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

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Title
Universal MS/MS Visualization and Retrieval with the Metabolomics Spectrum Resolver Web
Service
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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
Netabolomics Workbench and is integrated into several of these resources.

45 Introduction

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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 SPectraL hASH (SPLASH) identifier has been designed as an unambiguous, database-58 59 independent spectrum identifier¹. 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 Human Proteome Organization - Proteomics Standards Initiative (HUPO-PSI)² to provide a 63 64 standardized mechanism for encoding a virtual path to spectra contained in proteomics public 65 repositories³. Although USIs are easy to construct, the USI standard currently mainly supports 66 proteomics spectral data deposited via ProteomeXchange⁴ 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)⁵, the Interactive Peptide Spectral 71 Annotator (IPSA)⁶, and Lorikeet⁷ 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

We present here the Metabolomics Spectrum Resolver (<u>https://metabolomics-usi.ucsd.edu/</u>), 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.

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 PSI³. 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/usi).
- 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**): 101
 - Data repositories: MassIVE⁸, MetaboLights⁹, Metabolomics Workbench¹⁰.
- 102 Reference spectral library MassBank¹¹. MoNA resources: 103 (https://mona.fiehnlab.ucdavis.edu/), GNPS¹², and MS2LDA.org MOTIFDB¹³.
- Online informatics pipelines: GNPS Molecular Networking¹² / Library Search / MASST¹⁴ / 104 105 Feature-based Molecular Networking¹⁵, and MS2LDA.org¹³.
- 106

107 As such, the Metabolomics Spectrum Resolver provides a universal interface to more than 450M 108 MS/MS spectra from various public metabolomics repositories. It also supports linking back to the 109 source spectra in their original data resources to allow users to explore the original context of the 110 MS/MS spectra. Several resources (MassBank, GNPS, and MS2LDA.org) have already 111 integrated links to the Metabolomics Spectrum Resolver to facilitate bidirectional interoperability. 112 Additionally, SPLASH identifiers¹ are computed for all spectra retrieved through the Metabolomics 113 Spectrum Resolver to enable their comparison across different resources.

114

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

116 resources.

Resource	USI Format	Example USI	
MassBank	 collection: MASSBANK msRun: none index: accession:<spectrumid></spectrumid> 	<pre>mzspec:MASSBANK::accessi on:SM858102</pre>	
GNPS Spectral Library	 collection: GNPS msRun: GNPS-LIBRARY index: accession:<spectrumid></spectrumid> 	<pre>mzspec:GNPS:GNPS- LIBRARY:accession:CCMSLI B00005436077</pre>	
GNPS Molecular Networking Spectrum	 collection: GNPS msRun: TASK-<taskid></taskid> index: scan:<scannr></scannr> 	<pre>mzspec:GNPS:TASK- c95481f0c53d42e78a61bf89 9e9f9adb- spectra/specs_ms.mgf:sca n:1943</pre>	
MS2LDA MotifDB	 collection: MOTIFDB msRun: none index: accession:<motifid></motifid> 	<u>mzspec:MOTIFDB::accessio</u> n:171163	
MS2LDA Analysis Spectrum	 collection: MS2LDA msRun: TASK-<taskid></taskid> Index: accession:<spectrumid></spectrumid> 	<pre>mzspec:MS2LDA:TASK- 190:accession:270684</pre>	
MassIVE/GNPS Repository Spectrum	 collection:MassIVE/ProteomeXchan ge identifier msRun: filename index: scan:<scannr></scannr> 	<pre>mzspec:MSV000078547:1202 28 nbut 3610 it it take2 :scan:389</pre>	
Metabolights Repository Spectrum	 collection: MSV000082791 msRun: filename index: scan:<scannr></scannr> 	<pre>mzspec:MSV000082791:(-)- epigallocatechin:scan:2</pre>	
Metabolomics Workbench Repository Spectrum	 collection: MSV000082680 msRun: filename index: scan:<scannr></scannr> 	<pre>mzspec:MSV000082680:iPSC -T1R1:scan:3</pre>	

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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 generation¹⁶.

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 guality. 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 Plotting functionality is implemented in Python using spectrum utils¹⁷. Matplotlib¹⁸, and 142 Seaborn¹⁹. Additionally, NumPy²⁰, SciPy²¹, and Numba²² are used for efficient processing of 143 spectral data.

144





- Figure 1 Example MS/MS figure generation of (a) a single MS/MS spectrum and (b) a mirror 147
- 148 plot.
- 149



150

Metabolomics Spectrum Resolver - Release 6.8

151 *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.

- 154
- 155

156 Conclusion

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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

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

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- 175

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186

187 Conflict of Interests

188

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

- advisory board of Sirenas and Cybele Micro
- 191

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mzspec:MASSBANK::accession:SM858102 Precursor m/z: 271.1077 Charge: 0



b

a

Top: mzspec:GNPSTASK-3fbb9b6027aa483d8e63add5fe6d14d0:spectra/specs_ms.mgf:scan:2221 Precursor *m/z*: 898.4000 Charge: 1

Bottom: mzspec:GNPSLIBRARY:CCMSLIB00000075012 Precursor m/z: 898.0000 Charge: 1



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320.2680		
321.3200	D	
365.2860	D	
366.3500	D	
391.2960		
392.3110	D	
393.3690	O	
407.2610	D	
463.2970	Ref (
ng 1 to 10 of 43 entries	Showing	
1 2 3 4	Previous	
al places: 4	Decimal	Label precision
	90	Label rotation
dard	Standa	Cosine
1	320.2680 321.3200 365.2860 365.2860 366.3500 391.2960 392.3110 393.3690 407.2610 463.2970 1 to 10 of 43 entries 1 2 3 places: 4	□ 320.2680 □ 321.3200 □ 365.2860 □ 366.3500 □ 391.2960 □ 393.3690 □ 393.3690 □ 407.2610 ☑ 403.2970 Showing 1 to 10 of 43 entries Previous 1 2 3 Ø0 4 4

▲ 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!