METABOLOMICS WORKBENCH DATA DEPOSITION **RILEY BROOK / KANAREK LAB BOSTON CHILDREN'S HOSPITAL AND HARVARD MEDICAL SCHOOL**

STAGE 1:

EXCEL FILES FOR DATA DEPOSITION

STUDY DESIGN

Template for study design: Sheet 1

https://docs.google.com/spreadsheets/d/1SkFFhAYc1Ajp9OqGA8vEKKTXbl0nClt3Ft5Hbf-tbU/edit?usp=sharing

Steps

- 1) Fill out first column with sample names (you can use the same name as the raw file name). Include the pools.
- 2) Fill out second column with sample source (for example: mouse plasma).
- 3) Fill out the third column with a factor that identifies your groups. For the pool samples, you can put N/A. Example: this in this experiment we had plasma samples from mice with leptomeningeal metastasis (LM+) and without leptomeningeal metastasis (WT). I called the factor disease but you have some flexibility in terms of defining your samples (they will carefully review everything when you submit and they will communicate with you if something does not make sense and provide
- 4) Fill out the fourth column with the raw file names. Be careful that these exactly match the raw file names that you plan to upload AND the Sample_ID name from the first column.
- 5) Copy and paste from your excel sheet into this box, and it should look something like what you see in the image below.
- 6) Choose View/check study design.

mwTab Identifier: jrileyb_20241104_105910 Return to start

IMPORTANT!!

Make sure that sample names in submitted results table(s) or file(s) exactly match those in the study design table.

Otherwise you won't be able to complete the submission.

(One needs to be able to relate experimental conditions in the study-design section via sample names in ALL submitted datasets)

Input Study Design information. Sample names, experimental factor(s), sample source and raw data file names (if submitting raw data) are required. Subject name and additional sample data are optional.

First row must contain headings. Data must be tab-delimited.

```
Sample source Disease Raw file name
20240211 QEF1 HILIC mouseplasma serum polars XT288 WTplasma t
                                                                Mouse Plasma
                                                                                 WT
20240211_QEF1_HILIC_mouseplasma_serum_polars_XT288_WTplasma_t.raw
Mouse Plasma
                                                                                 WT
20240211_QEF1_HILIC_mouseplasma_serum_polars_XT290_WTplasma_t
20240211_QEF1_HILIC_mouseplasma_serum_polars_XT290_WTplasma_t.r
20240211_QEF1_HILIC_mouseplasma_serum_polars_XT291_LMplasma_t
20240211_QEF1_HILIC_mouseplasma_serum_polars_XT291_LMplasma_t.r
                                                                Mouse Plasma
                                                                                 I M+
20240211_QEF1_HILIC_mouseplasma_serum_polars_XT292_LMplasma_t
                                                                ...
Mouse Plasma
```

View/check study design See examples of study design layout

7) After choosing View/check study design, it will load something similar to the following table.

- 8) You can read the instructions for what is required, but you will need the following columns: Sample_ID, Sample Source, Factor, and Raw file name. You will see in the instructions that you can add additional columns, but these are optional. MAKE SURE YOU CHOOSE FROM THE DROP DOWN THE CORRECT IDENTIFICATION FOR THE COLUMN (see arrows in image below).
- 9) Choose Yes from the drop down for does this submission contain raw data? 10) Choose Process study design data.

Instructions:

Sample names/identifiers in the required 'Sample_ID' column should be unique and should exactly match those names used in the processed results. The required 'Sample source' column (e.g. blood, urine, HEK cells, blank, buffer) must be completed. This may be the same or different for all samples The required 'Raw file name' column must be completed when submitting raw data. The sample name to raw file name mapping is essential in order to enable re-analysis of raw data.

