**Supplementary Information**

**Cytoprotective organoselenium compounds for oligodendrocytes**

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**Content of supporting information**

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| --- | --- | --- |
| **1** | **Docking patterns (panel A) and surface maps (panel B) for compounds 4c, 12 and 15 against 3C1L protein** | **.** |
| **2** | **S 2. Docking patterns (panel A) and surface maps (panel B) for compounds 4c, 12, and 15 conformers against 2F8A protein** |  |
| **3** | **Copies of HRMS, 1H and 13C NMR spectra of new compounds** |  |

|  |  |
| --- | --- |
| **S1. Docking patterns (panel A) and surface maps (panel B) for selected conformers of compounds 4c, 12, and 15 against 3C1L protein** | |
| **A** | **B** |
| **4c** |  |
| **12** |  |
| **15** |  |

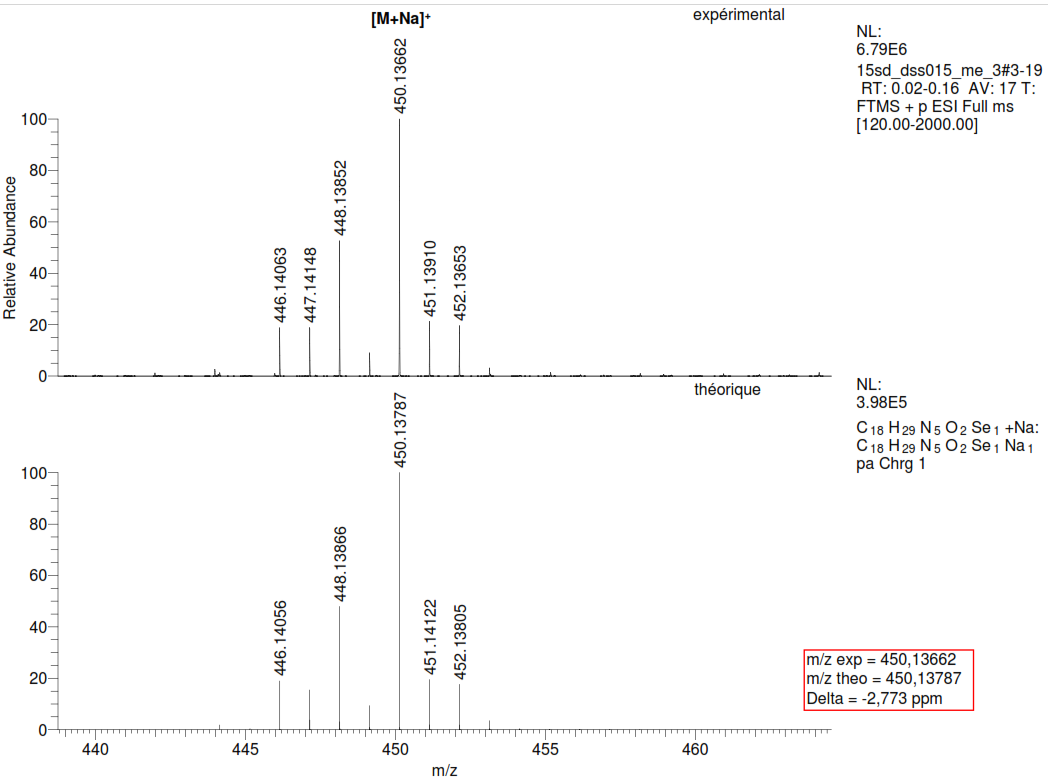
|  |  |
| --- | --- |
| **S 2. Docking patterns (panel A) and surface maps (panel B) for selected conformers of compounds 4c, 12, and 15 against 2F8A protein** | |
| **A** | **B** | **B** |
| **4c** |  |
| 12 |  |
| **15** |  |

