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Wout Bittremieux, Wout Bittremieux, Christopher Chen, Pieter C. Dorrestein ...+6 more authors

Institutions: University of Montana, University of Antwerp, University of Luxembourg, Leibniz Association ...+2 more institutions

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Title

Universal MS/MS Visualization and Retrieval with the Metabolomics Spectrum Resolver Web Service

Authors

Wout Bittremieux[1,2,*], Christopher Chen[1], Pieter C. Dorrestein[1], Emma L. Schymanski[3], Tobias Schulze[4], Steffen Neumann[5,6], Rene Meier[4], Simon Rogers[7,*], Mingxun Wang[1,*]

* These authors contributed equally

Affiliations

1. Skaggs School of Pharmacy and Pharmaceutical Sciences, UC San Diego, 9500 Gilman Dr., La Jolla CA 92093, USA.
2. Department of Computer Science, University of Antwerp, Middelheimlaan 1, 2020 Antwerpen, Belgium.
3. Luxembourg Centre for Systems Biomedicine (LCSB), University of Luxembourg, 6 Avenue du Swing, 4367 Belvaux, Luxembourg.
4. Leibniz Institute of Plant Biochemistry, Bioinformatics and Scientific Data, Weinberg 3, 06120 Halle, Germany.
5. German Centre for Integrative Biodiversity Research (iDiv) Halle-Jena-Leipzig, Deutscher Platz 5e, 04103 Leipzig, Germany.
6. Helmholtz Centre for Environmental Research – UFZ, Department of Effect Directed Analysis, Permoserstrasse 15, 04318 Leipzig, Germany.
7. School of Computing Science, University of Glasgow, Glasgow G12 8QQ, United Kingdom.

Abstract

The growth of online mass spectrometry metabolomics resources, including data repositories, spectral library databases, and online analysis platforms has created an environment of online/web accessibility. Here, we introduce the Metabolomics Spectrum Resolver (https://metabolomics-usi.ucsd.edu/), a tool that builds upon these exciting developments to allow for consistent data export (in human and machine-readable forms) and publication-ready visualisations of tandem mass spectrometry spectra. This tool supports the Human Proteome Organization – Proteomics Standards Initiative's Universal Spectrum Identifier (USI) specification, which has been extended to deal with the metabolomics use cases. To date, this resource already supports data formats from GNPS, MassBank, MS2LDA, MassIVE, MetaboLights, and Metabolomics Workbench and is integrated into several of these resources.

Introduction

The effective exchange and visualization of tandem mass spectrometry (MS/MS) information across a variety of resources is important in communicating and consequently building confidence in both data quality and molecule identification throughout the research and publication process. The inclusion of MS/MS spectra in scientific manuscripts and presentations to provide evidence of newly discovered molecules in a consistent manner is often challenging and labor intensive due to heterogeneous data availability and accessibility across public data resources, the variety of complex file formats in use to store mass spectrometry data, and the lack of suitable software tools available. Furthermore, it is often difficult to balance the ease of MS/MS figure generation with the level of customization possible.

A few approaches have been introduced to assign universal identifiers to MS/MS spectra. The SPectraL hASH (SPLASH) identifier has been designed as an unambiguous, database-independent spectrum identifier[1]. SPLASH identifiers can be used to determine spectral overlap between libraries and potentially query public data repositories. However, as generating a SPLASH identifier includes a complex hashing operation, these identifiers cannot be trivially produced. Alternatively, the Universal Spectrum Identifier (USI) was recently developed by the Human Proteome Organization – Proteomics Standards Initiative (HUPO-PSI)[2] to provide a standardized mechanism for encoding a virtual path to spectra contained in proteomics public repositories[3]. Although USIs are easy to construct, the USI standard currently mainly supports proteomics spectral data deposited via ProteomeXchange[4] and does not natively support spectral data stored in metabolomics repositories.

