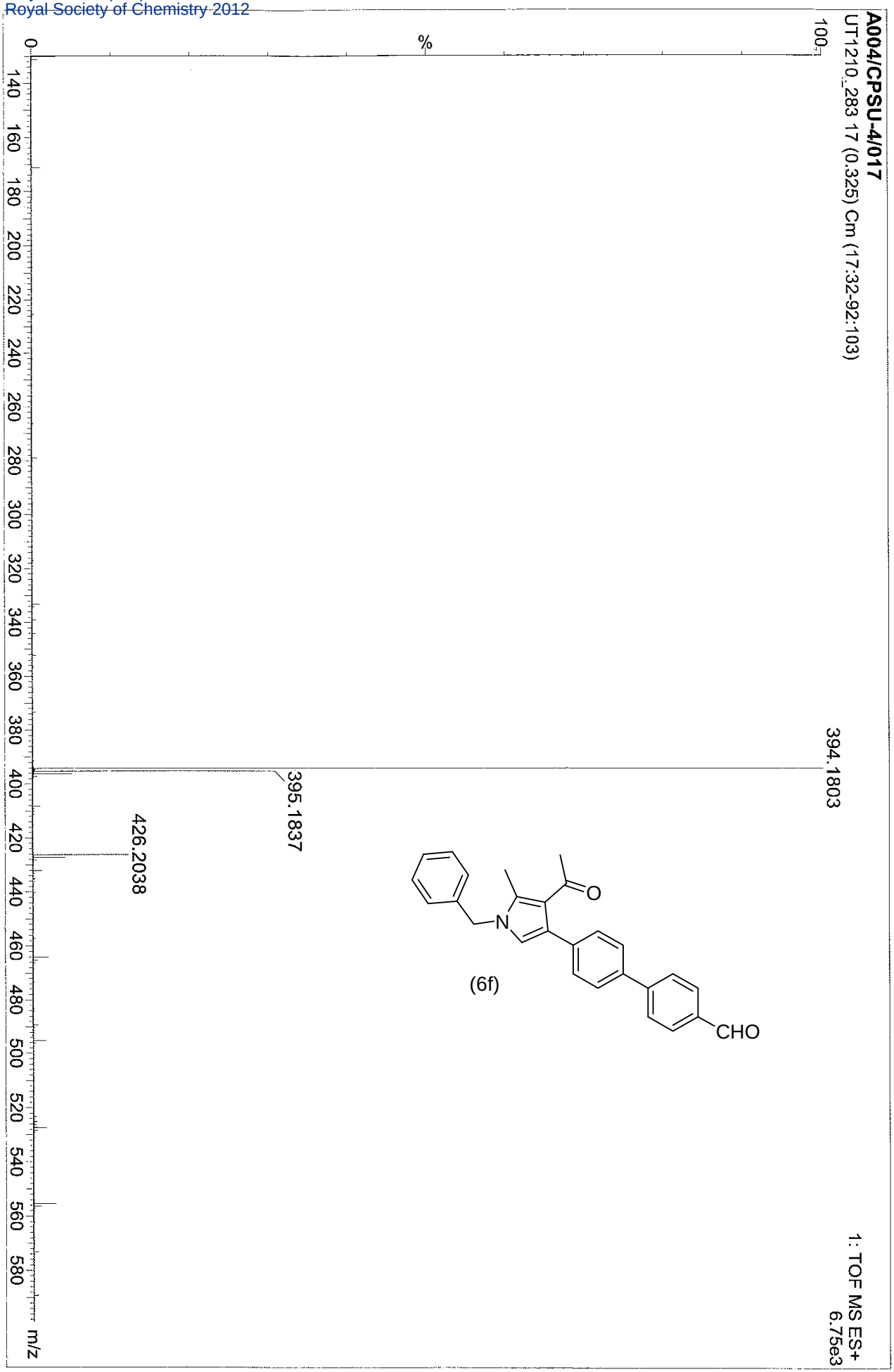


(6f)





(6f)

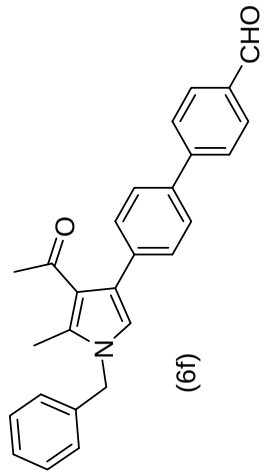


Elemental Composition Report

Single Mass Analysis

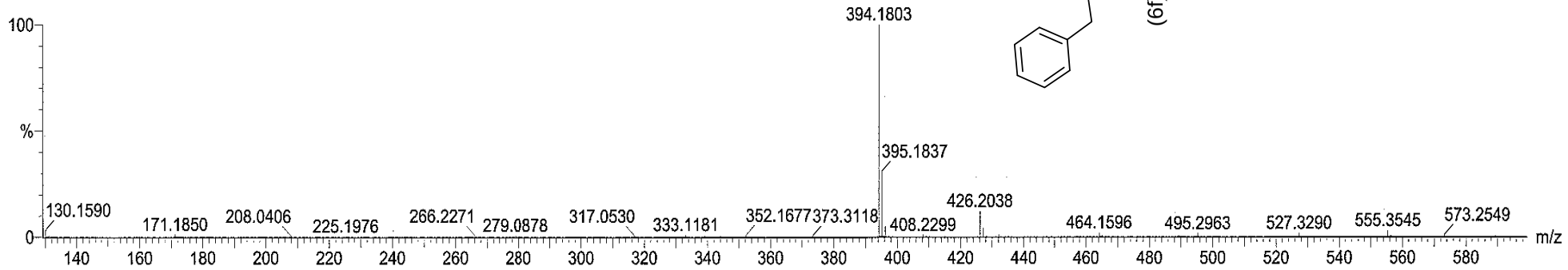
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
177 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-50 H: 0-75 N: 0-5 O: 0-5
A004/CPSU-4/017
UT1210_283 17 (0.325) Cm (17:32-92:103)

