

lesSDRF

Welcome to an overview of lesSDRF – a user-centric tool designed to streamline the creation of SDRF files.

Throughout this manual, we'll delve into its features, functionalities and how it simplifies the complex task of proteomics metadata annotation.

You can access the tool via: <https://lessdrf.streamlit.app/>

Home: Select SDRF template and input the raw file names

The home screen invites users to select an SDRF template, which is derived from the original SDRF initiative and is species-specific. By choosing this template, users can be assured that they will include the required columns for a valid SDRF.

Furthermore, the home screen offers an option to upload an intermediate SDRF file. This feature enables users to pause their annotation process and resume at a later time. Since it's a browser-based tool, the SDRF file isn't saved upon closing the browser. This capability also streamlines the annotation process for similar projects.

- Home
- 1. Mapping local metadata
- 2. Labeling
- 3. Required columns
- 4. Additional columns
- 5. Experiment types

 Data was loaded

Welcome to lesSDRF

The SDRF annotation tool, because spending less time on SDRF creates more time for amazing research

The Sample and Data Relationship Format (SDRF) is a crucial tool for maximizing the potential impact of your data. By making metadata available and machine-readable, other researchers can study your data more easily.

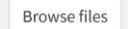
This tool will help you to annotate your data with the correct metadata in several steps for a maximum of 250 samples. First, on this homepage, you will need to select a default SDRF file based on the species of your sample and provide the raw file names. Then you can follow the steps in the sidebar.

- Step 1: If you have a local metadata file, you can upload it to map to the SDRF file
- Step 2: Provide information on potential labels in your sample
- Step 3: Fill in the columns that are required for a valid SDRF
- Step 4: Fill in columns with additional information to further optimise your SDRF file
- Step 5: For atypical experiment types, you can check community suggested columns

You are able to download the intermediate file at any given timepoint, so you can come back to the other steps whenever is suitable for you.

If this is the case right now, please upload your intermediate SDRF file here:

Upload intermediate SDRF file 

Drag and drop file here 
Limit 1GB per file • TSV 

In need of some inspiration? Download this example SDRF file to get an idea of the required output

[Download example SDRF](#)

Start here with a completely new SDRF file

Select a species for the SDRF template which will contain the basic columns to fill in for this specific species. If your species is not in the drop down list, you can always use the default template. 



You are able to download the intermediate file at any given timepoint, so you can come back to the other steps whenever is suitable for you.

If this is the case right now, please upload your intermediate SDRF file here:

Upload intermediate SDRF file

?



Drag and drop file here

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Browse files

Home

1. Mapping local metadata
2. Labeling
3. Required columns
4. Additional columns
5. Experiment types

Press to download SDRF file

In need of some inspiration? Download this example SDRF file to get an idea of the required output

Download example SDRF

Start here with a completely new SDRF file

Select a species for the SDRF template which will contain the basic columns to fill in for this specific species. If your species is not in the drop down list, you can always use the default [?](#)

human

input raw file names as a comma or tab separated list [?](#)

Prosser_1004.raw Prosser_1085.raw Prosser_1086.raw Prosser_1119.raw Prosser_1136.raw Prosser_1146.raw Prosser_1195.raw Prosser_1198.raw Prosser_1200.raw

Added filenames: ['Prosser_1004.raw', 'Prosser_1085.raw', 'Prosser_1086.raw', 'Prosser_1119.raw', 'Prosser_1136.raw', 'Prosser_1146.raw', 'Prosser_1195.raw', 'Prosser_1198.raw', 'Prosser_1200.raw', 'Prosser_1205.raw', 'Prosser_1209.raw', 'Prosser_1228.raw', 'Prosser_1273.raw', 'Prosser_1288.raw', 'Prosser_1290.raw', 'Prosser_1304.raw', 'Prosser_1311.raw', 'Prosser_1320.raw', 'Prosser_1325.raw', 'Prosser_1339.raw', 'Prosser_1356.raw', 'Prosser_1366.raw', 'Prosser_1375.raw', 'Prosser_1379.raw', 'Prosser_1383.raw', 'Prosser_1425.raw', 'Prosser_1427.raw', 'Prosser_1462.raw', 'Prosser_1467.raw', 'Prosser_1472.raw', 'Prosser_1510.raw', 'Prosser_1535.raw', 'Prosser_1602.raw', 'Prosser_1605.raw']

	licate]	technology type	assay name	comment[technical replicate]	comment[data file]	comment[fraction identifier]	comment[label]	comment[instrument]	comment
0		None	None	None	Prosser_1004.raw	None	None	None	None
1		None	None	None	Prosser_1085.raw	None	None	None	None
2		None	None	None	Prosser_1086.raw	None	None	None	None
3		None	None	None	Prosser_1119.raw	None	None	None	None
4		None	None	None	Prosser_1136.raw	None	None	None	None
5		None	None	None	Prosser_1146.raw	None	None	None	None
6		None	None	None	Prosser_1195.raw	None	None	None	None
7		None	None	None	Prosser_1198.raw	None	None	None	None
8		None	None	None	Prosser_1200.raw	None	None	None	None
9		None	None	None	Prosser_1205.raw	None	None	None	None



Step 1: Map local metadata file to SDRF columns

Recognizing that users frequently have some local metadata gathered during their experiments, the initial step in lesSDRF facilitates the uploading and mapping of this local metadata to the SDRF columns established on the Home screen. Once mapped, the system verifies the local metadata for ontology compatibility.



Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

[Press to download SDRF file](#)

1. Map local metadata to SDRF

If you have a local metadata file available, you can use this file to map the data to the required SDRF information.

Important: you can upload the file in csv, tsv or xlsx format.

The order of your raw file names should match the order in which you inputted them in the previous step

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry category]	characteristics[age]	characteristic
0	None	None	None	None	None	None	None
1	None	None	None	None	None	None	None
2	None	None	None	None	None	None	None
3	None	None	None	None	None	None	None
4	None	None	None	None	None	None	None
5	None	None	None	None	None	None	None
6	None	None	None	None	None	None	None
7	None	None	None	None	None	None	None
8	None	None	None	None	None	None	None
9	None	None	None	None	None	None	None

Upload your local metadata file (.csv, .tsv or .xls)



Drag and drop file here

Limit 1GB per file • CSV, TSV, XLSX

[Browse files](#)

local_metadata.xlsx 9.6KB



Your metadata file:

	source name	Organism	part	sample
0	Sample 1	Homo sapiens	heart LV	Prosser_1004.raw
1	Sample 2	Homo sapiens	heart LV	Prosser_1085.raw
2	Sample 3	Homo sapiens	heart LV	Prosser_1086.raw
3	Sample 4	Homo sapiens	heart LV	Prosser_1119.raw
4	Sample 5	Homo sapiens	heart LV	Prosser_1136.raw
5	Sample 6	Homo sapiens	heart LV	Prosser_1146.raw
6	Sample 7	Homo sapiens	heart LV	Prosser_1195.raw
7	Sample 8	Homo sapiens	heart LV	Prosser_1198.raw
8	Sample 9	Homo sapiens	heart LV	Prosser_1200.raw
9	Sample 10	Homo sapiens	heart LV	Prosser_1205.raw



9	None						
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Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

Press to download SDRF file

Upload your local metadata file (.csv, .tsv or .xls)