Additionally, producing high-quality figures of MS/MS spectra is challenging as well. On one hand, existing software such as the Proteomics Data Viewer (PDV)[5], the Interactive Peptide Spectral Annotator (IPSA)[6], and Lorikeet[7] proteomics data viewers, as well as vendor software, are able to draw MS/MS spectra, but are mainly aimed at interactive visualization. Three key features are often missing from such software: the ability to export vector graphics (to ensure high resolution), customization of spectral visualization, and high-throughput automated figure generation. On the other end of the spectrum are generic vector graphics editors such as Adobe Illustrator or Inkscape. While such generic editors are powerful, they lack MS/MS specific features and producing images ready for publication with these tools requires a significant time investment to achieve high levels of customization.

We present here the Metabolomics Spectrum Resolver (https://metabolomics-usi.ucsd.edu/), a web tool that enables: 1) integration with major metabolomics data repositories to retrieve MS/MS metabolomics data from various sources in a unified fashion, 2) high-quality and customizable vector graphics drawing, 3) direct integration with common online analysis tools, and 4) a web API to programmatically retrieve spectral data.

Results and Discussion

MS/MS Data Sources - Integration with Community Resources

The Metabolomics Spectrum Resolver builds upon the USI standard developed by the HUPO-PSI[3]. USIs are formatted as follows:

```
mzspec:<collection>:<msRun>:<indexType>:<indexNumber>:<optional interpretation>
```

For more details on the USI, including its formal specification, see the HUPO-PSI website (http://www.psidev.info/usi).

The USI standard has originally been developed for proteomics data, with only ProteomeXchange identifiers and related identifiers from its member repositories allowed in the "collection" field. We have extended the USI specification to support several major metabolomics resources as well. Concretely, the following metabolomics data services are currently supported (**Table 1**):

- Data repositories: MassIVE[8], MetaboLights[9], Metabolomics Workbench[10].
- Reference spectral library resources: MassBank[11], MoNA (https://mona.fiehnlab.ucdavis.edu/), GNPS[12], and MS2LDA.org MOTIFDB[13].
- Online informatics pipelines: GNPS Molecular Networking[12] / Library Search / MASST[14] / Feature-based Molecular Networking[15], and MS2LDA.org[13].

As such, the Metabolomics Spectrum Resolver provides a universal interface to more than 450M MS/MS spectra from various public metabolomics repositories. It also supports linking back to the source spectra in their original data resources to allow users to explore the original context of the MS/MS spectra. Several resources (MassBank, GNPS, and MS2LDA.org) have already integrated links to the Metabolomics Spectrum Resolver to facilitate bidirectional interoperability. Additionally, SPLASH identifiers[1] are computed for all spectra retrieved through the Metabolomics Spectrum Resolver to enable their comparison across different resources.

Table 1 - Examples of the Metabolomics Spectrum Resolver from various public data resources.

Resource	USI Format	Example USI
MassBank	• collection: `MASSBANK` • msRun: none • index: `accession:<spectrumId>`	`mzspec:MASSBANK::accession:SM858102`
GNPS Spectral Library	• collection: `GNPS` • msRun: `GNPS-LIBRARY` • index: `accession:<spectrumId>`	`mzspec:GNPS:GNPS-LIBRARY:accession:CCMSLIB00005436077`
GNPS Molecular Networking Spectrum	• collection: `GNPS` • msRun: `TASK-<taskId>` • index: `scan:<scanNr>`	`mzspec:GNPS:TASK-c95481f0c53d42e78a61bf899e9f9adb-spectra/specs_ms.mgf:scan:1943`
MS2LDA MotifDB	• collection: `MOTIFDB` • msRun: none • index: `accession:<motifId>`	`mzspec:MOTIFDB::accession:171163`
MS2LDA Analysis Spectrum	• collection: `MS2LDA` • msRun: `TASK-<taskId>` • Index: `accession:<spectrumId>`	`mzspec:MS2LDA:TASK-190:accession:270684`
MassIVE/GNPS Repository Spectrum	• collection:MassIVE/ProteomeXchange identifier • msRun: filename • index: `scan:<scanNr>`	`mzspec:MSV000078547:120228_nbut_3610_it_it_take2:scan:389`
Metabolights Repository Spectrum	• collection: `MSV000082791` • msRun: filename • index: `scan:<scanNr>`	`mzspec:MSV000082791:(-)-epigallocatechin:scan:2`
Metabolomics Workbench Repository Spectrum	• collection: `MSV000082680` • msRun: filename • index: `scan:<scanNr>`	`mzspec:MSV000082680:iPSC-T1R1:scan:3`

