



---

# Simple MassChroQ User Manual

---

Free and Open Source Mass Chromatogram  
Quantification Software

---

version: 2.4.30

Filippo Rusconi  
Edlira Nano  
Michel Zivy

Benoît Valot  
Olivier Langella

# Contents

<b>Introduction .....</b>	<b>3</b>
<b>Input format .....</b>	<b>3</b>
<b>Output format .....</b>	<b>3</b>
<b>Conclusion .....</b>	<b>5</b>

# Introduction

SimpleMassChroQ is designed to extract ion current of a list of peptide and measure the area under the curve on a single run. No match between run.

## Input format

*CSV input file format*

peptide proformat, charge, retention time

SLTNDWEDHLAVK, 2, 853.78

SLTNDWEDHLAVK, 3, 853.78

## Output format

Wouldn't be nice to try CBOR ? CBOR is supported in QT6

It could be something like that :

*output file format*

```
{
  "id": "msruna1",
  "msdatafile": "/gorgone/pappso",
  "quanti": [
    {
      "id": "pepala1",
      "proformat": "SLTNDWEDHLAVK",
      "charge": 2,
      "rt_target": 853.78,
      "xics": [
        {
          "mz": 764.3755373,
          "isotope": 0,
          "trace": {
            "x": [851.78, 852.78, 853.78, 854.78],
            "y": [851.78, 852.78, 853.78, 854.78]
          },
          "peak": {
            "area": 450245623,
            "max_intensity": 2345.456,
            "rt": [851.78, 852.78, 853.78],
            "aligned_rt": [851.78, 852.78, 853.78]
          }
        }
      ],
      "mz": 764.8769,
      "isotope": 1,
      "trace": {
        "x": [851.78, 852.78, 853.78, 854.78],
        "y": [851.78, 852.78, 853.78, 854.78]
      },
      "peak": {
        "area": 550245623,
```

```

    }
  }
]
},
{
}
]
}

```

Une mini introduction pour le TP...

## 0) La question 1 ?

Remarque personnalisée

### 1) Donne un exemple de code en python.

Voici le code nécessaire pour afficher “Hello, World!” en Python :

*HelloWorld en Python*

```
print('Hello, World!')
```

### Une question sans numéro !

La remarque par défaut est très sobre.

### 2) Passer du code via un fichier ?

```
def print_hello():
    print("Hello, world!")
```

*Classic SQL*

```
SELECT *
FROM Test
WHERE id = 1
AND name = 'John Doe'
OR name = 'Jane Doe';
```

Du texte entre les images.



Figure 2: Un exemple d’image avec une légende.

### 3) Une autre question ?

$$A = \pi r^2$$

area =  $\pi \cdot \text{radius}^2$

$\mathcal{A} := \{x \in \mathbb{R} \mid x \text{ is natural}\}$

$5 < 17$

4) Des matrices ?

$$\begin{pmatrix} 1 & 2 & \dots & 10 \\ 2 & 2 & \dots & 10 \\ \vdots & \vdots & \ddots & \vdots \\ 10 & 10 & \dots & 10 \end{pmatrix}$$

5) Du code inline !

What is `fn main()` in Rust would be `int main()` in C

6) Un tableau ?

	Area	Parameters
Une cellule	$\pi h \frac{D^2 - d^2}{4}$	<i>h</i> : height <i>D</i> : outer radius <i>d</i> : inner radius
Une autre cellule	$\frac{\sqrt{2}}{12} a^3$	<i>a</i> : edge length

Conclusion

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do.