Drag and drop file here

Limit 1GB per file • CSV, TSV, XLSX

Browse files



local_metadata.xlsx 9.6KB



Your metadata file:

	source name	Organism	part	sample
0	Sample 1	Homo sapiens	heart LV	Prosser_1004.raw
1	Sample 2	Homo sapiens	heart LV	Prosser_1085.raw
2	Sample 3	Homo sapiens	heart LV	Prosser_1086.raw
3	Sample 4	Homo sapiens	heart LV	Prosser_1119.raw
4	Sample 5	Homo sapiens	heart LV	Prosser_1136.raw
5	Sample 6	Homo sapiens	heart LV	Prosser_1146.raw
6	Sample 7	Homo sapiens	heart LV	Prosser_1195.raw
7	Sample 8	Homo sapiens	heart LV	Prosser_1198.raw
8	Sample 9	Homo sapiens	heart LV	Prosser_1200.raw
9	Sample 10	Homo sapiens	heart LV	Prosser_1205.raw

Select columns containing data that will be used in the SDRF data

 Ready to match?source name XOrganism Xpart XSelect column 1 to match in your metadata file:
Select column 2 to match in your metadata file:
Select column 3 to match in your metadata file:

9 | None | None

Upload your local metadata file (.csv, .tsv or .xlsx)

Drag and drop file here
Limit 1GB per file • CSV, TSV, XLSX

Browse files

local_metadata.xlsx 9.6KB

X

Your metadata file:

	source name	Organism	part	sample
0	Sample 1	Homo sapiens	heart LV	Prosser_1004.raw
1	Sample 2	Homo sapiens	heart LV	Prosser_1085.raw
2	Sample 3	Homo sapiens	heart LV	Prosser_1086.raw
3	Sample 4	Homo sapiens	heart LV	Prosser_1119.raw
4	Sample 5	Homo sapiens	heart LV	Prosser_1136.raw
5	Sample 6	Homo sapiens	heart LV	Prosser_1146.raw
6	Sample 7	Homo sapiens	heart LV	Prosser_1195.raw
7	Sample 8	Homo sapiens	heart LV	Prosser_1198.raw
8	Sample 9	Homo sapiens	heart LV	Prosser_1200.raw
9	Sample 10	Homo sapiens	heart LV	Prosser_1205.raw

Press to download SDRF file

Select columns containing data that will be used in the SDRF data

source name x Organism x part x

Ready to match?

Select column 1 to match in your metadata file:
source name

Select column 2 to match in your metadata file:
Organism

Select column 3 to match in your metadata file:
part

Select the corresponding column from the SDRF file:
source name

characteristics[organism]

characteristics[disease]

characteristics[individual]

characteristics[organism part]

characteristics[organism]

characteristics[sex]

characteristics[enrichment pro...]

characteristics[compound]

characteristics[concentration]

Match and check ontology

Match and check ontology

Match and check ontology

Great! The local metadata values are valid terms and are mapped to the SDRF file.

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Browse files

X

Upload your local metadata file (.csv, .tsv or .xls)



Drag and drop file here

Limit 1GB per file • CSV, TSV, XLSX



local_metadata.xlsx 9.6KB

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

Press to download SDRF file

Your metadata file:

	source name	Organism	part	sample
0	Sample 1	Homo sapiens	heart LV	Prosser_1004.raw
1	Sample 2	Homo sapiens	heart LV	Prosser_1085.raw
2	Sample 3	Homo sapiens	heart LV	Prosser_1086.raw
3	Sample 4	Homo sapiens	heart LV	Prosser_1119.raw
4	Sample 5	Homo sapiens	heart LV	Prosser_1136.raw
5	Sample 6	Homo sapiens	heart LV	Prosser_1146.raw
6	Sample 7	Homo sapiens	heart LV	Prosser_1195.raw
7	Sample 8	Homo sapiens	heart LV	Prosser_1198.raw
8	Sample 9	Homo sapiens	heart LV	Prosser_1200.raw
9	Sample 10	Homo sapiens	heart LV	Prosser_1205.raw

Select columns containing data that will be used in the SDRF data

source name x Organism x part x

 Ready to match?

Select column 1 to match in your metadata file:

source name

Select the corresponding column from the SDRF file:

source name

 Match and check ontology

Select column 2 to match in your metadata file:

Organism

Select the corresponding column from the SDRF file:

characteristics[organism]

 Match and check ontology

Select column 3 to match in your metadata file:

part

Select the corresponding column from the SDRF file:

characteristics[organism part]

 Match and check ontology

Great! The local metadata values are valid terms and are mapped to the SDRF file.

Great! The local metadata values are valid terms and are mapped to the SDRF file.

✗ {'heart LV'} are not ontology terms. Select the correct terms in the next steps directly from the ontology



Step 2: Select labeling approach

Labeling is an essential component of metadata. In this section, we'll illustrate both a label-free method and a TMT-labeled experiment using the same dataset to showcase the differential impact on the SDRF file structure.

When the label-free option is chosen, it's simply appended to the "comment[label]" column. In contrast, when a labeling method like TMT is selected, users must map each raw file to the appropriate label. Given that a single file can encompass multiple labels, this necessitates the generation of a new row in the SDRF file for each distinct file-label pairing.

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

Press to download SDRF file

2. Labeling

If a raw file contains multiple labels, every label will need to be annotated on a different row. Here you can map label information to your raw files. As a result, the raw file information will be duplicated with the correct label filled in

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry category]	characteristics[age]	characteristic
0	Sample 1	Homo sapiens	None	None	None	None	None
1	Sample 2	Homo sapiens	None	None	None	None	None
2	Sample 3	Homo sapiens	None	None	None	None	None
3	Sample 4	Homo sapiens	None	None	None	None	None
4	Sample 5	Homo sapiens	None	None	None	None	None
5	Sample 6	Homo sapiens	None	None	None	None	None
6	Sample 7	Homo sapiens	None	None	None	None	None
7	Sample 8	Homo sapiens	None	None	None	None	None
8	Sample 9	Homo sapiens	None	None	None	None	None
9	Sample 10	Homo sapiens	None	None	None	None	None

Input the label that was used in your experiment. If no label was added, indicate this using *label free sample*.

Select your matching ontology term using this autocomplete function

Or follow the ontology based drop down menu below

- label free sample
- > TMT
- > iTRAQ
- > SILAC
- > ICAT
- > metabolic label
- > Stable isotope dimethyl labeling

Match the filenames to the labels you selected above. Select ALL if the label is found in all raw files.

Ready?



Label free experiment

- Home
 - 1. Mapping local metadata
 - 2. Labeling**
 - 3. Required columns
 - 4. Additional columns
 - 5. Experiment types
- Press to download SDRF file**

2. Labeling

If a raw file contains multiple labels, every label will need to be annotated on a different row. Here you can map label information to your raw files. As a result, the raw file information will be duplicated with the correct label filled in

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry category]	characteristics[age]	characteristic
0	Sample 1	Homo sapiens	None	None	None	None	None
1	Sample 2	Homo sapiens	None	None	None	None	None
2	Sample 3	Homo sapiens	None	None	None	None	None
3	Sample 4	Homo sapiens	None	None	None	None	None
4	Sample 5	Homo sapiens	None	None	None	None	None
5	Sample 6	Homo sapiens	None	None	None	None	None
6	Sample 7	Homo sapiens	None	None	None	None	None
7	Sample 8	Homo sapiens	None	None	None	None	None
8	Sample 9	Homo sapiens	None	None	None	None	None
9	Sample 10	Homo sapiens	None	None	None	None	None

Input the label that was used in your experiment. If no label was added, indicate this using *label free sample*.

