

1    **Title**

2  
3    Universal MS/MS Visualization and Retrieval with the Metabolomics Spectrum Resolver Web  
4    Service

5  
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28  
29    **Abstract**

30  
31    The growth of online mass spectrometry metabolomics resources, including data repositories,  
32    spectral library databases, and online analysis platforms has created an environment of  
33    online/web accessibility. Here, we introduce the Metabolomics Spectrum Resolver  
34    (<https://metabolomics-usi.ucsd.edu/>), a tool that builds upon these exciting developments to allow  
35    for consistent data export (in human and machine-readable forms) and publication-ready  
36    visualisations of tandem mass spectrometry spectra. This tool supports the Human Proteome  
37    Organization – Proteomics Standards Initiative’s Universal Spectrum Identifier (USI) specification,  
38    which has been extended to deal with the metabolomics use cases. To date, this resource already  
39    supports data formats from GNPS, MassBank, MS2LDA, MassIVE, MetaboLights, and  
40    Metabolomics Workbench and is integrated into several of these resources.

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44

45 **Introduction**

46  
47 The effective exchange and visualization of tandem mass spectrometry (MS/MS) information  
48 across a variety of resources is important in communicating and consequently building confidence  
49 in both data quality and molecule identification throughout the research and publication process.  
50 The inclusion of MS/MS spectra in scientific manuscripts and presentations to provide evidence  
51 of newly discovered molecules in a consistent manner is often challenging and labor intensive  
52 due to heterogeneous data availability and accessibility across public data resources, the variety  
53 of complex file formats in use to store mass spectrometry data, and the lack of suitable software  
54 tools available. Furthermore, it is often difficult to balance the ease of MS/MS figure generation  
55 with the level of customization possible.

56  
57 A few approaches have been introduced to assign universal identifiers to MS/MS spectra. The  
58 SPectraL hASH (SPLASH) identifier has been designed as an unambiguous, database-  
59 independent spectrum identifier<sup>1</sup>. SPLASH identifiers can be used to determine spectral overlap  
60 between libraries and potentially query public data repositories. However, as generating a  
61 SPLASH identifier includes a complex hashing operation, these identifiers cannot be trivially  
62 produced. Alternatively, the Universal Spectrum Identifier (USI) was recently developed by the  
63 Human Proteome Organization – Proteomics Standards Initiative (HUPO-PSI)<sup>2</sup> to provide a  
64 standardized mechanism for encoding a virtual path to spectra contained in proteomics public  
65 repositories<sup>3</sup>. Although USIs are easy to construct, the USI standard currently mainly supports  
66 proteomics spectral data deposited via ProteomeXchange<sup>4</sup> and does not natively support spectral  
67 data stored in metabolomics repositories.

68  
69 Additionally, producing high-quality figures of MS/MS spectra is challenging as well. On one hand,  
70 existing software such as the Proteomics Data Viewer (PDV)<sup>5</sup>, the Interactive Peptide Spectral  
71 Annotator (IPSA)<sup>6</sup>, and Lorikeet<sup>7</sup> proteomics data viewers, as well as vendor software, are able  
72 to draw MS/MS spectra, but are mainly aimed at interactive visualization. Three key features are  
73 often missing from such software: the ability to export vector graphics (to ensure high resolution),  
74 customization of spectral visualization, and high-throughput automated figure generation. On the  
75 other end of the spectrum are generic vector graphics editors such as Adobe Illustrator or  
76 Inkscape. While such generic editors are powerful, they lack MS/MS specific features and  
77 producing images ready for publication with these tools requires a significant time investment to  
78 achieve high levels of customization.

79  
80 We present here the Metabolomics Spectrum Resolver (<https://metabolomics-usi.ucsd.edu/>), a  
81 web tool that enables: 1) integration with major metabolomics data repositories to retrieve MS/MS  
82 metabolomics data from various sources in a unified fashion, 2) high-quality and customizable  
83 vector graphics drawing, 3) direct integration with common online analysis tools, and 4) a web  
84 API to programmatically retrieve spectral data.

