

Copies of NMR and HRMS spectra

**Yb(OTf)₃ mediated MCR: a new and regioselective approach
towards polysubstituted pyrroles of pharmacological interest**

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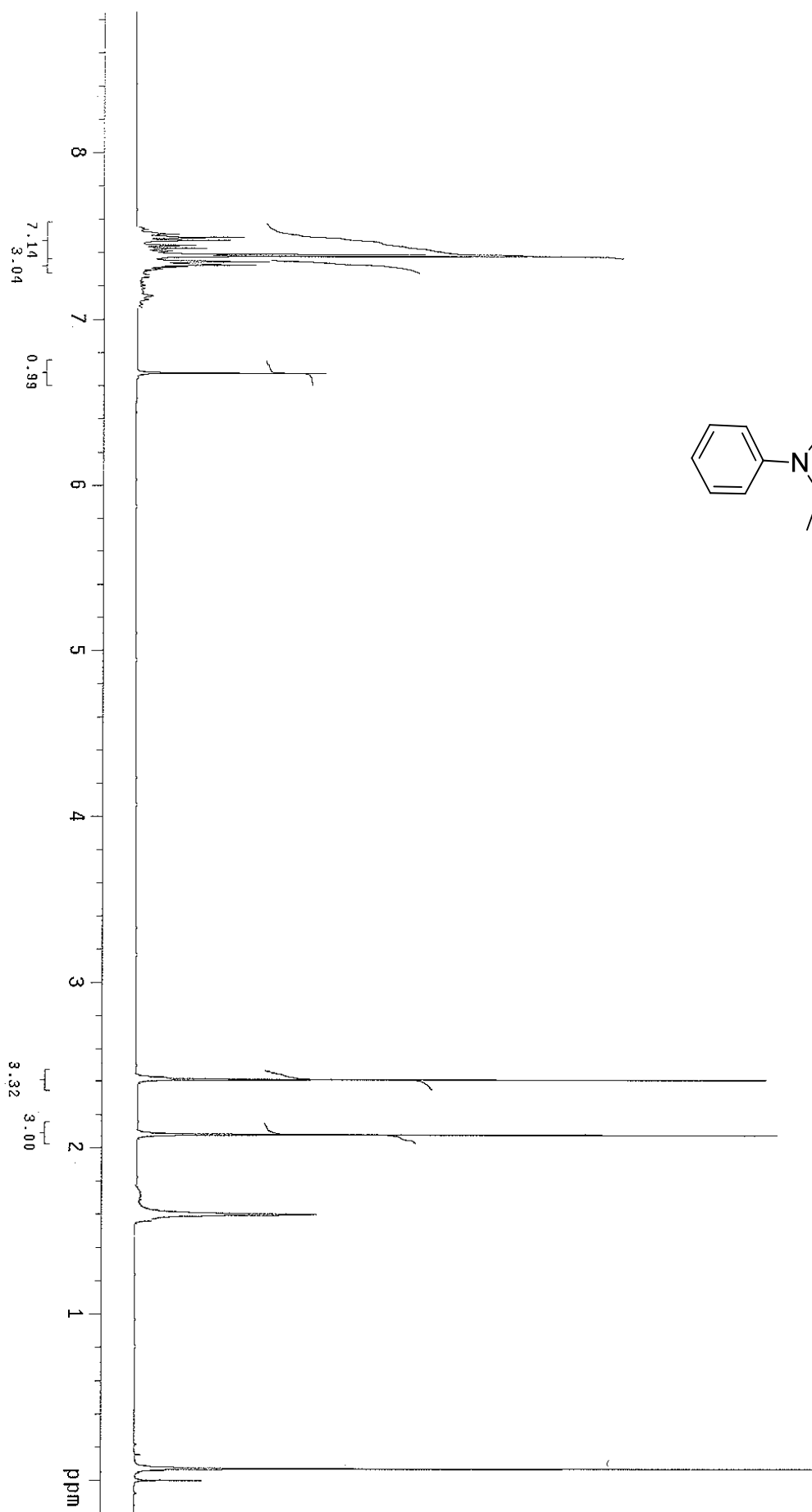
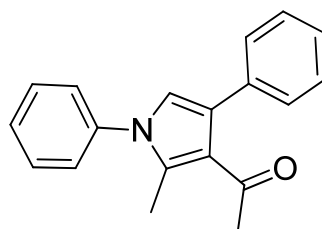
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India.*

^d*Department of Chemical Sciences, Indian Institute of Science Education and Research, Kolkata,
West Bengal, 741252, India.*

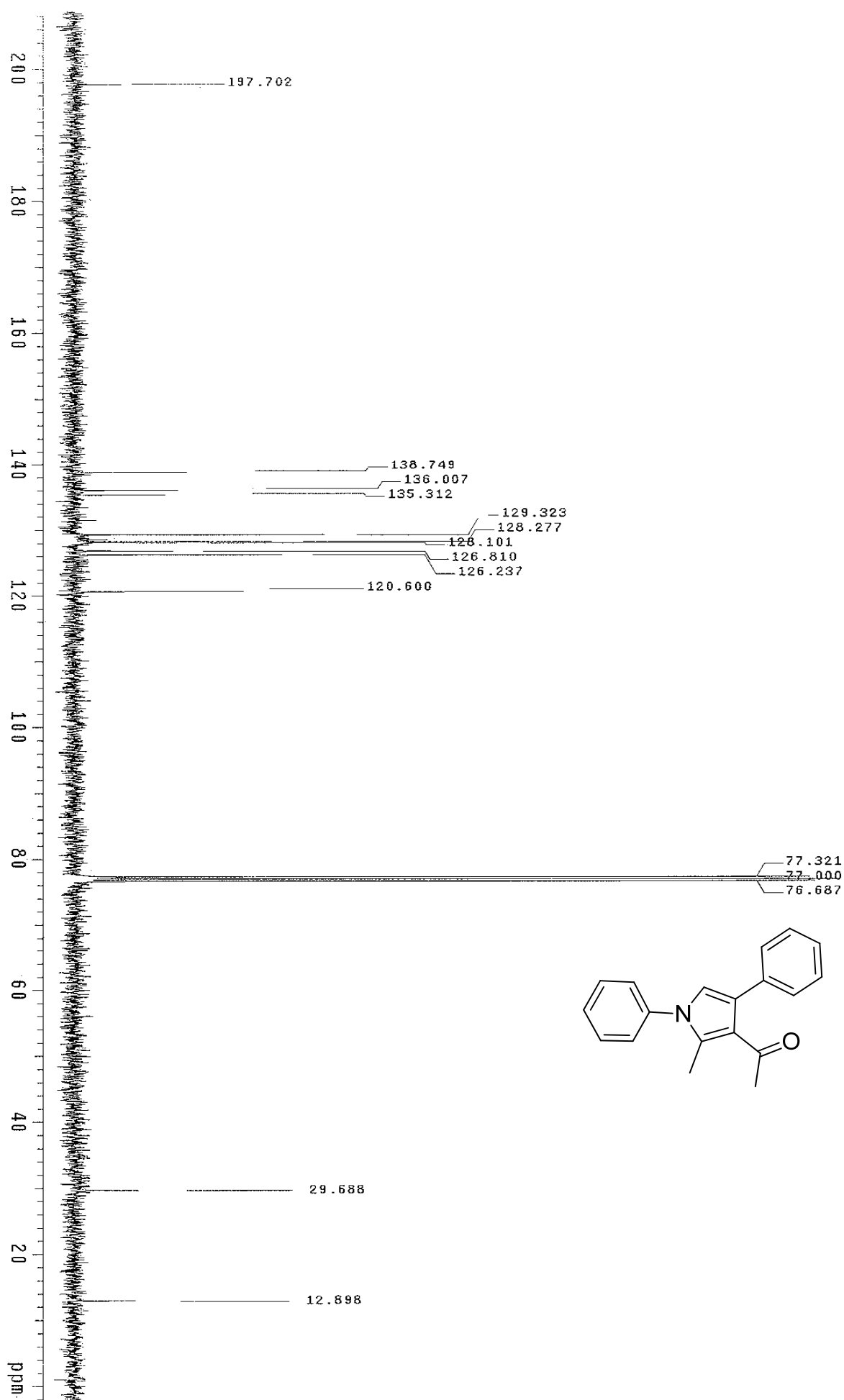
E-mail: manojitpal@rediffmail.com

4a ^1H NMR (400 MHz, CDCl_3)

A012/CCTP-1/001 in CDCl₃
NMR-400MHz

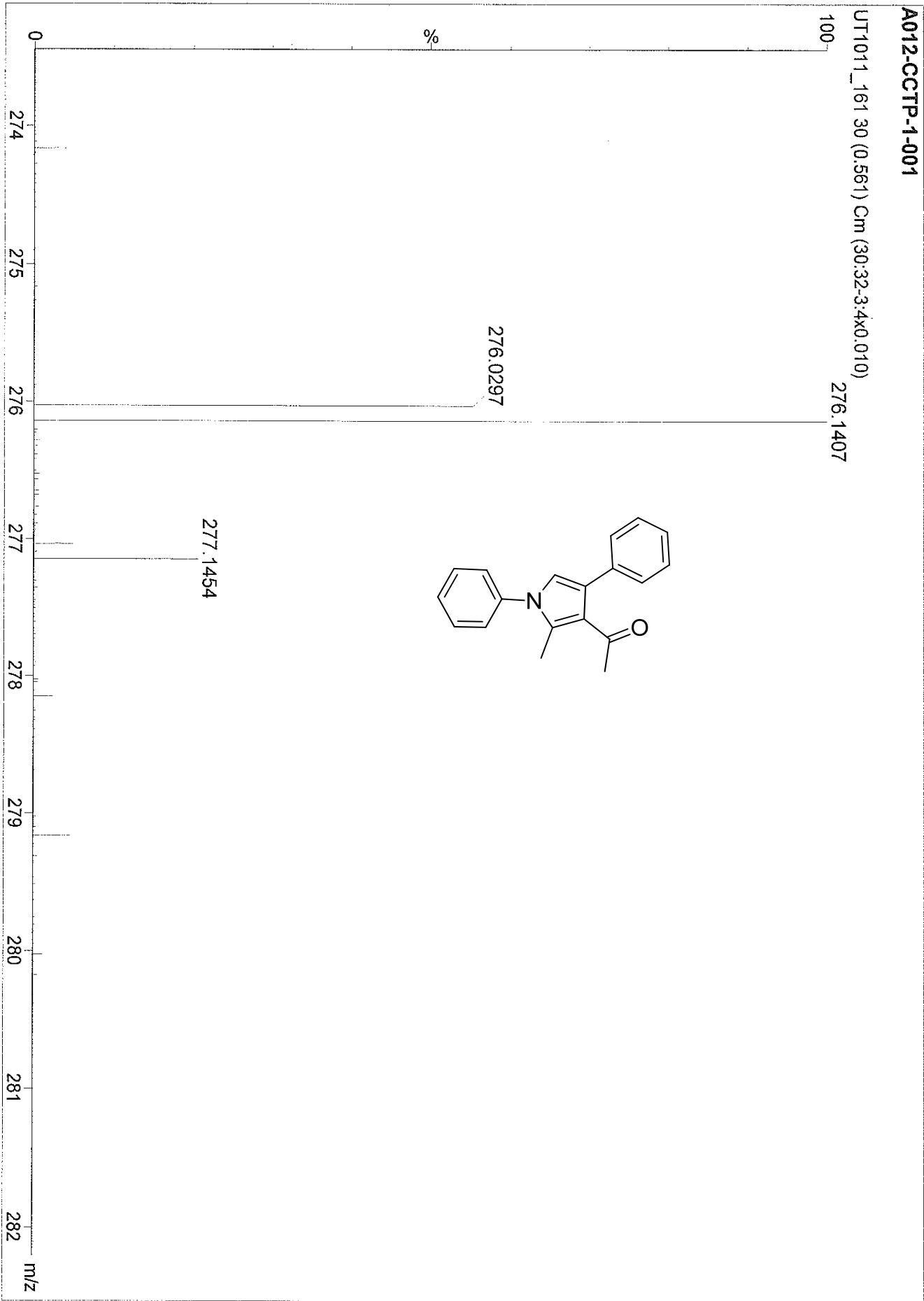


4a ^1H NMR (100 MHz, CDCl_3)



A012-CCTP-1-001 in CDCl_3
NMR-400MHz

4a HRMS



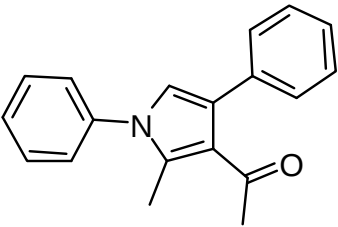
Elemental Composition Report

Single Mass Analysis

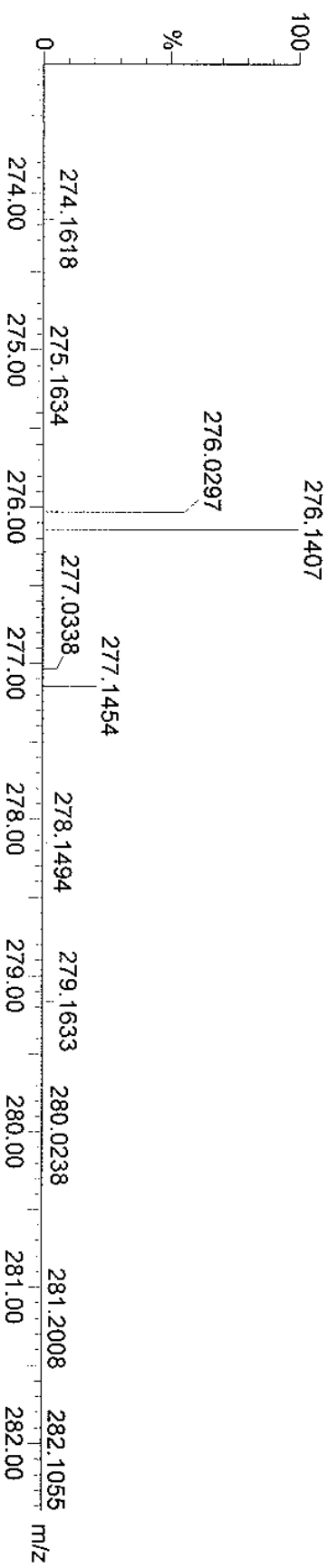
Tolerance = 10.0 PPM / DBE: min = 0.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
122 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)

Elements Used:
C: 0-50 H: 0-70 N: 0-2 O: 0-15
A012-CCTP-1-001
Dr.Reddy's Laboratories Ltd, ARD,TDC-1

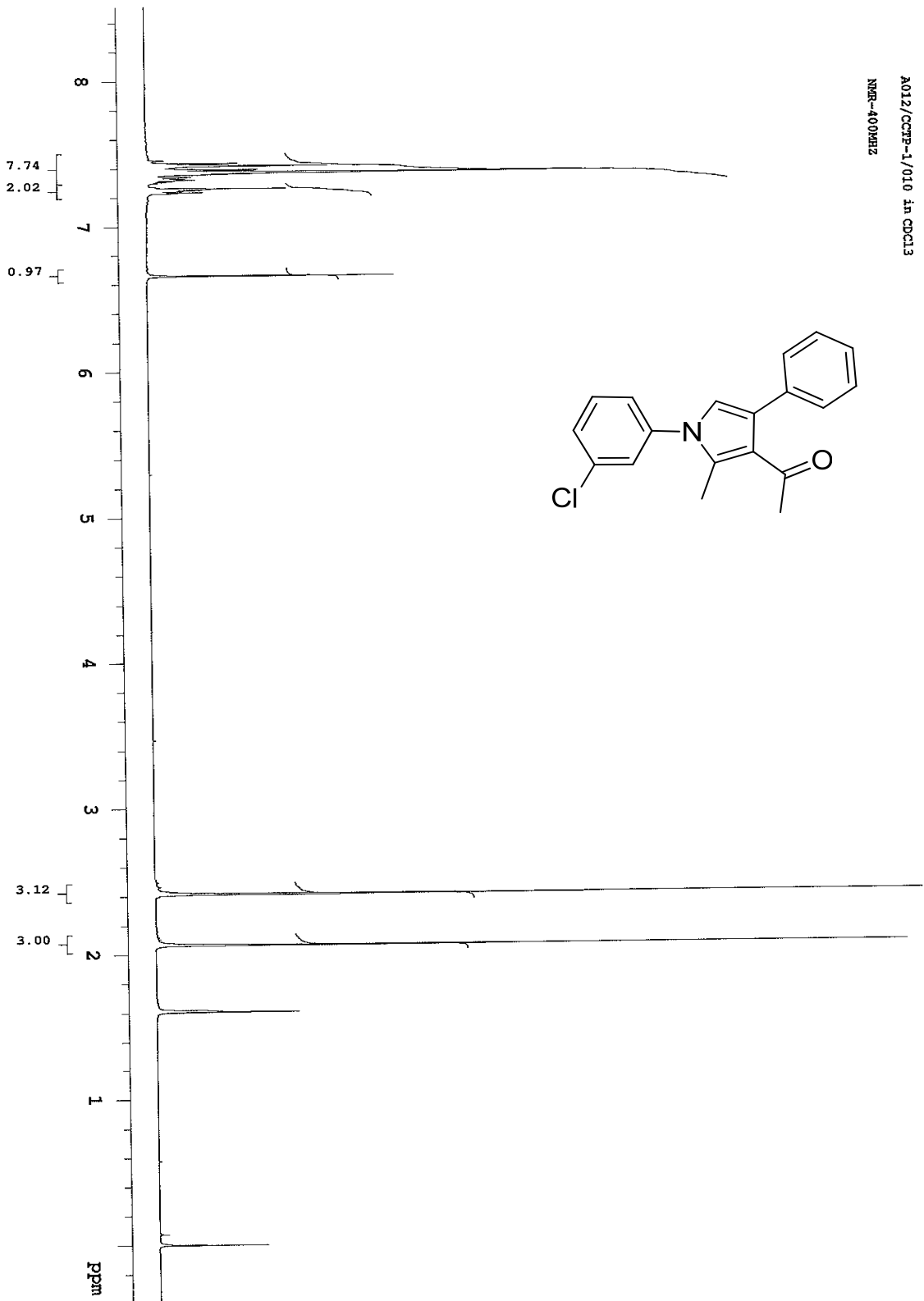


UT1011_161 30 (0.561) Cm (30:32-3:4x0.010)
1: TOF MS ES+
2.30e+003

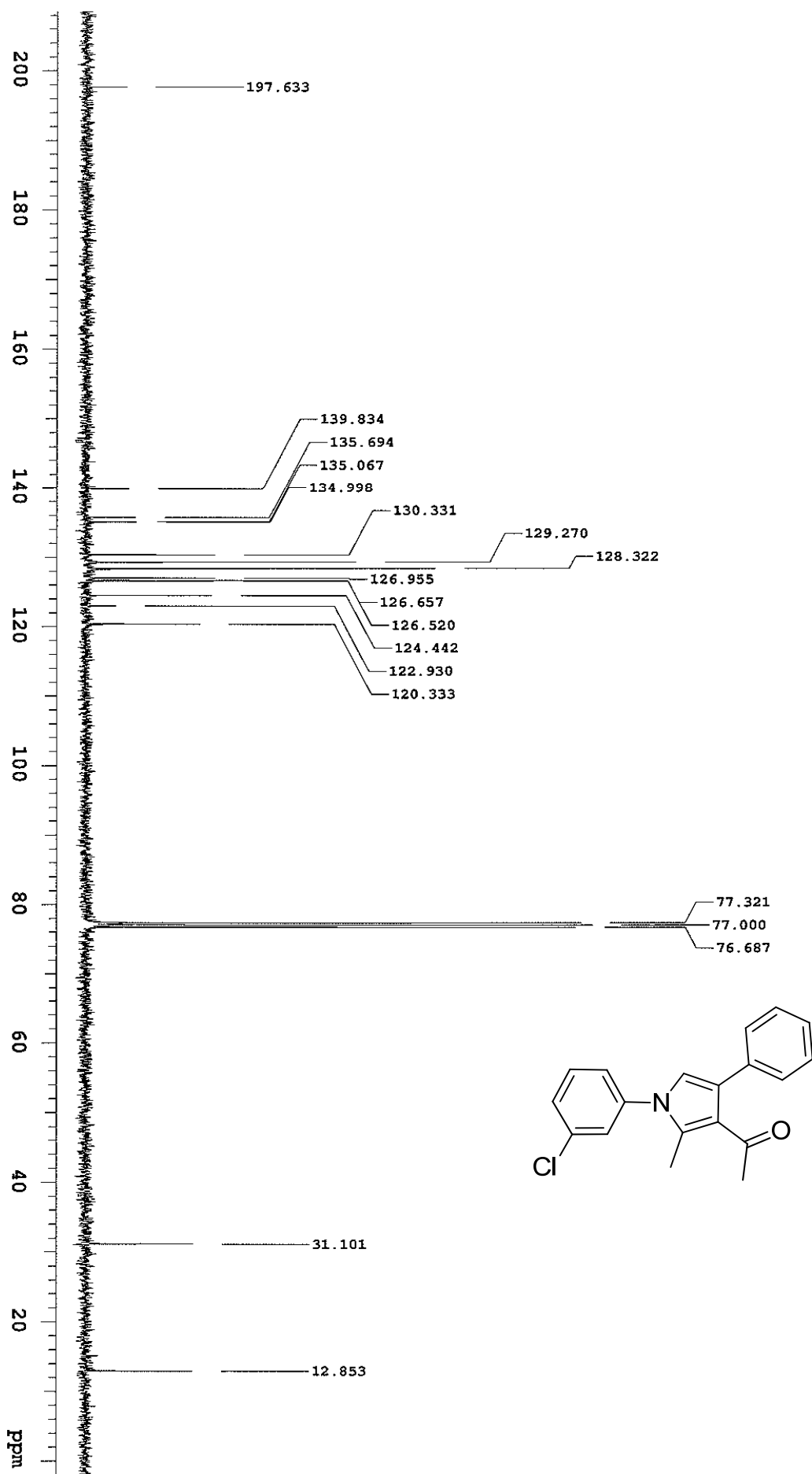


Minimum:						
Maximum:						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
276.1407	276.1388	1.9	6.9	11.5	50.9	C19 H18 N O

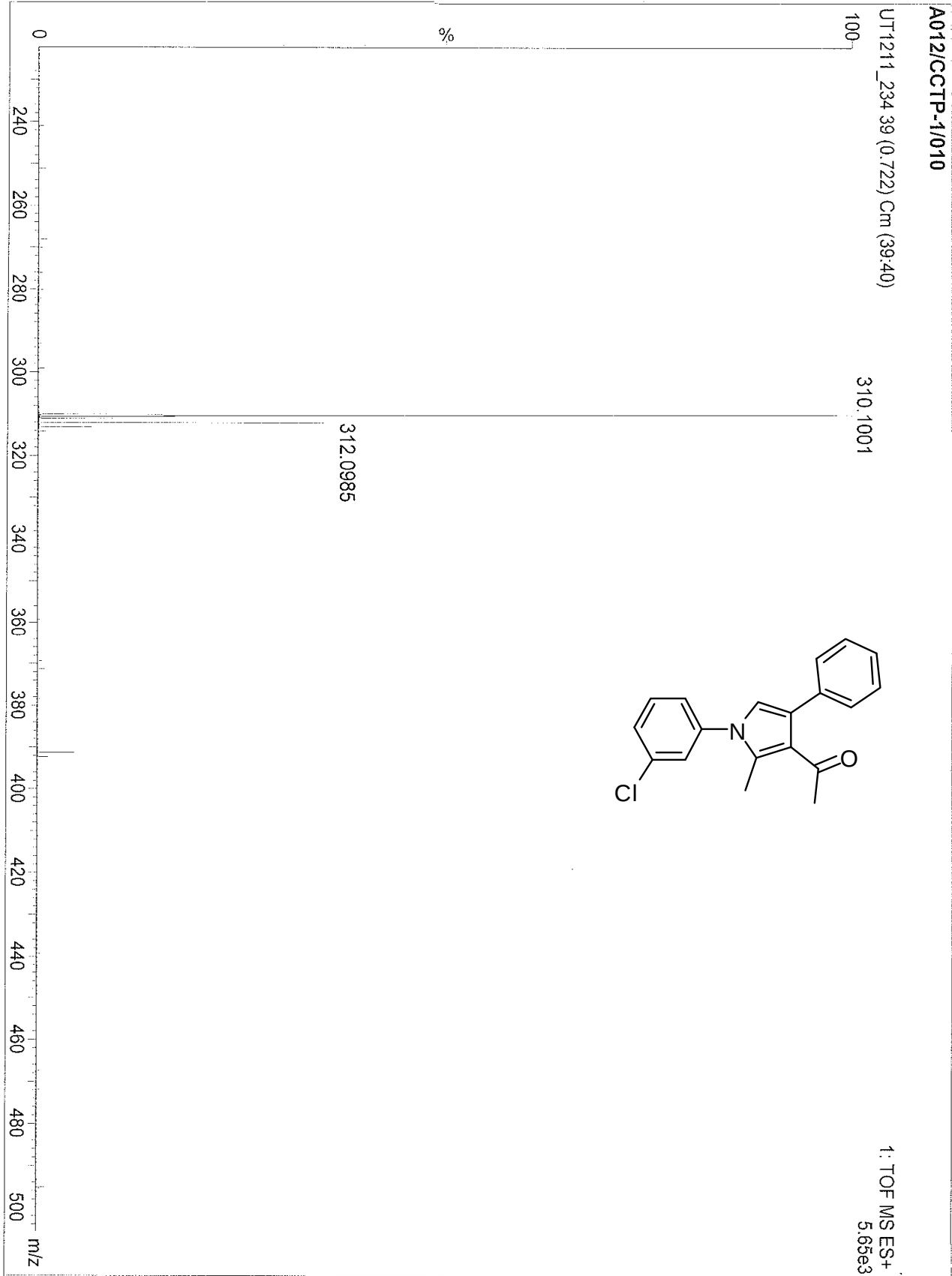
4b ¹H NMR (400 MHz, CDCl₃)