The Metabolomics Spectrum Resolver provides powerful visualization capabilities to plot spectral data (see below). Additionally, the raw spectral data can be retrieved directly in different machine readable formats (JSON or CSV) via web APIs. This enables inspection of the spectral data by both humans and automated tools, for example to provide visual evidence of newly discovered molecules in scientific manuscripts or to re-evaluate spectral identifications with alternative computational tools. Furthermore, using the programmatic web API, software developers are able to integrate high-throughput figure creation in a programming language-agnostic fashion. This functionality is already being used by members of the community to programmatically retrieve spectral data in a standardized fashion and facilitate figure generation[16].

Visualization Capabilities

The Metabolomics Spectrum Resolver enables users to plot individual MS/MS spectra (**Figure 1a**) and mirror matches between pairs of MS/MS spectra to show their similarity (e.g. between an experimental spectrum and its spectral library match; **Figure 1b**).The resulting figures can be modified by specifying mass ranges, intensity ranges, customizable peak labeling, figure size, decimal points for mass values, and an optional grid. Additionally, the similarity between the two spectra in a mirror plot can be displayed based on the standard cosine similarity or a “shifted cosine similarity” (i.e. also matching peaks that differ by the precursor mass difference between both spectra), with matching peaks between the two spectra highlighted to assess the match quality. The resulting drawing can be downloaded in the SVG (vector), PNG (raster), CSV (comma separated peaks), and JSON (machine readable peaks) formats (**Figure 2**).

Plotting functionality is implemented in Python using spectrum_utils[17], Matplotlib[18], and Seaborn[19]. Additionally, NumPy[20], SciPy[21], and Numba[22] are used for efficient processing of spectral data.

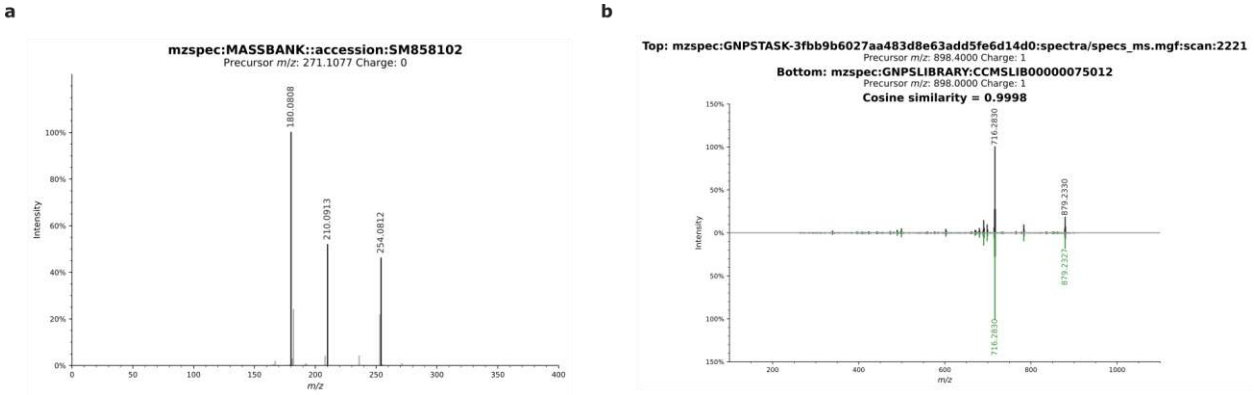

Figure 1 - Example MS/MS *figure generation of (a) a single MS/MS spectrum and (b) a mirror plot.*