The optional 'Subject_ID' column may be used to designate the submitter's source identifier for a given sample (e.g. subject/patient/animal identifer). The required 'Factor' column(s) are used to assign experimental variables (factors) to sample groups (e.g. treatment condition, time, genotype, phenotype, etc.). Use an appropriate name for the factor heading (e.g. Genotype, Time, Drug treatment) - don't use 'Factor' which is too vague. The optional 'Other' column(s) may be used to include additional data such as BMI, age, glucose measurements, etc. that are unique to each sample. These types of measurements should NOT be designated as factors.

Assign every column(below) as 'Subject ID'(optional), 'Sample ID'(required:1 and only 1), 'Sample source'(required:1 and only 1), 'Factor'(required:at least 1) or 'Other'(optional additional sample data). Columns assigned 'Ignore' will be ignored.

| Process study design data Does submission contain raw data?: Yes | | | |
|--|-----------------|----------|-------------------|
| Sample_ID V | Sample source V | Factor ~ | Raw file name V |
| Sample_ID | Sample source | Disease | Raw file name |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT288_WTplasma_t | Mouse Plasma | WT | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT289_WTplasma_t | Mouse Plasma | WT | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT290_WTplasma_t | Mouse Plasma | WT | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT291_LMplasma_t | Mouse Plasma | LM+ | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT292_LMplasma_t | Mouse Plasma | LM+ | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT293_LMplasma_t | Mouse Plasma | LM+ | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT294_plasma_pool1xa | Mouse Plasma | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT294_plasma_pool1xb | Mouse Plasma | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT294_plasma_pool1xc | Mouse Plasma | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT295_plasma_pool03xa | Mouse Plasma | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT295_plasma_pool03xb | Mouse Plasma | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT296_plasma_pool01xa | Mouse Plasma | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT296_plasma_pool01xb | Mouse Plasma | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT297_WTserum_t | Mouse Serum | WT | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT298_WTserum_t | Mouse Serum | WT | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT299_WTserum_t | Mouse Serum | WT | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT300_LMserum_t | Mouse Serum | LM+ | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT301_LMserum_t | Mouse Serum | LM+ | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT302_LMserum_t | Mouse Serum | LM+ | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT303_serum_pool1xa | Mouse Serum | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT303_serum_pool1xb | Mouse Serum | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT303_serum_pool1xc | Mouse Serum | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT304_serum_pool03xa | Mouse Serum | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT304_serum_pool03xb | Mouse Serum | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT305_serum_pool01xa | Mouse Serum | N/A | 20240211_QEF1_HIL |
| 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT305_serum_pool01xb | Mouse Serum | N/A | 20240211_QEF1_HIL |

ASSAYS

Template for Assay: Sheet 2

https://docs.google.com/spreadsheets/d/1SkFFhAYc1Ajp9OqGA8vEKKTXbl0-nClt3Ft5Hbf-tbU/edit?usp=sharing

Steps

- 1) Transpose your normalized data file so the metabolite names are in the first column of the excel sheet and the sample names are in the first row at the top of the excel sheet, and beneath them are all the normalized peak areas. To transpose, highlight the whole data set, copy, paste special > transpose. Since these are the normalized peak area values, you won't have your pool samples here.
- 2) Copy and paste the contents of the excel file into the box.
- 3) For the *Units of measurement (required)*, you can put a.u.
- 4) Choose View/check metabolite data.

mwTab Identifier: jrileyb_20241104_105910 Return to start Analysis: HILIC UNSPECIFIED (1) **OPTION 1:** Assays containing identified (named) metabolite species Input Data in tab-delimited format in the text area below. First column must contain metabolite names Subsequent columns must contain sample data with identical sample names as in Study Design submission. First row must contain sample names. metabolite_name 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT288_WTplasma_t 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT289_WTplasma_t 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT290_WTplasma_t 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT291_LMplasma_t 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT292_LMplasma_t 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT293_LMplasma_t 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT297_WTserum_t 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT298_WTserum_t 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT299_WTserum_t 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT300_LMserum_t Units of measurement (required): a.u. | View/check metabolite data | See examples of metabolite data layout | Delete existing metabolite data (this analysis only)

Note: I have not used OPTION 2, so I am not sure how this one works.

