The NIST DART-MS Database Search Tool (DST)

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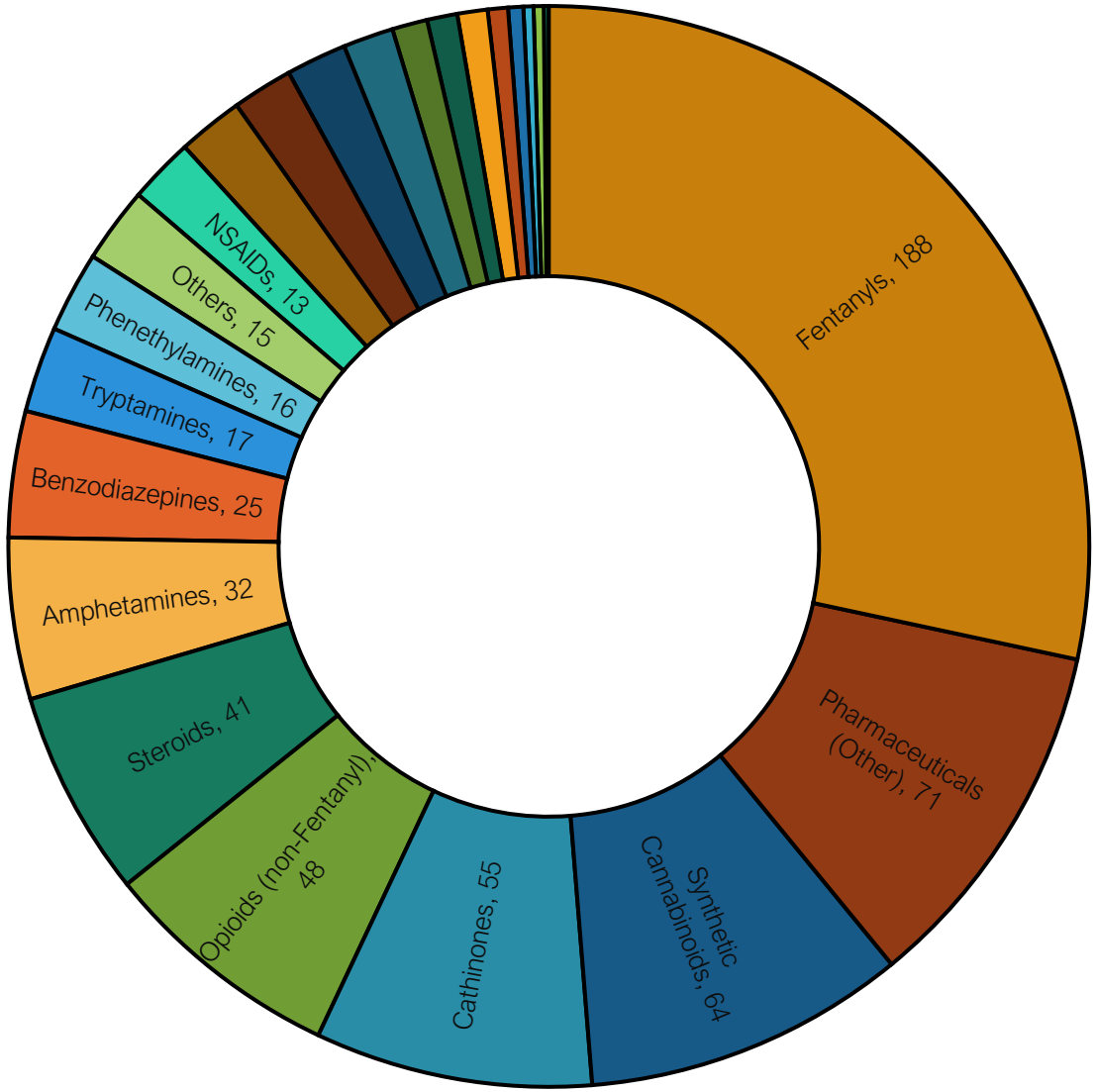
NIST National Institute of Standards and Technology U.S. Department of Commerce | Mass Spectrometry Data Center