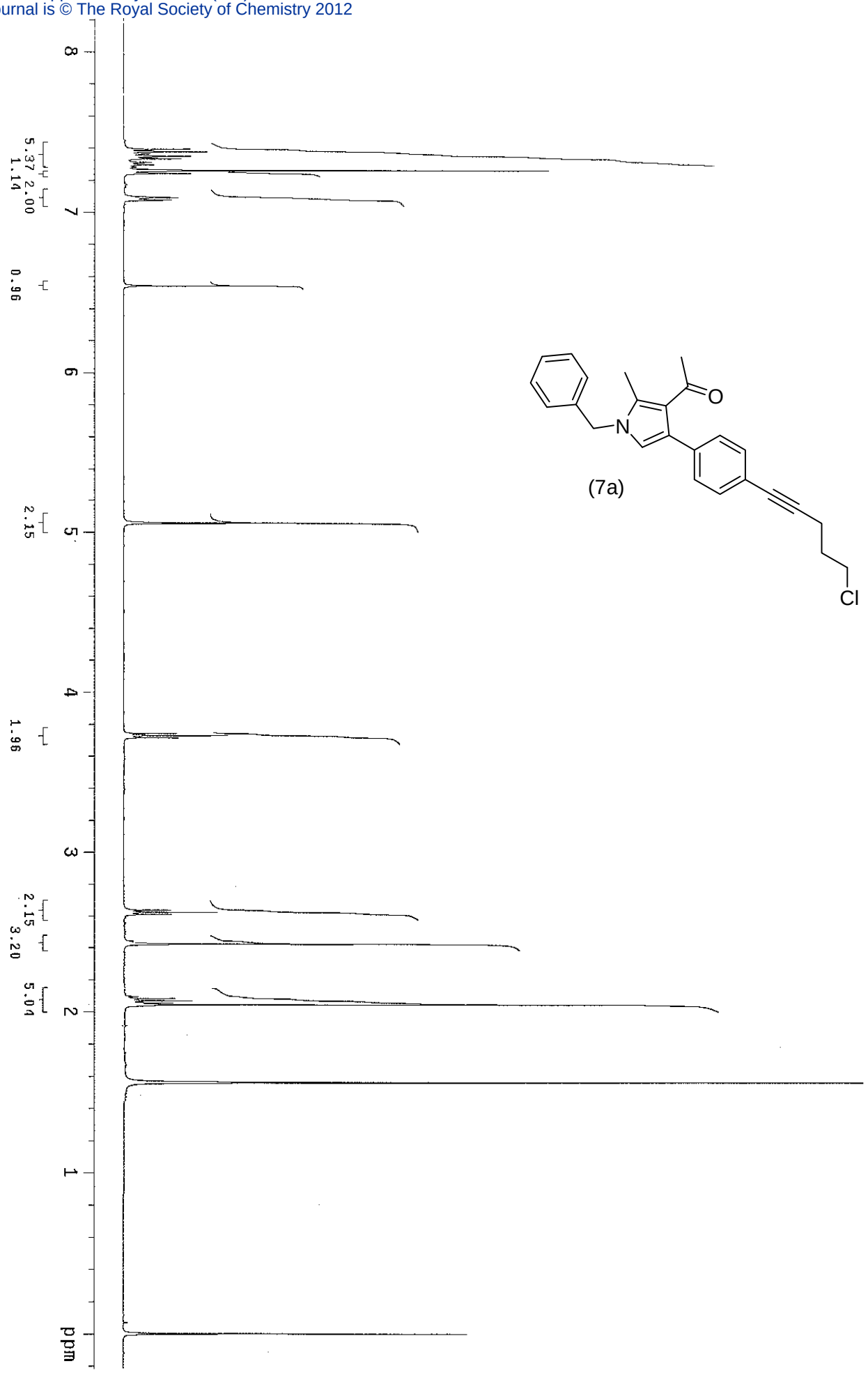


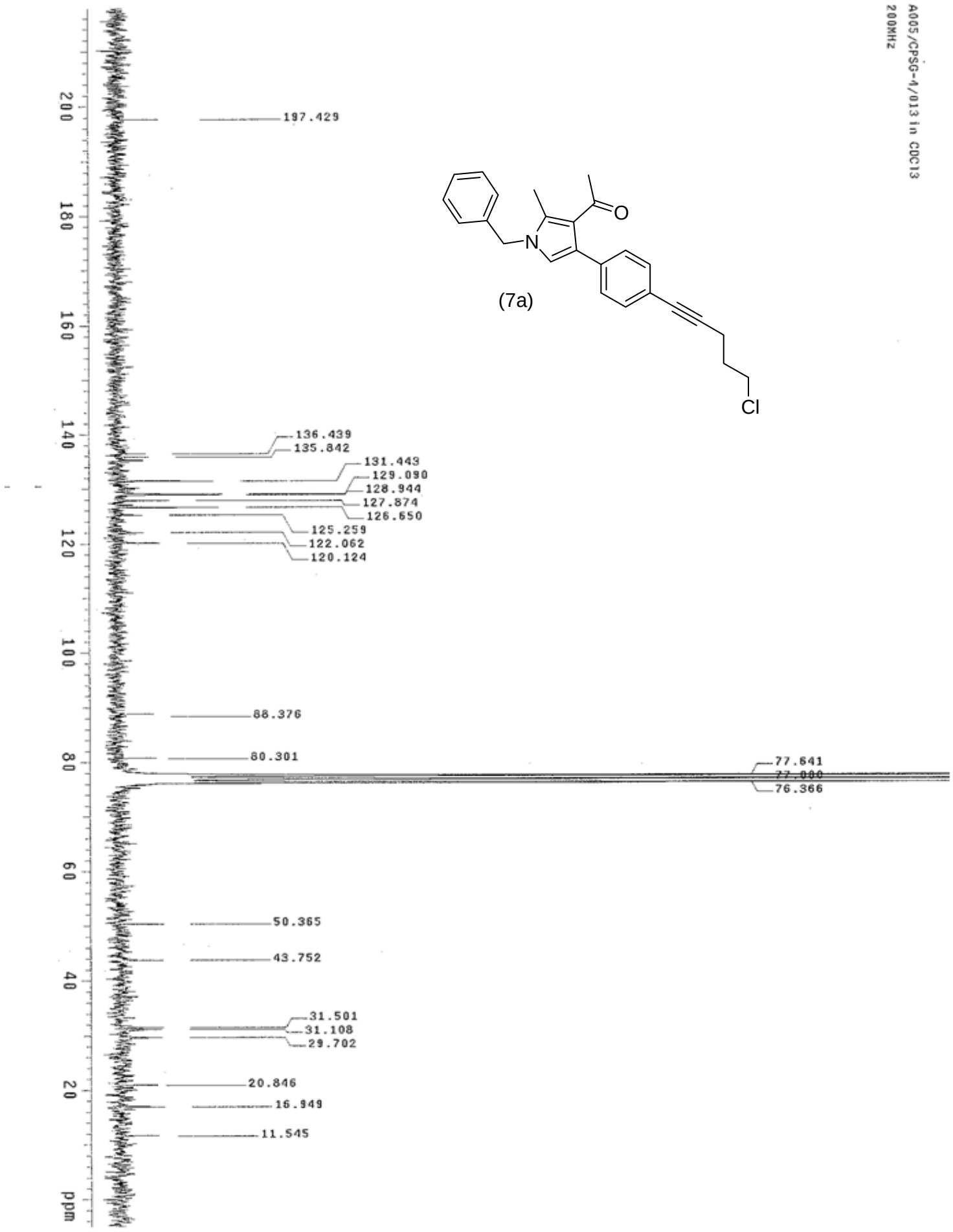
(6f)

1: TOF MS ES+
6.75e+003

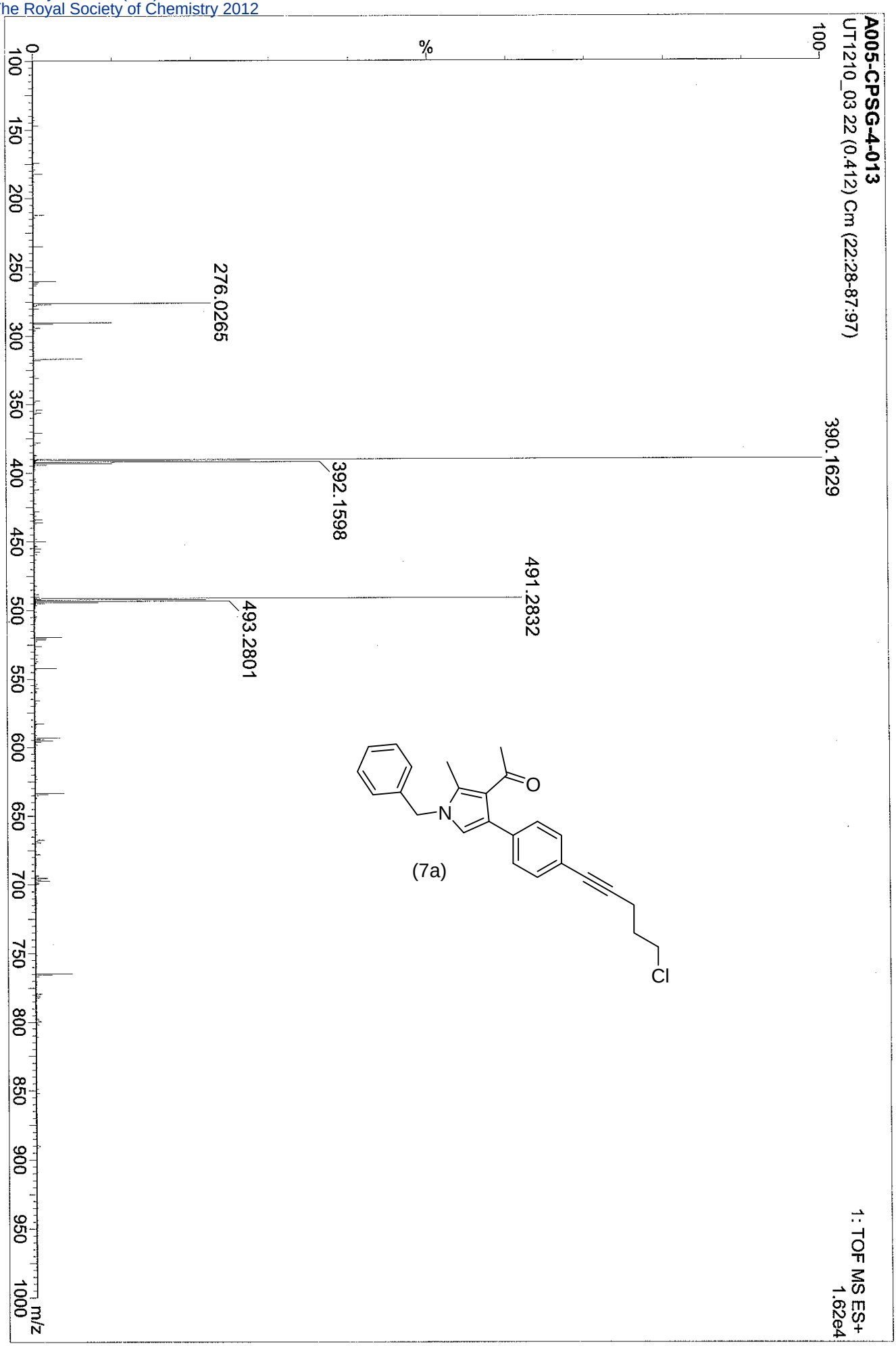


Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
394.1803	394.1807	-0.4	-1.0	16.5	0.1	C27 H24 N O2





(7a)