Select your matching ontology term using this autocomplete function

Choose an option

Or follow the ontology based drop down menu below

- label free sample
- TMT
- iTRAQ
- SILAC

ALL

Prosser_1004.raw

Prosser_1085.raw

Prosser_1086.raw

Prosser_1119.raw

Prosser_1136.raw

Prosser_1146.raw

Prosser_1195.raw

Choose an option

Ready?



	Sample ID	Homo sapiens	None	None	None	None	None	None
9	Sample 10	Homo sapiens	None	None	None	None	None	None

Input the label that was used in your experiment. If no label was added, indicate this using *label free sample*.

Select your matching ontology term using this autocomplete function

Or follow the ontology based drop down menu below

Choose an option

- label free sample
- TMT
- iTRAQ
- SILAC
- ICAT
- metabolic label
- Stable isotope dimethyl labeling

[Submit selection](#)

Match the filenames to the labels you selected above. Select ALL if the label is found in all raw files.

Select files labeled with label free sample.

ALL X

Ready?

SDRF file with label information

	ics[biological replicate]	technology type	assay name	comment[technical replicate]	comment[data file]	comment[fraction identifier]	comment[label]	comment[in]
0		None	None	None	Prosser_1004.raw	None	label free sample	None
1		None	None	None	Prosser_1085.raw	None	label free sample	None
2		None	None	None	Prosser_1086.raw	None	label free sample	None
3		None	None	None	Prosser_1119.raw	None	label free sample	None
4		None	None	None	Prosser_1136.raw	None	label free sample	None
5		None	None	None	Prosser_1146.raw	None	label free sample	None
6		None	None	None	Prosser_1195.raw	None	label free sample	None
7		None	None	None	Prosser_1198.raw	None	label free sample	None
8		None	None	None	Prosser_1200.raw	None	label free sample	None
9		None	None	None	Prosser_1205.raw	None	label free sample	None



Labeled experiment

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

Press to download SDRF file

	Sample ID	Species	None	None	None	None	None
1	Sample 11	Homo sapiens	None	None	None	None	None
2	Sample 12	Homo sapiens	None	None	None	None	None
3	Sample 14	Homo sapiens	None	None	None	None	None
4	Sample 18	Homo sapiens	None	None	None	None	None
5	Sample 24	Homo sapiens	None	None	None	None	None
6	Sample 26	Homo sapiens	None	None	None	None	None
7	Sample 28	Homo sapiens	None	None	None	None	None
8	Sample 31	Homo sapiens	None	None	None	None	None
9	Sample 33	Homo sapiens	None	None	None	None	None

Input the label that was used in your experiment. If no label was added, indicate this using *label free sample*.

Select your matching ontology term using this autocomplete function

Choose an option

Or follow the ontology based drop down menu below

label free sample

- TMT
 - TMT126
 - TMT127
 - TMT127C
 - TMT127N
 - TMT128
 - TMT128C
 - TMT128N
 - TMT129

- TMT129C
- TMT129N
- TMT130
- TMT130C
- TMT130N
- TMT131
- TMT131N
- TMT131C
- TMT132N
- TMT132C
- TMT133N
- TMT133C
- TMT134N

- > ITRAQ
- > SILAC
- > ICAT
- > metabolic label
- > Stable isotope dimethyl labeling

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

Press to download SDRF file

Submit selection

Match the filenames to the labels you selected above. Select ALL if the label is found in all raw files.

Select files labeled with TMT126.

Prosser_1205.raw x

Select files labeled with TMT127.

Prosser_1205.raw x

Select files labeled with TMT128.

Prosser_1205.raw x

Ready?

SDRF file with label information

characteristics[individual]	assay name	technology type	comment[data file]	comment[label]	comment[technical replicate]	comment[fraction i]
0 205	run 10	proteomic profiling by mass spectrometry	Prosser_1205.raw	TMT126	1	
1 205	run 10	proteomic profiling by mass spectrometry	Prosser_1205.raw	TMT127	1	
2 205	run 10	proteomic profiling by mass spectrometry	Prosser_1205.raw	TMT128	1	

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Step 3: Input required columns

Based on the SDRF template selected on the Home screen, users are provided with a list of required columns. Filling out these columns is crucial to generate a valid SDRF file.

Many columns require inputs that adhere to precise SDRF guidelines and formatting. To simplify this for users and to minimize errors, lesSDRF has integrated these requirements directly within the tool. This eliminates the need for users to sift through the extensive SDRF documentation. Additionally, the corresponding ontologies are embedded within lesSDRF, offering an easy navigation experience.

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are empty and required (?)

- start
- characteristics[organism part]
- characteristics[cell type]
- characteristics[ancestry category]
- characteristics[age]
- characteristics[sex]
- characteristics[disease]
- characteristics[individual]
- characteristics[biological replicate]
- technology type
- assay name
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[fragment mass tolerance]
- comment[precursor mass tolerance]
- undo column

Press to download SDRF file

3. Required columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry category]	characteristics[age]	characteristics[sex]
0	Sample 1	Homo sapiens	None	None	None	None	None
1	Sample 2	Homo sapiens	None	None	None	None	None
2	Sample 3	Homo sapiens	None	None	None	None	None
3	Sample 4	Homo sapiens	None	None	None	None	None
4	Sample 5	Homo sapiens	None	None	None	None	None
5	Sample 6	Homo sapiens	None	None	None	None	None
6	Sample 7	Homo sapiens	None	None	None	None	None
7	Sample 8	Homo sapiens	None	None	None	None	None
8	Sample 9	Homo sapiens	None	None	None	None	None
9	Sample 10	Homo sapiens	None	None	None	None	None

In the sidebar, all the empty columns that are required for your SDRF file are listed. Select the one you want to annotate first.

When a column is filled in, it will disappear from the sidebar so you can keep track on which columns still require input.

When you want to reannotate a previously filled in column, you can do so by clicking on the **undo column** button in the sidebar.

Every page will start with your current SDRF file and at the bottom of the page there is a button to download the intermediate SDRF file

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are
empty and required start characteristics[organism part] characteristics[cell type] characteristics[ancestry category] characteristics[age] characteristics[sex] characteristics[disease] characteristics[individual] characteristics[biological replicate] technology type assay name comment[technical replicate] comment[fraction identifier] comment[instrument] comment[cleavage agent details] comment[modification parameters] comment[fragment mass tolerance] comment[precursor mass tolerance] undo column

Press to download SDRF file

3. Required columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry category]	characteristics[age]	characteristic
0	Sample 1	Homo sapiens	None	None	None	None	None
1	Sample 2	Homo sapiens	None	None	None	None	None
2	Sample 3	Homo sapiens	None	None	None	None	None
3	Sample 4	Homo sapiens	None	None	None	None	None
4	Sample 5	Homo sapiens	None	None	None	None	None
5	Sample 6	Homo sapiens	None	None	None	None	None
6	Sample 7	Homo sapiens	None	None	None	None	None
7	Sample 8	Homo sapiens	None	None	None	None	None
8	Sample 9	Homo sapiens	None	None	None	None	None
9	Sample 10	Homo sapiens	None	None	None	None	None

Select the part of the organism that is present in your sample

Are there multiple characteristics[organism part] in your data?