4b ^1H NMR (100 MHz, CDCl_3)



4b HRMS



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 = 3

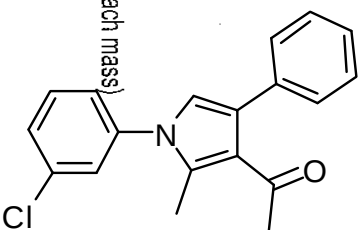
Monoisotopic Mass, Even Electron Ions

14 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

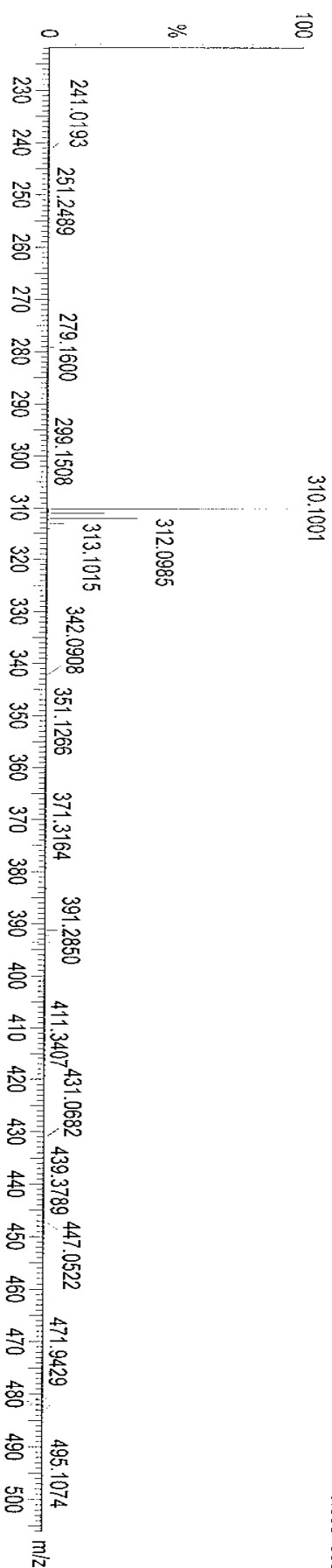
C: 0-25 H: 0-20 N: 0-1 O: 0-1 Cl: 0-1

A012/CTP-1/010



UT1211_234 39 (0.722) Cm (39.40)

1: TOF MS ES+
5.65e+003

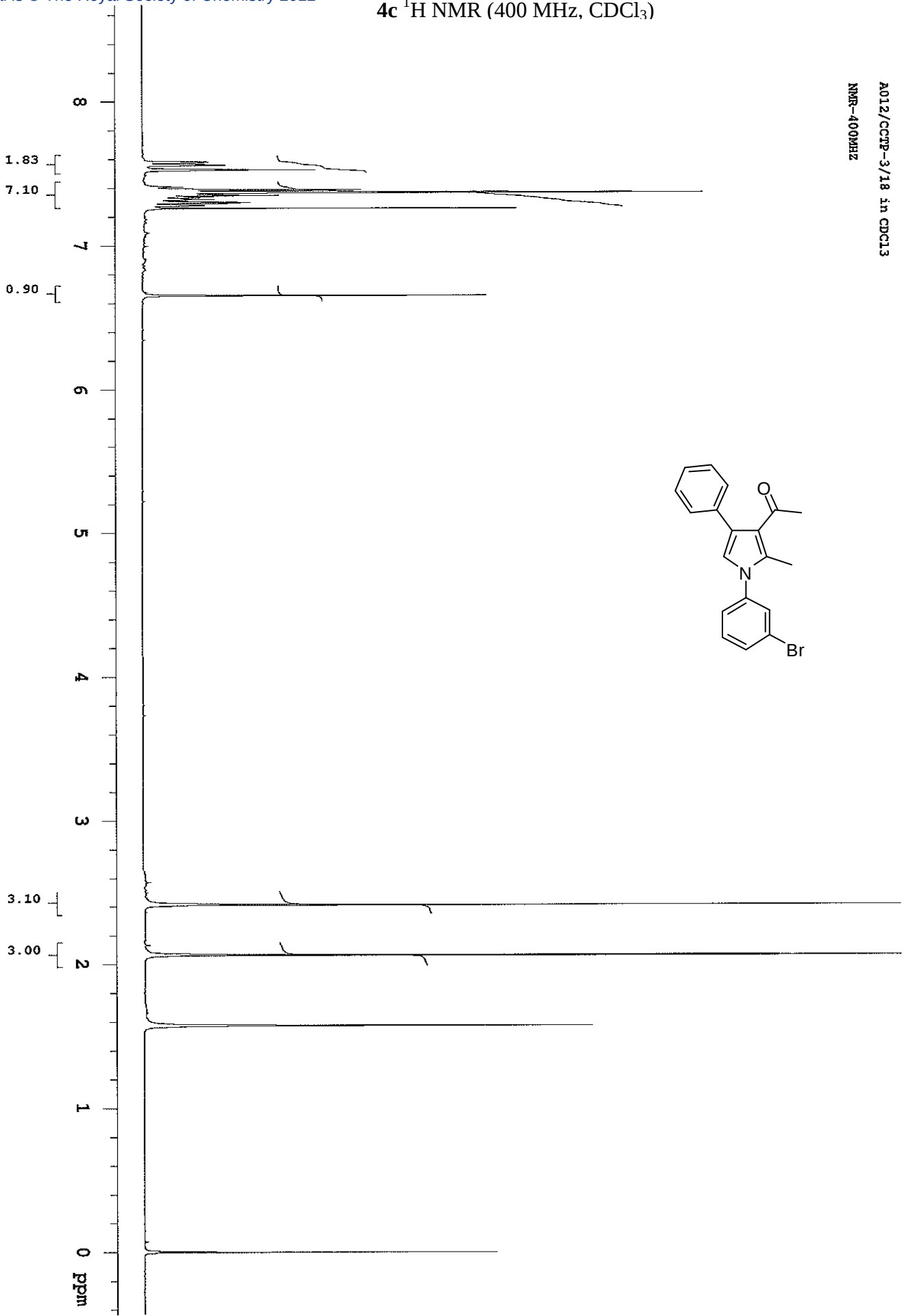


Minimum: -2.0
Maximum: 80.0

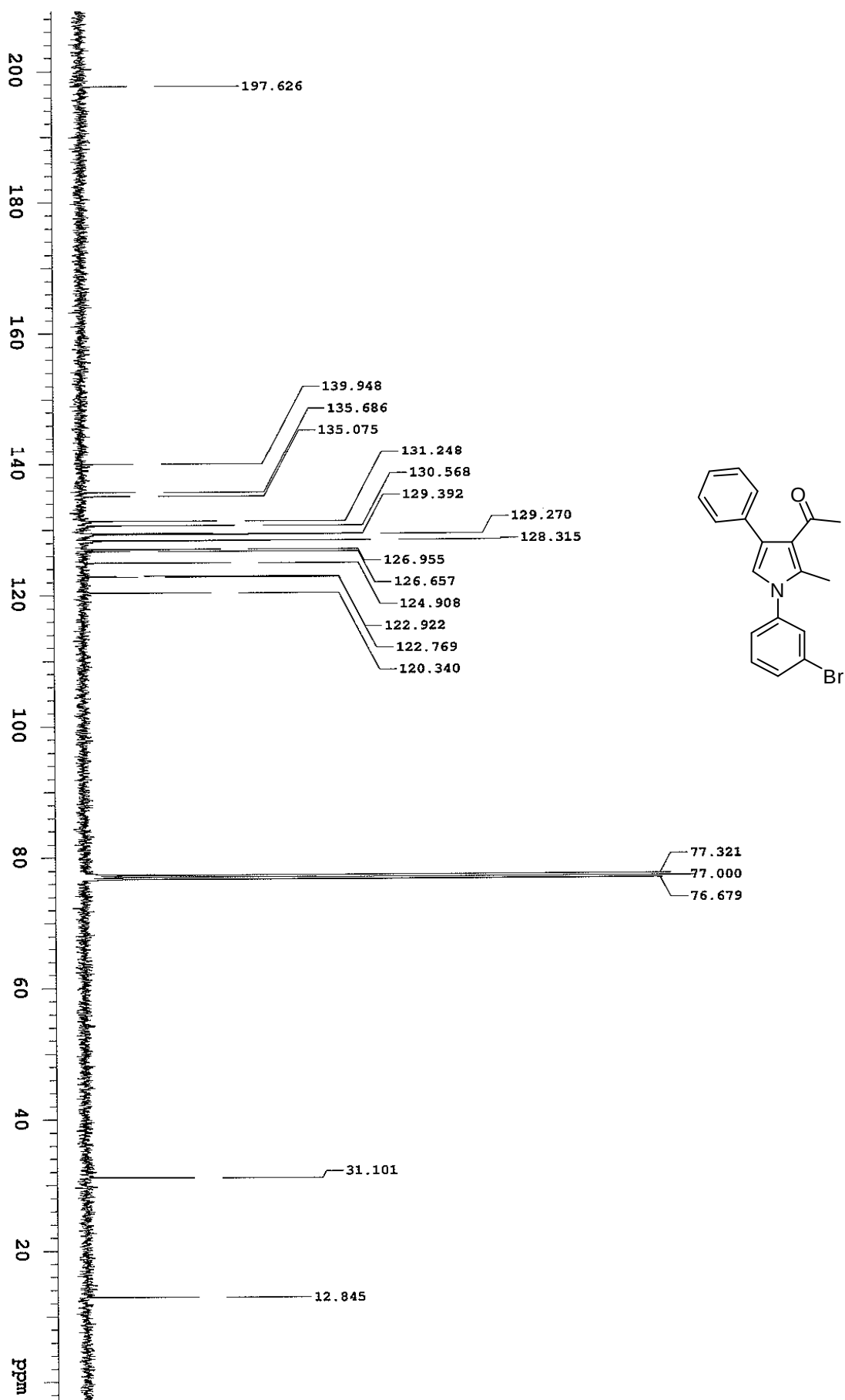
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
310.1001	310.0999	0.2	0.6	11.5	0.7	C19 H17 N O Cl

4c ¹H NMR (400 MHz, CDCl₃)

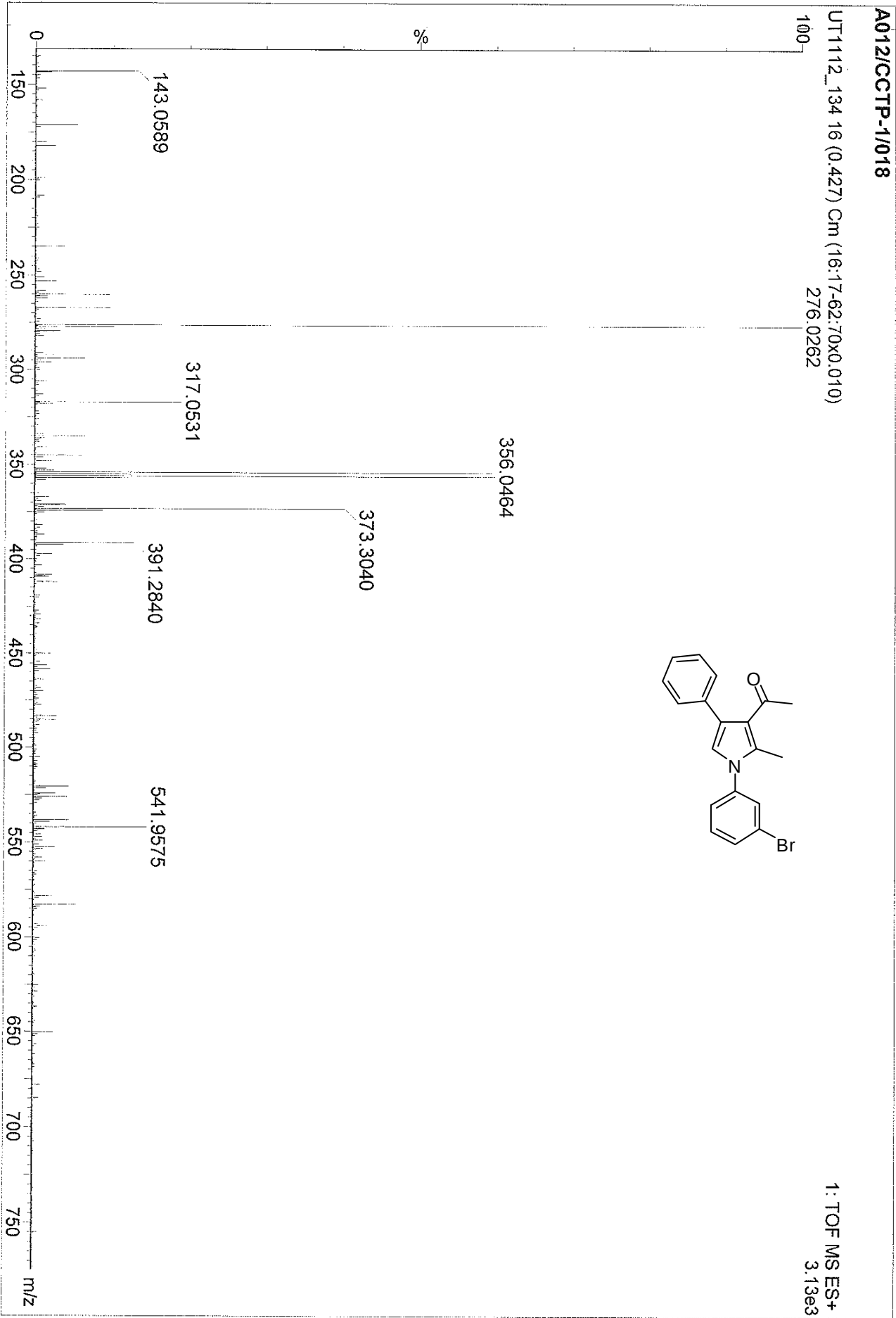
A012/CCTP-3/18 in CDCl₃
NMR-400MHZ



4c ^{13}C NMR (100 MHz, CDCl_3)



4c HRMS



4c HRMS

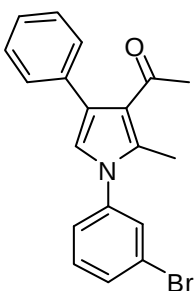
Elemental Composition Report

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 = 3



Monoisotopic Mass, Even Electron Ions

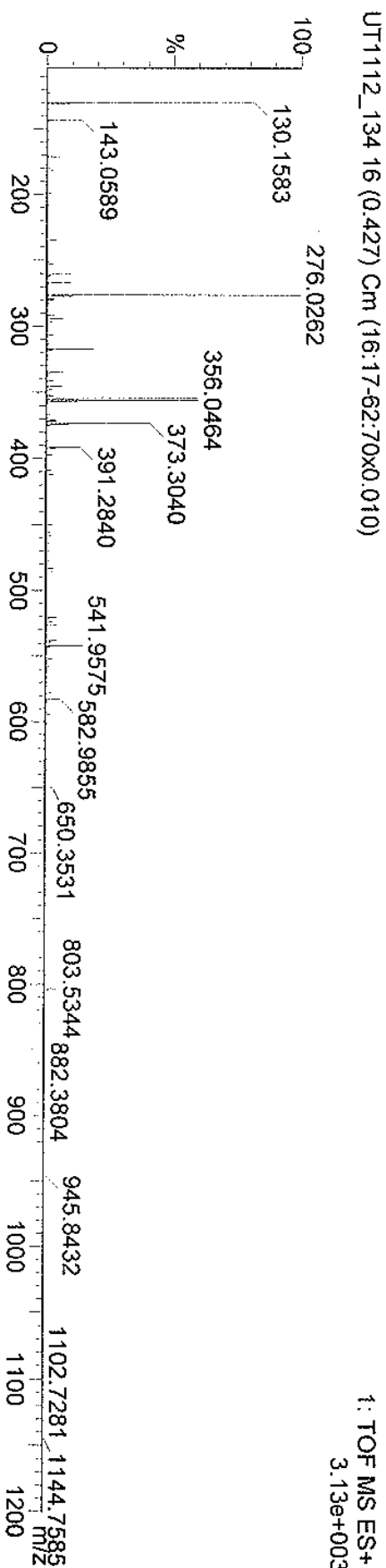
91 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-22 H: 0-22 N: 0-4 O: 0-5 Br: 0-1

A012/CCTP-1/018

UT1112_134 16 (0.427) Cm (16:17-62:70x0.010)

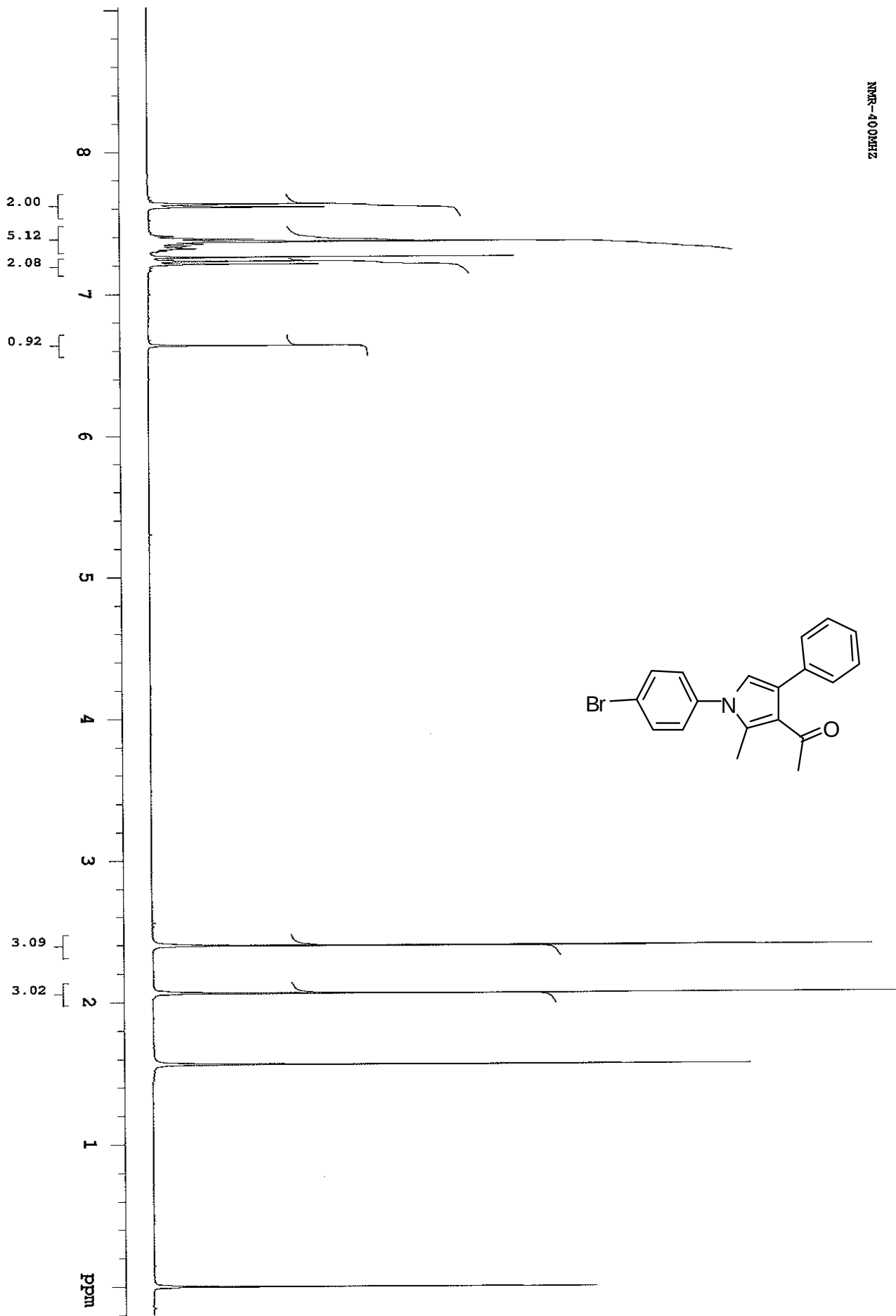


Minimum: 5.0
Maximum: 5.0

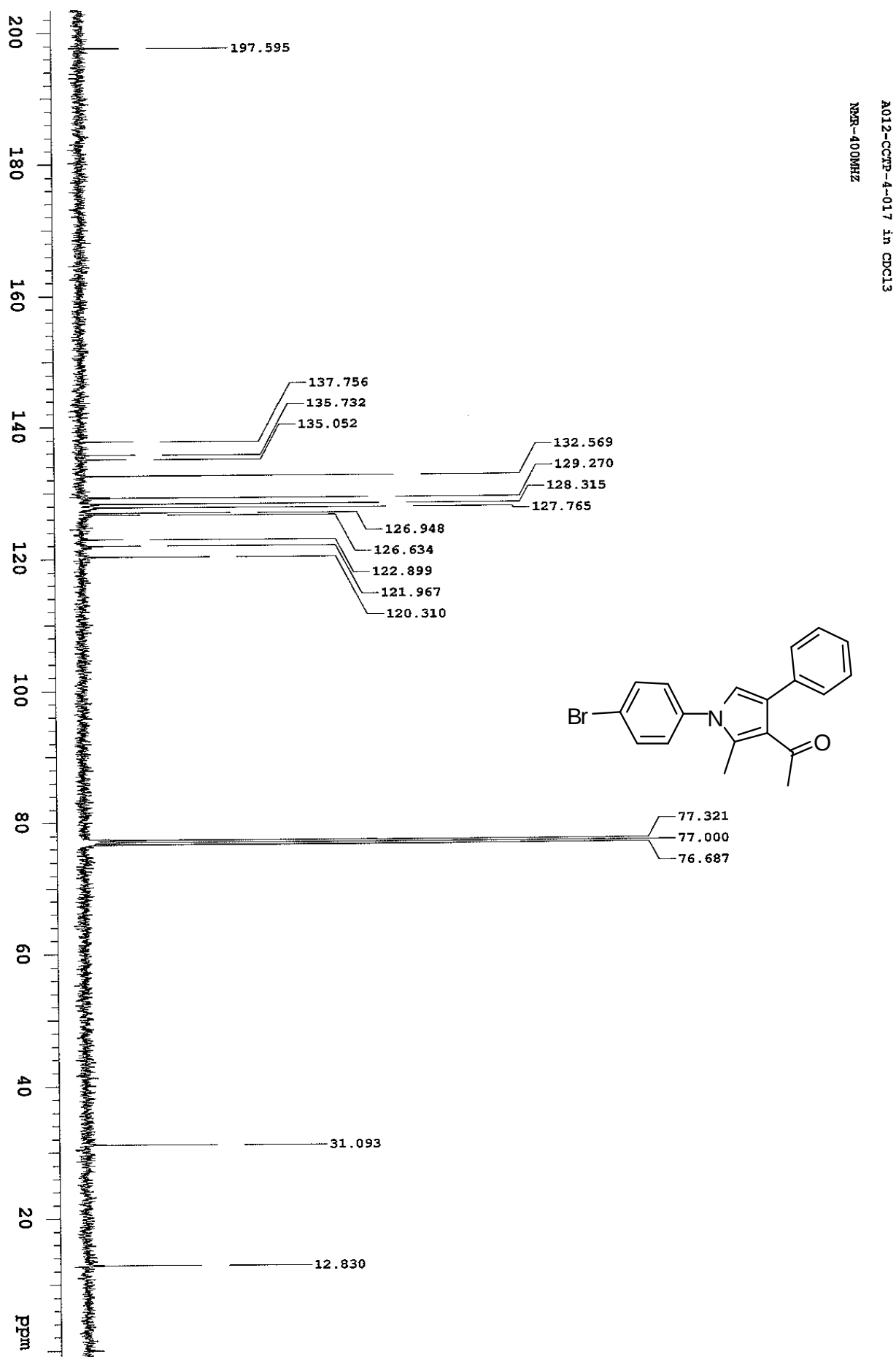
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
354.0484	354.0494	-1.0	-2.8	11.5	0.5	C19 H17 N O Br

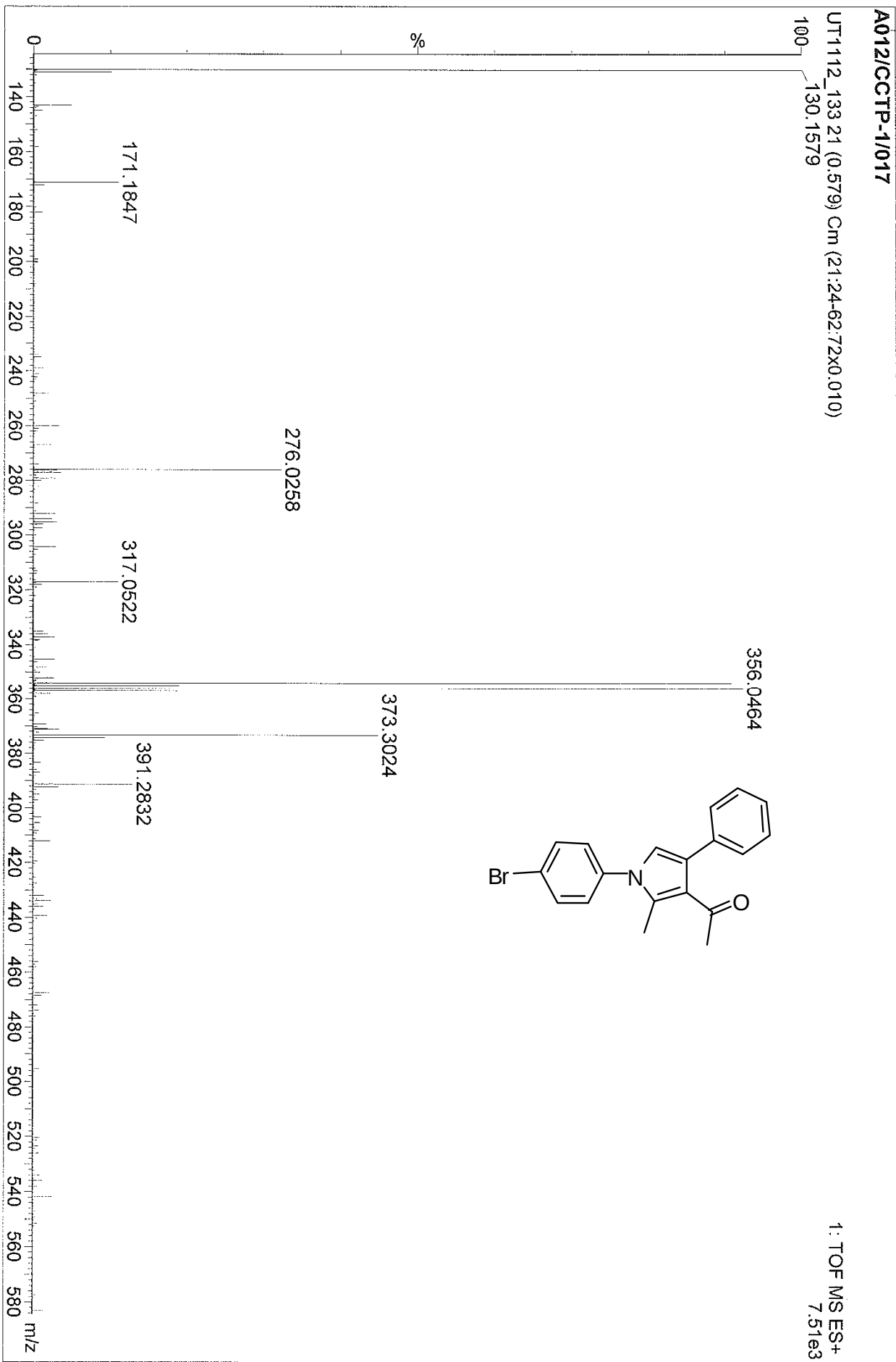
4d ¹H NMR (400 MHz, CDCl₃)