The Database

https://chemdata.nist.gov

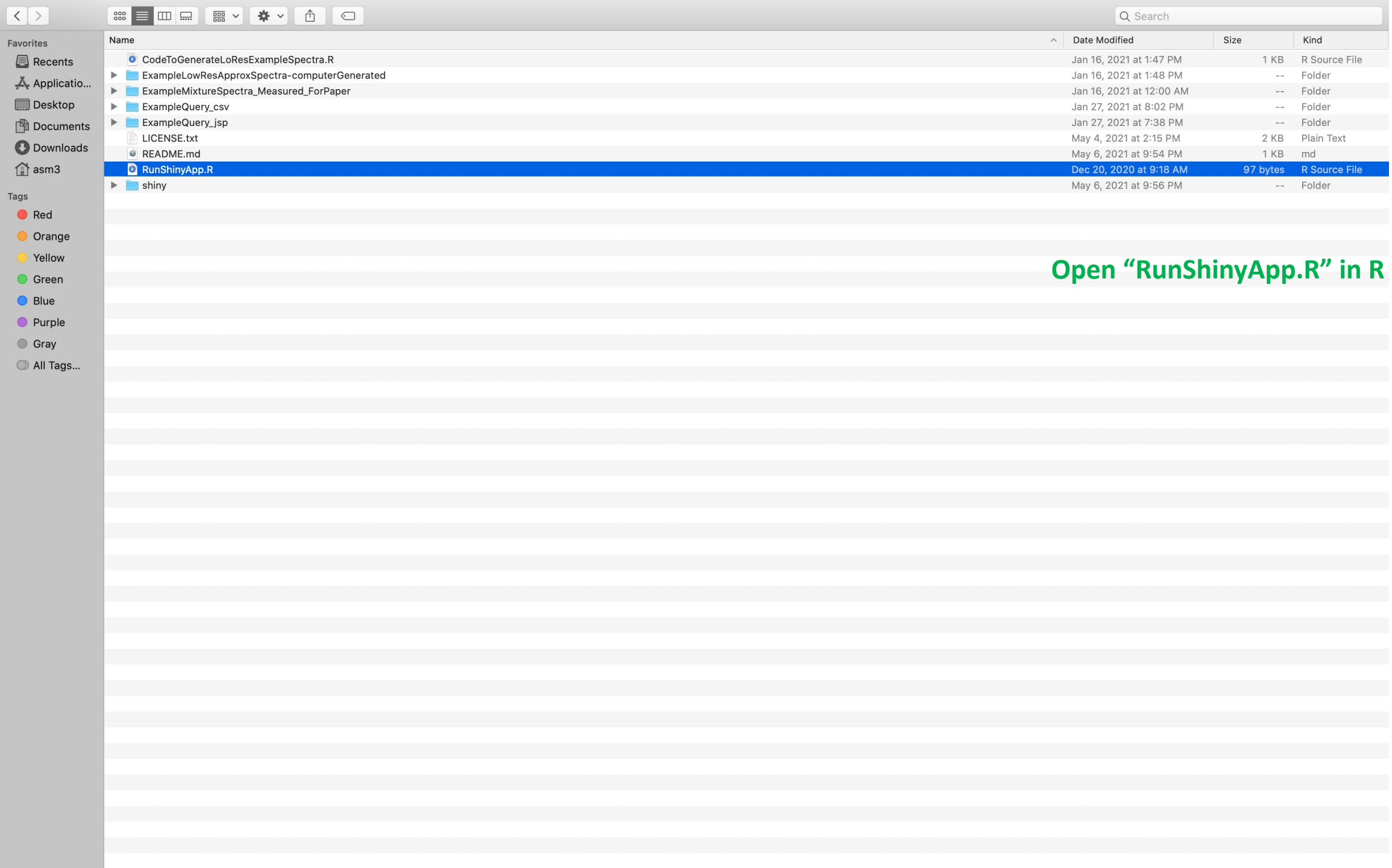
DART-MS Forensics Database

- A new database **available now**
  - focus on NPS's, synthetic opioids, cutting agents
  - spectra measured at multiple orifice 1 energies
- Developed new manual and **automated** evaluation workflow
- Implemented workflow to facilitate rapid updating of database
  - https://github.com/asm3-nist/NIST-MS-DBB
- Database available at https://chemdata.nist.gov



The Software

https://github.com/asm3-nist/DART-MS-DST


Search
Favorites
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Applicatio...
Desktop
Documents
Downloads
asm3
Tags
Red
Orange
Yellow
Green
Blue
Purple
Gray
All Tags...
Name
Date Modified
Size
Kind
CodeToGenerateLoResExampleSpectra.R
Jan 16, 2021 at 1:47 PM
1 KB
R Source File
ExampleLowResApproxSpectra-computerGenerated
Jan 16, 2021 at 1:48 PM
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LICENSE.txt
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2 KB
Plain Text
README.md
May 6, 2021 at 9:54 PM
1 KB
md
RunShinyApp.R
Dec 20, 2020 at 9:18 AM
97 bytes
R Source File
shiny
May 6, 2021 at 9:56 PM
--
Folder
Open “RunShinyApp.R” in R or Rstudio

~/Documents/Research/DART2020/ForGithub/DST/v02

Help Search

```
R version 4.0.5 (2021-03-31) -- "Shake and Throw"
Copyright (C) 2021 The R Foundation for Statistical Computing
Platform: x86_64-apple-darwin17.0 (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

  Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

[R.app GUI 1.74 (7950) x86_64-apple-darwin17.0]

[History restored from /Users/asm3/.Rapp.history]

> source("RunShinyApp.R")
```