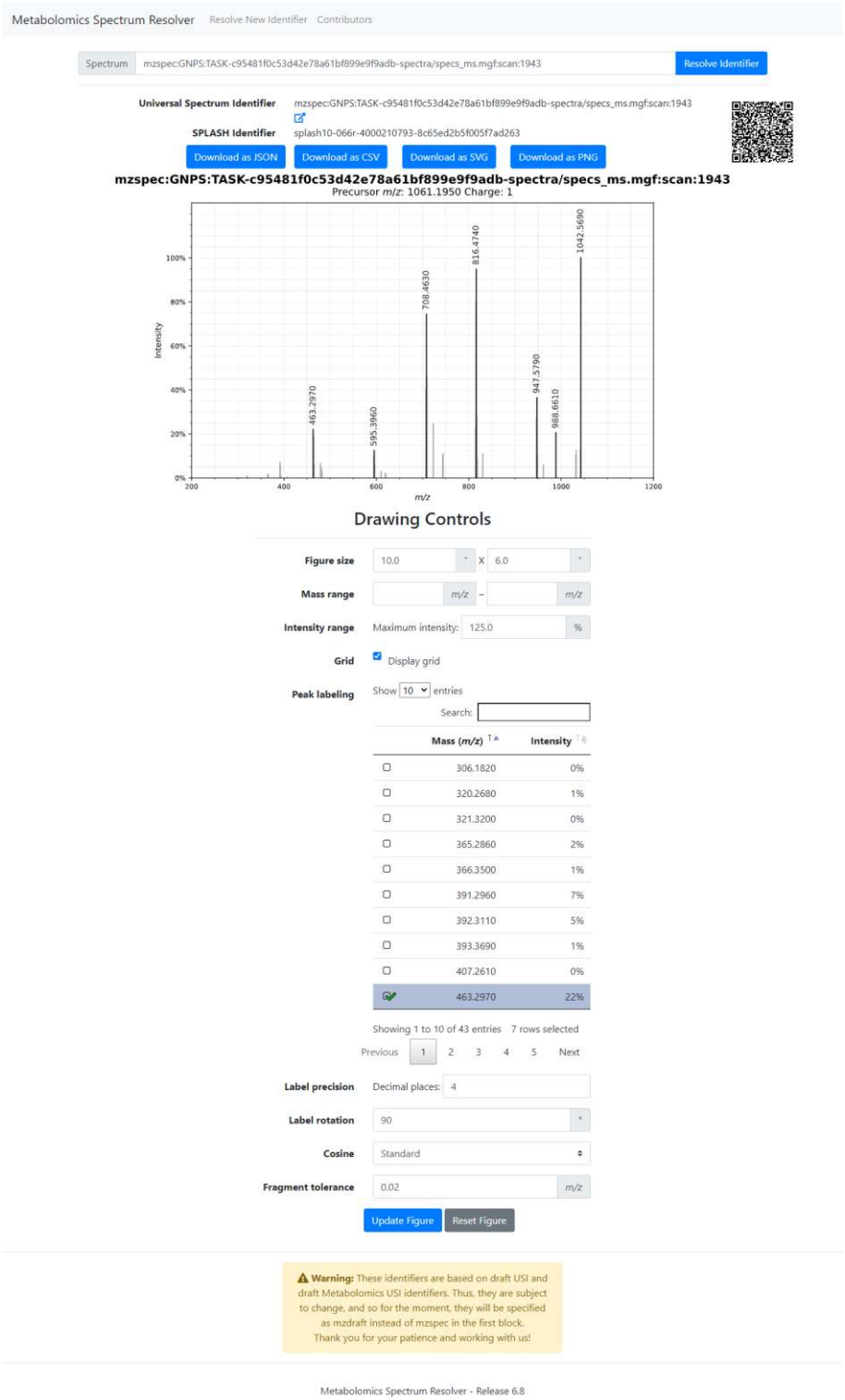

Figure 2 - Interactive User Interface with Drawing Options. Enables customizing the spectrum drawing, linking back to original spectral data via URL and a generated QR code, the spectrum's SPLASH identifier, spectrum peaks download, and programmatic data download.