 No Yes

Select your matching ontology term using this autocomplete function

- heart left ventricle
- heart right ventricle
- endothelial cell of respiratory system lymphatic vessel
- hepatopancreatic ampulla

If all cells are correctly filled in click twice on the update button

Or follow the ontology based drop down menu below

- anatomical entity
- anatomy basic component
- Not available

Update

source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry cat...]	characteristics
Sample 1	Homo sapiens	empty	empty	empty	empty
Sample 2	Homo sapiens	empty	empty	empty	empty
Sample 3	Homo sapiens	empty	empty	empty	empty
Sample 4	Homo sapiens	empty	empty	empty	empty
Sample 5	Homo sapiens	empty	empty	empty	empty
Sample 6	Homo sapiens	empty	empty	empty	empty
Sample 7	Homo sapiens	empty	empty	empty	empty



[Home](#)[1. Mapping local metadata](#)[2. Labeling](#)[3. Required columns](#)[4. Additional columns](#)[5. Experiment types](#)

The following columns are empty and required

- start
- characteristics[cell type]
- characteristics[ancestry category]
- characteristics[age]
- characteristics[sex]
- characteristics[disease]
- characteristics[individual]
- characteristics[biological replicate]
- technology type
- assay name
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[fragment mass tolerance]
- comment[precursor mass tolerance]
- undo column

[Press to download SDRF file](#)

3. Required columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry category]	characteristics[age]	characteristics[sex]
0	Sample 1	Homo sapiens	heart left ventricle	None	None	None	None
1	Sample 2	Homo sapiens	heart left ventricle	None	None	None	None
2	Sample 3	Homo sapiens	heart left ventricle	None	None	None	None
3	Sample 4	Homo sapiens	heart left ventricle	None	None	None	None
4	Sample 5	Homo sapiens	heart left ventricle	None	None	None	None
5	Sample 6	Homo sapiens	heart left ventricle	None	None	None	None
6	Sample 7	Homo sapiens	heart left ventricle	None	None	None	None
7	Sample 8	Homo sapiens	heart left ventricle	None	None	None	None
8	Sample 9	Homo sapiens	heart left ventricle	None	None	None	None
9	Sample 10	Homo sapiens	heart left ventricle	None	None	None	None

In the sidebar, all the empty columns that are required for your SDRF file are listed. Select the one you want to annotate first.

When a column is filled in, it will disappear from the sidebar so you can keep track on which columns still require input.

When you want to reannotate a previously filled in column, you can do so by clicking on the **undo column** button in the sidebar.

Every page will start with your current SDRF file and at the bottom of the page there is a button to download the intermediate SDRF file



4	Sample 5	Homo sapiens	heart left ventricle	cardiocyte	Not available	None	F
5	Sample 6	Homo sapiens	heart left ventricle	cardiocyte	Not available	None	F
6	Sample 7	Homo sapiens	heart left ventricle	cardiocyte	Not available	None	F
7	Sample 8	Homo sapiens	heart left ventricle	cardiocyte	Not available	None	M
8	Sample 9	Homo sapiens	heart left ventricle	cardiocyte	Not available	None	M
9	Sample 10	Homo sapiens	heart left ventricle	cardiocyte	Not available	None	M

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are empty and required

- start
- characteristics[age]
- characteristics[disease]
- characteristics[individual]
- characteristics[biological replicate]
- technology type
- assay name
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[fragment mass tolerance]
- comment[precursor mass tolerance]
- undo column

Press to download SDRF file

If you have healthy and control samples, indicate healthy samples using *normal*. Input the disease for the other samples using the ontology

Are there multiple characteristics[disease] in your data?

No

Yes

How many different characteristics[disease] are in your data?

4

- +

Select your matching ontology term using this autocomplete function

Or follow the ontology based drop down menu below

- > disease
- normal
- Not available
- Not applicable

Submit selection

If all cells are correctly filled in click twice on the update button

Update

source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry cat...]	characteristics
Sample 1	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 2	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 3	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 4	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 5	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 6	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 7	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 8	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 9	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 10	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 11	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 12	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 13	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 14	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 15	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 16	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 17	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty
Sample 18	Homo sapiens	heart left ventricle	cardiocyte	Not available	empty



Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are empty and required [?](#)

- start
- characteristics[age]
- characteristics[disease]
- characteristics[individual]
- characteristics[biological replicate]
- technology type
- assay name
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[fragment mass tolerance]
- comment[precursor mass tolerance]
- undo column

Press to download SDRF file

disease for the other samples using the ontology

Are there multiple characteristics[disease] in your data?

No

Yes

How many different characteristics[disease] are in your data?

4

-

+

Select your matching ontology term using this autocomplete function

Choose an option

Submit selection

Or follow the ontology based drop down menu below

- > disease
- normal
- Not available
- Not applicable

If all cells are correctly filled in click twice on the update button

Update

source name	characteristics[sex]	characteristics[disease]	characteristics[individual]	characteristics[biological re...	technology ty...
Sample 1	M	normal	empty	empty	empty
Sample 2	F	normal	empty	empty	empty
Sample 3	M	hypertrophic cardiomyopathy	empty	empty	empty
Sample 4	F	dilated cardiomyopathy	empty	empty	empty
Sample 5	F	ischemic cardiomyopathy	empty	empty	empty
Sample 6	F	normal	empty	empty	empty
Sample 7	F	normal	empty	empty	empty
Sample 8	M	normal	empty	empty	empty
Sample 9	M	normal	empty	empty	empty
Sample 10	M	normal	empty	empty	empty
Sample 11	F	normal	empty	empty	empty
Sample 12	M	normal	empty	empty	empty
Sample 13	M	normal	empty	empty	empty
Sample 14	F	normal	empty	empty	empty
Sample 15	M	normal	empty	empty	empty
Sample 16	F	normal	empty	empty	empty

2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available
6	Sample 26	Homo sapiens	heart left ventricle	40Y	adult	M	not available
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are
empty and required

- start
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[precursor mass tolerance]
- comment[fragment mass tolerance]
- undo column

Press to download SDRF file

Input the instrument that was used in your experiment

Are there multiple comment[instrument] in your data?

- No
- Yes

Select your matching ontology term using this autocomplete function

Choose an option

Or follow the ontology based drop down menu below

- > SCIEX instrument model
- > Bruker Daltonics instrument model
- > Shimadzu instrument model
- > Waters instrument model
- ✓ Thermo Fisher Scientific instrument model
 - > Thermo Finnigan instrument model
 - Thermo Electron instrument model
 - > Finnigan MAT instrument model
 - > Thermo Scientific instrument model
 - LTQ
 - LTQ FT
 - LTQ Orbitrap
 - LXQ
 - LTQ Orbitrap Discovery
 - LTQ Orbitrap XL
 - LTQ FT Ultra
 - Surveyor PDA
 - Accela PDA
 - ITQ 700
 - ITQ 900
 - ITQ 1100
 - LTQ XL ETD
 - LTQ Orbitrap XL ETD
 - DFS
 - DSQ II
 - MALDI LTQ XL



Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are
empty and required

- start
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[precursor mass tolerance]
- comment[fragment mass tolerance]
- undo column

[Press to download SDRF file](#)
[Submit selection](#)
[Update](#)

source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmen...]	characteristics
Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M

