

NIST/NIJ

DART-MS Data  
Interpretation Tool



User Manual – Version 1.0 (October 2021)

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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



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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

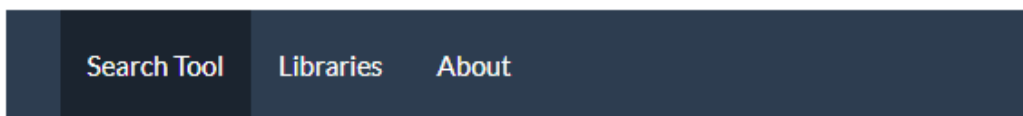
To start the DIT, open the “NIST-NIJ-DIT\_v#” folder. Double click on the “run-DIT.bat” file to start the program. The program will open in the default internet browser.

**Note:** The DIT does not require connection to the internet to operate. The program may take a few seconds to start.

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

### Navigating the application

The DIT is comprised of three different tabs, **Search Tool**, **Libraries**, 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 **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 threshold (e.g., 5 %). For each target  $m/z$  value, library compounds that have either a protonated molecule (or calculated base peak) within mass tolerance of the target  $m/z$  value are identified. Each library compound is then assigned two scores. The first score (FPIE) captures the *fraction of peak intensity* in the library spectrum that is *explained* by matching peaks with any non-zero intensity in the mixture spectrum. The second score is a *reverse match factor* (RevMF) which considers the intensity of peaks in the both the library spectrum and their matching peaks in the mixture mass spectrum. At present, either (or both) scores can be used for decision making, but extensive evaluation and optimization of the algorithm and scoring measures is on-going research. For a detailed description of the underlying algorithm, please see Moorthy & Sisco (2021), “A new library-search algorithm for mixture analysis using DART-MS”, *Journal of the American Society for Mass Spectrometry*, 32(7), 1725-1734. doi.org/10.1021/jasms.1c00097

### 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. At the top, there are navigation tabs for 'Search Tool', 'Libraries', and 'About'. Below this is a 'View' selector with 'Interactive' selected and 'Reporting' as an option. A date field shows '9/08/2021' and an instrument field shows 'Instrument 1'. A 'Comments...' field is present. Below these are buttons for 'Load Presets', 'Download Presets', and 'Restore Defaults'. The main interface is split into two panels. The left panel, 'Query Spectra', has a 'Settings' tab and a 'Reference Library' dropdown set to 'HeLibrary\_Cicada\_090721.RDS'. It includes instructions on selecting mass spectra and three 'Browse...' buttons for uploading 'L0004.jsp' files. A 'Search Database' button and a 'Clear Search' button are also present. The right panel, 'Results', shows a mass spectrum plot with 'Relative Intensity (%)' on the y-axis and 'm/z' on the x-axis. A table of 'All Peaks' is displayed, and a list of 'Potential matches' is shown below the plot.

**Area 1:** View:  Interactive  Reporting

**Area 2:** 9/08/2021 Instrument 1 L0004 1

**Area 3:** Load Presets Download Presets Restore Defaults

**Area 4:** Query Spectra Settings Reference Library: HeLibrary\_Cicada\_090721.RDS

Select centroided mass spectrum (txt, jsp, csv) measured at fragmentation levels of your choice. Low (30 V) fragmentation required.

Browse... L0004.jsp Upload complete

\*required

Browse... L0004.jsp Upload complete

Browse... L0004.jsp Upload complete

Search Database

Clear Search

References  
Moorthy & Sisco, DOI:10.1021/jasms.1c00097

**Area 5:** Low (30 V) Mid (60 V) High (90 V) Threshold Top 10

All Peaks

m/z	Rel. Int. (%)
389.2231	100.0
390.2259	35.3
297.1607	17.0
391.2292	7.9
389.3330	6.0

Target 1 Target 2 Target 3 Target 4 Target 5

Measured m/z: 389.2231  
Relative intensity: 100.0 %

Potential matches in HeLibrary\_Cicada\_090721 database by Protonated Molecule m/z targeting:  
ortho-methyl Furanyl Fentanyl: FPIE-based Index: 1 RevMF-based Index: 1  
para-Methyl Furanyl fentanyl: FPIE-based Index: 0.972 RevMF-based Index: 0.986  
meta-Methyl Furanyl fentanyl: FPIE-based Index: 0.943 RevMF-based Index: 0.987

- **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 parameters.
- **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.





