

Supporting Information- part 2

Synthesis of new fluorinated analogues of piperidine-type iminosugar as selective β -glucosidase inhibitors

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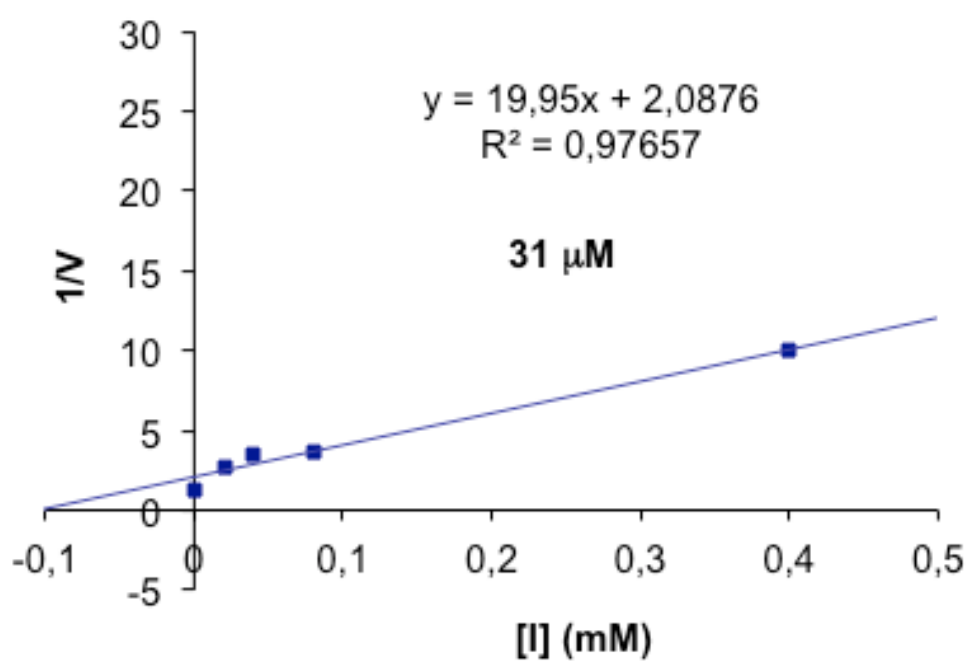
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HRMS for all new compounds	S2.6 to S2.47

% inhibition at 8, 16 and 80 μ M (bovine liver β -glucosidase)

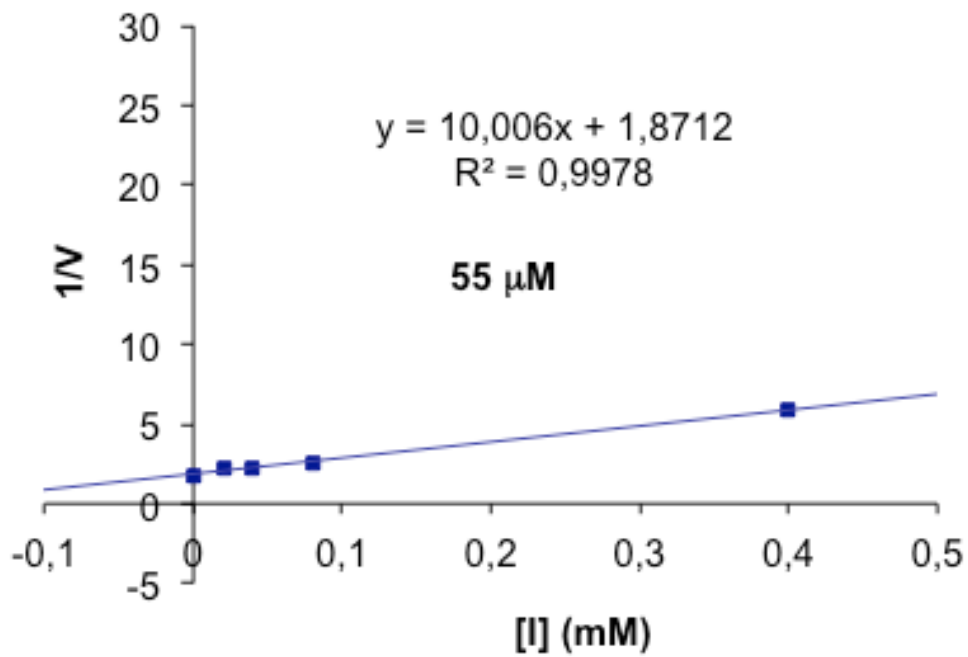
	Concentrations		
Compound	8 μM	16 μM	80 μM
5-Z	7%	8%	14%
5-E	7%	7%	16%
9a-Z	54%	62%	63%
9a-E	16%	19%	20%
9b-Z	11%	11%	18%
9b-E	16%	18%	36%
9c-Z	3%	6%	12%
9c-E	0%	0%	0%
10a-Z	5%	5%	11%
10a-E	15%	17%	34%
10b	21%	30%	54%
10c	10%	12%	21%
11a-Z	9%	16%	30%
11a-E	10%	12%	33%
11c	8%	17%	48%
12a-Z	13%	14%	24%
12a-E	20%	24%	41%
12b	27%	30%	48%
12c-E	10%	10%	21%

Dixon plot for 9a-(Z)