- LTQ Velos
- LTQ Velos ETD
- TSQ Vantage
- LTQ Orbitrap Velos
- ISQ
- Velos Plus
- LTQ Orbitrap Elite
- Q Exactive
- Orbitrap Fusion
- Orbitrap Fusion ETD
- TSQ Quantiva
- TSQ Endura
- Q Exactive HF
- TSQ 8000 Evo
- Exactive Plus
- Q Exactive Plus
- Orbitrap Fusion Lumos
- LTQ Orbitrap Classic
- TSQ Altis
- TSQ Quantis
- TSQ 9000
- Q Exactive HF-X
- Orbitrap Exploris 480
- Orbitrap Eclipse
- Orbitrap Exploris 240
- Orbitrap Exploris 120
- LTQ Orbitrap Velos Pro
- Orbitrap ID-X
- Q Exactive UHMR
- TSQ Altis Plus
- Hitachi instrument model
- Varian instrument model
- Agilent instrument model
- Dionex instrument model
- Applied Biosystems instrument model
- LECO instrument model



source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[category]	characteristics[age]	characteristics[sex]
3 Sample 4	Homo sapiens	heart left ventricle	None	None	None	None
4 Sample 5	Homo sapiens	heart left ventricle	None	None	None	None
5 Sample 6	Homo sapiens	heart left ventricle	None	None	None	None
6 Sample 7	Homo sapiens	heart left ventricle	None	None	None	None
7 Sample 8	Homo sapiens	heart left ventricle	None	None	None	None
8 Sample 9	Homo sapiens	heart left ventricle	None	None	None	None
9 Sample 10	Homo sapiens	heart left ventricle	None	None	None	None
10 Sample 11	Homo sapiens	heart left ventricle	None	None	None	None
11 Sample 12	Homo sapiens	heart left ventricle	None	None	None	None
12 Sample 13	Homo sapiens	heart left ventricle	None	None	None	None

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are empty and required

- start
- characteristics[cell type]
- characteristics[ancestry category]
- characteristics[age]
- characteristics[sex]
- characteristics[disease]
- characteristics[individual]
- characteristics[biological replicate]
- technology type
- assay name
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[fragment mass tolerance]
- comment[precursor mass tolerance]
- undo column

Press to download SDRF file

Input the cell type of your sample

Are there multiple characteristics[cell type] in your data?

- No
- Yes

Select your matching ontology term using this autocomplete function

Choose an option

Or follow the ontology based drop down menu below

- native cell
- cell in vitro
 - experimentally modified cell in vitro
 - cultured cell
 - primary cultured cell
 - protoplast
 - spheroplast
- abnormal cell

You need to select a total of 1.

Submit selection

Selection contains: ['primary cultured cell', 'spheroplast']

If all cells are correctly filled in click twice on the update button

Update

source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry cat...]	characteristics
Sample 1	Homo sapiens	heart left ventricle	empty	empty	empty
Sample 2	Homo sapiens	heart left ventricle	empty	empty	empty
Sample 3	Homo sapiens	heart left ventricle	empty	empty	empty
Sample 4	Homo sapiens	heart left ventricle	empty	empty	empty
Sample 5	Homo sapiens	heart left ventricle	empty	empty	empty



Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are
empty and required start characteristics[ancestry category]

- characteristics[age]
- characteristics[sex]
- characteristics[disease]
- characteristics[individual]
- characteristics[biological replicate]
- technology type
- assay name
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[fragment mass tolerance]
- comment[precursor mass tolerance]
- undo column

Press to download SDRF file

3. Required columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry category]	characteristics[age]	characteristic
0	Sample 1	Homo sapiens	heart left ventricle	cardiocyte		None	None
1	Sample 2	Homo sapiens	heart left ventricle	cardiocyte		None	None
2	Sample 3	Homo sapiens	heart left ventricle	cardiocyte		None	None
3	Sample 4	Homo sapiens	heart left ventricle	cardiocyte		None	None
4	Sample 5	Homo sapiens	heart left ventricle	cardiocyte		None	None
5	Sample 6	Homo sapiens	heart left ventricle	cardiocyte		None	None
6	Sample 7	Homo sapiens	heart left ventricle	cardiocyte		None	None
7	Sample 8	Homo sapiens	heart left ventricle	cardiocyte		None	None
8	Sample 9	Homo sapiens	heart left ventricle	cardiocyte		None	None
9	Sample 10	Homo sapiens	heart left ventricle	cardiocyte		None	None

Input the ancestry of your samples

Are there multiple characteristics[ancestry category] in your data?

 No Yes

Select your matching ontology term using this autocomplete function

Choose an option

Or follow the ontology based drop down menu below

- > European
- > Asian
- > African
- > Native American
- > Hispanic or Latin American
- > Greater Middle Eastern (Middle Eastern, North African or Persian)
- > African American or Afro-Caribbean
- > Oceanian
- > uncategorised population
- > genetically isolated population
- > Aboriginal Australian
- > undefined ancestry population
- Not available

Submit selection



X

#	Sample ID	Species	Tissue/Vehicle	Sex	Age	Gender	Last updated
30	Sample 20	Homo sapiens	heart left ventricle	36Y	adult	M	not available
31	Sample 21	Homo sapiens	heart left ventricle	51Y	adult	F	not available
32	Sample 25	Homo sapiens	heart left ventricle	59Y	adult	M	not available
33	Sample 9	Homo sapiens	heart left ventricle	48Y	adult	M	not available

- Home
- 1. Mapping local metadata
- 2. Labeling
- 3. Required columns**
- 4. Additional columns
- 5. Experiment types

The following columns are empty and required

- start
- assay name
- technology type
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[precursor mass tolerance]
- comment[fragment mass tolerance]
- undo column

Press to download SDRF file

The assay name is a name for the run file, this has to be a unique value eg. run 1 - run 2 - run 3_fraction1. If you did not add it using the previous mapping function, you can input it here manually.

Type the correct assay names in the corresponding column and click Update twice when finished

Update

s[disease]	characteristics[biological re...	characteristics[individual]	assay name	technology type	comment[data file]
hypertrophy		1 2	run 1	empty	Prosser_1205.raw
hypertrophy		1 3	run 10	empty	Prosser_1209.raw
hypertrophy		1 4	r	empty	Prosser_1228.raw
hypertrophy		1 6	empty	empty	Prosser_1288.raw
hypertrophy		1 10	empty	empty	Prosser_1320.raw
hypertrophy		1 17	empty	empty	Prosser_1379.raw
hypertrophy		1 19	empty	empty	Prosser_1425.raw
hypertrophy		1 21	empty	empty	Prosser_1462.raw
hypertrophy		1 25	empty	empty	Prosser_1510.raw
hypertrophy		1 27	empty	empty	Prosser_1602.raw
hypertrophy		1 29	empty	empty	Prosser_1119.raw
hypertrophy		1 30	empty	empty	Prosser_1136.raw
hypertrophy		1 31	empty	empty	Prosser_1146.raw
hypertrophy		1 15	empty	empty	Prosser_1366.raw
hypertrophy		1 16	empty	empty	Prosser_1375.raw
omyopathy		1 7	empty	empty	Prosser_1290.raw
omyopathy		1 8	empty	empty	Prosser_1304.raw
omyopathy		1 22	empty	empty	Prosser_1467.raw
omyopathy		1 24	empty	empty	Prosser_1472.raw
omyopathy		1 26	empty	empty	Prosser_1535.raw
omyopathy		1 28	empty	empty	Prosser_1605.raw
diomyopathy		1 1	empty	empty	Prosser_1004.raw
diomyopathy		1 9	empty	empty	Prosser_1311.raw
diomyopathy		1 20	empty	empty	Prosser_1427.raw
diomyopathy		1 23	empty	empty	Prosser_1086.raw
diomyopathy		1 32	empty	empty	Prosser_1195.raw
diomyopathy		1 33	empty	empty	Prosser_1198.raw
		1 5	empty	empty	Prosser_1273.raw
		1 11	empty	empty	Prosser_1325.raw
		1 12	empty	empty	Prosser_1085.raw
		1 13	empty	empty	Prosser_1339.raw
		1 14	empty	empty	Prosser_1356.raw
		1 18	empty	empty	Prosser_1383.raw
		1 34	empty	empty	Prosser_1200.raw