**S3. Copies of HRMS, 1H and 13C NMR spectra of new compounds**

***N-((1-(tert-butyl)-1H-tetrazol-5-yl)methyl)-4-((2,2-diethoxyethyl)selanyl)aniline (5)***



HRMS of compound 5



1HNMR of compound 5

Diagram, schematic

Description automatically generated

13CNMR of compound 5

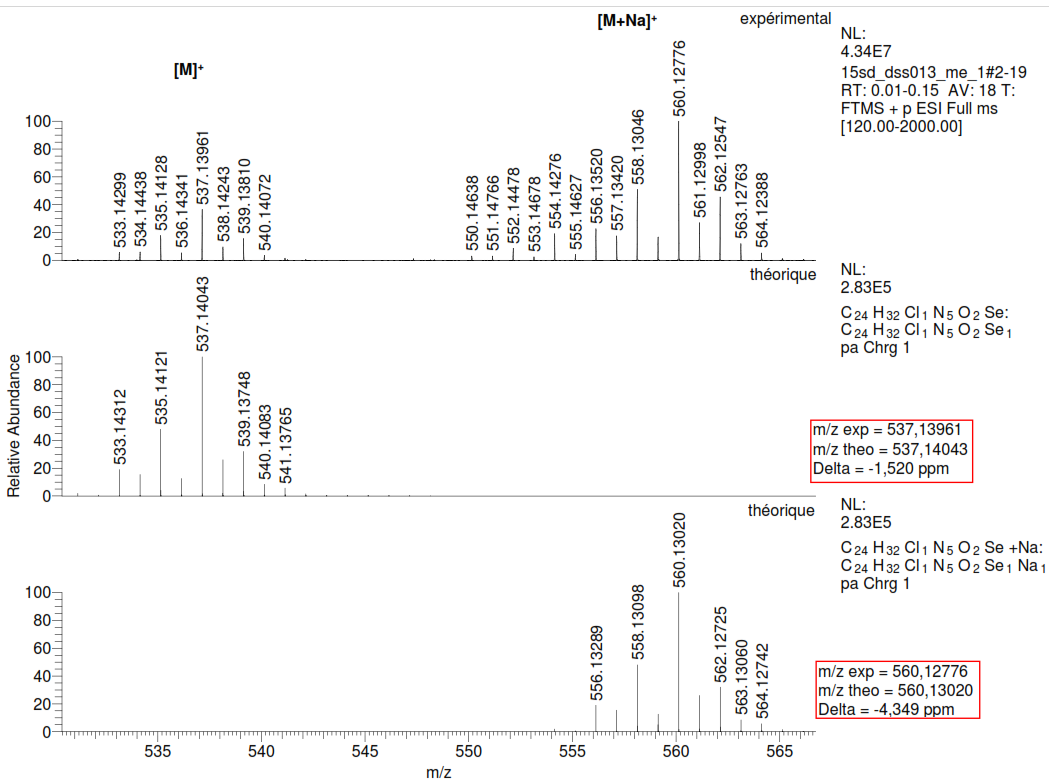
Chart, diagram

Description automatically generated with medium confidence

***N-((1-(tert-butyl)-1H-tetrazol-5-yl)(4-chlorophenyl)methyl)-4-((2,2-diethoxyethyl)selanyl)aniline*** *(****6****)*



HRMS of compound 6



1HNMR of compound 6

A picture containing small, sitting, boat, hanging

Description automatically generated

13CNMR of compound 6

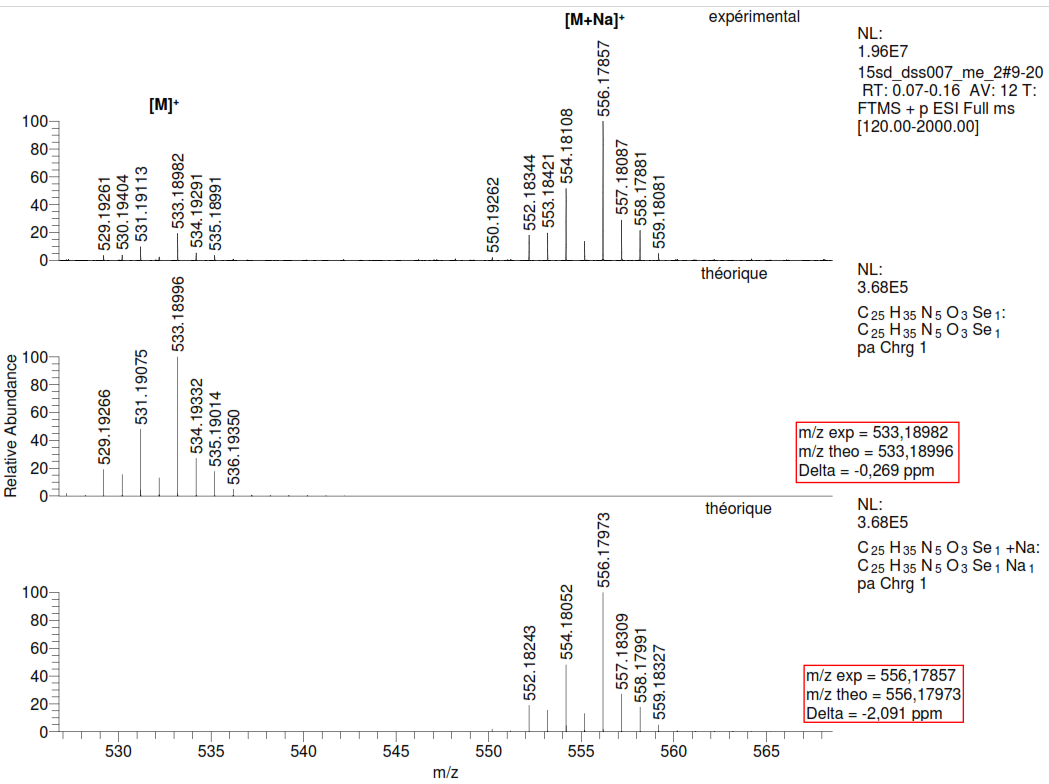
Chart

Description automatically generated

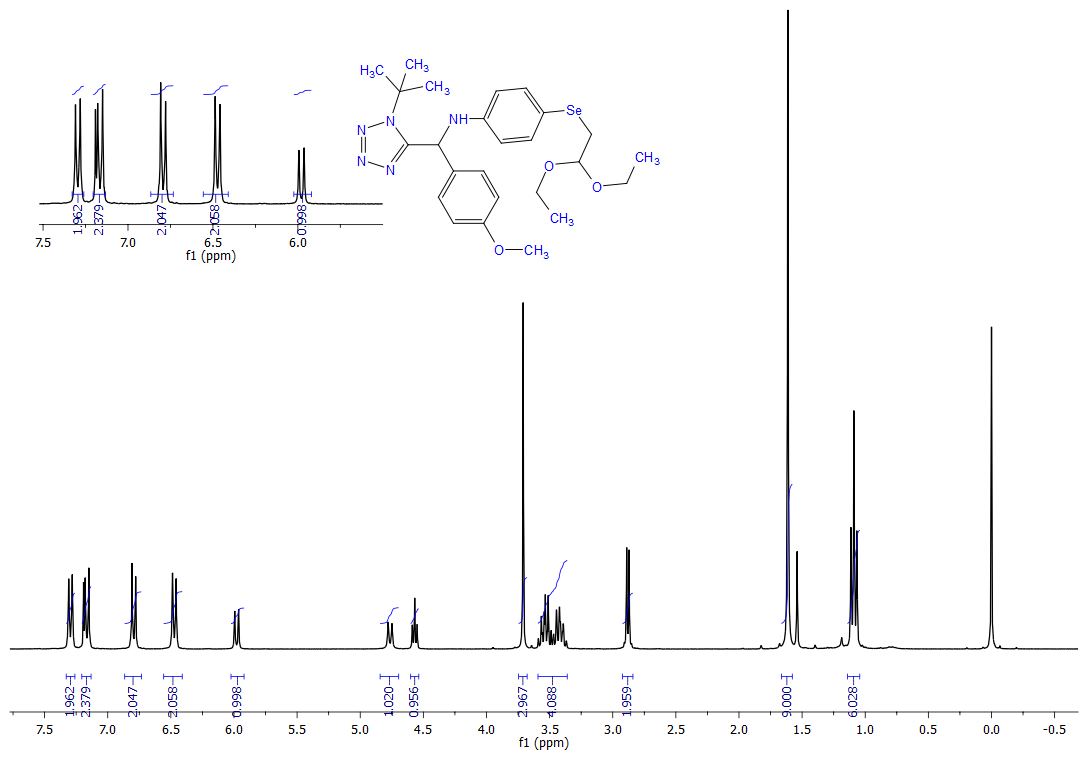
***N-((1-(tert-butyl)-1H-tetrazol-5-yl)(4-methoxyphenyl)methyl)-4-((2,2-diethoxyethyl)selanyl)aniline (7)***