If using base R, run the command *source("RunShinyApp.R")* to run the application. (shown here)

If using Rstudio, a button to "Run App" will be available. (not shown)

source(file, local = FALSE, echo = verbose, print.eval = echo, exprs, spaced = use_file, verbose = getOption("verbose"), prompt.echo = getOption("prompt"), max.deparse.length = 150, width.cutoff = 60L, deparseCtrl = "showAttributes", chdir = FALSE, encoding = getOption("encoding"), continue.echo = getOption("continue"), skip.echo = 0, keep.source = getOption("keep.source"))

The application will open in your browser and default to the “Viewer” tab.

Click through the available libraries.

Click through the available compounds in the navigator.

Select tabs to see spectra at a specific fragmentation energy.

NIST DART-MS | Viewer | Search Tool

The NIST DART-MS Database Search Tool (DST) is an open-source research tool for analyzing DART-MS spectra of seized drugs. The authors cannot guarantee the accuracy nor validate the claims of others using results generated by this software.

For help or more information: dartdata@nist.gov

Reference Library:

NIST-DARTMS-Forensics-2020-update1.RDS

Show 15 entries Search:

	Name	Formula	[M
1	1-(3-Chlorophenyl)piperazine	C10H13ClN2	1
2	1-(4-Methoxyphenyl)piperazine	C11H16N2O	19
3	1-Benzylpiperazine	C11H16N2	17
4	1B-LSD	C24H31N3O2	39
5	1-Demethyl Phenazolam	C16H10BrClN4	3
6	1P-LSD	C23H29N3O2	38
7	2,2,3,3-Tetramethyl-Cyclopropyl fentanyl	C27H36N2O	
8	2,3-Dimethylmethcathinone	C12H17NO	19
9	2,3-Pentylone	C13H17NO3	23
10	2,3-Seco-Fentanyl	C22H30N2O	33
11	2',5'-dimethoxy Fentanyl	C24H32N2O3	39
12	25B-NBOH	C17H20BrNO3	36
13	25B-NBOMe	C18H22BrNO3	38
14	25C-NBOMe	C18H22ClNO3	33
15	25I-NBOH	C17H20INO3	41

