

NIST/NIJ

# DART-MS Data Interpretation Tool



User Manual – Version 3.0 (March 2024)

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## Summary

Direct Analysis in Real Time Mass Spectrometry (DART-MS) is an analytical chemistry technology that is being increasingly employed in forensic applications. This form of mass spectrometry rapidly yields rich structural information about an analyte with minimal sample preparation. The challenge with DART-MS data, much like other data generated with high throughput technologies, lies in the data interpretation. This is especially true when the analyzed samples are multi-component mixtures like seized drug evidence.

The NIST/NIJ DART-MS Data Interpretation Tool (DIT) is a freely available and open-source software tool developed to support the interpretation of in-source collision induced dissociation (is-CID) DART-MS data. The NIST/NIJ DART-MS DIT can be used to view reference mass spectra from DART-MS spectral libraries, search query DART-MS mass spectra of mixtures against reference libraries, using the Inverted Library Search Algorithm, and generate printable reports from search results. Several of the features, including the formatting of generated reports, were iteratively designed with input from local, state, and federal forensic practitioners, ensuring that the program is intuitive and usable for the expected users.

**We would like to thank the laboratories that provided input on software features and design:**

- Maryland State Police Forensic Sciences Division
- Virginia Department of Forensic Science
- Harris County Institute of Forensic Sciences
- U.S. Customs and Border Protection, Laboratories and Scientific Services, INTERDICT Science Center
- U.S. Food and Drug Administration, Forensic Chemistry Center



## Update Overview

The following updates were made from v2 to v3.

### Search tool:

- Removed cap from search results, allowing for more than 10 results to be displayed per target.

### General:

- Updated source code to be compatible with R4.3.2
- Default library has been updated to HePos\_Inchworm\_v1

The following updates were made from v1 to v2.

### Inverted Library Search Algorithm (ILSA) (underlying search algorithm):

- A 1 % relative intensity noise filter has been included to minimize the effect of noise on spectral scoring
- For high-resolution measurements, the  $m/z$  window for comparing a reference spectrum to a query has been expanded to twice the user-defined mass tolerance to account for mass calibration variations. This setting will not affect target identification and is meant to provide more accurate scoring by addressing potential opposing mass drifts between query and library spectra.

### Search Tool:

- Search result lists have been replaced with search result tables
- Major isotopes and major fragment ions are now identified in the search result table when a protonated molecule or base peak is also identified.
  - The type of match that is made is now identified in the "Match Type" column of the result table
- The difference between the calculated and theoretical  $m/z$  values are now reported in the report table under  $\Delta m/z$
- A new metric, the isotope ratio difference, is now reported in the results table. The value is the difference between the observed and calculated major isotope ratios. A score of 0 indicates a perfect match.
- Peaks in the low fragmentation mass spectrum are now colored to indicate whether a target does (red) or does not (blue) have a possible match in the library
- A legend has been added to the mass spectra
- The target assumption setting has been removed. The DIT will automatically look for both protonated molecules and base peaks.
- The search type setting has been removed and is defaulted to mixture analysis. For a pure compound search, set the targeting threshold to 100 %.
- Peak list table is now sortable and labels which  $m/z$  values correspond to the respective targets

**Libraries Viewer:**

- Layout has been rearrange to allow users to see more columns within the library list
- Added class identification to the metadata for each entry
- Default library has been updated to Firefly

**Scoring Tab:**

- A new tab, titled “Scoring” has been added to provide a quick reference to how the ILSA scoring works and what the various scores and metrics represent



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## Download and installation

### Download

The latest version of the DIT can be downloaded directly from the NIST Public Data Repository, at DOI:10.18434/mds2-2448. On the website, download the latest “.zip” file. Alternatively, a USB flash drive version can be request by emailing [DARTdata@nist.gov](mailto:DARTdata@nist.gov).

The DIT requires approximately 0.5 GB of hard drive space and will run on 32 or 64-bit Windows system. The computer needs to have an internet browser (*i.e.*, Google Chrome, Microsoft Edge, etc.) to run from.

### Installation

If the DIT was downloaded from the NIST Public Data Repository, install it by extracting the “.zip” file onto a local directory or onto the desktop.