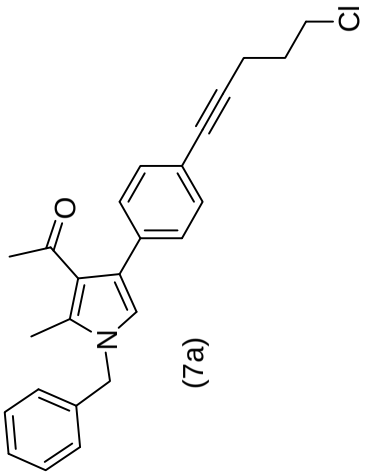
Elemental Composition Report

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

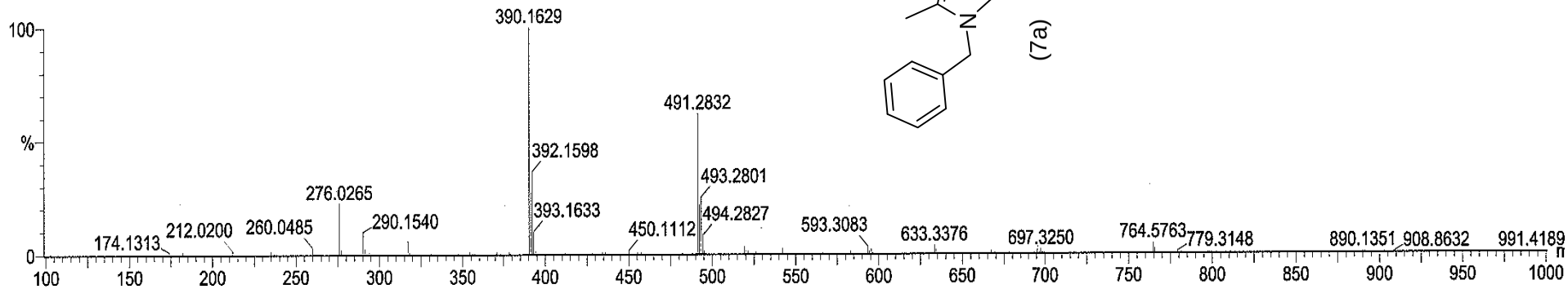
Monoisotopic Mass, Even Electron Ions
185 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-3 O: 0-4 Cl: 0-1

A005-CPSG-4-013
UT1210_03 22 (0.412) Cm (22:28-87:97)

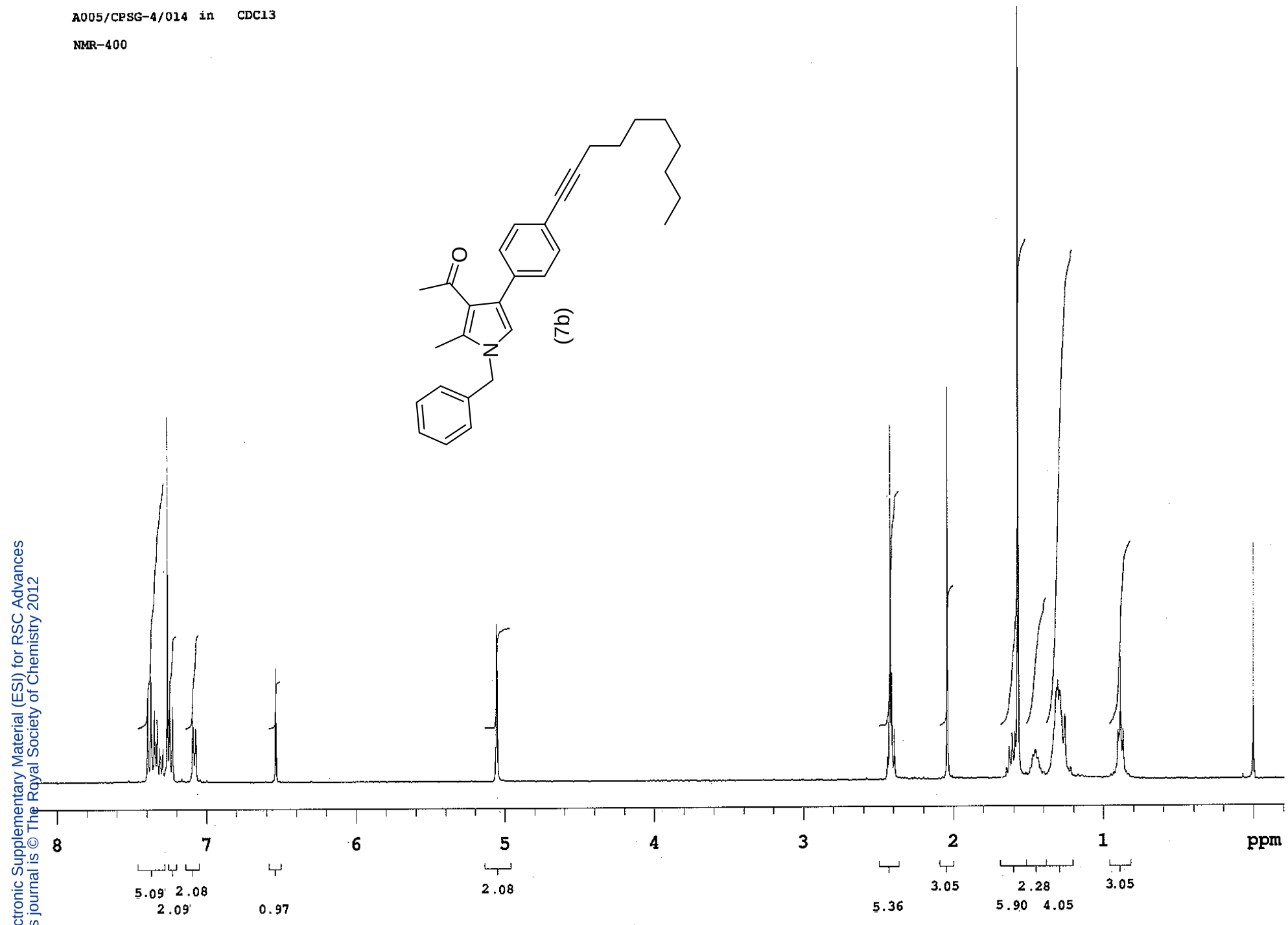


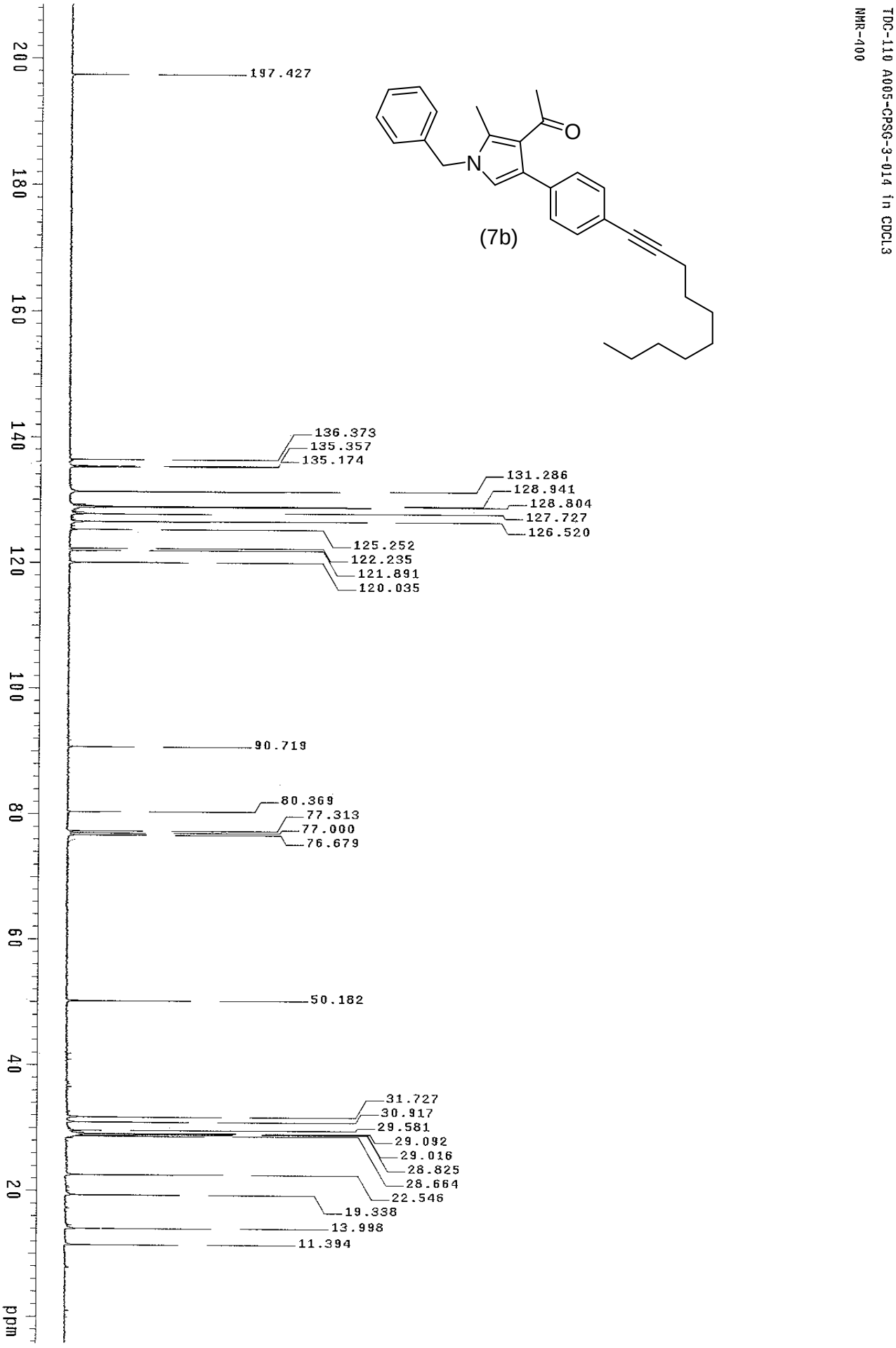
(7a)