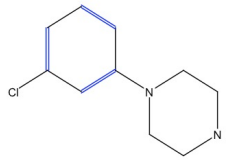
Showing 1 to 15 of 760 entries

Previous 1 2 3 4 5 ... 51 Next

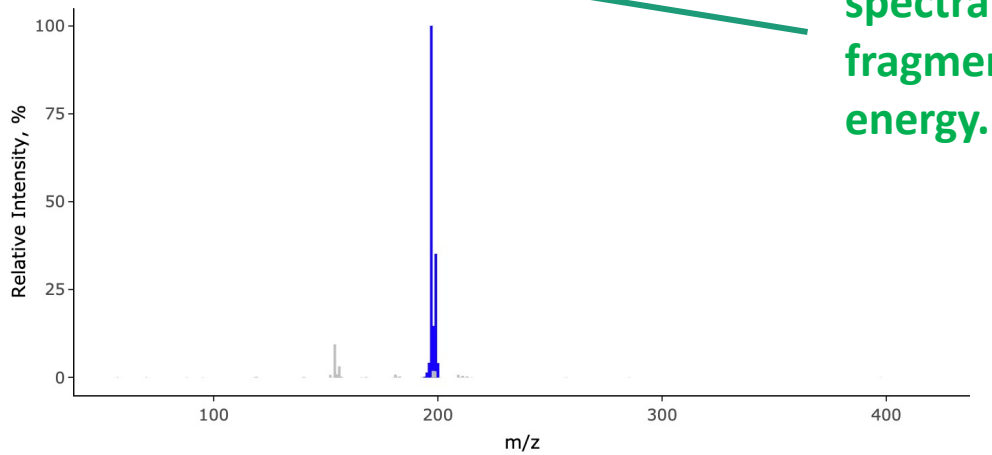
References

Sisco et. al. J. Am. Soc. Mass Spectrom. 2021, 32, 3, 685–689.

Name: 1-(3-Chlorophenyl)piperazine
Formula: C10H13ClN2
Exact Mass [Da]: 196.077
InChIKey: VHFVKMTVMIZMIK-UHFFFAOYSA-N
Contributor: NIST
Comment: None



+30 V | +60 V | +90 V



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CLICK HERE to transition to the Search Tool.

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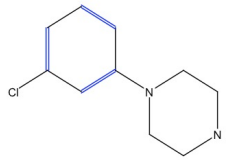

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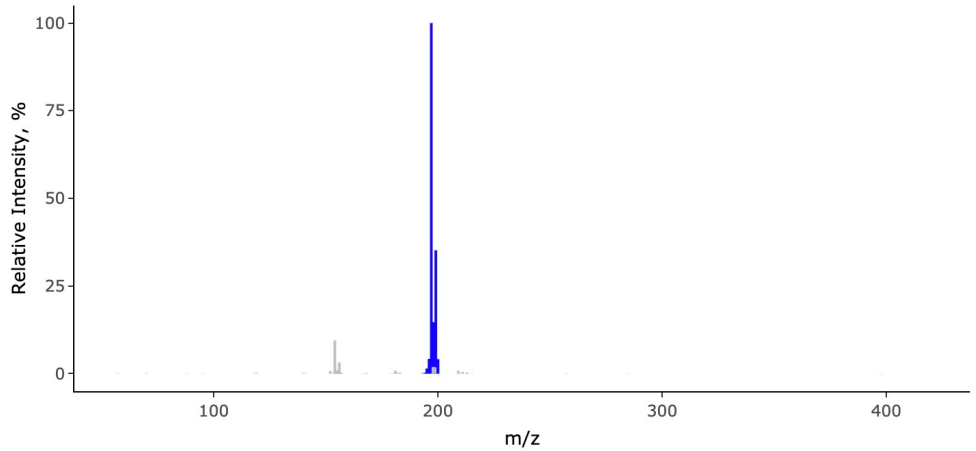

