

D-Tracer Web Version Instructions for Use

Noelle Reimers, Ryan Ostrander, Alyson Shoji, Chau Vuong
Contact: nreimers@uw.edu | GitHub: nreimers99/d-tracer
University of Washington Department of Medicinal Chemistry

D-Tracer is a program designed for the analysis of dual isotope labeling mass spectrometry data. The user provides a peaklist and D-Tracer will scan through the list to find pairs of compounds with the same retention time and collision cross section values and an m/z difference corresponding to the mass difference of the deuterium labels that were used. It will then adjust the mass of the labeled compounds to the corresponding unlabeled mass so that they can be identified.

User inputs:

- Peaklist.csv file with columns for m/z, RT, CCS, and normalized sample intensities
- Mass of each deuterium label
- Number of samples

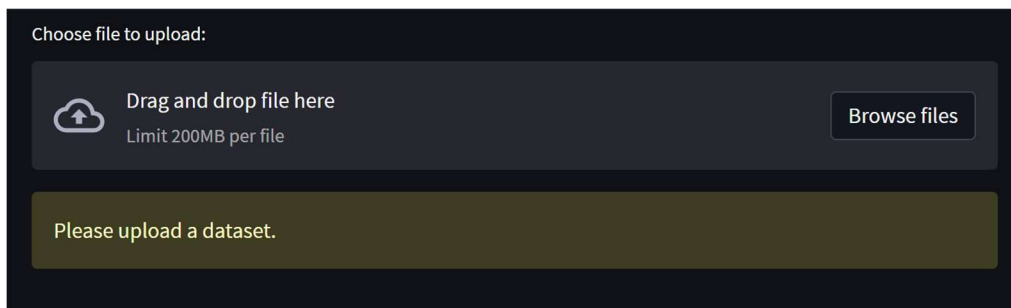
Output:

- .csv file containing labeled pairs and isotope-adjusted masses

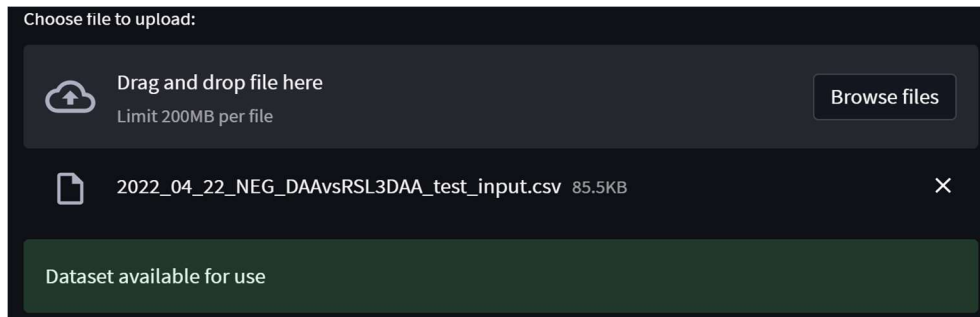
The web version of D-Tracer can be accessed at this URL:

<https://nreimers99-d-tracer-original-d-tracerapplication-xji04u.streamlit.app/>

Step 1: Upload dataset. The dataset must be a .csv peaklist containing columns named m/z, Retention time (min), and CCS (angstrom²). It was originally designed for use with .csv files exported from Waters Progenesis.



Step 2: The program will accept the file if it has all required columns. The program will raise an error if the file is not adequate for use. Once accepted, the following message will be displayed:



Step 3: Specify parameters. The program needs to know the mass adjustments (ie, the number of deuterium atoms in the two labels) used in the experiment. The first mass adjustment refers to the smaller label used. For example, if the experiment included a label with 5 deuterium atoms and 11 deuterium atoms, the inputs would be 5 for the first mass adjustment and 11 for the second mass adjustment. It also needs to know the number of samples to include intensity data in the output file.

Step 2: If you would like sample intensities included in the output file, enter the number of samples in your dataset

Enter number of samples:

- +

Step 3: To find isotope labeled pairs in the dataset, select 'Find pairs' in the dropdown menu

What would you like to do?

☒ Find pairs

☐ Find Standards

Step 4: Enter the number of deuterium atoms on each of the labeled compounds used in your experiment. Please enter the smaller number first. Values can be anywhere from 0 to 80.

Enter smaller number of deuterium atoms:

- +

Enter larger number of deuterium atoms:

- +

Step 4: Check 'Analyze' to run the pair picking algorithm on the provided dataset. If there are pairs found, the following message will be displayed:

☒ Analyze ?

17 pairs found | Runtime = 0.0 seconds

Pick One:

Show mass-adjusted data of pairs

Step 5: Select Show mass-adjusted data of pairs in the dropdown menu to display the pairs found. To download the .csv file to your device, select 'Export to CSV' in the bottom left corner.

Pick One:

Show mass-adjusted data of pairs

	Compound	m/z	m/z_adj	Retention time (min)	CCS (angstrom^2)	NEG_2022_04_22_NR
4	6.36_905.6896m/z	905.6896	894.6203	6.3618	304.433	
5	6.36_899.6525m/z	899.6525	894.621	6.3618	303.0519	
6	6.36_877.6611m/z	877.6611	866.5918	6.3618	296.0572	
7	6.36_871.6240m/z	871.624	866.5925	6.3618	296.089	
8	6.26_938.7460m/z	938.746	927.6767	6.2602	304.2722	
9	6.26_932.7086m/z	932.7086	927.6771	6.2602	304.3007	
9	6.26_932.7086m/z	932.7086	921.6393	6.2602	304.3007	
10	6.26_926.6708m/z	926.6708	921.6393	6.2602	302.9185	
17	5.17_805.6395m/z	805.6395	794.5702	5.1741	280.5054	
19	5.17_799.6012m/z	799.6012	794.5697	5.1741	279.0683	

Export to CSV

Step 6: If you would like to see a heatmap of intensities for each compound and sample in the dataset, check the 'Heatmap' box:

