

Sample and Data Relationship Format for Proteomics (SDRF- Proteomics)

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Table of Contents

| | |
|--|-----------|
| 1. Status of this document | 1 |
| 2. Abstract | 2 |
| 3. Motivation | 3 |
| 4. Quick Start | 5 |
| 4.1. Minimal Example | 5 |
| 4.2. Key Concepts | 5 |
| 4.3. Getting Started Steps | 5 |
| 5. Validating SDRF Files | 6 |
| 5.1. Installation | 6 |
| 5.2. Basic Validation | 6 |
| 5.3. Available Templates for Validation | 6 |
| 5.4. Additional Features | 6 |
| 6. Specification structure | 7 |
| 6.1. Versioning | 8 |
| 6.2. Notational Conventions | 8 |
| 6.3. Relationship to other specifications | 8 |
| 7. SDRF-Proteomics specification | 10 |
| 7.1. Format rules | 10 |
| 7.2. File-level metadata (Header comments) | 11 |
| 7.3. Column headers | 12 |
| 7.4. Cell values | 12 |
| 8. Ontologies and Controlled Vocabularies | 14 |
| 9. SDRF-Proteomics: Samples metadata | 16 |
| 9.1. BioSamples database integration | 17 |
| 9.2. Encoding sample technical and biological replicates | 18 |
| 9.3. Pooled samples | 20 |
| 9.3.1. Allowed values for characteristics[pooled sample] | 20 |
| 9.3.2. Example with pooled reference channel | 20 |
| 9.3.3. Metadata handling for pooled samples | 21 |
| 9.4. Spiked-in samples | 22 |
| 9.5. Sample Metadata Guidelines | 23 |
| 10. SDRF-Proteomics: data files metadata | 24 |
| 10.1. Sample preparation properties | 25 |
| 10.2. MS/MS properties | 25 |
| 10.3. Data acquisition | 25 |
| 10.4. Data File Metadata Guidelines | 26 |
| 11. Core Templates | 27 |
| 11.1. Default Template | 27 |
| 11.2. Human Template | 28 |
| 11.3. Vertebrates Template | 29 |
| 11.4. Invertebrates Template | 30 |
| 11.5. Plants Template | 31 |
| 11.6. Column Cardinality | 32 |

| | |
|--|-----------|
| 12. Factor Values (Study Variables) | 34 |
| 12.1. Column Format | 34 |
| 12.2. When to Use Factor Values | 34 |
| 12.3. Rules | 34 |
| 12.4. Example | 34 |
| 13. Experiment-specific Templates | 35 |
| 14. Examples of Annotated Datasets | 36 |
| 15. Ongoing template discussions | 37 |
| 16. Intellectual Property Statement | 38 |
| 17. Copyright Notice | 39 |
| 18. How to cite | 40 |
| 19. References | 41 |

Chapter 1. Status of this document

This document provides information to the proteomics community about a proposed standard for sample metadata annotations in public repositories called Sample and Data Relationship File (SDRF)-Proteomics format. Distribution is unlimited.

Version v1.1.0 - 2025-01

Chapter 2. Abstract

The Human Proteome Organisation (HUPO) Proteomics Standards Initiative (PSI) defines community standards for data representation in proteomics to facilitate data comparison, exchange, and verification. This document presents a specification for the Sample and Data Relationship Format (SDRF-Proteomics).

Further detailed information, including any updates to this document, implementations, and examples is available at [SDRF GitHub Repository](#). The official PSI web page for the document is the following: <http://psidev.info/sdrf>.

Chapter 3. Motivation

Many resources have emerged that provide raw or integrated proteomics data in the public domain. If these are valuable individually, their integration through re-analysis represents a huge asset for the community [1].

Unfortunately, proteomics experimental design and sample related information are often missing in public repositories or stored in very diverse ways and formats. For example:

- The [CPTAC Consortium](#) provides for every dataset a set of Excel files with the information on [each sample](#) including tumor size, origin, but also how every sample is related to a specific raw file (e.g. instrument configuration parameters).
- As a resource routinely re-analysing public datasets, ProteomicsDB, captures for each sample in the database a minimum number of properties to describe the sample and the related experimental protocol such as [tissue, digestion method and instrument](#).

Such heterogeneity often prevents data interpretation, reproducibility, and integration of data from different resources. For every proteomics dataset we propose to capture at least three levels of metadata:

- (i) dataset description
- (ii) the sample metadata and data files acquisition metadata.
- (iii) The relation between the sample and the data files. The experimental design.

The general description includes minimum information to describe the study overall: [title, description, date of publication, type of experiment](#). In ProteomeXchange partners this metadata is captured at the dataset level, in other omics resources this is captured as IDF file format (e.g. MAGE-TAB). Currently, all ProteomeXchange partners mandate this information for each dataset. However, the information regarding the sample and its relation to the data files (**Figure 1**) is mostly missing [1].

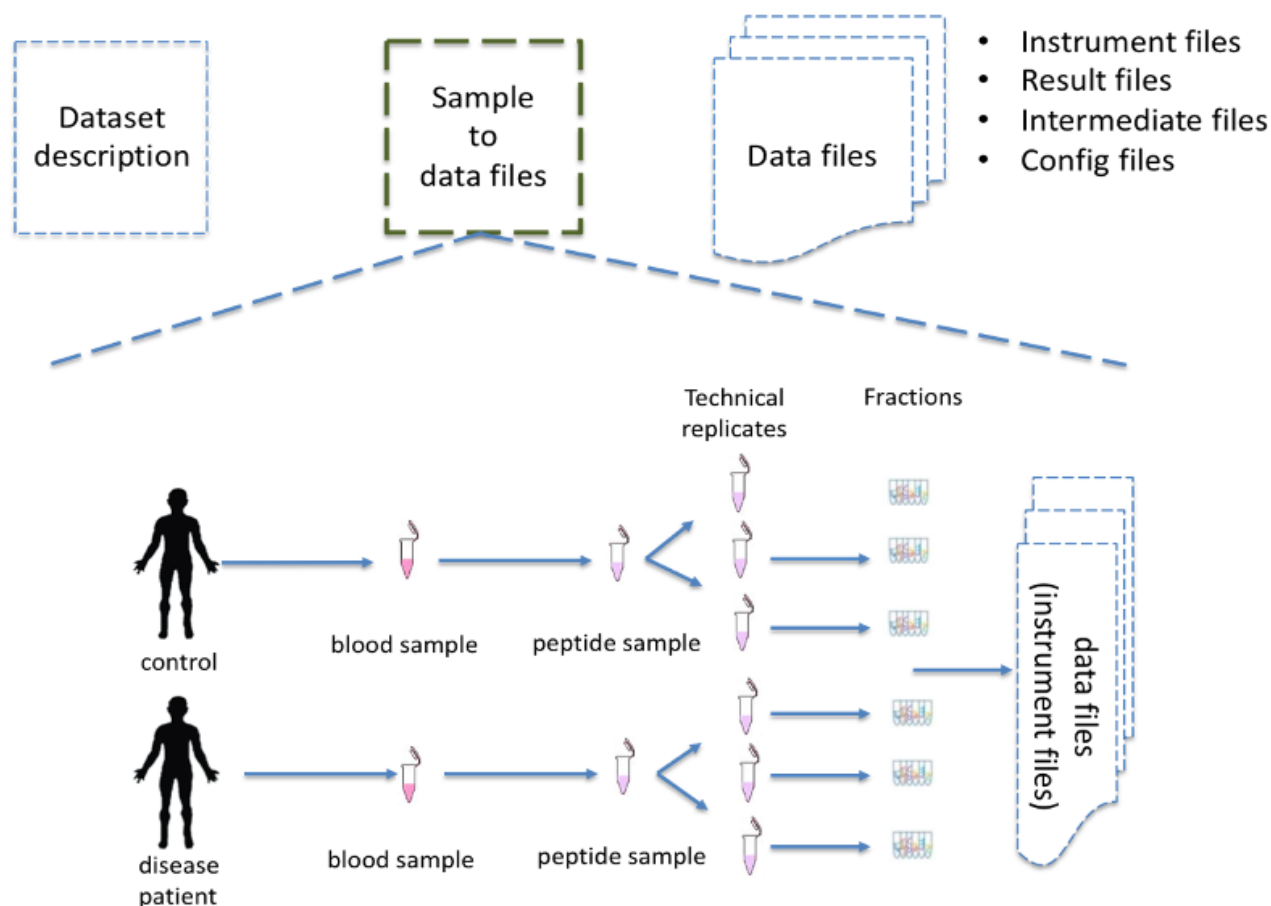


Figure 1: SDRF-Proteomics file format stores the information of the sample and its relation to the data files in the dataset. The file format includes not only information about the sample but also about how the data was acquired and processed.

