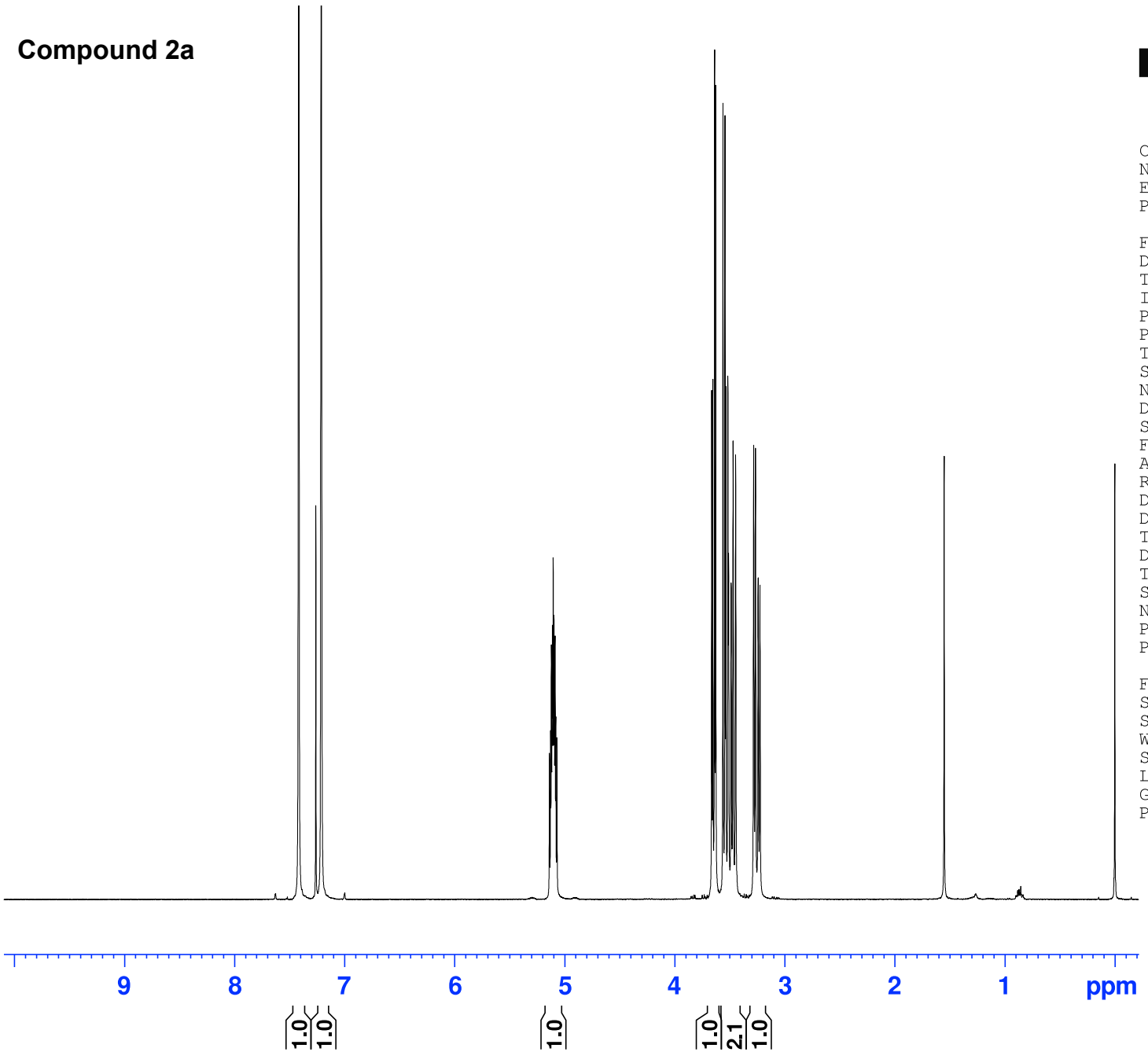
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for:

Synthesis Of 2-Bromomethyl-2,3-Dihydrobenzofurans From 2-Allylphenols Enabled By Organocatalytic Activation of N-Bromosuccinimide

Carolina G. Furst, Paulo H. P. Cota,[†] Taciano A. dos Santos Wanderley [†] and Eduardo E. Alberto*

Compound 2a

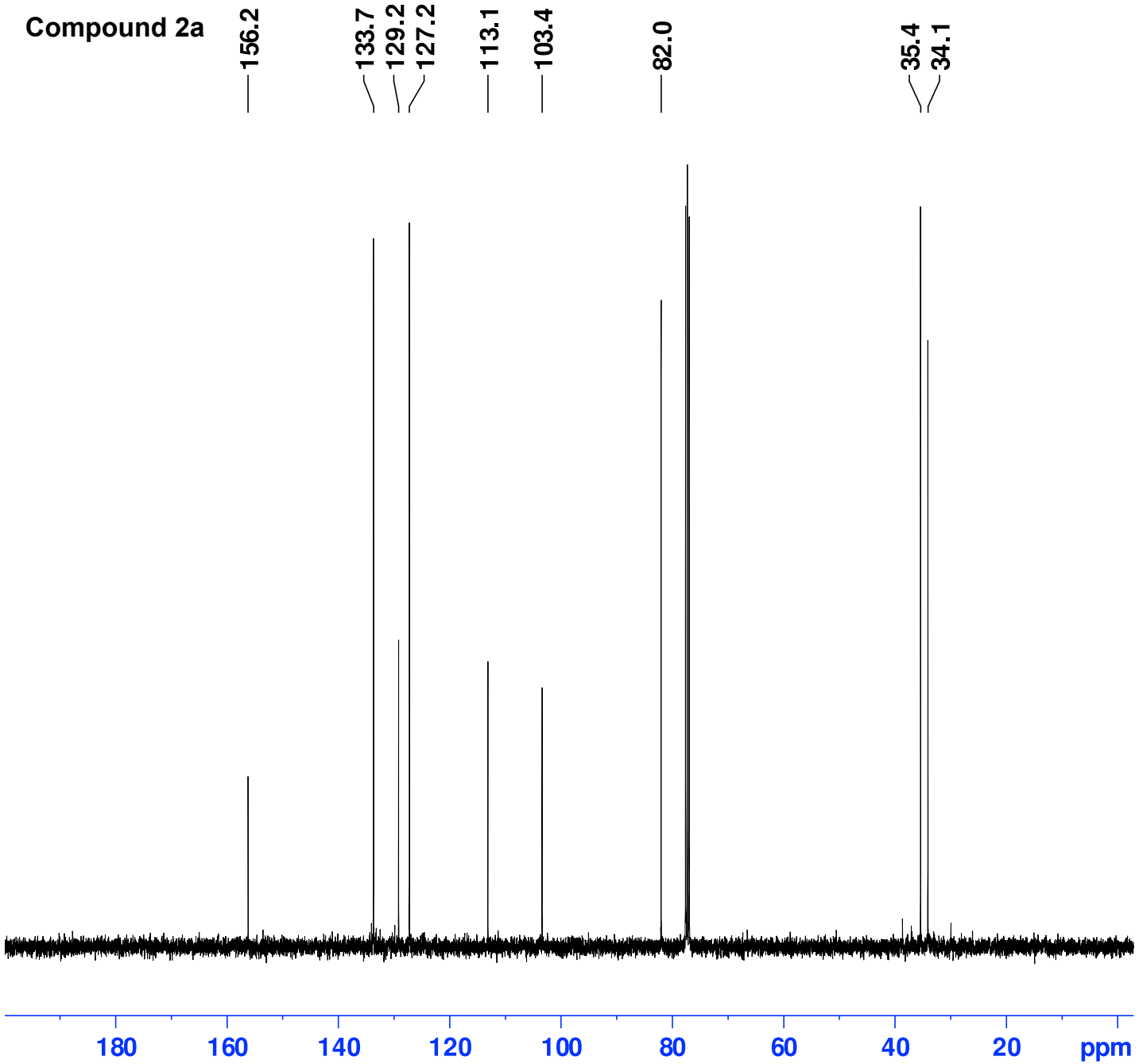



```
Current Data Parameters
NAME          I-CGF-29 R
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameter
Date_           20190516
Time              11.10 h
INSTRUM             spect
PROBHD   Z3756_0157 (5
PULPROG             zg30
TD                 65536
SOLVENT             CDC13
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES           0.244532 Hz
AQ              4.0894465 sec
RG                 175.09
DW                62.400 usec
DE                10.00 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1324708 MHz
NUC1                  1H
P1                11.42 usec
PLW1          11.19999981 W

F2 - Processing parameters
SI                 65536
SF            400.1300094 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Compound 2a




```
Current Data Parameters
NAME        I-CGF-29.II
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameter
Date_          20181003
Time             18.08 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  167
DS                    0
SWH           25252.525 Hz
FIDRES         1.541292 Hz
AQ            0.6488064 sec
RG               197.86
DW               19.800 usec
DE               10.00 usec
TE               300.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6198125 MHz
NUC1                 13C
P1                13.25 usec
PLW1         17.98900032 W
SFO2         400.1116004 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.19999981 W
PLW12         0.19090000 W
PLW13         0.09602200 W

F2 - Processing parameters
SI                32768
SF          100.6077179 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Compound 2a

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: **I-CGF-29**

Responsável pela amostra: Carolina Furst – UFMG (Prof. Eduardo Alberto)

e-mail do responsável: carolfurstg@gmail.com

Amostra submetida em: 28-jun-19

Aquisição e análise: 17-jul-19

Fórmula molecular: $C_9H_7Br_3O$

Massa exata calculada: $[M]^+$ 369.802124

(massa mais abundante) $[M+H]^+$ 370.809949

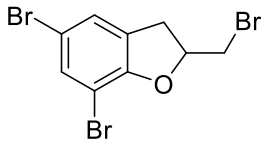
Íons observados: ☑ **$[M]^+$**

☐ **$[M+H]^+$**

☐ *outros:*

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações:

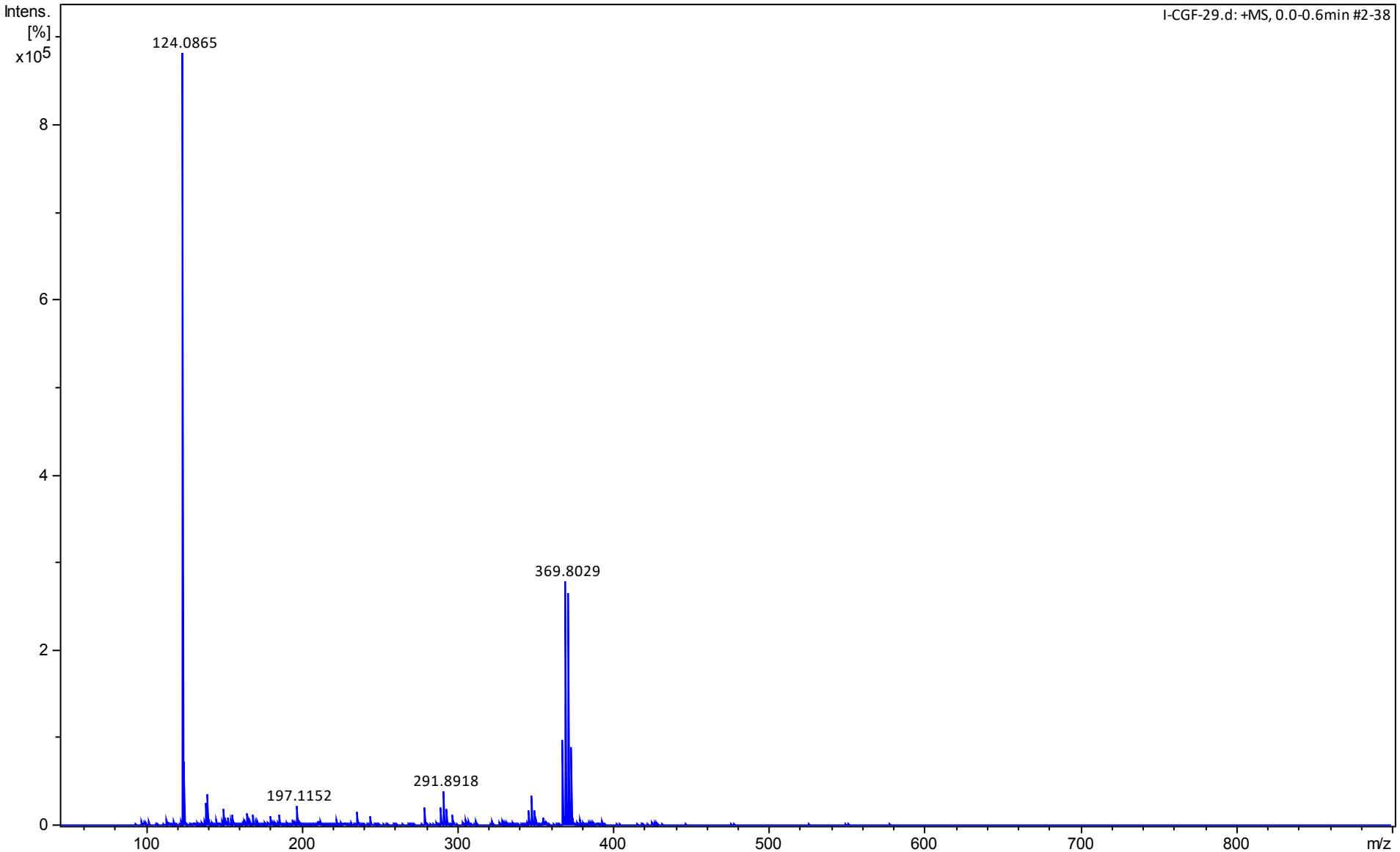
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

Compound 2a

Central de Análises - UCS

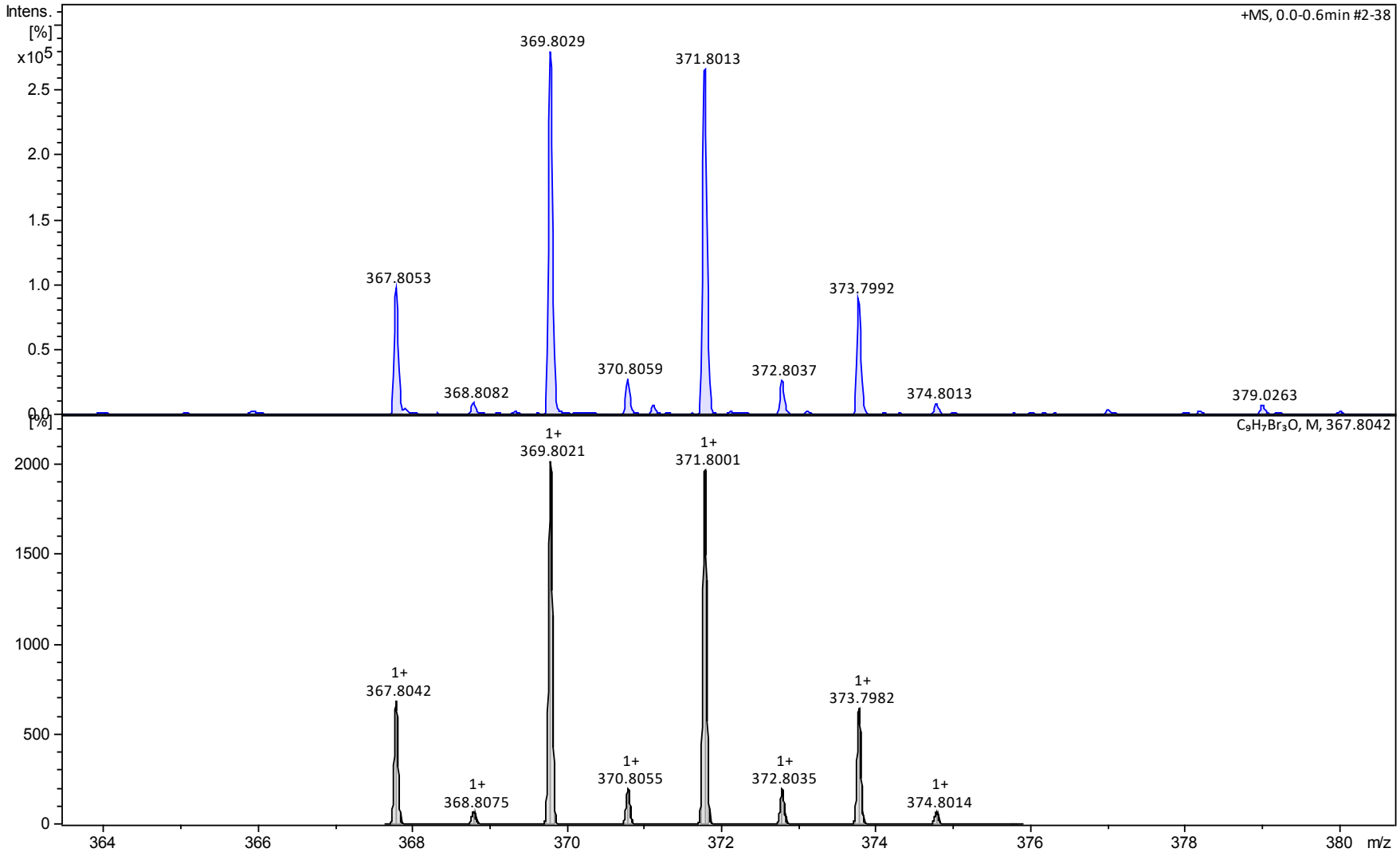
1. Espectro Obtido



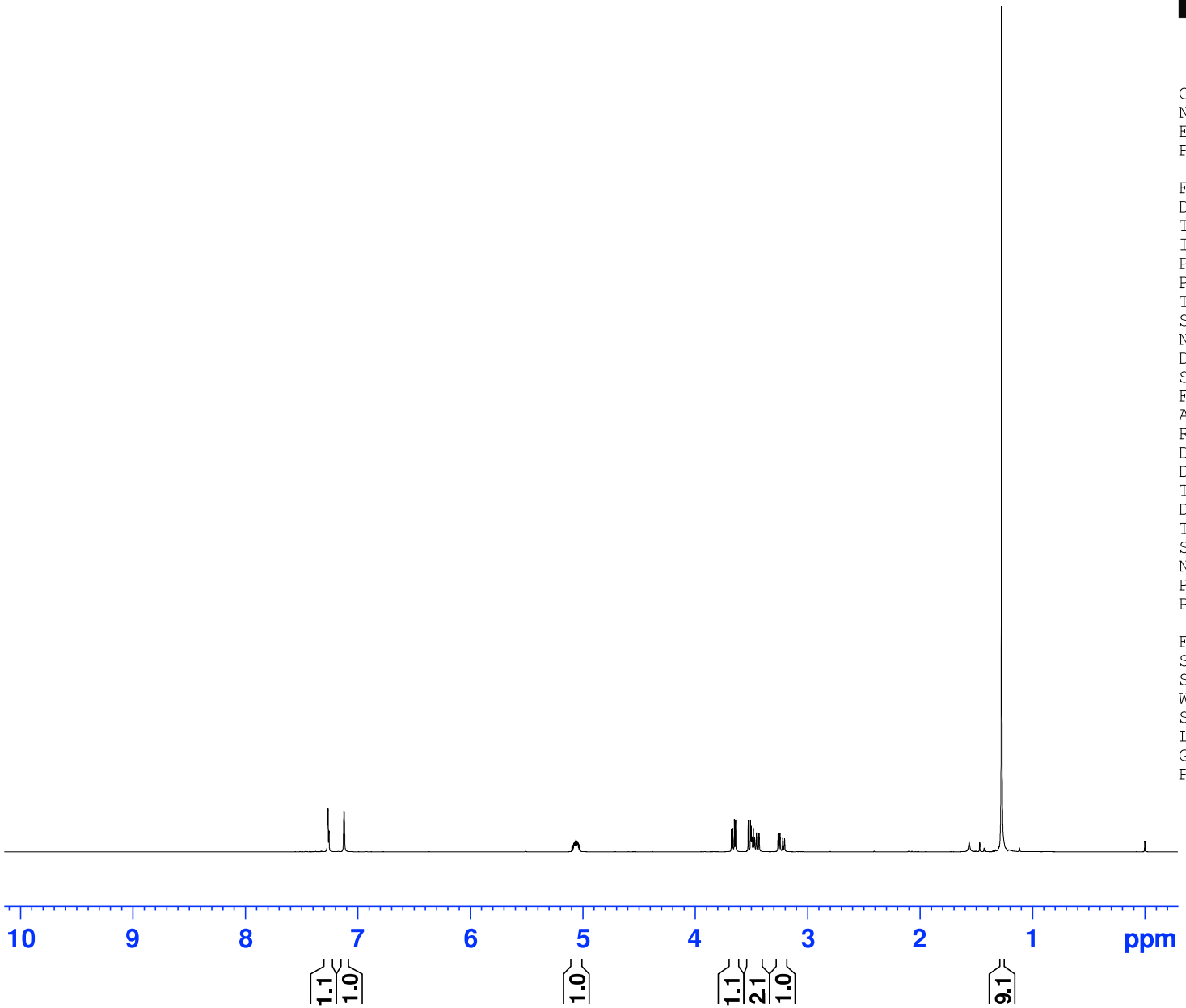
2. Expansão do espectro obtido incluindo os espectros simulados

Espectro obtido (expansão na região de *m/z* do íon de interesse)