Conclusion

The Metabolomics Spectrum Resolver has been designed to improve the accessibility and presentation of metabolomics data, both within supported public data resources and for the community. By extending the nascent USI standard developed by the HUPO-PSI to support metabolomics repositories and tools as well, it provides a universal interface to metabolomics spectral data from heterogeneous data resources. The Metabolomics Spectral Resolver supports a broad range of key online metabolomics resources, provides unified programmatic API access to spectral data, and facilitates high quality spectrum drawing. Implemented as a freely available and open source web service, it facilitates and democratizes public data access without the need to install specialized software.

Source Code

The Metabolomics Spectrum Resolver source code is released as open source under the MIT License and is available at this DOI: 10.5281/zenodo.4033442. Active development can be found on GitHub: https://github.com/mwang87/MetabolomicsSpectrumResolver.

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Conflict of Interests

Mingxun Wang is a founder of Ometa Labs LLC. Pieter C. Dorrestein is on the scientific advisory board of Sirenas and Cybele Microbiome.

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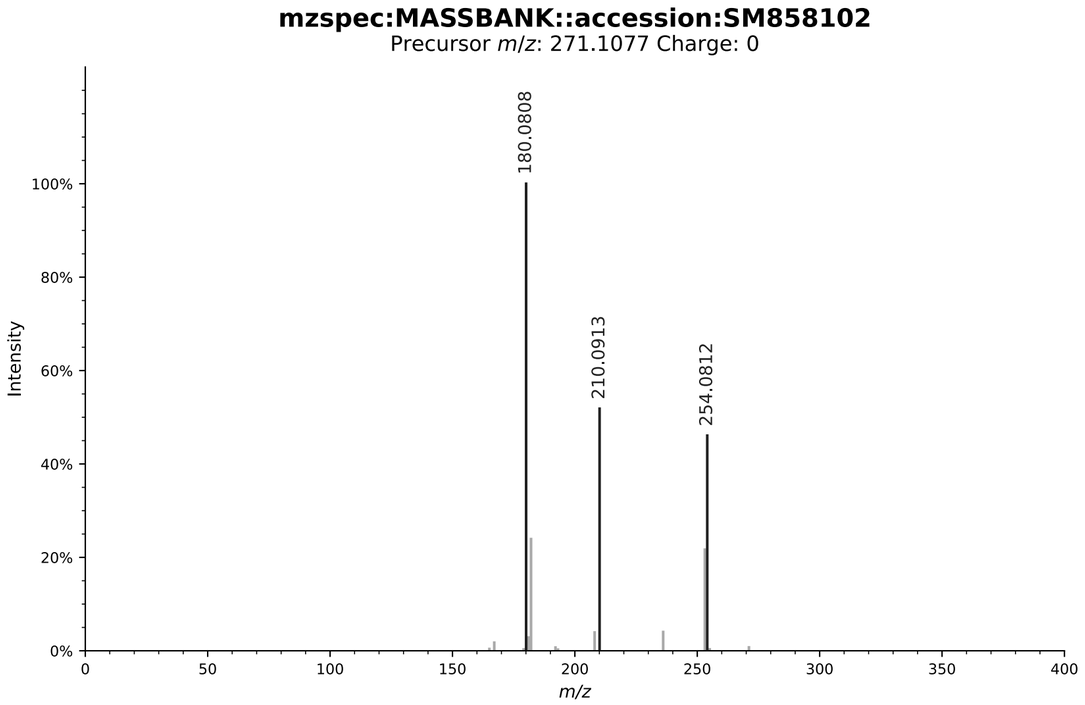
a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m/z