HRMS of compound 7



1HNMR of compound 7



13CNMR of compound 7

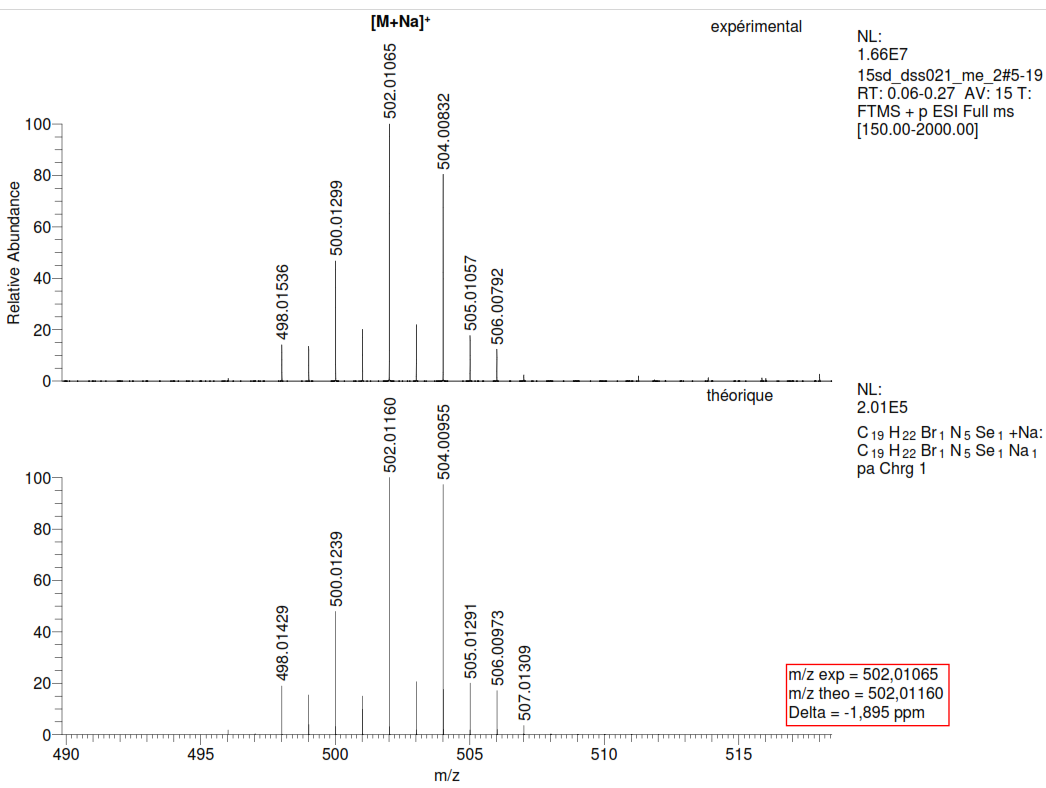
Chart, histogram

Description automatically generated

***4-((4-bromobenzyl)selanyl)-N-((1-(tert-butyl)-1H-tetrazol-5-yl)methyl)aniline (8)***



HRMS of compound 8



1HNMR of compound 8

Diagram

Description automatically generated

13CNMR of compound 8

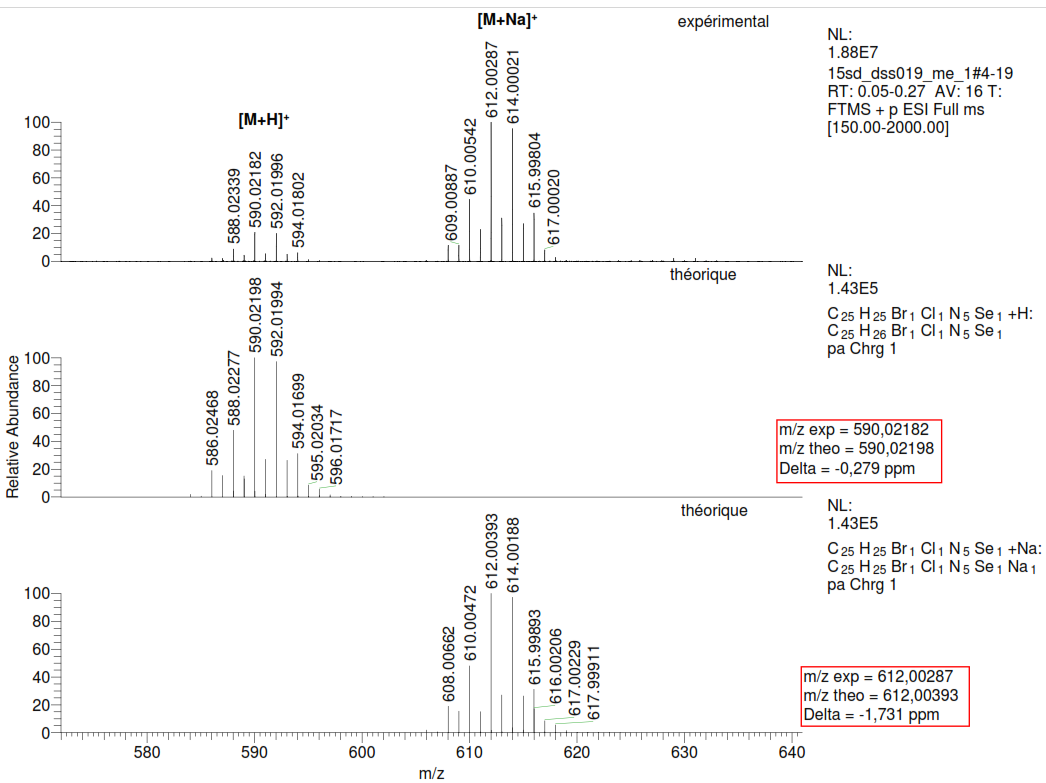
Chart

Description automatically generated

***4-((4-bromobenzyl)selanyl)-N-((1-(tert-butyl)-1H-tetrazol-5-yl)(4-chlorophenyl)methyl)aniline (9)***



HRMS of compound 9



1HNMR of compound 9