Here, we introduced the Sample and Data Relationship Format (SDRF-Proteomics) to capture the sample metadata and its relation to the data files for proteomics experiments. The SDRF-Proteomics format is a tab-delimited file format that describes the sample characteristics and the relationships between samples and data files included in a dataset.

This specification, which is a community effort, aims to provide a standard for the proteomics community to annotate the sample metadata and its relation to the data files.

Chapter 4. Quick Start

If you're new to SDRF-Proteomics, here's a minimal example to get you started. An SDRF file is a tab-separated file where each row represents a sample-to-data-file relationship.

4.1. Minimal Example

```
source name characteristics[organism]      characteristics[organism part]
characteristics[disease]      characteristics[biological replicate]  assay name
technology type comment[proteomics data acquisition method] comment[label]
comment[instrument] comment[cleavage agent details] comment[fraction identifier]
comment[technical replicate]      comment[data file]
sample_1      homo sapiens      liver      normal      1      run_1      proteomic profiling by mass
spectrometry      data-dependent acquisition label free sample      Q Exactive HF
NT=Trypsin;AC=MS:1001251      1      1      sample_1.raw
sample_2      homo sapiens      liver      hepatocellular carcinoma      1      run_2      proteomic
profiling by mass spectrometry      data-dependent acquisition label free sample      Q
Exactive HF      NT=Trypsin;AC=MS:1001251      1      1      sample_2.raw
```

4.2. Key Concepts

1. **Sample metadata** uses `characteristics[...]` columns (e.g., organism, disease)
2. **Data file metadata** uses `comment[...]` columns (e.g., instrument, label)
3. **Factor values** use `factor value[...]` columns to indicate variables under study
4. Each row links one sample to one data file

4.3. Getting Started Steps

1. Choose a [core template](#) (Human, Vertebrates, Plants, etc.)
2. Fill in sample metadata (characteristics columns)
3. Fill in data file metadata (comment columns)
4. Add factor values for your experimental variables
5. Validate your file using [sdrf-pipelines](#)

For detailed guidance, continue reading the full specification below.

Chapter 5. Validating SDRF Files

The official validator for SDRF-Proteomics files is **sdrf-pipelines**, a Python tool that checks your SDRF file for errors and compliance with the specification.

5.1. Installation

```
pip install sdrf-pipelines
```

5.2. Basic Validation

```
# Validate an SDRF file
parse_sdrf validate-sdrf --sdrf_file your_file.sdrf.tsv

# Validate with a specific template
parse_sdrf validate-sdrf --sdrf_file your_file.sdrf.tsv --template human
```

5.3. Available Templates for Validation

- `default` - Basic validation
- `human` - Human samples with clinical metadata
- `vertebrates` - Non-human vertebrates
- `invertebrates` - Invertebrates
- `plants` - Plant samples
- `cell_lines` - Cell line experiments

5.4. Additional Features

sdrf-pipelines can also convert SDRF files to configuration files for popular analysis tools:

```
# Convert to MaxQuant parameters
parse_sdrf convert-maxquant --sdrf_file your_file.sdrf.tsv --output_folder ./

# Convert to OpenMS parameters
parse_sdrf convert-openms --sdrf_file your_file.sdrf.tsv --output_folder ./
```

For more information, visit: [sdrf-pipelines on GitHub](#)

Chapter 6. Specification structure

This document describes the main specification of SDRF-Proteomics, the structure of the specification (**Figure 2**), how to contribute, and extend the specification. SDRF-Proteomics uses a three-tier system for organizing metadata requirements:

- **The SDRF-Proteomics core specification:** This document contains the main specification, requirements and rules for the SDRF-Proteomics format. It also includes the notational conventions and the relationship to other specifications.
- **Core templates:** Organism-based templates (human, vertebrates, plants, etc.) that define base schemas for common proteomics experiments. See the [Core Templates](#) section.
- **Specialized templates:** Complete schemas for specific experiment types (cell-lines, single-cell, affinity-proteomics, crosslinking, immunopectidomics, metaproteomics). Each template has its own directory containing:
 - A detailed README.adoc with checklists, and examples.
 - A template file ({name}-template.sdrf.tsv) with column headers.
- **Annotation guidelines:** Detailed documentation for specific metadata annotations (e.g., patient pre-existing condition, sample metadata, data file metadata).

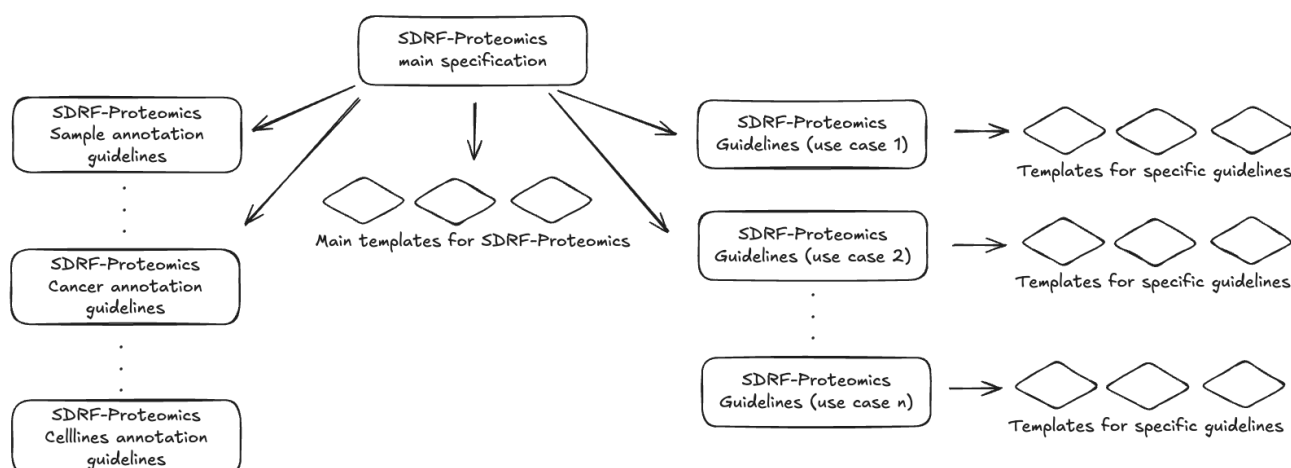


Figure 2: SDRF-Proteomics specification structure. The main specification defines the core rules and is extended by specific experiment templates and annotation guidelines.

NOTE

The main specification is in the [sdrf-proteomics](#) directory. Core templates (organism-based) are in [sdrf-proteomics/core-templates/](#) and specialized templates (experiment-type-specific) are in [sdrf-proteomics/templates/](#). Templates are extensions of the core specification, and should follow all the rules and requirements in the main specification. If a template rule is in conflict with the specification, a note should be done in the main specification to reflect the extension or conflict.

