Neurolipidomics Laboratory
India Taylor Lipidomics Research Platform
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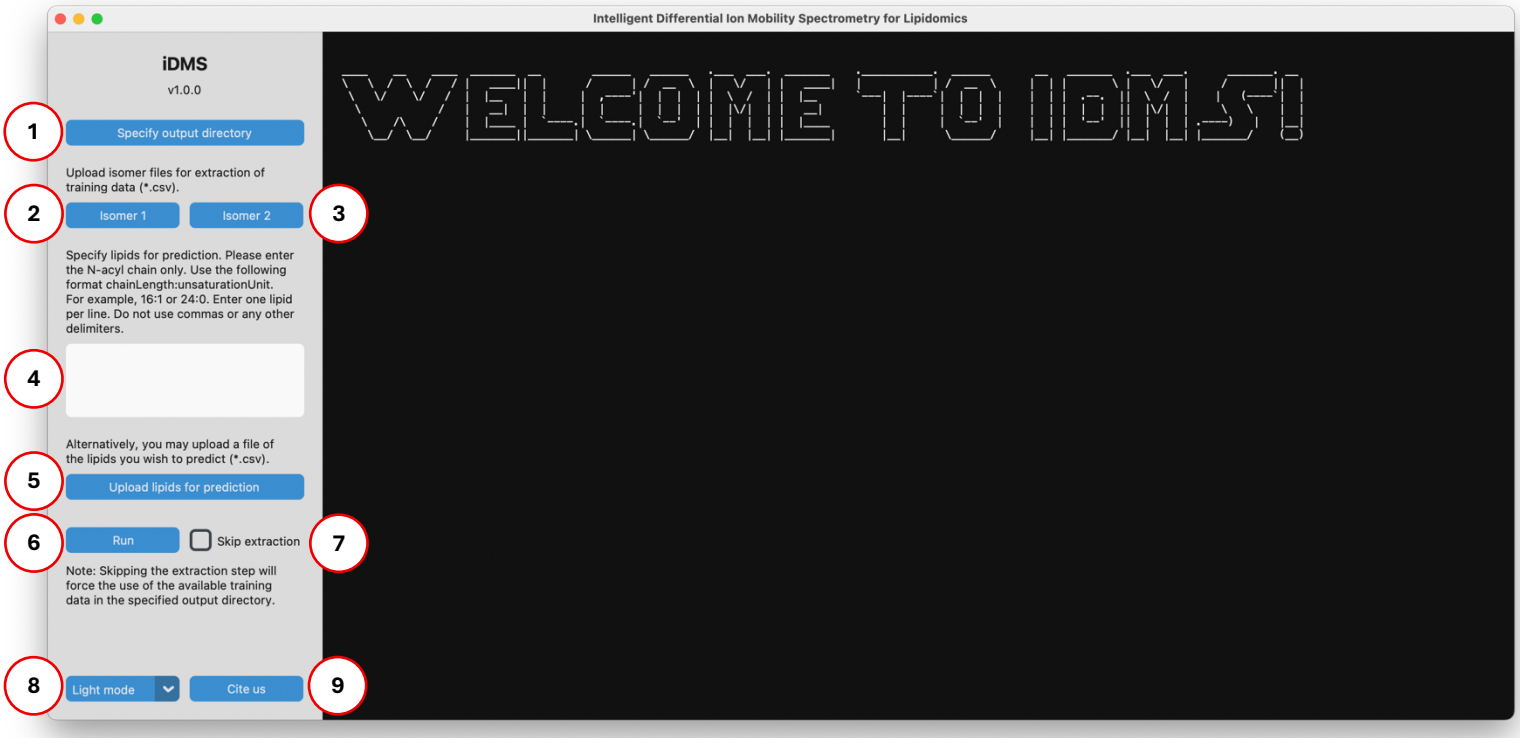
Understanding the iDMS Application Interface:



1. **Specify output directory:** Select the directory where iDMS will save extracted (training) data, predictions, and other output files.
2. **Isomer 1:** Upload the first isomer data file (.csv).
3. **Isomer 2:** Upload the second isomer data file (.csv).
4. **Lipid input field:** Enter the lipids you wish to predict. Provide only the *N*-acyl chain information using the format chainLength:unsaturationUnit (e.g.,14:0). Provide only one lipid per line. Do not include additional punctation (e.g., commas).

Good example:	Bad example 1:	Bad example 2:
14:0	14:0,	14:0,16:0,16:1
16:0	16:0,	
16:1	16:1	

5. **Upload lipids for prediction:** Alternatively, upload a file (.csv) containing the lipids for prediction. If uploading a list, do not enter the lipids manually. Format must match the format above with one lipid per line.
6. **Run:** Start the analysis pipeline.
7. **Skip extraction:** Select this option to bypass the data extraction step and to instead use existing extracted data (i.e., data extracted from your sample isomer datasets from the last full iDMS run made. If you close iDMS, you must re-extract your data).

8. **Theme selector:** Change the application appearance between light (default) and dark mode.
9. **Cite us:** Opens the iDMS website with citation information in a browser.

Understanding the iDMS Application Output:

iDMS generates two sub-directories and a .json file per run. Each sub-folder corresponds to a high-level analysis pipeline step:

- **Module 1 sub-directory:** Extracting and consolidating data from the two input isomer files.
- **Module 2 sub-directory:** Formatting consolidated data for neural network model training and predicting instrument parameters of queried lipids.

The .json file summarizes the input data of a given run and is critical, along with Module 1 results, for running the program while using the **Skip extraction** option.

These outputs are organized as follows:

```
Output directory                          Required for running with
├── lipid_data.json                          Skip extraction option
└── Module1_Outputs
      ├── CombinedAnalysis.csv
      ├── meanAllSigma.csv
      ├── Intersected_gauss.csv
      ├── extract_{isomer1}_MaxCov.csv
      ├── extract_{isomer2}_MaxCov.csv
      ├── norm_{isomer1}.csv
      ├── norm{isomer2}.csv
      ├── norm_{isomer1}_parameters.csv
      ├── norm{isomer2}_parameters.csv
      └── Plots
└── Module2_Outputs
      ├── iDMS_params.csv
      ├── iDMS_training_history.csv
      ├── TrainingSet.csv
      ├── PredictionResult.csv
      └── PredictedSetPlots
```

Note: Changing the names of the required files and sub-directories for the **Skip extraction** option will generate an error and exit the current run.

For more information on the iDMS analysis pipeline, please refer to the complete program documentation: https://github.com/Neurolipidomics/iDMS/tree/main