Diagram

Description automatically generated

13CNMR of compound 9

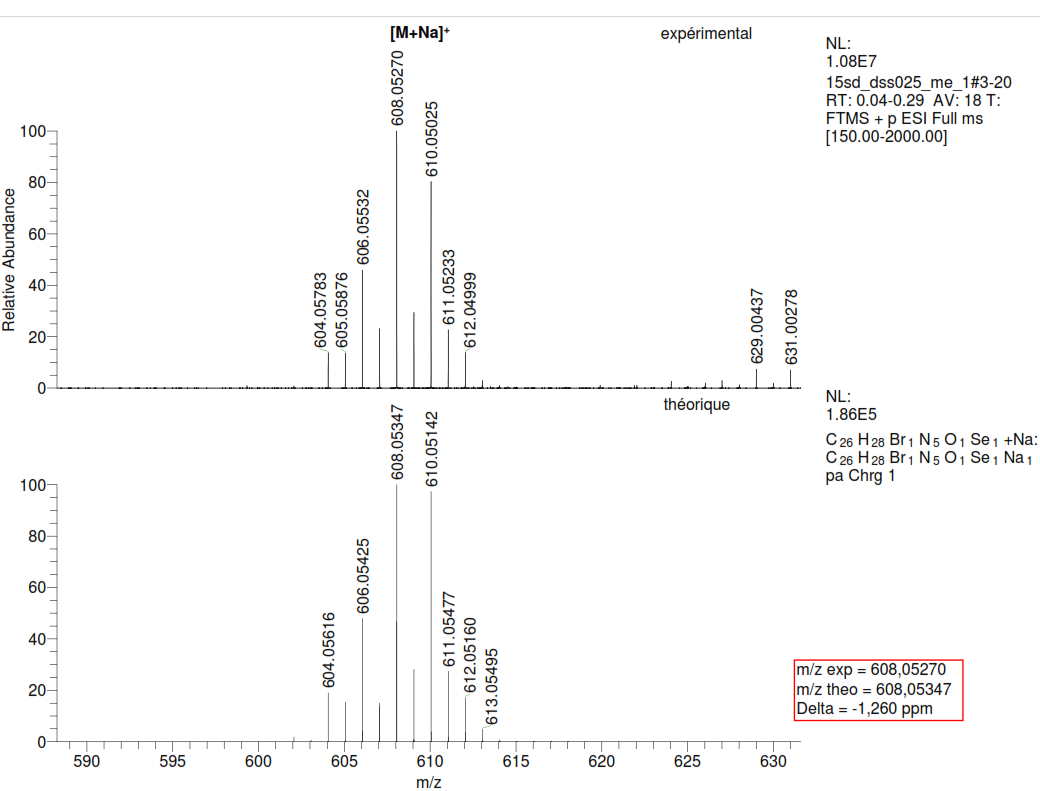
Chart, histogram

Description automatically generated

***4-((4-bromobenzyl)selanyl)-N-((1-(tert-butyl)-1H-tetrazol-5-yl)(4-methoxyphenyl)methyl)aniline (10)***



HRMS of compound 10



1HNMR of compound 10

Diagram

Description automatically generated

13CNMR of compound 10

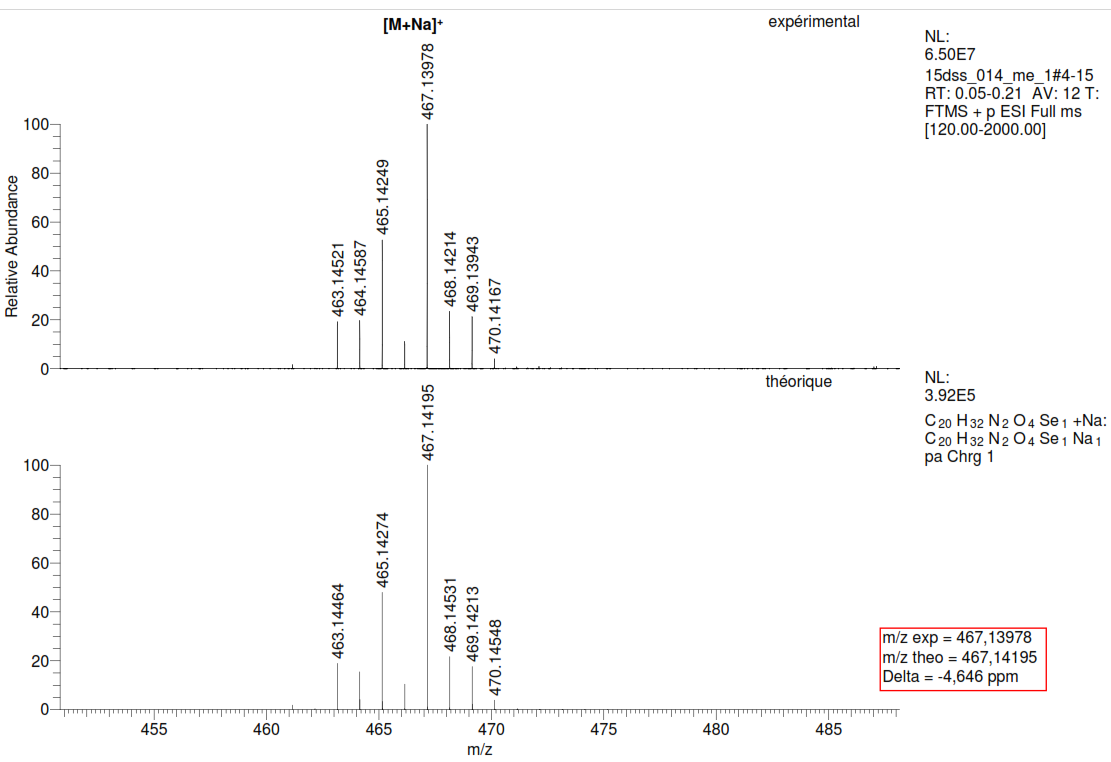
Chart

Description automatically generated

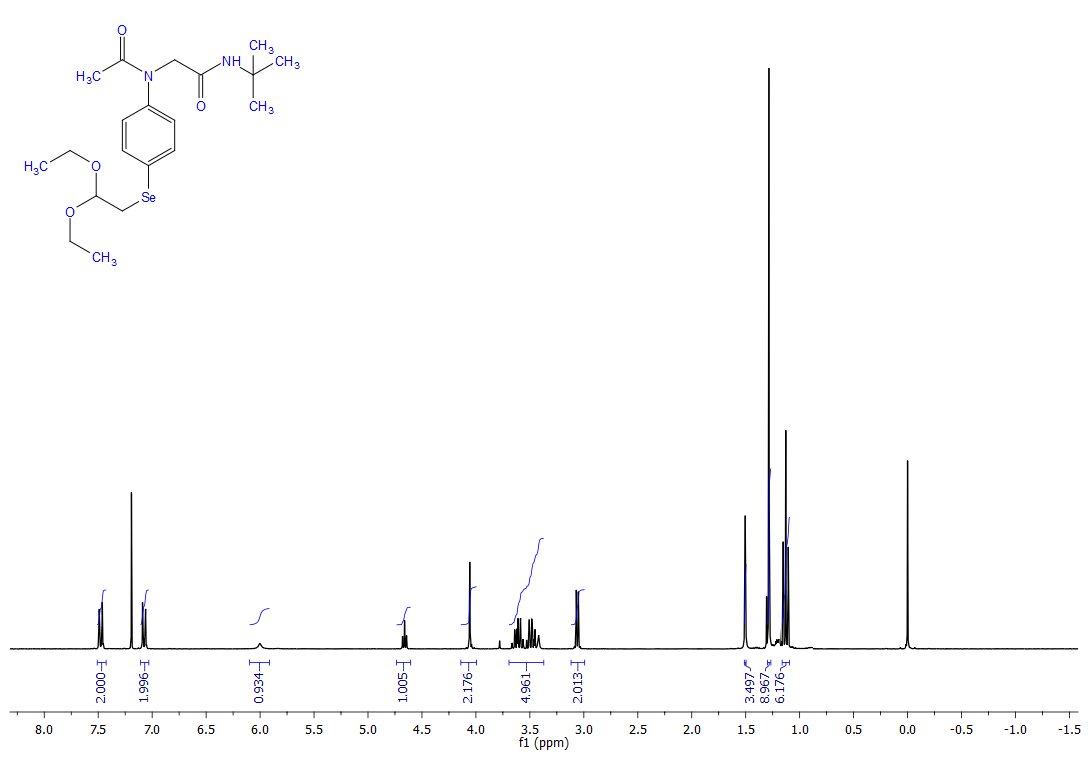
***N-(tert-butyl)-2-(N-(4-((2,2-diethoxyethyl)selanyl)phenyl)acetamido)acetamide (11)***