Espectro simulado: Íon $[M]^+$



Compound 2b

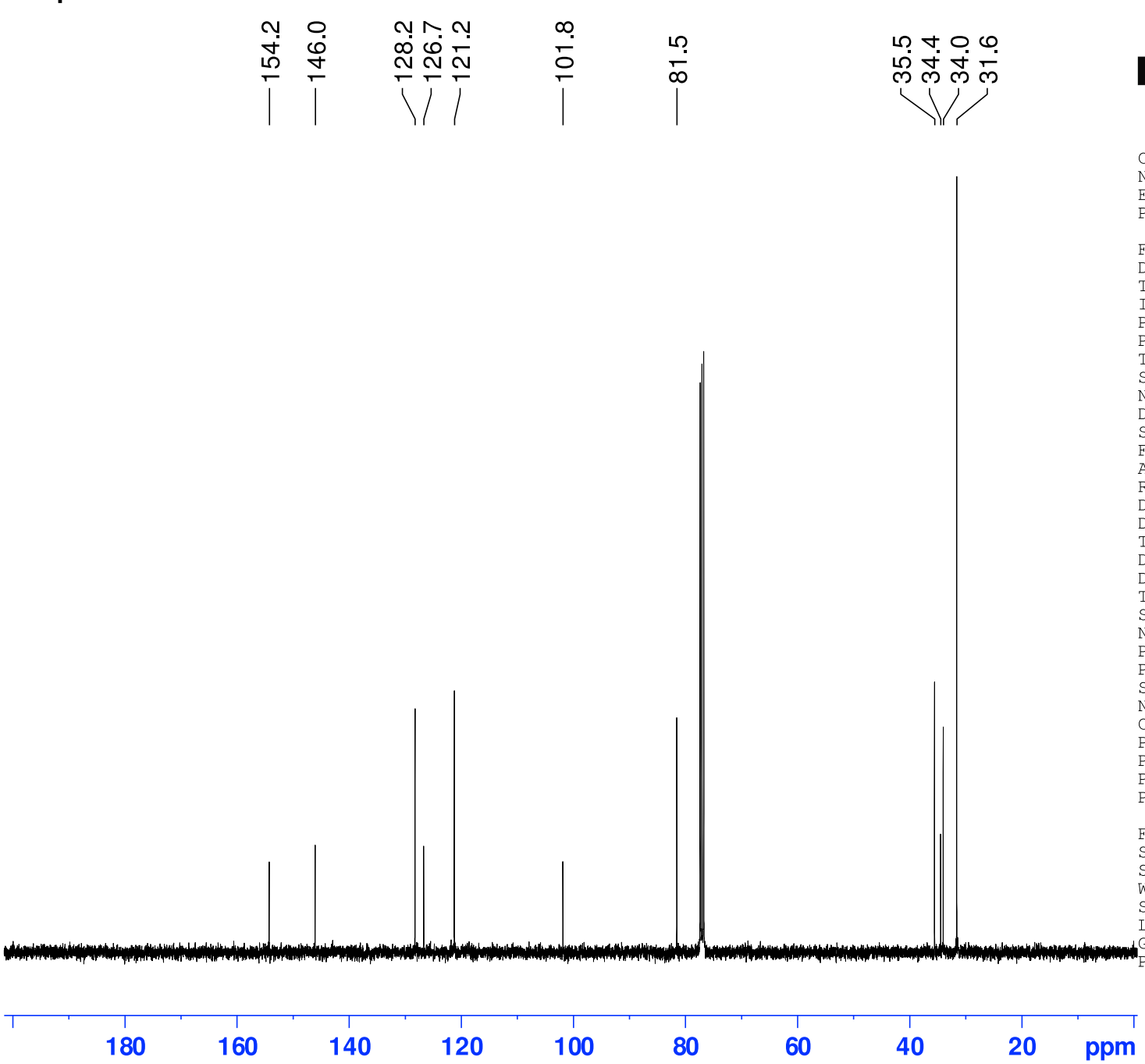



```
Current Data Parameters
NAME         I-CGF-34 C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameter
Date_          20190524
Time             16.45 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ           4.0894465 sec
RG                110.48
DW               62.400 usec
DE               10.00 usec
TE                300.1 K
D1           1.00000000 sec
TD0                   1
SFO1        400.1324708 MHz
NUC1                 1H
P1               11.42 usec
PLW1        11.19999981 W

F2 - Processing parameters
SI                65536
SF          400.1300115 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```

Compound 2b




```
Current Data Parameters
NAME          I-CGF-34 C
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameter
Date_           20190524
Time              16.53 h
INSTRUM             spect
PROBHD   Z3756_0157 (5
PULPROG           zgpg30
TD                65536
SOLVENT            CDCl3
NS                   128
DS                     2
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ            1.2582912 sec
RG                197.86
DW              19.200 usec
DE              10.00 usec
TE                300.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         100.6238359 MHz
NUC1                 13C
P1              13.25 usec
PLW1         17.98900032 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.19999981 W
PLW12         0.18032999 W
PLW13         0.09070400 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Compound 2b

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: **I-CGF-34**

Responsável pela amostra: Carolina Furst – UFMG (Prof. Eduardo Alberto)

e-mail do responsável: carolfurstg@gmail.com

Amostra submetida em: 28-jun-19

Aquisição e análise: 17-jul-19

Fórmula molecular: $C_{13}H_{16}Br_2O$

Massa exata calculada: $[M]^+$ 347.954244

(massa mais abundante) $[M+H]^+$ 348.962069

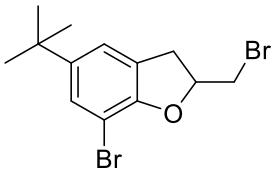
Íons observados: ☑ **$[M]^+$**

☐ **$[M+H]^+$**

☐ *outros:*

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações:

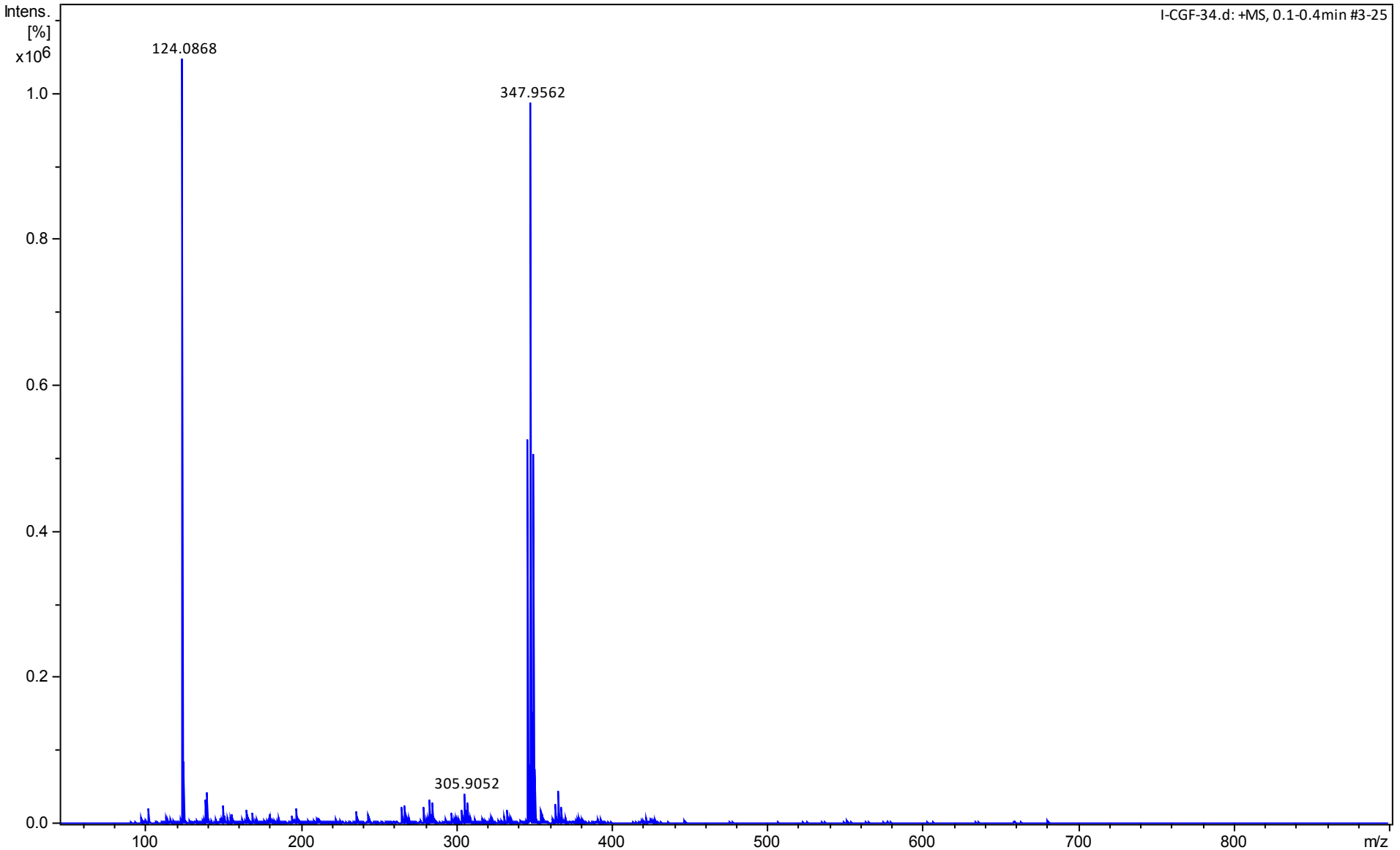
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

Compound 2b

Central de Análises - UCS

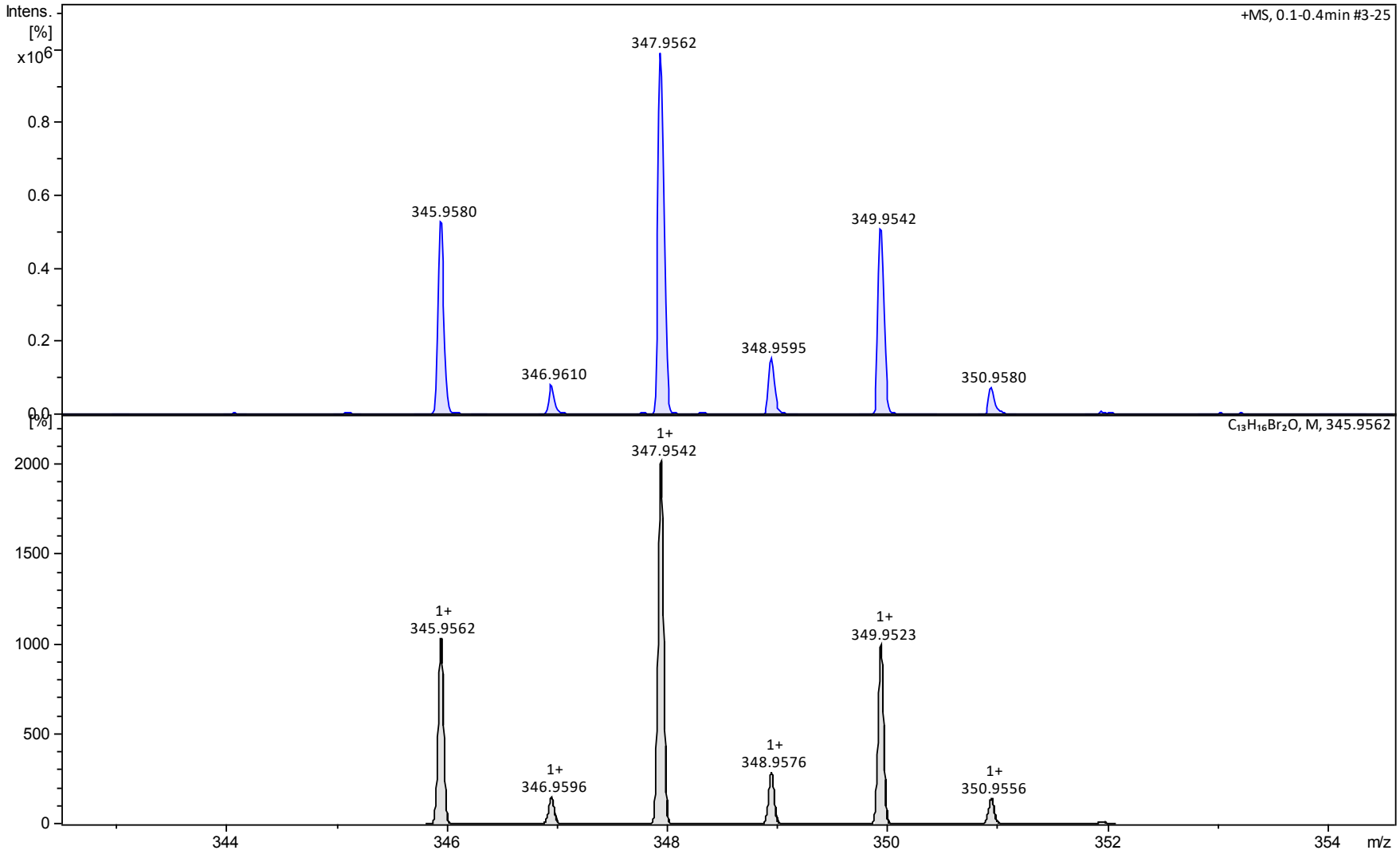
1. Espectro Obtido



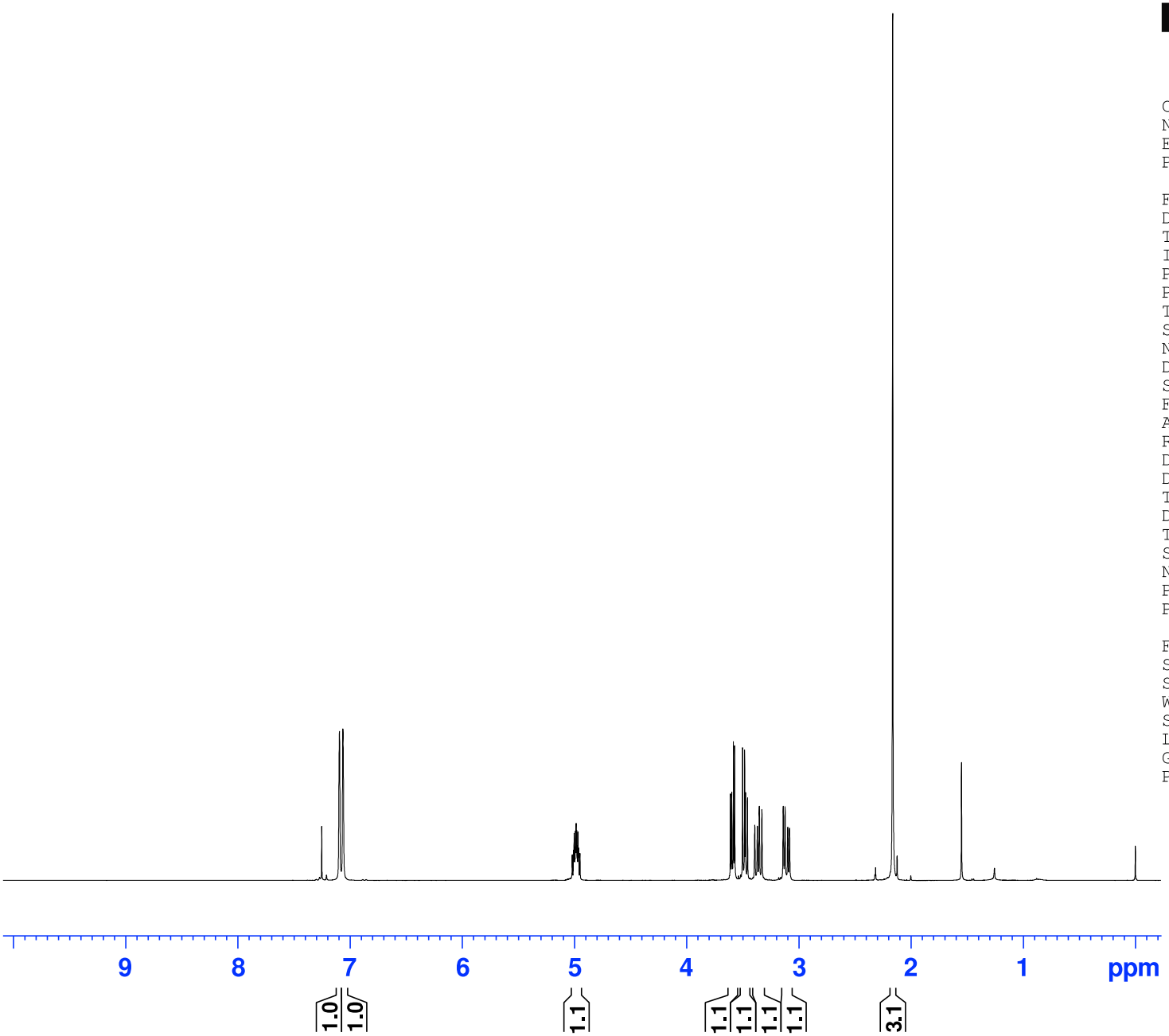
2. Expansão do espectro obtido incluindo os espectros simulados

Espectro obtido (expansão na região de *m/z* do íon de interesse)

Espectro simulado: Íon $[M]^+$



Compound 2c

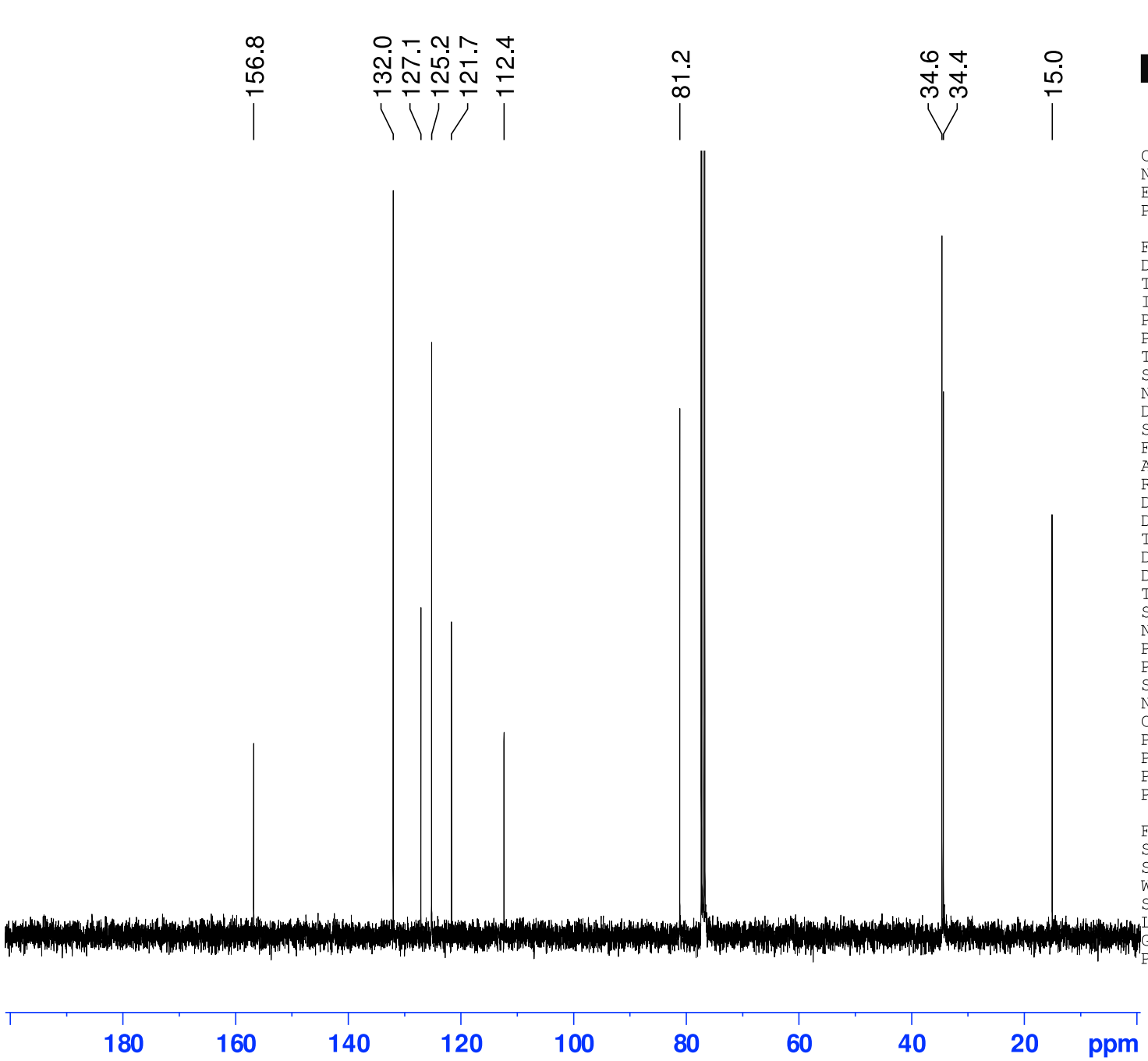



```
Current Data Parameters
NAME          I-CGF-54 C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameter
Date_          20190524
Time             16.23 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                125.16
DW                62.400 usec
DE                10.00 usec
TE                300.3 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                11.42 usec
PLW1         11.19999981 W

F2 - Processing parameters
SI                 65536
SF           400.1300125 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Compound 2c




```
Current Data Parameters
NAME          I-CGF-54 C
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameter
Date_           20190524
Time              16.34 h
INSTRUM             spect
PROBHD   Z3756_0157 (5
PULPROG           zgpg30
TD                65536
SOLVENT            CDCl3
NS                   128
DS                     2
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ            1.2582912 sec
RG                197.86
DW              19.200 usec
DE              10.00 usec
TE                300.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        100.6238359 MHz
NUC1                 13C
P1              13.25 usec
PLW1        17.98900032 W
SFO2        400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 use
PLW2        11.19999981 W
PLW12        0.18032999 W
PLW13        0.09070400 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Compound 2c