A012/CCTP4/017 in CDCl₃
NMR-400MHZ



4d ^{13}C NMR (100 MHz, CDCl_3)





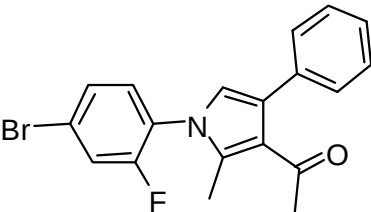
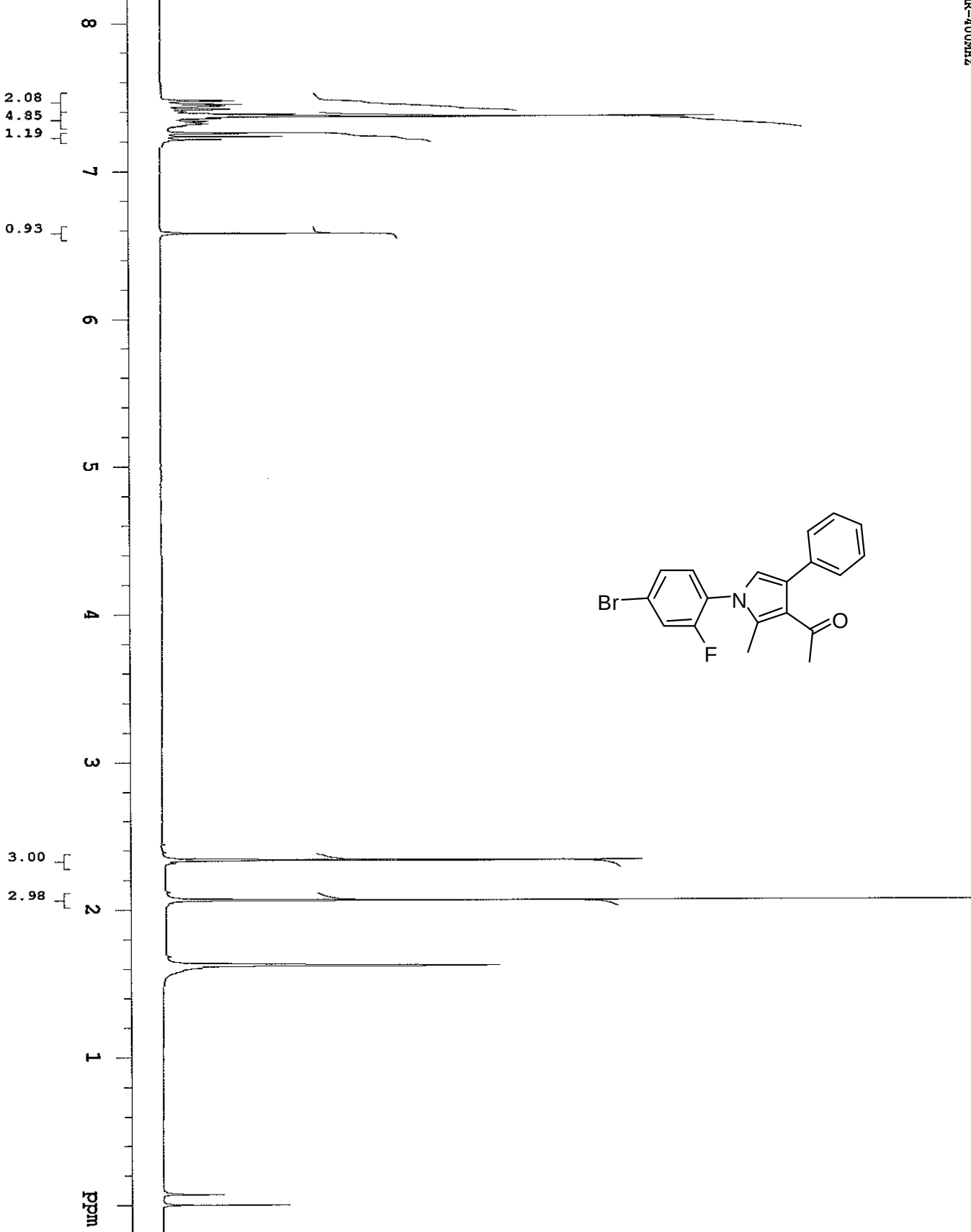
Mass spectrum of compound 10. The x-axis represents the mass-to-charge ratio (m/z) from 150 to 1200, and the y-axis represents the relative intensity in percent (%). The base peak is at m/z 356.0464. Other labeled peaks include:

m/z	Relative Intensity (%)
171.1847	~15
260.0477	~10
276.0258	~15
317.0522	~10
356.0464	100
373.3024	~15
391.2832	~10
433.9572	~10
541.9567	~10
582.9854	~10
684.6097	~10
752.4263	~10
803.5305	~10
861.7574	~10
900.7916	~10
1024.7203	~10
1102.7378	~10
1125.5229	~10

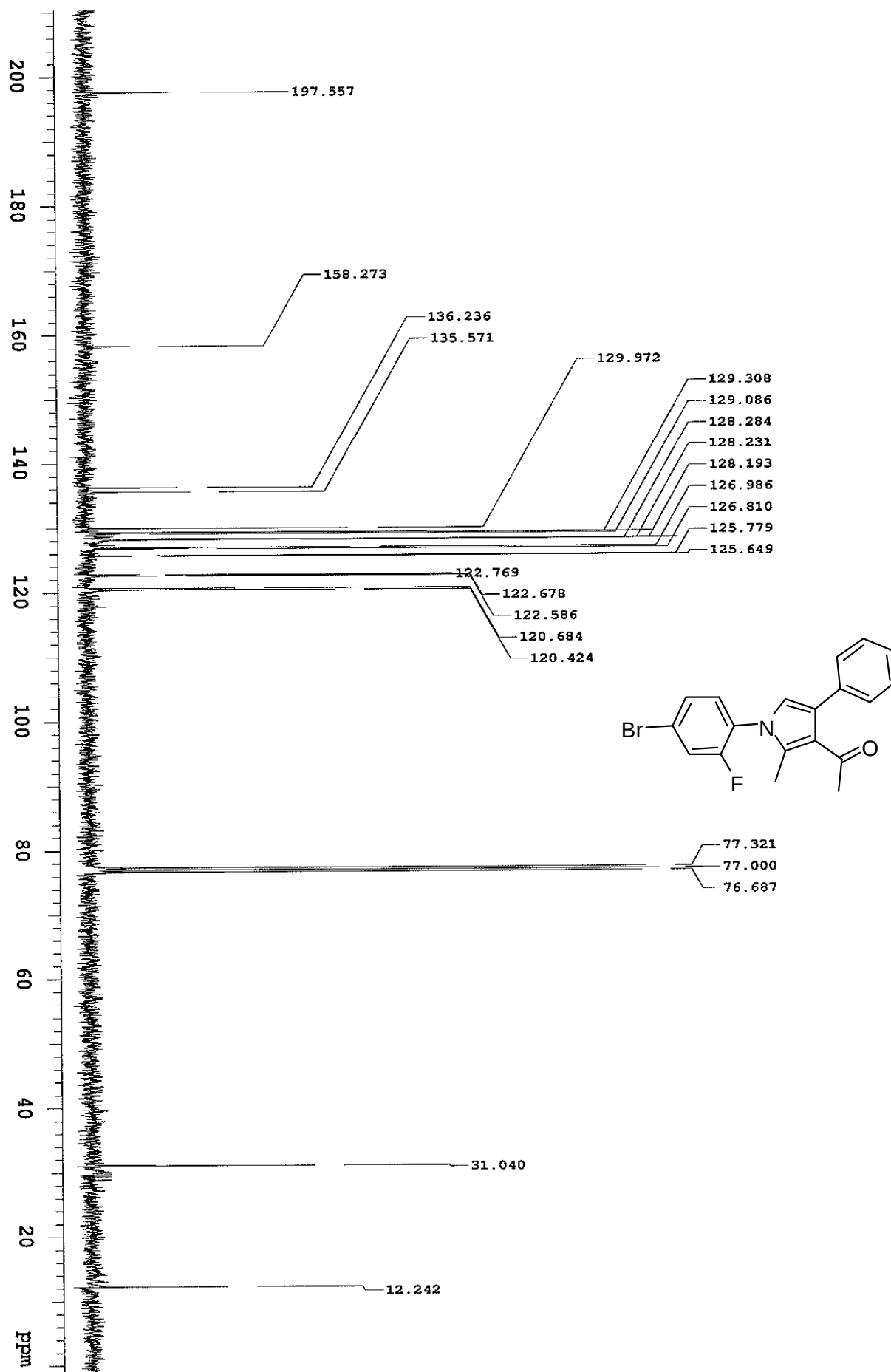
Minimum: Maximum:								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula		
354.0479	354.0494	-1.5	-4.2	11.5	2.6	C19 H17 N O Br		

4e ¹H NMR (400 MHz, CDCl₃)

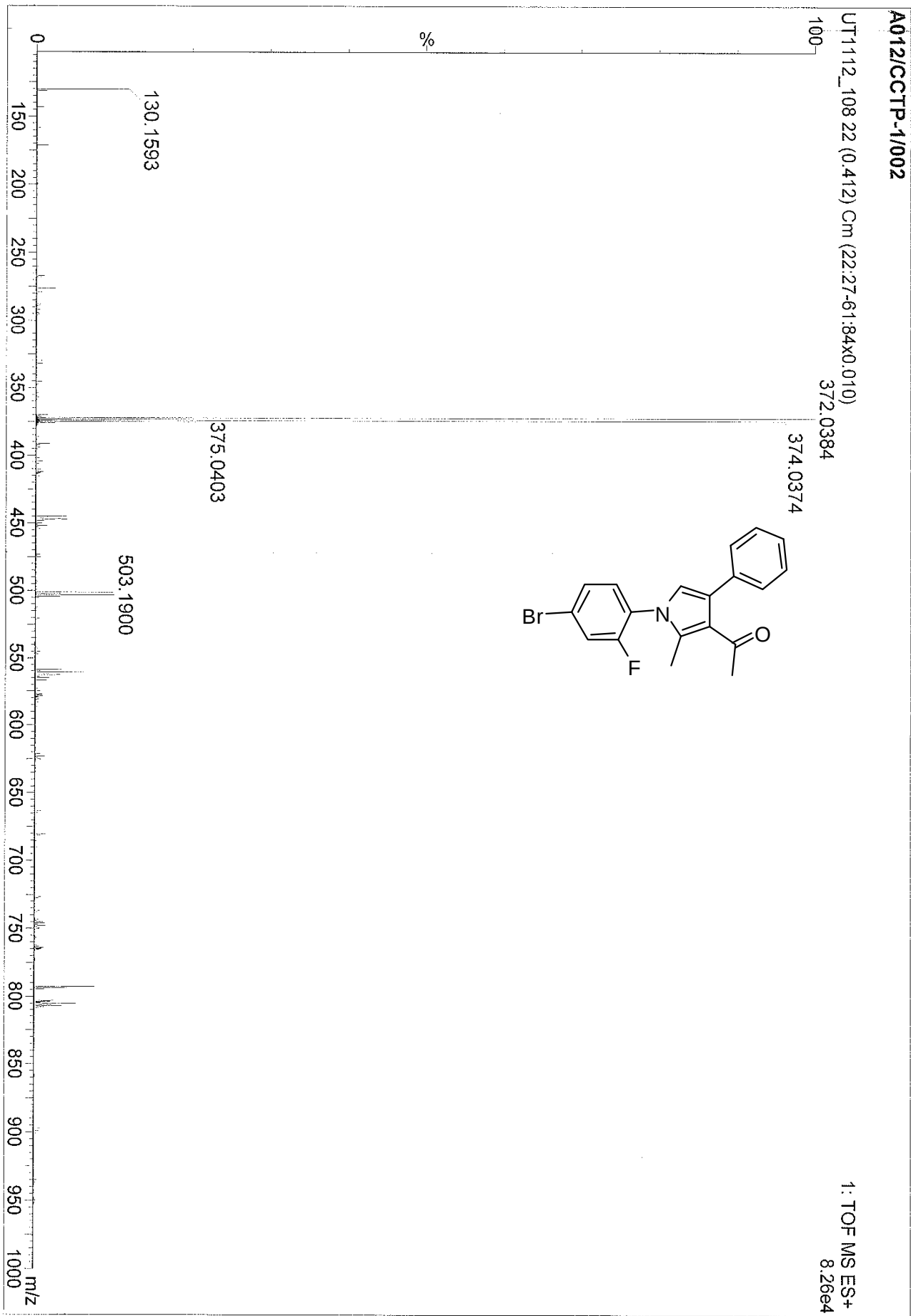
A012-CTP4-002 in CDCl₃
NMR-400MHz



4e ^{13}C NMR (100 MHz, CDCl_3)



4e HRMS



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

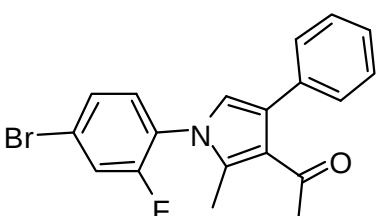
48 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

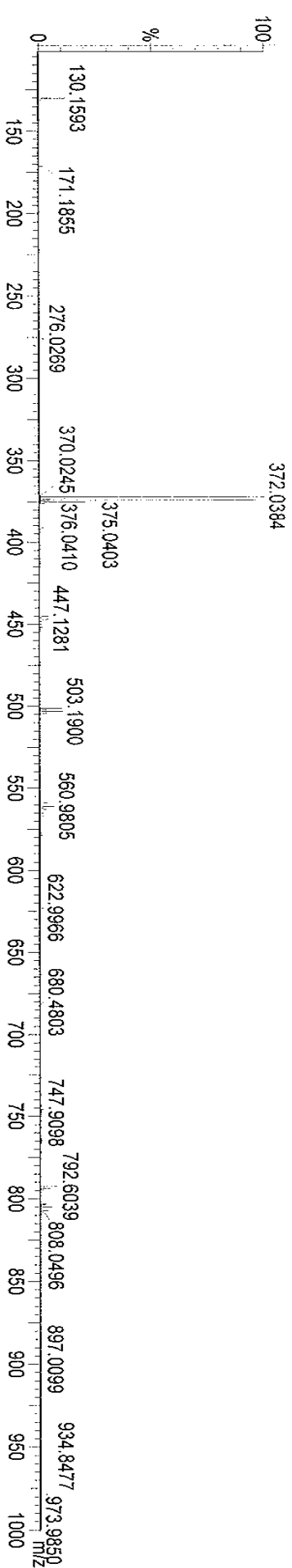
C: 0-20 H: 0-18 N: 0-2 O: 0-3 Br: 0-1 F: 0-1

A012CCTP-1/002

UT1112_108 22 (0.412) Cm (22.27-61.84x0.010)



1: TOF MS ES+
8.26e+004

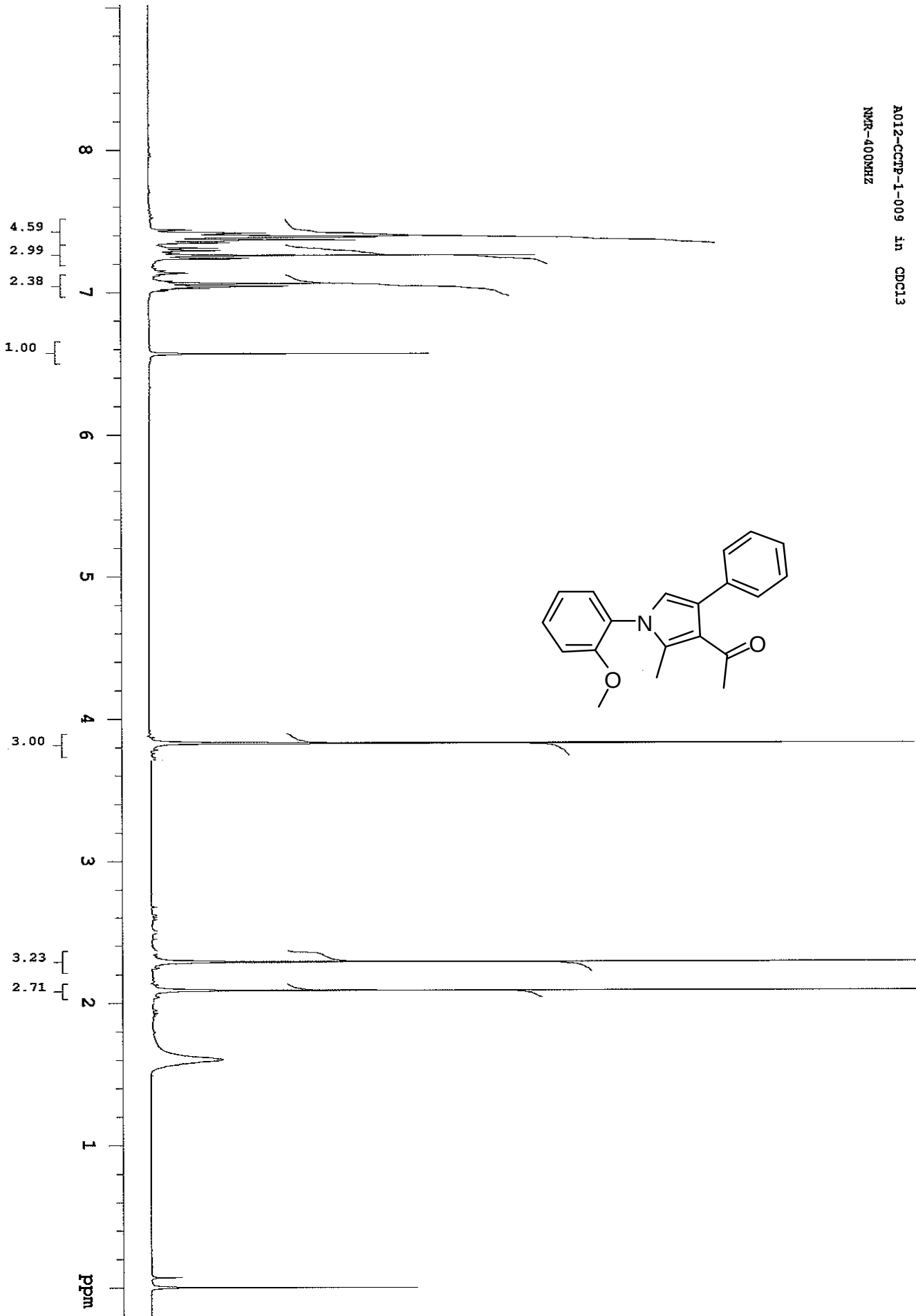


Minimum: -2.0
Maximum: 80.0

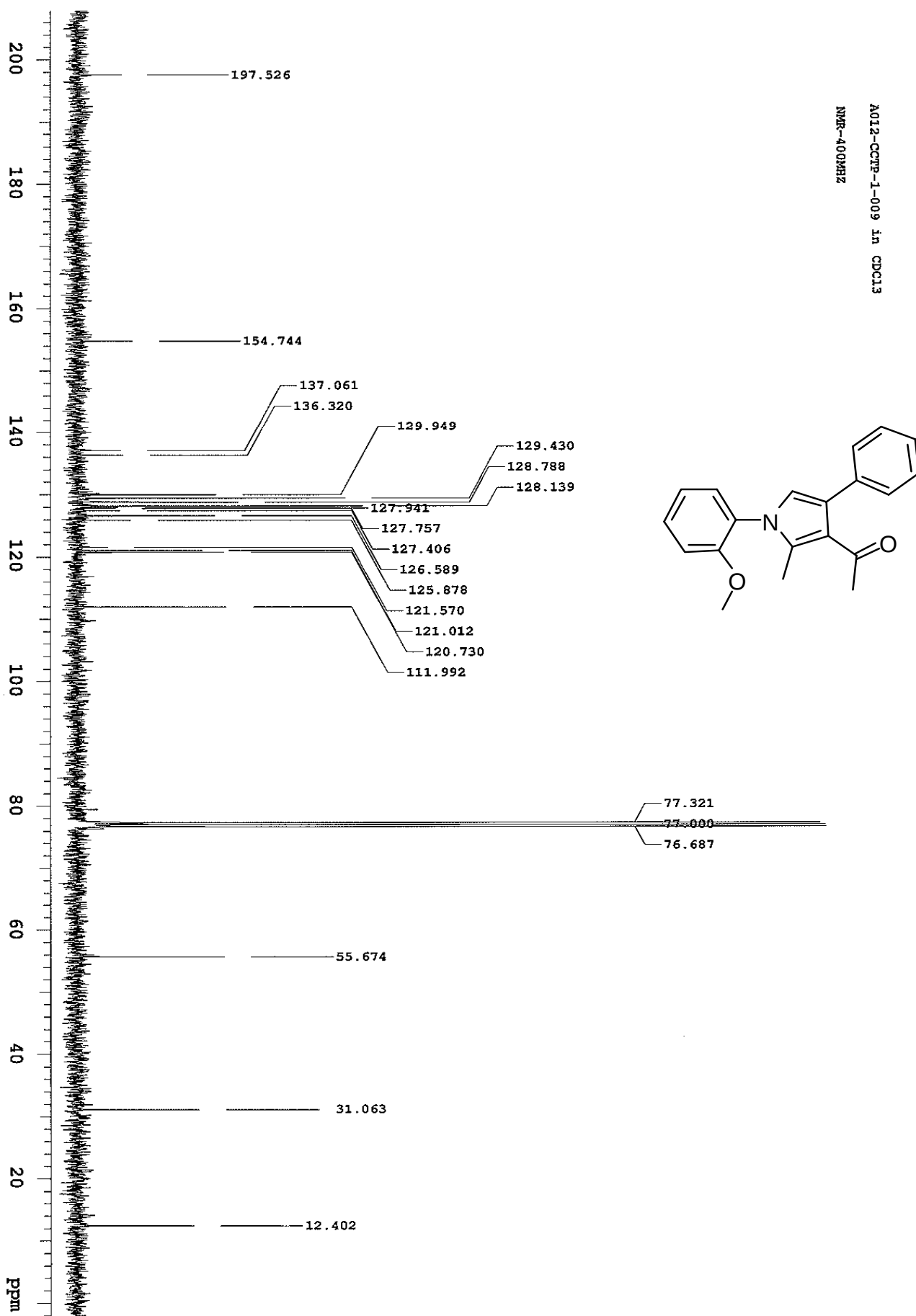
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
372.0384	372.0399	-1.5	-4.0	11.5	8.3	C19 H16 N O Br F

4f ¹H NMR (400 MHz, CDCl₃)