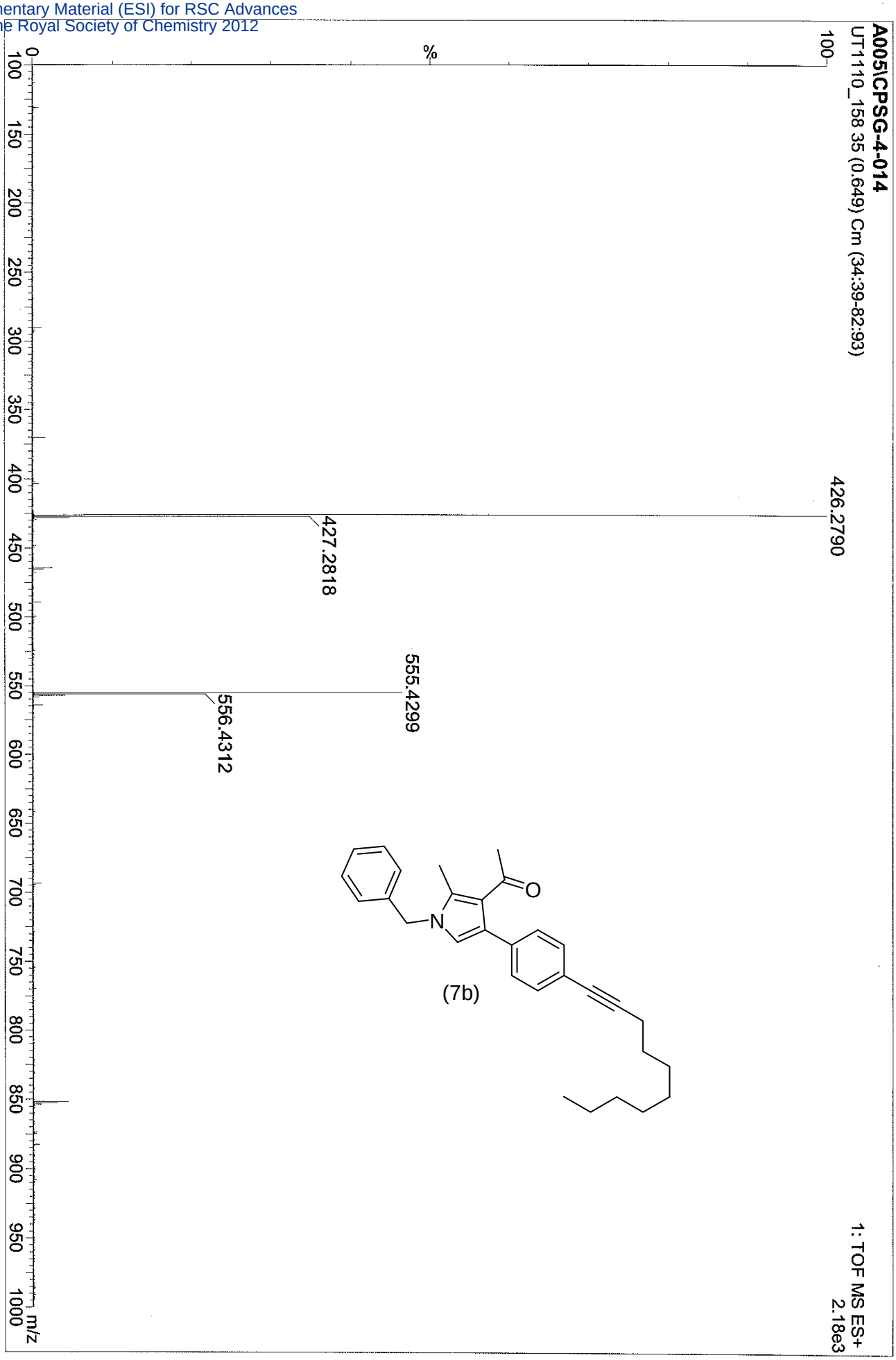
1: TOF MS E
1.62e+(



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
390.1629	390.1625	0.4	1.0	13.5	3.4	C25 H25 N O Cl





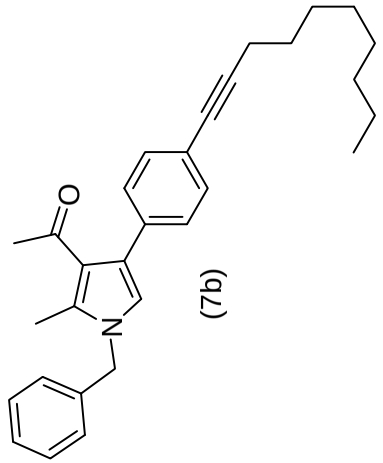


Elemental Composition Report

Single Mass Analysis

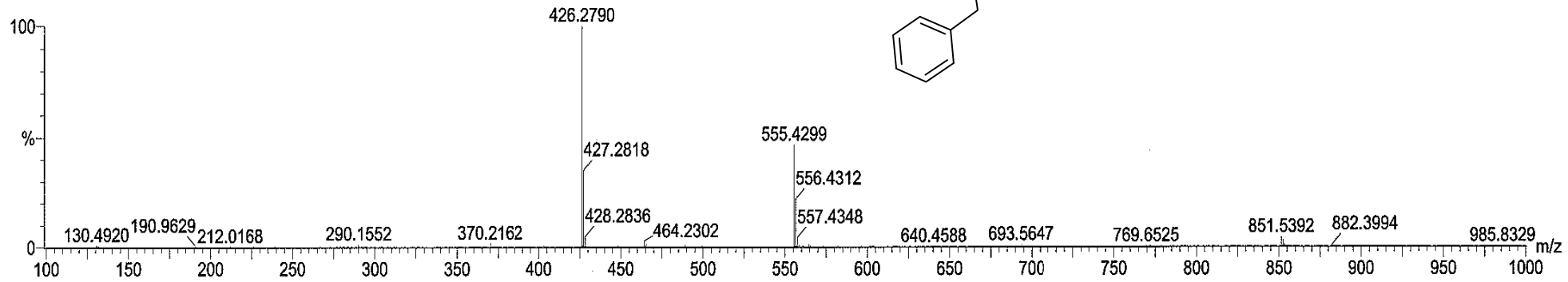
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
188 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-45 H: 0-65 N: 0-5 O: 0-5
A005\CPSG-4-014
UT1110_158 35 (0.649) Cm (34:39-82:93)