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: **I-CGF-54**

Responsável pela amostra: Carolina Furst – UFMG (Prof. Eduardo Alberto)

e-mail do responsável: carolfurstg@gmail.com

Amostra submetida em: 28-jun-19

Aquisição e análise: 17-jul-19

Fórmula molecular: $C_{10}H_{10}Br_2O$

Massa exata calculada: $[M]^+$ 305.907275

(massa mais abundante) $[M+H]^+$ 306.915100

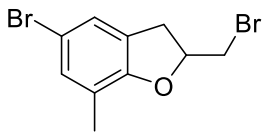
Íons observados: ☑ **$[M]^+$**

☐ **$[M+H]^+$**

☐ *outros:*

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações:

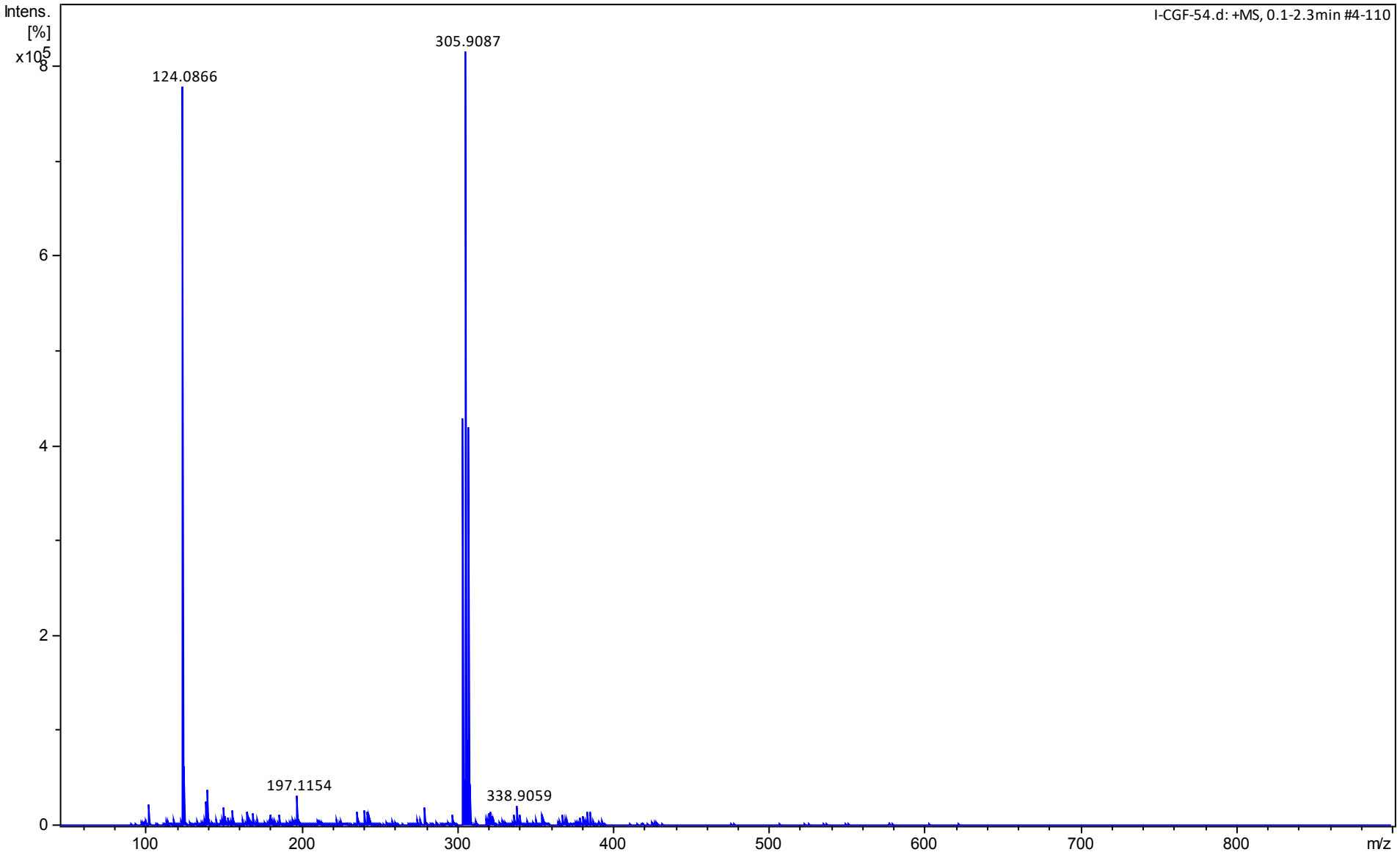
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

Compound 2c

Central de Análises - UCS

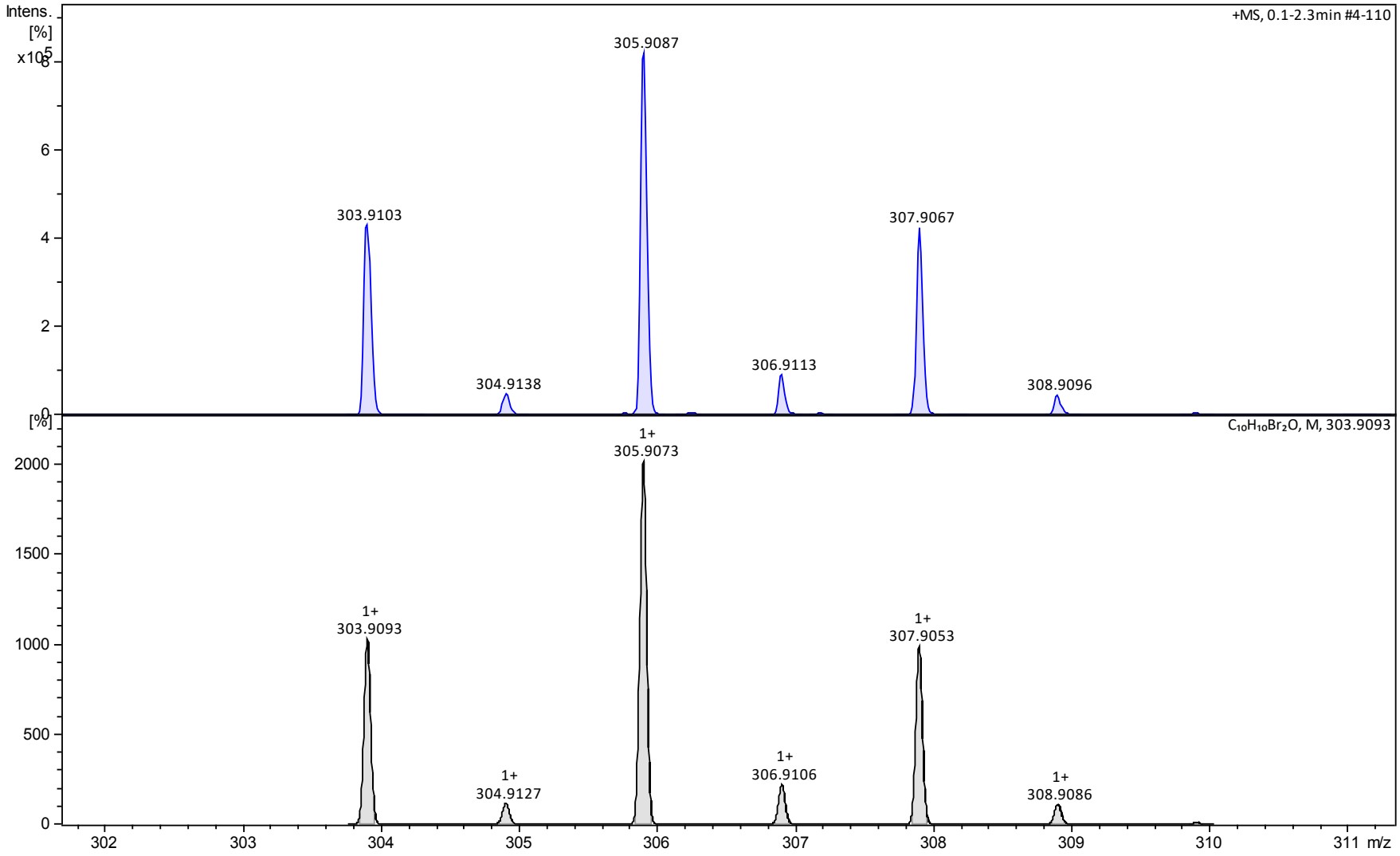
1. Espectro Obtido



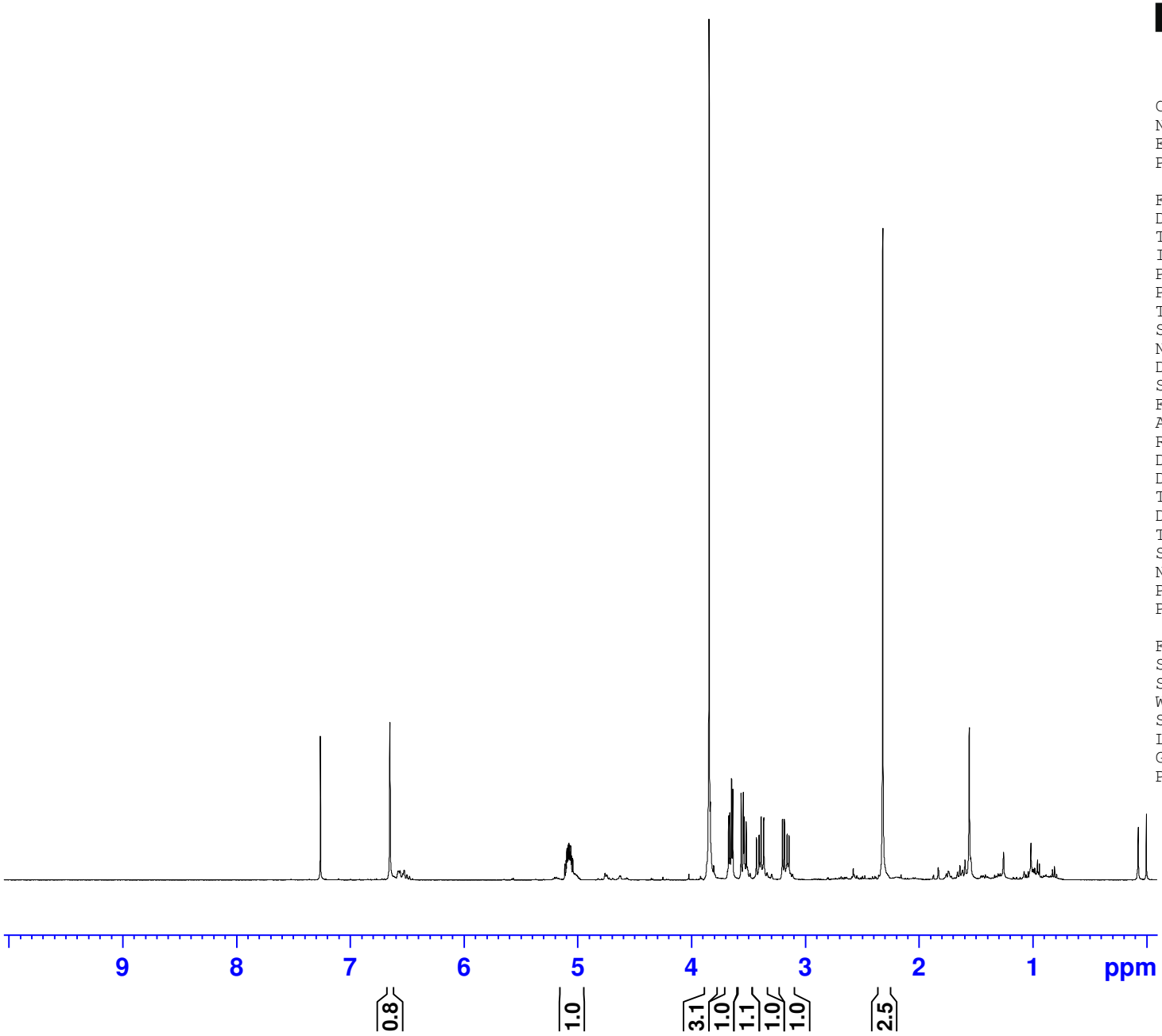
2. Expansão do espectro obtido incluindo os espectros simulados

Espectro obtido (expansão na região de *m/z* do íon de interesse)

Espectro simulado: Íon $[M]^+$



Compound 2d

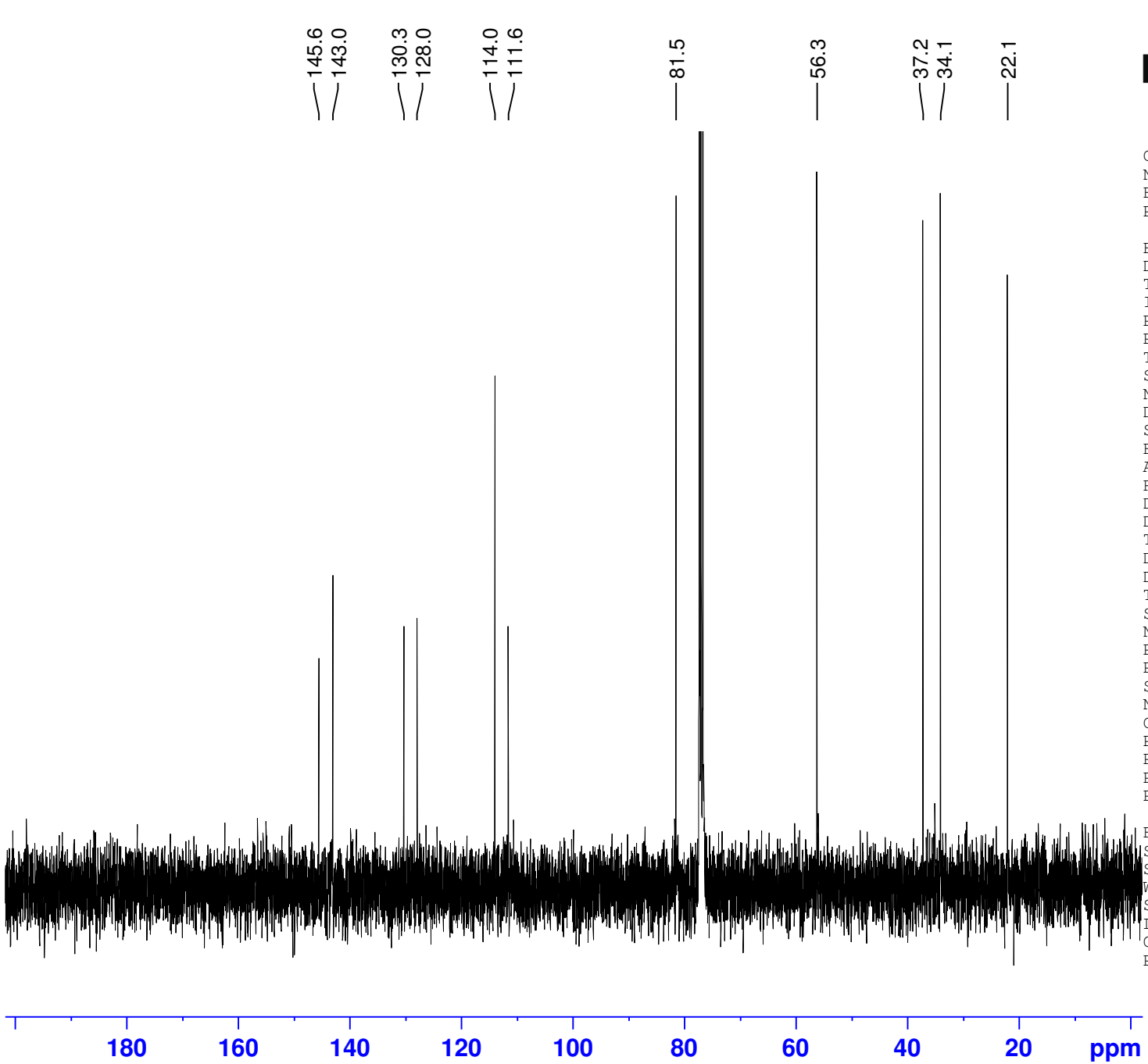



```
Current Data Parameters
NAME            I-CGF-92
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190822
Time               17.37 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                197.86
DW                62.400 usec
DE                10.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                11.34 usec
PLW1         11.19999981 W

F2 - Processing parameters
SI                 65536
SF           400.1300095 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Compound 2d




```
Current Data Parameters
NAME            I-CGF-92
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190822
Time               17.57 h
INSTRUM             spect
PROBHD   Z3756_0157 (5
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   256
DS                     2
SWH            26041.666 Hz
FIDRES          0.794729 Hz
AQ             1.2582912 sec
RG                197.86
DW                19.200 usec
DE                10.00 usec
TE                 300.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         100.6238359 MHz
NUC1                13C
P1                13.25 usec
PLW1         17.98900032 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.19999981 W
PLW12         0.17781000 W
PLW13         0.08943800 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Compound 2d

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: **I-CGF-95**

Responsável pela amostra: Prof. Eduardo E Alberto - UFMG

e-mail do responsável: albertoee.ufmg@gmail.com

Amostra submetida em: 6-jan-20

Aquisição e análise: 22-jan-20

Fórmula molecular: $C_{11}H_{13}BrO_2$

Massa exata calculada: $[M]^+$ 256.009343

(para o pico de maior intensidade) $[M+H]^+$ 257.017168

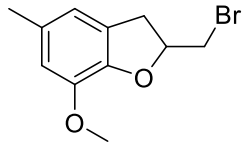
Íons observados: ☑ **$[M]^+$**

☐ **$[M+H]^+$**

☐ *outros*

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações:

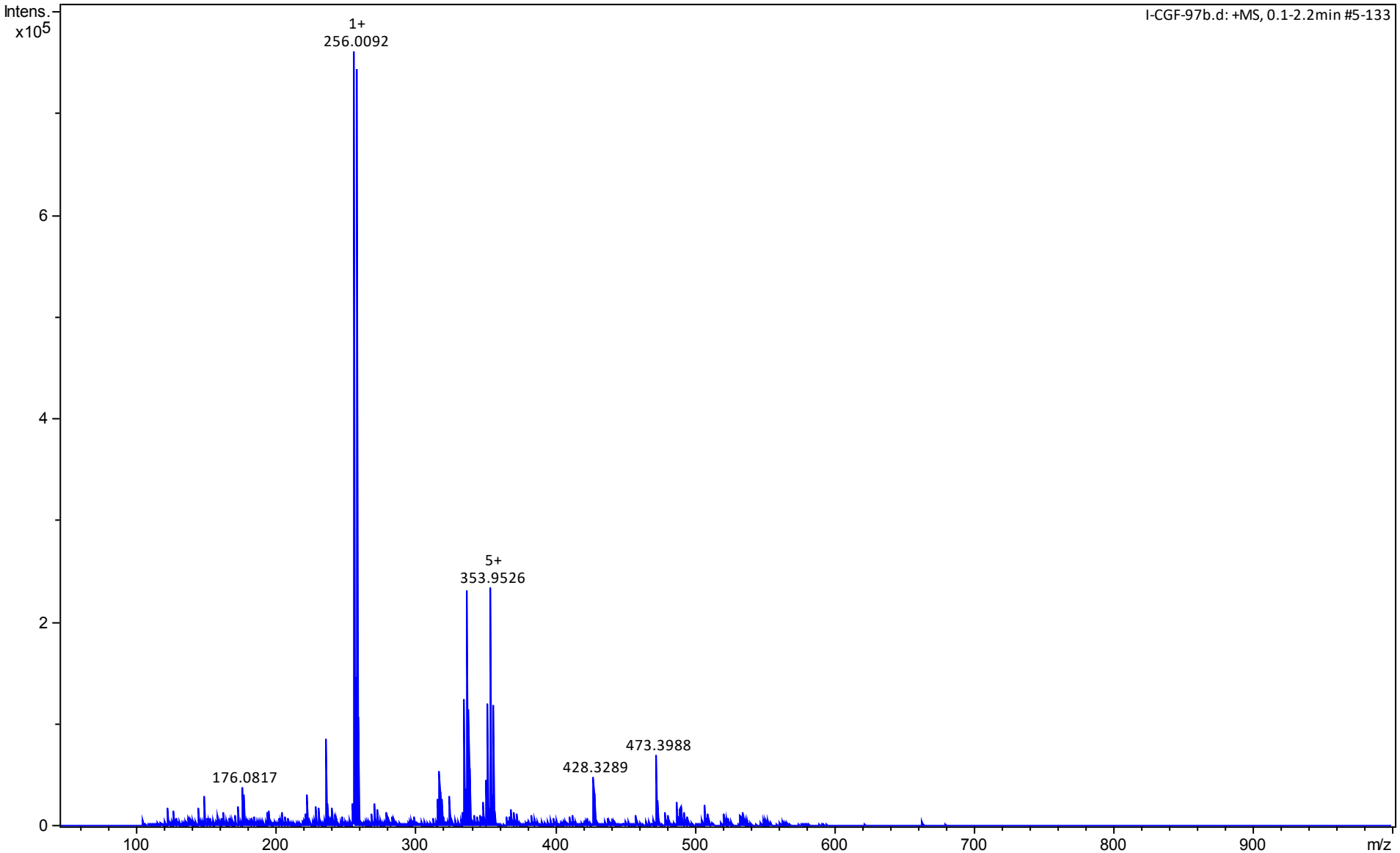
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