85  
86 **Results and Discussion**

87  
88 *MS/MS Data Sources - Integration with Community Resources*

89 The Metabolomics Spectrum Resolver builds upon the USI standard developed by the HUPO-  
90 PSI<sup>3</sup>. USIs are formatted as follows:

91

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

93

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

96

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

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

101

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

109

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

Resource	USI Format	Example USI
MassBank	<ul style="list-style-type: none"><li>● collection: MASSBANK</li><li>● msRun: none</li><li>● index: accession:&lt;spectrumId&gt;</li></ul>	<a href="#"><u>mzspec:MASSBANK::accession:SM858102</u></a>
GNPS Spectral Library	<ul style="list-style-type: none"><li>● collection: GNPS</li><li>● msRun: GNPS-LIBRARY</li><li>● index: accession:&lt;spectrumId&gt;</li></ul>	<a href="#"><u>mzspec:GNPS:GNPS-LIBRARY:accession:CCMSLI B00005436077</u></a>
GNPS Molecular Networking Spectrum	<ul style="list-style-type: none"><li>● collection: GNPS</li><li>● msRun: TASK-&lt;taskId&gt;</li><li>● index: scan:&lt;scanNr&gt;</li></ul>	<a href="#"><u>mzspec:GNPS:TASK-c95481f0c53d42e78a61bf899e9f9adb-spectra/specs_ms.mgf:scan:1943</u></a>
MS2LDA MotifDB	<ul style="list-style-type: none"><li>● collection: MOTIFDB</li><li>● msRun: none</li><li>● index: accession:&lt;motifId&gt;</li></ul>	<a href="#"><u>mzspec:MOTIFDB::accession:171163</u></a>
MS2LDA Analysis Spectrum	<ul style="list-style-type: none"><li>● collection: MS2LDA</li><li>● msRun: TASK-&lt;taskId&gt;</li><li>● Index: accession:&lt;spectrumId&gt;</li></ul>	<a href="#"><u>mzspec:MS2LDA:TASK-190:accession:270684</u></a>
MassIVE/GNPS Repository Spectrum	<ul style="list-style-type: none"><li>● collection:MassIVE/ProteomeXchange identifier</li><li>● msRun: filename</li><li>● index: scan:&lt;scanNr&gt;</li></ul>	<a href="#"><u>mzspec:MSV000078547:120228_nb1t_3610_it_it_take2:scan:389</u></a>
Metabolights Repository Spectrum	<ul style="list-style-type: none"><li>● collection: MSV000082791</li><li>● msRun: filename</li><li>● index: scan:&lt;scanNr&gt;</li></ul>	<a href="#"><u>mzspec:MSV000082791:(-)epigallocatechin:scan:2</u></a>
Metabolomics Workbench Repository Spectrum	<ul style="list-style-type: none"><li>● collection: MSV000082680</li><li>● msRun: filename</li><li>● index: scan:&lt;scanNr&gt;</li></ul>	<a href="#"><u>mzspec:MSV000082680:iPSC-T1R1:scan:3</u></a>

117  
118 The Metabolomics Spectrum Resolver provides powerful visualization capabilities to plot spectral  
119 data (see below). Additionally, the raw spectral data can be retrieved directly in different machine  
120 readable formats (JSON or CSV) via web APIs. This enables inspection of the spectral data by  
121 both humans and automated tools, for example to provide visual evidence of newly discovered  
122 molecules in scientific manuscripts or to re-evaluate spectral identifications with alternative  
123 computational tools. Furthermore, using the programmatic web API, software developers are able  
124 to integrate high-throughput figure creation in a programming language-agnostic fashion. This  
125 functionality is already being used by members of the community to programmatically retrieve  
126 spectral data in a standardized fashion and facilitate figure generation<sup>16</sup>.