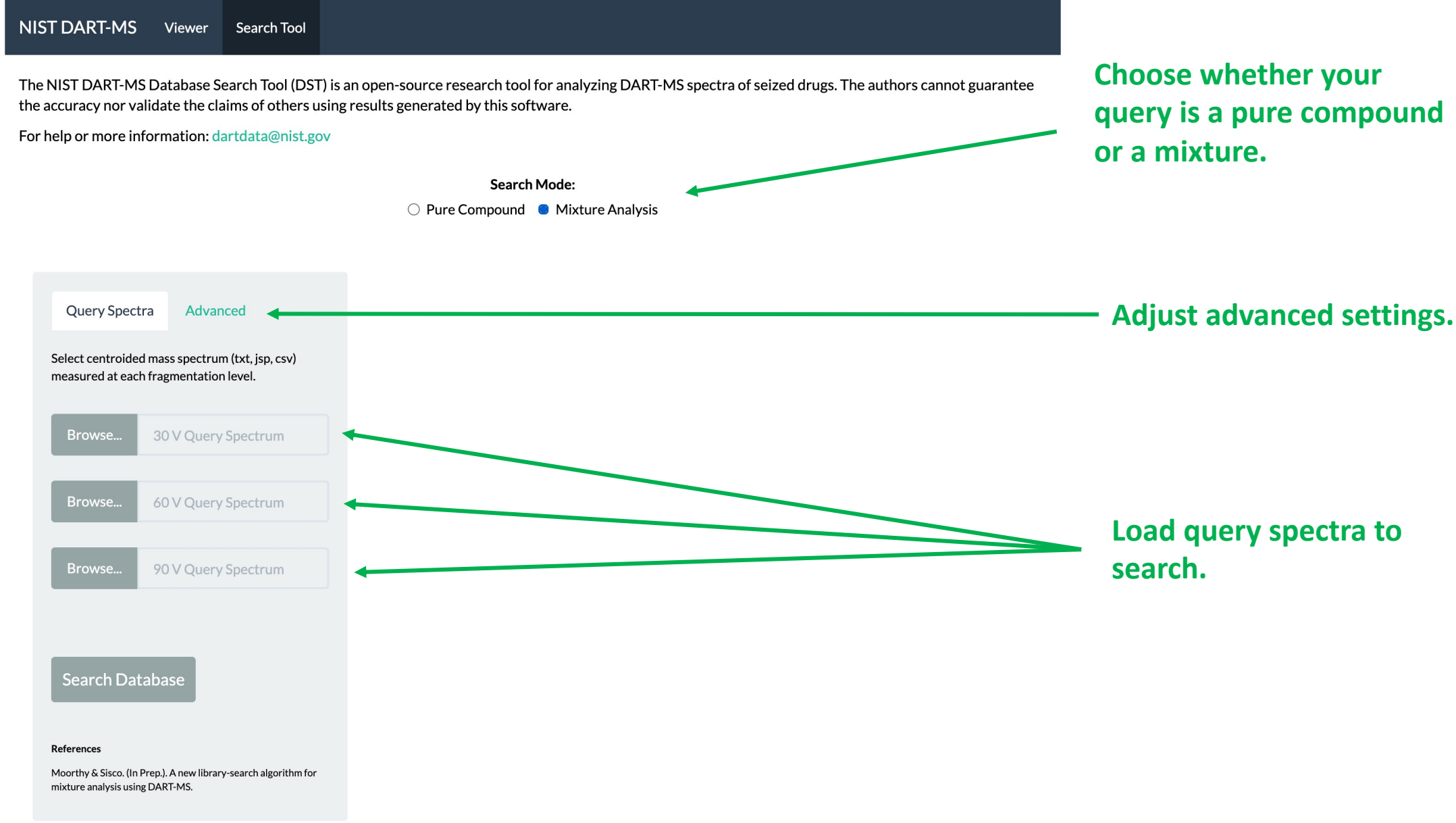
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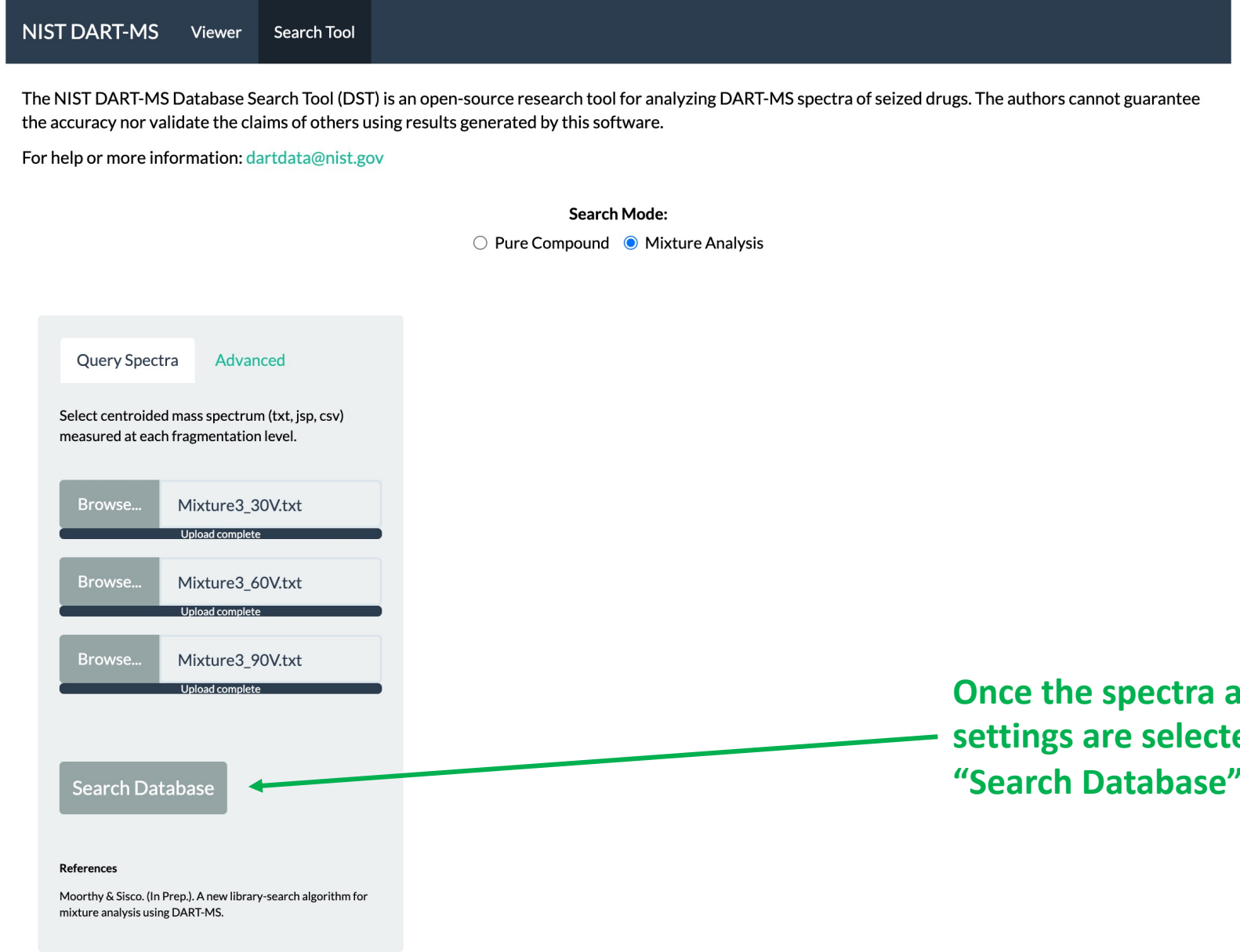
Search Mode:
Pure Compound
Mixture Analysis
Query Spectra
Advanced
Select centroided mass spectrum (txt, jsp, csv) measured at each fragmentation level.
Browse...
30 V Query Spectrum
Browse...
60 V Query Spectrum
Browse...
90 V Query Spectrum
Search Database
References
Moorthy & Sisco. (In Prep.). A new library-search algorithm for mixture analysis using DART-MS.
Choose whether your query is a pure compound or a mixture.
Adjust advanced settings.
Load query spectra to search.