Compound 2d

Central de Análises - UCS

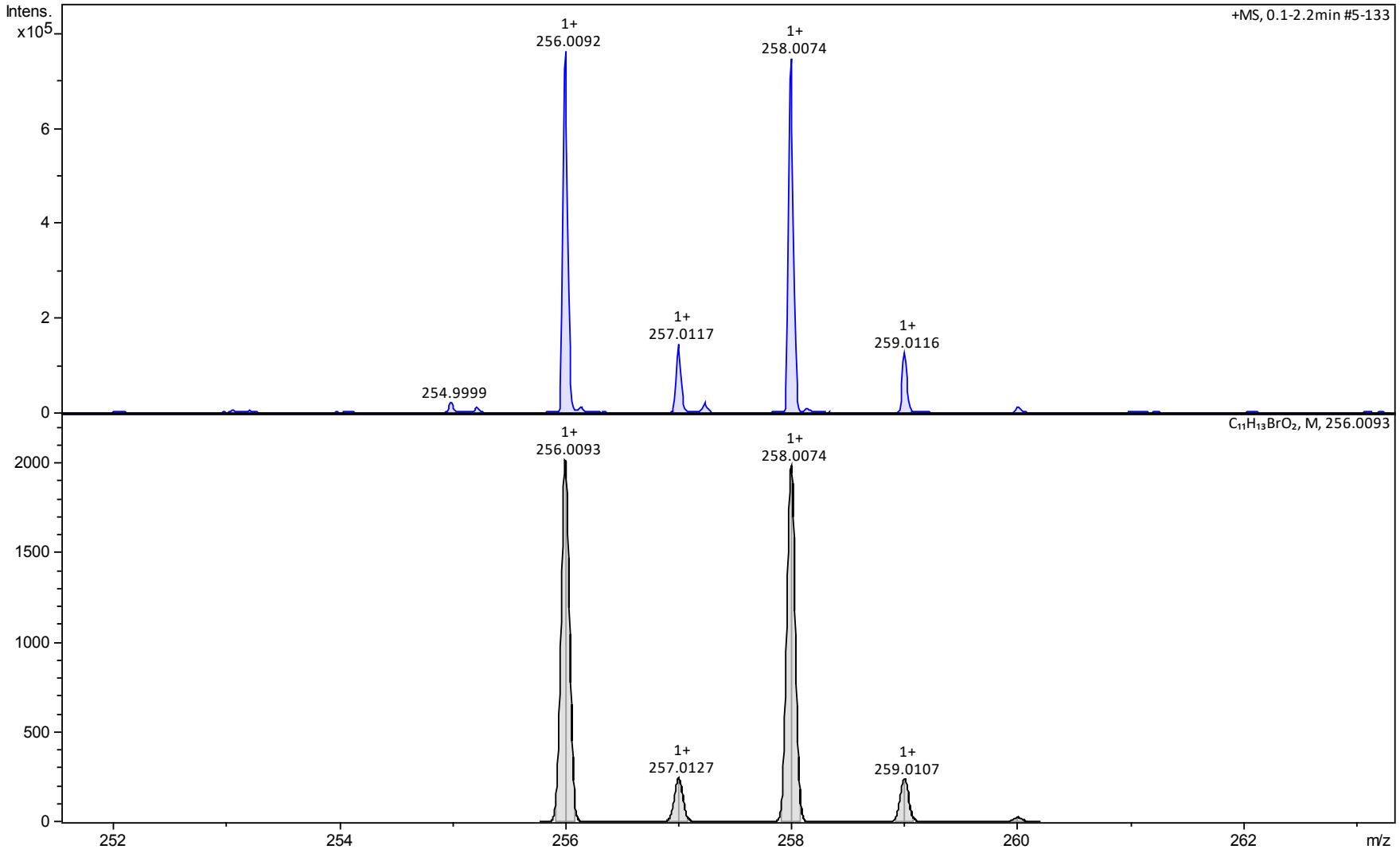
1. Espectro Obtido



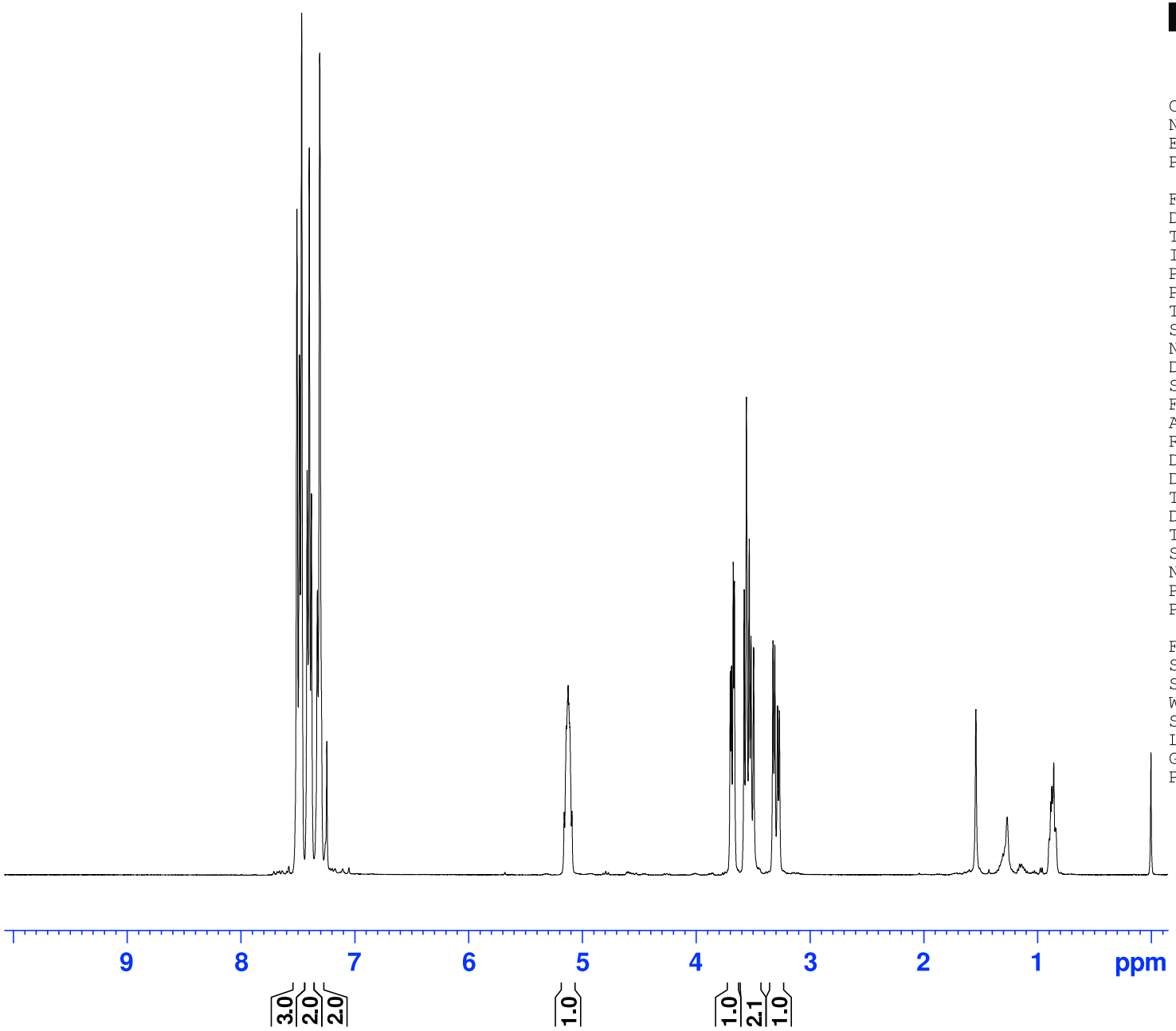
2. Expansão do espectro obtido incluindo os espectros simulados

Espectro obtido

Espectro simulado
Íon $[M]^+$



Compound 2e

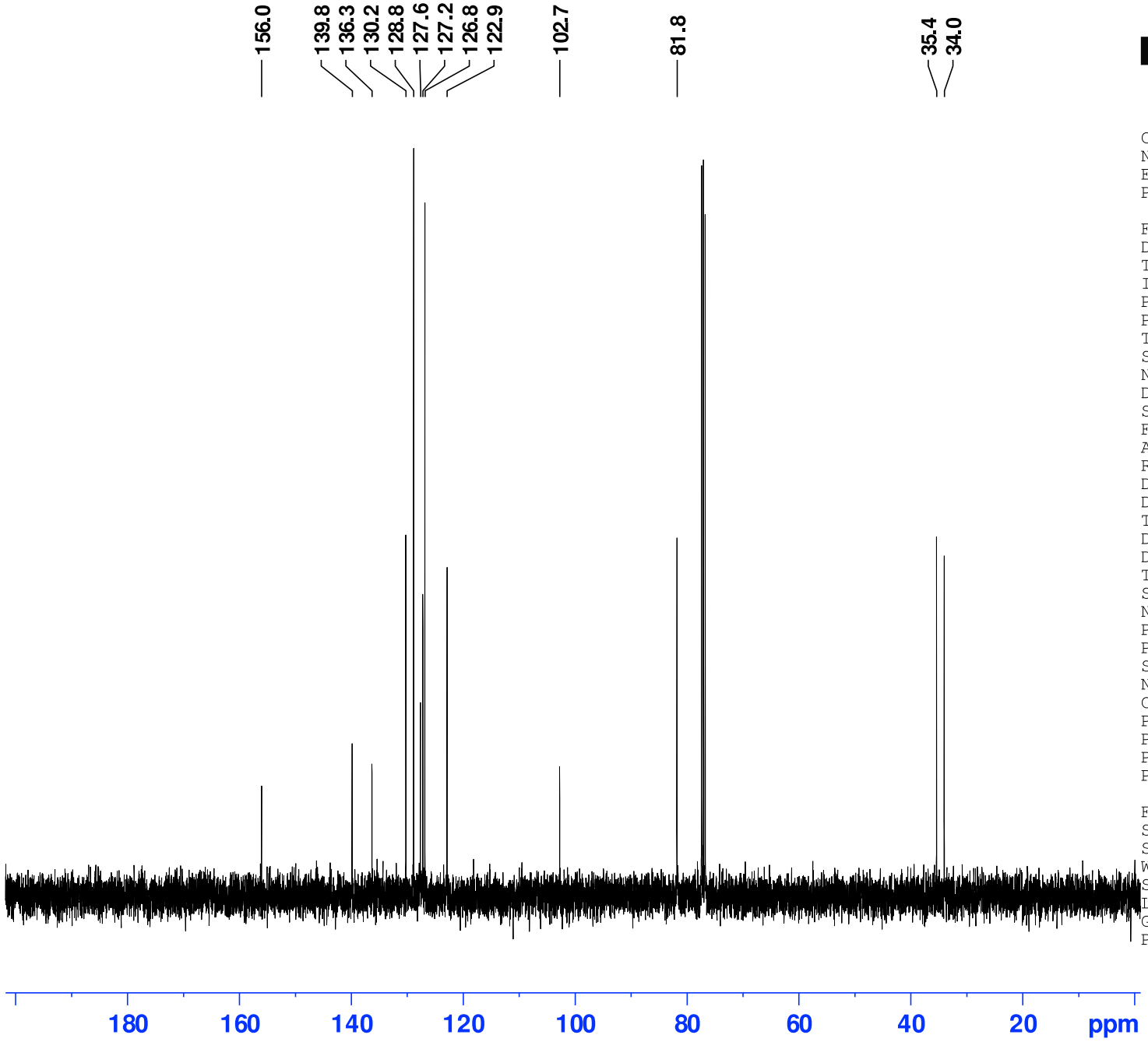



```
Current Data Parameters
NAME            I-CGF-46
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameter
Date_           20181207
Time              13.58 h
INSTRUM             spect
PROBHD   Z8057_0014 (5
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES           0.244532 Hz
AQ              4.0894465 sec
RG                 87.25
DW                62.400 usec
DE                 6.50 usec
TE                300.2 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1324708 MHz
NUC1                  1H
P1                 7.73 usec
PLW1          14.00000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300161 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Compound 2e




```
Current Data Parameters
NAME            I-CGF-46
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameter
Date_           20181207
Time              14.05 h
INSTRUM             spect
PROBHD   Z8057_0014 (5
PULPROG           zgpg30
TD                65536
SOLVENT            CDCl3
NS                   128
DS                     0
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ            1.2582912 sec
RG                197.86
DW               19.200 usec
DE                6.50 usec
TE                300.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         100.6248421 MHz
NUC1                 13C
P1                15.60 usec
PLW1        120.00000000 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         14.00000000 W
PLW12         0.10062000 W
PLW13         0.05061200 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Compound 2e

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: **I-CGF-46**

Responsável pela amostra: Carolina Furst – UFMG (Prof. Eduardo Alberto)

e-mail do responsável: carolfurstg@gmail.com

Amostra submetida em: 28-jun-19

Aquisição e análise: 17-jul-19

Fórmula molecular: $C_{15}H_{12}Br_2O$

Massa exata calculada: $[M]^+$ 367.922957

(massa mais abundante) $[M+H]^+$ 368.930782

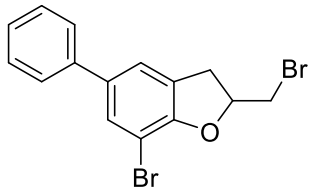
Íons observados: ☑ **$[M]^+$**

☐ **$[M+H]^+$**

☐ *outros:*

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações:

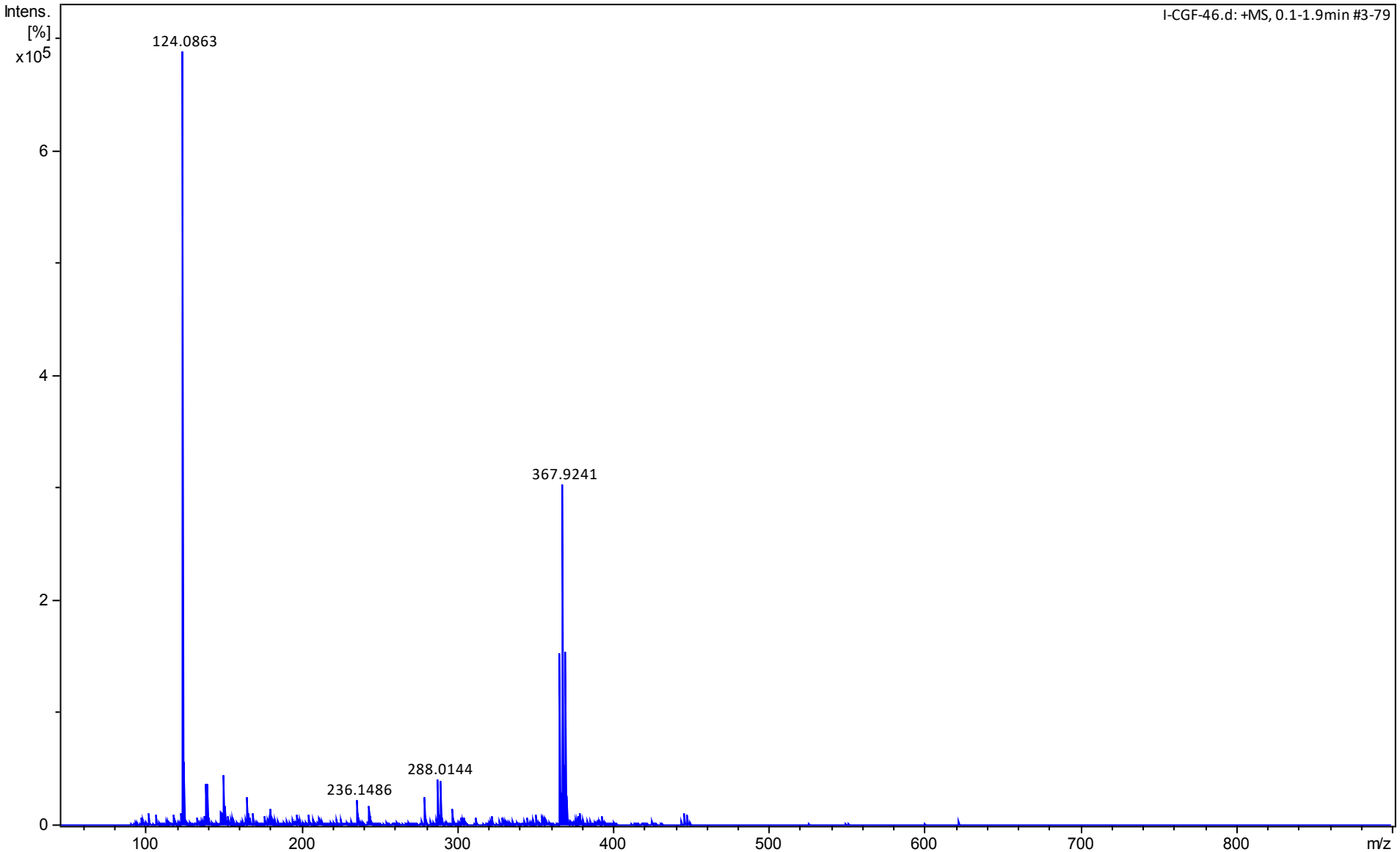
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