OPTION 2: Untargeted assays not containing identified (named) metabolite species

(e.g. datasets with m/z,retention time features from LC-MS experiments, NMR binned data)

| Add/replace results as a tab-delimited text file: Ideally, feature names should be formatted as 'm/z underscore retention time', e.g. 645.5327_24.91 IMPORTANTI:If unidentified features are listed by neutral mass rather than m/z ratio, this must be specified in the menu below This will enable analysis of the dataset by a larger number of tools on the Metabolomics Workbench | | | | | |
|--|--|--|--|--|--|
| | Feature names contain m/z values*? (required): | Feature names contain retention time values?(required): Time units: | | | |
| * By "m/z values" we are referring to mass-to-charge ratios and NOT neutral masses. | | | | | |
| Upload tab-delimited datafile Choose File No file chosen The first line in the submitted file should contain sample names exactly matching those that you submitted in the 'Study Design' section. | | | | | |
| Finalize or edit "jrileyb_20241104_105910" study submission | | | | | |

(In order to finalize the submission you must have added metabolite results for each analysis)

- 5) After choosing *View/check metabolite data* you should see something like the image below.
- 6) Choose Upload data.

| metabolite_name | 20240211_QEF1_HILIC_mouseplasma_serum_polars_XT288_WTplasma_t | 20240211_QEF1_HILIC_mousep |
|----------------------|---|----------------------------|
| alanine | 235725948.3 | 208723099.2 |
| Alpha.Ketoglutarate | 29129995.71 | 69576112.63 |
| arginine | 1923905734 | 1374443148 |
| aspartate | 44808354.86 | 28409108.43 |
| citrate | 1674833676 | 2527047406 |
| creatinine | 341056641.4 | 462367059.8 |
| cystine | 42125031.86 | 22883320.21 |
| fumarate | 30021472.76 | 50827173.19 |
| glutamate | 96097293.02 | 82396918.5 |
| glycine | 5214659.573 | 5111026.954 |
| histidine | 4106165758 | 3028936571 |
| hypoxanthine | 17064054.25 | 17376022.62 |
| INDOLE.3.ACETIC.ACID | 1325694.213 | 1065704.168 |
| isoleucine | 300943560 | 149276881.2 |
| leucine | 413157676.6 | 188764696 |
| lysine | 441215843.7 | 338650789.4 |
| methionine | 378529274.7 | 235421082.2 |
| niacinamide | 193042967.8 | 106431050.8 |
| palmitate | 3134077401 | 4368421210 |
| phenylalanine | 256558103 | 150457583.2 |
| proline | 827388111.8 | 771124821.8 |
| pyruvate | 2086900.267 | 9118605.507 |
| serine | 29286969.01 | 21354739.01 |
| threonine | 130967079.2 | 109325846.2 |
| THYMINE | 10968914.76 | 20585018.04 |
| tryptophan | 625637596 | 643796719.6 |
| tyrosine | 362582912.4 | 293030312.5 |
| valine | 535648125.9 | 235415679.2 |
| guanosine | N/A | N/A |

Template for Metabolite metadata: Sheet 3

https://docs.google.com/spreadsheets/d/1SkFFhAYc1Ajp9OqGA8vEKKTXbl0-nClt3Ft5Hbf-tbU/edit?usp=sharing

- 1) If you have specific metabolites for your experiment, you will need to fill this out with those metabolites. If you are looking generally at polar metabolites from HILIC, you can copy and paste from the template sheet the metabolites that you report from your assay (the sheet may not include all the polar metabolites, so you may need to add additional based on the metabolites you report).
- 2) Copy and paste the contents of the excel sheet in the box.
- 3) Choose View/check metabolite metadata.

mwTab Identifier: jrileyb_20241104_105910 Return to start

Analysis: HILIC UNSPECIFIED(1)

Metabolite metadata in tab-delimited format. First column must contain metabolite names.

