

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

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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 Format (SDRF)-Proteomics. Distribution is unlimited.

Version v1.1.0 - 2026-01

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: [HUPO-PSI SDRF](#).

Chapter 3. Motivation

Public proteomics data is valuable, but sample metadata is often missing or stored inconsistently across repositories (e.g., [CPTAC](#) uses Excel files, [ProteomicsDB](#) captures minimal properties) [1]. This heterogeneity prevents reproducibility and cross-dataset integration.

SDRF-Proteomics addresses this by providing a standard tab-delimited format to capture (**Figure 1**):

- Sample metadata and characteristics
- Data file acquisition parameters
- Sample-to-file relationships (experimental design)

[sample metadata] | <https://github.com/bigbio/proteomics-metadata-standard/raw/master/sdrf-proteomics/images/sample-metadata.png>

Figure 1: SDRF-Proteomics captures sample information and its relationship to data files.

The format is fully compatible with [MAGE-TAB](#) SDRF, enabling integration with transcriptomics metadata standards.

Chapter 4. Specification structure

SDRF-Proteomics uses a two-tier system: this **core specification** defines the format rules, and **templates** provide metadata checklists for specific experiment types (**Figure 2**). Templates are organized in the [templates/](#) directory, each with documentation and example files.

[Logo] | [images/sdrf-guidelines-structure.png](#)

Figure 2: SDRF-Proteomics specification structure. The main specification defines the core rules and is extended by sample templates (human, vertebrates, etc.) and experiment-type templates (crosslinking, immunopeptidomics, etc.).

The official repository is [GitHub](#), where you can find [annotated example projects](#) and the official validator [sdrf-pipelines](#).

IMPORTANT

Throughout this specification, the keywords "MUST", "REQUIRED", "SHOULD", "RECOMMENDED", and "OPTIONAL" are interpreted as described in [RFC 2119](#).

Chapter 5. The SDRF-Proteomics Format

SDRF-Proteomics is a **tab-delimited file** where:

- Each **row** = one sample linked to one data file
- Each **column** = a property (sample characteristic, data file attribute, or factor value)
- Each **cell** = the property value for that sample/file or a factor value.

Here's a 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] | factor value[disease] |
|-------------|---------------------------|--------------------------------|--------------------------|---------------------------------------|------------|--|---|-------------------|---------------------|---------------------------------|------------------------------|------------------------------|--------------------|--------------------------|
| 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 | normal |
| 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 | hepatocellular carcinoma |

| source name | characteristics[organism] | characteristics[organism part] | characteristics[disease] | characteristics[biological replicate] | assay name | technology type | comment[proteomic data acquisition method] | comment[label] | comment[instrument] | comment[cleavage agent details] | comment[fraction identifier] | comment[technical replicate] | comment[data file] | factor value[disease] |
|-------------|---------------------------|--------------------------------|--------------------------|---------------------------------------|------------|--|--|-------------------|---------------------|---------------------------------|------------------------------|------------------------------|--------------------|-----------------------|
| sample_3 | homo sapiens | not available | not available | 1 | run_3 | proteomic profiling by mass spectrometry | Data-dependent acquisition | label free sample | Q Exactive HF | NT=Trypsin;AC=MS:1001251 | 1 | 1 | sample_3.raw | not available |

The file is organized into three column sections:

1. **Sample metadata** (`characteristics[...]`) - organism, disease, tissue, etc.
2. **Data file metadata** (`comment[...]`) - instrument, label, fraction, data file
3. **Factor values** (`factor value[...]`) - variables under study for statistical analysis

NOTE

- This example shows **mass spectrometry** proteomics - see [MS-Proteomics template](#) for full requirements.
- For **affinity proteomics** (Olink, SomaScan), see [Affinity-Proteomics template](#).
- Unknown values use **reserved words**: `not available`, `not applicable`, or `pooled`.
- For a step-by-step tutorial, see the [Quick Start Guide](#).

5.1. Versioning

The SDRF-Proteomics specification uses [Semantic Versioning](#) (MAJOR.MINOR.PATCH). Version numbers are prefixed with "v" (e.g., v1.1.0). Changes are proposed via GitHub pull requests to the dev branch.

5.2. Format rules

- **Case sensitivity**: Text values are case-insensitive, but **column names are case-sensitive**. Use

lowercase for all column names (e.g., `source name`, `characteristics[organism]`, `comment[label]`). Incorrect casing like `Source Name` or `Characteristics[organism]` will cause validation failures.

- **Space sensitivity:** The SDRF is sensitive to spaces in column names (`sourcename` \neq `source name`). Column names must include appropriate spaces (e.g., `source name`, not `sourcename`) but must NOT have a space before the bracket (e.g., `characteristics[organism]`, not `characteristics [organism]`).
- **Column order:** The SDRF columns follows some structure; first the sample metadata columns in [Chapter 7](#); then the data file metadata columns in [Chapter 8](#); followed by the factor values columns in [\[study-variables\]](#).
- **Extension:** The extension of the SDRF file SHOULD be **sdrf.tsv (preferred)** or **.txt**.

5.3. Reserved words

There are general scenarios where cell values cannot be provided with actual data. The following reserved words MUST be used in these cases:

- **not available:** In some cases, the column is mandatory in the format, but for some samples the corresponding value is unknown or could not be determined. In those cases, users SHOULD use **not available**.
- **not applicable:** In some cases, the column is mandatory, but for some samples the corresponding value or concept does not apply. In those cases, users SHOULD use **not applicable**.
- **anonymized:** In some cases, the value exists but has been intentionally redacted for privacy protection (e.g., in clinical studies with de-identified patient data). In those cases, users SHOULD use **anonymized**.
- **pooled:** In some cases, the sample is a pool of multiple samples (e.g., TMT reference channels), and the value cannot be represented as a single value. In those cases, users SHOULD use **pooled**.

Table 1. Reserved words for SDRF cell values

| Term | Meaning | Example | Use Case |
|----------------|--|---|---|
| not available | Value exists but is unknown or could not be determined | <code>characteristics[age] = not available</code> | Patient age was not recorded in the study |
| not applicable | Value or concept does not apply to this sample | <code>characteristics[age] = not applicable</code> | Synthetic peptide library has no age |
| anonymized | Value exists but is redacted for privacy protection | <code>characteristics[age] = anonymized</code> | Clinical study with de-identified patient data |
| pooled | Value represents a mixture of multiple samples | <code>characteristics[biological replicate] = pooled</code> | TMT reference channel pooled from multiple replicates |

5.4. SDRF file-level metadata

Since version 1.1.0, SDRF-Proteomics supports file-level metadata using dedicated columns. These columns provide information about the SDRF file itself, such as the specification version, template(s) used, annotation tool, and validation status. This column-based approach maintains compatibility with spreadsheet applications (Excel, Google Sheets) and existing data processing tools.

The following metadata columns are supported:

| Column | Description | Example Value | Requirement | Ontology Term |
|--|--|--|-------------|---------------|
| <code>comment[sdrf version]</code> | SDRF-Proteomics specification version used. Should follow semantic versioning format (vMAJOR.MINOR.PATCH) | v1.1.0 | REQUIRED | PRIDE:0000839 |
| <code>comment[sdrf template]</code> | Template name and version used for annotation. Two formats are supported: simple format (<code>name vX.Y.Z</code>) or key=value format (<code>NT=name;VV=vX.Y.Z</code>). Multiple templates can be specified using multiple columns. | human v1.1.0 or NT=human;VV=v1.1.0 | OPTIONAL | PRIDE:0000832 |
| <code>comment[sdrf annotation tool]</code> | Software tool, script, or method used to generate or annotate the SDRF file. Two formats are supported: simple format (<code>name vX.Y.Z</code>) or key=value format (<code>NT=name;VV=vX.Y.Z</code>). | lesSDRF v0.1.0 or NT=lesSDRF;VV=v0.1.0 | OPTIONAL | PRIDE:0000840 |
| <code>comment[sdrf validation hash]</code> | Cryptographic hash (e.g., SHA-256) generated after successful validation | sha256:abc123... | OPTIONAL | PRIDE:0000834 |

NOTE

When combining multiple templates (e.g., `human` + `ms-proteomics`), use multiple `comment[sdrf template]` columns, one per template. The value in each row should be identical for all samples in the file.

Example of an SDRF file with metadata columns (simplified example showing only select columns; see [Chapter 10](#) for complete required columns):

```
<div class="sdrf-example-table">
<table>
<thead>
<tr>
<th class="sample-col">source name</th>
<th class="sample-col">characteristics[organism]</th>
<th class="sample-col">characteristics[disease]</th>
<th class="data-col">assay name</th>
<th class="data-col">comment[data file]</th>
<th class="data-col">comment[sdrf version]</th>
<th class="data-col">comment[sdrf template]</th>
<th class="data-col">comment[sdrf template]</th>
```

```

<th class="data-col">comment[sdrf annotation tool]</th>
</tr>
</thead>
<tbody>
<tr>
<td class="sample-col">sample_1</td>
<td class="sample-col">homo sapiens</td>
<td class="sample-col">normal</td>
<td class="data-col">run_1</td>
<td class="data-col">sample_1.raw</td>
<td class="data-col">v1.1.0</td>
<td class="data-col">human v1.1.0</td>
<td class="data-col">ms-proteomics v1.1.0</td>
<td class="data-col">lesSDRF v0.1.0</td>
</tr>
<tr>
<td class="sample-col">sample_2</td>
<td class="sample-col">homo sapiens</td>
<td class="sample-col">breast cancer</td>
<td class="data-col">run_2</td>
<td class="data-col">sample_2.raw</td>
<td class="data-col">v1.1.0</td>
<td class="data-col">human v1.1.0</td>
<td class="data-col">ms-proteomics v1.1.0</td>
<td class="data-col">lesSDRF v0.1.0</td>
</tr>
</tbody>
</table>
<div class="sdrf-legend">
<span class="legend-item"><span class="legend-color sample-bg"></span> Sample
metadata</span>
<span class="legend-item"><span class="legend-color data-bg"></span> Data file
metadata</span>
</div>
</div>

```

5.5. Table 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 12](#) section. On each section we also provide a list of properties that are supported.

5.6. Table 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.
- **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 6. 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.

Installation:

```
pip install sdrf-pipelines
```

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
```

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

Chapter 7. 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. Values MUST come from [NCBI Taxonomy](#).
- **characteristics[organism part]:** The part of organism's anatomy or substance arising from an organism from which the biomaterial was derived (e.g., liver). Values SHOULD come from [UBERON](#) or [BTO](#).
- **characteristics[disease]:** The disease under study in the Sample. Values SHOULD come from [MONDO](#), [EFO](#), or [DOID](#). For healthy/control samples, use [normal](#) (PATO:0000461) - see [Disease Annotation Guidelines](#).
- **characteristics[cell type]:** A cell type is a distinct morphological or functional form of cell (e.g., epithelial, glial). Values SHOULD come from [Cell Ontology \(CL\)](#) or [BTO](#).

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 per experiment type - see [SDRF-Proteomics templates](#) for required properties.
- Column headers SHOULD use EFO ontology terms (e.g., [characteristics\[organism\]](#)) - see [Disease Annotation Guidelines](#).
- Multiple columns with the same [characteristics](#) term are allowed (see [Section 9.1](#)), but RECOMMENDED to use more specific terms (e.g., "immunophenotype" instead of duplicate "phenotype").

7.1. BioSamples database integration

Use the OPTIONAL [characteristics\[biosample accession number\]](#) column to link samples to [BioSamples \[5\]](#), enabling cross-database integration with genomics and transcriptomics data. Formats: [SAMN*](#) (NCBI) or [SAMEA*](#) (EBI).

7.2. Encoding sample technical and biological replicates

SDRF-Proteomics uses two REQUIRED columns to track replicates [4]:

- **characteristics[biological replicate]**: Independent biological samples. Numbering restarts per experimental condition (factor value group).
- **comment[technical replicate]**: Repeated measurements of the same sample (e.g., multiple injections)

When no replicates are performed, set both columns to 1. For pooled samples, use [pooled](#) for biological replicate.

| source name | characteristics[biological replicate] | comment[fraction identifier] | comment[technical replicate] | comment[data file] |
|-------------|---------------------------------------|------------------------------|------------------------------|--------------------|
| patient_001 | 1 | 1 | 1 | P001_F1_TR1.raw |
| patient_001 | 1 | 1 | 2 | P001_F1_TR2.raw |
| patient_002 | 2 | 1 | 1 | P002_F1_TR1.raw |
| patient_002 | 2 | 1 | 2 | P002_F1_TR2.raw |

7.3. Pooled samples

When multiple samples are pooled into one (e.g., TMT/iTRAQ reference channels for normalization), use the *characteristics[pooled sample]* column to indicate pooling status. Allowed values:

- **not pooled**: Regular individual samples
- **pooled**: Sample is pooled but individual sources are unknown
- **SN=sample1;SN=sample2;...**: Lists source names of pooled samples when known

Example:

| source name | characteristics[pooled sample] | characteristics[organism] | characteristics[age] | comment[label] | comment[data file] |
|-------------|--------------------------------|---------------------------|----------------------|----------------|--------------------|
| sample_1 | not pooled | homo sapiens | 45Y | TMT126 | file01.raw |
| sample_2 | not pooled | homo sapiens | 52Y | TMT127N | file01.raw |
| pooled_ref | SN=sample_1;SN=sample_2 | homo sapiens | pooled | TMT131C | file01.raw |

TIP

For pooled samples, use [pooled](#) for individual-specific fields (biological replicate, age, sex) to indicate a mixture rather than a single sample.

7.4. 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, spiked-in samples, and other sample characteristics
- [Human Sample Metadata Guidelines](#) - Human-specific metadata including disease staging, treatment history, demographics, and lifestyle factors

Chapter 8. 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).

8.1. CV Term Format for Data File Metadata

For data file metadata (`comment` columns) that reference ontology terms, use the structured format: `NT={term name};AC={accession}`

Examples: `NT=HCD;AC=PRIDE:0000590`, `NT=Orbitrap;AC=MS:1000484`

This format enables automated validation and software extraction from raw files. Sample metadata (characteristics) can use simple term names since they are typically human-annotated.