Input the ages of your samples using the Years Months Days format, e.g. 1Y 2M 3D. Age ranges should be formatted as e.g. 1Y-3Y

Are there multiple ages in your data?



Yes

Update

source name	organism	characteristics[organism part]	characteristics[cell type]	characteristics[ancestry cat...]	characteristics[age]
Sample 1		heart left ventricle	cardiocyte	Not available	58Y
Sample 2		heart left ventricle	cardiocyte	Not available	54Y
Sample 3		heart left ventricle	cardiocyte	Not available	55Y
Sample 4		heart left ventricle	cardiocyte	Not available	52Y
Sample 5		heart left ventricle	cardiocyte	Not available	60Y
Sample 6		heart left ventricle	cardiocyte	Not available	55Y
Sample 7		heart left ventricle	cardiocyte	Not available	64Y
Sample 8		heart left ventricle	cardiocyte	Not available	55Y
Sample 9		heart left ventricle	cardiocyte	Not available	48Y
Sample 10		heart left ventricle	cardiocyte	Not available	44Y
Sample 11		heart left ventricle	cardiocyte	Not available	65Y
Sample 12		heart left ventricle	cardiocyte	Not available	35Y
Sample 13		heart left ventricle	cardiocyte	Not available	40Y
Sample 14		heart left ventricle	cardiocyte	Not available	53Y
Sample 15		heart left ventricle	cardiocyte	Not available	65Y
Sample 16		heart left ventricle	cardiocyte	Not available	63Y
Sample 17		heart left ventricle	cardiocyte	Not available	56Y
Sample 18		heart left ventricle	cardiocyte	Not available	26Y
Sample 19		heart left ventricle	cardiocyte	Not available	53Y
Sample 20		heart left ventricle	cardiocyte	Not available	36Y
Sample 21		heart left ventricle	cardiocyte	Not available	51Y
Sample 22		heart left ventricle	cardiocyte	Not available	42Y
Sample 23		heart left ventricle	cardiocyte	Not available	41Y
Sample 24		heart left ventricle	cardiocyte	Not available	42Y
Sample 25		heart left ventricle	cardiocyte	Not available	59Y
Sample 26		heart left ventricle	cardiocyte	Not available	40Y
Sample 27		heart left ventricle	cardiocyte	Not available	62Y
Sample 28		heart left ventricle	cardiocyte	Not available	51Y
Sample 29		heart left ventricle	cardiocyte	Not available	67Y
Sample 30		heart left ventricle	cardiocyte	Not available	41Y
Sample 31		heart left ventricle	cardiocyte	Not available	58Y
Sample 32		heart left ventricle	cardiocyte	Not available	58Y
Sample 33		heart left ventricle	cardiocyte	Not available	46Y
		heart left ventricle	cardiocyte	Not available	66

The age column is not in the correct format, please check and try again



X

	Sample ID	Host species	Heart left ventricle	cardiocyte	Not available	...
5	Sample 6	Homo sapiens	heart left ventricle	cardiocyte	Not available	55Y
6	Sample 7	Homo sapiens	heart left ventricle	cardiocyte	Not available	64Y
7	Sample 8	Homo sapiens	heart left ventricle	cardiocyte	Not available	55Y
8	Sample 9	Homo sapiens	heart left ventricle	cardiocyte	Not available	48Y
9	Sample 10	Homo sapiens	heart left ventricle	cardiocyte	Not available	44Y
10	Sample 11	Homo sapiens	heart left ventricle	cardiocyte	Not available	65Y
11	Sample 12	Homo sapiens	heart left ventricle	cardiocyte	Not available	35Y
12	Sample 13	Homo sapiens	heart left ventricle	cardiocyte	Not available	40Y

The following columns are empty and required

- start
- characteristics[sex]
- characteristics[disease]
- characteristics[individual]
- characteristics[biological replicate]
- technology type
- assay name
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[fragment mass tolerance]
- comment[precursor mass tolerance]
- undo column

Press to download SDRF file

Are there multiple sexes in your data?

Yes

Update

source name	characteristics[sex]	characteristics[disease]	characteristics[individual]	characteristics[biological re...	technolog...
Sample 1		empty	empty	empty	empty
Sample 2	empty	empty	empty	empty	empty
Sample 3	empty	empty	empty	empty	empty
Sample 4	empty	empty	empty	empty	empty
Sample 5	empty	empty	empty	empty	empty
Sample 6	empty	empty	empty	empty	empty
Sample 7	empty	empty	empty	empty	empty
Sample 8	empty	empty	empty	empty	empty
Sample 9	empty	empty	empty	empty	empty
Sample 10	empty	empty	empty	empty	empty
Sample 11	empty	empty	empty	empty	empty
Sample 12	empty	empty	empty	empty	empty
Sample 13	empty	empty	empty	empty	empty
Sample 14	empty	empty	empty	empty	empty
Sample 15	empty	empty	empty	empty	empty
Sample 16	empty	empty	empty	empty	empty
Sample 17	empty	empty	empty	empty	empty
Sample 18	empty	empty	empty	empty	empty
Sample 19	empty	empty	empty	empty	empty
Sample 20	empty	empty	empty	empty	empty
Sample 21	empty	empty	empty	empty	empty
Sample 22	empty	empty	empty	empty	empty
Sample 23	empty	empty	empty	empty	empty
Sample 24	empty	empty	empty	empty	empty
Sample 25	empty	empty	empty	empty	empty
Sample 26	empty	empty	empty	empty	empty
Sample 27	empty	empty	empty	empty	empty
Sample 28	empty	empty	empty	empty	empty
Sample 29	empty	empty	empty	empty	empty
Sample 30	empty	empty	empty	empty	empty
Sample 31	empty	empty	empty	empty	empty



Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are
empty and required

- start
- characteristics[biological replicate]
- characteristics[individual]
- assay name
- technology type
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[precursor mass tolerance]
- comment[fragment mass tolerance]
- undo column

Press to download SDRF file

3. Required columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[
0	Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M	not available
1	Sample 11	Homo sapiens	heart left ventricle	65Y	adult	F	not available
2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available
6	Sample 26	Homo sapiens	heart left ventricle	40Y	adult	M	not available
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available

Do you have biological replicates?