127

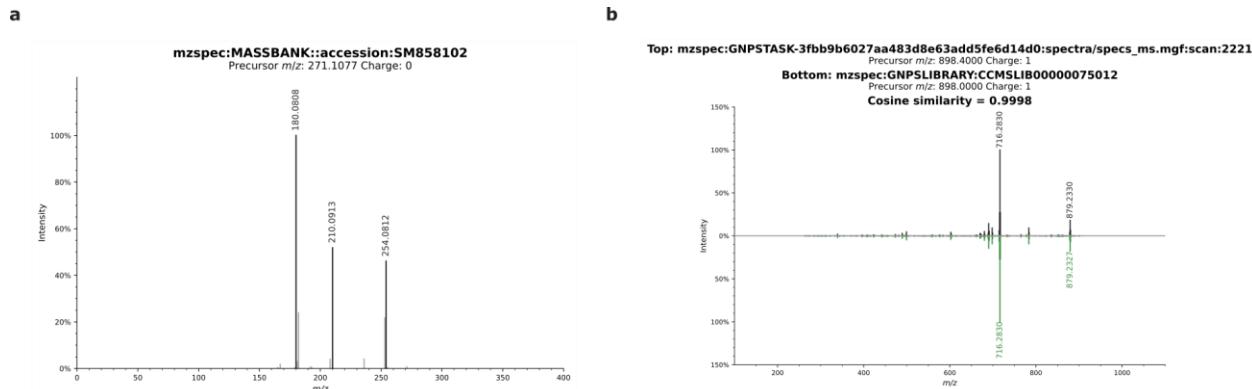
128 *Visualization Capabilities*

129

130 The Metabolomics Spectrum Resolver enables users to plot individual MS/MS spectra (**Figure**  
131 **1a**) and mirror matches between pairs of MS/MS spectra to show their similarity (e.g. between an  
132 experimental spectrum and its spectral library match; **Figure 1b**). The resulting figures can be  
133 modified by specifying mass ranges, intensity ranges, customizable peak labeling, figure size,  
134 decimal points for mass values, and an optional grid. Additionally, the similarity between the two  
135 spectra in a mirror plot can be displayed based on the standard cosine similarity or a “shifted  
136 cosine similarity” (i.e. also matching peaks that differ by the precursor mass difference between  
137 both spectra), with matching peaks between the two spectra highlighted to assess the match  
138 quality. The resulting drawing can be downloaded in the SVG (vector), PNG (raster), CSV (comma  
139 separated peaks), and JSON (machine readable peaks) formats (**Figure 2**).  
140