If a USB flash drive was provided copy and paste the entire folder “NIST-NIJ-DIT\_v#” onto a local directory or onto the desktop.



## Navigating the application

### Opening the application

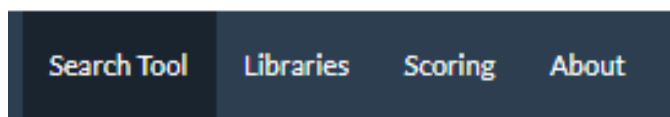
To start the DIT, open the “NIST-NIJ-DIT\_v#” folder. Double click on the “run-DIT.bat” file to start the program. The program will open in the default internet browser. The program may take a few seconds to start.

**Note:** The DIT does not require connection to the internet to operate.

**Note:** Multiple instances of the DIT can be run concurrently.

### Navigating the application

The DIT is comprised of three different tabs, **Search Tool**, **Libraries**, **Scoring**, and **About** which can be navigated using the blue banner at the top of the program.



Navigation bar.

The **Search Tool** tab allows users to upload and search query spectra using the Inverted Library Search Algorithm (ILSA). Within this tab users can also adjust search settings, input desired information for generating a report, and generate a printable report.

The **Libraries** tab allows users to view and search the libraries that are loaded into the DIT. Generation of printable reference data is also possible through this tab.

The **Scoring** tab provides a quick-look guide on how the ILSA works and the what the various scores and metrics represent.

The **About** tab contains relevant disclaimer information.





## Using the Search Tool

### How the search algorithm works

The inverted library search algorithm (ILSA) is a new multi-step search procedure that allows users to identify components of a mixture from a series of in-source collision induced dissociation (is-CID) mass spectra. First, “target”  $m/z$  values are identified from the low fragmentation (30 V) mixture mass spectrum as peaks with intensity greater than a user-prescribed relative intensity threshold (e.g., 5 %). For each target  $m/z$  value, library compounds within mass tolerance of the target  $m/z$  value are identified. The mass spectra of the identified library compounds are then compared to the query mass spectra. Two scores, the fraction of peak intensity explained (FPIE) and the reverse match factor (RevMF), as well as two metrics,  $\Delta m/z$  and isotope ratio difference (IRD), are defined for each potential library match. A table providing additional information on the scores and metrics is provided below.

Metric	Short Description	Output Range	Ideal Output
$\Delta m/z$	mass difference between the observed target $m/z$ and the calculated library reference $m/z$	$[-\epsilon, +\epsilon]$	0
Average FPIE (Fraction of Peak Intensity Explained)	The fraction of total peak intensity from the library spectrum that have a ‘matching’ peak in the corresponding mixture spectrum, where matching implies a peak in the mixture spectrum within a mass tolerance window ( $\pm 2\epsilon$ ) and with signal intensity above the noise threshold. The reported number is a simple arithmetic average computed based on number of available fragmentation spectra compared.	[0,1]	1
Average RevMF (Reverse Match Factor)	The cosine similarity between the vector constructed of relative intensities above the noise threshold from the library spectra and the vector constructed with relative intensities from ‘matching’ in the corresponding mixture spectrum, where matching implies the peak in the mixture closest (in $m/z$ ) to the library spectrum within a mass tolerance window ( $\pm 2\epsilon$ ). Note that the vector representing the mixture could have zero valued entries. The reported number is a simple arithmetic average computed based on number of available fragmentation spectra compared.	[0,1]	1
Average spread	The spread between the largest and smallest $m/z$ differences observed between reference spectrum peaks and ‘matching’ peaks in the mixture spectrum, where matching implies the mixture closest (in $m/z$ ) to the reference peak. If there are less than two matching peaks between the reference and mixture, the spread is reported as NA. The reported number is a simple arithmetic average computed based on number of available fragmentation spectra compared.	[0,4 $\epsilon$ ]	0
LFPM Isotope Ratio Difference (IRD) (Low Fragmentation Protonated Molecule)	The difference in calculated relative intensity isotope ratio $\left(\frac{M+i}{M}\right)$ between the reference protonated molecule and its major isotope ( $i = 1$ or $i = 2$ ) and the observed intensity values in the matching peaks in the mixture spectrum, where matching implies a peak in the mixture spectrum within a mass tolerance window ( $\pm \epsilon$ ) and with signal intensity above the noise threshold. If there is no peak matching the protonated molecule in the mixture spectrum, the LFPM Isotope Ratio Difference is reported as NA.	$[-9.99, +9.99]$	0