Once the spectra are loaded and settings are selected, press the "Search Database" button

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Search Mode:

○ Pure Compound ◉ Mixture Analysis

Query Spectra | Advanced

Select centroided mass spectrum (txt, jsp, csv) measured at each fragmentation level.

Browse... Mixture3_30V.txt
Upload complete

Browse... Mixture3_60V.txt
Upload complete

Browse... Mixture3_90V.txt
Upload complete

Search Database

References

Moorthy & Sisco. (In Prep.). A new library-search algorithm for mixture analysis using DART-MS.

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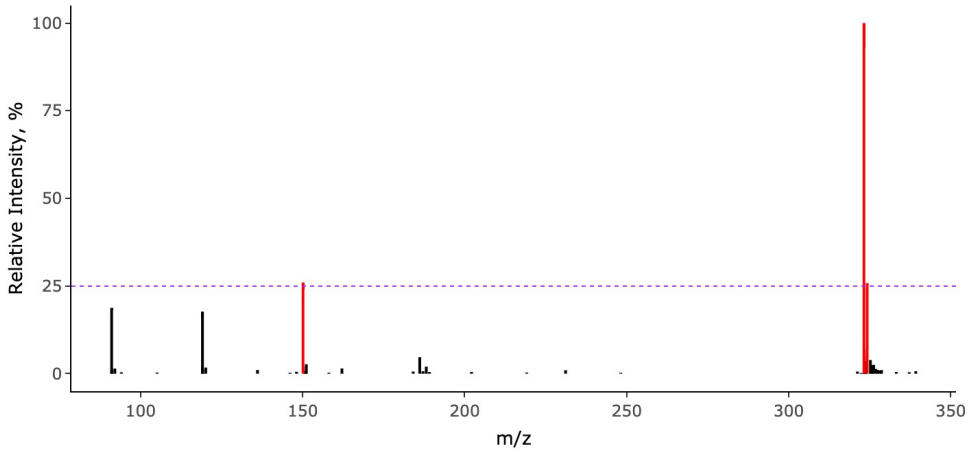