141

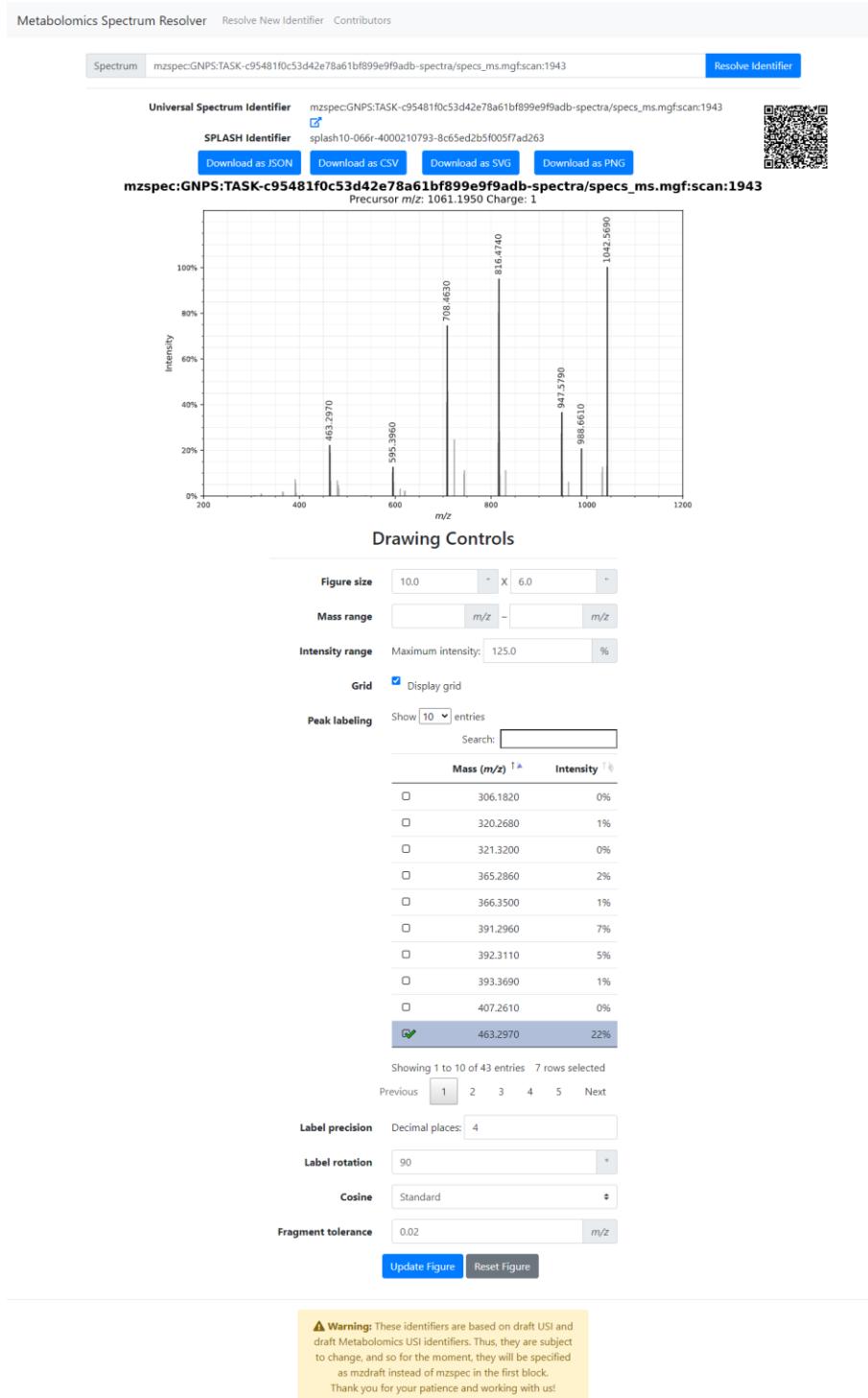
142 Plotting functionality is implemented in Python using `spectrum_utils`<sup>17</sup>, `Matplotlib`<sup>18</sup>, and  
143 `Seaborn`<sup>19</sup>. Additionally, `NumPy`<sup>20</sup>, `SciPy`<sup>21</sup>, and `Numba`<sup>22</sup> are used for efficient processing of  
144 spectral data.  
145



146

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

149



150  
151 **Figure 2 - Interactive User Interface with Drawing Options.** Enables customizing the  
152 spectrum drawing, linking back to original spectral data via URL and a generated QR code, the  
153 spectrum's SPLASH identifier, spectrum peaks download, and programmatic data download.  
154  
155

156 **Conclusion**

157

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

167

168 **Source Code**

169

170 The Metabolomics Spectrum Resolver source code is released as open source under the MIT  
171 License and is available at this DOI: [10.5281/zenodo.4033442](https://doi.org/10.5281/zenodo.4033442). Active development can be found  
172 on GitHub: <https://github.com/mwang87/MetabolomicsSpectrumResolver>.