Compound 2e

Central de Análises - UCS

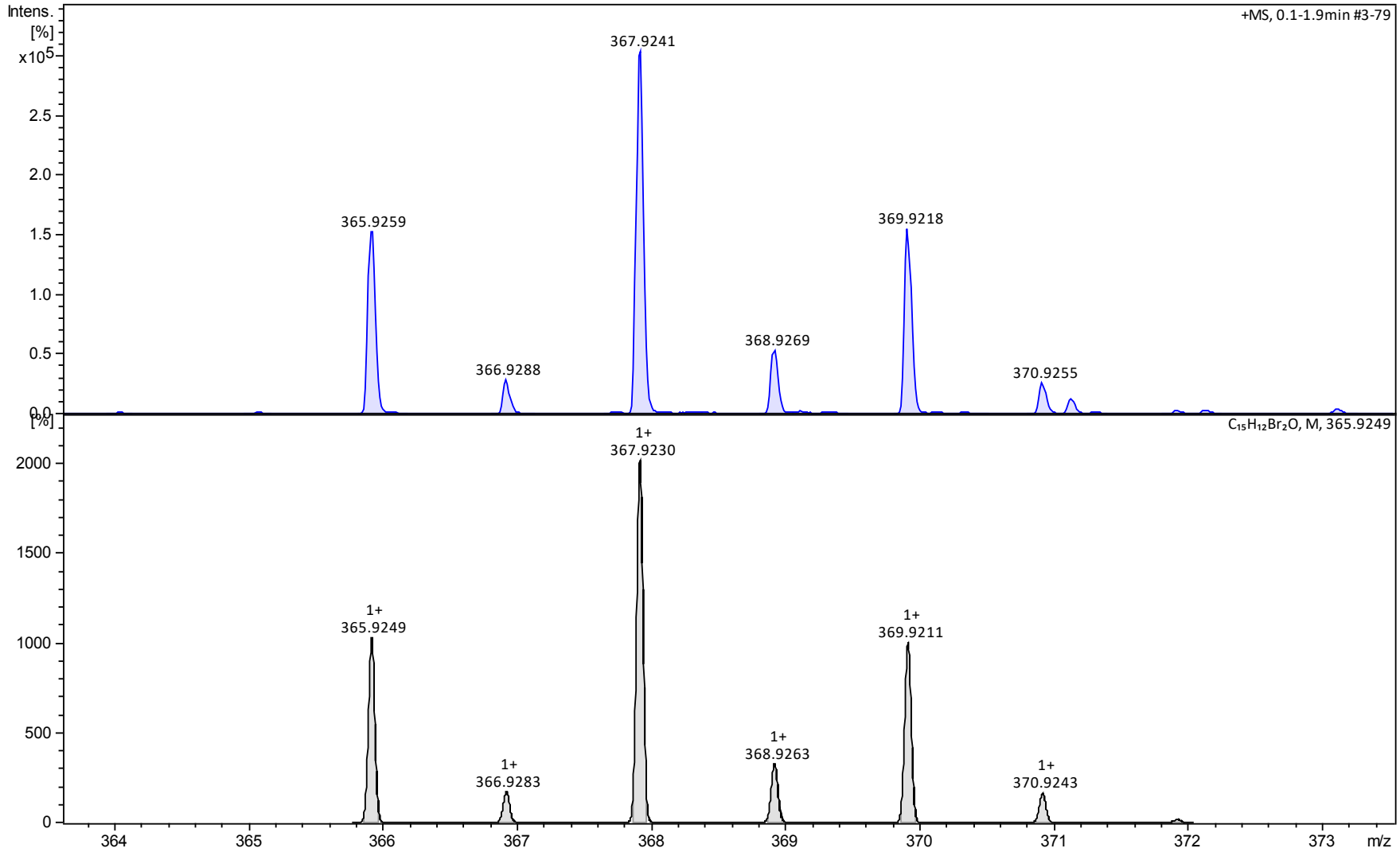
1. Espectro Obtido



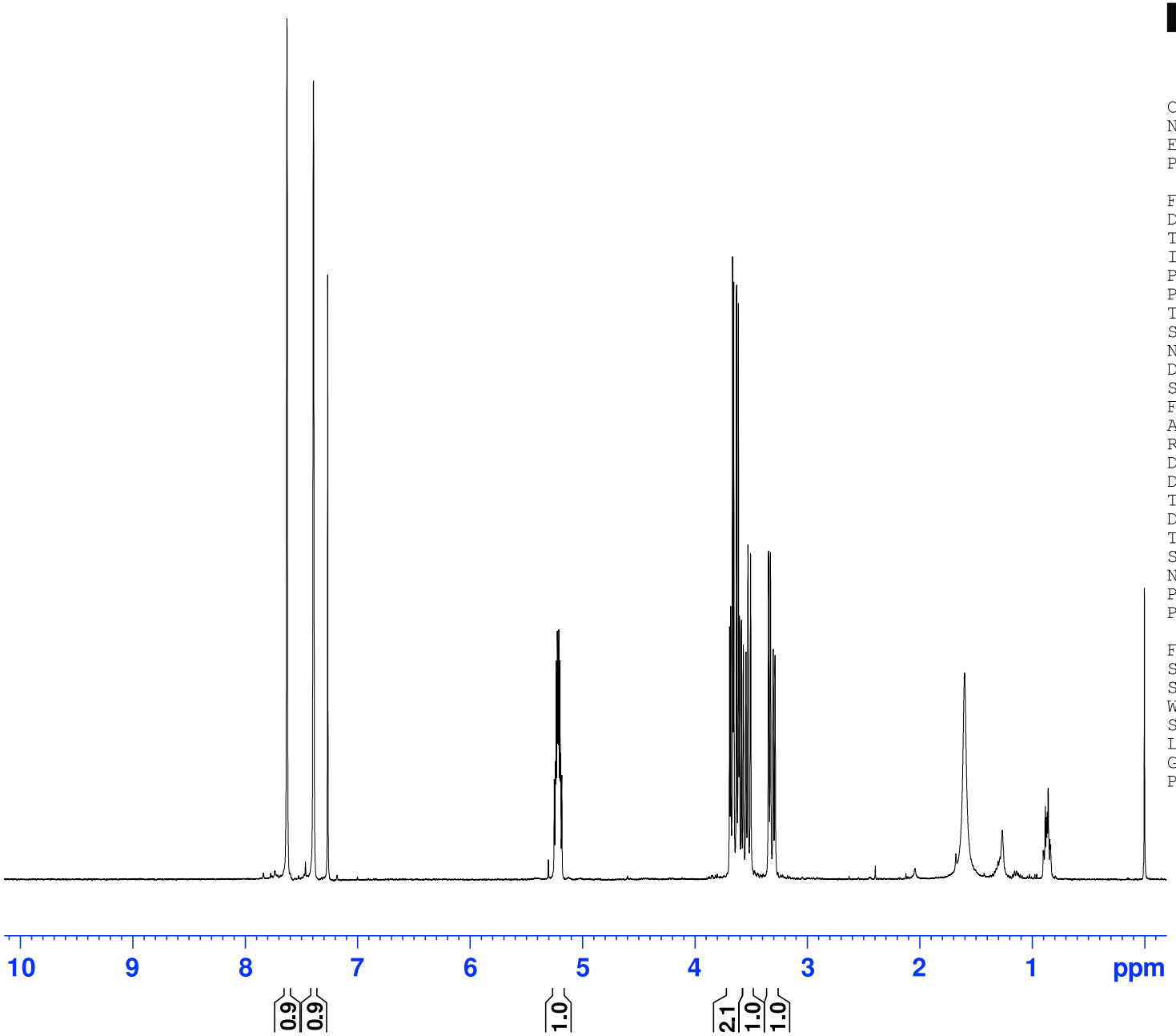
2. Expansão do espectro obtido incluindo os espectros simulados

Espectro obtido (expansão na região de *m/z* do íon de interesse)

Espectro simulado: Íon $[M]^+$



Compound 2f

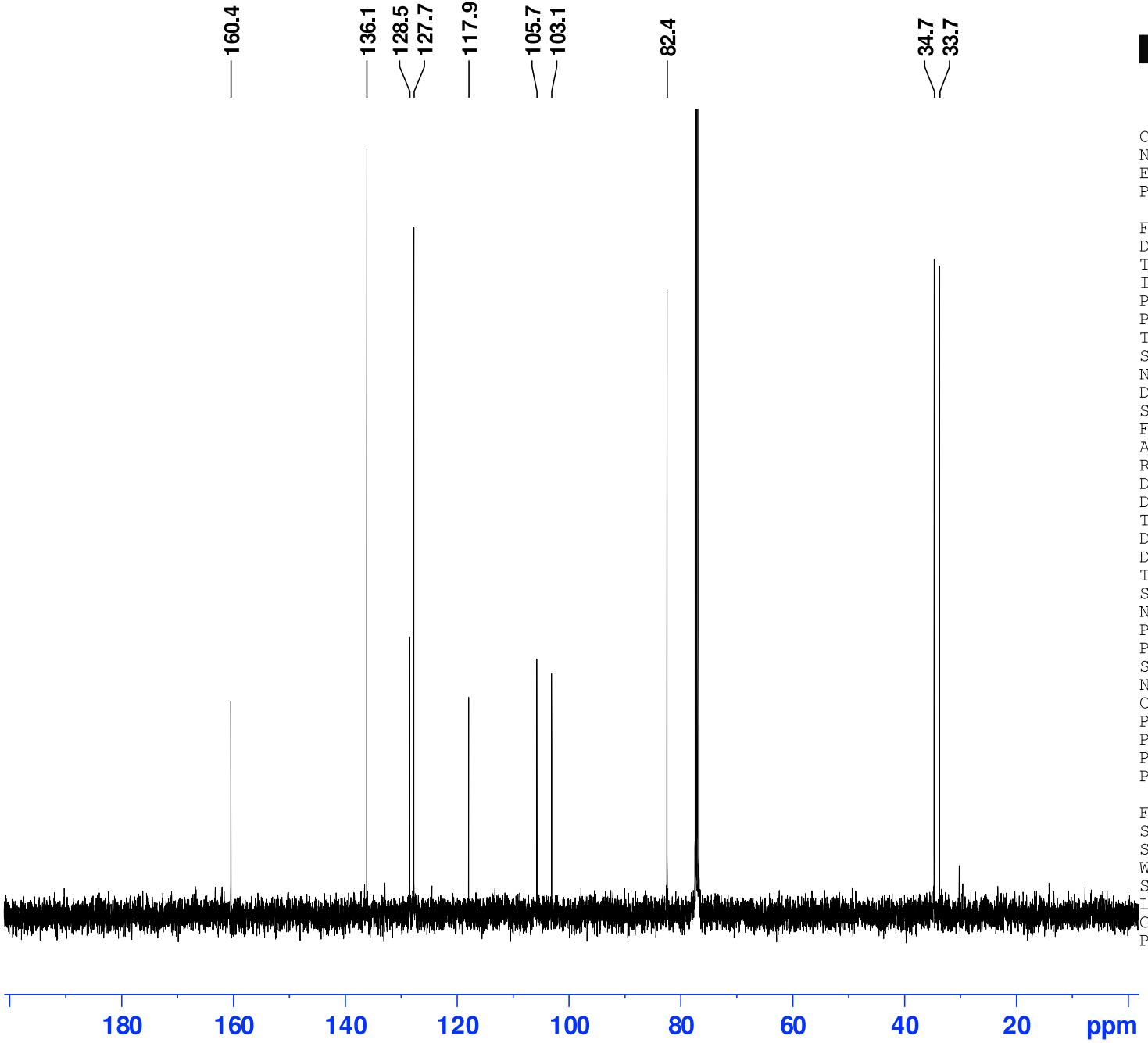



```
Current Data Parameters
NAME      II-CGF-05 ALIX
EXPNO                1
PROCNO               1

F2 - Acquisition Parameter
Date_         20200312
Time              11.55 h
INSTRUM             spect
PROBHD   Z3756_0157 (5
PULPROG             zg30
TD                65536
SOLVENT           CDC13
NS                   16
DS                    0
SWH            8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                197.86
DW                62.400 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                   1
SFO1         400.1324708 MHz
NUC1                 1H
P1                11.34 usec
PLW1         11.19999981 W

F2 - Processing parameters
SI                65536
SF           400.1300076 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Compound 2f



BRUKER

```
Current Data Parameters
NAME          II-CGF-05
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameter
Date_          20191204
Time             12.31 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    2
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ            1.2582912 sec
RG               197.86
DW               19.200 usec
DE               10.00 usec
TE               300.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6238359 MHz
NUC1               13C
P1               13.25 usec
PLW1        17.98900032 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        11.19999981 W
PLW12        0.17781000 W
PLW13        0.08943800 W

F2 - Processing parameters
SI                32768
SF          100.6127685 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Compound 2f

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: II-CGF-05

Responsável pela amostra: Prof. Eduardo E Alberto - UFMG

e-mail do responsável: albertoee.ufmg@gmail.com

Amostra submetida em: 6-jan-20

Aquisição e análise: 22-jan-20

Fórmula molecular: $C_{10}H_7Br_2NO$

Massa exata calculada: $[M]^+$ 316.886874

$[M+H]^+$ 317.894700

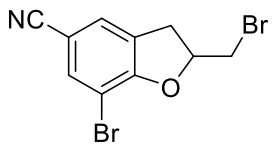
Íons observados: ☑ **$[M]^+$**

☑ **$[M+H]^+$**

☐ *outros*

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações:

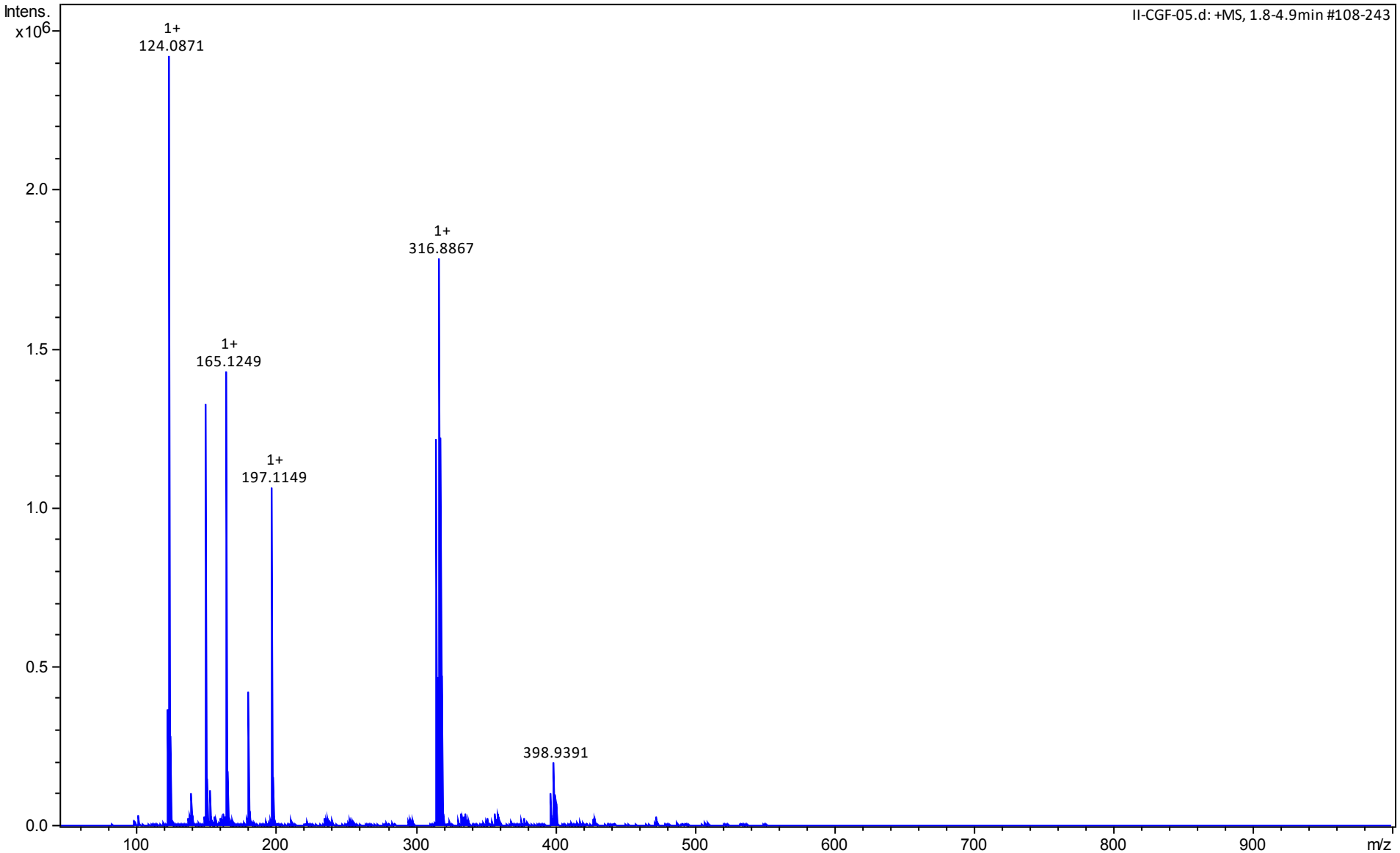
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