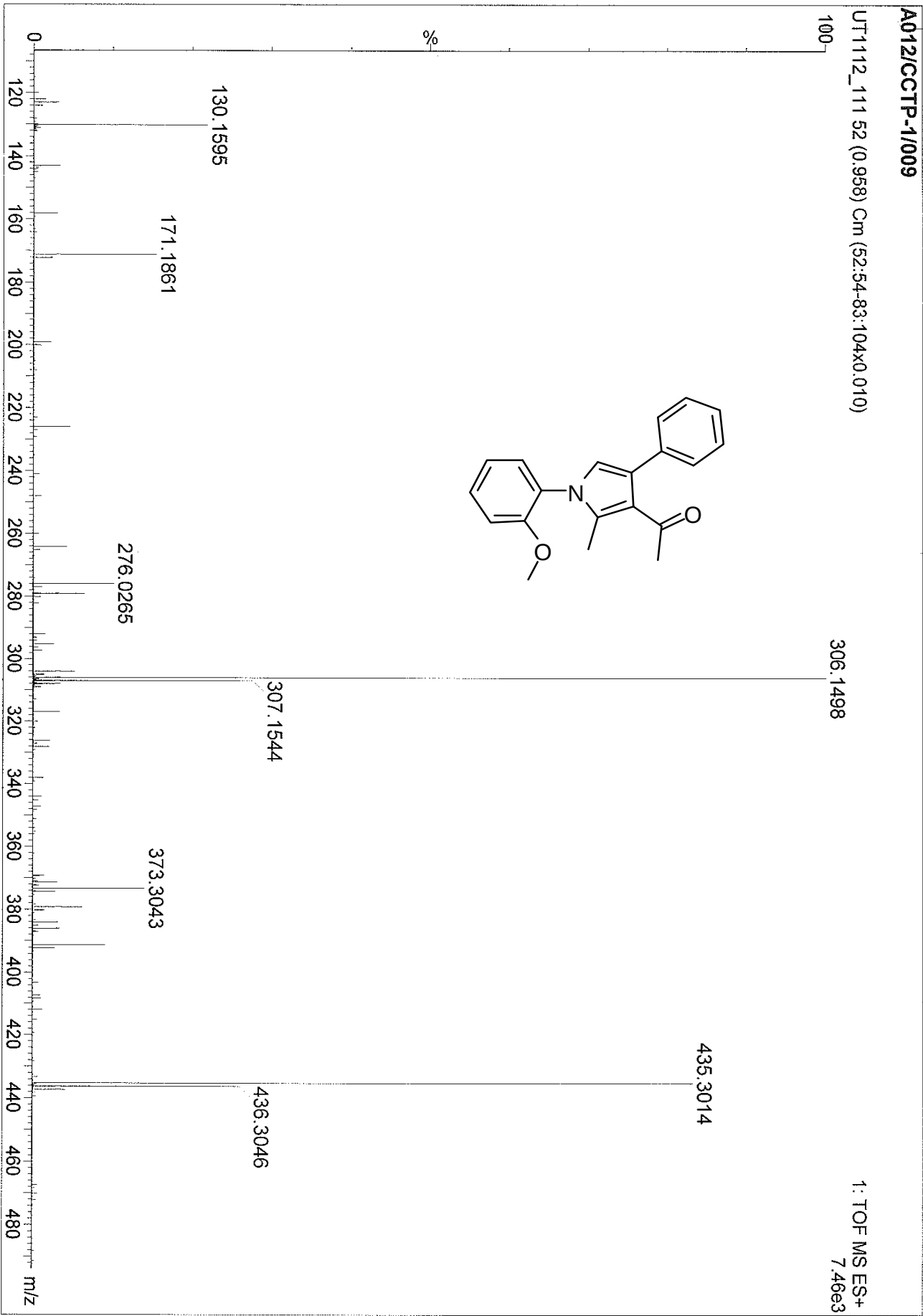
A012-CCTP-1-009 in CDCl₃
NMR-400MHz



4f ^{13}C NMR (100 MHz, CDCl_3)



4f HRMS



Elemental Composition Report

Single Mass Analysis

Tolerance = 30.0 PPM / DBE: min = -2.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FTT = 2

Monoisotopic Mass, Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

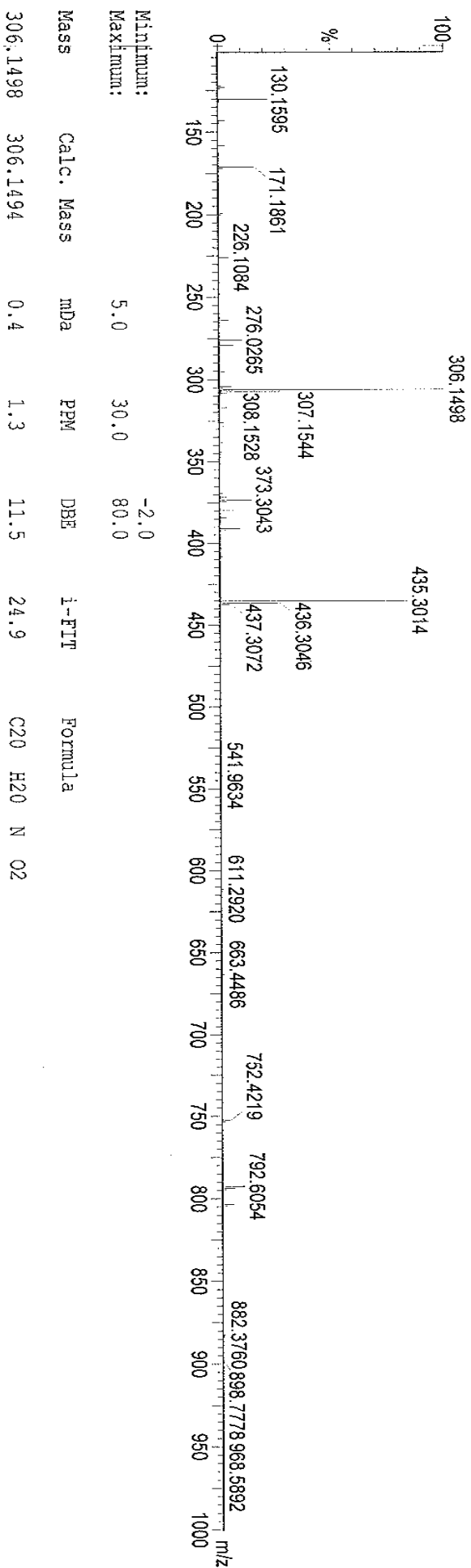
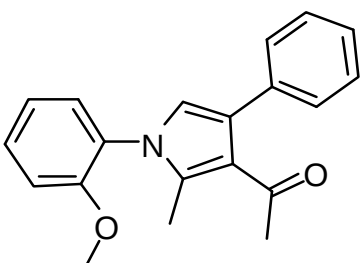
Elements Used:

C: 0-25 H: 0-23 N: 0-2 O: 0-2

A012/CCTP-1/009

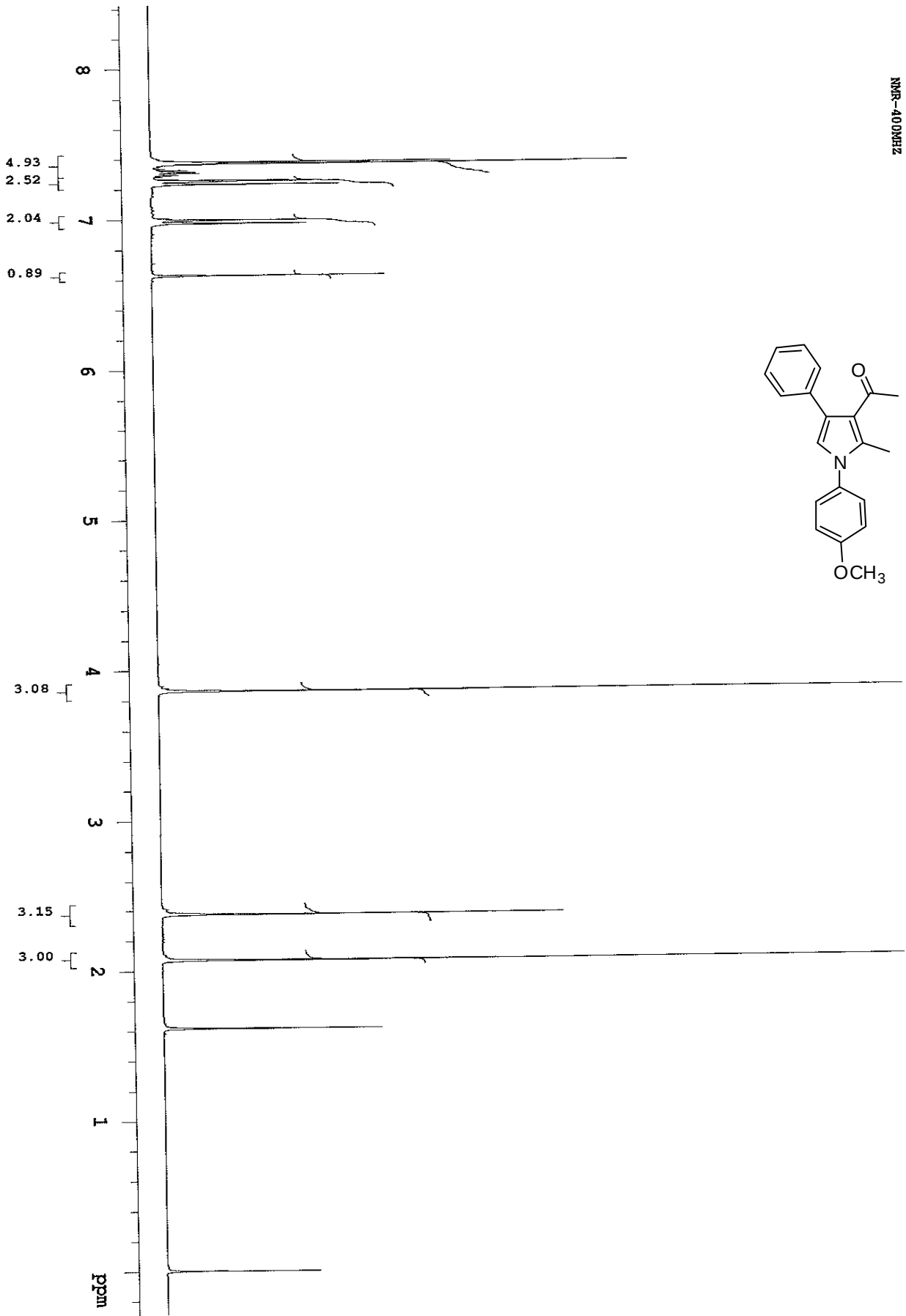
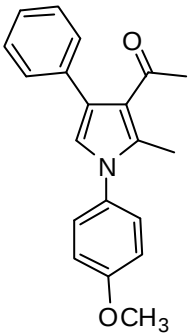
UT1112_111 52 (0.958) Cm (52:54:83:104x0.010)

1: TOF MS ES+
7.46e+003

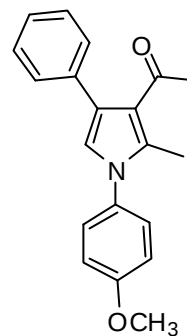
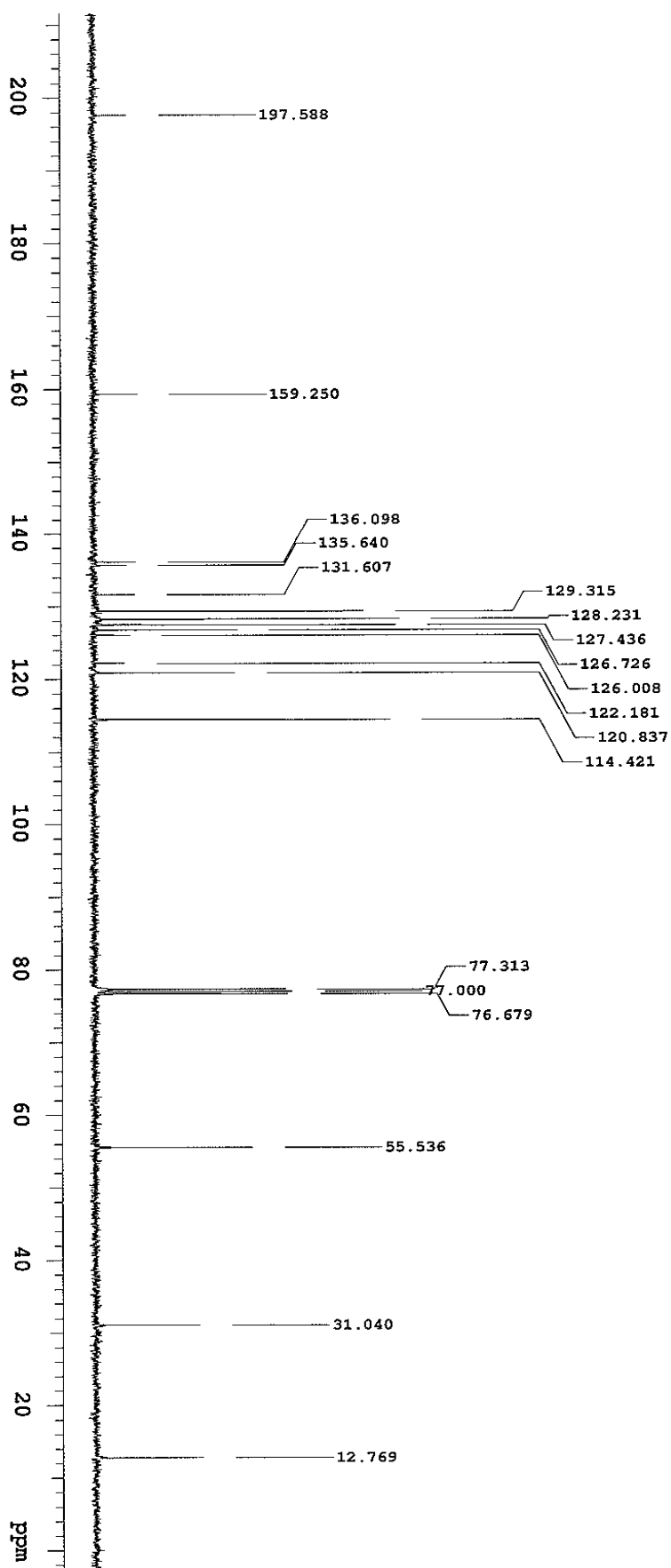


4g ¹H NMR (400 MHz, CDCl₃)

A012/CCP-1/015 in CDCl₃
NMR-400MHz

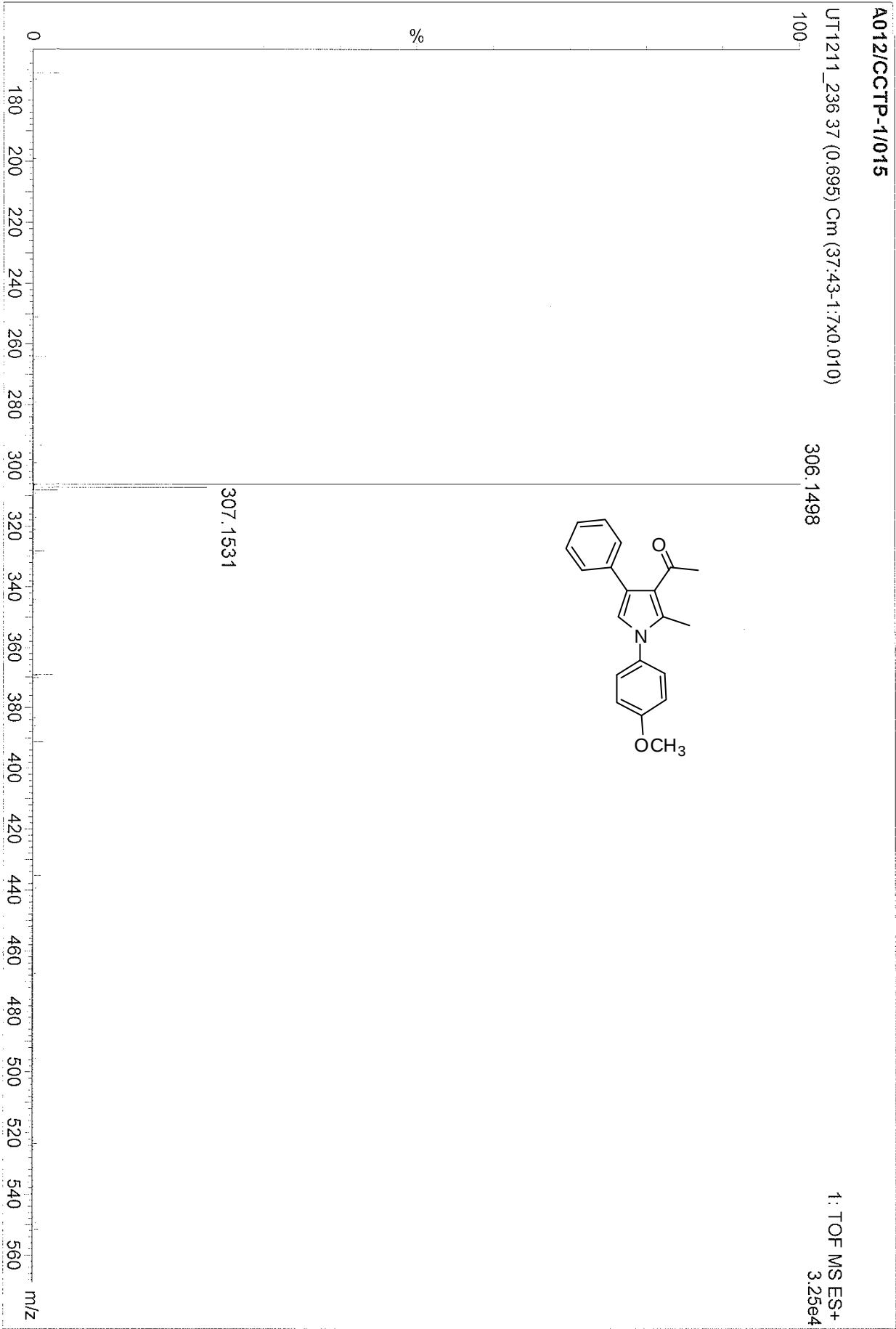


4g ^{13}C NMR (100 MHz, CDCl_3)



A012-CTFP-1-015 in CDCl_3
NMR-400MHz

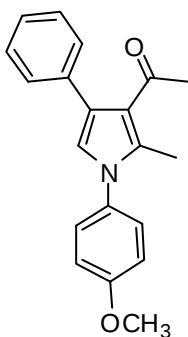
4g HRMS



Single Mass Analysis

Element prediction: Off

Number of isotope peaks used for i-FT = 3



Monoisotopic Mass, Even Electron Ions

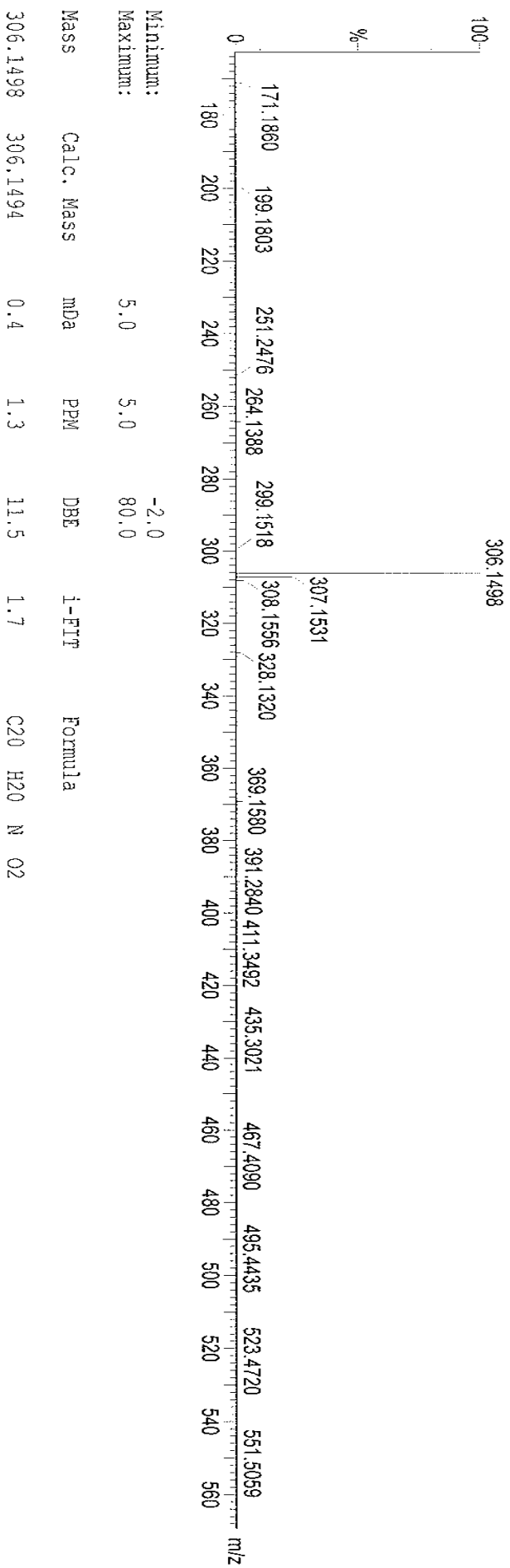
13 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

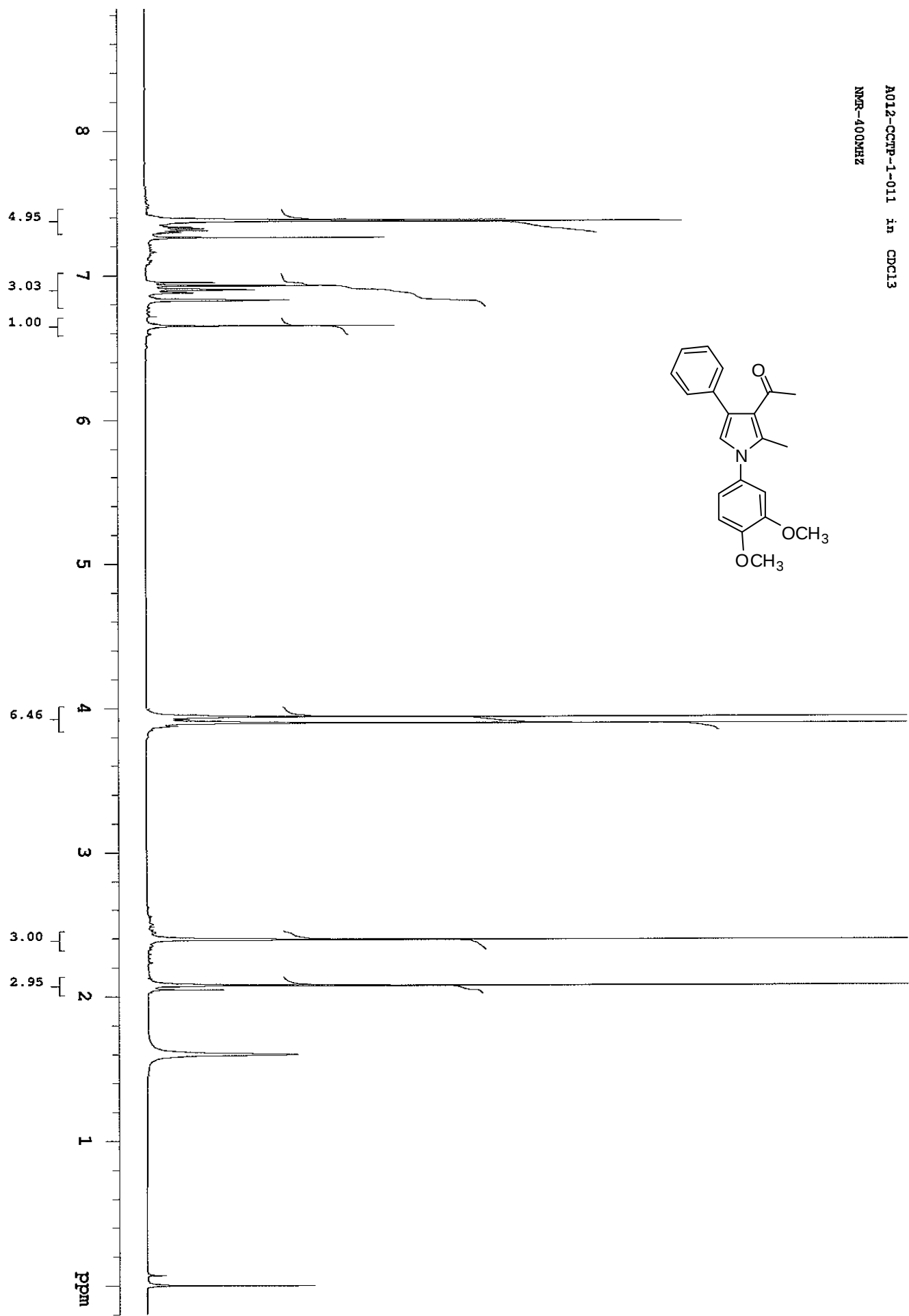
C: 0-25 H: 0-25 N: 0-1 O: 0-2

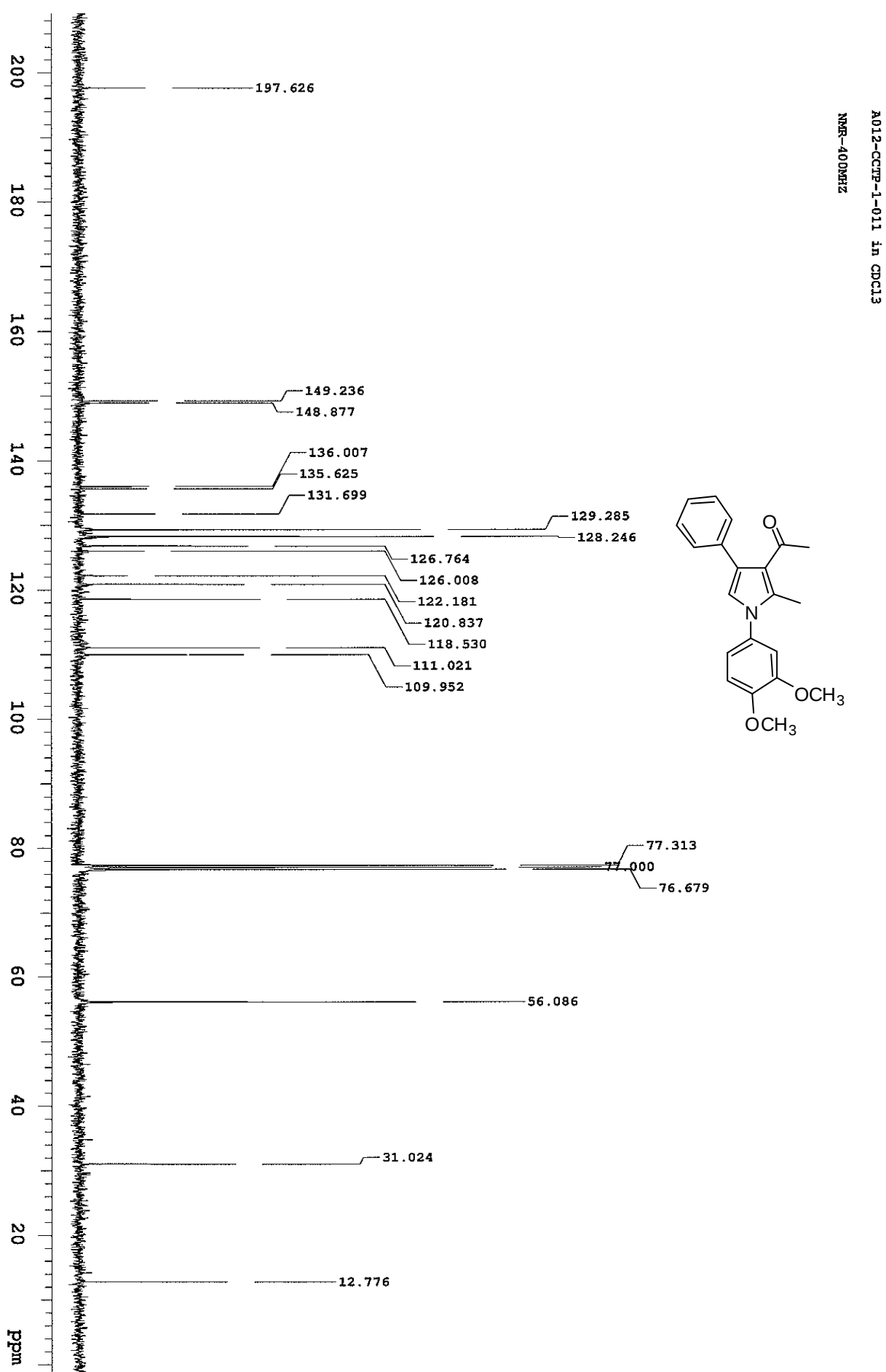
A012/CCTP-1/015

UT1211_236 37 (0.695) Cm (37:43-1:7x0.010)