HRMS of compound 11



1HNMR of compound 11



13CNMR of compound 11

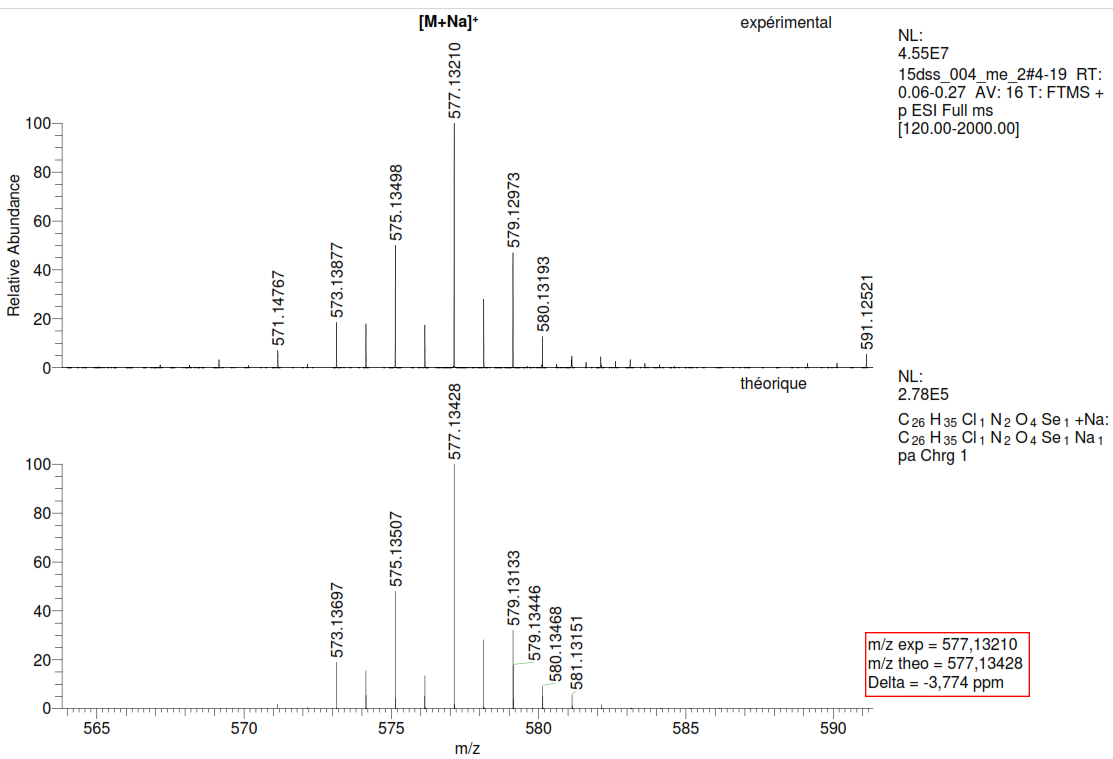
Chart, histogram

Description automatically generated

***N-(tert-butyl)-2-(4-chlorophenyl)-2-(N-(4-((2,2-diethoxyethyl)selanyl)phenyl)acetamido)acetamide (12)***



HRMS of compound 12



1HNMR of compound 12

Diagram

Description automatically generated

13CNMR of compound 12

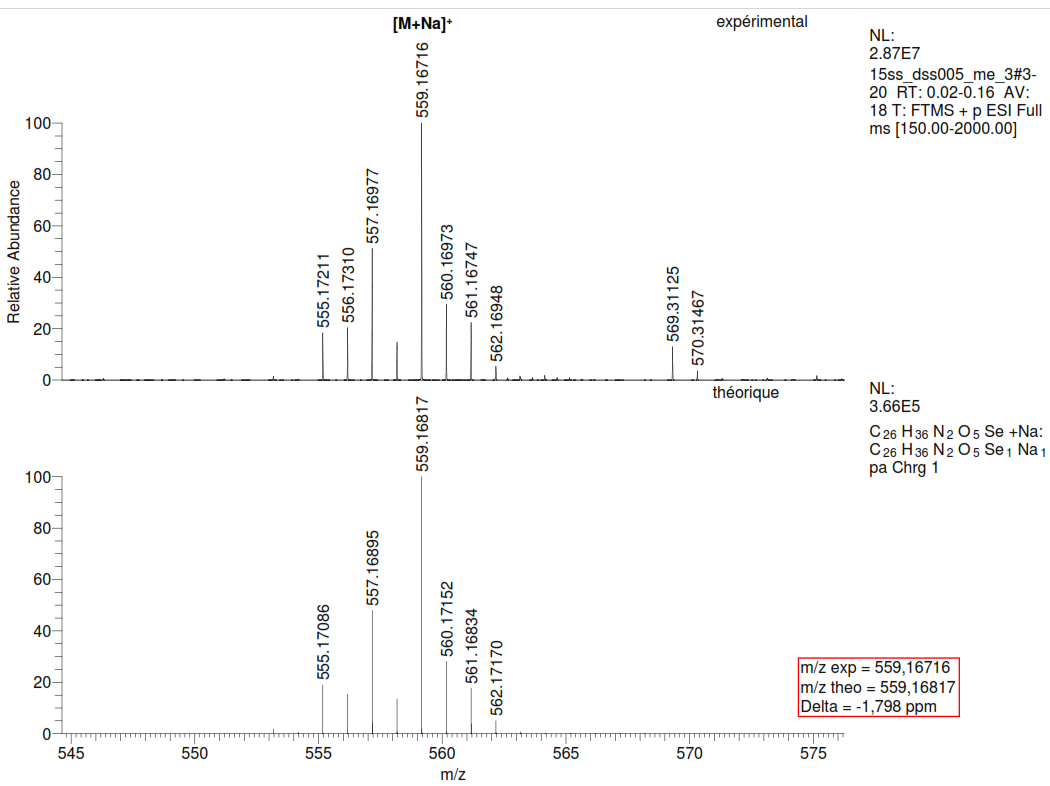
A picture containing chart

Description automatically generated

***N-(tert-butyl)-2-(N-(4-((2,2-diethoxyethyl)selanyl)phenyl)acetamido)-2-(4-hydroxyphenyl)acetamide (13)***



HRMS of compound 13



1HNMR of compound 13

Diagram

Description automatically generated