Compound 2f

Central de Análises - UCS

1. Espectro Obtido

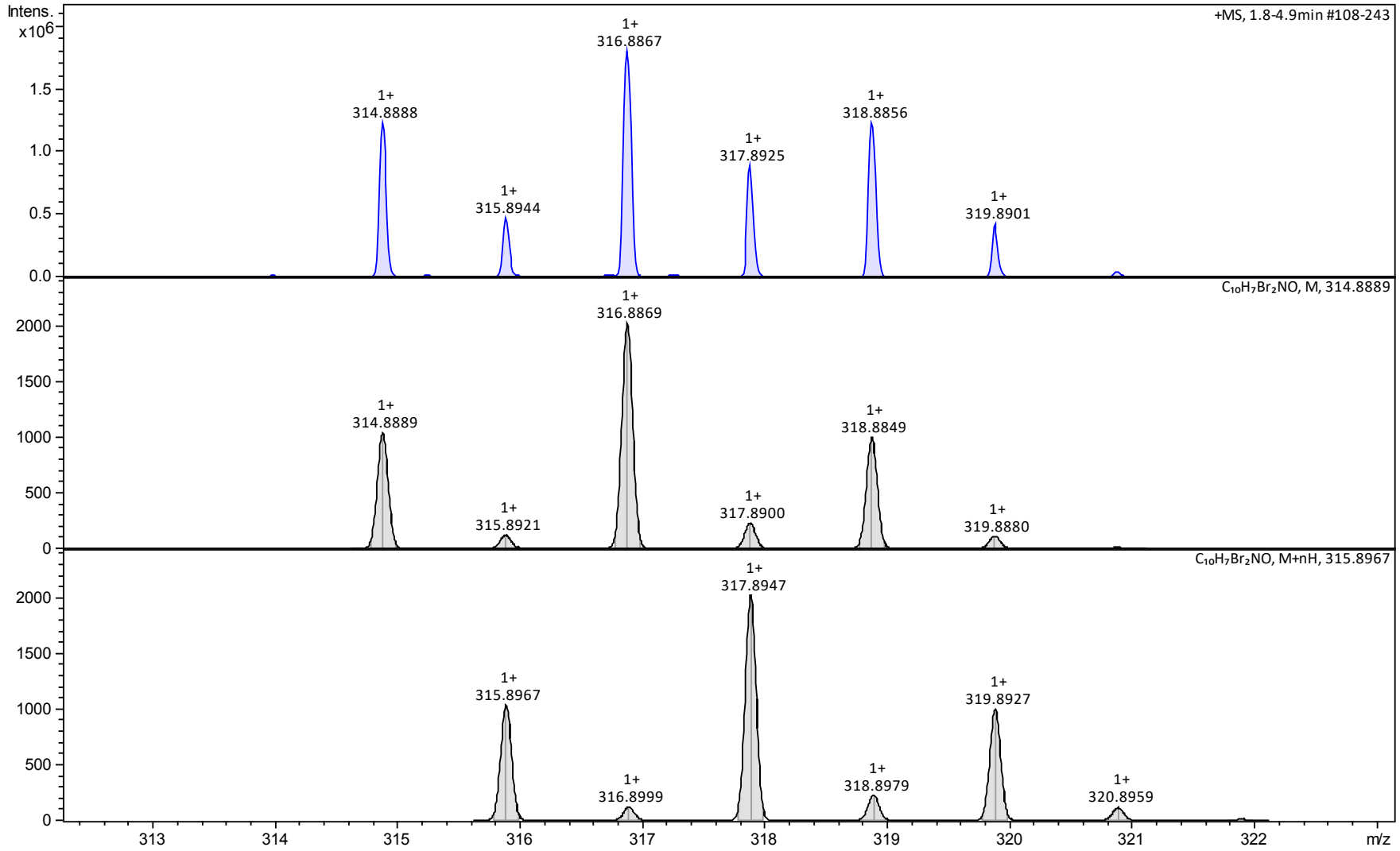


2. Expansão do espectro obtido incluindo os espectros simulados

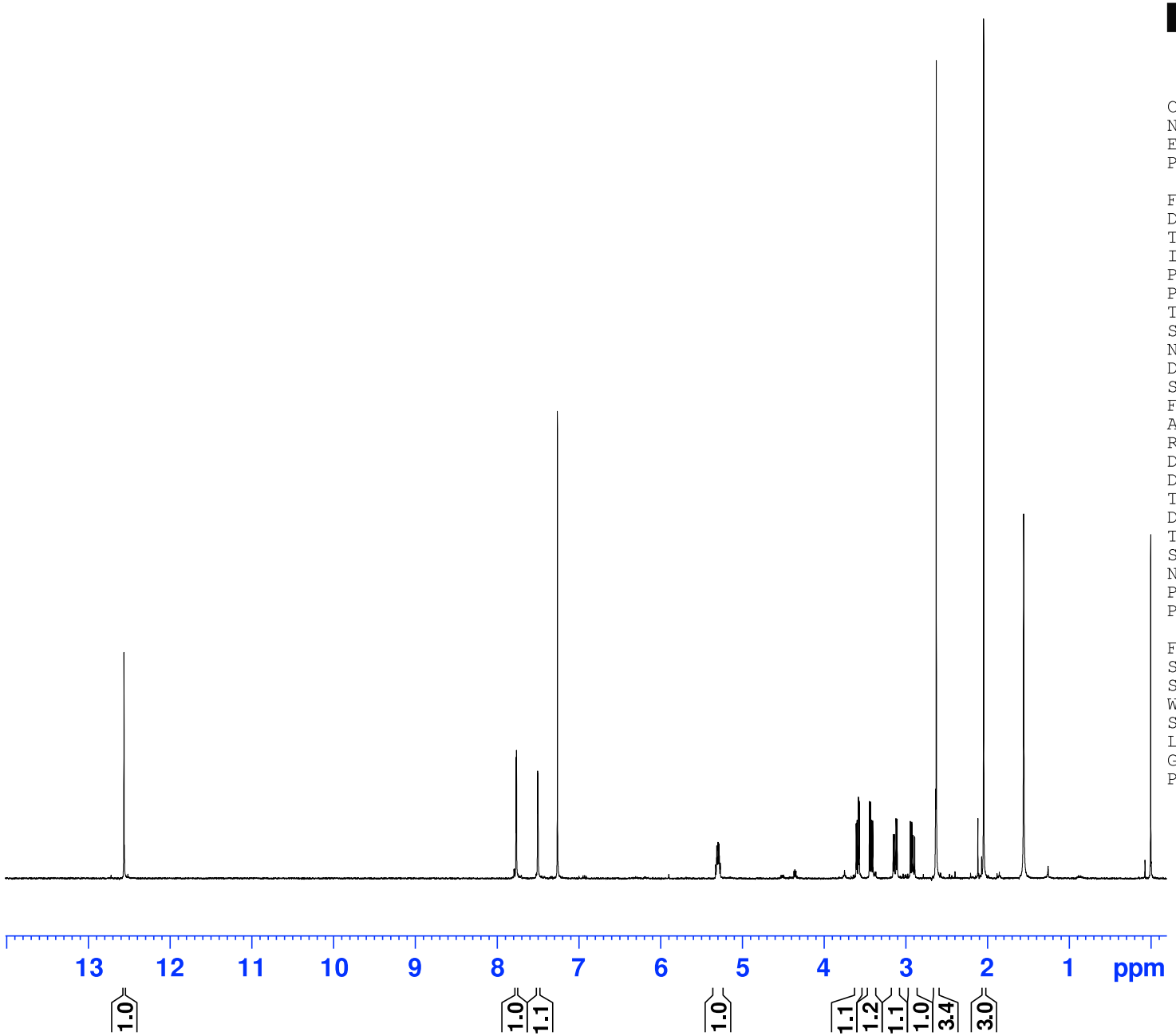
Espectro obtido

Espectro simulado Íon $[M]^+$

Espectro simulado Íon $[M+H]^+$



Compound 2g

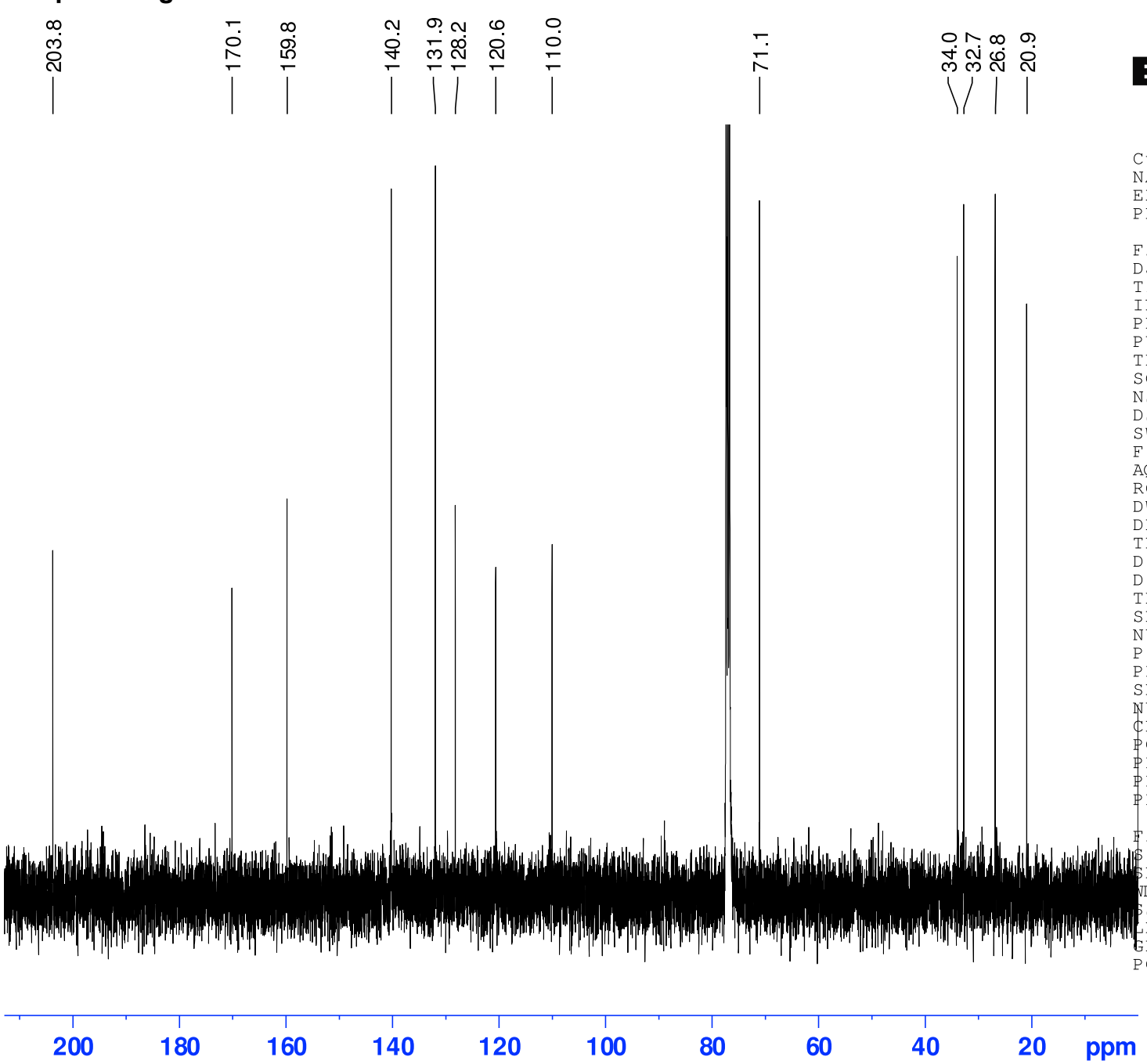



```
Current Data Parameters
NAME     I-CGF-97 solido
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameter
Date_          20190930
Time             16.10 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG            zg30
TD                65536
SOLVENT            CDCl3
NS                    4
DS                    0
SWH            8012.820 Hz
FIDRES          0.244532 Hz
AQ            4.0894465 sec
RG               197.86
DW               62.400 usec
DE               10.00 usec
TE               300.1 K
D1            1.00000000 sec
TD0                   1
SFO1         400.1324708 MHz
NUC1                 1H
P1               11.34 usec
PLW1         11.19999981 W

F2 - Processing parameters
SI                65536
SF           400.1300092 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Compound 2g




```
Current Data Parameters
NAME         i1080_c97s
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameter
Date_          20191003
Time              22.11 h
INSTRUM           spect
PROBHD   Z3750_0125 (5
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 8192
DS                    0
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ            1.2582912 sec
RG               204.69
DW               19.200 usec
DE               12.00 usec
TE               300.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6374161 MHz
NUC1               13C
P1               13.00 usec
PLW1        70.00000000 W
SFO2        400.1816007 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        10.47099972 W
PLW12        0.06889100 W
PLW13        0.03465200 W

F2 - Processing parameters
SI                65536
SF          100.6253400 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

Compound 2g

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: **I-CGF-97**

Responsável pela amostra: Prof. Eduardo E Alberto - UFMG

e-mail do responsável: albertoee.ufmg@gmail.com

Amostra submetida em: 6-jan-20

Aquisição e análise: 22-jan-20

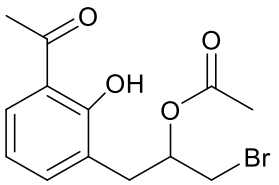
Fórmula molecular: $C_{13}H_{15}BrO_4$

Massa exata calculada: (para o pico de maior intensidade)
$[M]^+$ 314.014822
$[M+H]^+$ 315.022648
$[M-H]^+$ 313.006997

Íons observados:
☐ **$[M]^+$**
☐ **$[M+H]^+$**
☑ *outros* **$[M-H]^+$**

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações: **A formação do íon [M-H]+ quando adquirido no modo de ionização positivo não é comum.**

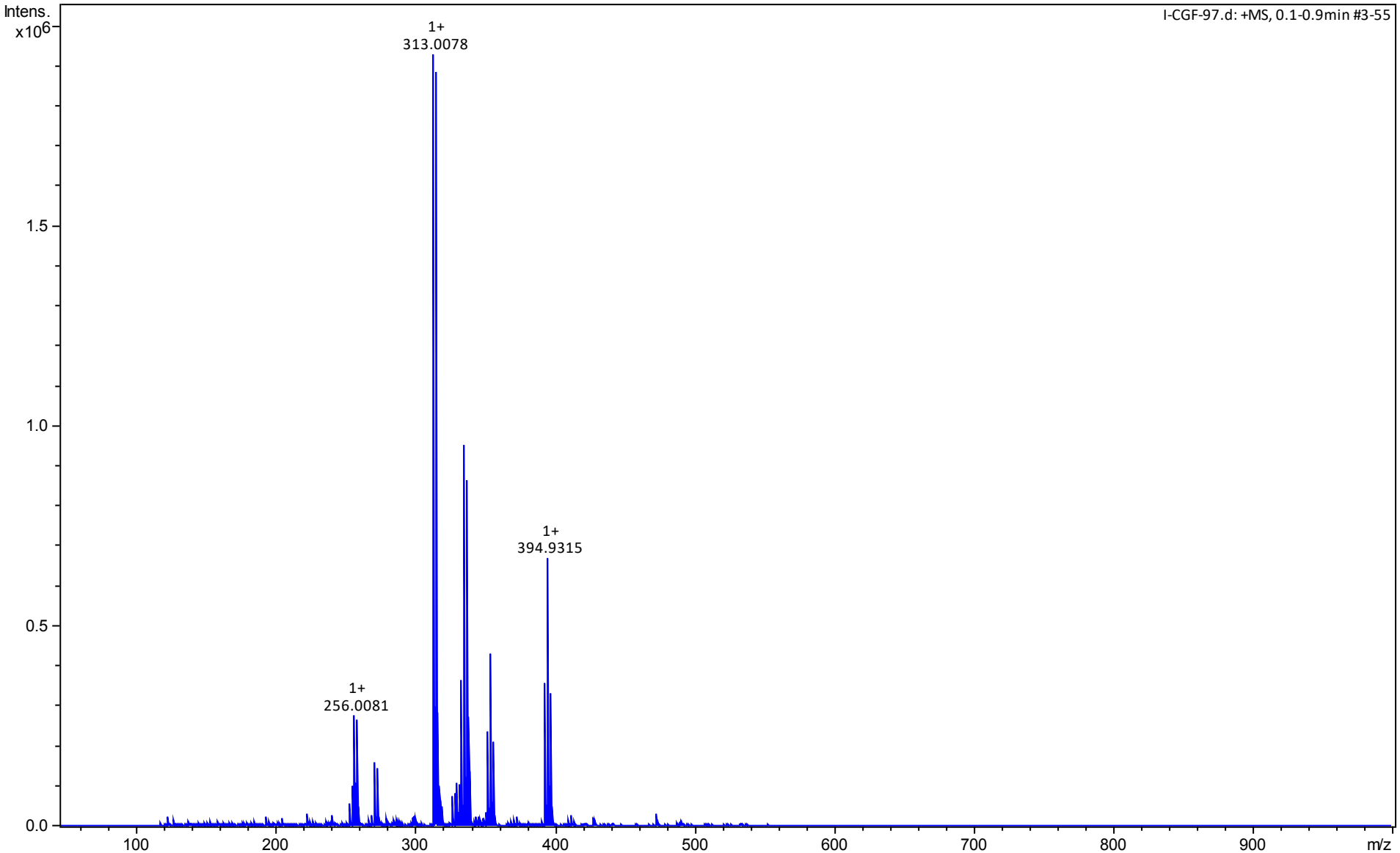
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

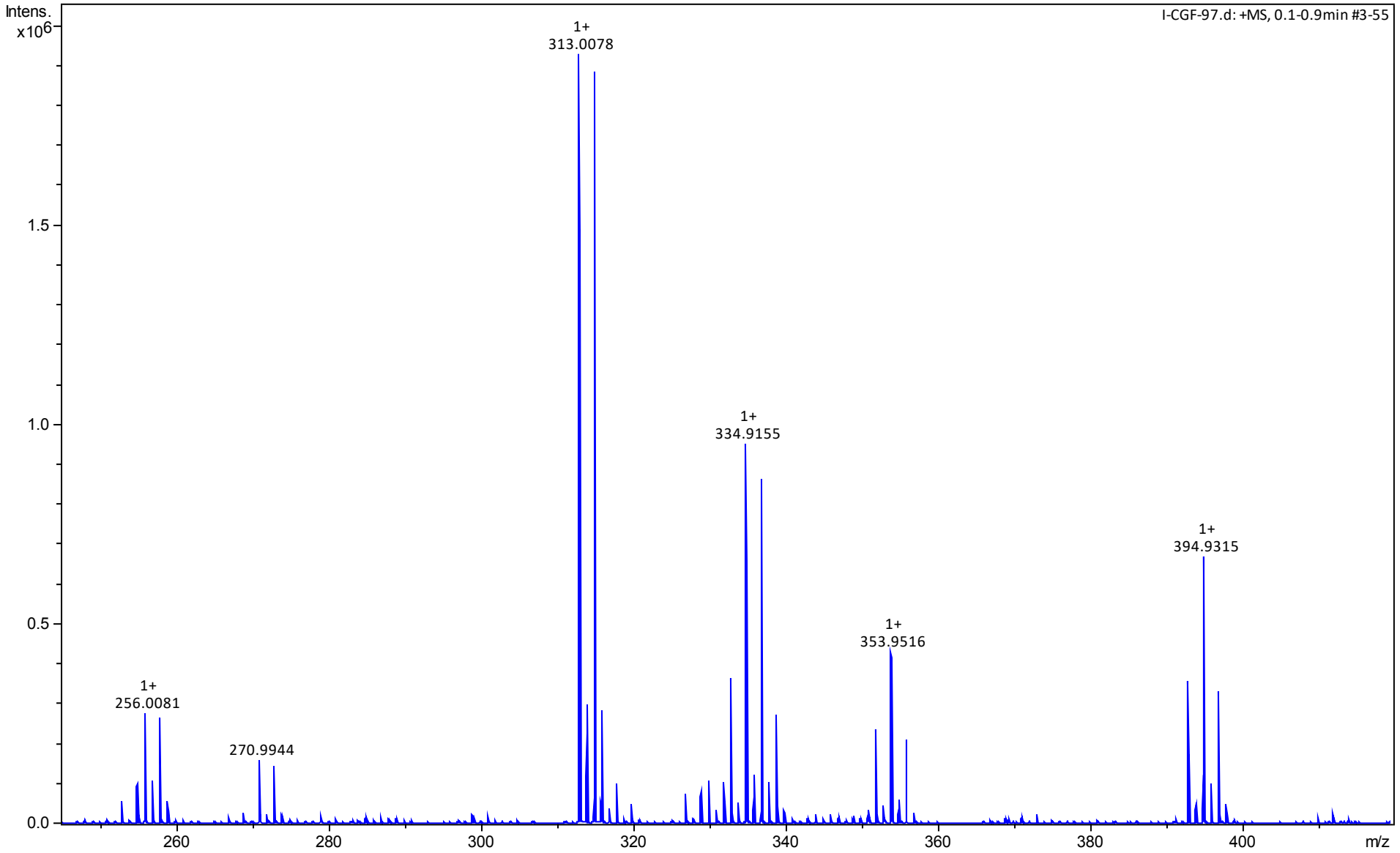
Compound 2g

Central de Análises - UCS

1. Espectro Obtido



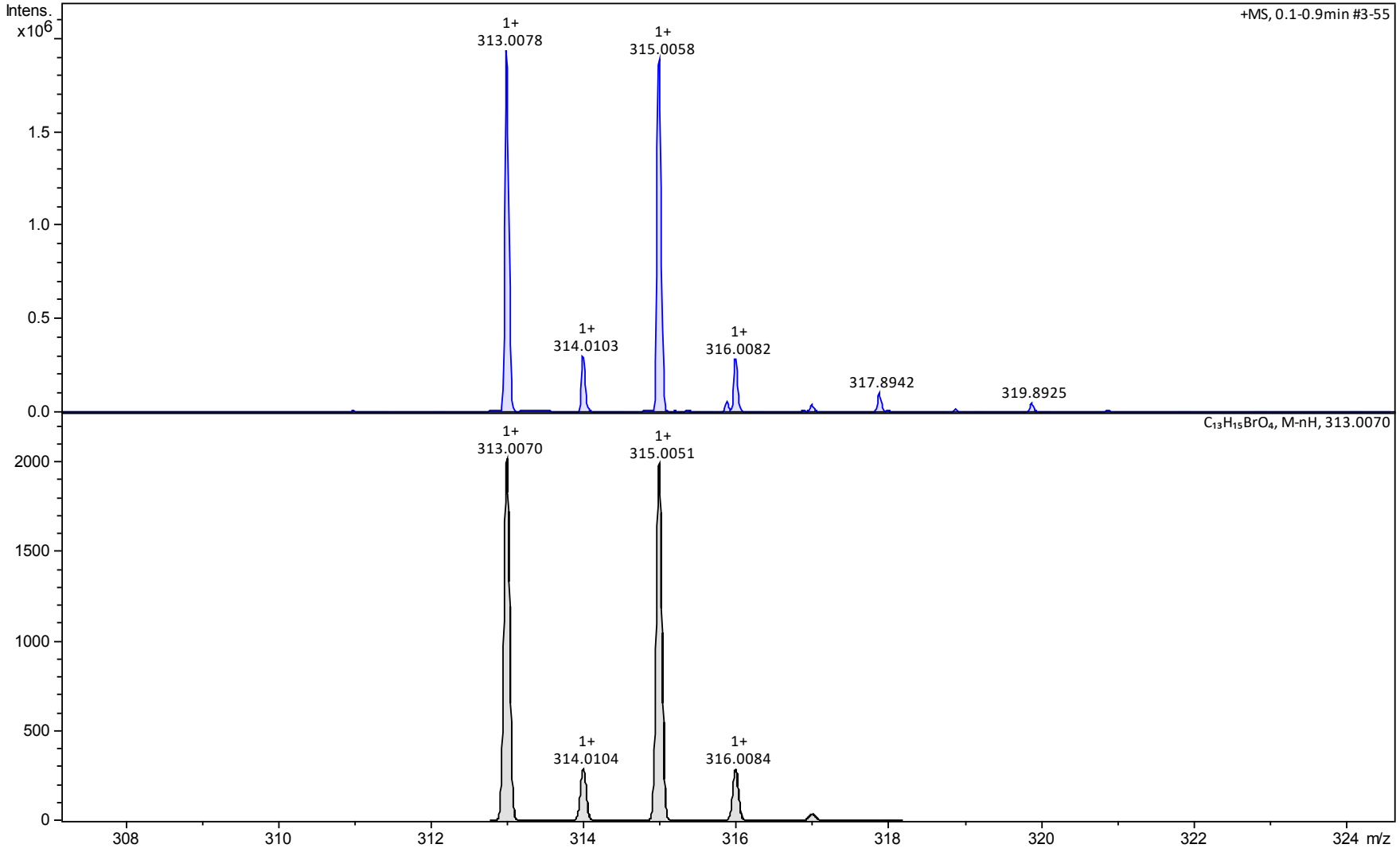
2. Expansão do espectro obtido



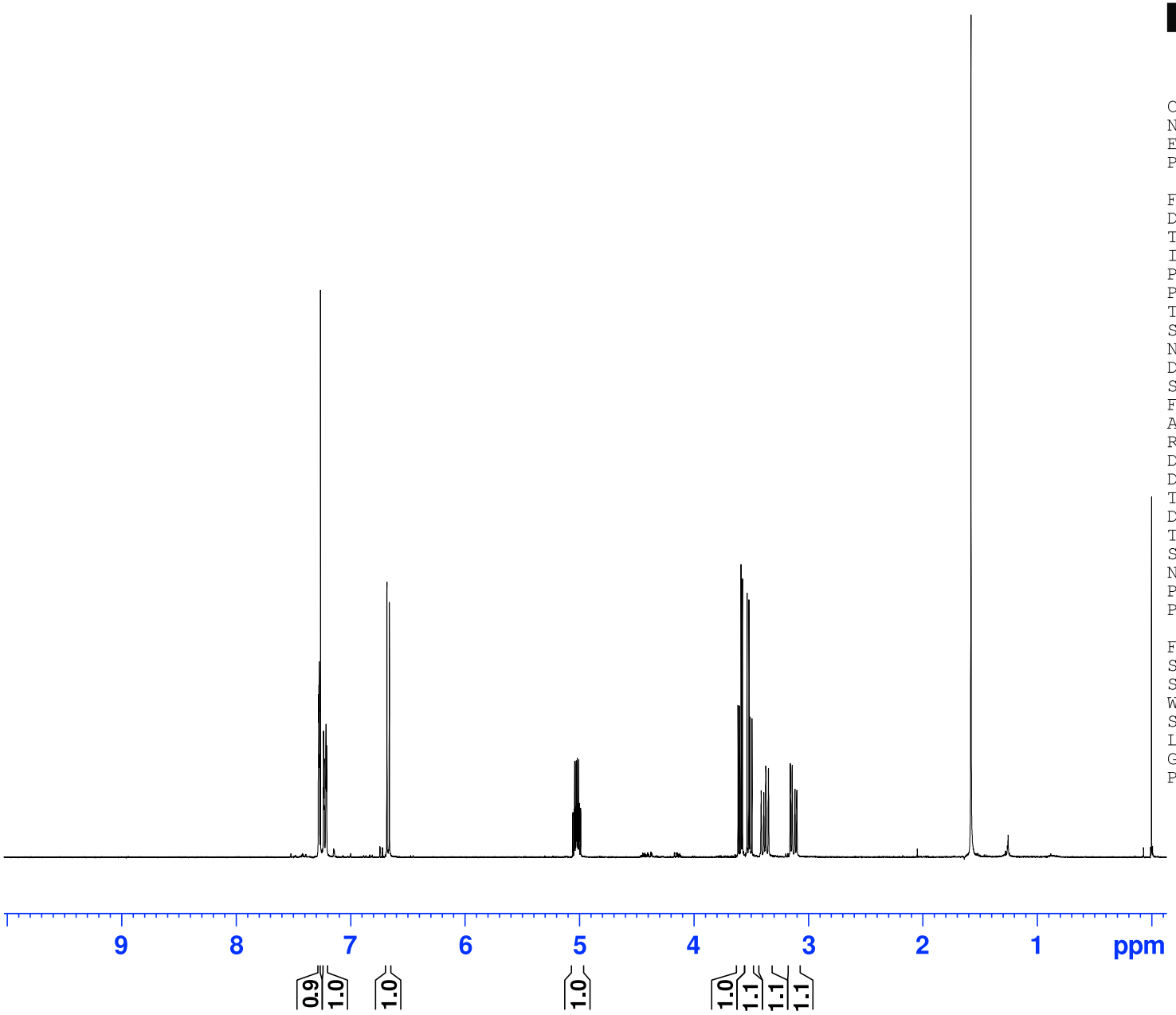
3. Expansão do espectro obtido incluindo os espectros simulados