Subsequent columns should contain KEGG,PubChem identifiers, retention index,quantitated m/z, etc.

First row must contain headings.

```
quantified m/z PubChem KEGG
                                                                 HMDB
metabolite_name retention time
                                                                          Compound Formula
                90.055 5950
                                 C00041 HMDB0000161
                                                         C3H7N02
alanine 9.02
Alpha.Ketoglutarate
                        10.57
                                 145.0143
                                                                          C5H605
arginine
                14.23
                        175.119 6322 (ARGININE) C00062 (ARGININE)
                                                                          HMDB0000517 (ARGININE) C6H14N402
aspartate
                9.93
                        132.0302
                                         5960
                                                 C00049
                                                         HMDB0000191
                                                                          C4H7N04
citrate 12.3
                191.0197
                                         C00158
                                                 HMDB0000094
                                                                  C6H807
creatinine
                4.86
                       114.0662
                                         588
                                                 C00791
                                                         HMDB0000562
                                                                          C4H7N30
cystine 10.41 fumarate
                                 67678
                241.0311
                                         C00491
                                                         HMDB0000192
                                                                          C6H12N2O4S2
                        115.0037
                10.74
                                         444972
                                                 C00122
                                                         HMDB0000134
                                                                          C4H404
glutamate
                9.78
                        146.0459
                                         33032
                                                 C00025
                                                         HMDB0000148
                                                                          C5H9N04
```

View/check metabolite metadata See examples of metabolite metadata layout

- 4) After clicking View/check metabolite metadata you should see something like the image below.
- 5) Choose Upload metabolite metadata.

Upload metabolite metadata

| metabolite_name | retention time | quantified m/z | PubChem | KEGG | НМОВ | Compound Formula |
|----------------------|-------------------|-------------------|--------------------|----------------------|---------------------------|---------------------|
| alanine | 9.02 | 90.055 | 5950 | C00041 | HMDB0000161 | C3H7NO2 |
| Alpha.Ketoglutarate | 10.57 | 145.0143 | | | | C5H6O5 |
| arginine | 14.23 | 175.119 | 6322 (ARGININE) | C00062 (ARGININE) | HMDB0000517 (ARGININE) | C6H14N4O2 |
| aspartate | 9.93 | 132.0302 | 5960 | C00049 | HMDB0000191 | C4H7NO4 |
| citrate | 12.3 | 191.0197 | 311 | C00158 | HMDB0000094 | C6H8O7 |
| creatinine | 4.86 | 114.0662 | 588 | C00791 | HMDB0000562 | C4H7N3O |
| cystine | 10.41 | 241.0311 | 67678 | C00491 | HMDB0000192 | C6H12N2O4S2 |
| fumarate | 10.74 | 115.0037 | 444972 | C00122 | HMDB0000134 | C4H4O4 |
| glutamate | 9.78 | 146.0459 | 33032 | C00025 | HMDB0000148 | C5H9NO4 |
| glycine | 9.84 | 76.0393 | 750 | C00037 | HMDB0000123 | C2H5NO2 |
| histidine | 8.94 | 156.0768 | 6274 | C00135 | HMDB0000177 | C6H9N3O2 |
| hypoxanthine | 5.5 | 137.0458 | 790 | C00262 | HMDB0000157 | C5H4N4O |
| INDOLE.3.ACETIC.ACID | 4.55 | 174.0561 | | | | C3H5O6P |
| isoleucine | 6.18 | 132.1019 | 6306 | C00407 | HMDB0000172 | C6H13NO2 |
| leucine | 5.58 | 132.1019 | 6106 | C00123 | HMDB0000687 | C6H13NO2 |
| lysine | 13.89 | 147.1128 | 5962 (LYSINE) | C00047 (LYSINE) | HMDB0000182 (LYSINE) | C6H14N2O2 |
| methionine | 6.32 | 150.0583 | 6137 | C00073 | HMDB0000696 | C5H11NO2S |
| niacinamide | 3.03 | 123.0553 | | | | C6H6N2O |
| palmitate | 1.85 | 255.233 | 985 | C00249 | HMDB0000220 | C16H32O2 |
| phenylalanine | 4.9 | 164.0717 | 6140 | C00079 | HMDB0000159 | C9H11NO2 |
| proline | 7.33 | 116.0706 | 145742 | C00148 | HMDB0000162 | C5H9NO2 |
| pyruvate | 4.2 | 87.0088 | 1060 | C00022 | HMDB0000243 | C3H4O3 |
| serine | 9.69 | 106.0499 | 5951 | C00065 | HMDB0000187 | C3H7NO3 |
| threonine | 8.81 | 120.0655 | 6288 | C00188 | HMDB0000167 | C4H9NO3 |
| THYMINE | 3.3 | 125.0357 | 1135 | C00178 | HMDB0000262 | C5H6N2O2 |
| tryptophan | 6.36 | 205.0972 | 9060 | C00525 | HMDB0013609 | C11H12N2O2 |
| tyrosine | 7.68 | 182.0812 | 6057 | C00082 | HMDB0000158 | C9H11NO3 |
| valine | 7.2 | 118.0863 | 6287 | C00183 | HMDB0000883 | C5H11NO2 |
| guanosine | 7.43 | 284.0989 | 6802 | C00387 | HMDB0000133 | C10H13N5O5 |