173

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175

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186

187 **Conflict of Interests**

188

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

191

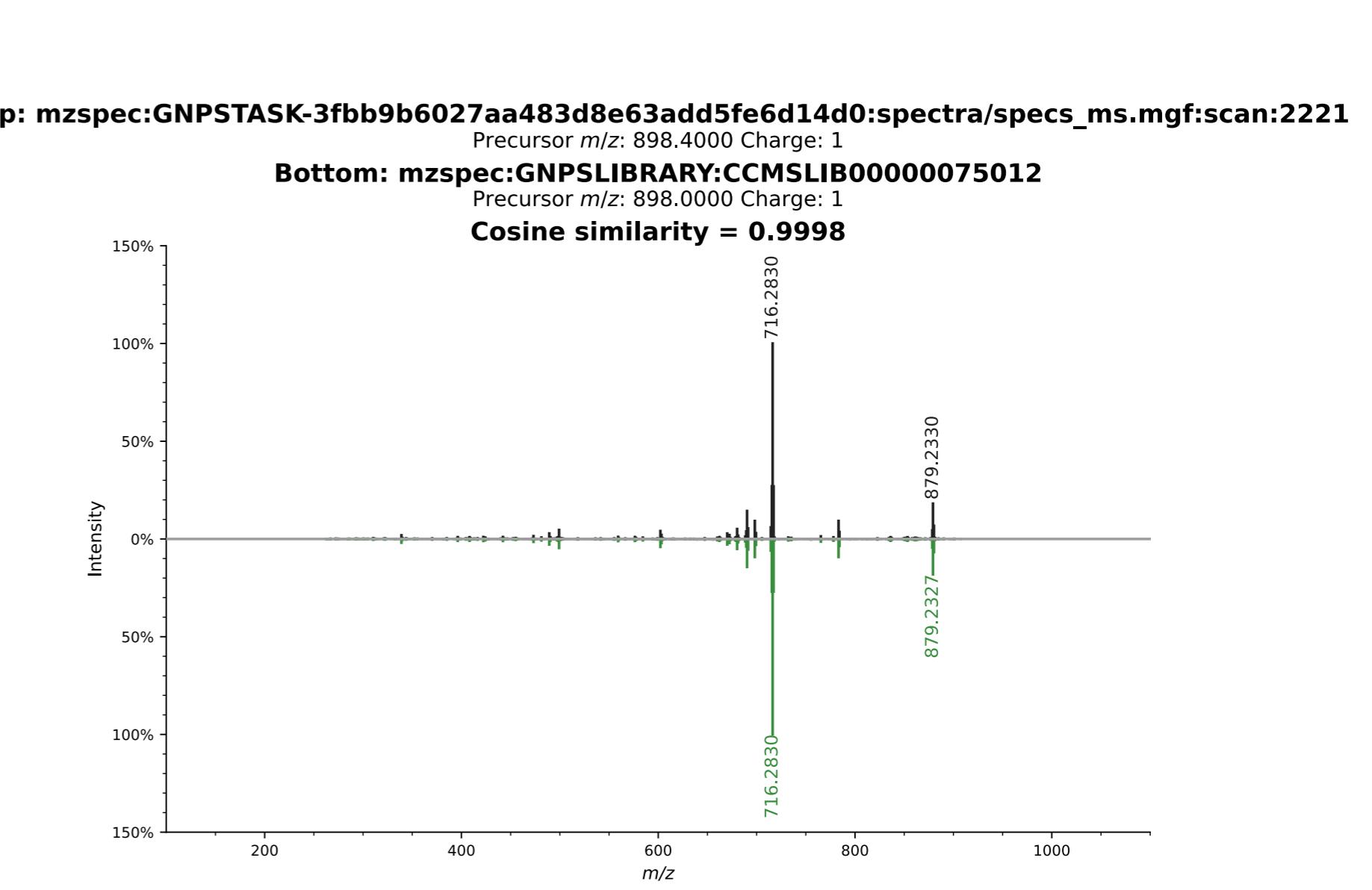
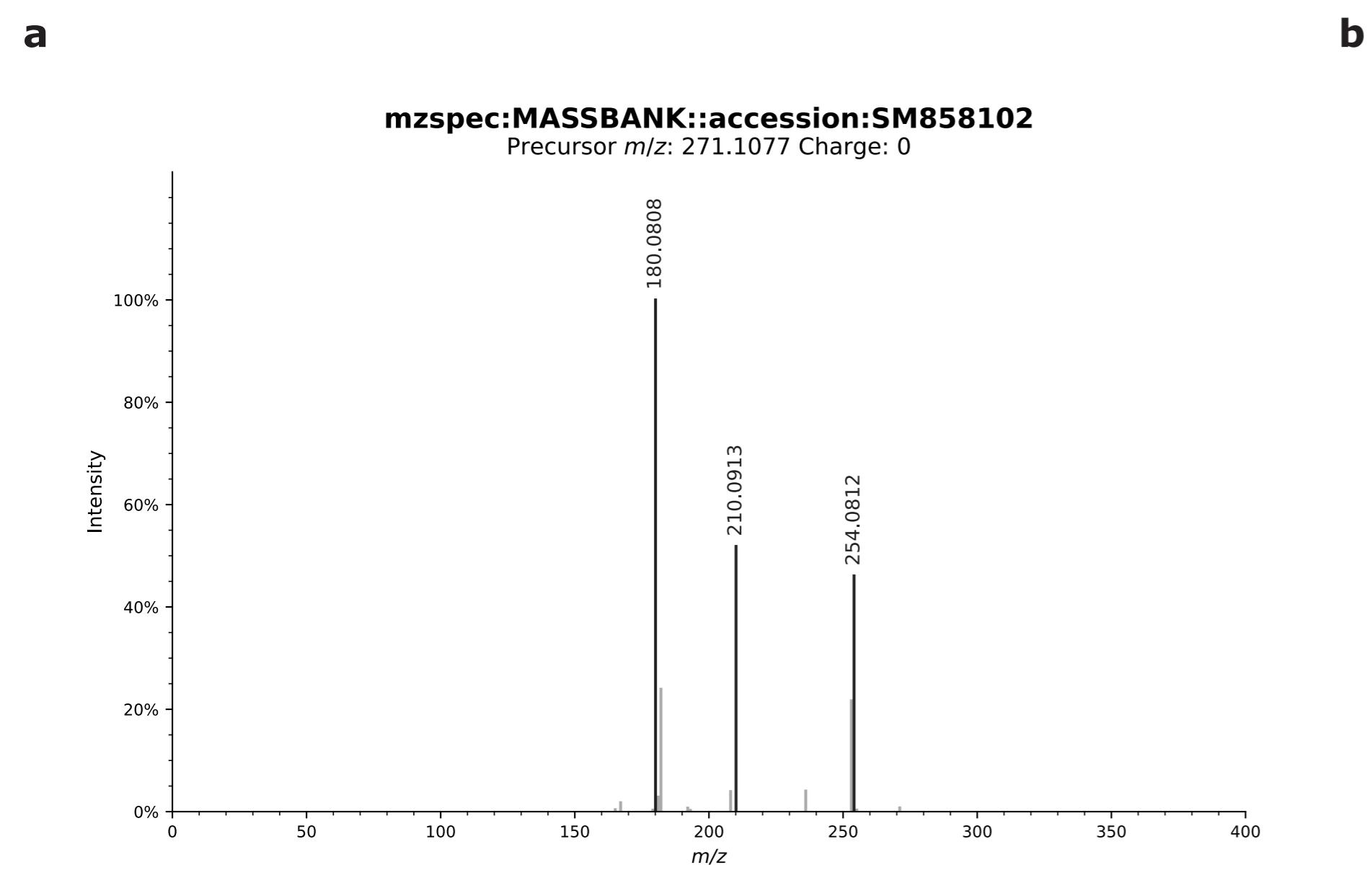
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Spectrum