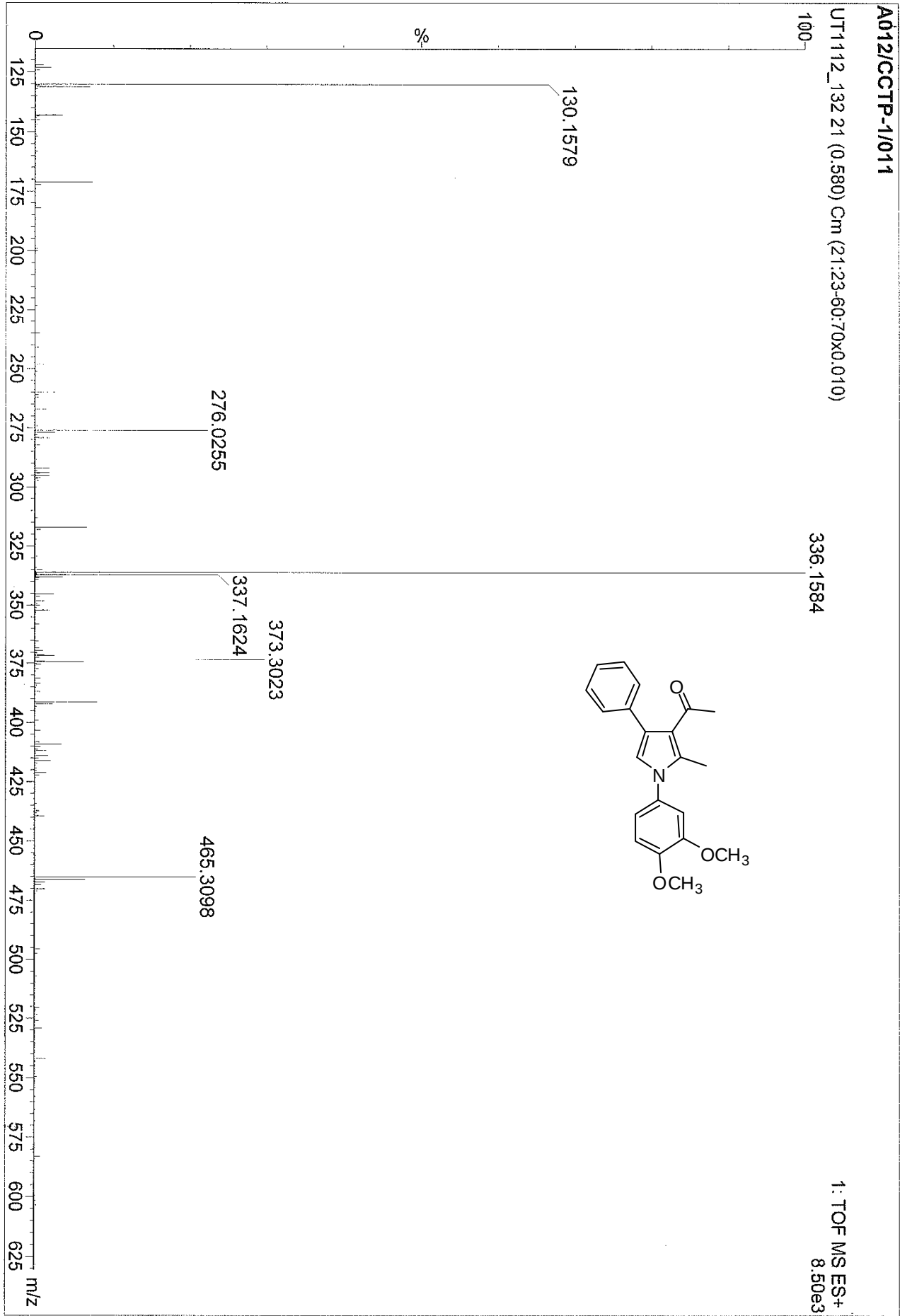
1: TOF MS ES+
3.25e+004

4h ^1H NMR (400 MHz, CDCl_3)





4h HRMS

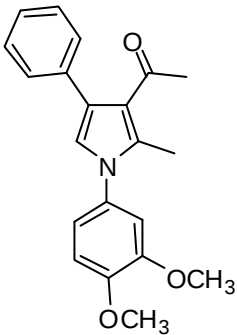


4h HRMS

Elemental Composition Report

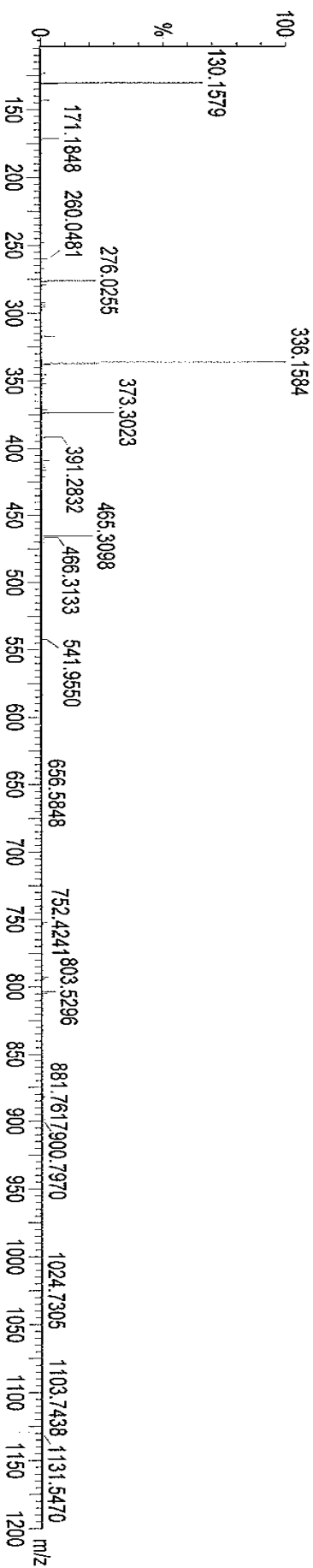
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -2.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions
38 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-22 N: 0-4 O: 0-5
A012/CCTP-1/011

UT1112_132.21 (0.580) Cm (21:23-60:70x0.010)

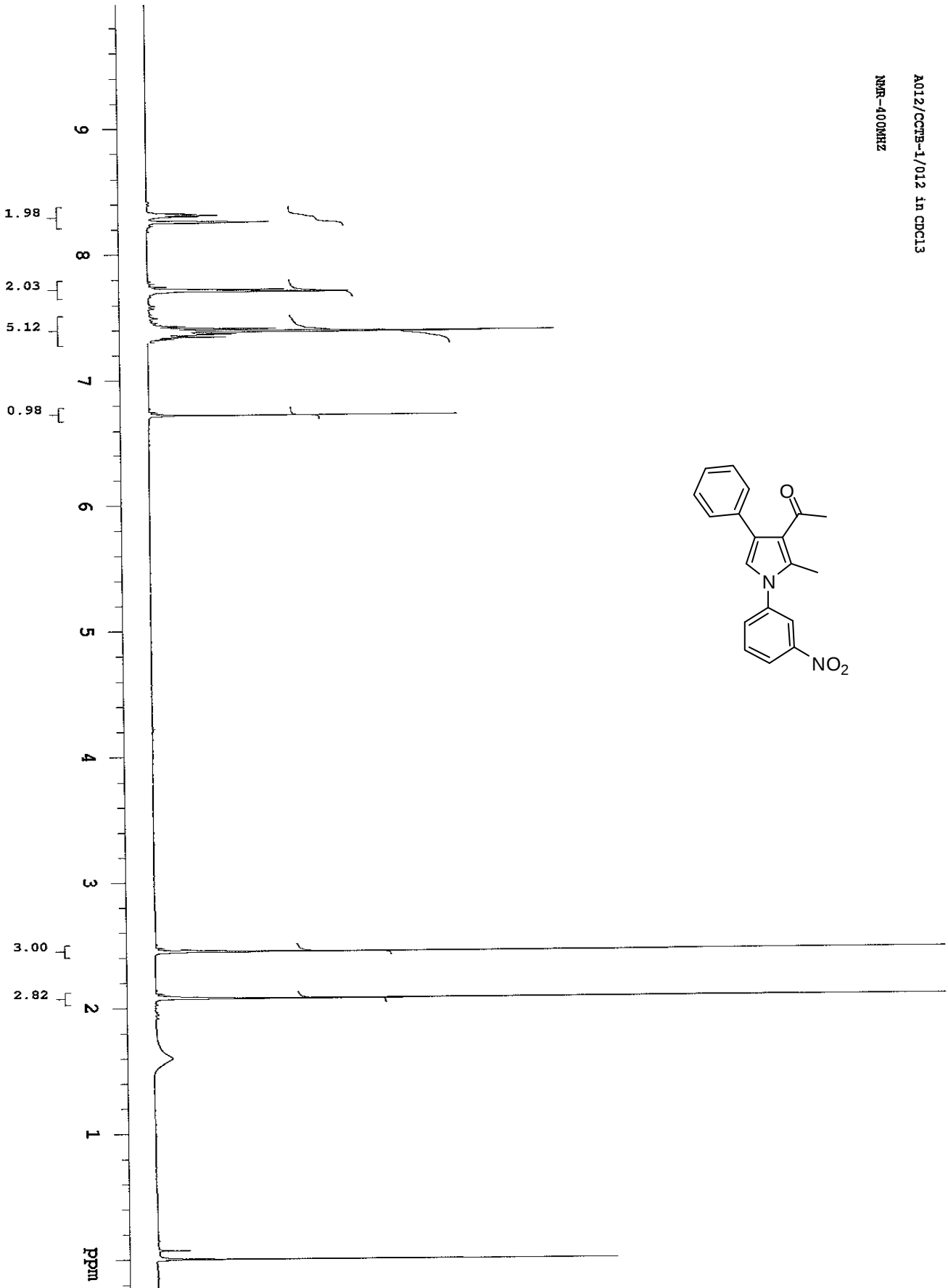


1: TOF MS ES+
8.50e+003

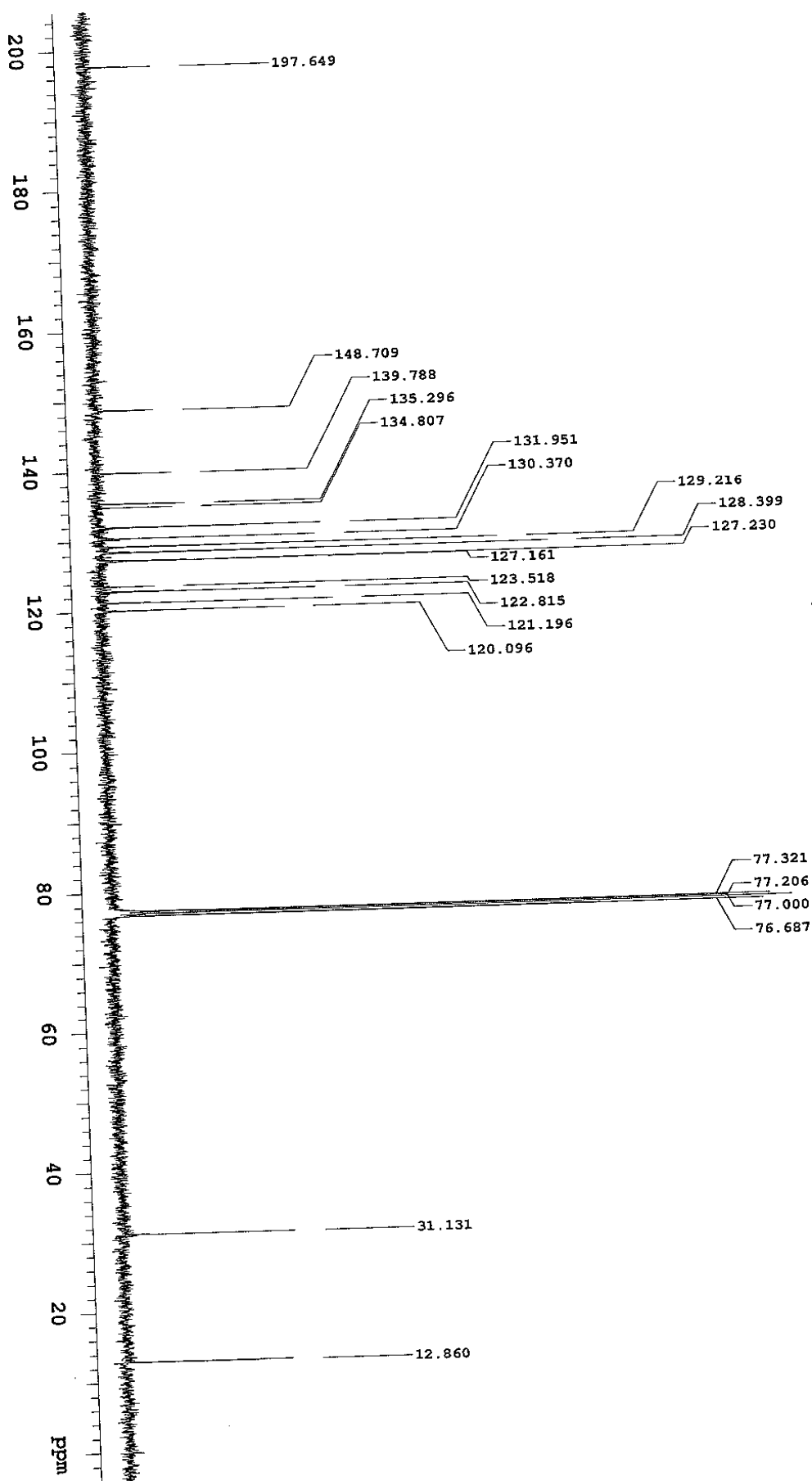
Minimum:						
Maximum:						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
336.1584	336.1600	-1.6	-4.8	11.5	1.4	C21 H22 N O3

4i ¹H NMR (400 MHz, CDCl₃)

A012/CCTB-1/012 in CDCl₃
NMR-400MHZ

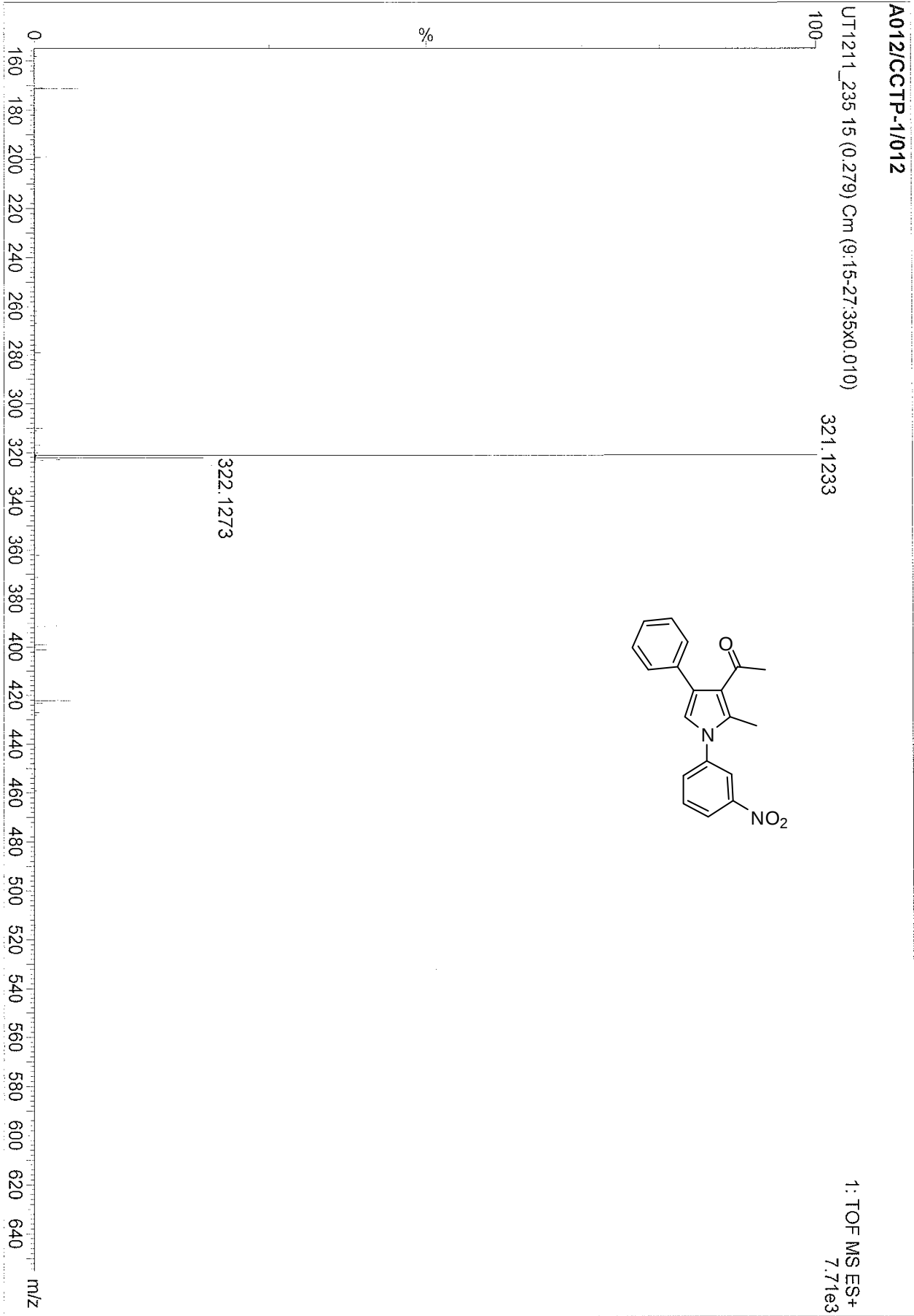


4i ^{13}C NMR (100 MHz, CDCl_3)



A012-CCTP-1-012 in CDCl_3
NMR-400MHz

4i HRMS



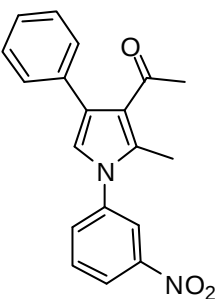
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -2.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FTT = 3



Monoisotopic Mass, Even Electron Ions

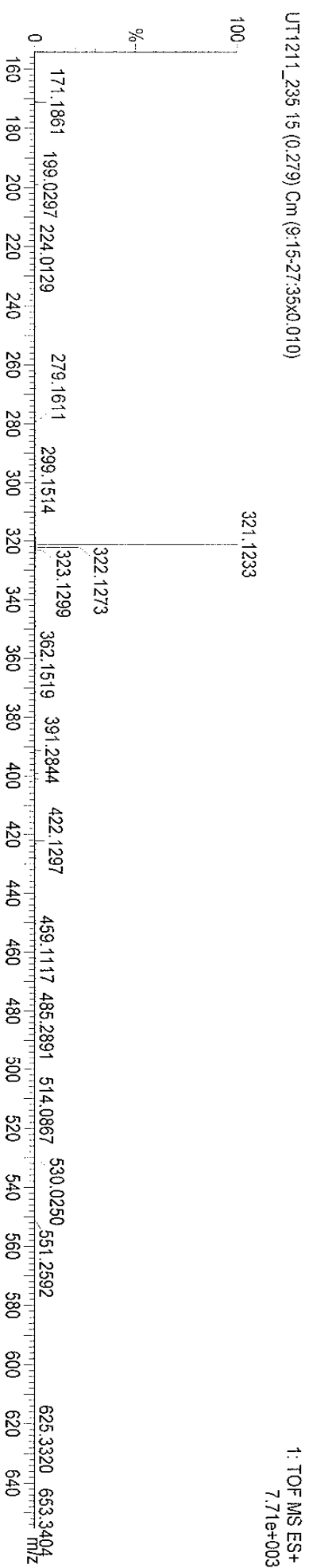
35 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-3

A012/CCTP-1/012

UT1211_235 15 (0.279) Cm (9:15-27:35x0.010)

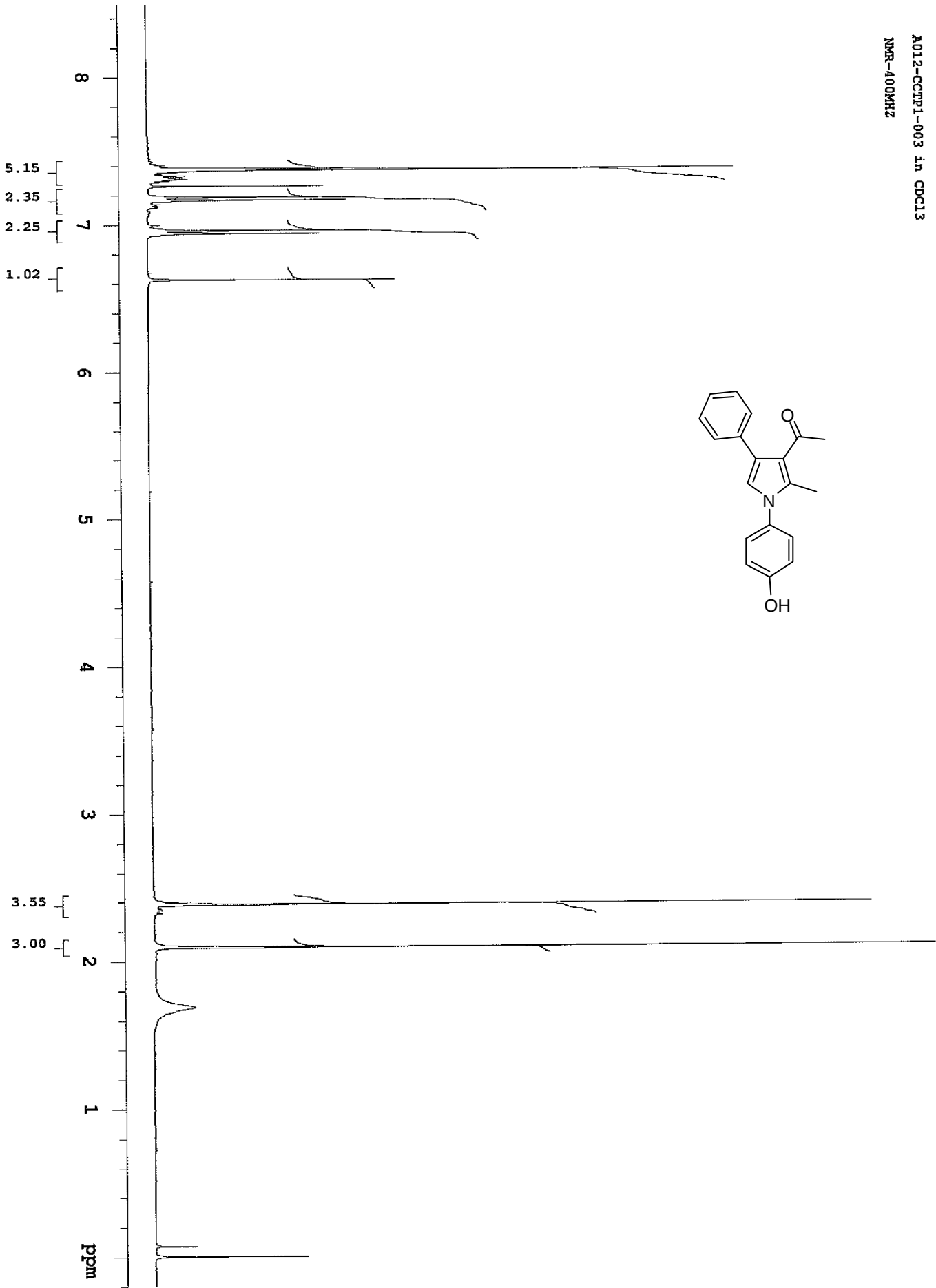


Minimum: 5.0
Maximum: 5.0
-2.0
80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FTT	Formula
321.1233	321.1239	-0.6	-1.9	12.5	1.3	C19 H17 N2 O3