## Layout

The **Search Tab** has two different views – *Interactive* and *Reporting*. The *Interactive* view allows users to interface with the DIT to upload files, change search settings, etc. The *Reporting* view allows users to obtain a printable version of the search results. The *Interactive* view is separated into five different areas, each with their own purpose. An example of this layout is provided below, with red boxes outlining the different areas.

The screenshot shows the DIT Search Tool interface. The top navigation bar includes 'Search Tool', 'Libraries', 'Scoring', and 'About'. Below this, a 'View:' section has radio buttons for 'Interactive' (selected) and 'Reporting'. A row of input fields contains '03/28/2022', 'Instrument 1', '1234', and 'Item No...'. Below these are 'Comments...' and buttons for 'Load Presets', 'Download Presets', and 'Restore Defaults'. The main area is divided into two panels. The left panel, labeled '4.', contains a 'Query Spectra' section with a 'Reference Library' dropdown set to 'HeFirefly\_Collapsed.RDS', polarity and source gas settings, and three file upload sections for 'Mixture10\_30V.txt', 'Mixture10\_60V.txt', and 'Mixture10\_90V.txt'. The right panel, labeled '5.', displays a mass spectrum plot with 'Relative Intensity (%)' on the y-axis and 'm/z' on the x-axis. It includes a table of peaks with columns for 'm/z', 'Relative Intensity', and 'Target'. Below the plot, it shows 'Measured m/z: 323.2131' and 'Relative Intensity: 100.0 %'. A 'Potential matches' table lists compounds like 'Acetyl fentanyl' and 'Benzylfentanyl' with their respective  $\Delta m/z$ , FPIE, RevMF, and IRD values. A search bar is also present.

- **Area 1:** Allows users to change between the *Interactive* and *Reporting* views.
- **Area 2:** Allows users to enter text to assist in generating a printable report.
- **Area 3:** Allows users to manage setting configurations.
- **Area 4:** Allows users to upload spectra for searching and select relevant search settings.
- **Area 5:** Allows users to view results.



## Selecting a reference library (Area 4)

The reference library is the library that query spectra will be searched against. When opening the DIT the program will default to the reference library that was used in the last session. If a different reference library is desired, choose the appropriate one from the dropdown in the **Query Spectra** tab on the left-hand side of the application. The default library contains spectra collected on JEOL AccuTOF mass spectrometers. Once a library is chosen, the ionization polarity and source gas used to generate the library are displayed.

## Changing the settings (Area 4)

Prior to completing a search, users have the ability to select settings based on the query data and their preferences. All search settings can be found in the **Settings** tab in the grey box on the left-hand side of the application (shown below). A description of each setting is provided below.

The screenshot shows the 'Settings' tab in the DIT application. It features three main settings sections. The first is 'Target Display' with a checkbox labeled 'Display only targets with potential matches' which is currently unchecked. The second is 'Targeting Threshold (%)' with a horizontal slider ranging from 0 to 100, with the current value set at 10. The third is 'm/z Tolerance (± Da)' with a checkbox labeled 'Integer Resolution Spectra' which is unchecked, and a horizontal slider ranging from 0 to 0.1, with the current value set at 0.005. At the bottom of the settings panel is a blue button labeled 'Update Search'.

**Target Display:** This setting determines whether all targets are shown after a search is completed (unchecked) or only targets that have potential matches in the selected reference library (checked).

**Identification Threshold:** This setting allows users to select the minimum relative intensity for peak identification and peak searching. Integer values between 1 and 100 can be chosen.

***m/z* Tolerance:** This setting allows users to select the *m/z* tolerance that is appropriate for their data. If the data was collected using a unit mass resolution instrument, check the *Integer Resolution Spectra* box. Otherwise, a tolerance value matching that of the instrument the data was collected on can be selected, ranging from  $\pm 0.001$  Da to  $\pm 0.1$  Da.