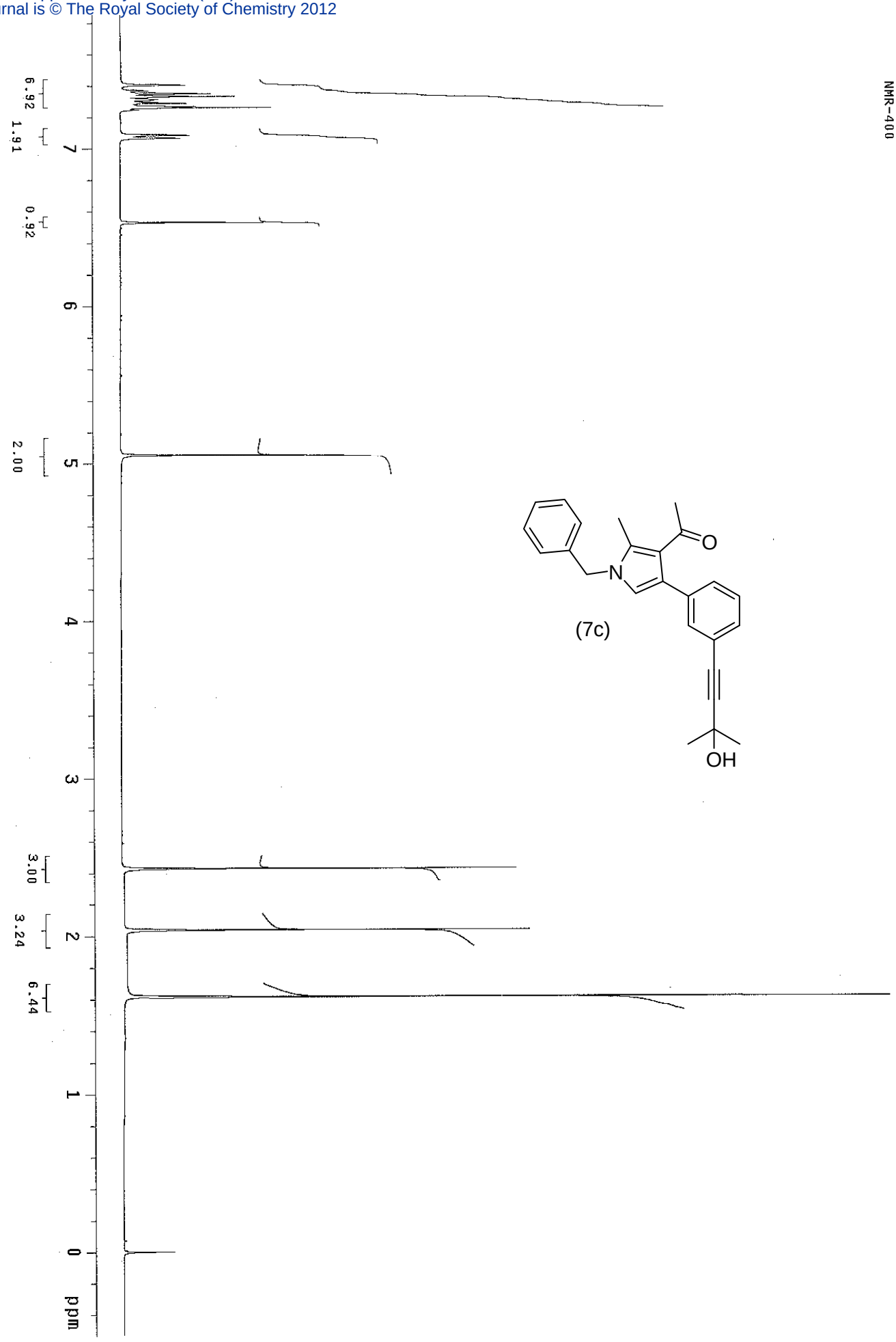


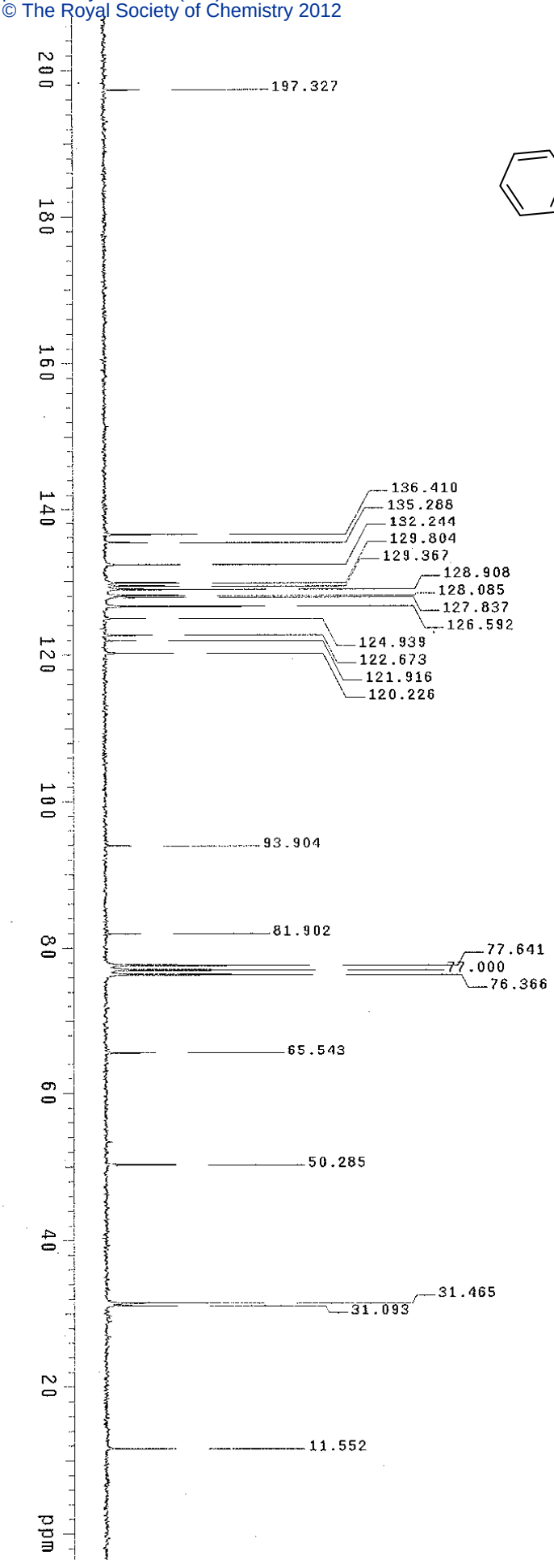
(7b)

1: TOF MS ES+
2.18e+003

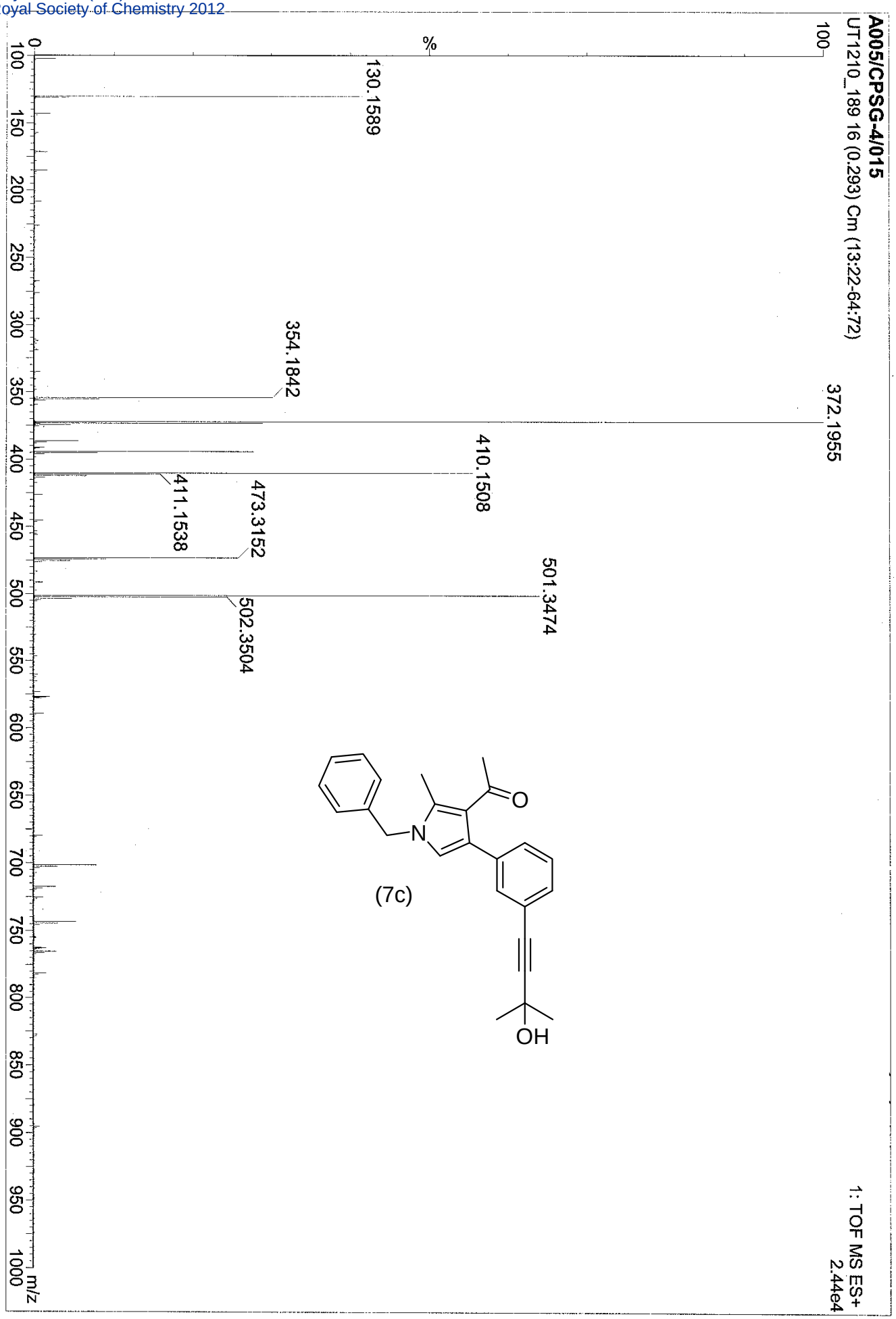


Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
426.2790	426.2797	-0.7	-1.6	13.5	0.1	C30 H36 N O





(7c)



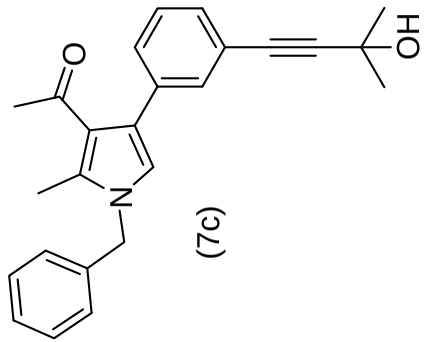
(7c)

Elemental Composition Report

Single Mass Analysis

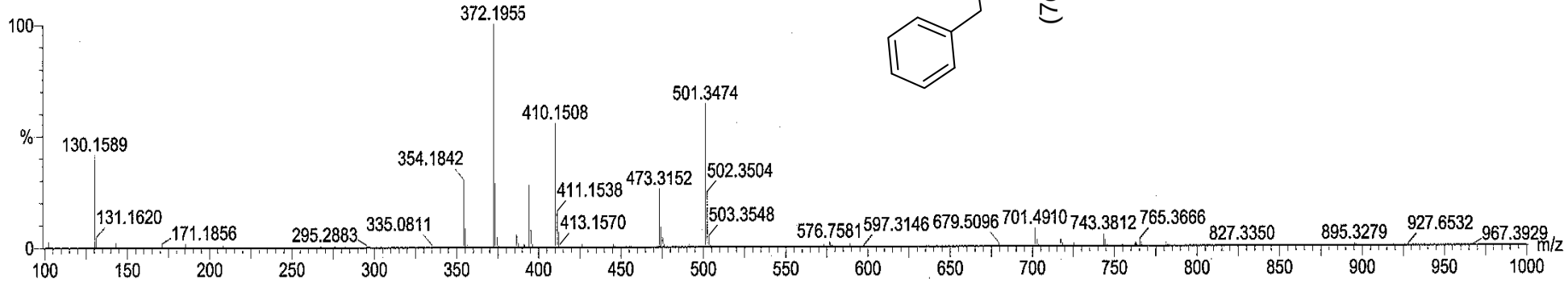
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
117 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-60 N: 0-4 O: 0-4
A005/CPSG-4/015
UT1210_189 16 (0.293) Cm (13:22-64:72)