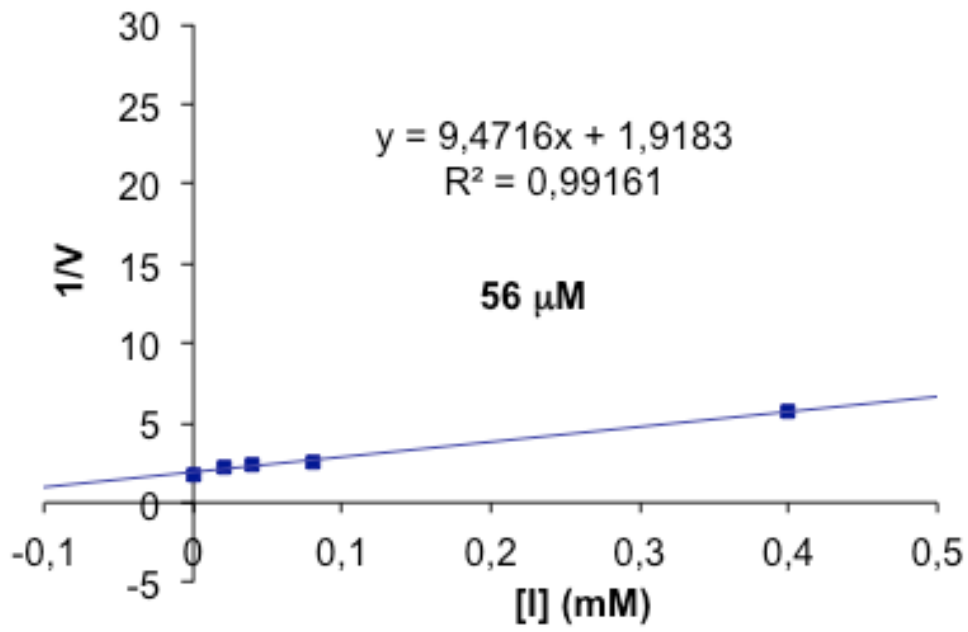
enzyme : bovine liver β -glucosidase

Dixon plot for 10b



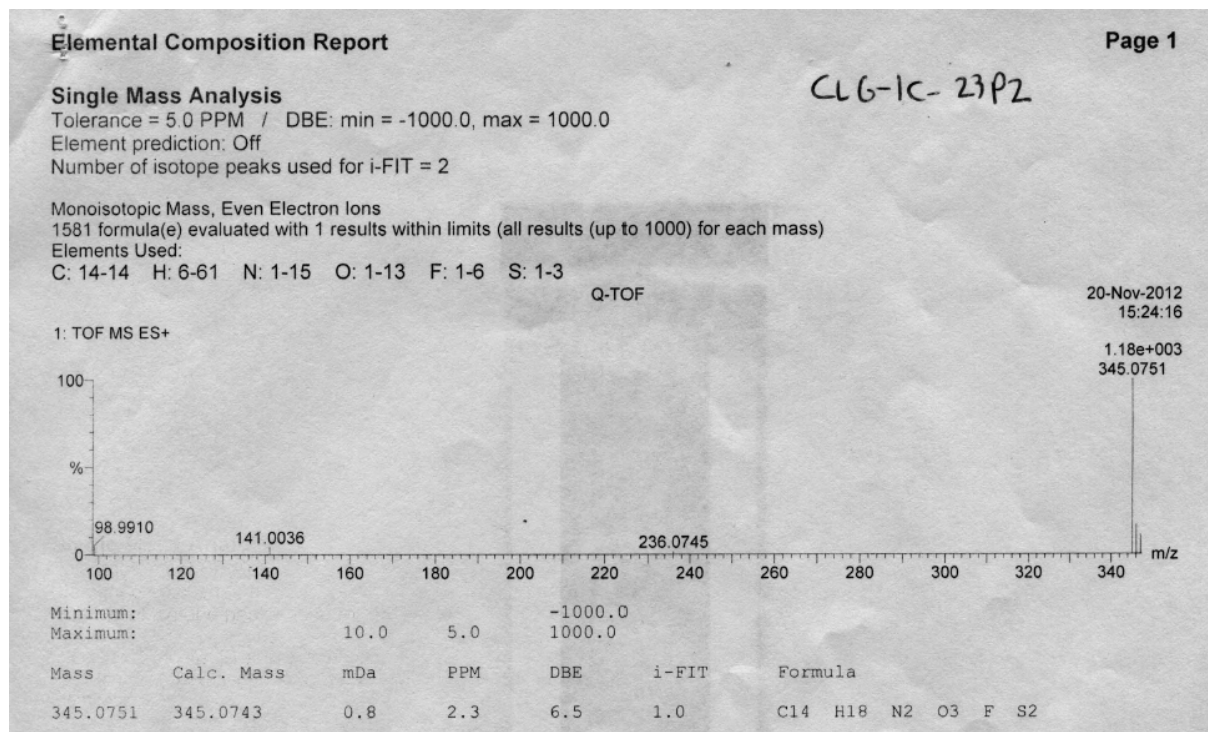
enzyme : bovine liver β -glucosidase

Dixon plot for 12b

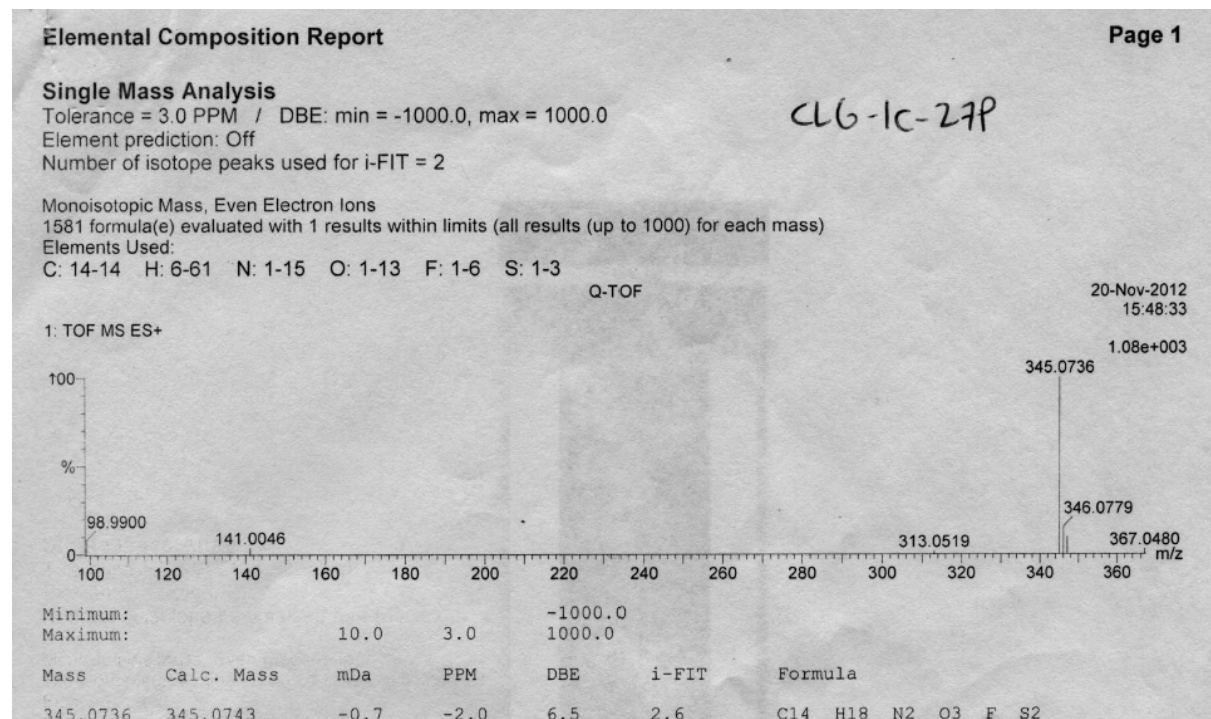


enzyme : bovine liver β -glucosidase

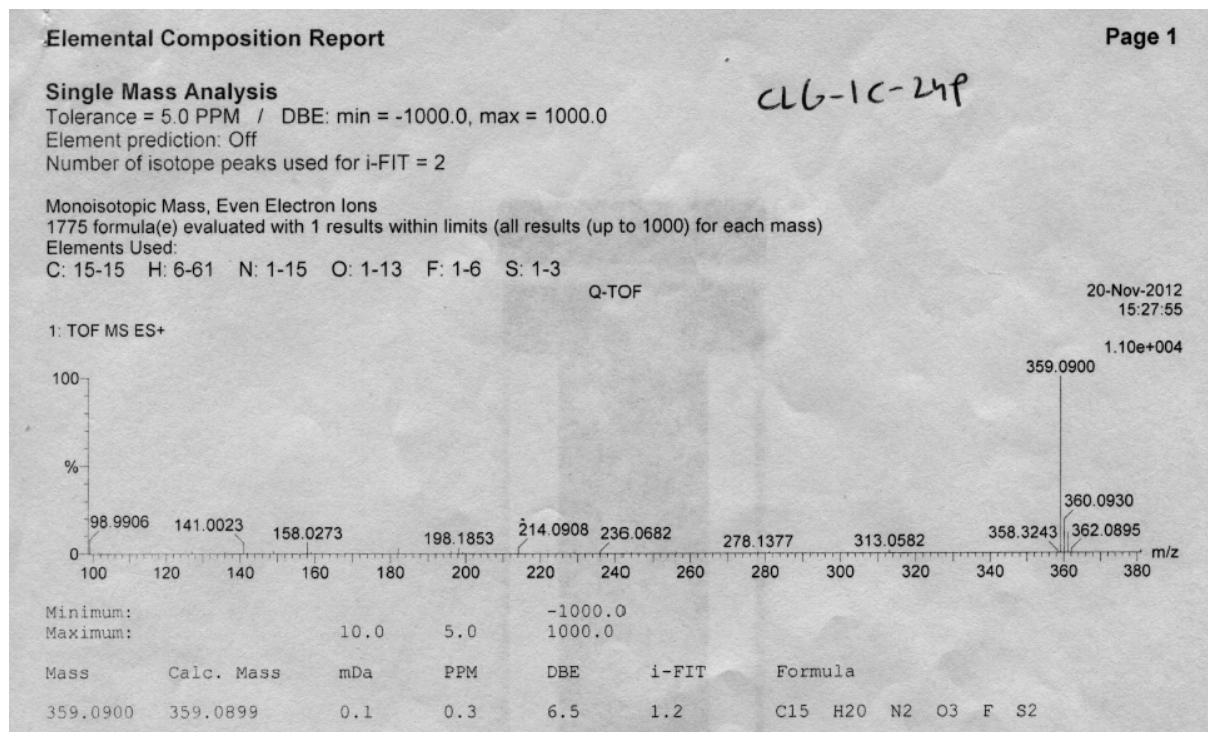
N-[(2-Fluoro-2-benzothiazolylsulfonyl)-ethyl]-4-hydroxypiperidine 2b



***N*-[(2-Fluoro-2-benzothiazolylsulfonyl)-ethyl]-3-hydroxypiperidine 2c**



N-[(2-Fluoro-2-benzothiazolylsulfonyl)-ethyl]-2-(hydroxymethyl)piperidine 2d



***N*-[(2-Fluoro-2-benzothiazolylsulfonyl)ethyl]-4-[(*tert*-butyldimethylsilyl)oxy]-piperidine 3b**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1000.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

235 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

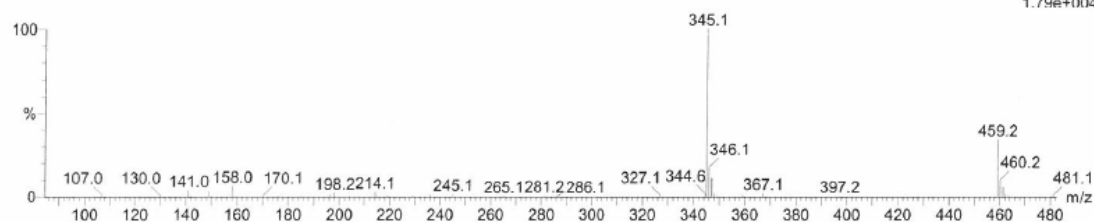
C: 1-20 H: 1-70 N: 1-2 O: 1-5 F: 1-1 Si: 1-1 S: 1-2 ³⁵Cl: 0-2

Q-TOF

30-Aug-2013
16:03:28

1.79e+004

1: TOF MS ES+



Minimum: -1000.0
Maximum: 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
459.1618	459.1608	1.0	2.2	6.5	1.6	C20 H32 N2 O3 F Si S2

***N*-[(2-Fluoro-2-benzothiazolysulfonyl)ethyl]-3-[(*tert*-butyldimethylsilyl)oxy]-piperidine 3c**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1000.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

235 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

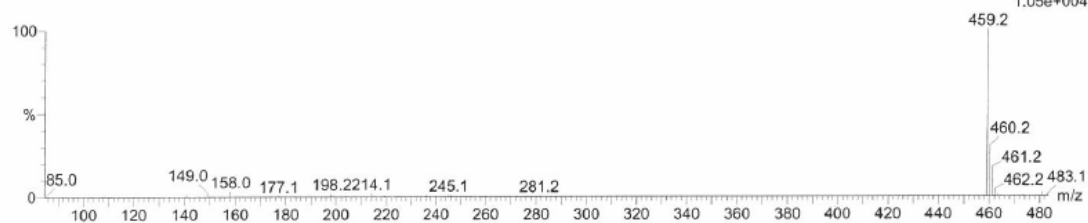
C: 1-20 H: 1-70 N: 1-2 O: 1-5 F: 1-1 Si: 1-1 S: 1-2 35Cl: 0-2

Q-TOF

30-Aug-2013

15:48:46

1: TOF MS ES+



Minimum: -1000.0
Maximum: 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
459.1617	459.1608	0.9	2.0	6.5	0.5	C20 H32 N2 O3 F Si S2

***N*-[(2-Fluoro-2-benzothiazolylsulfonyl)-ethyl]-2-[(*tert*-butyldiphenyl)oxymethyl]piperidine 3d**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1000.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

104 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

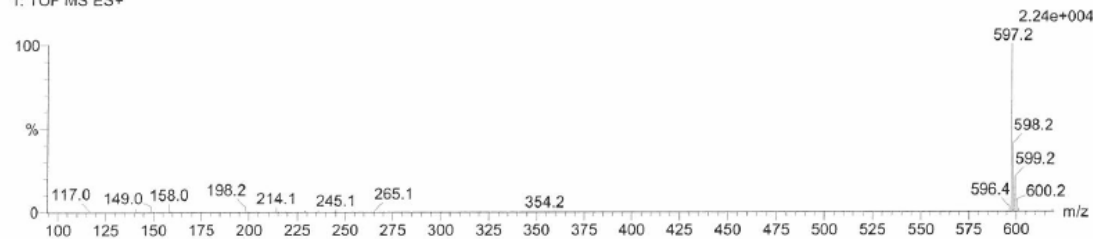
Elements Used:

C: 1-31 H: 1-70 N: 1-2 O: 1-3 F: 1-1 Si: 1-1 S: 1-2 35Cl: 0-2

Q-TOF

30-Aug-2013
16:15:03

1: TOF MS ES+



Minimum: -1000.0
Maximum: 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
597.2078	597.2077	0.1	0.2	14.5	5.4	C31 H38 N2 O3 F Si S2