13CNMR of compound 13

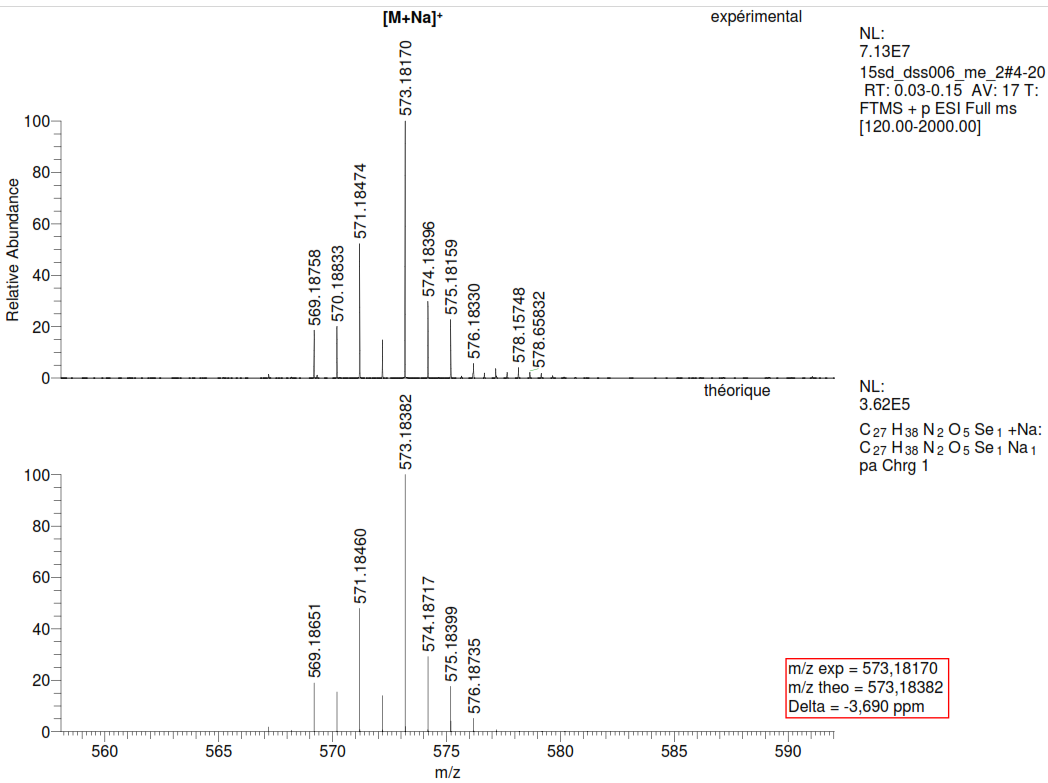
Chart, histogram

Description automatically generated

***N-(tert-butyl)-2-(N-(4-((2,2-diethoxyethyl)selanyl)phenyl)acetamido)-2-(4-methoxyphenyl)acetamide (14)***



HRMS of compound 14



1HNMR of compound 14

Diagram

Description automatically generated

13CNMR of compound 14

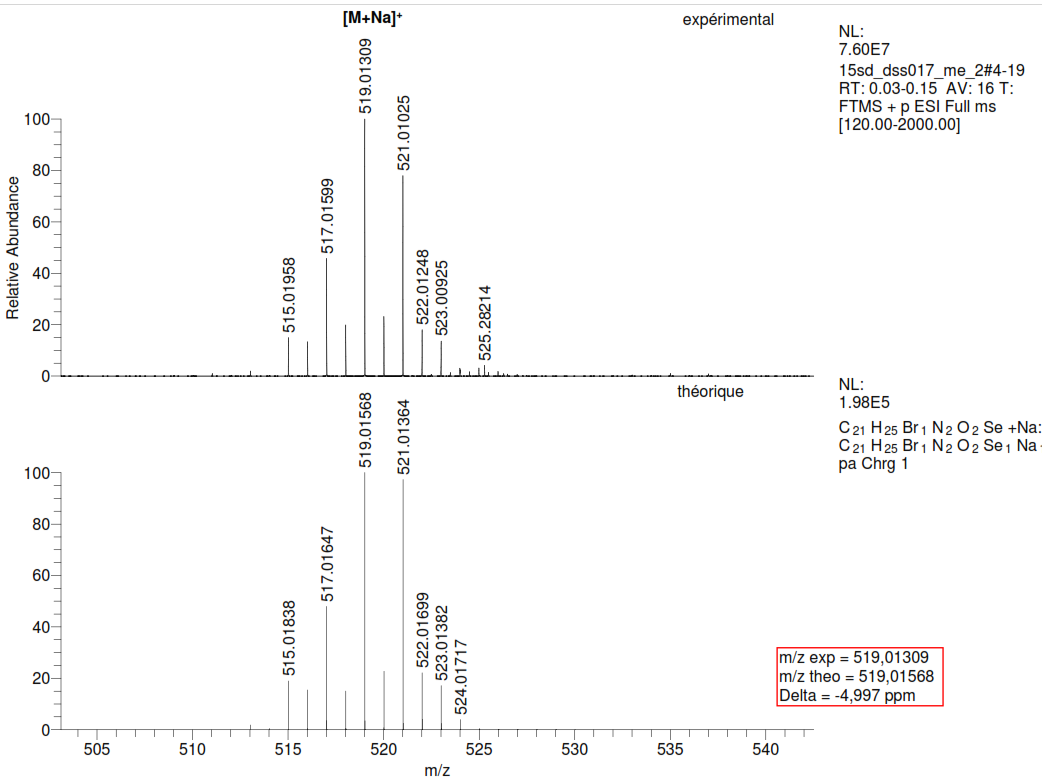
Chart

Description automatically generated

***N-(4-((4-bromobenzyl)selanyl)phenyl)-N-(2-(tert-butylamino)-2-oxoethyl)acetamide (15)***



HRMS of compound 15



1HNMR of compound 15

Diagram

Description automatically generated

13CNMR of compound 15

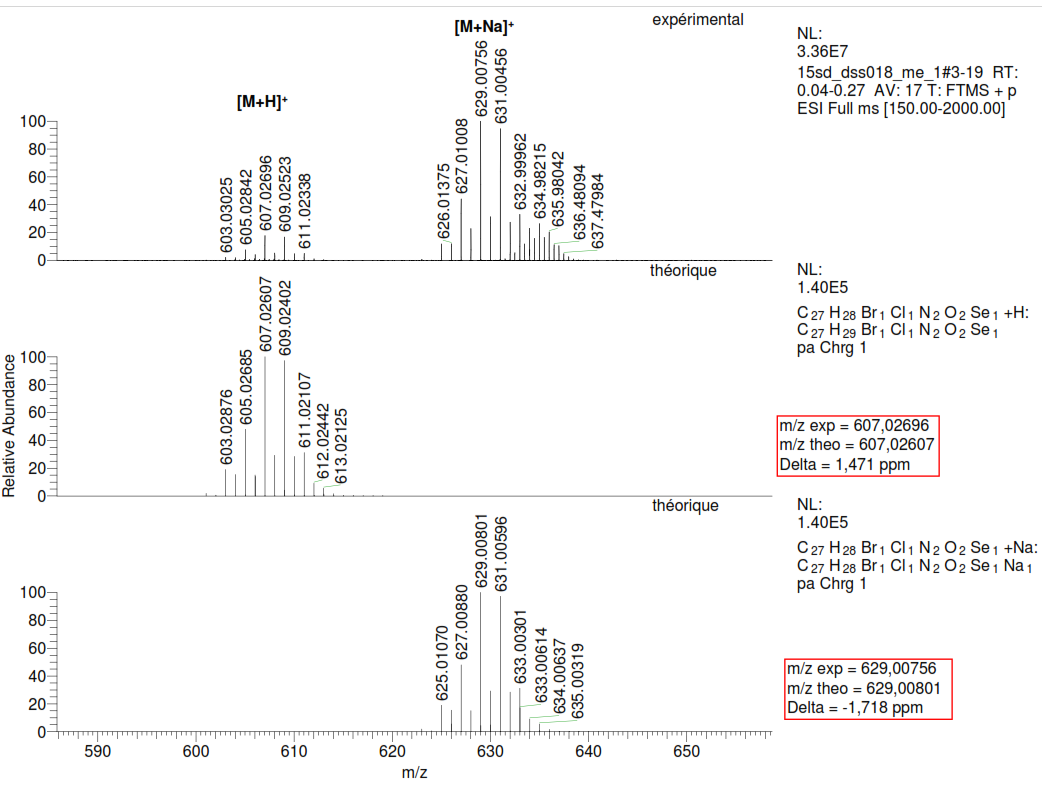