The official website for SDRF-Proteomics project is <https://github.com/bigbio/proteomics-metadata-standard>. New use cases, changes to the specification and examples can be added by using Pull requests or issues in GitHub (see introduction to GitHub - <https://lab.github.com/githubtraining/introduction-to-github>).

A set of examples and annotated projects from ProteomeXchange can be found here: <https://github.com/bigbio/proteomics-metadata-standard/tree/master/annotated-projects>

Multiple tools have been implemented to validate, annotate and convert SDRF-Proteomics files. The official validator of SDRF-Proteomics is sdrf-pipelines (Python - <https://github.com/bigbio/sdrf-pipelines>). This tool allows to validate an SDRF-Proteomics file. In addition, it allows converting SDRF to other popular pipelines and software configure files such as MaxQuant or OpenMS.

6.1. Versioning

The SDRF-Proteomics specification is versioned using the Semantic Versioning 2.0.0 (<https://semver.org/>) scheme. The version number is in the format MAJOR.MINOR.PATCH, where:

- MAJOR version is incremented for incompatible changes to the specification, when major changes are done to the specification.
- MINOR version is incremented for new features that are backward compatible with the previous version. Guidelines and templates are added or modified.
- PATCH version is incremented for bug fixes and minor changes that do not affect the specification or the templates. This includes typos, formatting changes, and other minor updates.

Every change in the specification should be done in GitHub using pull requests into the dev branch. The pull request should include a description of the changes and the reason for the changes. The pull request will be reviewed by the community and merged into the main branch when approved. After the merge, the version number will be updated according to the changes made, the release will be performed, and the Zenodo record will be updated.

NOTE

We added the prefix v to the version number to indicate that it is the version of the specification that was used to create the file. Examples: v1.1.0, v2.0.0, v3.0.0.

6.2. Notational Conventions

The key words “MUST”, “MUST NOT”, “REQUIRED”, “SHALL”, “SHALL NOT”, “SHOULD”, “SHOULD NOT”, “RECOMMEND/RECOMMENDED”, “MAY”, “COULD BE”, and “OPTIONAL” are to be interpreted as described in RFC 2119 (<https://www.rfc-editor.org/rfc/rfc2119>).

6.3. Relationship to other specifications

SDRF-Proteomics is fully compatible with the SDRF file format part of [MAGE-TAB](#). MAGE-TAB is the file format used to store metadata and sample information for transcriptomics experiments. When the ProteomeXchange project file is converted to idf file (project description in MAGE-TAB) and is combined with the SDRF-Proteomics a valid MAGE-TAB is obtained.

SDRF-Proteomics sample information can be embedded into mzTab metadata files. The sample metadata in mzTab contains properties as the columns in the SDRF-Proteomics and values as Sample cell values.

The SDRF-Proteomics aims to capture the sample metadata and its relationship with the data files (e.g. raw files from mass spectrometers). The SDRF-Proteomics do not aim to capture the downstream analysis part of the experimental design such as what samples should be compared, how they can be combined or parameters for the downstream analysis (FDR or p-values thresholds). The HUPO-PSI community will work in the future to include this information in other file formats such as mzTab or a new type of file format.

Chapter 7. SDRF-Proteomics specification

The SDRF-Proteomics file format describes the sample characteristics and the relationships between samples and data files. The file format is a tab-delimited one where each **ROW** corresponds to a relationship between a Sample and a Data file (in an ms proteomics experiment the data file containing the mass spectra), each **COLUMN** corresponds to an attribute/property of the Sample, the Data file, or the Factor values; and the value in each **CELL** is the specific value of the property for a given Sample/Data file/Factor value (**Figure 3**).

| sample properties | | | | | data file properties | | | study variables | |
|-------------------|---------------------------|--------------------------|----------------------------|-----|----------------------|------------------------------|----------------|------------------------|-------------------------|
| source name | characteristics[organism] | characteristics[disease] | characteristics[phenotype] | ... | assay name | comment[fraction identifier] | comment[label] | comment[data file] | factor value[phenotype] |
| sample 1 | homo sapiens | gastric carcinoma | control | | Run 1 | 1 | label free | fileRAW_Control_F1.raw | control |
| sample 2 | homo sapiens | gastric carcinoma | primary tumor | | Run 2 | 1 | label free | fileRAW_Tumor_F1.raw | primary tumor |
| | | | | | | | | | |

Figure 3: SDRF-Proteomics in a nutshell. The file format is a tab-delimited one where columns are properties of the sample, the data file or the variables under study. The rows are the samples of origin and the cells are the values for one property in a specific sample.

The SDRF-Proteomics format contains three main sections:

- The first section contains the [sample metadata](#).
- The second section contains the [data file metadata](#).
- The third section contains the [factor values](#) properties.

7.1. Format rules

There are general scenarios/use cases that are addressed by the following rules:

- **Unknown values:** In some cases, the column is mandatory in the format, but for some samples the corresponding value is unknown. In those cases, users SHOULD use **not available**.
- **Not Applicable values:** In some cases, the column is mandatory, but for some samples the corresponding value is not applicable. In those cases, users SHOULD use **not applicable**.

Table 1. When to use "not available" vs "not applicable"

| Term | Meaning | Example Scenario | Example |
|----------------|-------------------------------------|---|--|
| not available | Value exists but is unknown | Patient age was not recorded in the clinical data | characteristics[age] = not available |
| not applicable | Value does not apply to this sample | Cell line sample has no meaningful "age" | characteristics[age] = not applicable |
| not available | Information could not be determined | Disease status could not be confirmed | characteristics[disease] = not available |

| Term | Meaning | Example Scenario | Example |
|----------------|------------------------|---|---|
| not applicable | Concept does not apply | Asking for "cell type" of a whole tissue homogenate | characteristics[cell type] = not applicable |

- **Case sensitivity:** By specification the SDRF is case-insensitive for text values, but we RECOMMEND using lowercase characters throughout all the text (Column names and values).
- **Space sensitivity:** By specification the SDRF is sensitive to spaces in column names (sourcename != source name).
- **Column order:** The SDRF columns follows some structure; first the sample metadata columns in [Chapter 9](#); then the data file metadata columns in [Chapter 10](#); followed by the factor values columns in [Chapter 12](#).
- **Extension:** The extension of the SDRF file SHOULD be sdrf.tsv (preferred) or .txt.

7.2. File-level metadata (Header comments)

SDRF-Proteomics supports optional file-level metadata using header comments at the beginning of the file. These header comments provide information about the SDRF file itself, such as the format version, template used, and validation status. This approach is inspired by VCF (Variant Call Format) file headers and is fully compatible with pandas and other tabular data processing tools.

Header comments MUST:

- Start with # (single hash) followed by a key-value pair
- Appear at the very beginning of the file, before the column header row
- Use the format `#key=value`

The following header fields are supported:

| Key | Description | Example | Requirement |
|------------------|--|----------------------------|-------------|
| fileformat | Identifier for the file format | SDRF | RECOMMENDED |
| version | SDRF-Proteomics specification version used | v1.1.0 | RECOMMENDED |
| template | Name of the template used | human, cell_lines, default | OPTIONAL |
| template_version | Version of the template | v1.0.0 | OPTIONAL |
| source | Origin or creator of the file | PRIDE, user-generated | OPTIONAL |
| validation_hash | Hash from validator certification | sha256:abc123... | OPTIONAL |

Example of an SDRF file with header comments (simplified example showing only select columns; see [Chapter 11](#) for complete required columns):

```
#fileformat=SDRF
#version=v1.1.0
#template=human
#template_version=v1.0.0
#source=PRIDE
source name characteristics[organism] characteristics[organism part]
characteristics[disease] assay name comment[data file]
sample_1 homo sapiens liver normal run_1 sample_1.raw
```

NOTE

Header comments are OPTIONAL. SDRF files without header comments are still valid. When present, header comments provide valuable provenance information and enable tools to handle version-specific features appropriately.