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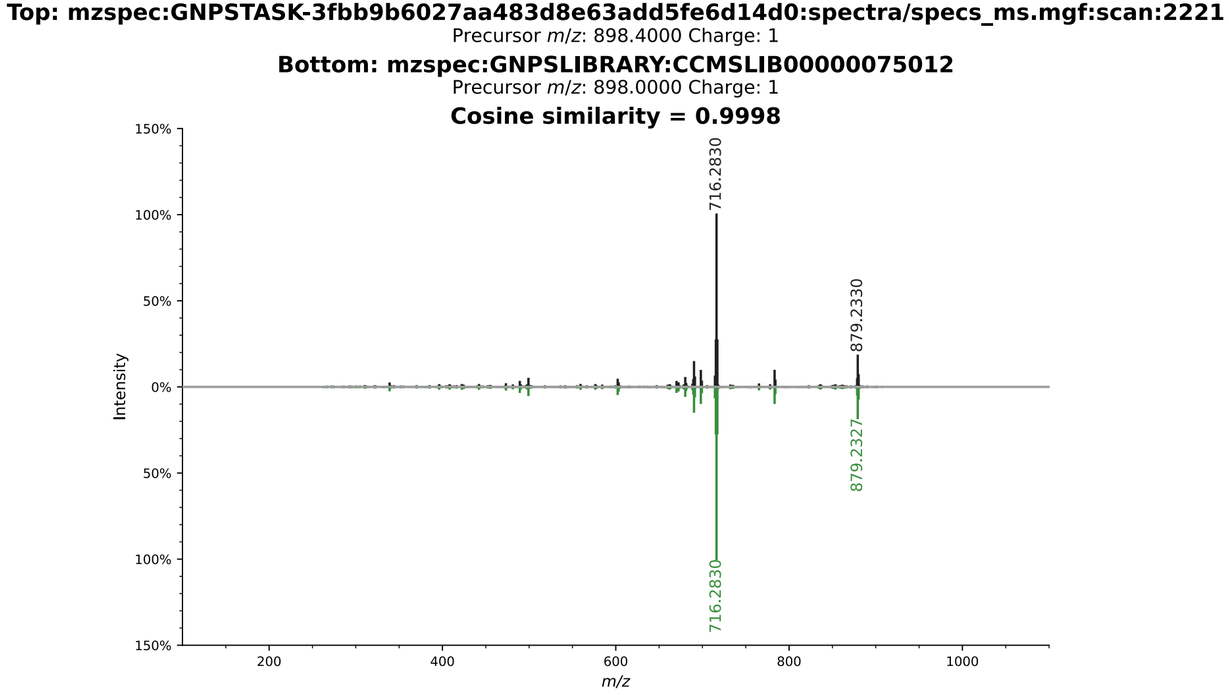
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Bottom: mzspec:GNPSLIBRARY:CCMSLIB00000075012
Precursor m/z: 898.0000 Charge: 1
Cosine similarity = 0.9998
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879.2330
879.2327
716.2830
Intensity
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100%
50%
0%
50%
100%
150%
200
400
600
800
1000
m/z

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Universal Spectrum Identifier mzspec:GNPS:TASK-c95481f0c53d42e78a61bf899e9f9adb-spectra/specs_ms.mgf:scan:1943