Chart, histogram

Description automatically generated

***2-(N-(4-((4-bromobenzyl)selanyl)phenyl)acetamido)-N-(tert-butyl)-2-(4-chlorophenyl)acetamide (16)***



HRMS of compound 16



1HNMR of compound 16

Diagram

Description automatically generated

13CNMR of compound 16

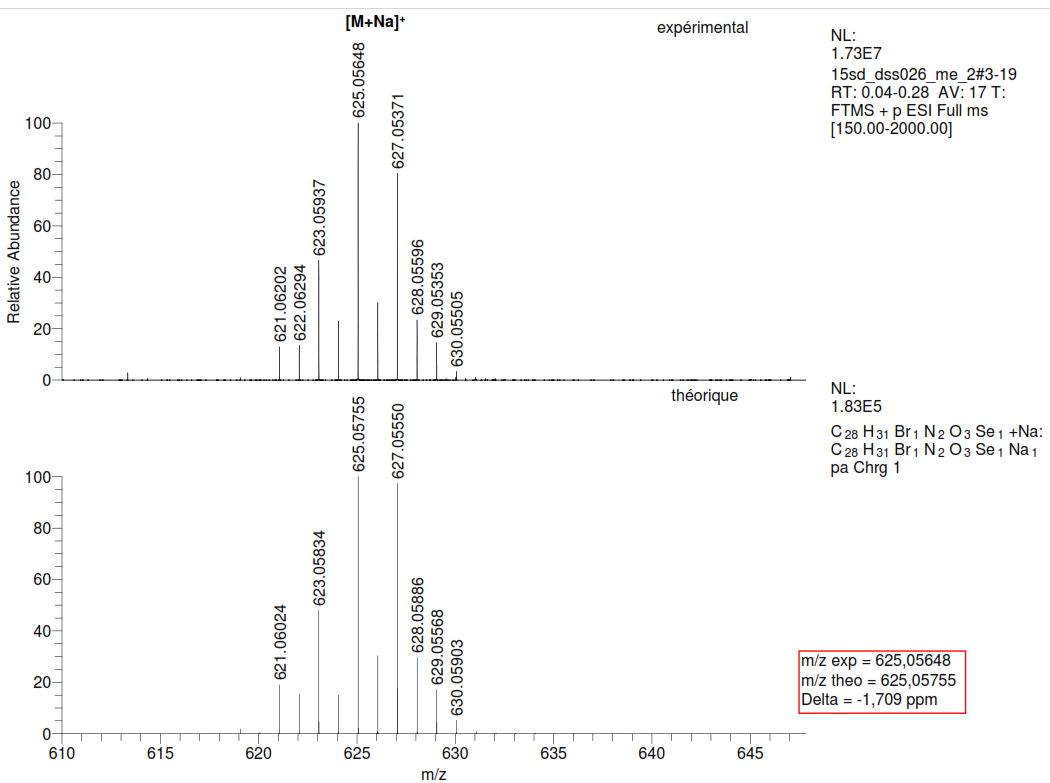
A picture containing diagram

Description automatically generated

***2-(N-(4-((4-bromobenzyl)selanyl)phenyl)acetamido)-N-(tert-butyl)-2-(4-methoxyphenyl)acetamide (17)***



HRMS of compound 17



1HNMR of compound 17

A picture containing boat, small, sitting, table

Description automatically generated

13CNMR of compound 17

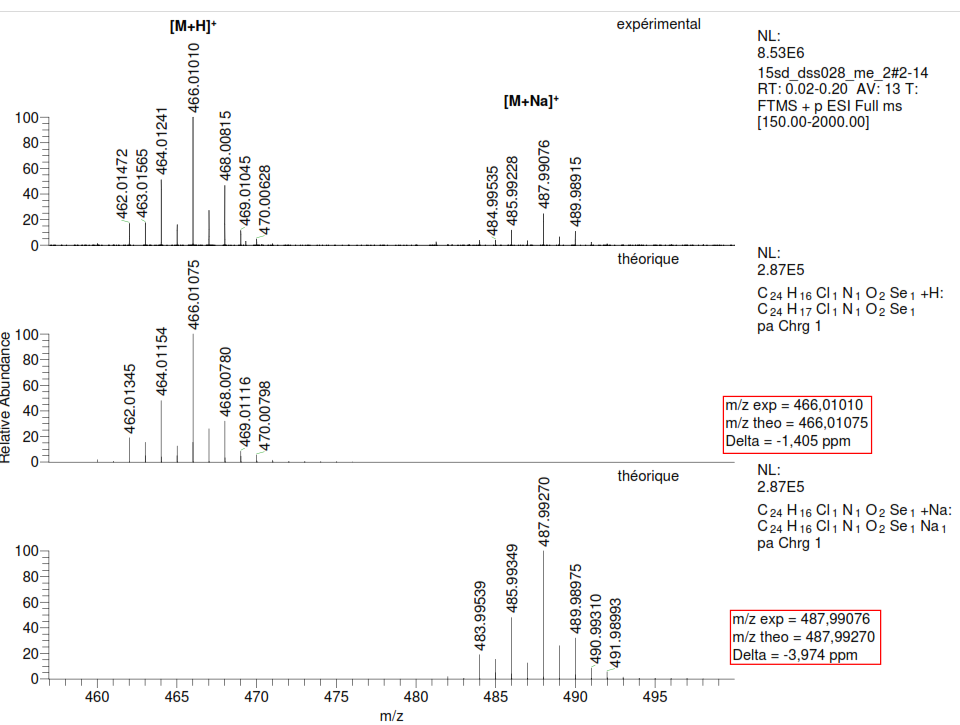