## Changing the settings (Area 4)

Prior to completing a search, users have the ability to select a number of parameters 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.

- **Search Mode:** This setting dictates whether or not a user-defined relative intensity threshold is used for compound identification. If *Pure Compound* is chosen, the relative intensity threshold is fixed at 100 %, and only the most abundant peak in the Low (30 V) spectrum will be used for initial target identification. If *Mixture Analysis* is chosen, the user will be able to set a defined relative intensity threshold. In this mode all peaks above the threshold in the Low (30 V) spectrum will be used for initial target identification.
- **Target Assumption:** This setting determines the way the initial target identification is completed for the peaks above the defined threshold in the Low (30 V) spectrum. *Protonated Molecule* indicates that peaks are identified using the theoretical protonated molecule  $m/z$  values for all compounds in the reference library. *Base Peak* indicates that peaks are identified using the calculated  $m/z$  values for base peaks from the Low (30 V) spectra for all compounds in the selected reference library.
- **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 the user to select the minimum relative intensity for peak identification and peak searching. Integer values between 1 and 100 can be chosen. Note that if *Pure Compound* is chosen as the **Search Mode**, this option will be unavailable.
- **$m/z$  Tolerance:** This setting allows the user to select the  $m/z$  tolerance that is appropriate for the data that will be searched. The selected tolerance will be incorporated into the initial target identification step. 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 opened again.

## 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 saving presets, text entered into any of the reporting fields (discussed in the next section) will also be saved. For example, if a user only has one instrument, the *Instrument ID...* field could be filled in prior to downloading the presets. Then, every time the presets are loaded, this field will be auto-populated.

## Inputting reporting information (Area 2)

The **Search Tool** contains a number of text fields at the top of the screen where users can enter relevant information for report generation. Boxes are open text and allow for users to enter a date, an instrument name, a case number, an item number, and any additional information. Inputting text into these boxes is not required. Text entered into these boxes will be used to generate the downloadable / printable report, discussed in more detail in the “Report viewing & printing” section.

## 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 collisional induced dissociation (is-CID) spectra. ***At a minimum, the Low (30 V) spectrum needs to be uploaded.*** Uploading the Mid (60 V) and High (90 V) spectra are optional. **Note:** 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 Database* 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. These are peaks that were used to make an initial compound identification.

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 listed in order of 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, potential matches are listed based on decreasing FPIE scores. For each potential compound both an FPIE and RevMF score is listed. Refer to the “How the search algorithm works” section for more information on what these scores represent. If a target was found to have no corresponding compounds in the reference library, the message “No matches in <Library> database...” will be displayed.

To the right of the 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).

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.

**View:**  
 Interactive  Reporting

<b>Parameter</b>	<b>Value</b>
Date:	09/08/2021
Instrument ID:	Instrument 1
Case Number:	L0004
Item Number:	1
Filename of Low (30 V) Spectrum:	L0004.jsp
Filename of Mid (60 V) Spectrum:	No file selected
Filename of High (90 V) Spectrum:	No file selected
Search Mode:	Mixture Analysis
Target Assumption:	Protonated Molecule
Display only targets with potential matches:	No
Identification threshold (%):	5%
m/z Tolerance ( $\pm$ Da):	0.005
Comments:	None

**Low (30 V) L0004.jsp**

**Legend**  
--- Threshold

**Threshold**

index	m/z	Rel. Intensity	Target
1	389.2231	100.0	T1
2	390.2259	35.3	T2
3	297.1607	17.0	T3
4	391.2292	7.9	T4
5	389.3330	6.0	T5

**Target 1**  
 Measured m/z: 389.2231  
 Relative intensity: 100.0 %.

Potential matches in He\_Pos\_Dragonfly database by Protonated Molecule m/z targeting:  
 ortho-methyl Furanyl Fentanyl: FPIE-based Index: 1 RevMF-based Index: 1  
 meta-Methyl Furanyl fentanyl: FPIE-based Index: 0.971 RevMF-based Index: 0.987  
 para-Methyl Furanyl fentanyl: FPIE-based Index: 0.97 RevMF-based Index: 0.987

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



### 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.

New spectra can also be loaded without clearing the spectra, if desired, and this will clear the current search.