Summary of uploaded data sets

Please select an appropriate **Datatrack ID** from the table below to upload additional raw data files or select an appropriate **mwTab Filename** to edit metadata and results for already registered data.

| DataTrack ID (upload raw data) | Study ID | Date Submitted | Release date | Data Type | mwTab FileName (edit study) | Archive Filename | Data Review Status | Uploaded Files |
|--------------------------------|-------------|-------------------|-----------------|----------------|---|--|-----------------------|---|
| 5342 Upload | | 2024-11-04 | - | Target edMS | jrileyb_20241 104_105910_mw tab.txt Edit study | retinoids_mou se_plamsa_ser um_HILIC_XT4. zip | Response under review | HILIC_Plasma_Serum .zip (3.5G) |
| 5326 Upload | - | 2024-10-31 | - | Target edMS | jrileyb_20241 031_113710_mw tab.txt Edit study | retinoids_mou se_CSF_HILIC_ XT3.zip | Response under review | CSF_HILIC.zip (2.1G) |
| 5286 Upload | - | 2024-10-11 | - | Target edMS | jrileyb_20241 011_095004_mw tab.txt Edit study | retinoids_mou se_plamsa_ser um_XT2.zip | Response under review | C18_Serum_Plasma_R etinoids.zip (4.1G) |
| 5267 Upload | - | 2024-10-07 | 2027-01-01 | | jrileyb_20241 007_120309_mw tab.txt Edit study | retinoids_mou se_XT1.zip | Response under review | C18_CSF_retinoids. zip (3.2G) |

Showing results 1 to 4 of 4

Results per page: 10 V

STAGE 2:

ORGANIZING YOUR SUBMISSIONS

- You will create a new submission for every metabolomics experiment that you reference in your publication.
 - You can include two different columns as a part of one submission (for example: if you ran mouse plasma on both C18 to detect folates and HILIC to detect polar metabolites, this can be part of one submission).
 - Metabolomics Workbench prefers that you separate submissions based on tissue-type (for example: if you ran mouse plasma and mouse CSF on both C18 to detect folates and HILIC to detect polar metabolites, the mouse plasma would be one submission and the mouse CSF would be a separate submission).
- For multi-part studies (several experiments all belonging to the same project), you
 can indicate on the first page that it is a multi-part study. Despite what it says, you
 do not need to include in the comments "Study part m of n" unless you know.
 - Metabolomics Workbench reviewers will know something is a multi-part study if there are several submissions with identical Project Titles and Project Summaries.
- Submissions that are all a part of one project should have identical Project Titles and Project Summaries.
 - The Project Title and Project Summary are more generic and describe overarching goals and results, while the Study Title and Study Summary are more detailed. The Study Summary should clearly highlight the differences/how the study is unique and is included within the project.