Diagram, histogram

Description automatically generated

***(E)-2-((4-((4-chlorobenzylidene)amino)phenyl)selanyl)-3-methylnaphthalene-1,4-dione (18)***



HRMS of compound 18



1HNMR of compound 18

Diagram

Description automatically generated

13CNMR of compound 18

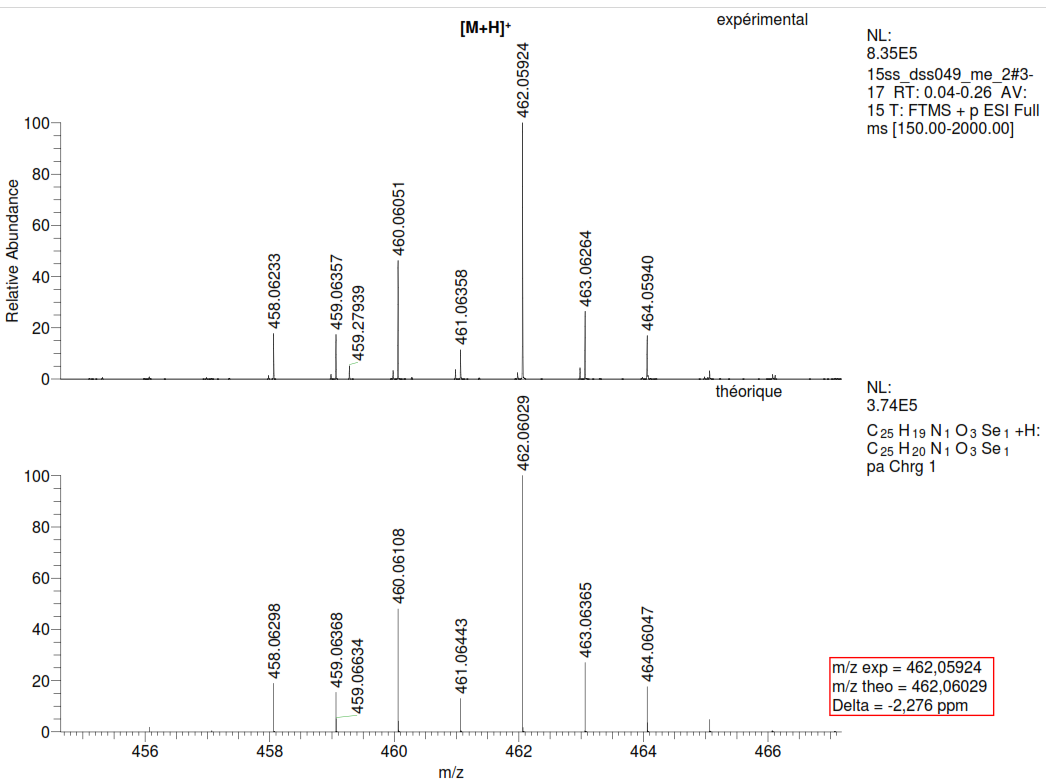
**Diagram

Description automatically generated**

***(E)-2-((4-((4-methoxybenzylidene)amino)phenyl)selanyl)-3-methylnaphthalene-1,4-dione (19)***



HRMS of compound 19



1HNMR of compound 19

Diagram

Description automatically generated

13CNMR of compound 19

Diagram

Description automatically generated

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