7.3. Column headers

Depending on each section the column headers (property names) will be prefixed with the following prefixes:

- **characteristics**: Sample metadata (e.g. *characteristics[organism]*)
- **comment**: Data file metadata (e.g. *comment[data file]*)
- **factor value**: Factor values properties (e.g. *factor value[disease]*)

Each property name MUST be a valid ontology term or a valid controlled vocabulary term. Each section will have some specific order for column headers.

NOTE

A list of all controlled vocabularies and ontologies supported are in the [Chapter 8](#) section. On each section we also provide a list of properties that are supported.

7.4. Cell values

The value for each property, (e.g. characteristics, comment, factor value) corresponding to each sample or data file can be represented in multiple ways.

- **Free Text (Human readable)**: In the free text representation, the value is provided as text without Ontology support (e.g. colon or providing accession numbers). This is only RECOMMENDED when the text inserted in the table is the exact name of an ontology/CV term in EFO. If the term is not in EFO, other ontologies can be used.

| source name | characteristics[organism] |
|-------------|---------------------------|
| sample 1 | homo sapiens |
| sample 2 | homo sapiens |

- **Ontology url (Computer readable)**: Users can provide the corresponding URI (Uniform Resource Identifier) of the ontology/CV term as a value. This is recommended for enriched files where the user does not want to use intermediate tools to map from free text to ontology/CV terms.

| source name | characteristics[organism] |
|-------------|---|
| Sample 1 | http://purl.obolibrary.org/obo/NCBITaxon_9606 |
| Sample 2 | http://purl.obolibrary.org/obo/NCBITaxon_9606 |

- Key=value representation (Human and Computer readable): The current representation aims to provide a mechanism to represent the complete information of the ontology/CV term including Accession, Name and other additional properties. In the key=value pair representation, the Value of the property is represented as an Object with multiple properties, where the key is one of the properties of the object and the value is the corresponding value for the particular key. An example of key value pairs is post-translational modification (see [Protein Modifications](#)):

```
NT=Glu->pyro-Glu;MT=fixed;PP=Anywhere;AC=Unimod:27;TA=E
```

Chapter 8. Ontologies and Controlled Vocabularies

SDRF-Proteomics uses ontologies and controlled vocabularies (CVs) to standardize metadata values. The following ontologies are supported:

| Category | Ontology/CV | Description | Notes |
|-------------------------------|------------------------------------|-----------------------------------|------------------------|
| General Purpose | | | |
| General | Experimental Factor Ontology (EFO) | General experimental metadata | |
| General | PATO | Phenotype and Trait Ontology | |
| Organism and Taxonomy | | | |
| Taxonomy | NCBI Taxonomy (NCBITaxon) | Organism classification | |
| Taxonomy | Rat Strain Ontology | Rat strains and breeds | |
| Anatomy and Cell Types | | | |
| Anatomy | UBERON | Cross-species anatomy ontology | |
| Cell Type | Cell Ontology (CL) | Cell type classification | |
| Anatomy | BRENDA Tissue Ontology (BTO) | Tissues and cell lines | |
| Anatomy | Plant Ontology (PO) | Plant anatomy and development | For plant samples |
| Anatomy | FlyBase Anatomy (FBbt) | Drosophila anatomy | For Drosophila samples |
| Anatomy | WormBase Anatomy (WBbt) | C. elegans anatomy | For C. elegans samples |
| Anatomy | Zebrafish Anatomy (ZFA) | Zebrafish anatomy and development | For zebrafish samples |
| Disease | | | |
| Disease | Mondo Disease Ontology (MONDO) | Unified disease ontology | RECOMMENDED |
| Disease | Human Disease Ontology (DOID) | Human diseases | |
| Cell Lines | | | |
| Cell Lines | Cellosaurus | Cell line knowledge resource | RECOMMENDED |

| Category | Ontology/CV | Description | Notes |
|---|-------------------------------------|--|---------------------|
| Cell Lines | Cell Line Ontology (CLO) | Cell line ontology | Legacy support only |
| Mass Spectrometry and Proteomics | | | |
| MS/Proteomics | PSI Mass Spectrometry CV (PSI-MS) | Instruments, methods, parameters | |
| MS/Proteomics | PRIDE Controlled Vocabulary | Proteomics-specific terms | |
| Modifications | Unimod | Protein modifications database | |
| Modifications | PSI-MOD CV | Protein modifications ontology | |
| Other | | | |
| Chemistry | ChEBI | Chemical Entities of Biological Interest | |
| Environment | Environment Ontology (ENVO) | Environmental sample classification | For metaproteomics |
| Ancestry | Human Ancestry Ontology (HANCESTRO) | Human ancestry categories | For human samples |

Chapter 9. SDRF-Proteomics: Samples metadata

The Sample metadata section provides information about the samples of origin and their characteristics. Each sample contains a *source name* (unique identifier) and a set of *characteristics* columns. The first column of the file should be the *source name* and the following columns should be the characteristics of the sample. For example, for any proteomics experiment (human, vertebrate, cell line), the following characteristics should be provided:

- **source name:** Unique sample name (it can be present multiple times if the same sample is used several times in the same dataset)
- **characteristics[organism]:** The organism of the Sample of origin.
- **characteristics[organism part]:** The part of organism's anatomy or substance arising from an organism from which the biomaterial was derived, (e.g., liver)
- **characteristics[disease]:** The disease under study in the Sample.
- **characteristics[cell type]:** A cell type is a distinct morphological or functional form of cell. Examples are epithelial, glial etc.

Example:

| source name | characteristics[organism] | characteristics[organism part] | characteristics[disease] | characteristics[cell type] |
|----------------|---------------------------|--------------------------------|--------------------------|----------------------------|
| sample_treat | homo sapiens | liver | liver cancer | not available |
| sample_control | homo sapiens | liver | liver cancer | not available |

NOTE

Additional characteristics can be added depending on the type of the experiment and sample. The [SDRF-Proteomics templates](#) defines a set of templates and checklists of properties that should be provided depending on the proteomics experiment. In the core guidelines and templates, main document of SDRF-Proteomics, we explain the major sample properties for different experiments. However, SDRF-Proteomics can be extended using guidelines for specific experiments.

Some important notes:

- Each characteristic name in the column header SHOULD be a CV term from the EFO ontology. For example, the header *characteristics[organism]* corresponds to the ontology term Organism. However the values could be from EFO or other ontologies. For example, we RECOMMEND to use MONDO for diseases because it has better coverage than EFO.
- Multiple values (columns) for the same characteristics term are allowed in SDRF-Proteomics. However, it is RECOMMENDED not to use the same column in the same file. If you have multiple phenotypes, you can specify what it refers to or use another more specific term, e.g., "immunophenotype".

9.1. BioSamples database integration

BioSamples databases are reference databases that store information about biological samples used in research. There are two main BioSamples services: the EBI BioSamples (<https://www.ebi.ac.uk/biosamples/>) and the NCBI BioSample (<https://www.ncbi.nlm.nih.gov/biosample>). Both provide persistent identifiers for samples that can be referenced across multiple studies and databases. SDRF-Proteomics supports linking samples to BioSamples entries from either service through the use of BioSample accession numbers.

To integrate with a BioSamples database, use the optional *characteristics[biosample accession number]* column to specify the BioSamples accession identifier for each sample. This characteristic provides a direct link between the proteomics sample metadata and the corresponding BioSamples database entry. Note that BioSample accession numbers must be requested from one of the BioSamples services (NCBI or EBI) before they can be used, and this can be done by users directly or by proteomics services like PRIDE on behalf of users.