The settings that are selected when the DIT is closed will be restored when the program is reopened.

## Saving presets (Area 3)

If there are settings that will be frequently used for searching, users can save those presets as a downloadable .csv file and reload them when necessary. To save a preset, change all settings to the desired values and then select the *Download Presets* button at the top center of the screen. A .csv file titled "DST\_preset-XXXXX.csv" will be created and saved in the "Downloads" folder on the computer. This file can be moved to a different directory and/or renamed, if desired. To retrieve the preset, click the *Load Presets* button at the top center of the screen. This will open a file explorer for the user to locate and select the desired preset file.

**Note:** When downloading presets, any text that is entered into the reporting text boxes (discussed in the next section) will also be saved. For example, if a user always reports the same instrument in the "Instrument ID" text box, that preset along with all other settings can be downloaded and loaded during another session. Each time the presets are loaded, this field will be pre-populated.



**Note:** Preset files from version 1 of the DIT will not work on this version.

## Inputting reporting information (Area 2)

The **Search Tool** contains five text fields at the top of the screen where users can enter relevant information that will appear in the *Reporting view*. These text entry boxes allow users to enter information that will appear in the downloadable / printable report, including the date, an instrument name, a case number, an item number, and any additional information in a comment field. Inputting text into these boxes is not required. More details about the *Reporting view* can be found in the “Report viewing & printing” section on page 7.

## Uploading & searching spectra (Area 4)

The **Search Tool** will accept .txt, .csv, and .jsp files of mass spectral data. Users have the ability to upload up to three in-source collision induced dissociation (is-CID) spectra. ***At a minimum, the Low (30 V) spectrum needs to be uploaded.*** The 30 V, 60 V, and 90 V designations correspond to the orifice 1 voltages on the JEOL AccuTOF mass spectrometers and may not translate to other systems.

To upload files, click the *Browse* button next to the desired fragmentation level under the *Query Spectra* tab in the grey box. Once the desired spectrum or spectra are loaded, click *Search Library* to complete the search. There are example query spectra in the “ExampleQuery” sub-folders in the main “NIST-NIJ-DIT\_v#” folder.

If a Low (30 V) spectrum is not uploaded, an error will be displayed asking the user to upload a file. If the same file is uploaded as two or more spectra an error will be displayed that tells the user which files are identical and the search will not be completed.

## Completing a search & viewing results (Area 5)

Upon completing a search, the uploaded mass spectrum or spectra and the results will be displayed to the right of the grey *Query Spectra* box. Peaks that are indicated in red in the Low (30 V) spectrum represent targets that were above the user-defined threshold and have one or more possible matches in the library. Peaks that are indicated in blue in the Low (30 V) spectrum represent targets that were above the user-defined threshold and did not have a possible match in the library. The dotted purple line represents the selected relative intensity threshold.

The mass spectrum plot is interactive so users can hover over peaks of interest to see their  $m/z$  values, and relative intensities. Hovering the mouse over the mass spectrum will display a set of additional tools at the top of the plot that allow users to manipulate the plot (*i.e.*, zoom in and zoom out) and save the plot as a picture.

Below the spectrum are the Targets that were identified. Targets are numbered based on decreasing relative intensity in the Low (30 V) spectrum. To select different targets, click the *Target 1*, *Target 2*, etc. tabs. Within each target tab the measured  $m/z$  of the peak and the relative intensity are listed. Below that, the results table for the peak is shown. Within this data table, the potential library match(es), the  $\Delta m/z$  between the measured and theoretical values, the FPIE and RevMF spectral



similarity scores, the isotope ratio difference, and the match type are shown. Possible match types include Protonated Molecule, Base Peak, +1 Isotope (PM), +1 Isotope (BP), and Major Fragment Ion. If a target was found to have no corresponding compounds in the reference library, the message “No matches in database.” will be displayed.

To the right of the mass spectrum is the peak list. Multiple options exist for peak list display including *Threshold* (displays the  $m/z$  values of all peaks above the user-defined threshold), *Top 10* (displays the ten most abundant  $m/z$  values), and *All Peaks* (displays the  $m/z$  values for all peaks in the spectrum). This list is sortable by relative intensity,  $m/z$ , or target number.