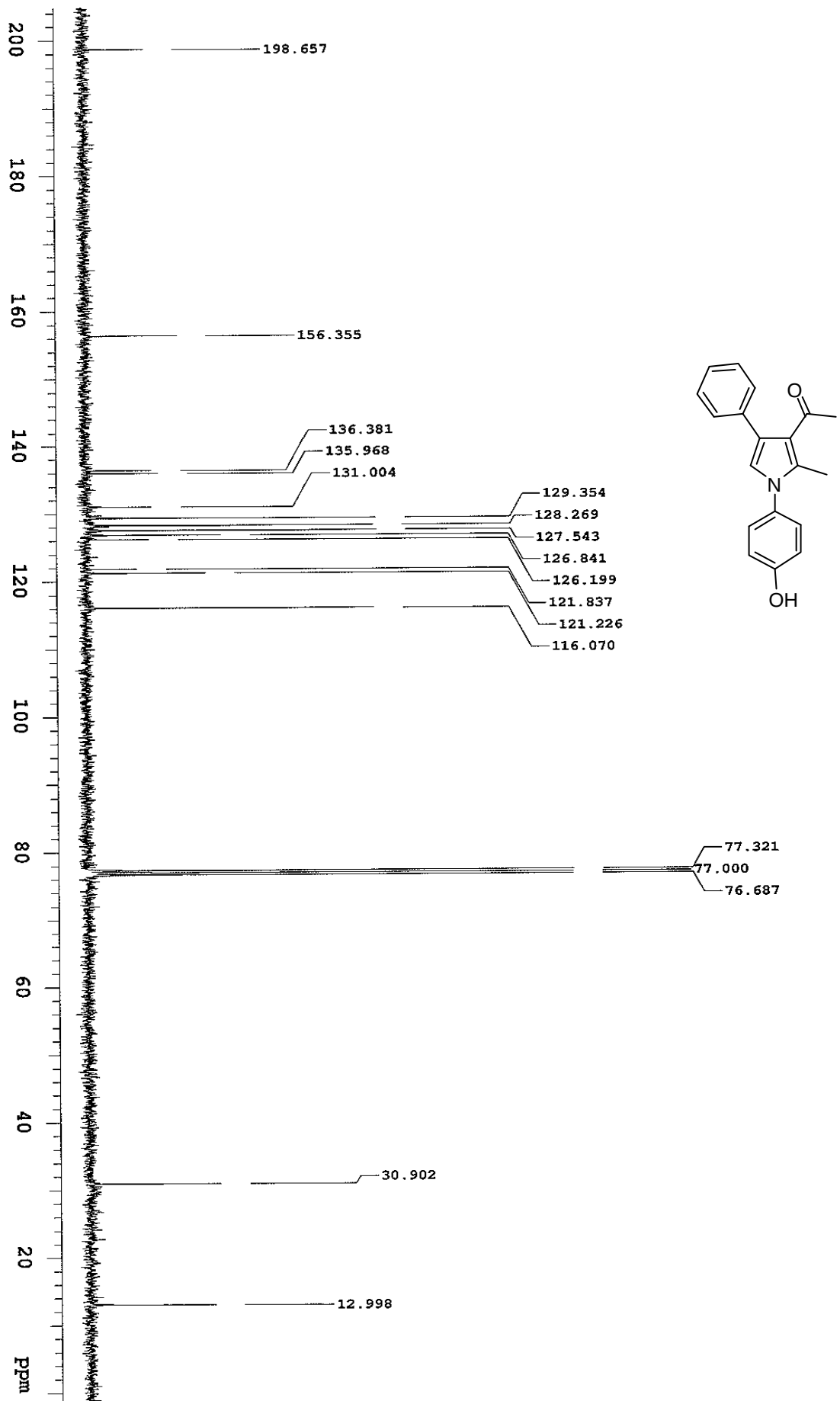
4j ¹H NMR (400 MHz, CDCl₃)

A012-CCTP1-003 in CDCl₃
NMR-400MHZ

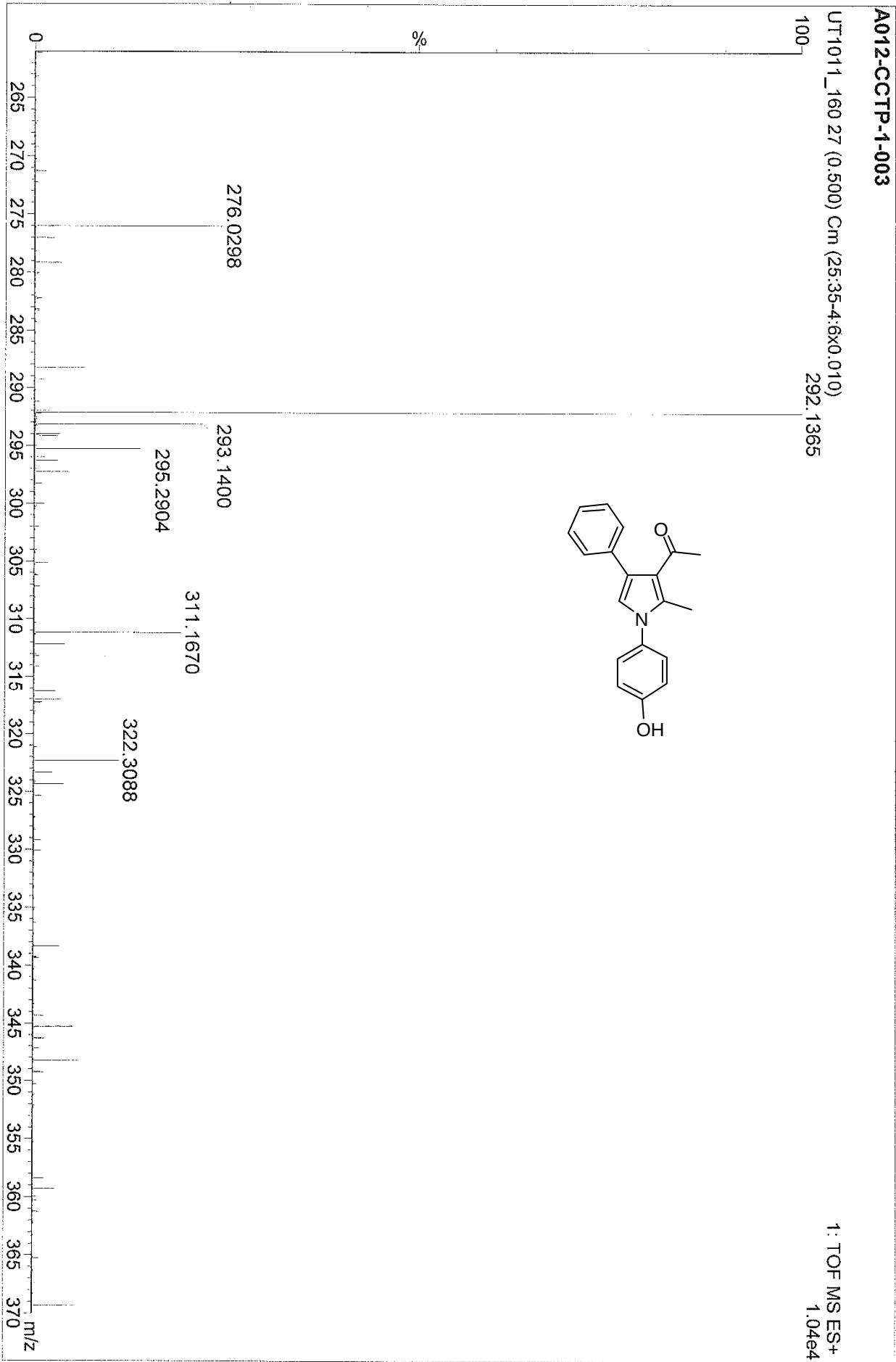


4j ¹³C NMR (100 MHz, CDCl₃)

A012-CTP1-003 in CDCl₃
NMR-400MHZ



4j HRMS



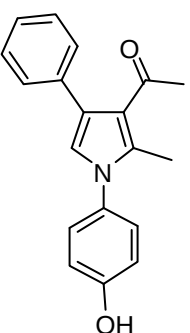
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.0, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4



Monoisotopic Mass, Even Electron Ions

4 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)

Elements Used:

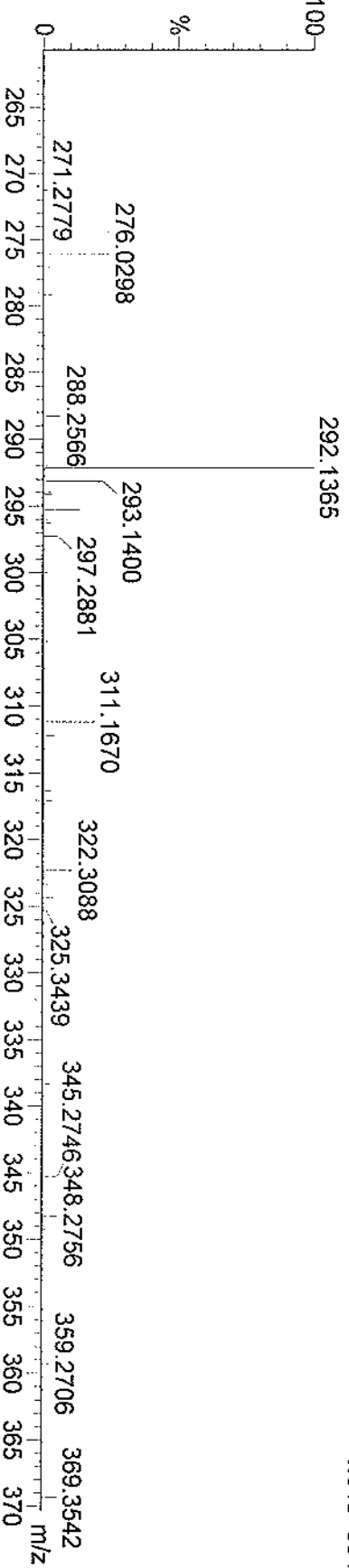
C: 0-20 H: 0-20 N: 0-1 O: 0-2

A012-CCTP-1-003

UT1011_160 27 (0.500) Cm (25:35-4:6x0.010)

1: TOF MS ES+
1.04e+004

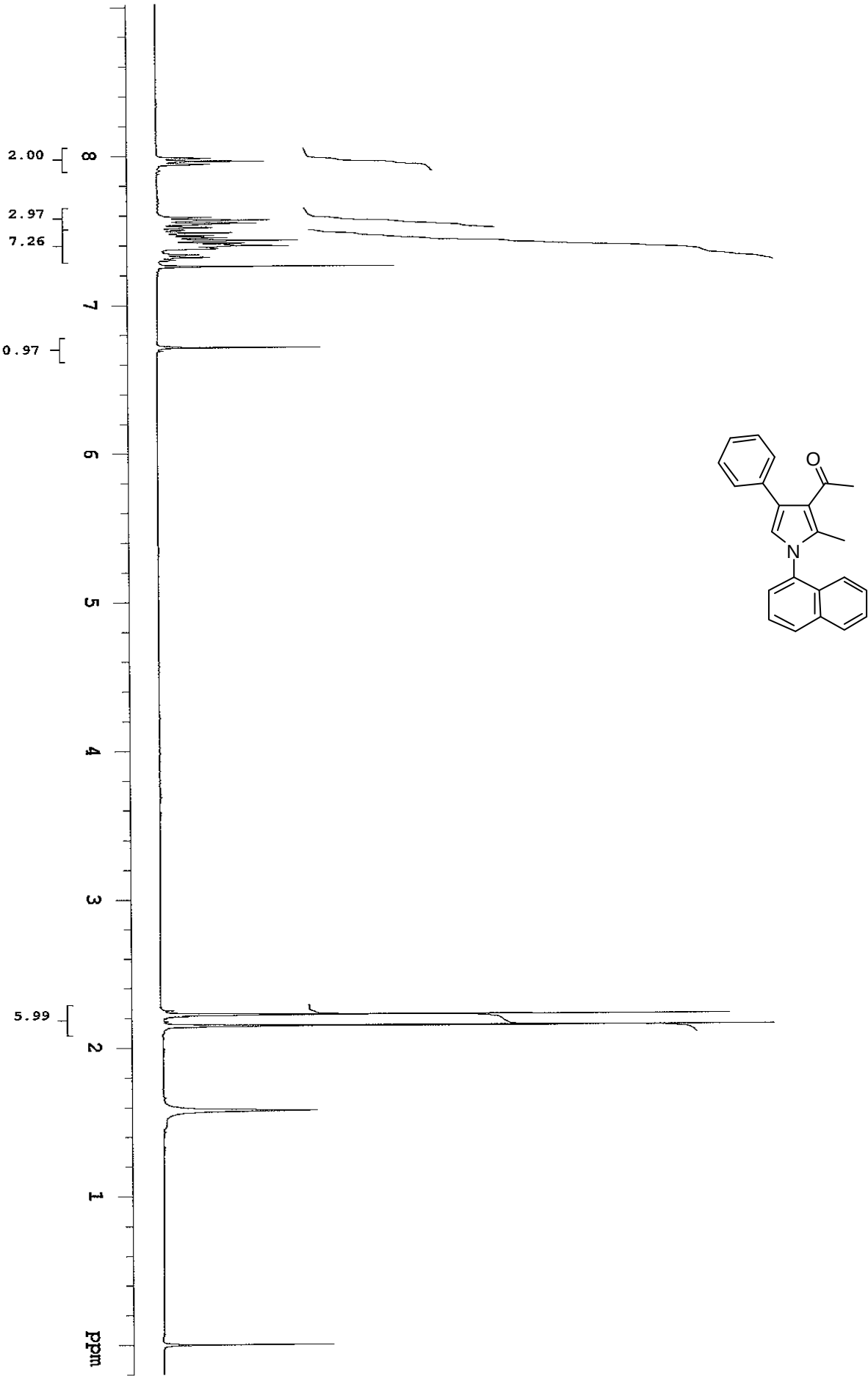
4j HRMS



Minimum: 0.0
Maximum: 50.0

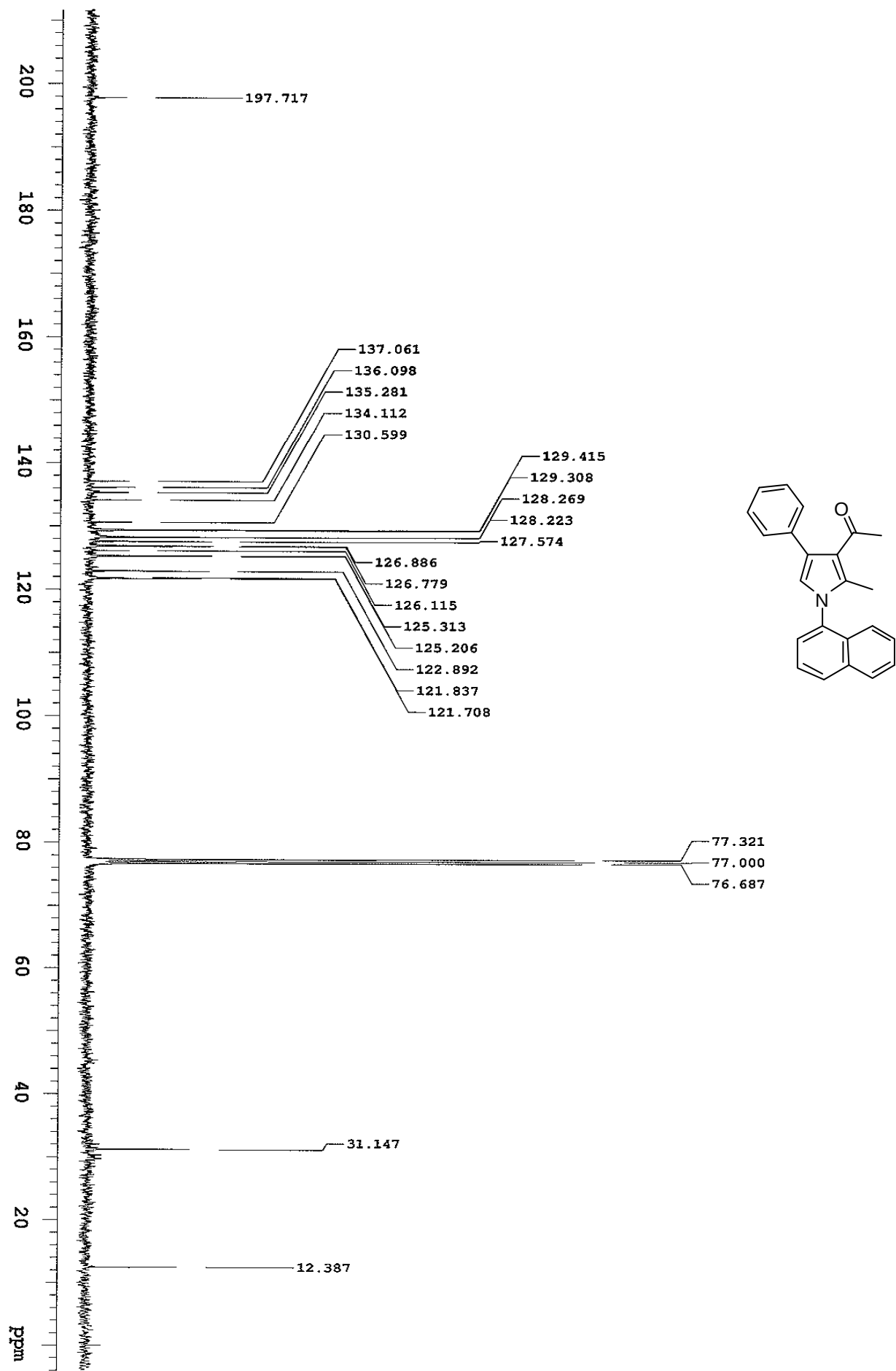
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
292.1365	292.1338	2.7	9.2	11.5	7.4	C19 H18 N O2

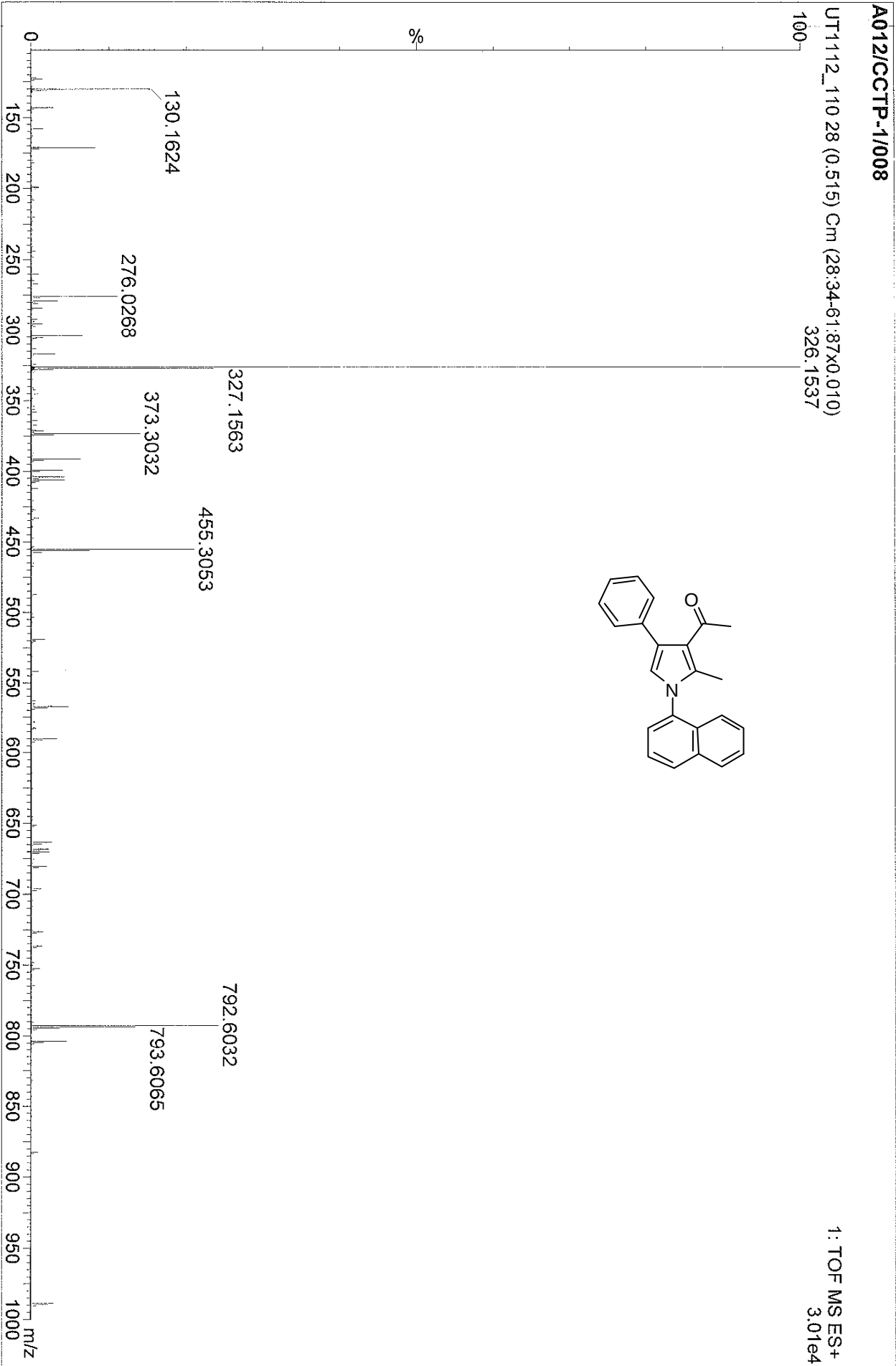
4k ¹H NMR (400 MHz, CDCl₃)



A012-CCTP-1-008 in CDCl₃
NMR-400MHz

4k ¹³C NMR (100 MHz, CDCl₃)





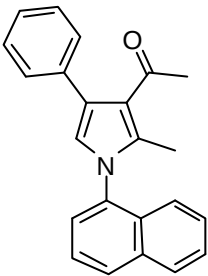
Elemental Composition Report

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
15 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

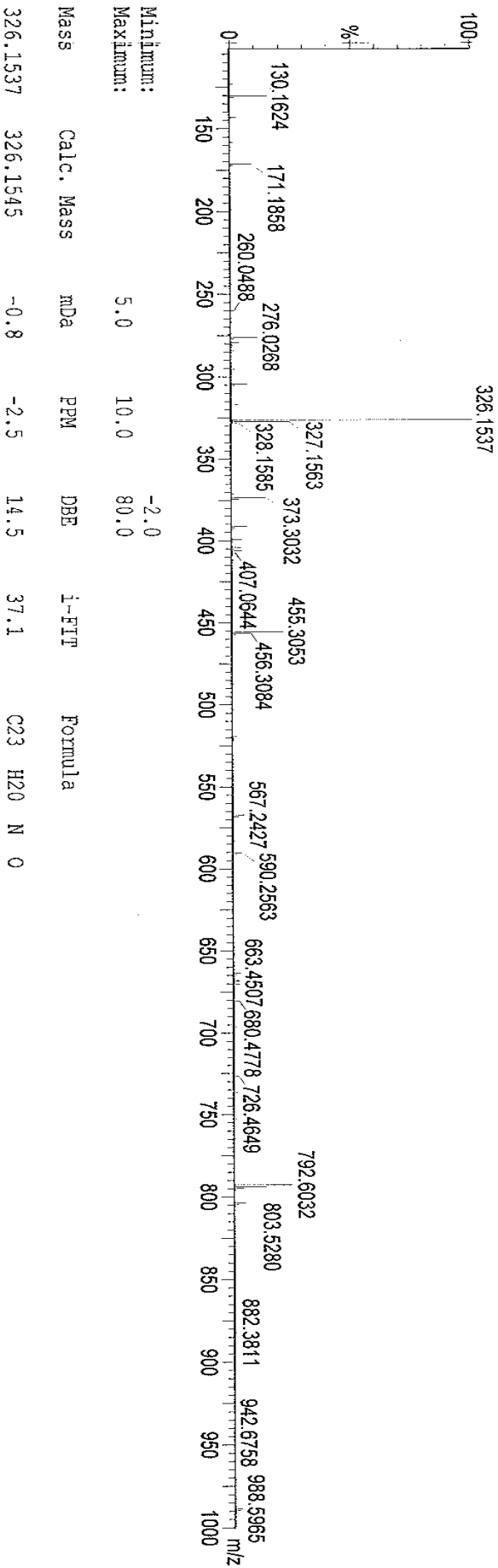
Elements Used:

C: 0-25 H: 0-23 N: 0-2 O: 0-2

A012CCTP-1/008

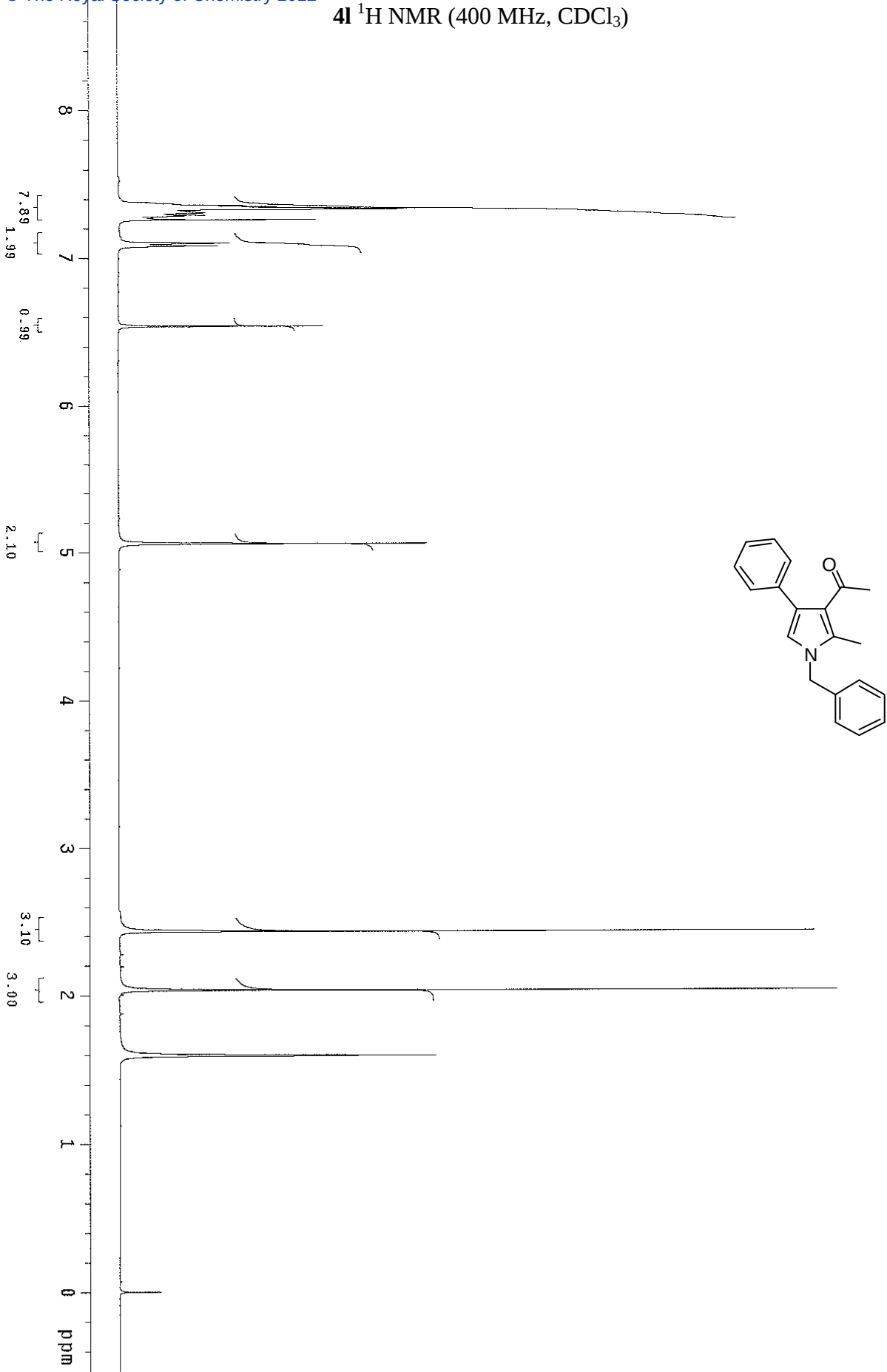
UT1112_110 28 (0.515) Cm (28.34-61.87x0.010)