N-[(2-Fluoro-2-benzothiazolylsulfonyl)-ethyl]-4-(benzyloxy)piperidine 4

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

129 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

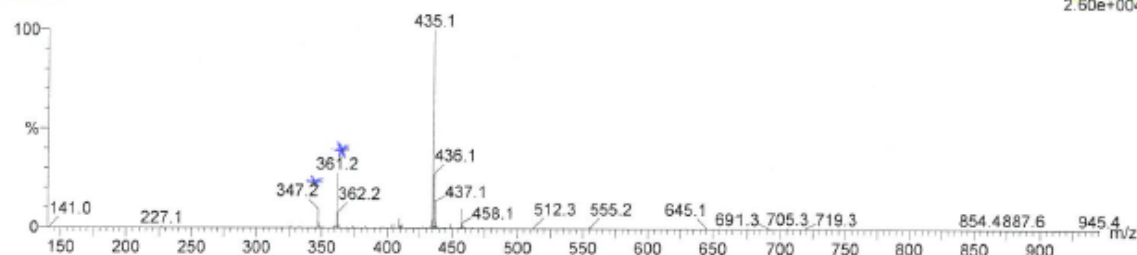
Elements Used:

C: 0-21 H: 0-70 N: 1-3 O: 1-3 F: 1-1 S: 0-2 79Br: 0-1

04-Sep-2014

CLG 1C 102P 11 (0.205) AM (Cen.6, 80.00, Ar.5000.0,361.19,0.70); Cm (6:11)

11:20:51
1: TOF MS ES+
2.60e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
435.1216	435.1212	0.4	0.9	10.5	10.0	C21 H24 N2 O3 F S2

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 1C 102P
 $C_{23}H_{24}N_2O_2$ $n = 360$

Analyse dans $H_2O/CH_3COOH + 0,2\% HCO_2H$

**¹H and ¹³C NMR spectra of compounds 5-(Z)-9c-(E)
(Z)-1-[3-(4-Bromophenyl)-2-fluoroprop-2-enyl]-piperidine 5-(Z)**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

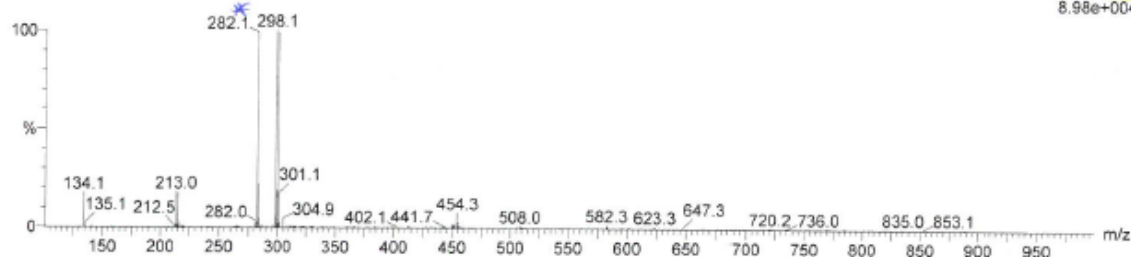
C: 0-14 H: 0-70 N: 1-1 F: 1-1 79Br: 0-1

05-Sep-2014

CLG2138F2 16 (0.297) AM (Cen, 6, 80.00, Ar, 5000.0, 282.15, 0.70); Cm (2:21)

15:16:43

1: TOF MS ES+
8.98e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
298.0609	298.0607	0.2	0.7	5.5	43494.3	C14 H18 N F 79Br

* Référence utilisée pour la mesure de la masse exacte
et mise en mélange avec l'échantillon CLG 2138 p2
 $C_{18}H_{19}NO_2$ $n = 281$

Analyse dans H_2O/CH_3CN + 0,2% HCO_2H

(E)-1-[3-(4-Bromophenyl)-2-fluoroprop-2-enyl]-piperidine 5-E

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

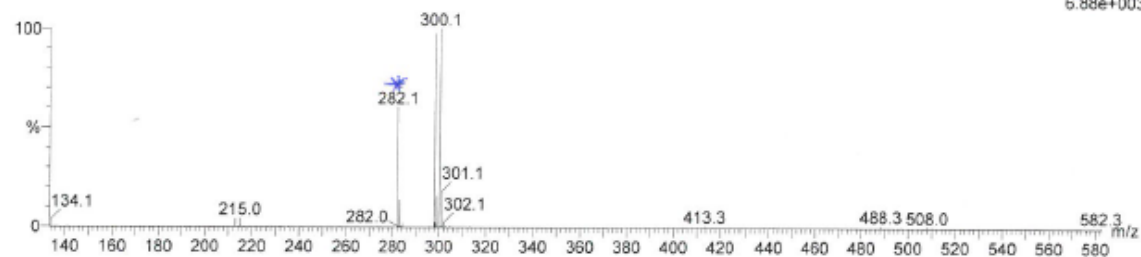
Elements Used:

C: 0-14 H: 0-70 N: 1-1 F: 1-1 79Br: 0-1

05-Sep-2014

CLG2138F1 2 (0.037) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (2:5)

15:03:12
1: TOF MS ES+
6.88e+003



Minimum:

Maximum:

5.0

5.0

-1.5

50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
298.0613	298.0607	0.6	2.0	5.5	3369.5	C14 H18 N F 79Br

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG2138F1
 $C_{18}H_{19}NO_2$, $n = 281$

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(E)-1-[3-(4-Bromophenyl)-2-fluoroprop-2-enyl]-4-[(*tert*-butyldimethylsilyl)oxy]piperidine 6a-E

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1000.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-20 H: 1-80 N: 1-1 O: 1-2 F: 1-1 Si: 1-1 79Br: 0-2

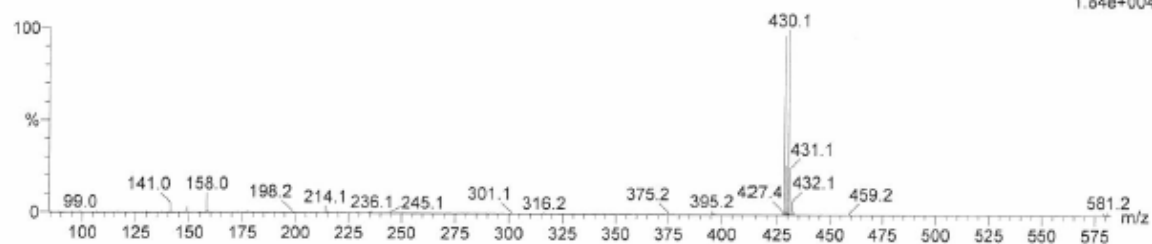
Q-TOF

21-Oct-2013

10:14:23

1.84e+004

1: TOF MS ES+



Minimum: -1000.0
Maximum: 2.0 5.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.1419	428.1421	-0.2	-0.5	5.5	2.7	C20 H32 N O F Si 79Br

(Z)-1-[3-(4-Bromophenyl)-2-fluoroprop-2-enyl]-4-[(*tert*-butyldimethylsilyl)oxy]piperidine 6a-Z

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1000.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

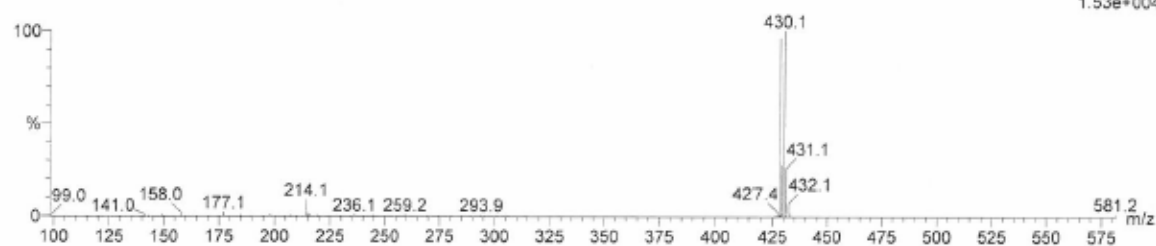
C: 1-20 H: 1-80 N: 1-1 O: 1-2 F: 1-1 Si: 1-1 79Br: 0-2

Q-TOF

21-Oct-2013
09:56:51

1: TOF MS ES+

1.53e+004



Minimum: -1000.0
Maximum: 2.0 5.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.1435	428.1421	1.4	3.3	5.5	1.6	C20 H32 N O F Si 79Br

(Z/E)-1-(2-Fluoronon-2-enyl)-4-[(tert-butyl dimethylsilyl)oxy]piperidine 6b

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

86 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

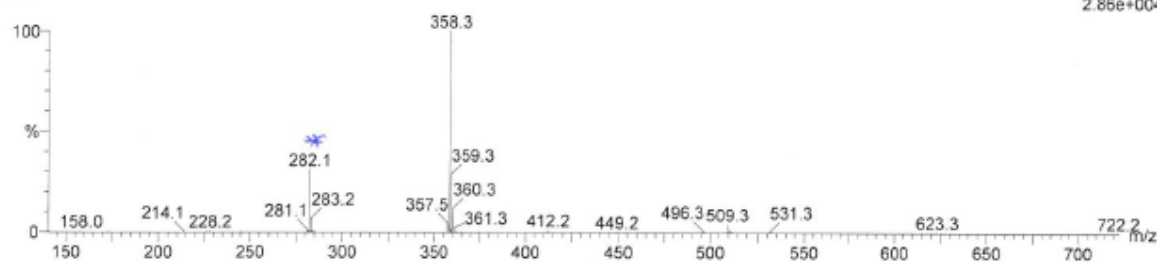
C: 0-20 H: 0-100 N: 1-4 O: 1-2 F: 1-1 Si: 0-1 I: 0-1

16-Sep-2014

CLG3188P 47 (0.874) AM (Cen, 6, 80.00, Ar, 5000.0, 282.15, 0.70); Cm (39:56)

11:04:20

1: TOF MS ES+
2.86e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
358.2931	358.2941	-1.0	-2.8	1.5	228.6	C20 H41 N O F Si

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG3188P

Analyse dans H₂O / CH₃CO + 0,2% H₂O

(Z/E)-1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-4-[(*tert*-butyldimethylsilyl)oxy]piperidine 6c

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

52 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

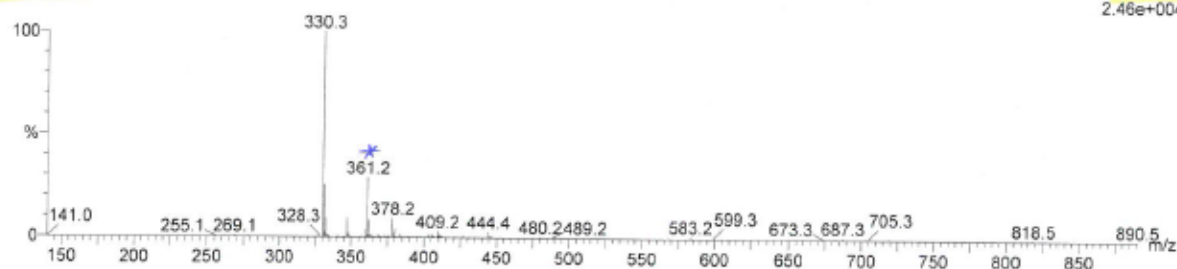
C: 0-18 H: 0-70 N: 1-3 O: 1-2 F: 1-1 Si: 0-2

02-Sep-2014

CLG3092B 247 (4.577) AM (Cen,6, 80.00, Ar,5000.0,361.19,0.70); Cm (229.251)

16:02:06

1: TOF MS ES+
2.46e+004



Minimum:

Maximum:

5.0 5.0 -1.5
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
330.2636	330.2628	0.8	2.4	1.5	64.9	C18 H37 N O F Si

* Référence utilisée pour la mesure de masse exacte
et mise en relation avec l'échantillon CLG 3092B
 $C_{23}H_{24}N_2O_2$, $n=360$

Analyse dans $H_2O/U_3O_8 + 0,2\% H_2O_2$

(Z)-1-[3-(4-Bromophenyl)-2-fluoroprop-2-enyl]-3-[(*tert*-butyldimethylsilyl)oxy]piperidine 7a-Z

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

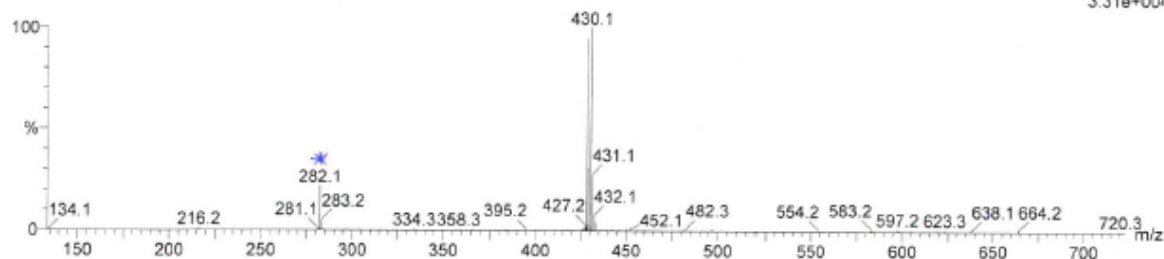
Elements Used:

C: 0-20 H: 0-70 N: 1-1 O: 1-1 F: 1-1 79Br: 0-1 Si: 0-1

11-Sep-2014

CLG 3096F3 6 (0.111) AM (Cen, 6, 80.00, Ar, 5000.0, 282.15, 0.70); Cm (3.14)

14:27:11
1: TOF MS ES+
3.31e+004



Minimum:

Maximum: 5.0 5.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.1417	428.1421	-0.4	-0.9	5.5	14302.8	C20 H32 N O F 79Br Si

* Référence utilisée pour la mesure de masse exacte et mise en mélange avec l'échantillon à analyser
CLG 3096 f3 (C₁₈H₁₉NO₂, n = 281)

Analyse dans H₂O / CH₃CN + 0,2 % HCO₂H

(E)-1-[3-(4-Bromophenyl)-2-fluoroprop-2-enyl]-3-[(*tert*-butyldimethylsilyl)oxy]piperidine 7a-E

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-20 H: 0-70 N: 1-1 O: 1-1 F: 1-1 Si: 0-1 79Br: 0-1

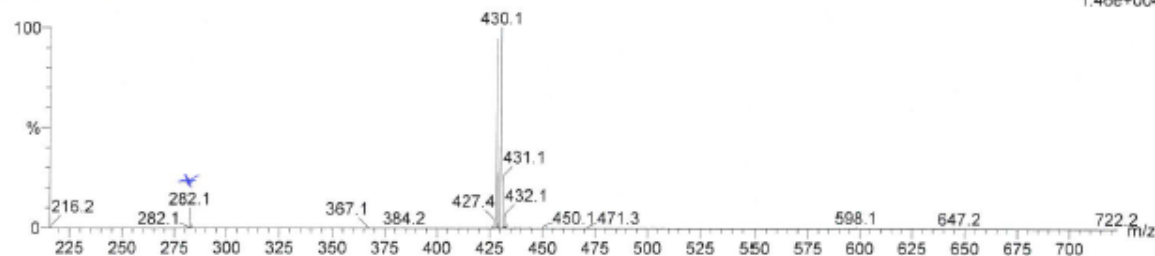
11-Sep-2014

CLG 236F1 19 (0.354) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (12:19)

14:43:24

1: TOF MS ES+

1.46e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.1425	428.1421	0.4	0.9	5.5	6306.2	C20 H32 N O F Si 79Br

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 236 f1
($C_{18}H_{19}NO_2$, $n=281$)

Analyse dans H_2O / CH_3CN + 0,2% HCO_2H

(Z/E)-1-(2-Fluoronon-2-enyl)-3-[(*tert*-butyldimethylsilyl)oxy]piperidine 7b

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

93 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

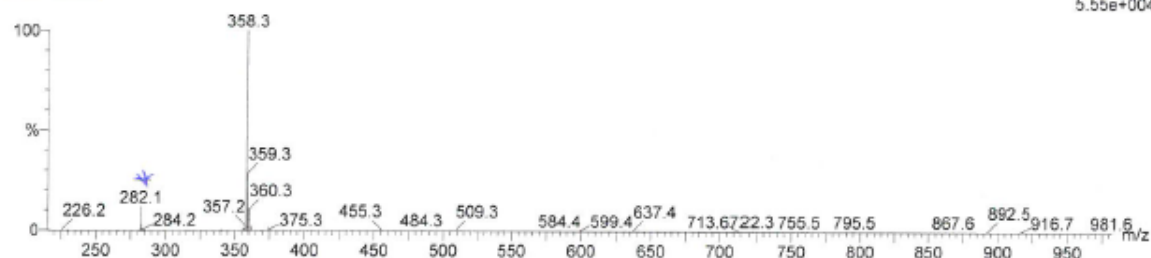
C: 0-24 H: 0-70 N: 1-1 O: 1-4 F: 1-1 Si: 0-2 ⁵⁶Fe: 0-1

09-Sep-2014

CLG275F1 49 (0.913) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (41:56)

10:20:35

1: TOF MS ES+
5.55e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
358.2932	358.2941	-0.9	-2.5	1.5	227.9	C20 H41 N O F Si

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 275 f1
(C₁₈H₁₉N₂O₂, n=281)

Analyse dans H₂O / CH₃COOH, 2% HCO₂H

(Z)-1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-3-[(*tert*-butyldimethylsilyl)oxy]piperidine 7c-Z

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

58 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

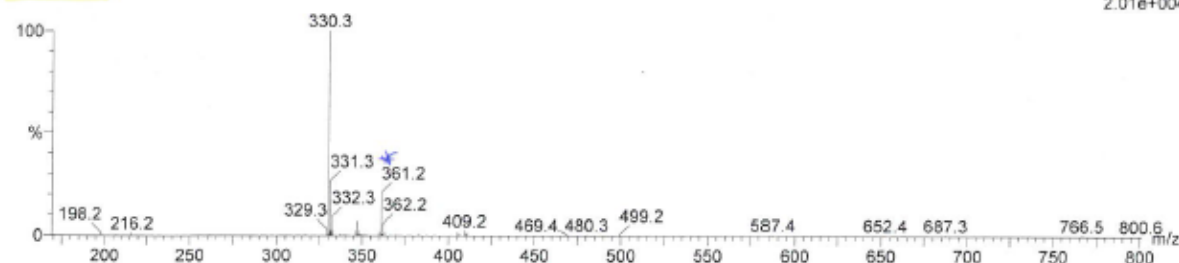
C: 0-19 H: 0-70 N: 1-3 O: 1-2 F: 1-1 Si: 0-2

02-Sep-2014

CLG3127F3 22 (0.410) AM (Cen,6, 80.00, Ar,5000.0,361.19,0.70); Cm (19:22)

14:52:35

1: TOF MS ES+
2.01e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
330.2629	330.2628	0.1	0.3	1.5	48.5	C18 H37 N O F Si

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG3127F3
 $C_{23}H_{26}N_2O_2$, $n=360$

Analyse dans H_2O/CH_3CN + 0,2% HCO_2H

(E)-1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-3-[(*tert*-butyldimethylsilyl)oxy]piperidine 7c-E

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

58 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

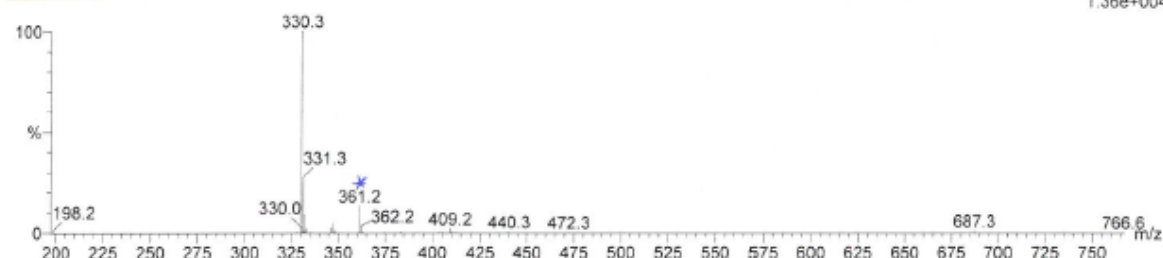
Elements Used:

C: 0-19 H: 0-70 N: 1-3 O: 1-2 F: 1-1 Si: 0-2

02-Sep-2014

CLG3127F1 10 (0.185) AM (Cen,6, 80.00, Ar,5000.0,361.19,0.70); Cm (10:13)