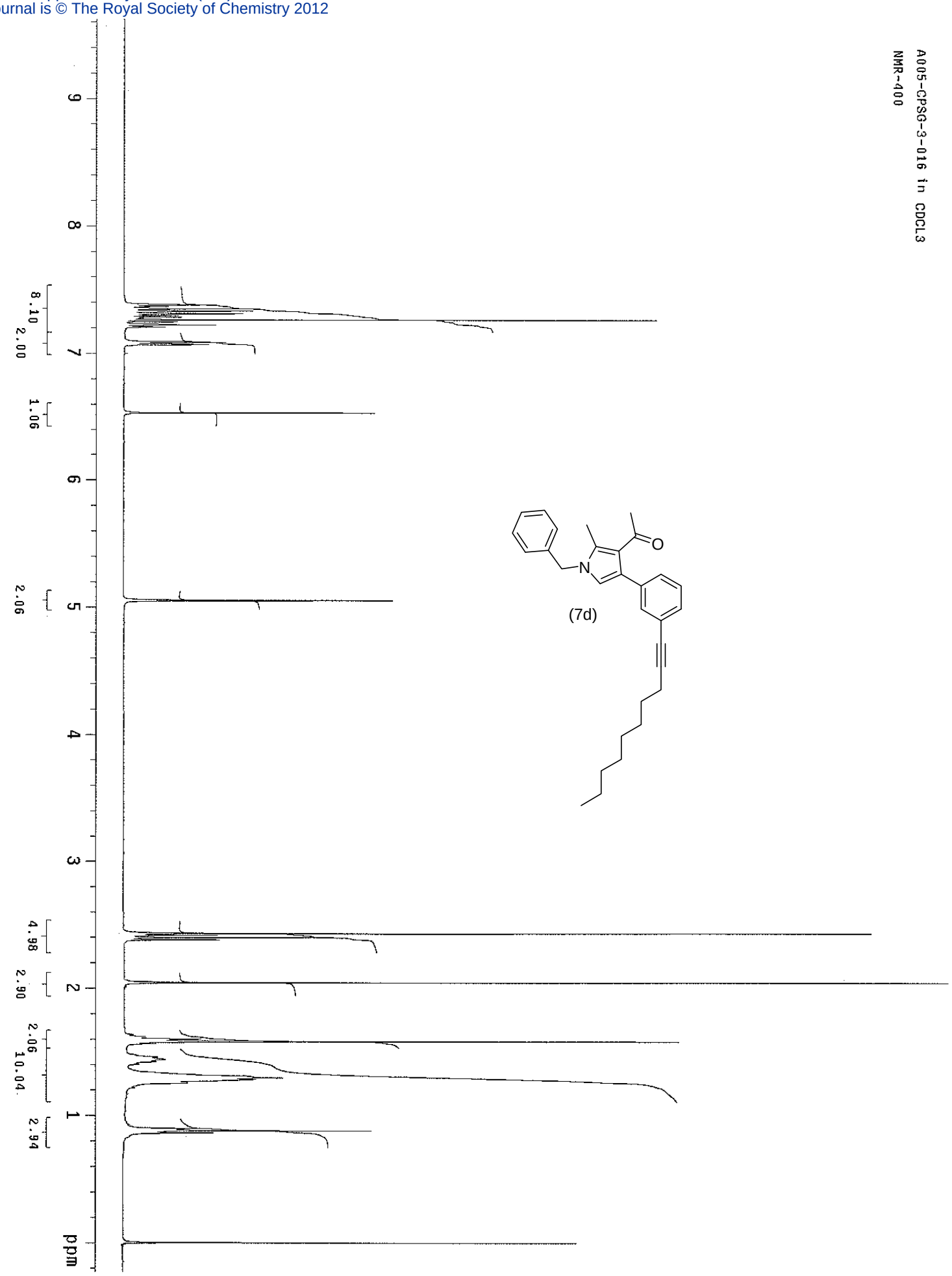


(7c)