1: TOF MS ES+
3.01e+004

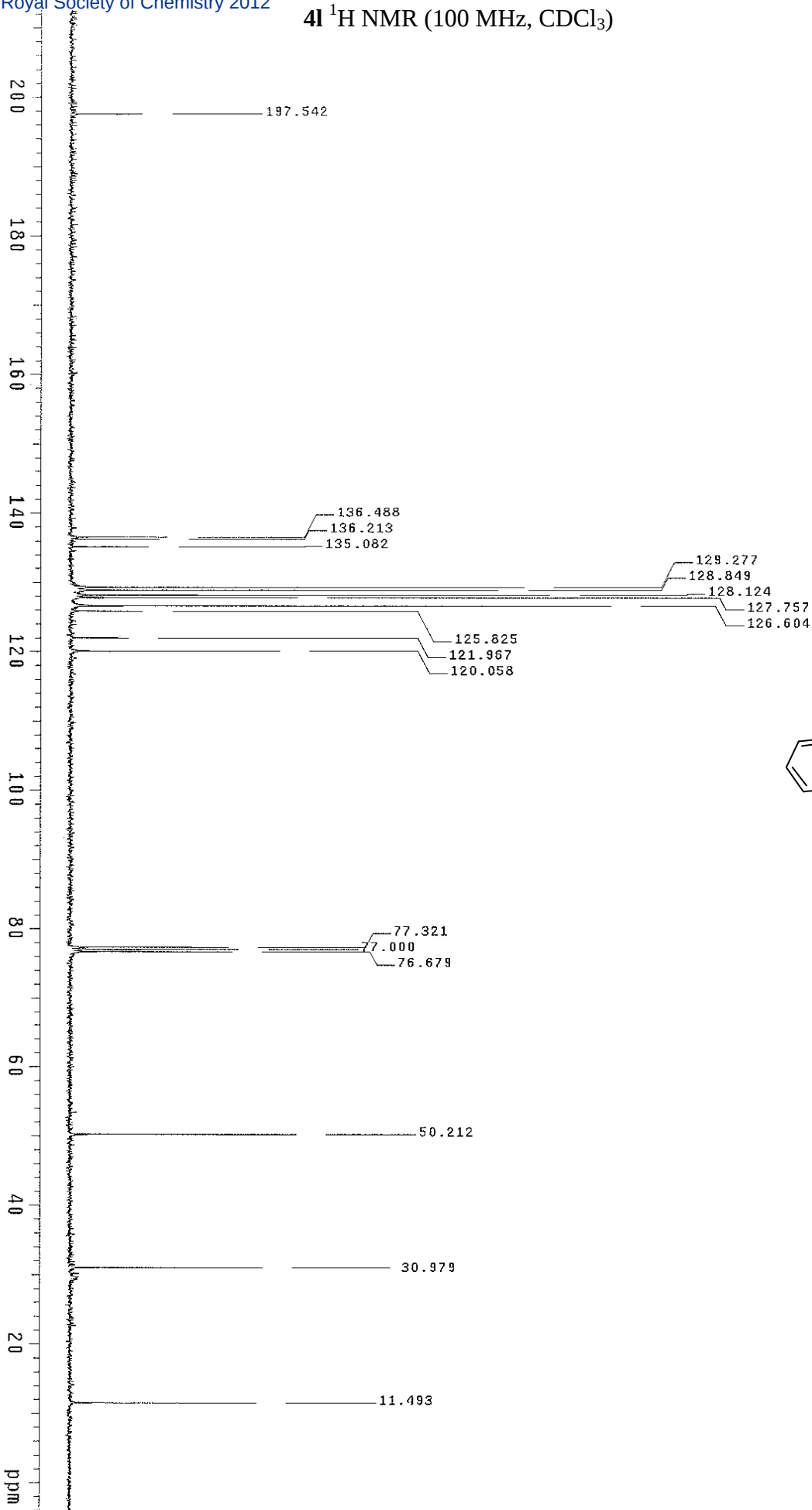


A012/CC1P-1/006 in CDCl3
NMR-400MHZ

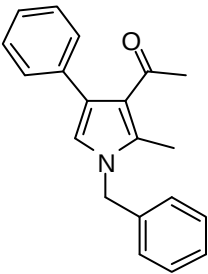
4l ¹H NMR (400 MHz, CDCl₃)



4l ¹H NMR (100 MHz, CDCl₃)



A012-CCIP-1-006 in CDCl₃
NMR-400MHz



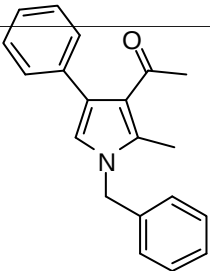
41 HRMS

A012-CCTP-1-006

UT1011_158 26 (0.487) Cm (26.32-3.8x0.010)

290.1572

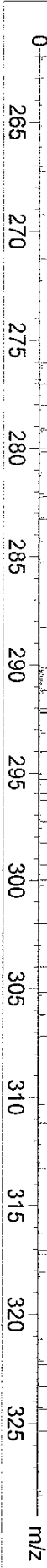
1: TOF MS ES+
3.55e3



276.0302

295.2910

322.3096



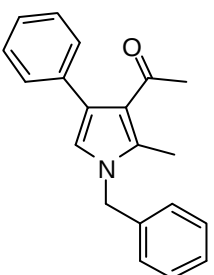
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.0, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4



Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)

Elements Used:

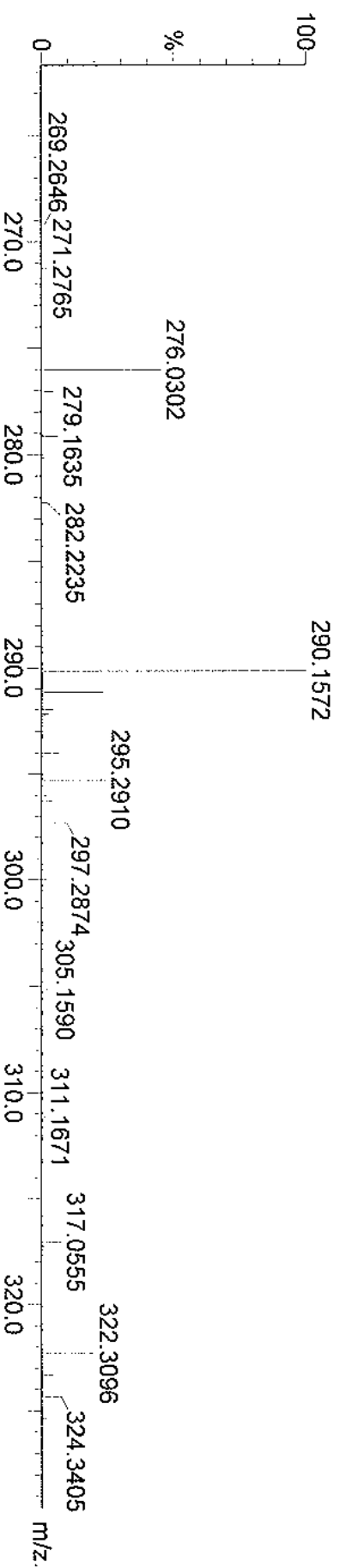
C: 0-20 H: 0-20 N: 0-1 O: 0-2

A012-CCTP-1-006

UT1011_158 26 (0.487) Cm (26:32-3:8x0.010)

1: TOF MS ES+
3.55e+003

41 HRMS

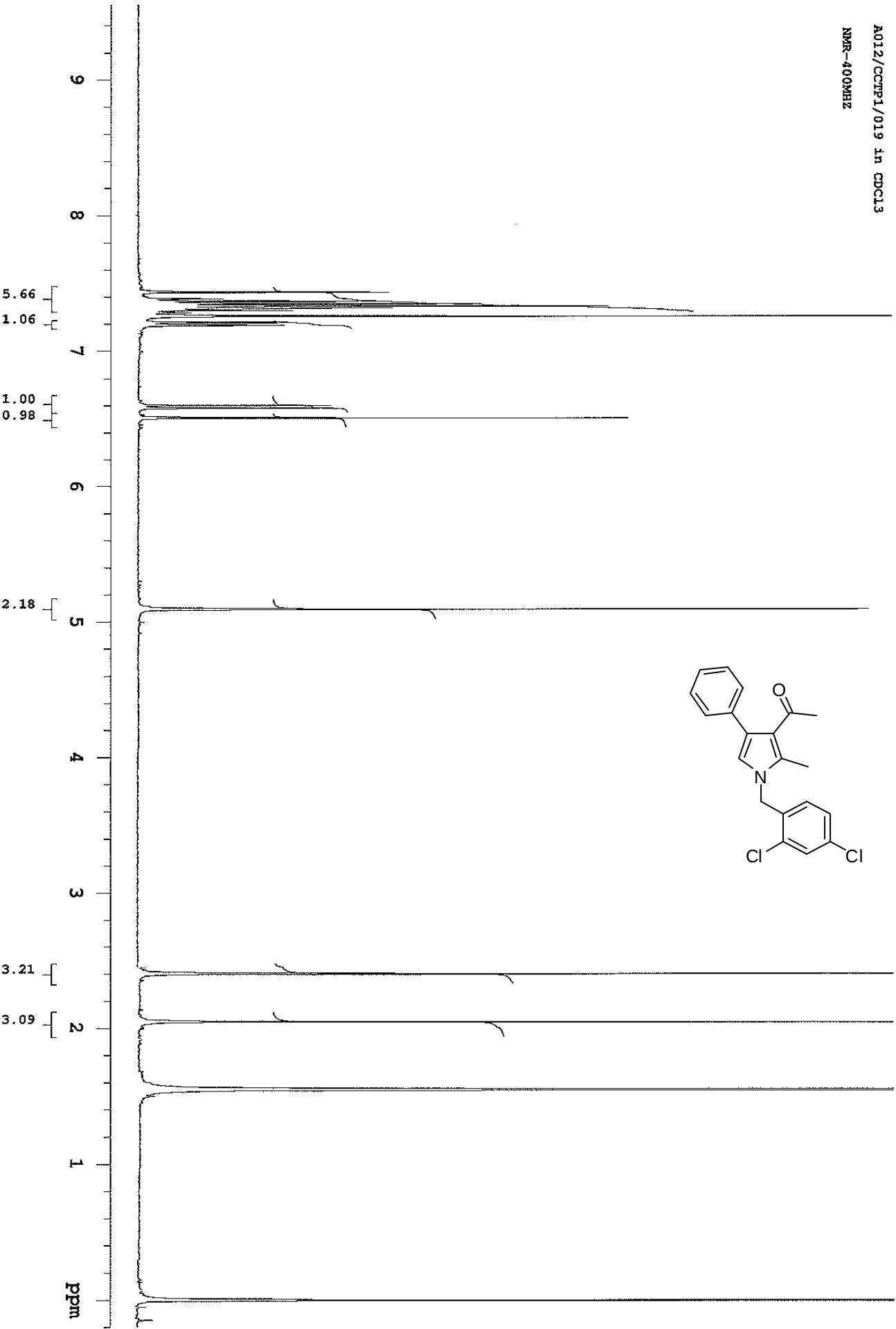


Minimum: 5.0
Maximum: 10.0
0.0
50.0

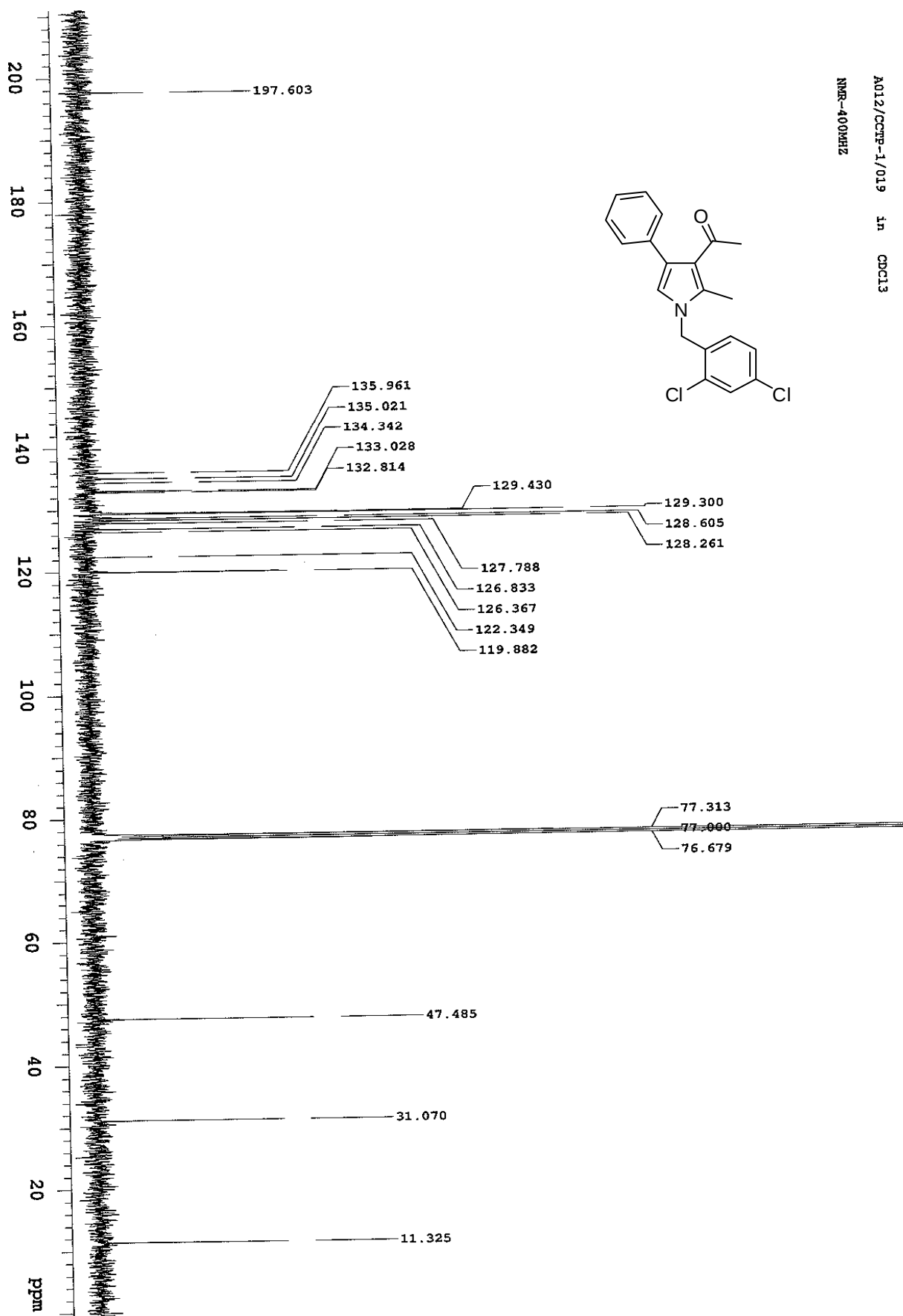
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.1572	290.1545	2.7	9.3	11.5	5.1	C20 H20 N O

4m ¹H NMR (400 MHz, CDCl₃)

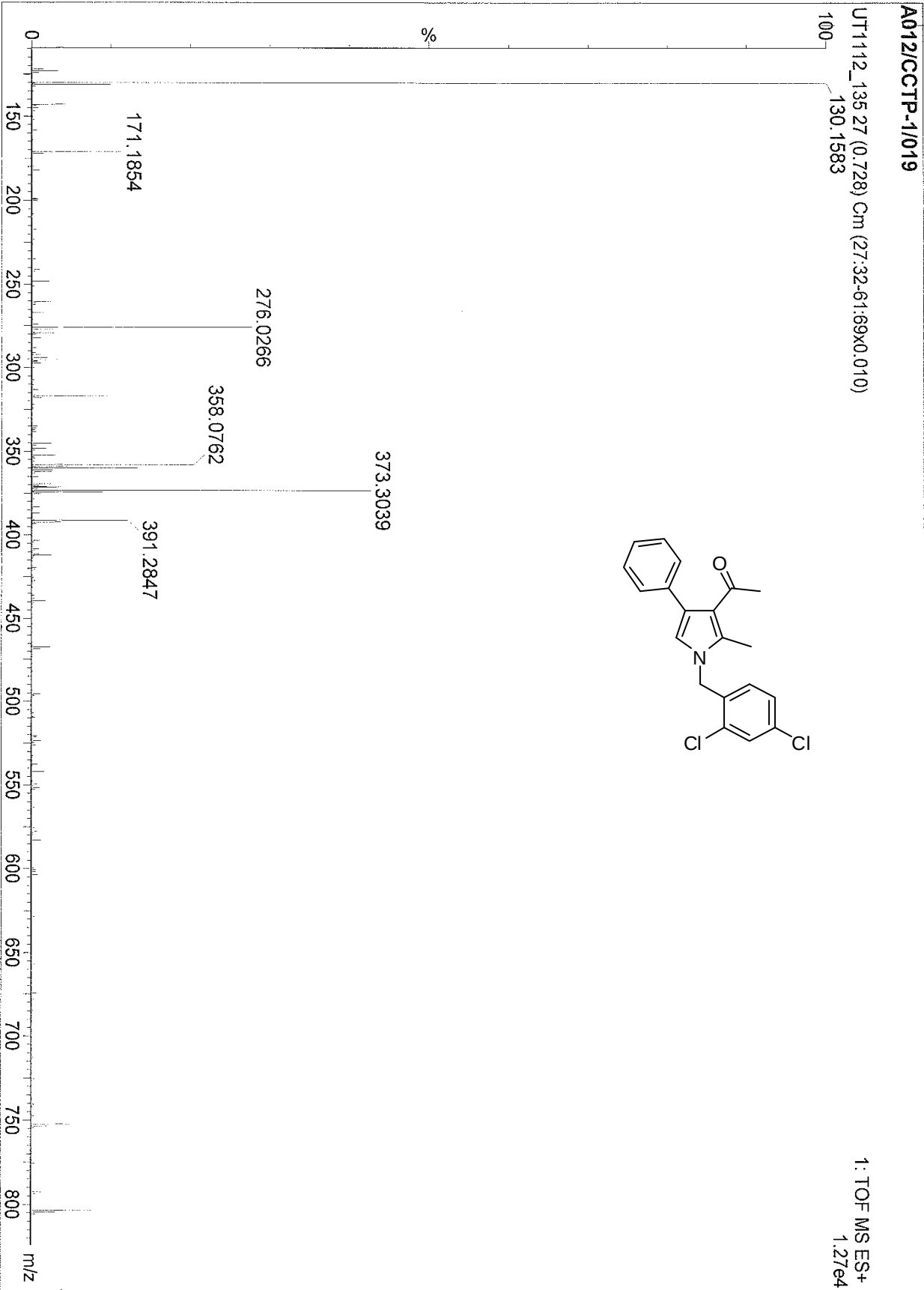
A012/CCTP1/019 in CDCl₃
NMR-400MHZ



4m ^1H NMR (100 MHz, CDCl_3)



4m HRMS



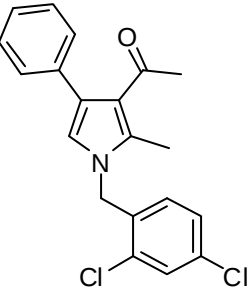
Elemental Composition Report

Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -2.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

194 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

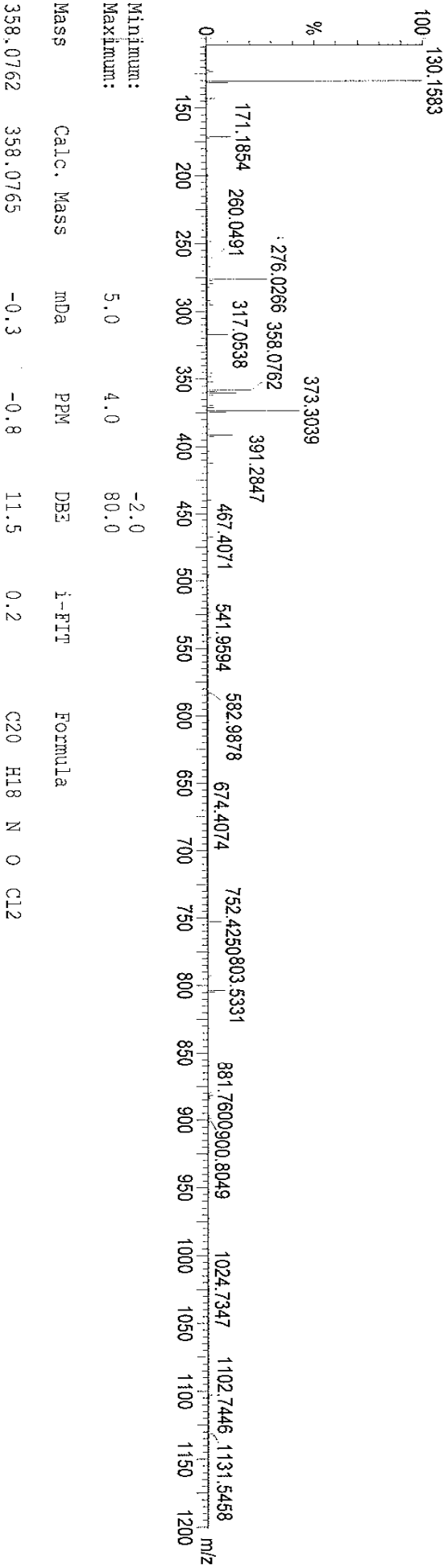
Elements Used:

C: 0-22 H: 0-22 N: 0-4 O: 0-5 Cl: 0-3

A012/CCTP-1/019

UT1112_135 27 (0.728) Cm (27.3261;69x0.010)