15:06:57
1: TOF MS ES+
1.36e+004



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
330.2643	330.2628	1.5	4.5	1.5	40.4	C18 H37 N O F Si

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 3127F1
 $C_{23}H_{24}N_2O_2$, $n = 360$

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(Z)-1-[3-(4-Bromophenyl)-2-fluoroallyl]-2-[(*tert*-butyldiphenyl)oxymethyl]piperidine 8a-Z

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

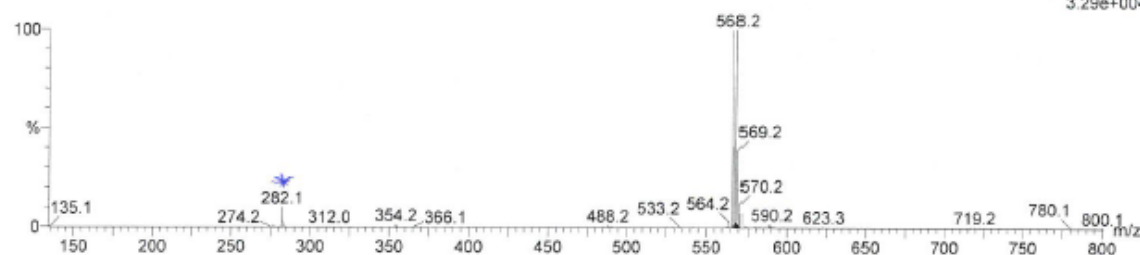
C: 0-31 H: 0-70 N: 1-1 O: 1-1 F: 1-1 Na: 0-1 Si: 0-1 79Br: 0-1

11-Sep-2014

CLG3170F2 23 (0.427) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (13:23)

16:12:08

1: TOF MS ES+
3.29e+004



Minimum:

Maximum: 5.0 5.0 -1.5

Mass Calc. Mass mDa PPM DBE i-FIT Formula

566.1902 566.1890 1.2 2.1 13.5 12781.0 C31 H38 N O F Si 79Br

* Référence utilisée pour la mesure de masse exacte et
mise en mélange avec l'échantillon CLG3170F2

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(E)-1-[3-(4-Bromophenyl)-2-fluoroallyl]-2-[(*tert*-butyldiphenyl)oxymethyl]piperidine 8a-E

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

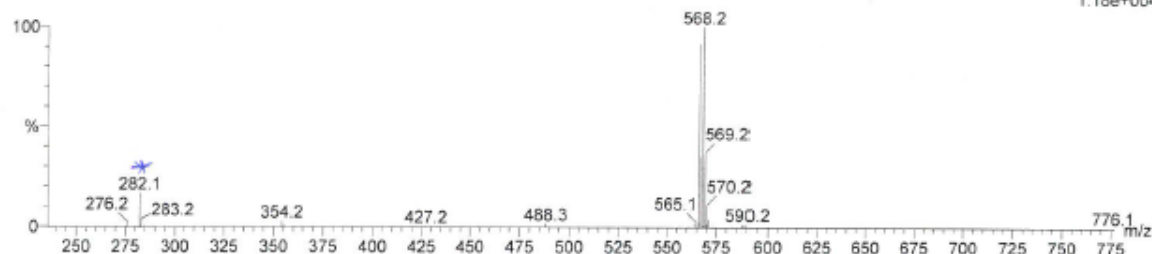
C: 0-31 H: 0-70 N: 1-1 O: 1-1 F: 1-1 Si: 0-1 79Br: 0-1

11-Sep-2014

CLG 3170F1 111 (2.068) AM (Cen, 6, 80.00, Ar, 5000.0, 282.15, 0.70); Cm (109:113)

15:00:09

1: TOF MS ES+
1.18e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
566.1895	566.1890	0.5	0.9	13.5	4706.6	C31 H38 N O F Si 79Br

* Référence utilisée pour la mesure de masse exacte et mise en mélange avec l'échantillon CLG3170 f1 (C₁₈H₁₉NO₂, n = 281)

Analyse dans H₂O/CH₃COOH + 0,2% HCO₂H

(Z/E)-(2-Fluoronon-2-enyl)-2-[(*tert*-butyldiphenyl)oxy]piperdinemethanol 8b

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

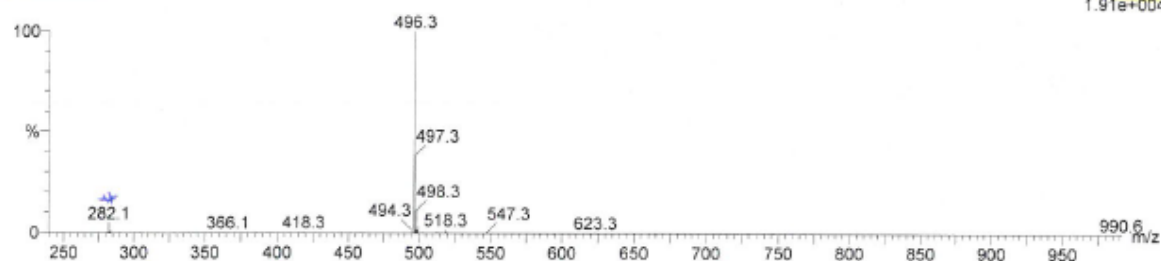
Elements Used:

C: 0-31 H: 0-70 N: 1-1 O: 1-1 F: 1-1 Si: 0-1

11-Sep-2014

CLG 3174P 25 (0.465) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (23:27)

11:30:40
1: TOF MS ES+
1.91e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
496.3419	496.3411	0.8	1.6	9.5	9.2	C31 H47 N O F Si

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG3174P
($C_{18}H_{19}NO_2$, n=281)

Analyse dans H_2O/CH_3COOH 0,2% HCO_2H

(Z)-1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-2-[(*tert*-butyldiphenyl)oxy]piperdinemethanol 8c-Z

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

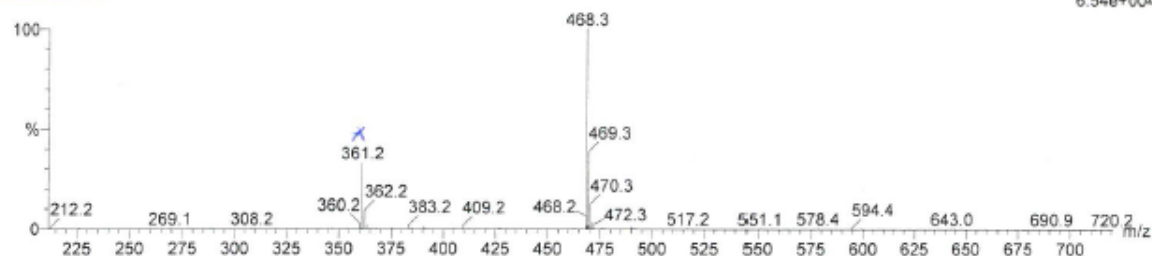
C: 0-29 H: 0-50 N: 1-1 O: 1-1 F: 1-1 Si: 0-1

30-Jun-2014

CLG 2160F3 18 (0.335) AM (Cen,6, 80.00, Ar,5000.0,361.19,0.70); Cm (15:25)

15:48:28

1: TOF MS ES+
6.54e+004



Minimum:

Maximum: 5.0 5.0 -1.5

Mass Calc. Mass mDa PPM DBE i-FIT Formula

468.3098 468.3098 0.0 0.0 9.5 60.3 C29 H43 N O F Si

* Référence utilisée pour la mesure de masse exacte



composé mis en mélange avec l'échantillon CLG 2160 f3

Analyse dans $H_2O/CH_3CN + 0,2\% HCl$

(E)-1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-2-[(*tert*-butyldiphenyl)oxy]piperdinemethanol 8c-E

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

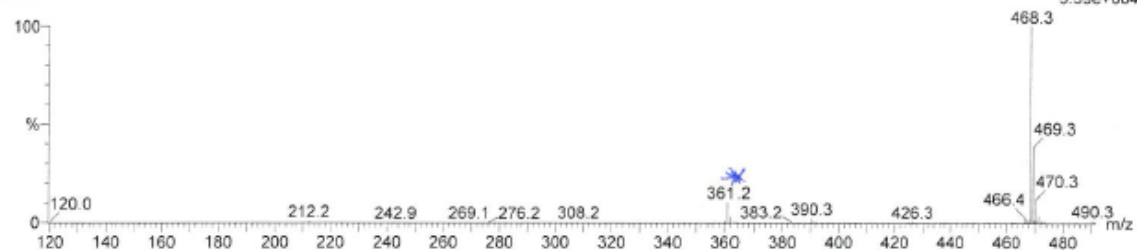
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-29 H: 0-50 N: 1-1 O: 1-1 F: 1-1 Si: 0-1

30-Jun-2014

CLG 2160F1 482 (8.953) AM (Cen,6, 80.00, Ar,5000.0,361.19,0.70); Cm (470.483)



Minimum: -1.5
Maximum: 5.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
468.3093	468.3098	-0.5	-1.1	9.5	24.0	C ₂₉ H ₄₃ N O F Si

* Référence utilisée pour la mesure de masse exacte
C₂₃H₂₄N₂O₂ n = 360

Composé mis en mélange avec l'échantillon CLG 2160F1

Analyse dans H₂O/CH₃CO + 0,2% HCl

(Z)-1-[3-(4-Bromophenyl)-2-fluoroallyl]-4-(benzyloxy)piperidine 9a-Z

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-21 H: 0-70 N: 1-1 O: 1-1 F: 1-1 79Br: 0-1

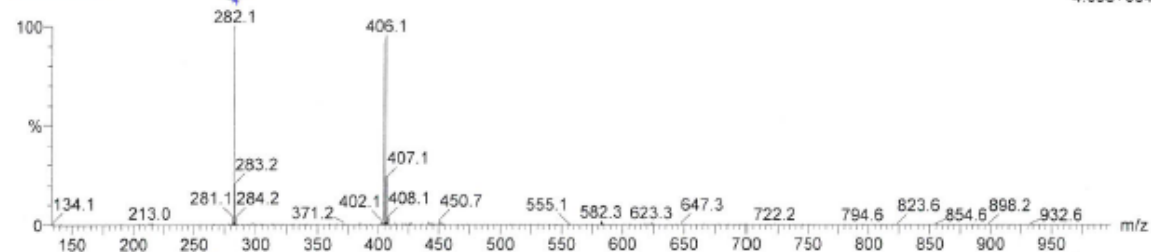
05-Sep-2014

CLG 1C 159F3 8 (0.148) AM (Cen.6, 80.00, Ar.5000.0,282.15,0.70); Cm (2:12)