mzspec:GNPS:TASK-c95481f0c53d42e78a61bf899e9f9adb-spectra/specs\_ms.mgf:scan:1943

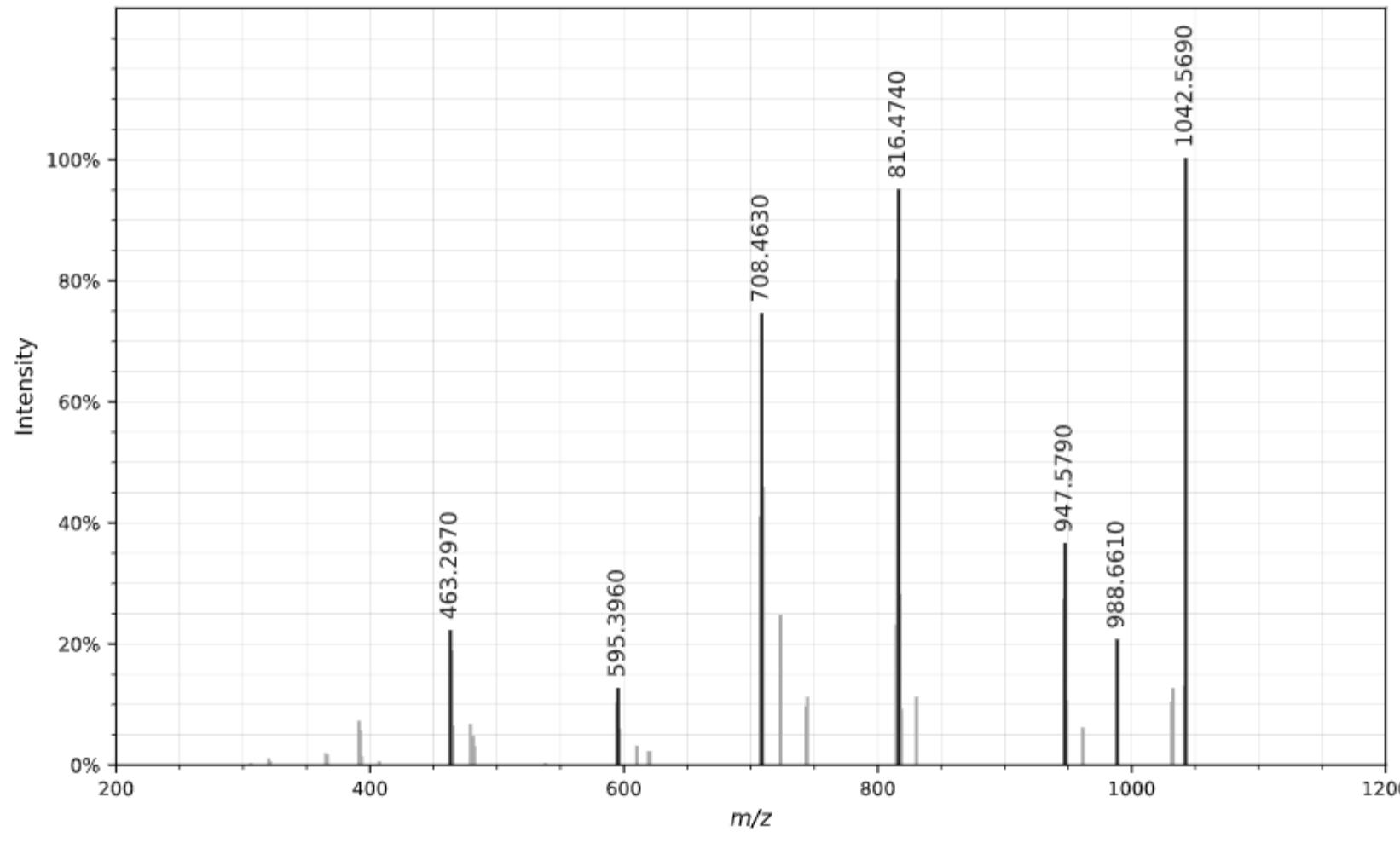
Resolve Identifier

**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](#)**mzspec:GNPS:TASK-c95481f0c53d42e78a61bf899e9f9adb-spectra/specs\_ms.mgf:scan:1943**Precursor  $m/z$ : 1061.1950 Charge: 1**Drawing Controls****Figure size** 10.0 " X 6.0 "**Mass range**  $m/z$  –  $m/z$ **Intensity range** Maximum intensity: 125.0 %**Grid**  Display grid**Peak labeling** Show 10 entriesSearch: **Mass ( $m/z$ ) ↑** **Intensity ↑**

06.1820	0%
320.2680	1%
321.3200	0%
365.2860	2%
366.3500	1%
391.2960	7%
392.3110	5%
393.3690	1%
407.2610	0%
463.2970	22%

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!