It is RECOMMENDED to place the *characteristics[biosample accession number]* column immediately after the *source name* column in the SDRF file. Additionally, each unique *source name* should have a unique biosample accession number. It's important to note that *source name* is unique to the individual sample/data file, not to the entire SDRF file, as a sample may be repeated in the file. The combination of *source name* and *assay name* is unique to the SDRF file.

| Property | Column Name | Example Value | Description |
|---------------------|--|---------------|--|
| BioSample Accession | <i>characteristics[biosample accession number]</i> | SAMN12345678 | The unique BioSamples database accession number for the sample (NCBI format) |
| BioSample Accession | <i>characteristics[biosample accession number]</i> | SAMEA12345678 | The unique BioSamples database accession number for the sample (EBI format) |

Example usage:

| source name | <i>characteristics[biosample accession number]</i> | <i>characteristics[organism]</i> | <i>characteristics[organism part]</i> | <i>characteristics[disease]</i> |
|-------------|--|----------------------------------|---------------------------------------|---------------------------------|
| sample_001 | SAMN12345678 | homo sapiens | liver | liver cancer |
| sample_002 | SAMN12345679 | homo sapiens | liver | normal |
| sample_003 | SAMEA12345680 | mus musculus | brain | normal |

The BioSamples accession number enables:

- **Cross-database linking:** Connect proteomics datasets with genomics, transcriptomics, and other omics data that reference the same biological samples

- **Enhanced metadata:** Access additional sample metadata stored in the BioSamples database
- **Data provenance:** Trace the origin and history of biological samples across multiple studies
- **Improved findability:** Enable discovery of related datasets through shared sample identifiers

When a BioSample accession number is provided, the full sample metadata from the corresponding BioSamples database becomes available and can complement the information provided in the SDRF-Proteomics file. If there are discrepancies between the SDRF-Proteomics metadata and the BioSamples metadata, the SDRF-Proteomics values take precedence for the specific proteomics experiment context.

NOTE

BioSample accession numbers from NCBI follow the format [SAMNxxxxxxxxxx](#) and from EBI follow the format [SAMEAxxxxxxxxxx](#), where [x](#) represents digits. Either NCBI or EBI BioSample accession numbers can be used depending on where the sample is registered. The *characteristics[biosample accession number]* column is optional, but when available, providing BioSample accession numbers is RECOMMENDED to enhance data integration and reusability. Users must first request BioSample accession numbers from the appropriate service (NCBI or EBI) before including them in their SDRF files.

9.2. Encoding sample technical and biological replicates

Different measurements of the same biological sample are often categorized as (i) Technical or (ii) Biological replicates, based on whether they are (i) matched on all variables, e.g. same sample and same protocol; or (ii) different samples matched on explanatory variable(s), e.g. different patients receiving a placebo, in a placebo vs. drug trial. Technical and biological replicates have different levels of independence, which must be taken into account during data interpretation.

For a given experiment, there are different levels to which samples can be matched - e.g., same sample, sample protocol, covariates - the definition of technical replicate can therefore vary based on the number of variables included. In addition, an experiment might be used in multiple models with different explanatory variable(s), and biological replicates in one model would not be replicates in another. Therefore, Technical vs. Biological considerations, while sometimes relevant to analytical and statistical interpretation, fall beyond the scope of the SDRF-Proteomics format. However, data providers are encouraged to provide any identifier - e.g. Biological_replicate_1, Technical_replicate_2 - that would help link the samples to their analytical and statistical analysis as comments. A good starting point for the SDRF-Proteomics specification is the following:

technical replicate: It is defined as repeated measurements of the same sample that represent independent measures of the random noise associated with protocols or equipment [4].

In MS-based proteomics, a technical replicate can be, for example, doing the full sample preparation from extraction to MS multiple times to control variability in the instrument and sample preparation. Another valid example would be to replicate only one part of the analytical method, for example, run the sample twice on the LC-MS/MS. technical replicates indicate if measurements are scientifically robust or noisy, and how large the measured effect must be to stand out above that noise.

Biological replicate: parallel measurements of biologically distinct samples that capture biological variation, which may itself be a subject of study or a source of noise. Biological replicates address if and

how widely the results of an experiment can be generalized. For example, repeating a particular assay with independently generated samples, individuals or samples derived from various cell types, tissue types, or organisms, to see if similar results can be observed. Context is critical, and appropriate biological replicates will indicate whether an experimental effect is sustainable under a different set of biological variables or an anomaly itself.

The following example shows an experiment with 2 biological replicates (different samples from 2 patients), each with 2 fractions and 2 technical replicates:

| source name | characteristics[biological replicate] | assay name | comment[label] | comment[fraction identifier] | comment[technical replicate] | comment[data file] |
|--------------------|---------------------------------------|------------|-------------------|------------------------------|------------------------------|--------------------|
| patient_001_sample | 1 | run_01 | label free sample | 1 | 1 | P001_F1_TR 1.raw |
| patient_001_sample | 1 | run_02 | label free sample | 2 | 1 | P001_F2_TR 1.raw |
| patient_001_sample | 1 | run_03 | label free sample | 1 | 2 | P001_F1_TR 2.raw |
| patient_001_sample | 1 | run_04 | label free sample | 2 | 2 | P001_F2_TR 2.raw |
| patient_002_sample | 2 | run_05 | label free sample | 1 | 1 | P002_F1_TR 1.raw |
| patient_002_sample | 2 | run_06 | label free sample | 2 | 1 | P002_F2_TR 1.raw |
| patient_002_sample | 2 | run_07 | label free sample | 1 | 2 | P002_F1_TR 2.raw |
| patient_002_sample | 2 | run_08 | label free sample | 2 | 2 | P002_F2_TR 2.raw |

In this example:

- **Biological replicates:** `patient_001_sample` and `patient_002_sample` are different biological samples (different source names), annotated with `characteristics[biological replicate]` values 1 and 2
- **Technical replicates:** Each biological sample is measured twice (`comment[technical replicate]` = 1 and 2)
- **Fractions:** Each technical replicate has 2 fractions (`comment[fraction identifier]` = 1 and 2)

IMPORTANT

Both `characteristics[biological replicate]` and `comment[technical replicate]` columns are REQUIRED. When no replicates are performed in a study, set both columns to 1 (i.e., each sample is biological replicate 1 and technical replicate 1).

Some examples with explicit annotation of the biological replicates can be found here:

- <https://github.com/bigbio/proteomics-metadata-standard/blob/c3a56b076ef381280dfcb0140d2520126ace53ff/annotated-projects/PXD006401/sdrf.tsv>

9.3. Pooled samples

When multiple samples are pooled into one, the general approach is to annotate them separately, abiding by the general rule: one row stands for one sample-to-file relationship. In this case, multiple rows are created for the corresponding data file, much like in multiplexed labeling experiments (see [Label Annotations](#)).

One possible exception is made for the case when one channel (e.g., in a TMT/iTRAQ multiplexed experiment) is used for a sample pooled from all other channels, typically for normalization purposes. In this case, it is not necessary to repeat all sample annotations. Instead, the *characteristics[pooled sample]* column SHOULD be used.

9.3.1. Allowed values for characteristics[pooled sample]

The *characteristics[pooled sample]* column accepts the following values:

| Value | Description | When to Use |
|---------------------------|--|---|
| not pooled | Sample is not pooled, represents a single biological sample | Regular individual samples |
| pooled | Sample is pooled but individual source samples cannot be annotated | When pooling details are unknown or samples are from external sources |
| SN=sample1;SN=sample2;... | Structured format listing source names of pooled samples | When individual samples are known and annotated in the same SDRF file |

NOTE

The [SN](#) key stands for "source name" and lists the [source name](#) values of samples that are annotated in the same file and used in the same experiment and same MS run. Use semicolons to separate multiple entries.