If multiple spectra were uploaded and searched, the additional spectra can be viewed by clicking the desired tab at the top of the mass spectrum (Low (30 V), Mid (60 V), and High (90 V)). In the other mass spectra, peaks indicated in orange have the same  $m/z$  as one of the targets in the Low (30 V) spectrum.

### Updating search settings (Area 4)

Search settings can be updated after a search has been completed by clicking on the *Settings* tab in the grey box, adjusting the desired settings, and the clicking *Update Search*.

### Reporting viewing & printing (Area 1)

To view a static report of the search results, click the *Reporting* button under *View* at the top of the screen. Selecting *Reporting* will display a printable or pdf-able version of the data, settings, and populated text fields. To print or save the report, use the printing and/or saving features of the web browser in which the DIT is running. An example of the report that is generated is shown on the following page.

To switch back to the dynamic search tool, select the *Interactive* button, under *View*, at the top of the screen.

Parameter	Value
Date:	3/28/2022
Instrument ID:	Instrument 1
Case Number:	1234
Item Number:	None
Library:	HeFirefly_Collapsed.RDS
Library Polarity:	Positive
Library Source Gas:	He
Filename of Low (30 V) Spectrum:	Mixture10_30V.txt
Filename of Mid (60 V) Spectrum:	No file selected
Filename of High (90 V) Spectrum:	No file selected
Display only targets with potential matches:	No
Targetting threshold (%):	5 %
m/z Tolerance ( $\pm$ Da):	0.005
Comments:	None

Low (30 V) Mixture10\_30V.txt

Show 10 entries

m/z	Relative Intensity	Target
323.2131	100.0	T1
324.2161	26.4	T2
91.0556	15.9	T3
150.1294	15.0	T4
119.0879	14.6	T5
323.3091	4.9	
323.9190	3.6	
172.1136	3.5	
325.2191	2.9	
323.4129	2.6	

Previous 1 2 3  
4 5 Next

**Target 1**

Measured m/z: 323.2131  
Relative Intensity: 100.0 %

Potential matches:

	Compound	Class	$\Delta$ m/z	FPIE	RevMF	IRD	Match Type
1	Acetyl fentanyl	Fentanyl	0.0008	0.355	0.471	0.037	Protonated Molecule
2	Benzylfentanyl	Fentanyl	0.0008	0.931	0.694	0.037	Protonated Molecule



### Clearing a search (Area 4)

To clear the uploaded query mass spectrum or spectra from the DIT, click the *Clear Search* button located in the *Query Spectra* tab in the grey box.

### Restoring defaults (Area 3)

To restore all settings to their original defaults, and clear any search spectra that were loaded, click the *Restore Defaults*. In order to reload user-defined defaults, click the *Load Presets* button and then locate and load the .csv file containing the desired settings.



## Using the Libraries Viewer

### Layout

The **Libraries Tab** also has two different views – *Interactive* and *Reporting*. The *Interactive* view allows users to interface with the DIT to view and search entries in the reference libraries. The *Reporting* view allows users to obtain a printable version of a library entry. The *Interactive* view is separated into three different areas, each with their own purpose. An example of this layout is provided below, with red boxes outlining the different areas.

**Area A: View Controls**

Search Tool Libraries Scoring About

View: ☒ Interactive ☐ Reporting

Library: HePos\_Firefly\_v1.RDS

Polarity: Positive

Source Gas: He

Name: 1B-LSD

Class: Lysergamides

Formula:  $C_{24}H_{21}N_3O_2$

Exact Mass (Da): 393.2416

$[M+H]^+$  (m/z): 394.2495

30 V Base Peak (m/z): 394.2495

InChIKey: [SVRFNPSPIQUBC](#)  
[DYFSRHJHSA-N](#)

Contributor: NIST

Synonyms: 1-butanoyl LSD

**Area B: Spectral Data and Chemical Structure**

Low (30 V) Mid (60 V) High (90 V)

Relative Intensity (%)

m/z

Chemical Structure:

Show 10 entries

m/z	Relative Intensity
394.2478	100.0
395.2499	37.3
396.2528	5.6
410.2416	4.3
351.2052	4.1
393.2386	4.1
394.3706	3.4
411.2478	2.5
394.4814	2.4
392.2311	2.0

Previous 1 2 3 4 5 ... 111 Next

**Area C: Reference Library Search Results**

Reference Library: HePos\_Firefly\_v1.RDS

Show 10 entries

Previous 1 2 3 4 5 ... 111 Next Search:

Name	Formula	$[M+H]^+$	Synonyms	Base Peak
1	1-(3-Chlorophenyl)piperazine	$C_{10}H_{12}ClN_2$	m-CPD; meta-Chlorophenylpiperazine	197.0846
2	1-(4-Methoxyphenyl)piperazine	$C_{11}H_{14}N_2O$	4-MeOPP; p-Methoxyphenylpiperazine; 4-MPP; pMPP; Parapearlaine	193.1341
3	1-Androstenedione	$C_{19}H_{28}O_2$	$\Delta^1$ -5 $\alpha$ -Androstene-3,17-dione	287.2011
4	1-Benzylpiperazine	$C_{11}H_{14}N_2$	BZP; N-Benzylpiperazine; 1-Phenylmethylpiperazine; 4-Benzylpiperazine	177.1392
5	1B-LSD	$C_{24}H_{21}N_3O_2$	1-butanoyl LSD	394.2495
6	1-Demethyl Phenazolin	$C_{14}H_{12}BrClN_4$		372.9856
7	1P-LSD	$C_{23}H_{21}N_3O_2$	1-Propionyl-lysergic acid diethylamide; 1P-LAD; 1-Propionyl-lsd	380.2338
8	2,2,3,3-Tetramethyl-Cyclopropyl fentanyl	$C_{27}H_{34}N_2O$		405.2906
9	2,3-dimethoxy Fentanyl	$C_{24}H_{22}N_2O_2$		397.2491
10	2,3-Dimethylcathinone	$C_{11}H_{13}NO$	2,3-DMEC	206.1545

References

Sisco et al. DOI:10.1021/jams.0c00416

- **Area A:** Allows users to change between the *Interactive* and *Reporting* views.
- **Area B:** Allows users to view spectra and metadata for entries in the reference library.
- **Area C:** Allows users to select a reference library and search entries within it.





## Selecting a reference library (Area C)

To select a reference library, click the drop-down menu in the grey box titled *Reference Library*. A list of available reference libraries will be displayed. The default library contains spectra collected on JEOL AccuTOF mass spectrometers.

## Searching the library (Area C)

Within the grey box is a data table containing information on all compounds in the selected reference library. For each entry, the name, chemical formula,  $m/z$  value of the protonated molecule,  $m/z$  value of the base peak in the Low (30 V) spectrum, and synonyms are displayed. To search the table, type a name, chemical formula, or  $m/z$  value into the search bar located at the top of the table. Once the entry of interest has been identified, click on it to display the associated spectra and reference data,

## Viewing reference data (Area B)

When a compound of interest is selected from the table, the metadata and mass spectral data for the compound will be displayed. The metadata is displayed to the left of the mass spectra and includes information about the library, the contributor of the reference data, and the compound. If the DIT is being used on a computer connected to the internet, users can click on the InChi Key to open the PubChem entry for the compound.

To the right of the metadata is the mass spectra for the is-CID mass spectra collected at Low (30 V), Mid (60 V), and High (90 V) energies. Peaks that are blue indicate those that are either the protonated molecular ion or have potential chemical formulas explained by a single bond break in the molecule. Grey peaks cannot be explained by single bond breakages. The mass spectrum viewer is interactive, and users can hover over peaks of interest to see  $m/z$  values, relative intensities, and chemical formulae (for blue peaks). Hovering the mouse over the mass spectrum will display a set of additional tools at the top of the plot that allow users to manipulate the plot (*i.e.*, zoom in and zoom out) and save the plot as a picture.

To the right of the spectrum is the peak list. The peak list can be displayed as either *Top 10* (displays the ten most abundant  $m/z$  values) or *All peaks* (displays the  $m/z$  values for all peaks in the spectrum). This list is sortable.