15:43:27

1: TOF MS ES+

4.09e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
404.1010	404.1025	-1.5	-3.7	9.5	18386.1	C21 H24 N O F 79Br

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 1C 159F3
 $C_{18}H_{19}N_2$, $\eta = 281$

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(E)-1-[3-(4-Bromophenyl)-2-fluoroallyl]-4-(benzyloxy)piperidine 9a-E

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

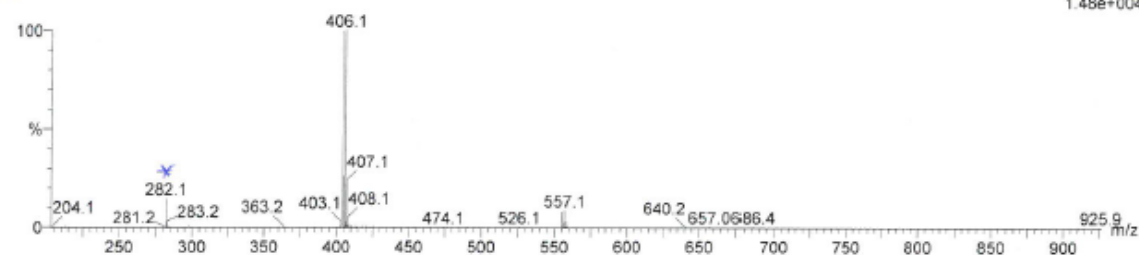
C: 0-21 H: 0-70 N: 1-1 O: 1-1 F: 1-1 79Br: 0-1

05-Sep-2014

CLG 1C 159F1 71 (1.328) AM (Cen, 6, 80.00, Ar, 5000.0, 282.15, 0.70); Cm (69:78)

15:29:54

1: TOF MS ES+
1.48e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
404.1009	404.1025	-1.6	-4.0	9.5	7007.8	C21 H24 N O F 79Br

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 1C 159F1
 $C_{18}H_{19}NO_2$, $n=281$

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(Z)-1-(2-Fluoronon-2-en-1-yl)-4-(benzyloxy)piperidine) 9b-Z

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

27 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-21 H: 0-70 N: 1-2 O: 1-4 F: 1-1

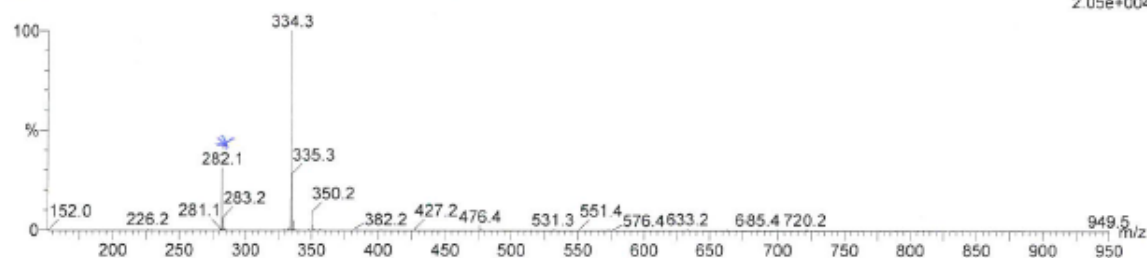
09-Sep-2014

CLG254F2 37 (0.689) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (26:38)

10:49:41

1: TOF MS ES+

2.05e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
334.2539	334.2546	-0.7	-2.1	5.5	91.1	C21 H33 N O F

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG254_F2
($C_{18}H_{19}NO_2$, $n = 281$)

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(E)-1-(2-Fluoronon-2-en-1-yl)-4-(benzyloxy)piperidine 9b-E

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

27 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

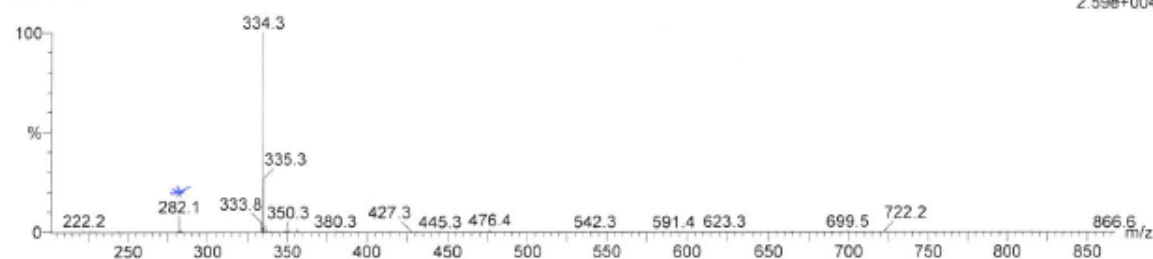
C: 0-21 H: 0-70 N: 1-2 O: 1-4 F: 1-1

09-Sep-2014

CLG254F1 16 (0.297) AM (Cen, 6, 80.00, Ar, 5000.0, 282.15, 0.70); Cm (11:16)

11:02:04

1: TOF MS ES+
2.59e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
334.2557	334.2546	1.1	3.3	5.5	27.6	C21 H33 N O F

* Référence utilisée pour la mesure de masse exacte et mise en mélange avec l'échantillon CLG254 f1 (C₁₈H₁₉N₂O₂, n=281)

Analyse dans H₂O/CH₃CN + 0,2% H₂CO

(Z)-1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-4-(benzyloxy)piperidine 9c-Z

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

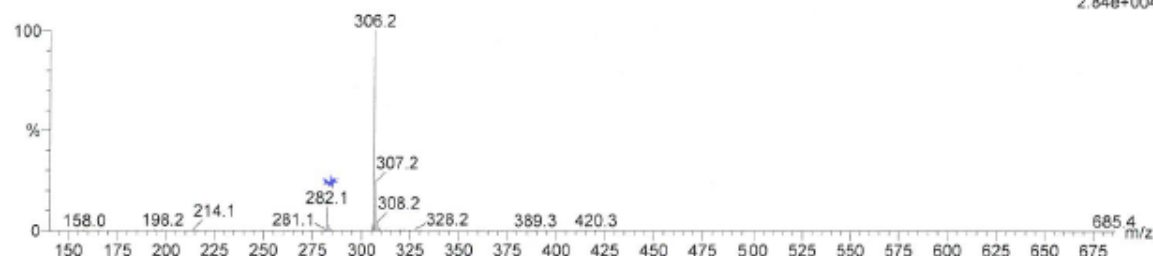
C: 0-19 H: 0-70 N: 1-2 O: 1-4 F: 1-1

09-Sep-2014

CLG2152F2 34 (0.633) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (33:53)

14:52:28

1: TOF MS ES+
2.84e+004



Minimum:

Maximum: 5.0 5.0 -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
306.2230	306.2233	-0.3	-1.0	5.5	100.4	C19 H29 N O F

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 2152 p2
($C_{18}H_{19}NO_2$, $n = 281$)

Analyse dans $H_2O/CH_3CN + 0,2\% HCl$

(E)-1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-4-(benzyloxy)piperidine 9c-E

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

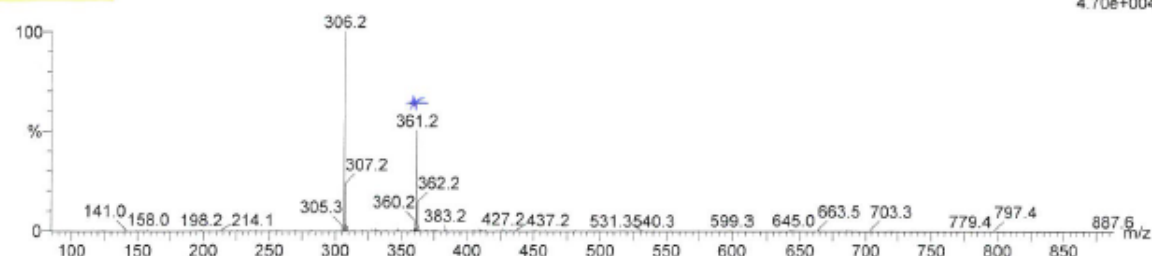
Elements Used:

C: 0-19 H: 0-40 N: 1-1 O: 1-4 F: 1-1

30-Jun-2014

CLG 2152 F1 160 (2.983) AM (Cen.6, 80.00, Ar.5000.0,361.19,0.70); Cm (147:169)

14:11:49
1: TOF MS ES+
4.70e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
306.2234	306.2233	0.1	0.3	5.5	69.3	C19 H29 N O F

* Référence utilisée pour la mesure de masse exacte
 $C_{23}H_{24}N_2O_2$ $n=360$

Composé mis en mélange avec l'échantillon CLG 2152 F1

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$.