Yes

No



Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are empty and required
②

 start characteristics[individual] assay name technology type comment[technical replicate] comment[fraction identifier] comment[instrument] comment[cleavage agent details] comment[modification parameters] comment[precursor mass tolerance] comment[fragment mass tolerance] undo column

Press to download SDRF file

7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available
10	Sample 4	Homo sapiens	heart left ventricle	52Y	adult	F	not available
11	Sample 5	Homo sapiens	heart left ventricle	60Y	adult	F	not available
12	Sample 6	Homo sapiens	heart left ventricle	55Y	adult	F	not available

Do you have multiple individuals in your data?

How many individuals are in your data?

 Ready for input?

Yes

35



Update

source name ↑	try cat...	characteristics[cell type]	characteristics[disease]	characteristics[biological re...	characteristics[individual]
Sample 1		cardiocyte	ischemic cardiomyopathy	1	1
Sample 10		cardiocyte	cardiac hypertrophy	1	2
Sample 11		cardiocyte	cardiac hypertrophy	1	3
Sample 12		cardiocyte	cardiac hypertrophy	1	4
Sample 13		cardiocyte	normal	1	5
Sample 14		cardiocyte	cardiac hypertrophy	1	6
Sample 15		cardiocyte	dilated cardiomyopathy	1	7
Sample 16		cardiocyte	dilated cardiomyopathy	1	8
Sample 17		cardiocyte	ischemic cardiomyopathy	1	9
Sample 18		cardiocyte	cardiac hypertrophy	1	10
Sample 19		cardiocyte	normal	1	11
Sample 2		cardiocyte	normal	1	12
Sample 20		cardiocyte	normal	1	13
Sample 21		cardiocyte	normal	1	14
Sample 22		cardiocyte	cardiac hypertrophy	1	15
Sample 23		cardiocyte	cardiac hypertrophy	1	16
Sample 24		cardiocyte	cardiac hypertrophy	1	17
Sample 25		cardiocyte	normal	1	18
Sample 26		cardiocyte	cardiac hypertrophy	1	19
Sample 27		cardiocyte	ischemic cardiomyopathy	1	20
Sample 28		cardiocyte	cardiac hypertrophy	1	21
Sample 29		cardiocyte	dilated cardiomyopathy	1	22
Sample 3		cardiocyte	ischemic cardiomyopathy	1	23
Sample 30		cardiocyte	dilated cardiomyopathy	1	empty
Sample 31		cardiocyte	cardiac hypertrophy	1	empty
Sample 32		cardiocyte	dilated cardiomyopathy	1	empty
Sample 33		cardiocyte	cardiac hypertrophy	1	empty
Sample 34		cardiocyte	dilated cardiomyopathy	1	empty
Sample 4		cardiocyte	cardiac hypertrophy	1	empty
Sample 5		cardiocyte	cardiac hypertrophy	1	empty
Sample 6		cardiocyte	cardiac hypertrophy	1	empty
Sample 7		cardiocyte	ischemic cardiomyopathy	1	empty
Sample 8		cardiocyte	ischemic cardiomyopathy	1	empty



[Home](#)[1. Mapping local metadata](#)[2. Labeling](#)[3. Required columns](#)[4. Additional columns](#)[5. Experiment types](#)

The following columns are
empty and required

- start
- technology type
- comment[technical replicate]
- comment[fraction identifier]
- comment[instrument]
- comment[cleavage agent details]
- comment[modification parameters]
- comment[precursor mass tolerance]
- comment[fragment mass tolerance]
- undo column

[Press to download SDRF file](#)

3. Required columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[
0	Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M	not available
1	Sample 11	Homo sapiens	heart left ventricle	65Y	adult	F	not available
2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available
6	Sample 26	Homo sapiens	heart left ventricle	40Y	adult	M	not available
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available

Choose the technology type from these options:

- proteomic profiling by mass spectrometry
- metabolomics profiling by mass spectrometry
- other

[Submit](#)

Home
1. Mapping local metadata
2. Labeling
3. Required columns
4. Additional columns
5. Experiment types

The following columns are empty and required [?](#)

- start
- comment[cleavage agent details]
- comment[modification parameters]
- comment[precursor mass tolerance]
- comment[fragment mass tolerance]
- undo column

Press to download SDRF file

3. Required columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[available]
0	Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M	not available
1	Sample 11	Homo sapiens	heart left ventricle	65Y	adult	F	not available
2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available
6	Sample 26	Homo sapiens	heart left ventricle	40Y	adult	M	not available
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available

Input the cleavage agent details of your sample

Select the cleavage agents used in your sample If no cleavage agent was used e.g. in top down proteomics, choose *NoEnzyme*

Choose an option

- NoEnzyme
- NT=2-iodobenzoate; CS='(?<=W)'
- NT=Arg-C; CS='(?<=R)(?!\P)'
- NT=Asp-N; CS='(?=[BD])'
- NT=Asp-N ambic; CS='(?=[DE])'
- NT=CNBr; CS='(?<=M)'
- NT=Chymotrypsin; CS='(?<=[FYWL])(?!\P)'
- NT=Formic acid; CS='((?<=D))((?<=D))'

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

The following columns are empty and required

- start
- comment[cleavage agent details]
- comment[modification parameters]
- comment[precursor mass tolerance]
- comment[fragment mass tolerance]
- undo column

Press to download SDRF file

3. Required columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[
0	Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M	not available
1	Sample 11	Homo sapiens	heart left ventricle	65Y	adult	F	not available
2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available
6	Sample 26	Homo sapiens	heart left ventricle	40Y	adult	M	not available
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available

Input the cleavage agent details of your sample

Select the cleavage agents used in your sample If no cleavage agent was used e.g. in top down proteomics, choose *NoEnzyme*

NT=Trypsin/P; CS='(?<=[KR])'

 NT=Trypsin; CS='(?<=[KR])(?!\P)'

 NT=Chymotrypsin; CS='(?<=[FYWL])(?!\P)'

 NT=TrypChymo; CS='(?<=[FYWLKR])(?!\P)'



	profiling by mass spectrometry	Prosser_1420.raw	NT=label free sample	1	Q Exactive	NT=Tryp
7	profiling by mass spectrometry	Prosser_1462.raw	NT=label free sample	1	Q Exactive	NT=Tryp
8	profiling by mass spectrometry	Prosser_1510.raw	NT=label free sample	1	Q Exactive	NT=Tryp
9	profiling by mass spectrometry	Prosser_1602.raw	NT=label free sample	1	Q Exactive	NT=Tryp
10	profiling by mass spectrometry	Prosser_1119.raw	NT=label free sample	1	Q Exactive	NT=Tryp

3. Required columns

- 4. Additional columns
- 5. Experiment types

The following columns are empty and required

- start
- comment[modification parameters] comment[modification parameters]
- comment[precursor mass tolerance]
- comment[fragment mass tolerance]
- undo column

Press to download SDRF file

First select the modifications that are in your sample using the drop down autocomplete menu. After selection you will need to choose the modification type, position and target amino acid.

Modification type can be fixed, variable or annotated. Annotated is used to search for all the occurrences of the modification into an annotated protein database file like UNIPROT XML or PEFF.

Position can be anywhere, protein N-term, protein C-term, any N-term or any C-term.

Target amino acid can be any amino acid or X if it's not in the list. You can also select multiple amino acids.

If the modification of your choice is not available in the drop down list, select "Other" and input the modification name, chemical formula and mass of your custom modification.

The final modification will be formatted following the SDRF guidelines after which you can click on "Submit modifications".