9.3.2. Example with pooled reference channel

| source name | characteristics[pooled sample] | characteristics[organism] | characteristics[age] | characteristics[sex] | assay name | comment[label] | comment[data file] |
|-------------|--------------------------------|---------------------------|----------------------|----------------------|------------|----------------|--------------------|
| sample_1 | not pooled | homo sapiens | 45Y | male | run_1 | TMT126 | file01.raw |
| sample_2 | not pooled | homo sapiens | 52Y | female | run_1 | TMT127N | file01.raw |

| source name | characteristics[pooled sample] | characteristics[organism] | characteristics[age] | characteristics[sex] | assay name | comment[label] | comment[data file] |
|-------------|-------------------------------------|---------------------------|----------------------|----------------------|------------|----------------|--------------------|
| sample_3 | not pooled | homo sapiens | 38Y | male | run_1 | TMT127C | file01.raw |
| pooled_ref | SN=sample_1;SN=sample_2;SN=sample_3 | homo sapiens | not applicable | not applicable | run_1 | TMT131C | file01.raw |

9.3.3. Metadata handling for pooled samples

When a sample is pooled from multiple individuals, certain sample-specific metadata fields are no longer meaningful at the individual level. For pooled samples, the following metadata handling rules apply:

Fields that **SHOULD** use "not applicable" for pooled samples:

- `characteristics[age]` - Age is not applicable when samples from multiple individuals of different ages are pooled
- `characteristics[sex]` - Sex is not applicable when samples from individuals of different sexes are pooled
- `characteristics[individual]` - Individual identifier is not applicable for pooled samples
- `characteristics[ancestry category]` - Ancestry is not applicable when samples from individuals of different ancestries are pooled

Fields that **SHOULD** still be annotated for pooled samples:

- `characteristics[organism]` - The organism **SHOULD** still be specified (all pooled samples should be from the same organism)
- `characteristics[organism part]` - The tissue/organ **SHOULD** be specified if consistent across pooled samples
- `characteristics[disease]` - Disease status **SHOULD** be specified if consistent across pooled samples, otherwise use "not applicable"
- `characteristics[cell type]` - Cell type **SHOULD** be specified if consistent across pooled samples

IMPORTANT

When `characteristics[pooled sample]` contains "pooled" or an "SN=..." value, validators **SHOULD** accept "not applicable" for individual-specific metadata fields (age, sex, individual, ancestry category). This enables proper annotation of reference/normalization channels in multiplexed experiments.

TIP

If all pooled samples share the same value for a characteristic (e.g., all from females, or all age 40-50Y), that shared value **MAY** be used instead of "not applicable".

9.4. Spiked-in samples

There are multiple scenarios when a sample is spiked with additional analytes. Peptides, proteins, or mixtures can be added to the sample as controlled amounts to provide a standard or ground truth for quantification, or for retention time alignment, etc.

To include information about the spiked compounds, use *characteristics[spiked compound]*. The information is provided in key-value pairs. Here are the keys and values that **SHOULD** be provided:

| Key | Meaning | Examples | Peptide | Protein | Mixture | Other |
|-----|----------------------------|---|----------|----------|----------|----------|
| CT | Compound type | protein, peptide, mixture, other | Required | Required | Required | Required |
| QY | Quantity (molar or mass) | 10 mg, 20 nmol | Required | Required | Required | Required |
| PS | Peptide sequence | PEPTIDESE Q | Required | - | - | - |
| AC | Uniprot Accession | A9WZ33 | - | Required | - | - |
| CN | Compound name | iRT mixture, substance name | Optional | Optional | Optional | Optional |
| SP | Species | Escherichia coli K-12 | Optional | Optional | Optional | Optional |
| CV | Compound vendor | in-house or vendor name | Optional | Optional | Required | Optional |
| CS | Compound specification URI | http://vendor.web.site/specs/kit.xlsx | Optional | Optional | Optional | Optional |
| CF | Compound formula | C ₂ H ₂ O | - | - | - | Optional |

In addition to specifying the component and its quantity, the injected mass of the main sample **SHOULD** be specified as *characteristics[mass]*.

An example of SDRF-Proteomics for a sample spiked with a peptide would be:

| | |
|-----------------------|-------------------------------------|
| characteristics[mass] | characteristics[spiked compound] |
| 1 ug | CT=peptide;PS=PEPTIDESEQ;QY=10 fmol |

For multiple spiked components, the column *characteristics[spiked compound]* may be repeated.

If the spiked component is another biological sample (e.g. *E. coli* lysate spiked into human sample), then the spiked component MUST be annotated in its own row. Both components of the sample SHOULD have `characteristics[mass]` specified. Inclusion of `characteristics[spiked compound]` is optional in this case; if provided, it SHOULD be the string `spiked` for the spiked sample.

9.5. Sample Metadata Guidelines

For detailed guidance on annotating sample metadata, refer to the following conventions documents:

- [Sample Metadata Guidelines](#) - Detailed guidelines for age, sex, disease, organism part, cell type, developmental stage, and other sample characteristics
- [Human Sample Metadata Guidelines](#) - Human-specific metadata including disease staging, treatment history, demographics, and lifestyle factors

Chapter 10. SDRF-Proteomics: data files metadata

The connection between samples and data files is done using properties annotated with the **comment** prefix. All properties referring to a data file (e.g., MS run file) are annotated with the category `comment`. This differentiates data file properties from sample properties (characteristics).

The following properties **MUST** be provided for each data file:

| Column | Requirement | Description |
|---|-------------|--|
| assay name | REQUIRED | Unique identifier for an MS run/data file |
| technology type | REQUIRED | Technology used to capture the data |
| comment[proteomics data acquisition method] | REQUIRED | DDA, DIA, PRM, SRM |
| comment[label] | REQUIRED | Label applied to sample (or "label free sample") |
| comment[instrument] | REQUIRED | Mass spectrometer model |
| comment[cleavage agent details] | REQUIRED | Enzyme information |
| comment[fraction identifier] | REQUIRED | Fraction number (1 if not fractionated) |
| comment[technical replicate] | REQUIRED | Technical replicate number (1 if none) |
| comment[data file] | REQUIRED | Name of the raw file |

IMPORTANT

The combination of source name + assay name + comment[label] **MUST** be unique within the SDRF file.

Example:

| source name | assay name | technology type | comment[proteomics data acquisition method] | comment[label] | comment[instrument] | comment[data file] |
|-------------|---------------|--|---|-------------------|---------------------|--------------------|
| sample_1 | sample1_run 1 | proteomic profiling by mass spectrometry | data-dependent acquisition | label free sample | Q Exactive HF | sample1.raw |

10.1. Sample preparation properties

In order to encode sample preparation details, we strongly RECOMMEND specifying the following parameters:

- **comment[depletion]:** The removal of specific components of a complex mixture of proteins or peptides based on some specific property of those components. The values of the columns will be [no depletion](#) or [depletion](#). In the case of depletion [depleted fraction](#) or [bound fraction](#) can be specified.
- **comment[reduction reagent]:** The chemical reagent that is used to break disulfide bonds in proteins. The values of the column are under the term [reduction reagent](#). For example, DTT.
- **comment[alkylation reagent]:** The alkylation reagent that is used to covalently modify cysteine SH-groups after reduction, preventing them from forming unwanted novel disulfide bonds. The values of the column are under the term [alkylation reagent](#). For example, IAA.
- **comment[fractionation method]:** The fraction method used to separate the sample. The values of this term can be read under PRIDE ontology term [Fractionation method](#). For example, Off-gel electrophoresis.

10.2. MS/MS properties

- **comment[collision energy]:** Collision energy can be added as non-normalized (10000 eV) or normalized (1000 NCE) value.
- **comment[dissociation method]:** This property will provide information about the fragmentation method, like HCD, CID. The values of the column are under the term [dissociation method](#).