NEW SUBMISSION

Steps

- 1) Create account and login
- 2) Go to New Submission tab and fill out the information (see below)
 - a. Name of raw data file(s) to be uploaded: give your project a name (for example: retinoids_mouse_CSF_HILIC.zip)
 - b. Data type being submitted: choose among MS, Targeted MS, Untargeted MS, Targeted and untargeted MS (for Kanarek Lab projects, for the most part it will be Targeted MS)
 - c. Protocol/methods filename(s): protocol.docx
 - d. MS/NMR instrument manufacturer: Thermo
 - e. MS/NMR instrument model: Q Exactive Orbitrap
 - f. Binary data format: .RAW
 - g. Open source text formats: mzML
 - h. MS level in raw data (if MS data): choose MS2 only if applicable
 - i. Multi-part study: choose Yes or No
 - j. Samples analyzed by Metabolon: No
 - k. Embargo: choose Yes or No (generally yes if the paper has not been published yet)
 - l. Embargo until: provide date in the future

3) Submit

| Overview New Submission | List your submissions Test FTP Upload Tutorials |
|---|--|
| | |
| NOTE: Please do not use multiple tabs | or browsers to do multiple simultaneous uploads. |
| Please tell us about the data you plan to | upload. (* = required) |
| * mwTab file name | jrileyb_20250102_102526_mwtab.txt (Automatically assigned name) |
| * Name of raw data file(s) to be uploaded | (e.g. MyData.zip, MyData.7z) |
| * Data type being submitted | (Use separate submissions for studies containing both MS and NMR data) |
| * Protocol/methods filename(s) | |
| | |
| * MS/NMR instrument manufacturer | |
| * MS/NMR instrument model | |
| * Binary data format | (e.gWIFF (ABI/Sciex), .RAW (Thermo) or .d (Agilent)) |
| * Open source text formats | (e.g. mzML, mzXML, CDF) |
| MS level in raw data (if MS data) | ✓ (Specify the MS acqusition level in raw data files) |
| * Multi-part study | (For multi-part studies, add additional information such as "Study part m of n" in comments field) |
| Samples analyzed by Metabolon | (For studies analyzed by Metabolon, you must use the Metabolon template during submission) |
| * Embargo | (If Yes, then please specify date below) |
| Embargo until | (e.g. 1 year, 6 months, or YYYY-MM-DD) |
| HHEAR/CHEAR study | ☐ (For NIH's HHEAR/CHEAR & program only, Add any additional information in comments field) |
| HHEAR/CHEAR project ID | (Required for HHEAR/CHEAR program only) |
| | |
| NIH funding source | ✓ (For NIH programs only) |
| NIH Common Fund component | (For NIH programs only) |
| Comments | |
| | |
| | |
| Submit Reset | |

UPLOAD AND MANAGE EXPERIMENTAL DATA AND METADATA

Steps

- 1) Choose New online study submission.
- 2) You will see a page that asks whether you want to start a new online study submission or use another study as a template, choose *Start a new online study submission*.
 - a. After creating your first experiment submission, it will appear as an option to use as a template in future submissions, which may be helpful for creating additional submissions that are part of the same project. If it is the first submission for the project, choose *Start a new online study submission*.