SPLASH Identifier splash10-066r-4000210793-8c65ed2b5f005f7ad263

Download as JSON | Download as CSV | Download as SVG | Download as PNG

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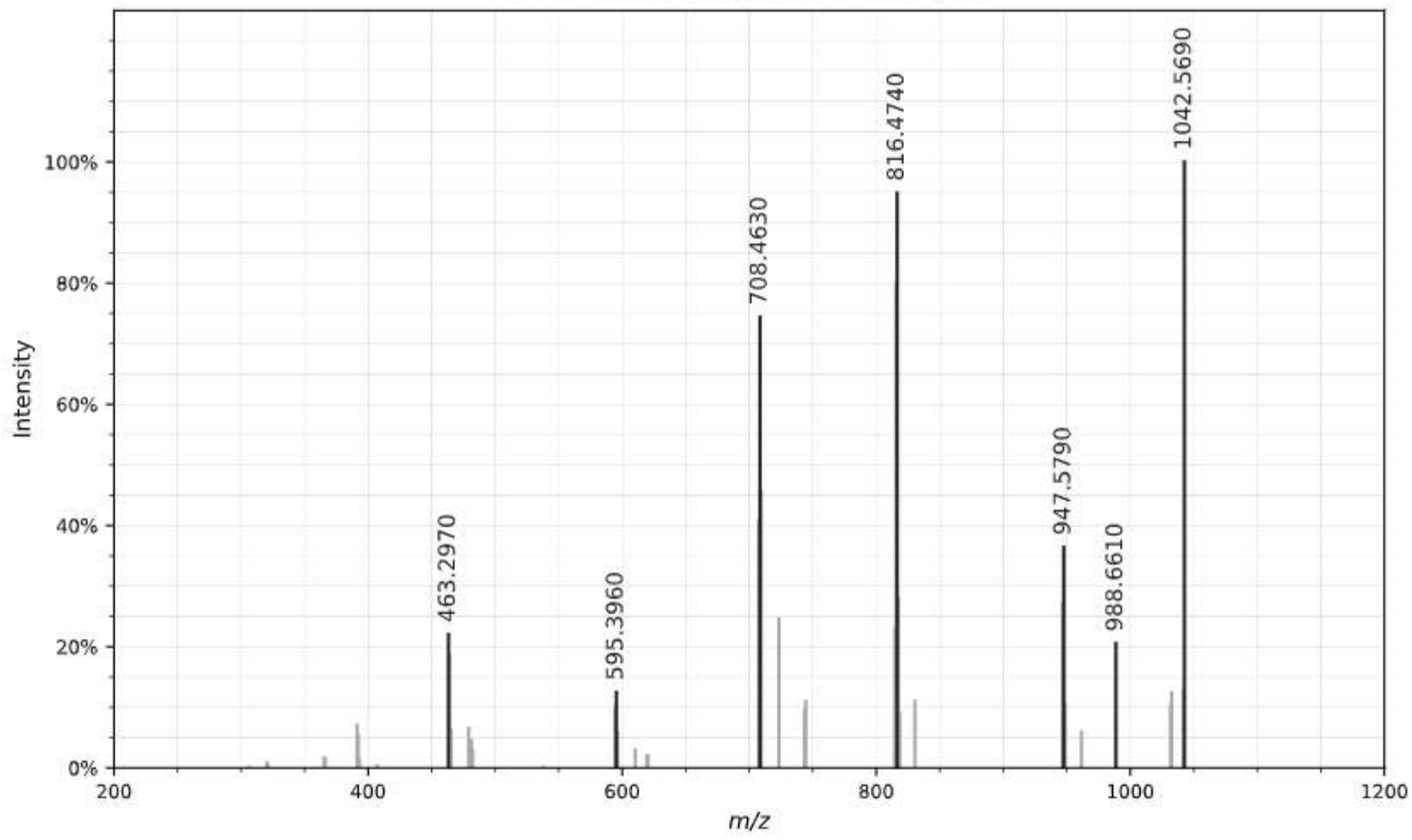

Drawing Controls

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Mass range m/z – m/z

Intensity range Maximum intensity: 125.0 %

Grid Display grid

Peak labeling

Show 10 entries Search:

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☐	306.1820	0%
☐	320.2680	1%
☐	321.3200	0%
☐	365.2860	2%
☐	366.3500	1%
☐	391.2960	7%
☐	392.3110	5%
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Showing 1 to 10 of 43 entries 7 rows selected

Previous 1 2 3 4 5 Next

Label precision Decimal places: 4

Label rotation 90 °

Cosine Standard

Fragment tolerance 0.02 *m/z*

Update Figure | Reset Figure

⚠ **Warning:** These identifiers are based on draft USI and draft Metabolomics USI identifiers. Thus, they are subject to change, and so for the moment, they will be specified as mzdraft instead of mzspec in the first block.
Thank you for your patience and working with us!