(Z)-1-(3-(4-Bromophenyl)-2-fluoroallyl)-4-hydroxypiperidine 10a-Z

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

22 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

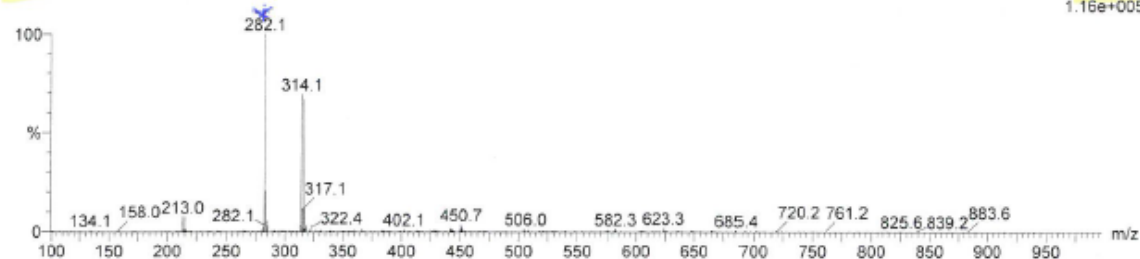
Elements Used:

C: 0-14 H: 0-70 N: 1-3 O: 1-2 F: 1-1 79Br: 0-1

02-Sep-2014

CL2156P 52 (0.968) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (22:58)

16:50:56
1: TOF MS ES+
1.16e+005



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.0558	314.0556	0.2	0.6	5.5	37601.0	C14 H18 N O F 79Br

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon à
analyser CLG2156P
 $C_{18}H_{19}NO_2$, n = 281

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(E)-1-(3-(4-Bromophenyl)-2-fluoroallyl)-4-hydroxypiperidine 10a-E

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

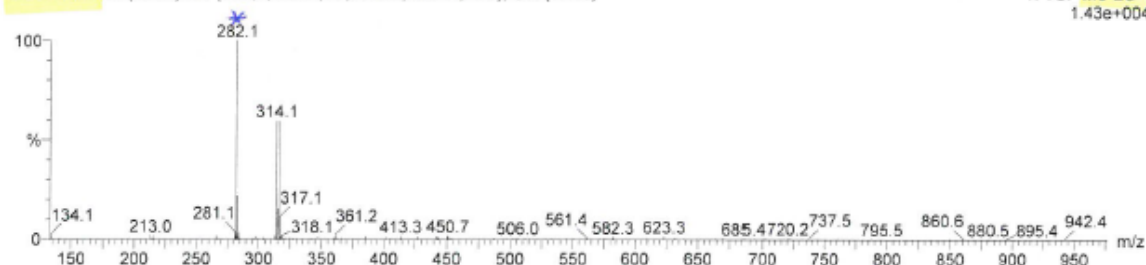
Elements Used:

C: 0-14 H: 0-70 N: 1-1 O: 1-1 F: 1-1 79Br: 0-1

04-Sep-2014

CLG 2155P 16 (0.299) AM (Cen.6, 80.00, Ar.5000.0,282.15,0.70); Cm (11:16)

11:44:15
1: TOF MS ES+
1.43e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.0560	314.0556	0.4	1.3	5.5	4233.6	C14 H18 N O F 79Br

* Référence utilisée pour la mesure de masse exacte et mise en mélange avec l'échantillon CLG 2155P
 $C_{18}H_{19}NO_2$ $n = 281$

Analyse dans $H_2O/CH_3CN + 0,2\% HCl$

(Z/E)-1-(2-Fluoronon-2-en-1-yl)-4-hydroxypiperidine 10b

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1000.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

137 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-14 H: 1-70 N: 1-4 O: 1-6 F: 1-1

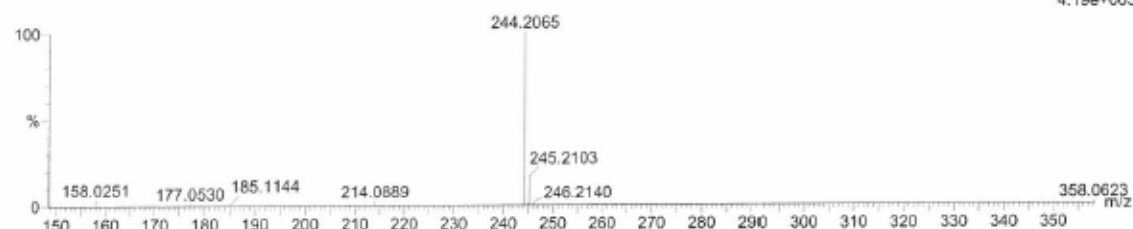
Q-TOF

03-Sep-2013

16:32:55

4.19e+003

1: TOF MS ES+



Minimum: -1000.0
Maximum: 2.0 5.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
244.2065	244.2077	-1.2	-4.9	1.5	0.4	C14 H27 N O F

(Z/E)-1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-4-hydroxypiperidine 10c

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

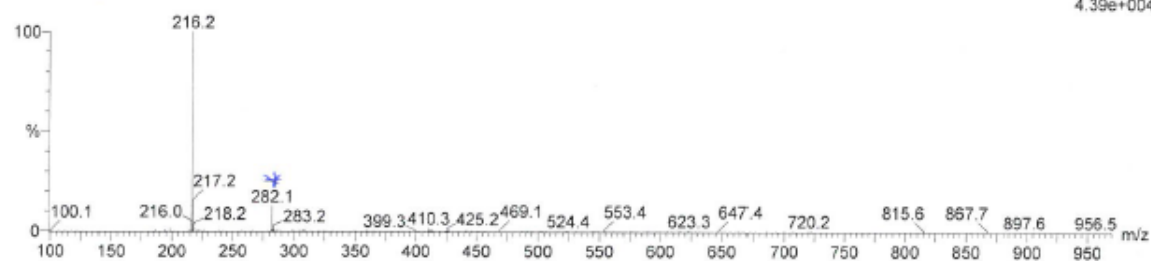
Elements Used:

C: 0-12 H: 0-70 N: 1-3 O: 1-2 F: 1-1

29-Aug-2014

CLG 3095P 8 (0.149) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (2:9)

11:51:06
1: TOF MS ES+
4.39e+004



Minimum:
Maximum: 5.0 5.0 -1.5
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
216.1774	216.1764	1.0	4.6	1.5	485.7	C12 H23 N O F

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 3095P
 $C_{18}H_{19}NO_2$, $n = 281$

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(Z)-1-[3-(4-Bromophenyl)-2-fluoroallyl]-3-hydroxypiperidine 11a-Z

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

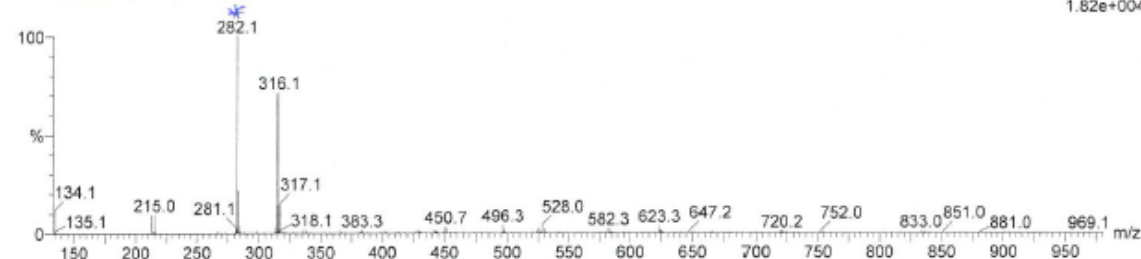
C: 0-14 H: 0-70 N: 1-1 O: 1-1 F: 1-1 79Br: 0-1

11-Sep-2014

CLG 3097P 11 (0.205) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (10:14)

11:47:18

1: TOF MS ES+
1.82e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.0552	314.0556	-0.4	-1.3	5.5	6358.0	C14 H18 N O F 79Br

* Référence utilisée pour la mesure de la masse exacte
et mise en mélange avec l'échantillon CLG3097P
($C_{18}H_{19}NO_2$, $n = 281$)

Analyse dans $H_2O/CH_3CO + 0,2\% HCO_2H$

(E)-1-[3-(4-bromophenyl)-2-fluoroallyl]-3-hydroxypiperidine 11a-E

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-14 H: 0-70 N: 1-1 O: 1-1 F: 1-1 79Br: 0-1

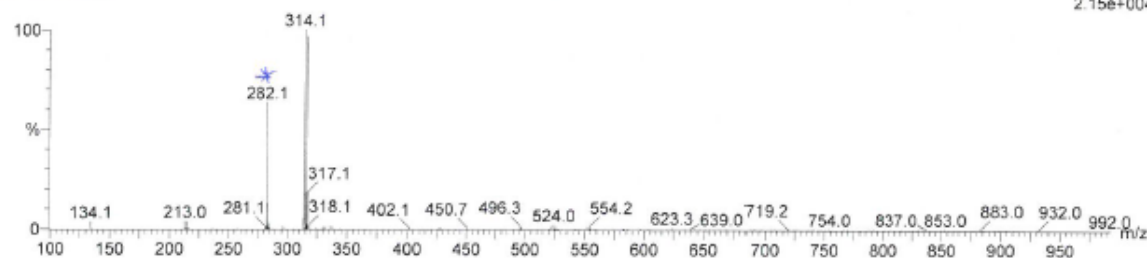
11-Sep-2014

CLG 3098P 18 (0.336) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (13:20)

14:13:10

1: TOF MS ES+

2.15e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.0549	314.0556	-0.7	-2.2	5.5	10140.6	C14 H18 N O F 79Br

* Référence utilisée pour la mesure de masse exacte et mise en mélange avec l'échantillon CLG 3098P (C₁₈H₁₉NO₂, n = 281)

Analyse dans H₂O/CH₃CN + 0,2% HCO₂H

(Z/E)-N-(2-Fluoronon-2-enyl)-3-hydroxypiperidine 11b

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

70 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

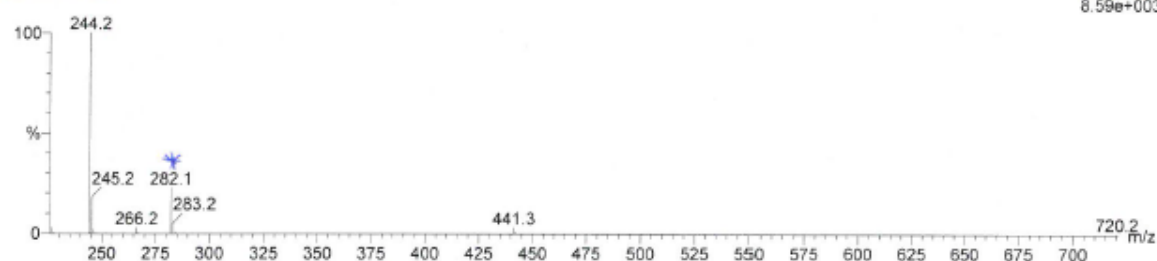
C: 0-15 H: 0-70 N: 1-2 O: 1-4 F: 1-1 Si: 0-2

11-Sep-2014

CLG 3177P 12 (0.223) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (8:12)

11:16:31

1: TOF MS ES+
8.59e+003



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
244.2077	244.2077	0.0	0.0	1.5	5.4	C14 H27 N O F

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 3177P
($C_{18}H_{19}NO_2$, $n = 281$)

Analyse dans $H_2O/CH_3CN + 0,2\% HCl$

(Z/E)-1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-3-hydroxypiperidine 11c