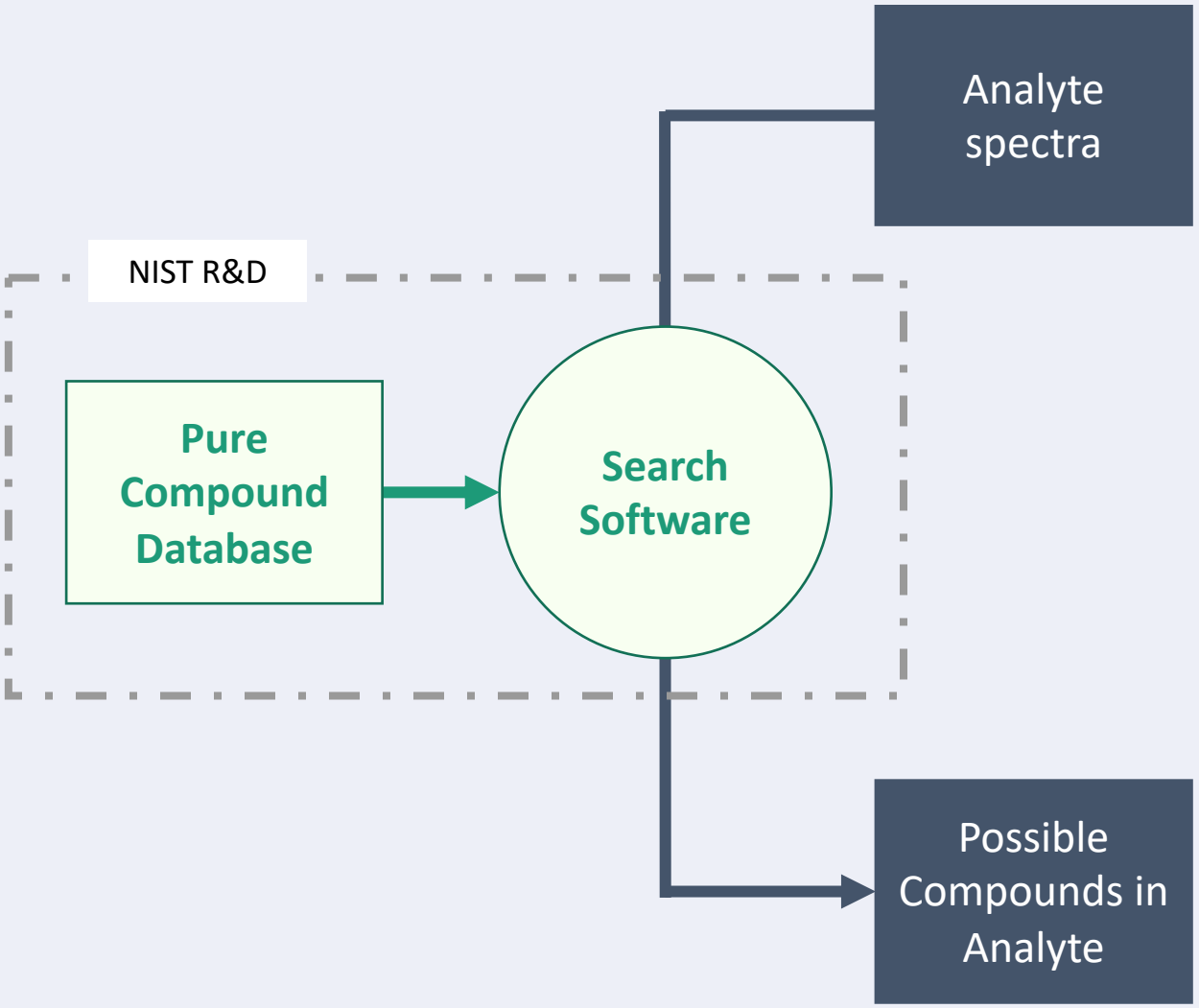
Target 1 | Target 2 | Target 3

Mass-to-charge: 323.214
Relative intensity: 100.0 %.

Potential matches in **NIST-DARTMS-Forensics-2020-update1** database by *protonated molecule* m/z targeting:
Acetyl fentanyl : FPIE-based Index: **0.928** RevMF-based Index: **0.974**
Benzylfentanyl : FPIE-based Index: **0.535** RevMF-based Index: **0.644**

Look through all the fragmentation spectra of the query by switching between these tabs

Look through all the search results by switching between these tabs



Summary

1. New NIST DART-MS Forensics Database (Library)
   a. Plan to provide regular updates as more compounds and spectra are acquired
   b. Suggestions for new or missing compounds, or corrections to entries should be submitted to DARTdata@nist.gov
   c. Most updated database available at https://chemdata.nist.gov

2. New NIST DART-MS Database Search Tool (DST)
   a. Plan to provide updated software based on user feedback
   b. Suggestions of new or improved features should be submitted to DARTdata@nist.gov
   c. DART-MS Search Tool (DST) available at https://github.com/asm3-nist/DART-MS-DST

DARTdata@nist.gov