### 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.

The screenshot displays the Libraries Viewer interface. At the top, there are tabs for "Search Tool", "Libraries", and "About". The "Libraries" tab is active. Below the tabs, there are three main areas outlined in red:

- Area A:** View:  Interactive  Reporting
- Area B:** Reference Library: HeLibrary\_Cicada\_090721.RDS. A search bar shows "Show 15 Entries" and "Search:". A table lists library entries with columns for Name, Formula, and [M]. The first entry is highlighted: 1-(3-Chlorophenyl)piperazine, C<sub>10</sub>H<sub>13</sub>ClN<sub>2</sub>, 197.1.
- Area C:** Metadata and Spectrum for 1-(3-Chlorophenyl)piperazine. It includes fields for Library, Polarity, Source Gas, Name, Formula, Exact Mass, [M+H]<sup>+</sup>, 30V Base Peak, InChIKey, Contributor, and Synonyms. A chemical structure is shown. Below is a mass spectrum plot for "Mid (60 V)" showing Relative Intensity (%) vs m/z. A table of peaks is provided:

m/z	Rel. Intensity
197.0832	100.0
199.0793	35.2
198.0844	14.7
154.0405	9.5
196.0738	4.2
200.0825	4.1
156.0383	3.2
197.7846	1.9
198.8113	1.8
195.0665	1.4

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



## Selecting a reference library (Area B)

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 B)

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 C)

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 above 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.

Below 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).

## 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*. (Note that this is a hidden folder, so users may have to unhide folders to access it). 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.





## Waters QDa File Converter

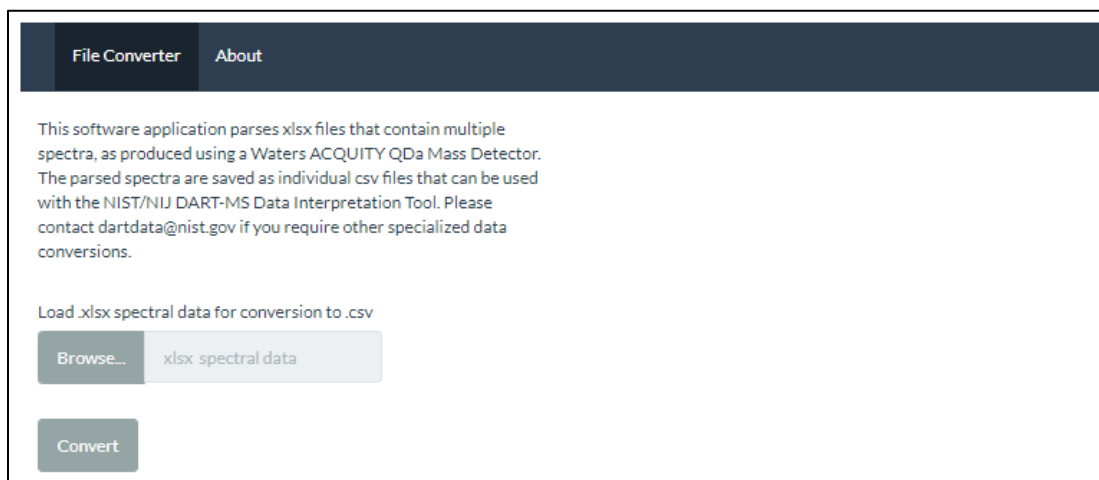
Data collected from the Waters Acquity QDa that is exported as single .xlsx file containing mass spectra from multiple is-CID voltages must be converted prior to upload into the DIT. This file converter will separate the mass spectra contained in the .xlsx into individual files for upload into the DIT.

### 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.