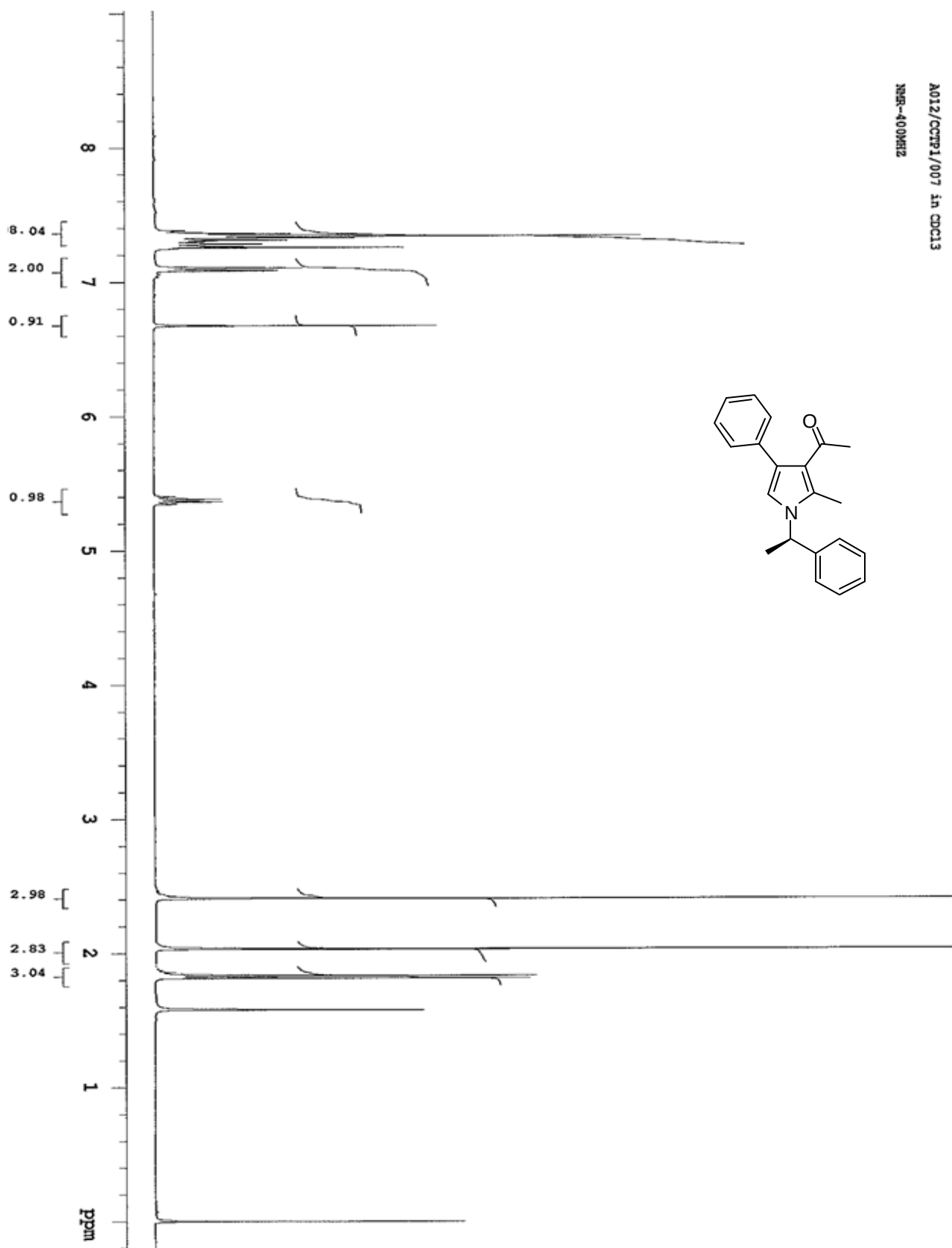
1: TOF MS ES+
1.27e+004



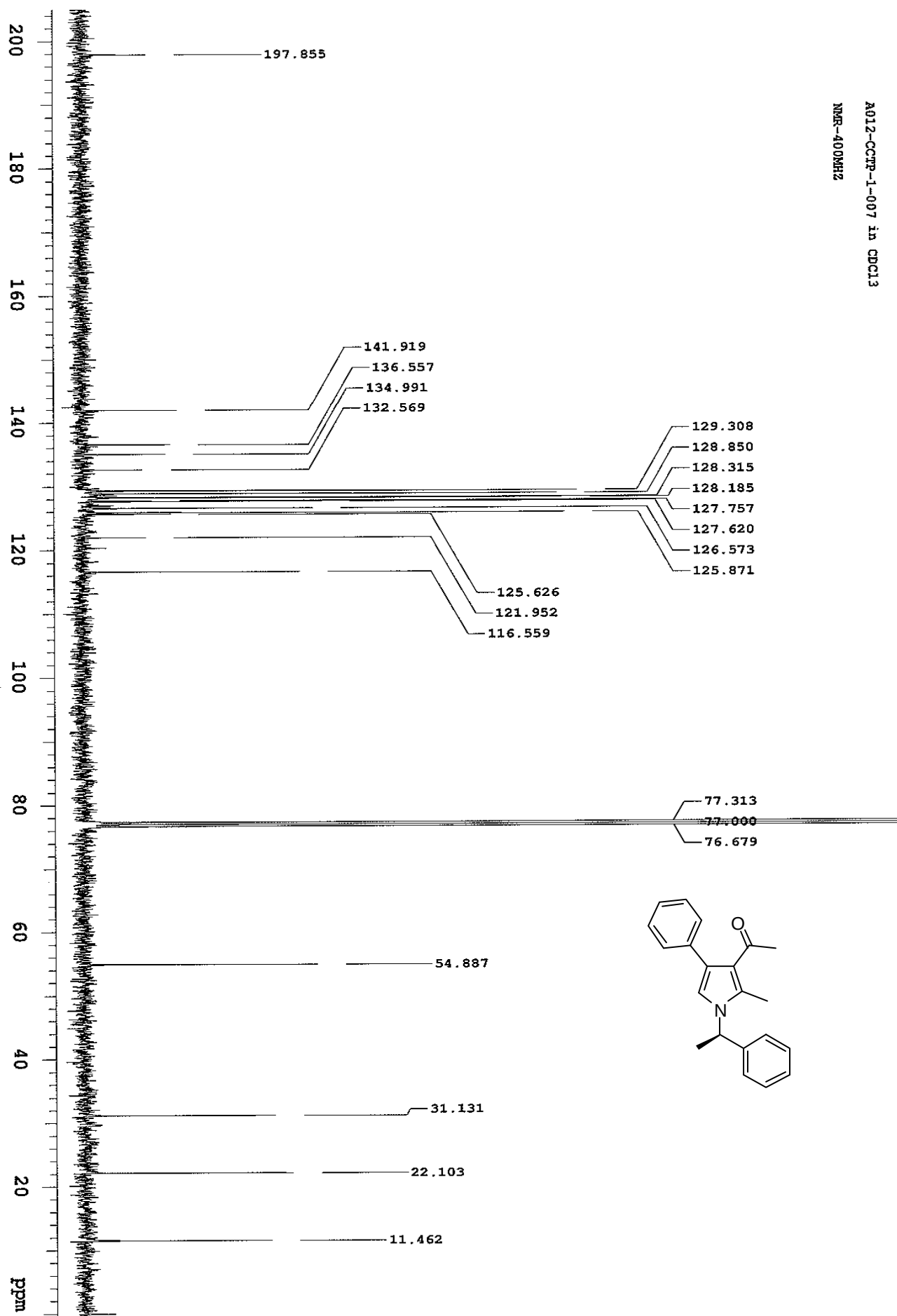
Minimum: 5.0
Maximum: 4.0
-2.0
80.0

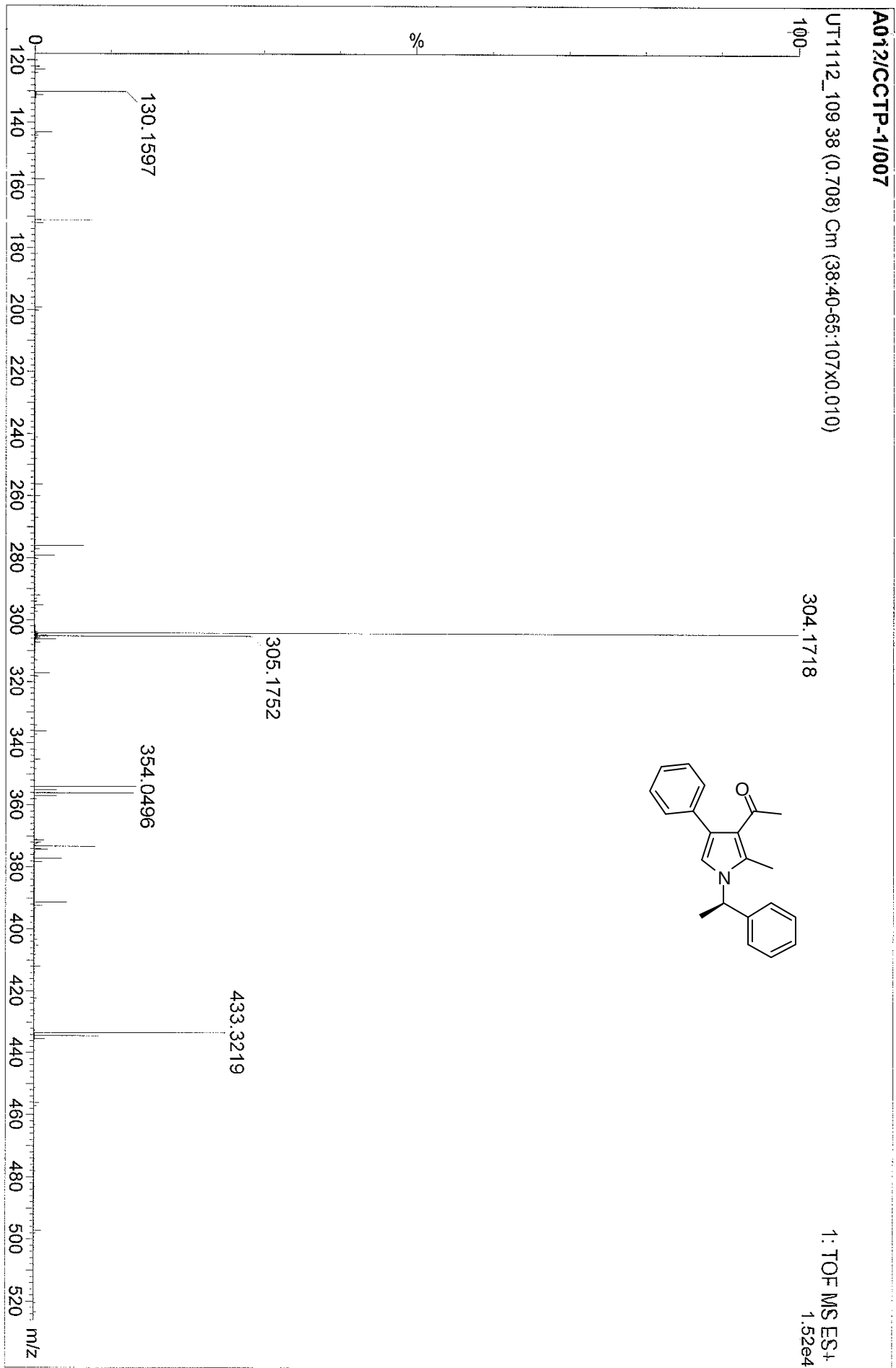
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
358.0762	358.0765	-0.3	-0.8	11.5	0.2	C20 H18 N O Cl2

4n ^1H NMR (400 MHz, CDCl_3)



4n ^1H NMR (100 MHz, CDCl_3)





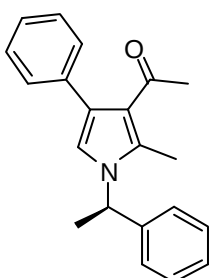
Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -2.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

33 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

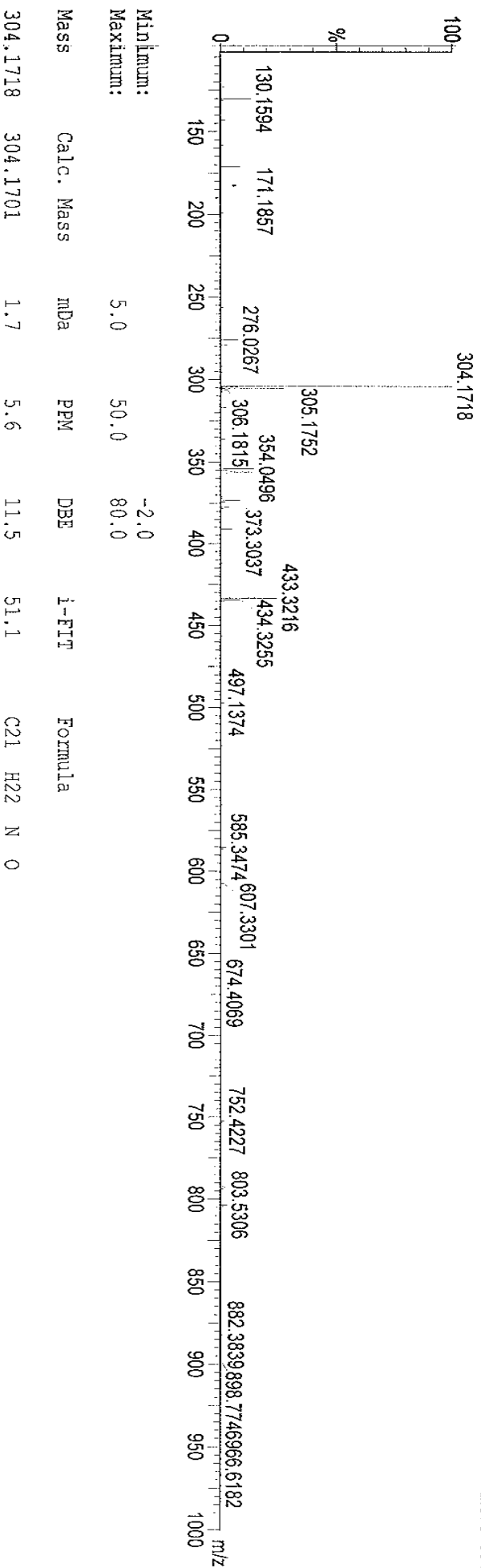
C: 0-25 H: 0-42 N: 0-2 O: 0-2

A012/CTP-1/007

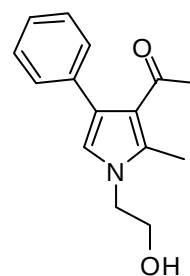
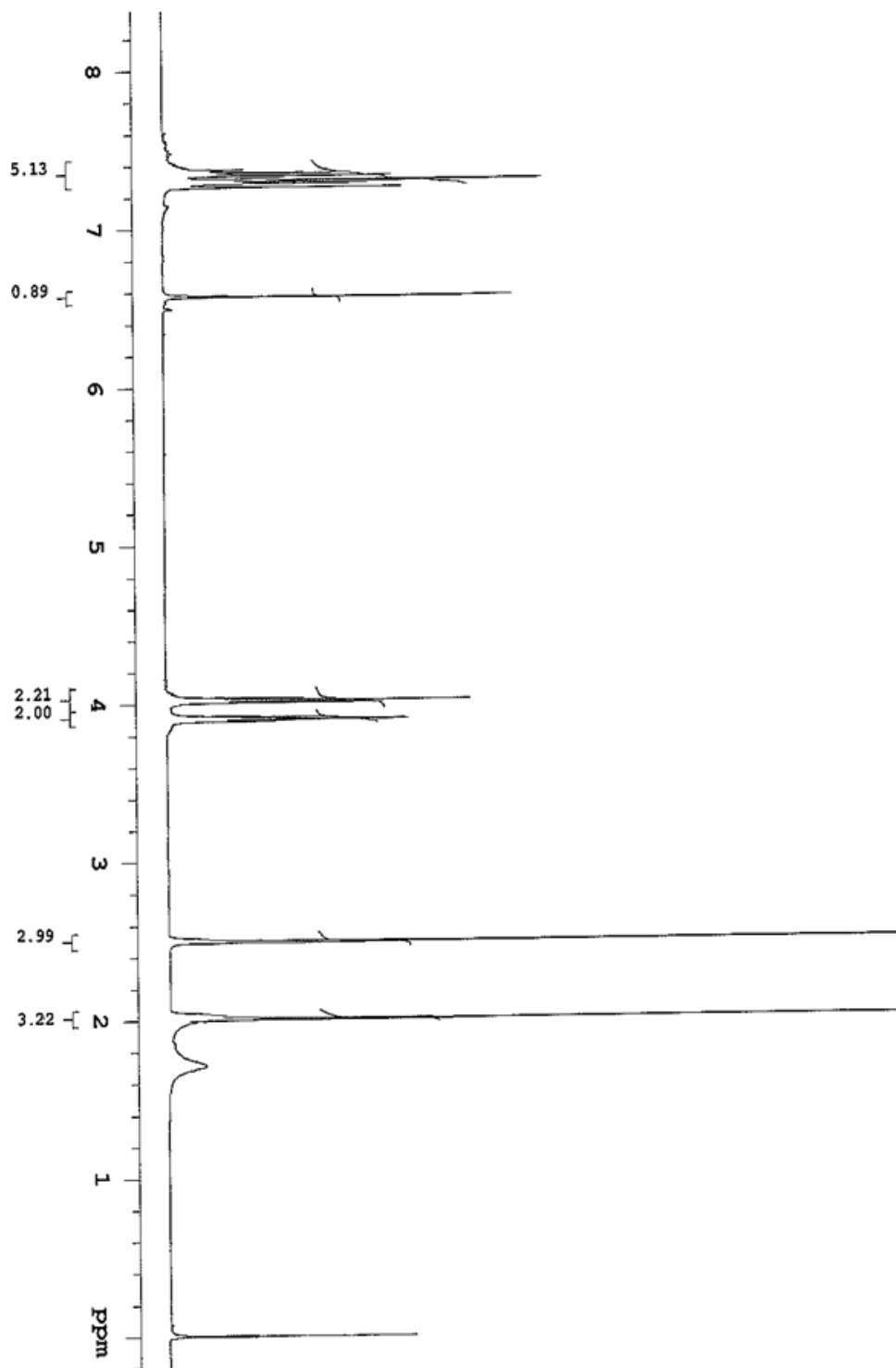
UT1112_109.37 (0.695) Cm (37.41-74.103x0.010)

1: TOF MS ES+
2.57e+004

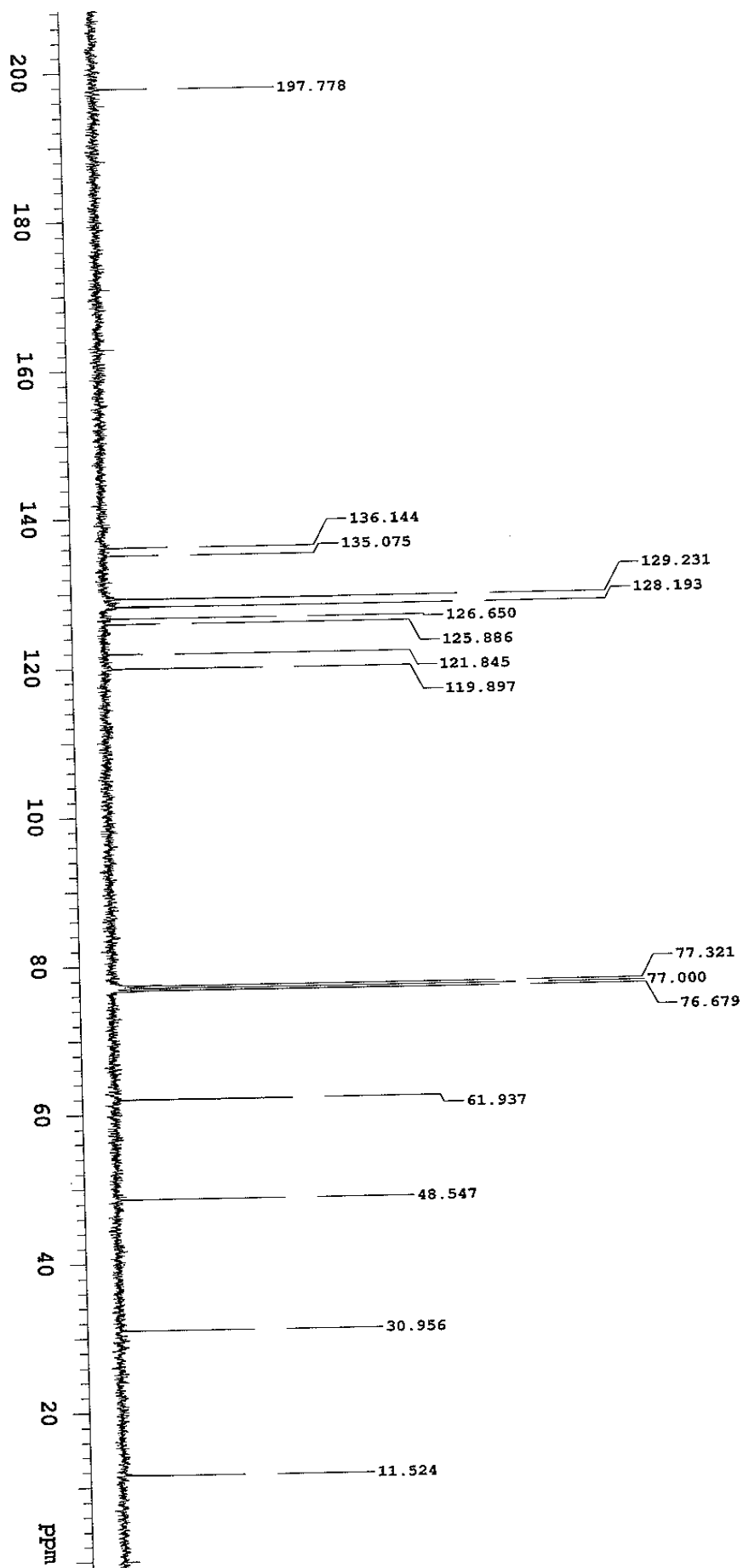
4n HRMS



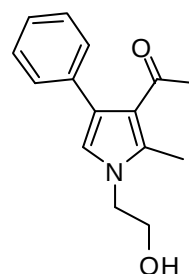
4o ^1H NMR (400 MHz, CDCl_3)



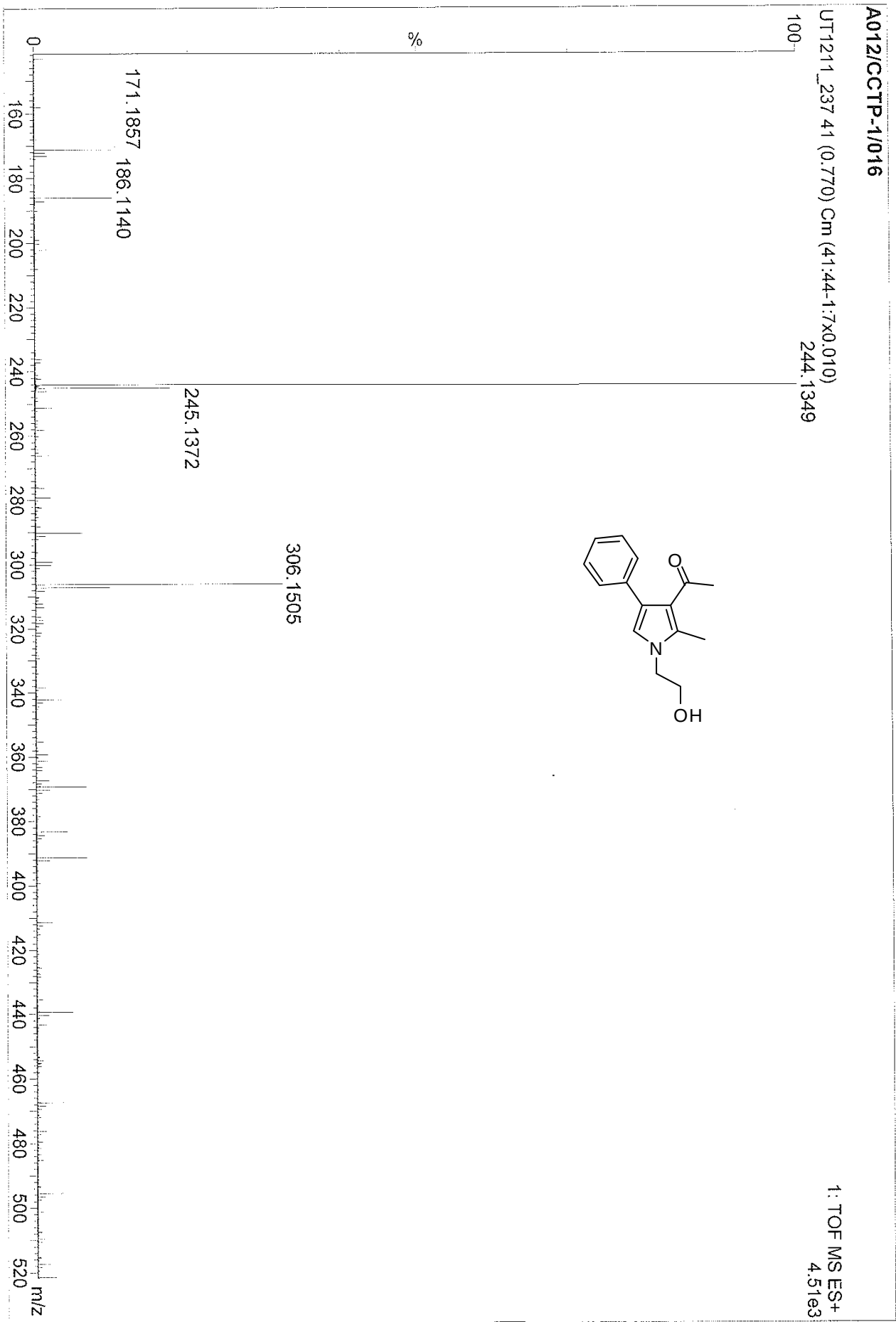
40 ^1H NMR (100 MHz, CDCl_3)



A012-CCTP-1-016 in CDCl_3
NMR-400MHZ



4o HRMS



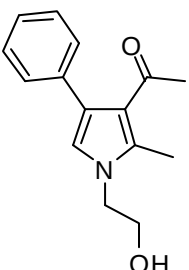
Elemental Composition Report

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 = 3



Monoisotopic Mass, Even Electron Ions

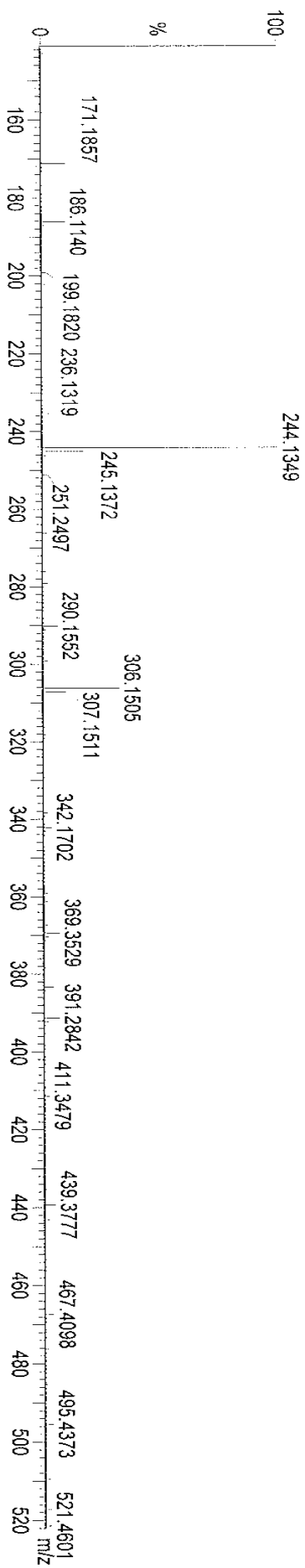
11 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-1 O: 0-2

A012/CCTP-1/016

UT1211_237 41 (0.770) Cm (41:44-1:7x0.010)



1: TOF MS ES+
4.51e+003

Minimum: -2.0
Maximum: 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
244.1349	244.1338	1.1	4.5	7.5	2.0	C15 H18 N O2