## Printing a reference data report (Area A)

To view a static report of the reference data click the *Reporting* button under *View* at the top of the screen. Selecting *Reporting* will display a printable or pdf-able version of the metadata and three reference mass spectra. To print or save the report use the printing and/or saving features of the web browser in which the DIT is running.

To switch back to the dynamic Libraries Viewer, select the *Interactive* button, under *View*, at the top of the screen.



## Adding a new library

Libraries exist as .RDS datafiles that can be generated using the DART-MS Database Builder (Reference: <https://dx.doi.org/10.1021/jasms.0c00416>, Source Code: <https://github.com/asm3-nist/DART-MS-DBB>). Alternatively, new and updated databases can be downloaded from <https://data.nist.gov/od/id/mds2-2313>. To add a new reference library, navigate to the *Libraries* subfolder using the following path: *DIT\_v# > shiny\_DIT > Libraries*. Paste the new .RDS file into this folder. If the DIT is running during this process, the program will have to be restarted in order for the new library to be recognized.

**Note:** Due to the new features added to the ILSA, previous library versions (Cicada and Dragonfly) are not compatible with the new version of the DIT.



## Waters QDa File Converter

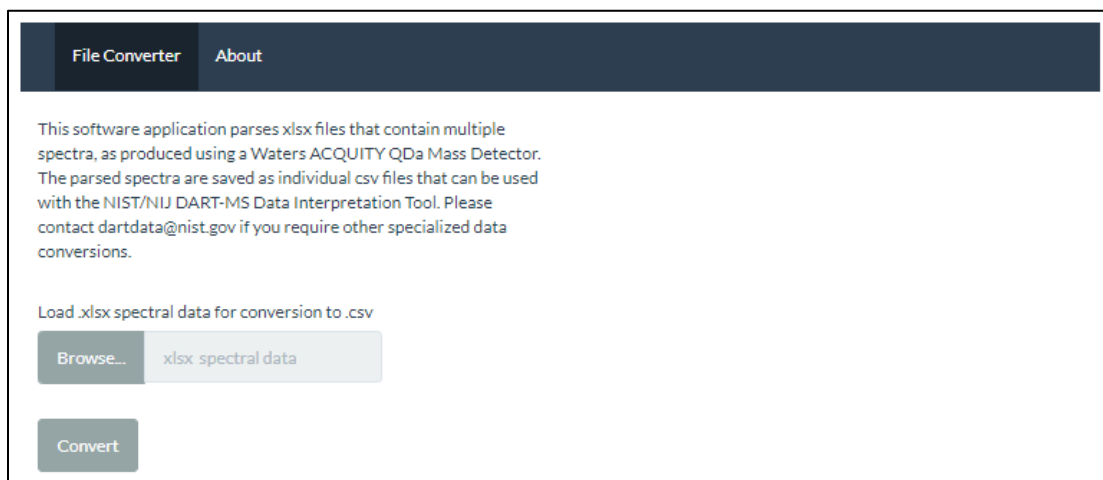
Data collected from the Waters Acquity QDa that is exported as single .xlsx file containing mass spectra from multiple is-CID voltages must be converted prior to upload into the DIT. This file converter will separate the mass spectra contained in the .xlsx into individual files for upload into the DIT.

### Opening the application

To start the file converter, open the “NIST-NIJ-DIT\_v#” folder. Double click on the “run-xlsx2csv.bat” file to start the program. The program will open in the default internet browser.

### Layout

The file converter consists of a **File Converter** tab and an **About** tab, as shown below.



### Uploading & converting files

To convert a .xlsx containing multiple mass spectra into individual .csv files for each spectrum, select *Browse* then locate and upload the desired .xlsx file. Once uploaded click convert. An example .xlsx is included in the “Example\_QDa\_Xlsx” subfolder in the main “NIST-NIJ-DIT\_v#” folder.

Once the file has been converted a message will pop up saying the file has been converted to parsed .csv files. The new files are automatically saved in the “DIT\_v#” folder. New .csv files are saved with the same name as the original .xlsx file with an “\_F#” extension.