Espectro obtido

Espectro simulado
Íon $[M-H]^+$



Compound 3

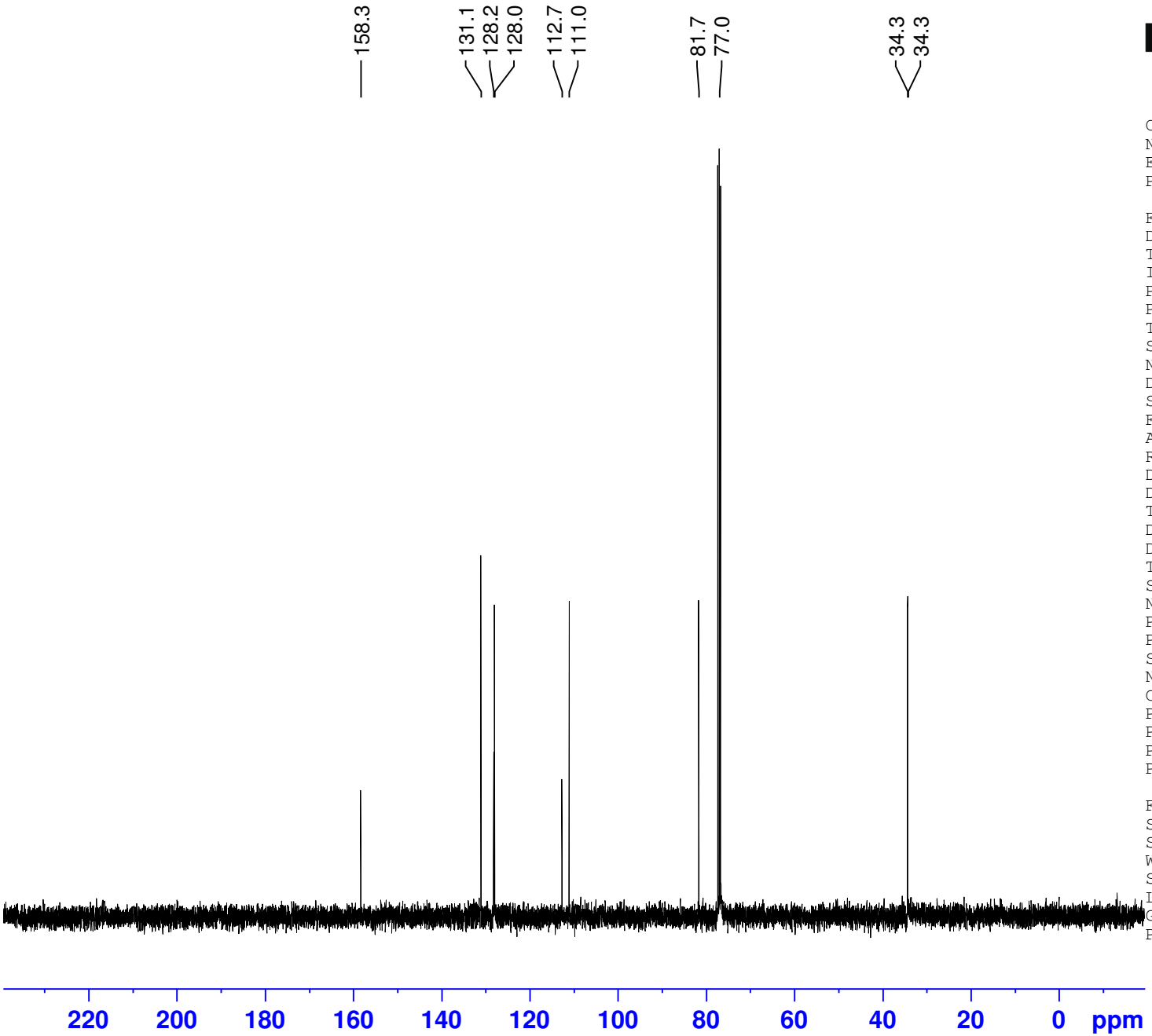



```
Current Data Parameters
NAME       I-CGF-75 6-6
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameter
Date_          20190606
Time               9.07 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8012.820 Hz
FIDRES        0.244532 Hz
AQ            4.0894465 sec
RG               197.86
DW               62.400 usec
DE               10.00 usec
TE               295.7 K
D1            1.00000000 sec
TD0                   1
SFO1         400.1324708 MHz
NUC1                 1H
P1               11.42 usec
PLW1         11.19999981 W

F2 - Processing parameters
SI                65536
SF           400.1300089 MHz
WDW                  GM
SSB      0
LB                -0.30 Hz
GB                  0.2
PC                 1.00
```

Compound 3




```
Current Data Parameters
NAME            I-CGF-75
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190502
Time               18.21 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     2
SWH            26041.666 Hz
FIDRES          0.794729 Hz
AQ             1.2582912 sec
RG                197.86
DW                19.200 usec
DE                10.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         100.6238359 MHz
NUC1                13C
P1                13.25 usec
PLW1         17.98900032 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.19999981 W
PLW12         0.18032999 W
PLW13         0.09070400 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Compound 3

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: **I-CGF-75**

Responsável pela amostra: Carolina Furst – UFMG (Prof. Eduardo Alberto)

e-mail do responsável: carolfurstg@gmail.com

Amostra submetida em: 28-jun-19

Aquisição e análise: 17-jul-19

Fórmula molecular: $C_9H_8Br_2O$

Massa exata calculada: $[M]^+$ 291.891620

(massa mais abundante) $[M+H]^+$ 292.899445

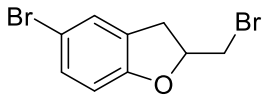
Íons observados: ☑ **$[M]^+$**

☐ **$[M+H]^+$**

☐ *outros:*

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações:

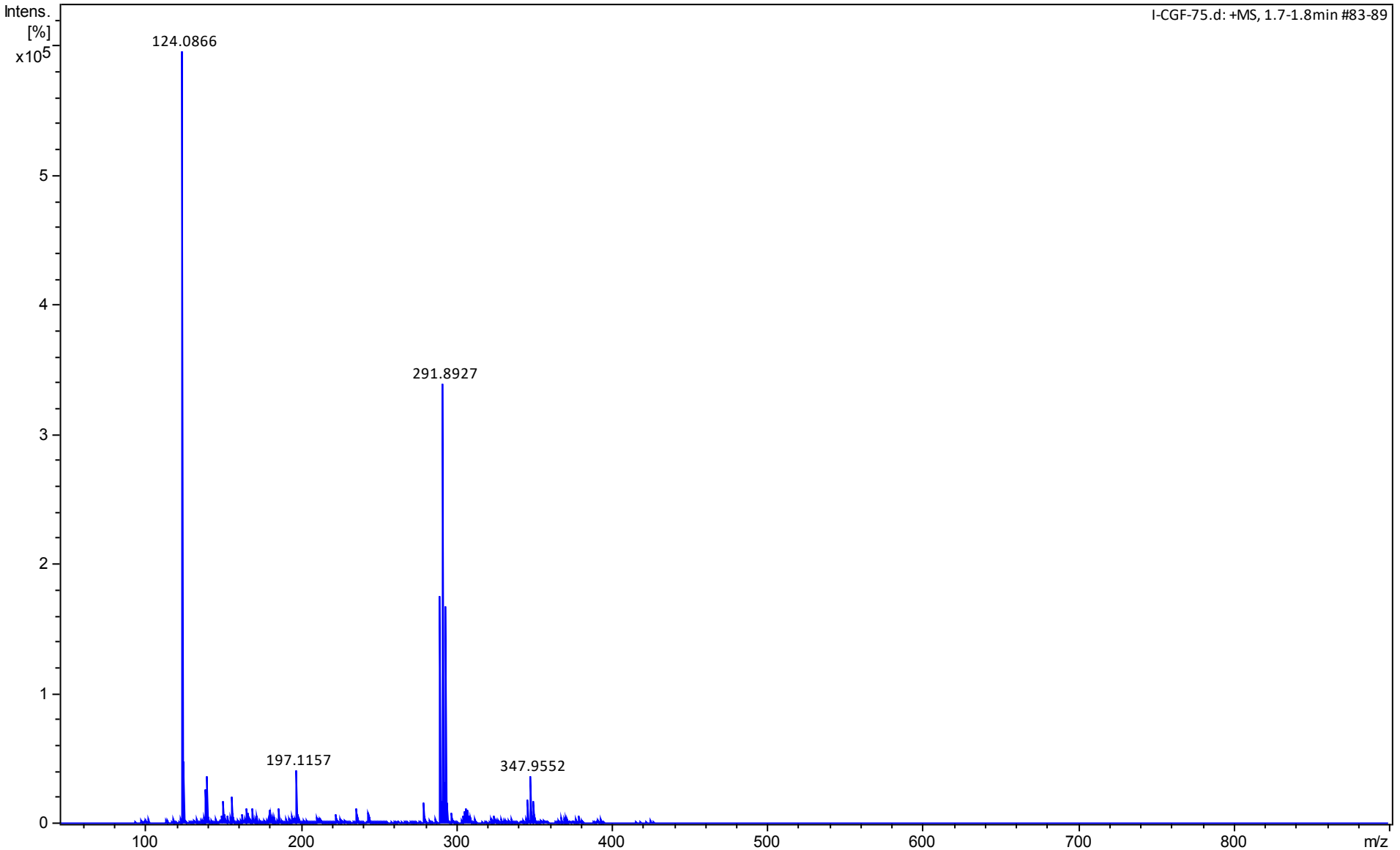
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

Compound 3

Central de Análises - UCS

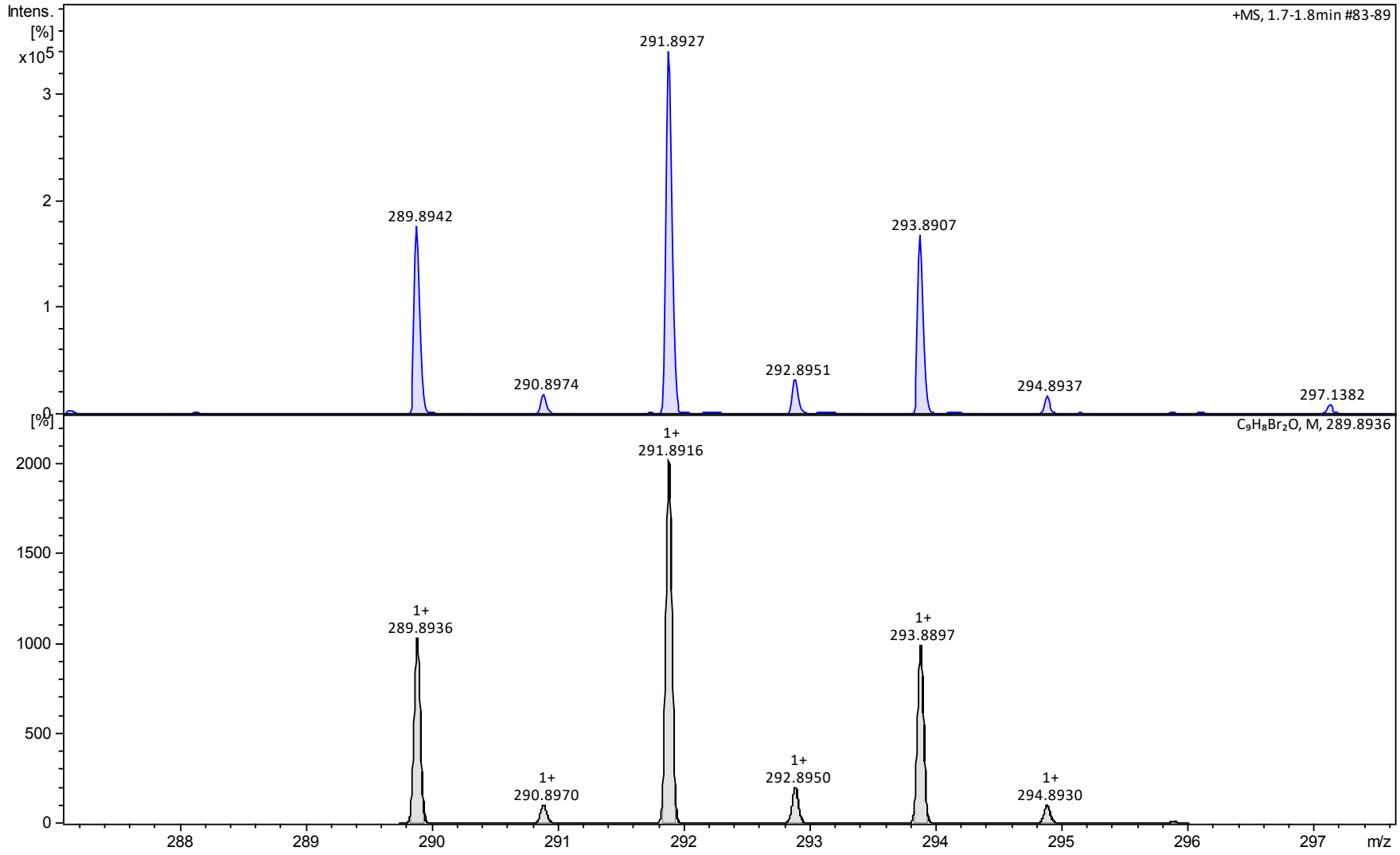
1. Espectro Obtido



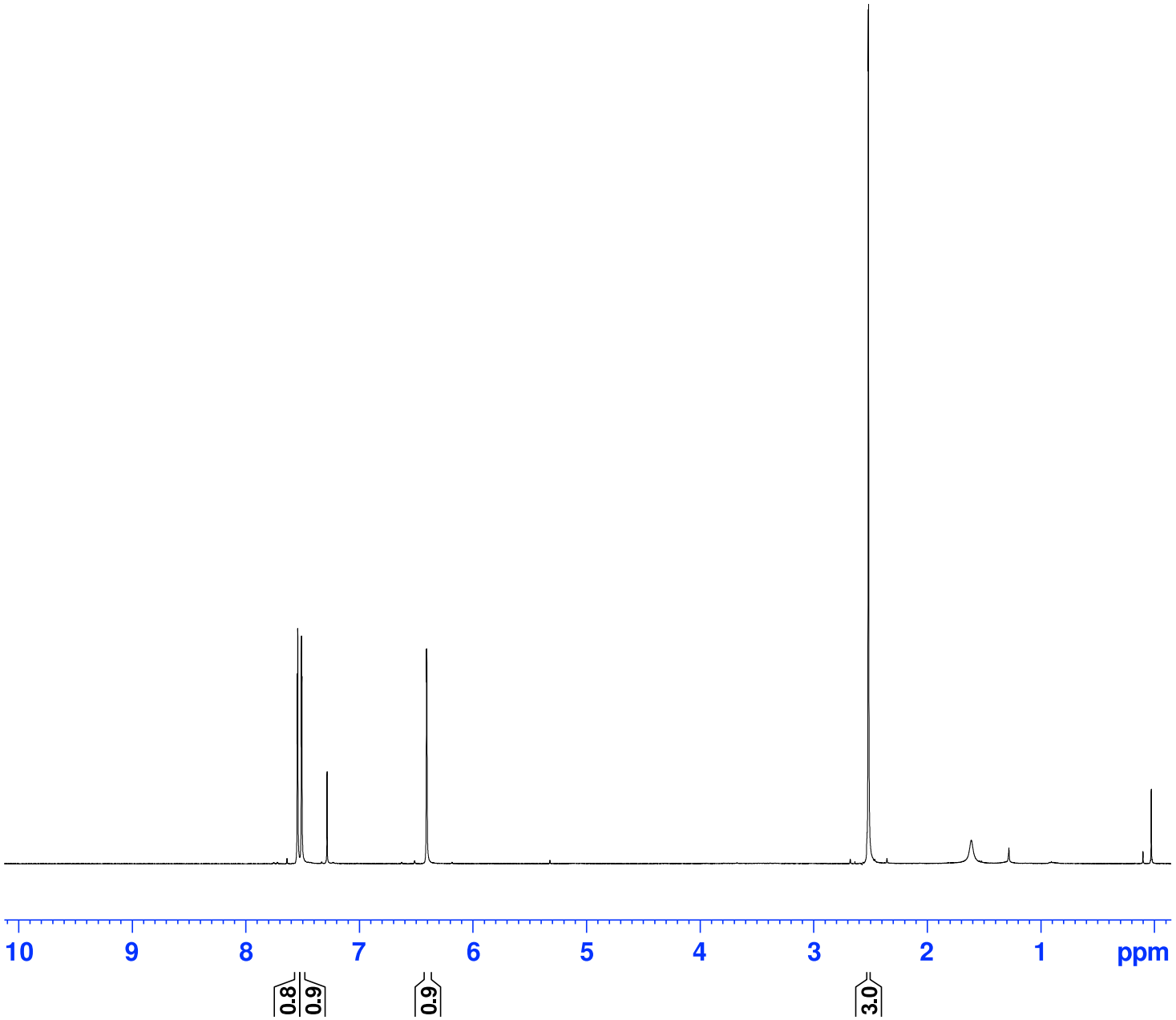
2. Expansão do espectro obtido incluindo os espectros simulados

Espectro obtido (expansão na região de *m/z* do íon de interesse)

Espectro simulado: Íon $[M]^+$



Compound 4a

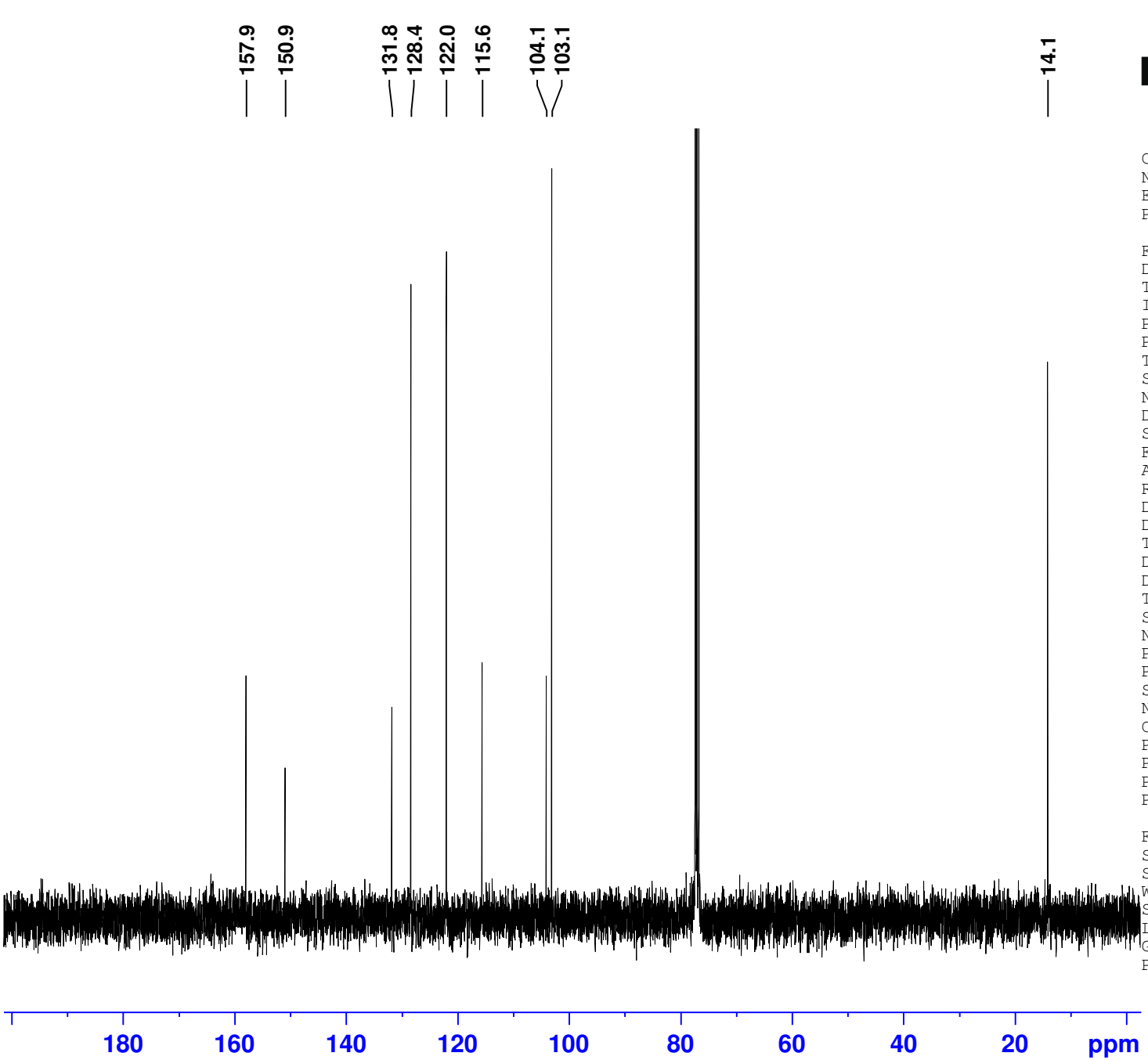



```
Current Data Parameters
NAME          II-CGF-03
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameter
Date_          20191122
Time             10.40 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG            zg30
TD                65536
SOLVENT            CDCl3
NS                    4
DS                    0
SWH            8012.820 Hz
FIDRES          0.244532 Hz
AQ            4.0894465 sec
RG                197.86
DW                62.400 usec
DE                10.00 usec
TE                300.2 K
D1           1.00000000 sec
TD0                   1
SFO1         400.1324708 MHz
NUC1                  1H
P1                11.34 usec
PLW1         11.19999981 W