Upload and Manage Experimental Data and Metadata

| Overview New Submission List your submissions Test FTP Upload Tutorials |
|---|
| Please click New online study submission button to start a new study submission and enter metadata and results for your study with DataTrack ID 5504 and mwTab file name jrileyb_20250103_135859 . You will be prompted to upload an archive file after successful completion of the online submission process. New online study submission |
| UCSD Metabolomics Workbench, a resource sponsored by the Common Fund of the National Institutes of Health Terms of use Site map Contact NMDR Personnel |
| UC San Diego |

PROJECT METADATA

- 1) Fill out all fields highlighted in red.
 - a. Project Title: may want to use your paper title (this will be identical for all submissions for this project)
 - b. Project Summary: may want to use your paper abstract (this will be identical for all submissions for this project)
- 2) BCH Address: 61 Binney St Boston, MA 02115
- 3) Choose Add project metadata.

Start/Edit Data Submission | Examples of study design and data layouts | Online Study Submission Tutorial(pdf)

mwTab identifier: jrileyb_20250103_135859

Jump to: Study Subject Study Design Collection Treatment SamplePrep MS/NMR Data Finalize

| project information | Add project metadata Reset |
|----------------------|---|
| Project Title: | |
| Project Type: | |
| Project Summary: | |
| Institute: | Boston Children's Hospital |
| Department: | |
| Laboratory: | |
| Last Name: | Brook |
| First Name: | Jeannette |
| Address: | 61 Binney St, Boston, MA, 02115, USA |
| Email: | jeannette.brook@childrens.harvard.edu |
| Phone: | |
| Funding Source: | |
| Project Comments: | |
| Publications: | |
| contributors: | |
| project information | Add project metadata Reset |
| Display all proto | ocol/methods files uploaded in previous submissions |

STUDY METADATA

- 1) Fill out all fields highlighted in red.
 - a. Subject Type: choose an option from the drop-down menu
 - b. Study Title: should be more specific to the specific experiment/submission
 - c. Study Summary: should be more specific to the specific experiment/submission
- 2) BCH Address: 61 Binney St Boston, MA 02115
- 3) Choose Add study metadata.

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mwTab Identifier: jrileyb_20250103_135859 Return to start

Jump to: Project Study Subject Study Design Collection Treatment SamplePrep MS/NMR Data Finalize

| study information | Add study metadata Reset |
|-------------------------|---|
| Subject Type: | Mammalian subjects → This choice dictates which context-specific metadata items appear in subsequent sections |
| Study Title: | |
| Study Type: | |
| Study Summary: | |
| Institute: | Boston Children's Hospital |
| Department: | |
| Laboratory: | |
| Last Name: | Brook |
| First Name: | Jeannette |
| Address: | 61 Binney St, Boston, MA 02115, USA |
| Email: | jeannette.brook@childrens.harvard.edu |
| Phone: | 3035493341 |
| Number of Groups: | |
| Total Subjects: | |
| Number of Males: | |
| Number of Females: | |
| Study Comments: | |
| Publications: | |
| chear_study: | |
| analysis_type_detail: | |
| study information | Add study metadata Reset |
| Display all protocol/me | thods files uploaded in previous submissions |

SUBJECT METADATA

- 1) Fill out all fields highlighted in red.
 - a. Subject Species: choose option from drop-down menu
- 2) Choose Add subject metadata.

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mwTab Identifier: jrileyb_20250103_135859 Return to start Jump to: Project Study Subject Study Design Collection Treatment SamplePrep MS/NMR Data Finalize subject information Add subject metadata Reset Subject Type: Mammal (entered in Study page) Subject Species: Mouse (Mus musculus) Taxonomy ID: 10090 Genotype/Bacterial Strain: Age or Age Range: Weight or Weight Range: Height or Height Range: Animal Animal Supplier: Animal Housing: Animal Light Cycle: Animal Feed: Animal Water: Animal Inclusion Criteria: Species Group: subject information Add subject metadata Reset Display all protocol/methods files uploaded in previous submissions

STUDY DESIGN

See How To Create Metabolomics Workbench Excel Files document.