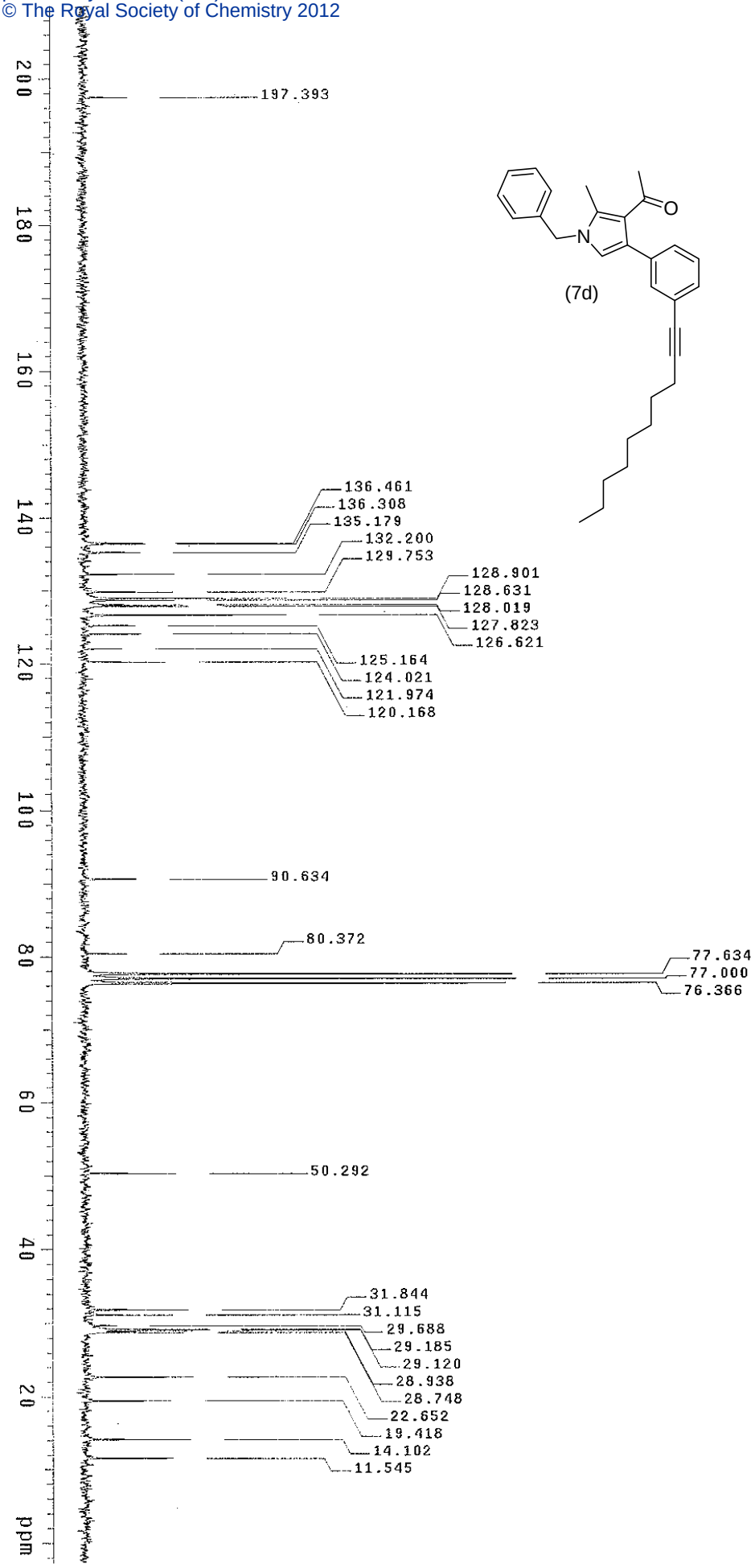
1: TOF MS ES+
2.44e+004



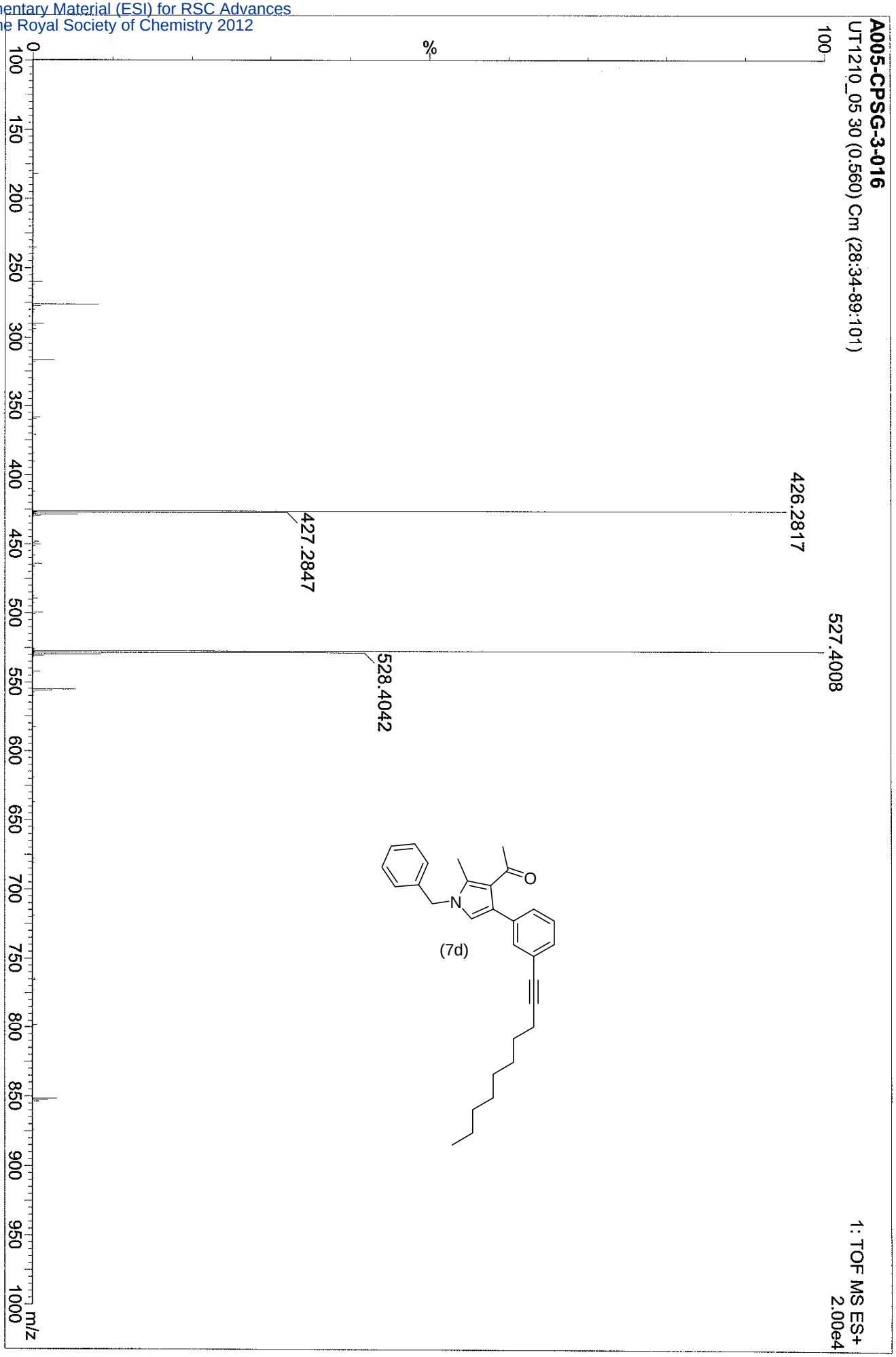
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
372.1955	372.1964	-0.9	-2.4	13.5	2.2	C25 H26 N O2



A005/CPSG-3/016 in CDCl3
200MHz



(7d)



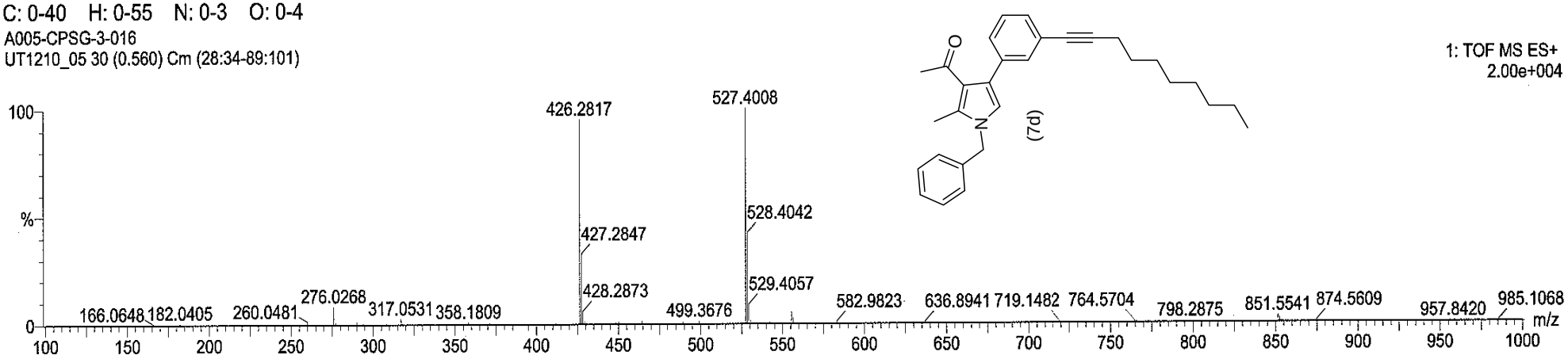
Elemental Composition Report

Single Mass Analysis

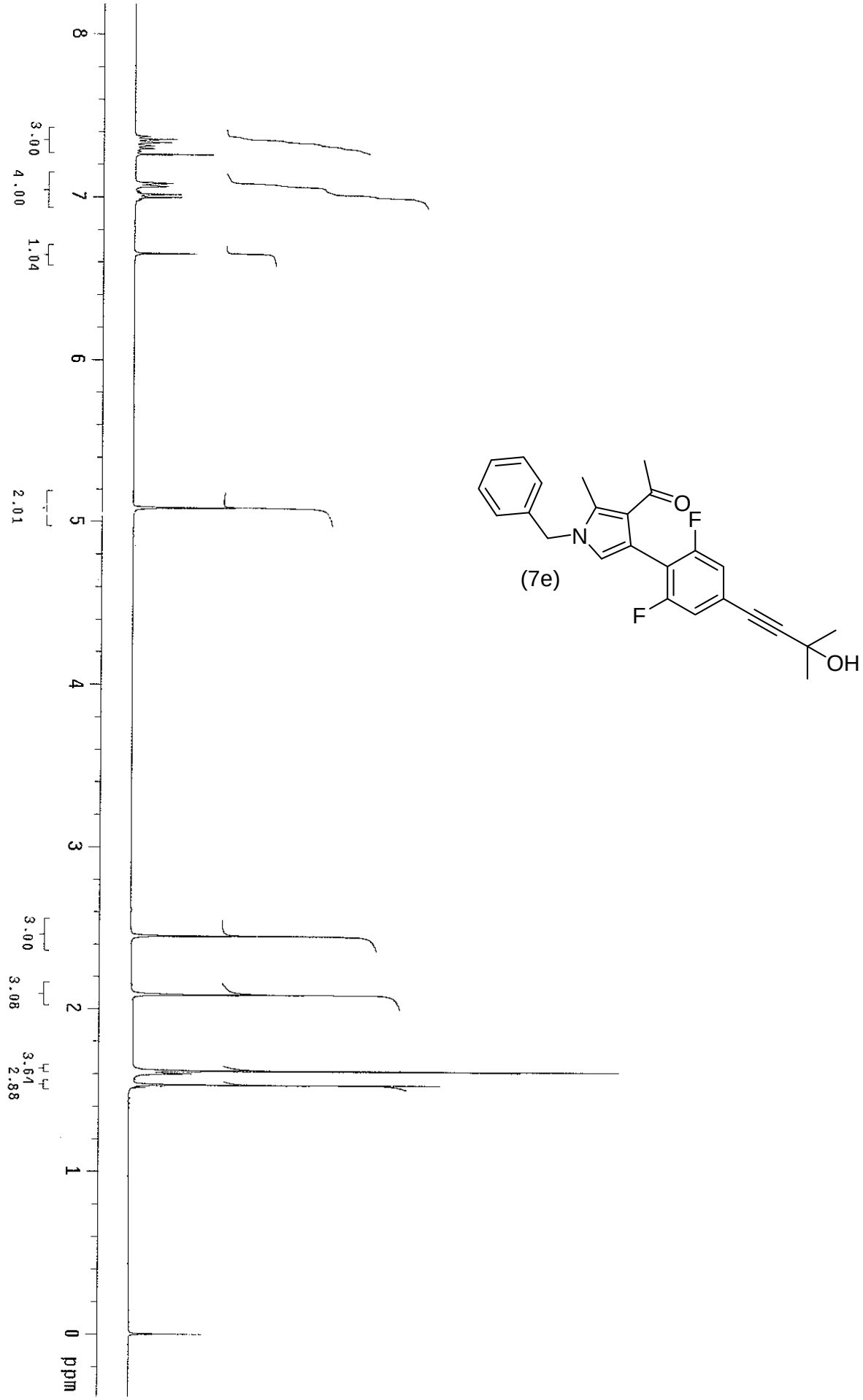
Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
94 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-3 O: 0-4

