



MASSCHROQ₃ USER MANUAL

FREE AND OPEN SOURCE PEPTIDE QUANTIFICATION SOFTWARE

version: 1.2.0

Benoît Valot
Edlira Nano

Olivier Langella
Filippo Rusconi

CONTENTS

1	<i>MASSCHROQ</i> ₃	5
2	<i>MASSCHROQ</i> EXPORT TOOL	6
2.1	Export alignment data to JSON	6
2.2	Generate PDF alignment data report using Typst	6
	BIBLIOGRAPHY	7

LIST OF FIGURES

I *MASSCHROQ₃*

2 *MASSCHROQ* EXPORT TOOL

MassChroQ3 comes with a CLI tool *masschroq-export* to extract data from the CBOR *MassChroQ3* output file

masschroq-export online help

```
$ masschroq-export -h RETURN
```

2.1 EXPORT ALIGNMENT DATA TO JSON

extracting alignment data to JSON file

```
$ masschroq-export --json alignment_data.json mcq_quantification_results.cbor RETURN
```

2.2 GENERATE PDF ALIGNMENT DATA REPORT USING TYPST

You need the JSON alignment data file generated in [SECTION 2.1 “EXPORT ALIGNMENT DATA TO JSON”](#).

Prepare a simple Typst file (text file with .typ extension) called “alignment.typ” with this content:

```
#import "@preview/proteograph:0.2.0": *  
  
= Display retention time alignment informations  
  
#let mcq3_json = json("alignment_data.json")  
#mcq3-alignment-summary(mcq3_json)
```

And compile this file using :

Compile alignment typst file

```
$ typst compile alignment.typ RETURN
```

BIBLIOGRAPHY