Select the modifications present in your data

Oxidation X Carbamidomethyl X

Oxidation

Select the modification type

Fixed

Select the position of the modification

Anywhere

Select the target amino acid

M X

X

G

A

L

F

W

K

Final SDRF notation of modification:

NT=Oxidation;AC=35;CF=O;MM=15.994915;MT=Fixed;PP=Anywhere;TA=['M']

Carbamidomethyl

Select the modification type

Fixed

Select the position of the modification

Anywhere

Final SDRF notation of modification:

NT=Carbamidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere;TA=[]

Confirmed modifications contain: ["NT=Oxidation;AC=35;CF=O;MM=15.994915;MT=Fixed;PP=Anywhere;TA=['M']", "NT=Carbamidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere;TA=[]"]

Submit modifications ?

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[status]
0	Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M	not available
1	Sample 11	Homo sapiens	heart left ventricle	65Y	adult	F	not available
2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available



Step 4: Input additional columns

Beyond the required columns needed for a valid SDRF, there are other optional columns available. To prevent overwhelming users with choices, these are incorporated into step 4 and are distinctly labeled as "additional columns". This design choice ensures clarity while providing users the flexibility to include any supplementary data they deem relevant.

Examples of such columns are compound, enrichment, collision energy, etc.

Of these columns, the 'factor value' stands out as particularly significant. This column represents the study variable, essentially highlighting the main focus or subject of investigation in the study.

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

These are all possible columns you may want to add:

- start
- factor value
- characteristics[cell line]
- characteristics[compound]
- characteristics[concentration of compound]
- characteristics[enrichment process]
- comment[collision energy]
- comment[depletion]
- comment[dissociation method]
- undo column

Press to download SDRF file

4. Additional columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[
0	Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M	not available
1	Sample 11	Homo sapiens	heart left ventricle	65Y	adult	F	not available
2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available
6	Sample 26	Homo sapiens	heart left ventricle	40Y	adult	M	not available
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available

You can choose one or multiple columns that define the **factor value** in your experiment.

This column indicates which experimental factor/variable is used as the hypothesis to perform the data analysis.

If there are multiple factor values, we ask the user to take care in assigning biological and technical replicates.

Select a factor value:

Choose an option

source name

- characteristics[organism]
- characteristics[organism part]
- characteristics[age]
- characteristics[developmental stage]
- characteristics[sex]
- characteristics[ancestry category]
- characteristics[cell type]

 Save factor value?

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available





Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

These are all possible columns you may want to add:

- start
- factor value
- characteristics[cell line]
- characteristics[compound]
- characteristics[concentration of compound]
- characteristics[enrichment process]
- comment[collision energy]
- comment[depletion]
- comment[dissociation method]
- undo column

Press to download SDRF file

4. Additional columns

This is your current SDRF file.

it[modification parameters]_1	comment[precursor mass tolerance]	comment[fragment mass tolerance]	↑ factor value[disease]
1 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
2 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
3 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
4 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
5 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
6 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
7 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
8 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
9 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
10 \amidomethyl;AC=4;CF=H(3) C(2) N O;MM=57.021464;MT=Fixed;PP=Anywhere	20 ppm	20 ppm	cardiac hypertrophy
..

You can choose one or multiple columns that define the **factor value** in your experiment.

This column indicates which experimental factor/variable is used as the hypothesis to perform the data analysis.

If there are multiple factor values, we ask the user to take care in assigning biological and technical replicates.

Select a factor value:

Save factor value?

Choose an option

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[
0	Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M	not available
1	Sample 11	Homo sapiens	heart left ventricle	65Y	adult	F	not available
2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available
6	Sample 26	Homo sapiens	heart left ventricle	40Y	adult	M	not available
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available



[Home](#)[1. Mapping local metadata](#)[2. Labeling](#)[3. Required columns](#)[4. Additional columns](#)[5. Experiment types](#)

These are all possible columns you may want to add:

- start
- factor value
- characteristics[cell line]
- characteristics[compound]
- characteristics[concentration of compound]
- characteristics[enrichment process]
- comment[collision energy]
- comment[depletion]
- comment[dissociation method]
- undo column

[Press to download SDRF file](#)

4. Additional columns

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[
0	Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M	not available
1	Sample 11	Homo sapiens	heart left ventricle	65Y	adult	F	not available
2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available
6	Sample 26	Homo sapiens	heart left ventricle	40Y	adult	M	not available
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available

There are still columns that you can add to your SDRF file.

Similar to the previous section, you can select a column to annotate in the sidebar. When a column is filled, it will disappear from the sidebar so you can keep track on which columns you can still add.

When you want to reannotate a previously filled in column, you can do so by clicking on the **undo column** button in the sidebar.

At the bottom of the page there are now two download buttons. The first one will download your intermediate SDRF file.

The second button will download your final SDRF file after some final checks.



Step 5: Experiment types

The final segment of lesSDRF is the "Experiment types" tab. Currently, this section is in development and heavily relies on feedback from the community. The ultimate aim is to enable users to specify the kind of experiment they've conducted. Subsequently, they can then fill out columns suggested by the community. This feature is particularly beneficial for studies that are relatively new to the field of proteomics, like metaproteomics or single cell proteomics. The community-driven approach ensures that the tool remains up-to-date and relevant to emerging research trends.

Home

1. Mapping local metadata

2. Labeling

3. Required columns

4. Additional columns

5. Experiment types

Join the community
effort

This is your current SDRF file.

	source name	characteristics[organism]	characteristics[organism part]	characteristics[age]	characteristics[developmental stage]	characteristics[sex]	characteristics[biome]
0	Sample 10	Homo sapiens	heart left ventricle	44Y	adult	M	not available
1	Sample 11	Homo sapiens	heart left ventricle	65Y	adult	F	not available
2	Sample 12	Homo sapiens	heart left ventricle	35Y	adult	M	not available
3	Sample 14	Homo sapiens	heart left ventricle	53Y	adult	F	not available
4	Sample 18	Homo sapiens	heart left ventricle	26Y	adult	M	not available
5	Sample 24	Homo sapiens	heart left ventricle	42Y	adult	M	not available
6	Sample 26	Homo sapiens	heart left ventricle	40Y	adult	M	not available
7	Sample 28	Homo sapiens	heart left ventricle	51Y	adult	M	not available
8	Sample 31	Homo sapiens	heart left ventricle	58Y	adult	M	not available
9	Sample 33	Homo sapiens	heart left ventricle	46Y	adult	M	not available

🚧 Under development 🚧

5. Experiment types

⚠️ This application is currently in development and the current page is not yet finalized. We are in touch with several members of the involved communities, but we have not yet decided on a strict template. If you would like to be a part of this discussion, please use the button in the sidebar to get involved.

Some experiment types have an atypical SDRF structure. Here you can find the community-suggested SDRF columns for such experiments.

Metaproteomics

Single cell proteomics

Immunopeptidomics

✓ The suggested column characteristics[organism] is already in your SDRF file.

✗ The suggested column characteristics[environmental material] is not in your SDRF file. Do you want to add it?

✗ The suggested column characteristics[diet] is not in your SDRF file. Do you want to add it?

✗ The suggested column characteristics[biome] is not in your SDRF file. Do you want to add it?

Suggested columns:

Add characteristics[environmental material] to SDRF file

Add characteristics[diet] to SDRF file

Add characteristics[biome] to SDRF file

Add characteristics[environmental condition] to SDRF file