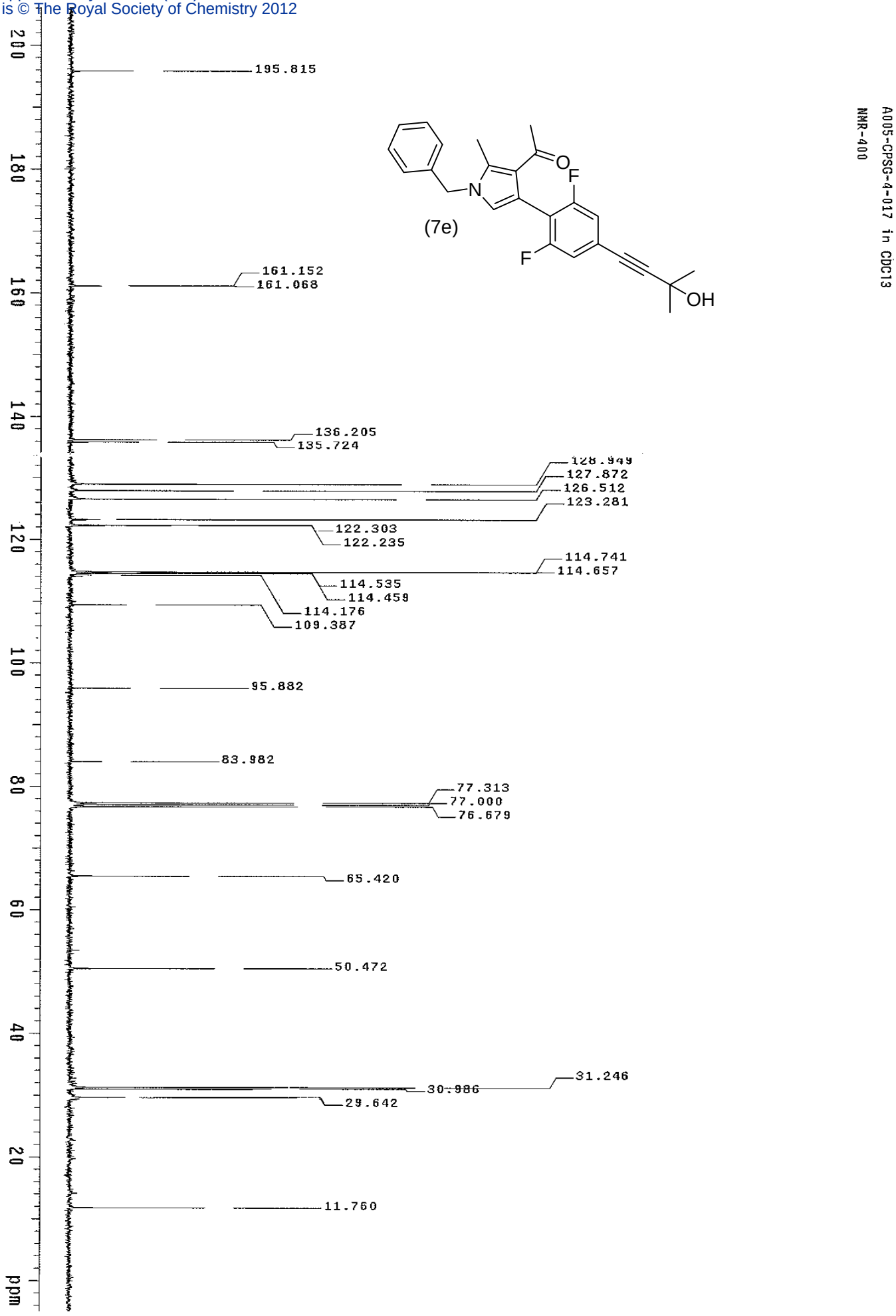
A005-CPSG-3-016
UT1210_05 30 (0.560) Cm (28:34-89:101)

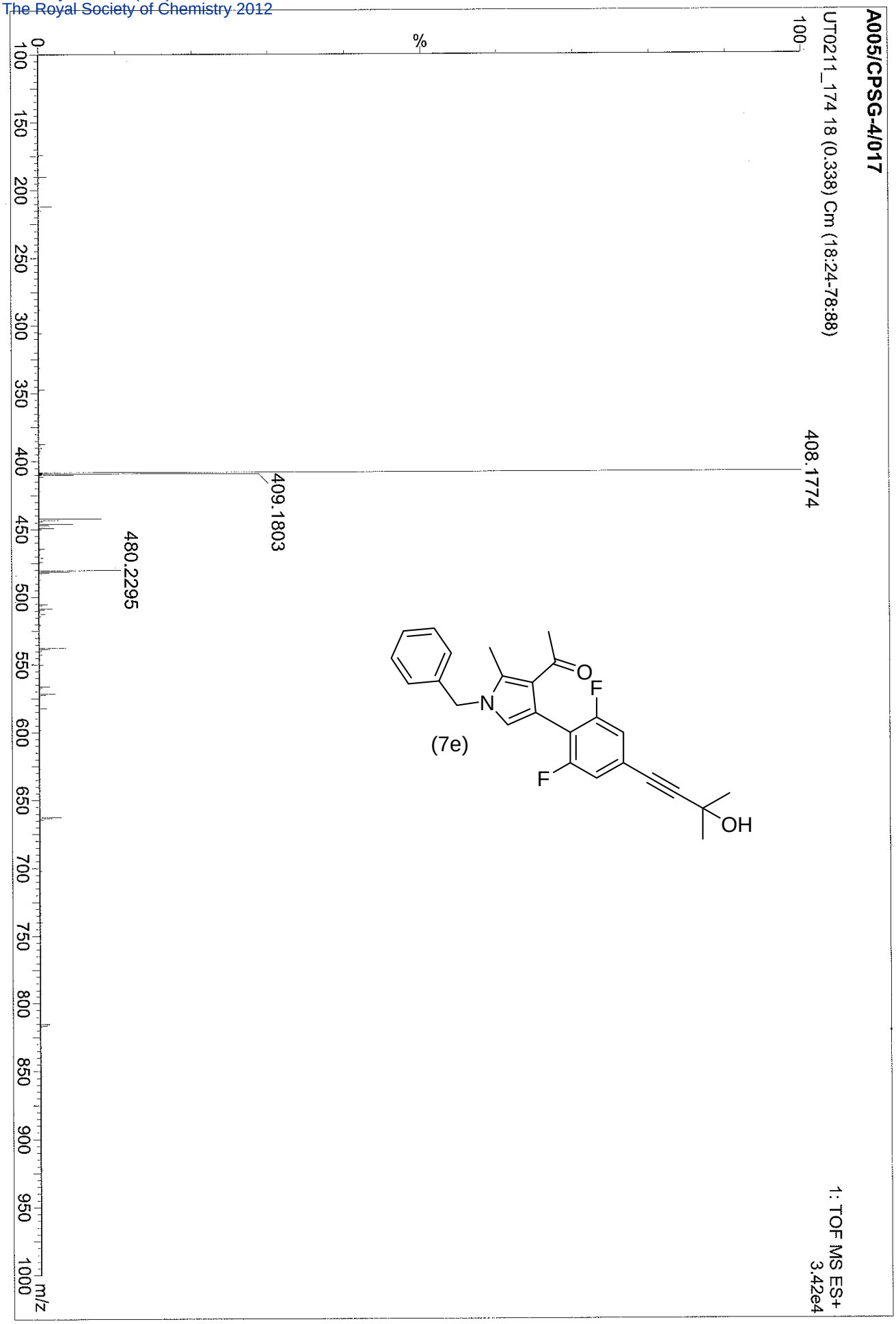


Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
426.2817	426.2797	2.0	4.7	13.5	2.4	C30 H36 N O



(7e)





Elemental Composition Report

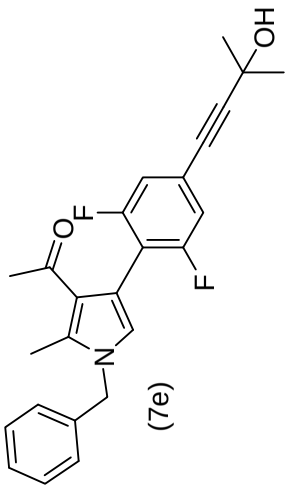
Single Mass Analysis

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
105 formula(e) evaluated with 3 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-28 H: 0-35 N: 0-2 O: 0-3 F: 0-3

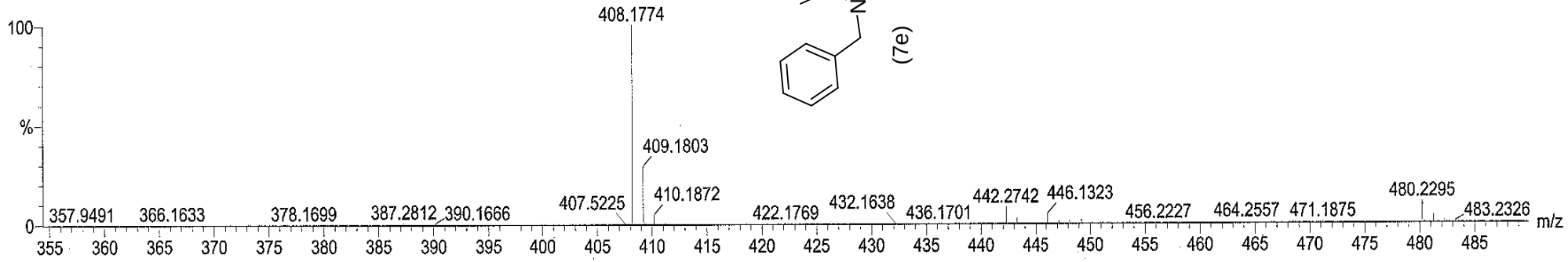
A005/CPSG-4/017

UT0211_174 18 (0.338) Cm (18:24-78:88)



(7e)

1: TOF MS ES+
3.42e+004



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
408.1774	408.1775	-0.1	-0.2	13.5	1.6	C25 H24 N O2 F2

Electronic Supplementary Material (ESI) for RSC Advances