F2 - Processing parameters
SI                65536
SF           400.1300000 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Compound 4a




```
Current Data Parameters
NAME          II-CGF-03
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20191122
Time              10.32 h
INSTRUM           spect
PROBHD   Z3756_0157 (5
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    2
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ            1.2582912 sec
RG               197.86
DW               19.200 usec
DE               10.00 usec
TE                300.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6238359 MHz
NUC1               13C
P1               13.25 usec
PLW1        17.98900032 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        11.19999981 W
PLW12        0.17781000 W
PLW13        0.08943800 W

F2 - Processing parameters
SI                32768
SF          100.6127685 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Compound 4a

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: **II-CGF-03**

Responsável pela amostra: Prof. Eduardo E Alberto - UFMG

e-mail do responsável: albertoee.ufmg@gmail.com

Amostra submetida em: 6-jan-20

Aquisição e análise: 22-jan-20

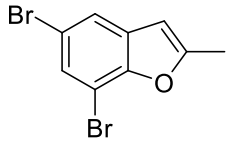
Fórmula molecular: $C_9H_6Br_2O$

Massa exata calculada: $[M]^+$ 289.875970
(para o pico de maior intensidade) $[M+H]^+$ 290.883795

Íons observados: ☐ **$[M]^+$**
☑ **$[M+H]^+$**
☐ *outros*

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações:

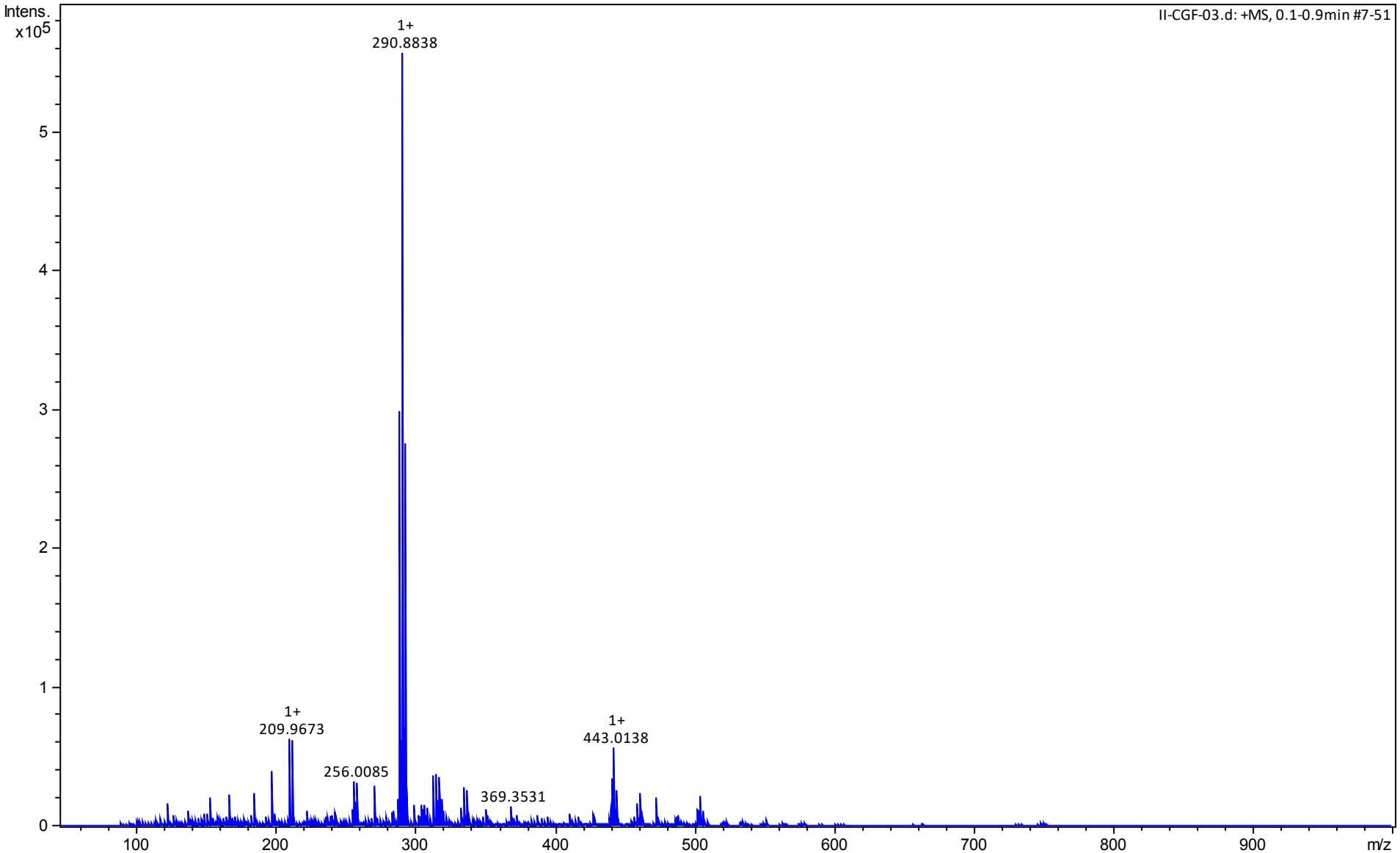
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

Compound 4a

Central de Análises - UCS

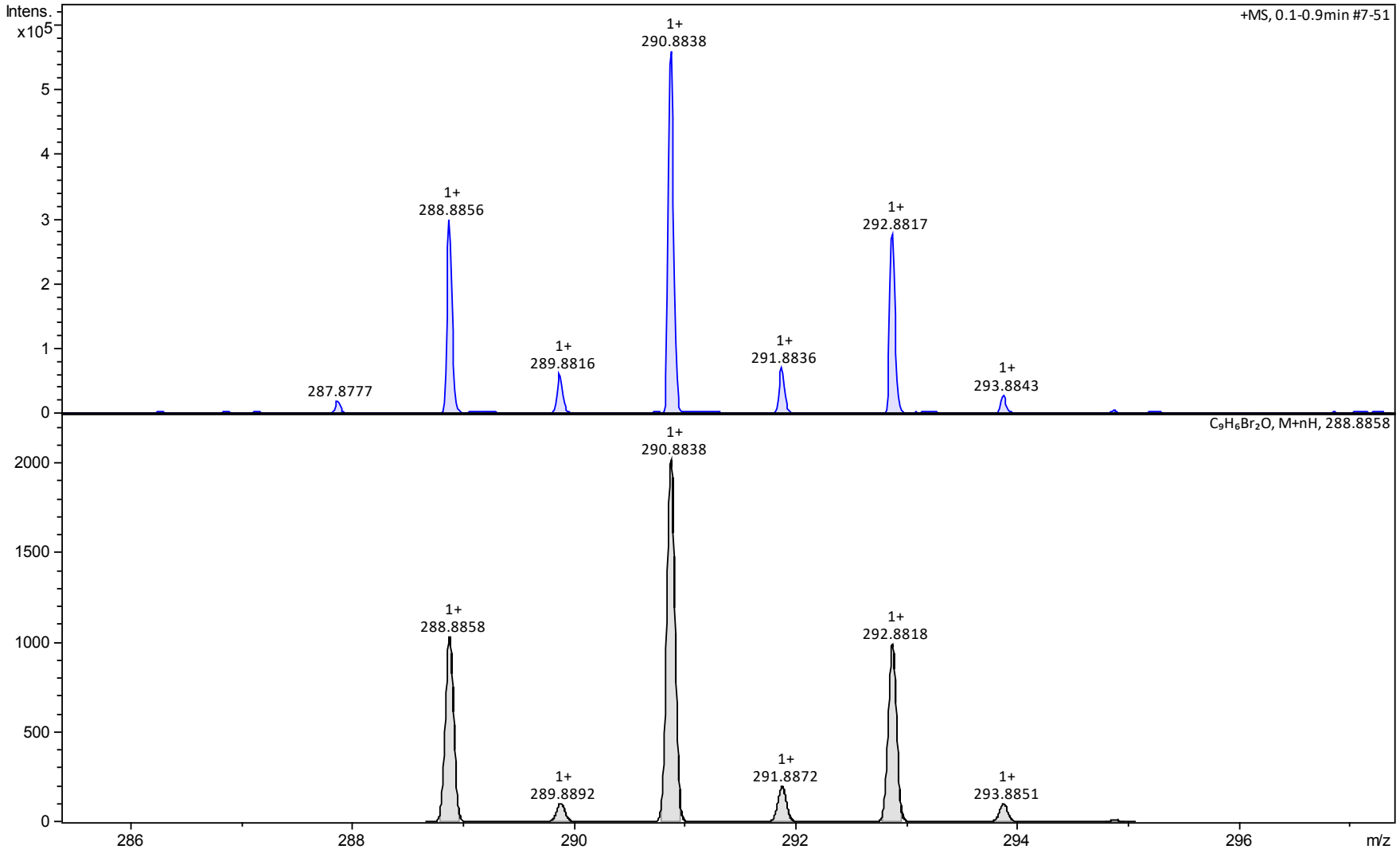
1. Espectro Obtido



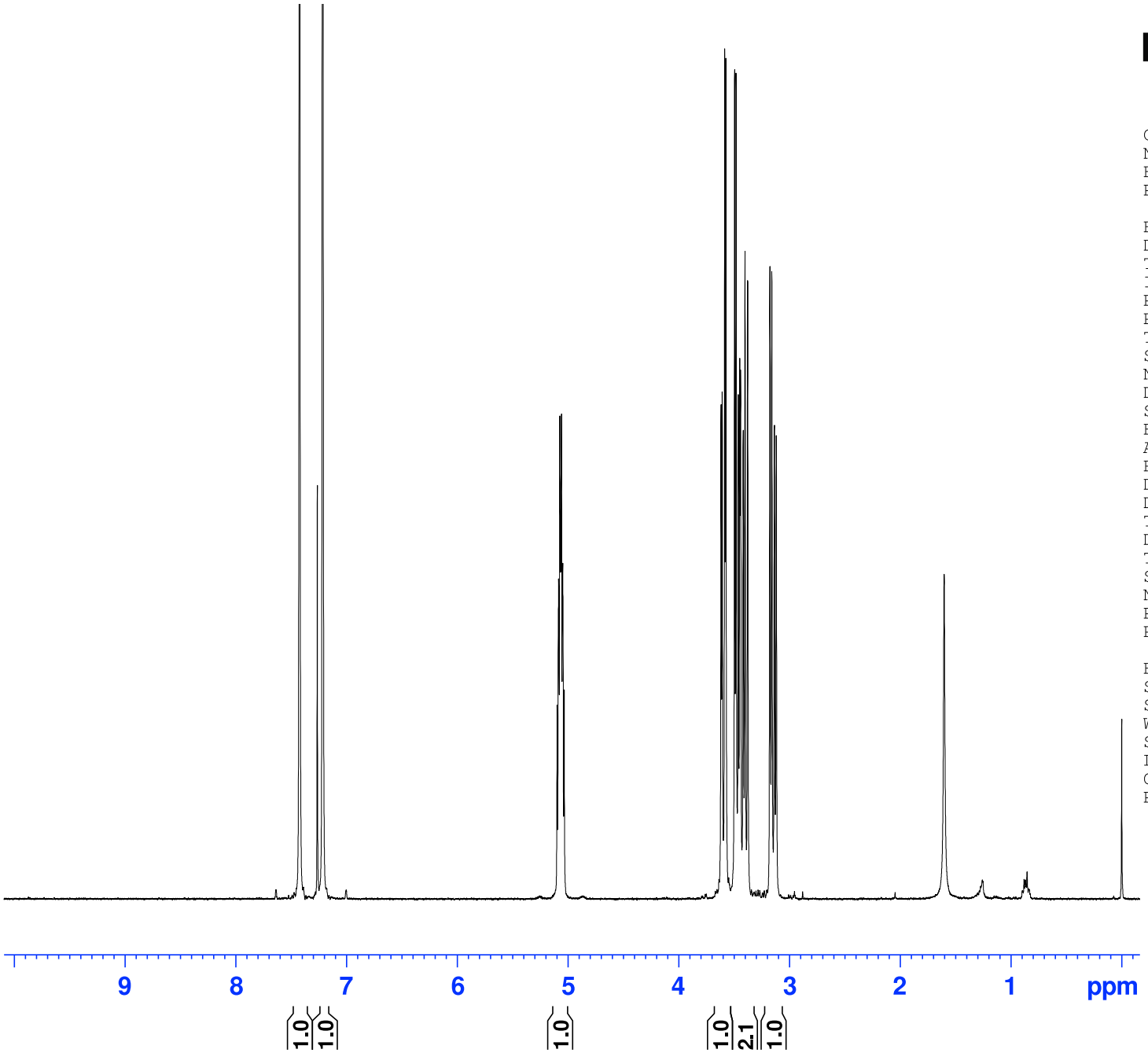
2. Expansão do espectro obtido incluindo os espectros simulados

Espectro obtido

Espectro simulado
Íon $[M+H]^+$



Compound 5a

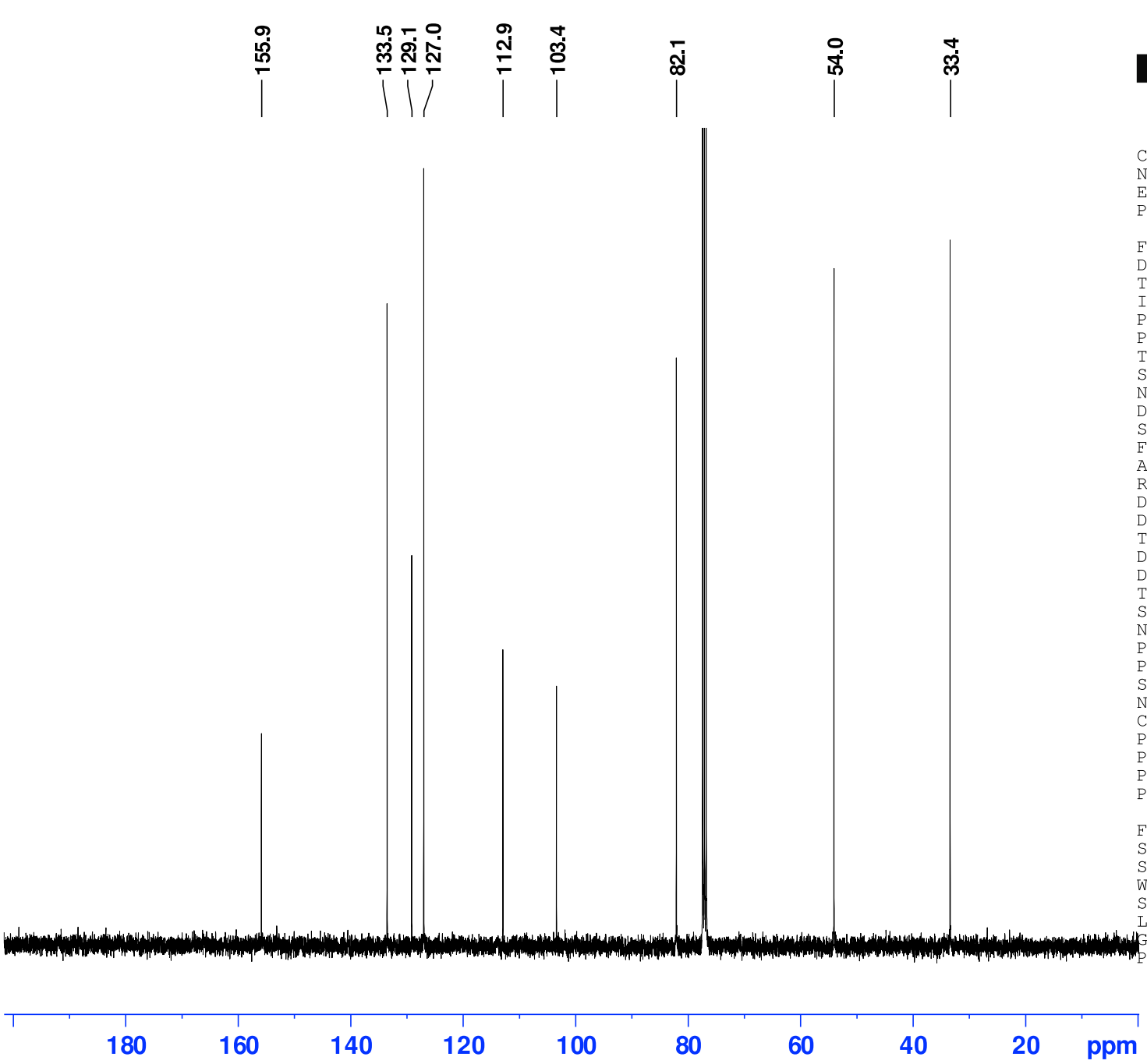



```
Current Data Parameters
NAME            I-CGF-80
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameter
Date_           20190610
Time                9.27 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                154.14
DW                62.400 usec
DE                10.00 usec
TE                294.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                11.42 usec
PLW1         11.19999981 W

F2 - Processing parameters
SI                 65536
SF           400.1300078 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Compound 5a




```
Current Data Parameters
NAME            I-CGF-80
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameter
Date_           20190610
Time                9.50 h
INSTRUM            spect
PROBHD   Z3756_0157 (5
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   256
DS                     2
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ            1.2582912 sec
RG                197.86
DW              19.200 usec
DE              10.00 usec
TE                294.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         100.6238359 MHz
NUC1                  13C
P1              13.25 usec
PLW1         17.98900032 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.19999981 W
PLW12         0.18032999 W
PLW13         0.09070400 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Compound 5a

Central de Análises - UCS

Espectrometria de massas de alta resolução

(Bruker micrOTOF-QII)

Dados da amostra

Código da amostra: **I-CGF-86**

Responsável pela amostra: Prof. Eduardo E Alberto - UFMG

e-mail do responsável: albertoee.ufmg@gmail.com

Amostra submetida em: 6-jan-20

Aquisição e análise: 22-jan-20

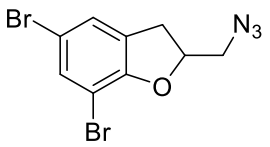
Fórmula molecular: $C_9H_7Br_2N_3O$

Massa exata calculada: $[M]^+$ 332.893018
(para o pico de maior intensidade) $[M+H]^+$ 331.885193
$[M-N_2+H]^+$ 305.894695

Íons observados: ☐ **$[M]^+$**
☐ **$[M+H]^+$**
☑ *outros* **$[M-N_2+H]^+$**

Erro experimental **< 5 ppm**

Inserir abaixo a estrutura molecular (imagem do ChemDraw)



Observações:

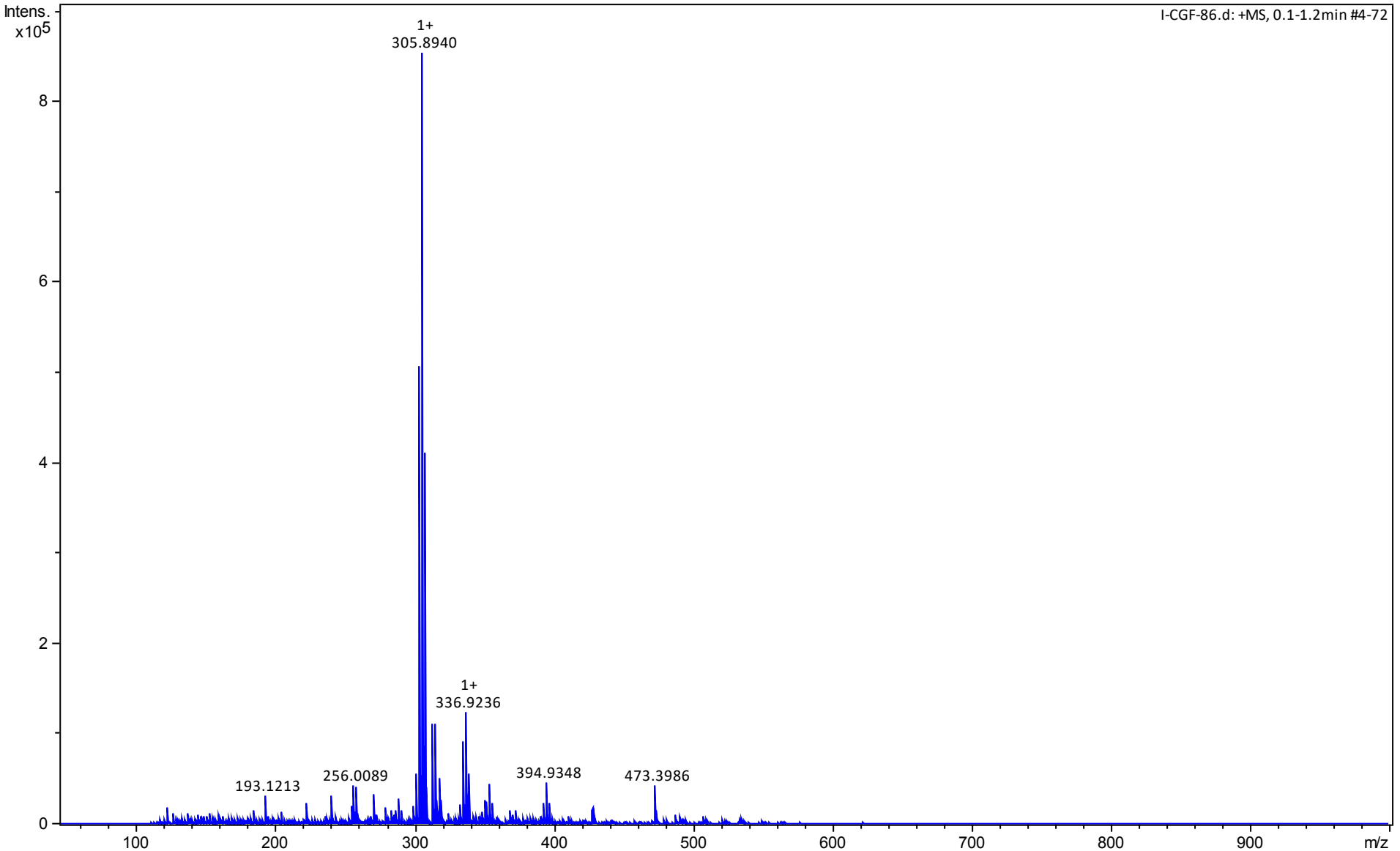
Parâmetros de Aquisição

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

Compound 5a

Central de Análises - UCS

1. Espectro Obtido



2. Expansão do espectro obtido incluindo os espectros simulados

Espectro obtido

Espectro simulado
Íon $[M-N_2+H]^+$