10.3. Data acquisition

Proteomics data acquisition method can happen in multiple ways: Data Dependent Acquisition (DDA), Data Independent Acquisition (DIA), and targeted approaches. The SDRF-Proteomics file format REQUIRES capturing the method used for the data acquisition in the *comment[proteomics data acquisition method]* column. The values MUST be children of the PRIDE ontology term [proteomics data acquisition method](#) (PRIDE:0000659). The following values are commonly used:

- [data-dependent acquisition](#)
- [data-independent acquisition](#)
 - [diaPASEF](#)
 - [SWATH MS](#)
- [parallel reaction monitoring](#)
- [selected reaction monitoring](#)

IMPORTANT

The *comment[proteomics data acquisition method]* column is REQUIRED for all mass spectrometry-based SDRF files. This field must be explicitly specified and cannot be omitted or assumed.

You can find an example of a DIA experiment in the following link: [DIA example](#)

TIP

For DIA experiments, additional properties like MS1 scan range can be captured. See [DIA Scan Window Limits](#) in the Data File Metadata Guidelines.

10.4. Data File Metadata Guidelines

For detailed guidance on data file metadata, refer to the conventions document:

- [Data File Metadata Guidelines](#) - Detailed guidelines for labels, instruments, modifications, cleavage agents, mass tolerances, RAW file URIs, and other data file properties

Chapter 11. Core Templates

SDRF-Proteomics provides core templates that define the required and recommended metadata columns based on the sample organism. Each template includes both **sample metadata** (characteristics) and **data file metadata** (comments) - everything needed to create a complete SDRF file.

Choose the appropriate template based on your sample organism:

- [Default template](#): Basic template for any proteomics experiment
- [Human template](#): For human samples with additional clinical metadata (age, sex, ancestry)
- [Vertebrates template](#): For non-human vertebrate species (mouse, rat, zebrafish)
- [Invertebrates template](#): For insects (*Drosophila*), nematodes (*C. elegans*), and other invertebrates
- [Plants template](#): For plant species (*Arabidopsis*, crops)

For detailed explanations of each column, see [sample metadata](#) for sample properties and [data file metadata](#) for data file properties.

11.1. Default Template

The default template is the most basic template that can be used for any proteomics experiment. Use this when no other template is applicable.

Checklist:

| Column | Category | Requirement | Example |
|---|----------|-------------|--|
| Sample Metadata | | | |
| source name | Sample | Required | sample_1 |
| characteristics[organism] | Sample | Required | homo sapiens |
| characteristics[organism part] | Sample | Required | liver |
| characteristics[disease] | Sample | Required | normal |
| characteristics[biological replicate] | Sample | Required | 1 |
| Data File Metadata | | | |
| assay name | Data | Required | run_1 |
| technology type | Data | Required | proteomic profiling by mass spectrometry |
| comment[proteomics data acquisition method] | Data | Required | data-dependent acquisition |

| Column | Category | Requirement | Example |
|---|----------|-------------|--------------------------|
| comment[label] | Data | Required | label free sample |
| comment[instrument] | Data | Required | Q Exactive HF |
| comment[cleavage agent details] | Data | Required | NT=Trypsin;AC=MS:1001251 |
| comment[fraction identifier] | Data | Required | 1 |
| comment[technical replicate] | Data | Required | 1 |
| comment[data file] | Data | Required | sample_1.raw |

Template file: [sdrf-default.sdrf.tsv](#)

NOTE

The [characteristics\[cell type\]](#) column is RECOMMENDED across all templates when the cell type is known or can be determined. Use [not available](#) if the cell type cannot be determined (e.g., whole tissue samples, mixed cell populations). For cell line experiments, use the cell-lines template which provides more specific guidance.

11.2. Human Template

The human template extends the default template with clinical and demographic metadata required for human samples.

Checklist:

| Column | Category | Requirement | Example |
|---|----------|-------------|--------------------------|
| Sample Metadata | | | |
| source name | Sample | Required | patient_001 |
| characteristics[organism] | Sample | Required | homo sapiens |
| characteristics[organism part] | Sample | Required | liver |
| characteristics[disease] | Sample | Required | hepatocellular carcinoma |
| characteristics[cell type] | Sample | Recommended | hepatocyte |
| characteristics[biological replicate] | Sample | Required | 1 |
| characteristics[age] | Sample | Required | 45Y |
| characteristics[sex] | Sample | Required | male |

| Column | Category | Requirement | Example |
|---|----------|-------------|--|
| characteristics[ancestry category] | Sample | Recommended | European |
| characteristics[individual] | Sample | Recommended | P001 |
| Data File Metadata | | | |
| assay name | Data | Required | patient_001_run1 |
| technology type | Data | Required | proteomic profiling by mass spectrometry |
| comment[proteomics data acquisition method] | Data | Required | data-dependent acquisition |
| comment[label] | Data | Required | label free sample |
| comment[instrument] | Data | Required | Orbitrap Exploris 480 |
| comment[cleavage agent details] | Data | Required | NT=Trypsin;AC=MS:1001251 |
| comment[fraction identifier] | Data | Required | 1 |
| comment[technical replicate] | Data | Required | 1 |
| comment[data file] | Data | Required | patient_001.raw |

Template file: [sdrf-human.sdrf.tsv](#)

NOTE

The [characteristics\[individual\]](#) column is optional and is only used when a code for the individual is available; if not, use **not available**. For age encoding format, see [Sample Metadata Guidelines](#).

11.3. Vertebrates Template

The vertebrates template is used for non-human vertebrate species such as mouse, rat, zebrafish, and other model organisms.

Checklist:

| Column | Category | Requirement | Example |
|---|----------|-------------|--------------|
| Sample Metadata | | | |
| source name | Sample | Required | mouse_001 |
| characteristics[organism] | Sample | Required | mus musculus |

| Column | Category | Requirement | Example |
|---|----------|-------------|--|
| characteristics[organism part] | Sample | Required | brain |
| characteristics[disease] | Sample | Required | normal |
| characteristics[cell type] | Sample | Recommended | neuron |
| characteristics[biological replicate] | Sample | Required | 1 |
| characteristics[developmental stage] | Sample | Recommended | adult |
| Data File Metadata | | | |
| assay name | Data | Required | mouse_001_run1 |
| technology type | Data | Required | proteomic profiling by mass spectrometry |
| comment[proteomics data acquisition method] | Data | Required | data-dependent acquisition |
| comment[label] | Data | Required | label free sample |
| comment[instrument] | Data | Required | timsTOF Pro |
| comment[cleavage agent details] | Data | Required | NT=Trypsin;AC=MS:1001251 |
| comment[fraction identifier] | Data | Required | 1 |
| comment[technical replicate] | Data | Required | 1 |
| comment[data file] | Data | Required | mouse_001.raw |

Template file: [sdrf-vertebrates.sdrf.tsv](#)

11.4. Invertebrates Template

The invertebrates template is used for non-vertebrate animal species such as insects (*Drosophila*), nematodes (*C. elegans*), and other invertebrate model organisms.

Checklist:

| Column | Category | Requirement | Example |
|------------------------|----------|-------------|--------------|
| Sample Metadata | | | |
| source name | Sample | Required | fly_sample_1 |

| Column | Category | Requirement | Example |
|---|----------|-------------|--|
| characteristics[organism] | Sample | Required | drosophila melanogaster |
| characteristics[organism part] | Sample | Required | head |
| characteristics[disease] | Sample | Required | normal |
| characteristics[cell type] | Sample | Recommended | neuron |
| characteristics[biological replicate] | Sample | Required | 1 |
| Data File Metadata | | | |
| assay name | Data | Required | fly_sample_1_run1 |
| technology type | Data | Required | proteomic profiling by mass spectrometry |
| comment[proteomics data acquisition method] | Data | Required | data-dependent acquisition |
| comment[label] | Data | Required | label free sample |
| comment[instrument] | Data | Required | Q Exactive Plus |
| comment[cleavage agent details] | Data | Required | NT=Trypsin;AC=MS:1001251 |
| comment[fraction identifier] | Data | Required | 1 |
| comment[technical replicate] | Data | Required | 1 |
| comment[data file] | Data | Required | fly_sample_1.raw |

Template file: [sdrf-invertebrates.sdrf.tsv](#)

NOTE

For Drosophila samples, use [FBbt](#) (FlyBase anatomy ontology) for organism part. For C. elegans, use [WBbt](#) (WormBase anatomy ontology).