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

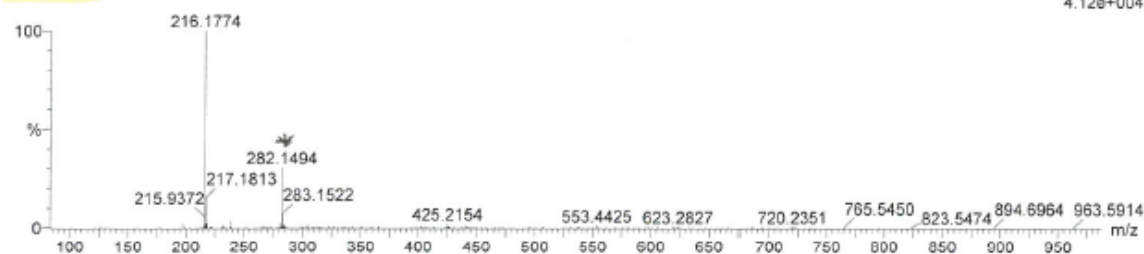
C: 0-12 H: 0-70 N: 1-3 O: 1-2 F: 1-1

29-Aug-2014

CLG 3139P 29 (0.541) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (12:34)

11:20:59

1: TOF MS ES+
4.12e+004



Minimum:

Maximum: 5.0 5.0 -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
216.1774	216.1764	1.0	4.6	1.5	96.2	C12 H23 N O F

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG 3139P
 $C_{18}H_{19}NO_2$, $n = 281$

Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(Z)-1-[3-(4-Bromophenyl)-2-fluoroprop-2-enyl]-2-(hydroxymethyl)piperidine 12a-Z

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

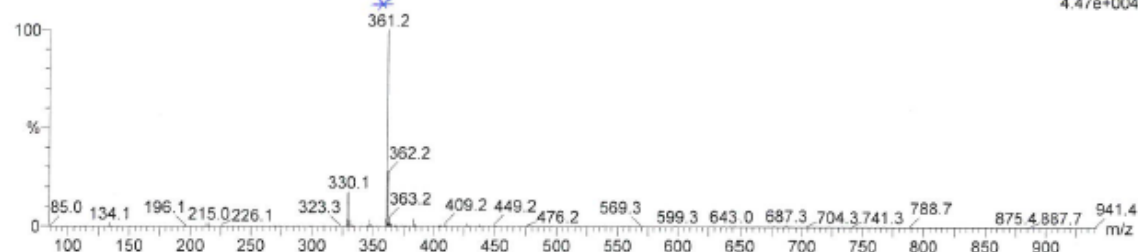
Elements Used:

C: 0-15 H: 0-40 N: 1-1 O: 1-1 F: 1-1 79Br: 0-1

30-Jun-2014

CLG2114 F2 5 (0.093) AM (Cen,6, 80.00, Ar,5000.0,361.19,0.70); Cm (3:10)

10:57:08
1: TOF MS ES+
4.47e+004



Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
328.0722	328.0712	1.0	3.0	5.5	3790.2	C15 H20 N O F 79Br

* Référence utilisée pour la mesure de masse exacte
 $C_{23}H_{25}N_2O_2$ $nn=360$
composé mis en mélange avec l'échantillon CLG2114 F2
Analyse dans $H_2O/CH_3CN + 0,2\% HCO_2H$

(E)-1-[3-(4-Bromophenyl)-2-fluoroprop-2-enyl]-2-(hydroxymethyl)piperidine 12a-E

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

29 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

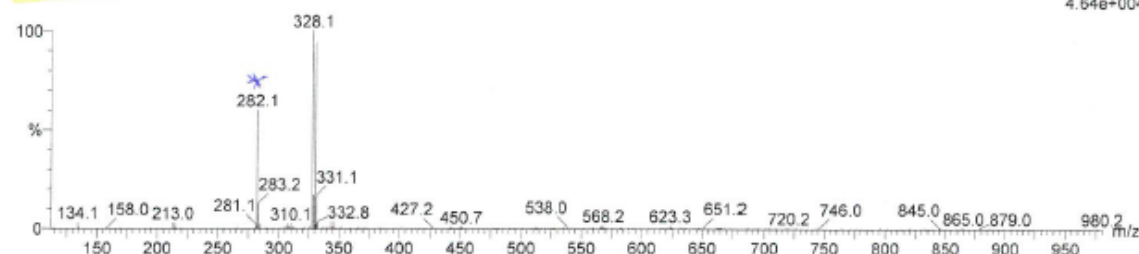
C: 0-15 H: 0-70 N: 1-2 O: 1-4 F: 1-1 79Br: 0-1

09-Sep-2014

CLG2113F2 9 (0.168) AM (Cen, 6, 80.00, Ar, 5000.0, 282.15, 0.70); Cm (4:18)

15:47:17

1: TOF MS ES+
4.64e+004



Minimum:

Maximum: 5.0 5.0 -1.5

Maximum: 5.0 5.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

328.0709 328.0712 -0.3 -0.9 5.5 21114.3 C15 H20 N O F 79Br

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG2113F2
(C₁₈H₁₉NO₂, n = 281)

Analyse dans H₂O / CH₃CN + 0,2% HCO₂H

(Z/E)-1-(2-Fluoronon-2-enyl)-2-(hydroxymethyl)piperidine 12b

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

71 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

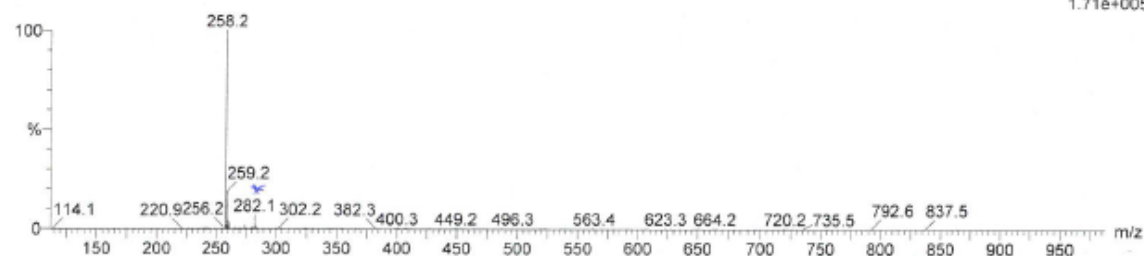
C: 0-15 H: 0-70 N: 1-2 O: 1-4 F: 1-1 Si: 0-2

11-Sep-2014

CLG 142F2 271 (5.027) AM (Cen:6, 80.00, Ar:5000.0,282.15,0.70); Cm (257:291)

10:42:19

1: TOF MS ES+
1.71e+005



Minimum:

Maximum:

-1.5

5.0

5.0

50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
258.2231	258.2233	-0.2	-0.8	1.5	1145.1	C15 H29 N O F

* Référence utilisée pour la mesure de masse exacte et mise en mélange avec l'échantillon CLG 142F2 (C₁₈H₁₉NO₂, n = 281)

Analyse dans H₂O/CH₃CN + 0,2% HCO₂H

(Z)-[1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-2(hydroxymethyl)piperidine 12c-Z

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-21 H: 0-70 N: 1-2 O: 1-4 F: 1-1

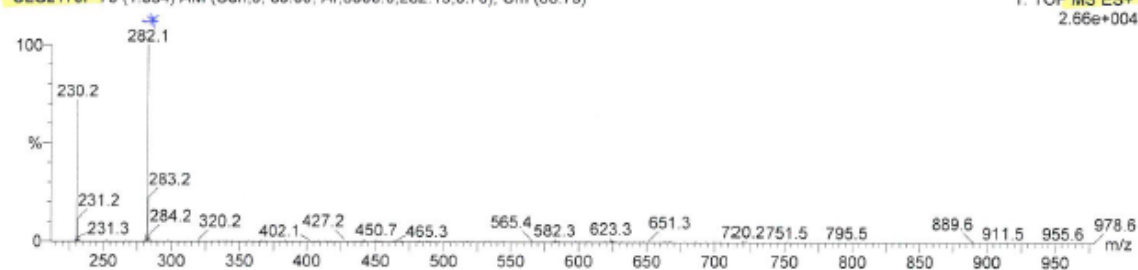
09-Sep-2014

CLG2170P 73 (1.354) AM (Cen,6, 80.00, Ar,5000,0,282.15,0.70); Cm (68.79)

14:40:49

1: TOF MS ES+

2.66e+004



Minimum:

Maximum: 5.0 5.0 -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
230.1930	230.1920	1.0	4.3	1.5	11.5	C13 H25 N O F

* Référence utilisée pour la mesure de masse exacte
et mise en mélange avec l'échantillon CLG2170P
(C₁₈H₁₉NO₂, n=281)

Analyse dans H₂O / CH₃OH + 0,2% HCl

(E)-[1-(2-Fluoro-4,4-dimethylpent-2-en-1-yl)-2(hydroxymethyl)piperidine 12c-E

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

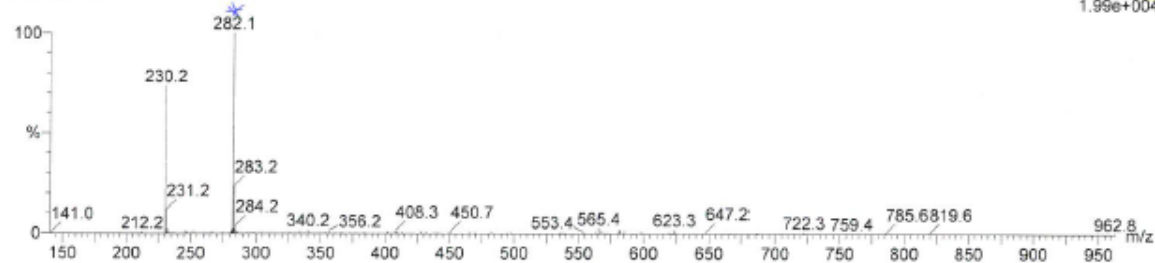
Elements Used:

C: 0-21 H: 0-70 N: 1-2 O: 1-4 F: 1-1

09-Sep-2014

CLG2169P 143 (2.644) AM (Cen,6, 80.00, Ar,5000.0,282.15,0.70); Cm (135.143)

14:26:45
1: TOF MS ES+
1.99e+004



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
230.1930	230.1920	1.0	4.3	1.5	68.9	C13 H25 N O F

* Référence utilisée pour la mesure de masse exacte et mise en mélange avec l'échantillon
(C₁₈H₁₉NO₂, n=281)

Analyse dans H₂O / CH₃CO + 0,2% HCO₂H