11.5. Plants Template

The plants template is used for plant species including model organisms like Arabidopsis thaliana and crop species.

Checklist:

| Column | Category | Requirement | Example |
|------------------------|----------|-------------|---------|
| Sample Metadata | | | |

| Column | Category | Requirement | Example |
|---|----------|-------------|--|
| source name | Sample | Required | arabidopsis_col0_1 |
| characteristics[organism] | Sample | Required | arabidopsis thaliana |
| characteristics[organism part] | Sample | Required | leaf |
| characteristics[disease] | Sample | Required | normal |
| characteristics[cell type] | Sample | Recommended | guard cell |
| characteristics[biological replicate] | Sample | Required | 1 |
| Data File Metadata | | | |
| assay name | Data | Required | arabidopsis_col0_run1 |
| technology type | Data | Required | proteomic profiling by mass spectrometry |
| comment[proteomics data acquisition method] | Data | Required | data-dependent acquisition |
| comment[label] | Data | Required | label free sample |
| comment[instrument] | Data | Required | Orbitrap Fusion Lumos |
| comment[cleavage agent details] | Data | Required | NT=Trypsin;AC=MS:1001251 |
| comment[fraction identifier] | Data | Required | 1 |
| comment[technical replicate] | Data | Required | 1 |
| comment[data file] | Data | Required | arabidopsis_col0.raw |

Template file: [sdrf-plants.sdrf.tsv](#)

NOTE | For plant samples, use [PO](#) (Plant Ontology) for organism part and cell type annotations.

11.6. Column Cardinality

Some columns can appear multiple times for the same sample. The cardinality rules are:

- **Single (1):** Column appears exactly once per sample (e.g., biological replicate)
- **Multiple (*):** Column can appear multiple times (e.g., organism part can specify both "heart" and "heart left ventricle")

Example of multiple organism part columns:

| source name | characteristics[organism part] | characteristics[organism part] |
|-------------|--------------------------------|--------------------------------|
| sample-1 | heart | heart left ventricle |

The template files can be downloaded from the [core-templates](#) folder.

Chapter 12. Factor Values (Study Variables)

Factor values identify the experimental variables being studied - the conditions you want to compare in your analysis. They highlight which sample characteristics are the focus of your experiment.

12.1. Column Format

```
factor value[{variable name}]
```

12.2. When to Use Factor Values

Use factor values to indicate:

- The primary variable(s) under investigation
- Conditions being compared (e.g., disease vs. control, treated vs. untreated)
- Variables that define experimental groups

12.3. Rules

- Factor value columns SHOULD appear after all characteristics and comment columns
- Multiple factor values can be used when studying multiple variables
- The value in a factor value column typically mirrors a characteristics column value

12.4. Example

In an experiment comparing tumor vs. normal tissue across different cancer stages:

| source name | characteristics[disease] | characteristics[disease stage] | factor value[disease] | factor value[disease stage] |
|-----------------|--------------------------|--------------------------------|-----------------------|-----------------------------|
| tumor_sample_1 | breast carcinoma | stage II | breast carcinoma | stage II |
| normal_sample_1 | normal | not applicable | normal | not applicable |
| tumor_sample_2 | breast carcinoma | stage III | breast carcinoma | stage III |

In this example, both `disease` and `disease stage` are factor values because the experiment aims to compare expression differences between disease states and across cancer stages.

Chapter 13. Experiment-specific Templates

For specialized proteomics experiments that require additional metadata beyond the core templates, experiment-specific templates provide detailed guidelines and checklists. These templates define experiment-specific metadata fields while maintaining full compatibility with the core SDRF-Proteomics format.

Choose the appropriate template based on your experiment type:

- **Affinity Proteomics:** Olink, SomaScan, Luminex, and other affinity-based methods
- **Cell Lines:** Standardized cell line annotation using Cellosaurus
- **Crosslinking:** XL-MS structural proteomics experiments
- **Immunopeptidomics:** MHC-bound peptide identification
- **Metaproteomics:** Microbial community proteomics
- **Single Cell:** Single cell proteomics experiments

For detailed specifications and examples, visit the [Experiment-specific Templates](#) documentation.

Chapter 14. Examples of Annotated Datasets

The following table provides links to example SDRF files for different experiment types. These can serve as references when creating your own SDRF files.

| Experiment Type | Dataset | Description | SDRF URL |
|-------------------|-----------|--|---------------------------|
| Label-free | PXD008934 | Human proteome label-free quantification | View SDRF |
| TMT | PXD017710 | TMT-labeled quantitative proteomics | View SDRF |
| SILAC | PXD000612 | SILAC-based quantification | View SDRF |
| DIA | PXD018830 | Data-independent acquisition | View SDRF |
| Phosphoproteomics | PXD000759 | PTM enrichment study | View SDRF |
| Cell lines | PXD001819 | Cell line proteomics | View SDRF |

A comprehensive collection of annotated projects is available at: [Annotated Projects Repository](#)

Chapter 15. Ongoing template discussions

We have created a file in GitHub [Ongoing template discussions](#) where we aggregate all the ongoing discussions about the format and new templates.

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Dai C, Füllgrabe A, Pfeuffer J, Solovyeva EM, Deng J, Moreno P, Kamatchinathan S, Kundu DJ, George N, Fexova S, Grüning B, Föll MC, Griss J, Vaudel M, Audain E, Locard-Paulet M, Turewicz M, Eisenacher M, Uszkoreit J, Van Den Bossche T, Schwämmle V, Webel H, Schulze S, Bouyssié D, Jayaram S, Duggineni VK, Samaras P, Wilhelm M, Choi M, Wang M, Kohlbacher O, Brazma A, Papatheodorou I, Bandeira N, Deutsch EW, Vizcaíno JA, Bai M, Sachsenberg T, Levitsky LI, Perez-Riverol Y. A proteomics sample metadata representation for multiomics integration and big data analysis. Nat Commun. 2021 Oct 6;12(1):5854. doi: 10.1038/s41467-021-26111-3. PMID: 34615866; PMCID: PMC8494749. [Manuscript - <https://www.nature.com/articles/s41467-021-26111-3>]

Chapter 19. References

- [1] Y. Perez-Riverol, S. European Bioinformatics Community for Mass, Toward a Sample Metadata Standard in Public Proteomics Repositories, *J Proteome Res* 19(10) (2020) 3906-3909.
- [2] A. Gonzalez-Beltran, E. Maguire, S.A. Sansone, P. Rocca-Serra, linkedISA: semantic representation of ISA-Tab experimental metadata, *BMC Bioinformatics* 15 Suppl 14 (2014) S4.
- [3] T.F. Rayner, P. Rocca-Serra, P.T. Spellman, H.C. Causton, A. Farne, E. Holloway, R.A. Irizarry, J. Liu, D.S. Maier, M. Miller, K. Petersen, J. Quackenbush, G. Sherlock, C.J. Stoeckert, Jr., J. White, P.L. Whetzel, F. Wymore, H. Parkinson, U. Sarkans, C.A. Ball, A. Brazma, A simple spreadsheet-based, MIAME-supportive format for microarray data: MAGE-TAB, *BMC Bioinformatics* 7 (2006) 489.
- [4] P. Blainey, M. Krzywinski, N. Altman, Points of significance: replication, *Nat Methods* 11(9) (2014) 879-80.