The following properties **MUST** be provided for each data file in **mass spectrometry-based proteomics** experiments. For **affinity-based proteomics** (Olink, SomaScan), see the [Affinity-Proteomics template](#) for different required columns.

| Column | Requirement | Description | Ontology |
|--|-------------|---|--------------------------|
| <code>assay name</code> | REQUIRED | Unique identifier for an MS run/data file | Free text |
| <code>technology type</code> | REQUIRED | Technology used to capture the data | Fixed values |
| <code>comment[proteomics data acquisition method]</code> | REQUIRED | DDA, DIA, PRM, SRM | PRIDE:0000659 |
| <code>comment[label]</code> | REQUIRED | Label applied to sample (or "label free sample") | PRIDE - Labels |
| <code>comment[instrument]</code> | REQUIRED | Mass spectrometer model | PSI-MS - Instruments |
| <code>comment[cleavage agent details]</code> | REQUIRED | Enzyme information (use "not applicable" for top-down/undigested samples) | PSI-MS - Cleavage agents |
| <code>comment[fraction identifier]</code> | REQUIRED | Fraction number (1 if not fractionated) | Integer |
| <code>comment[technical replicate]</code> | REQUIRED | Technical replicate number (1 if none) | Integer |
| <code>comment[data file]</code> | REQUIRED | Name of the raw file | Free text |

Example:

| source name | assay name | technology type | comment[proteomics data acquisition method] | comment[label] | comment[instrument] | comment[data file] |
|-------------|--------------|--|---|-------------------|---------------------|--------------------|
| sample_1 | sample1_run1 | proteomic profiling by mass spectrometry | data-dependent acquisition | label free sample | Q Exactive HF | sample1.raw |

8.2. Sample Preparation and Fragmentation (MS-based only)

NOTE

This section applies to **mass spectrometry-based proteomics** experiments only. For affinity-based proteomics, these properties do not apply.

For detailed documentation of sample preparation and MS/MS fragmentation properties, see the [MS-Proteomics Template](#):

- **Sample preparation:** depletion, reduction reagent, alkylation reagent
- **Fractionation:** fractionation method (used with `comment[fraction identifier]`)
- **Fragmentation:** collision energy, dissociation method

8.3. Proteomics data acquisition method

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 MS-Proteomics Template.

8.4. MS-Proteomics Template

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

- [MS-Proteomics Template](#) - Detailed guidelines for labels, instruments, modifications, cleavage agents, mass tolerances, RAW file URIs, and other data file properties

Chapter 9. Additional SDRF Rules

9.1. 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., `characteristics[biological replicate]`)
- **Multiple (*):** Column can appear multiple times (e.g., `comment[modification parameters]` can specify multiple post-translational modifications)

Example of multiple `comment[modification parameters]` columns:

| source name | characteristics[...] | comment[modification parameters] | comment[modification parameters] | ... |
|-------------|----------------------|--|--|-----|
| sample-1 | ... | NT=Carbamidomethyl;AC=UNIMOD:4;TA=C;MT=fixed;PP=Anywhere | NT=Oxidation;AC=UNIMOD:35;TA=M;MT=variable;PP=Anywhere | ... |

9.2. Row Uniqueness Requirements

Uniqueness constraints ensure data integrity:

- **MUST be unique** (error): `source name + assay name + comment[label]`
- **SHOULD be unique** (warning): `source name + assay name`
- **Assay name:** Each data file MUST have a unique `assay name`

NOTE

For multiplexed experiments (TMT, iTRAQ), multiple rows share the same `assay name` since samples are in one MS run. The `comment[label]` distinguishes samples within the run.

Chapter 10. Templates

A **template** is a predefined set of metadata columns that ensures consistent annotation for specific experiment types. Templates define REQUIRED, RECOMMENDED, and OPTIONAL columns to make datasets FAIR-compliant.

10.1. Template Architecture

Templates follow a layered hierarchy:

| Layer | Templates | Description |
|------------------------------|---|---------------------------------|
| TECHNOLOGY (required) | ms-proteomics , affinity-proteomics | Minimum valid SDRF - choose one |
| SAMPLE (recommended) | human , vertebrates , invertebrates , plants | Organism-specific metadata |
| EXPERIMENT (optional) | cell-lines , crosslinking , dda-acquisition , dia-acquisition , single-cell , immunopeptidomics | Methodology-specific columns |

Child templates inherit all columns from parents and may add new columns or strengthen requirements (e.g., [optional](#) → [required](#)).

10.2. Specifying Templates in SDRF Files

Declare templates using `comment[sdrf template]` columns. Only list leaf templates (parents are implied). When using multiple templates, add multiple columns with the same name. Two formats are supported:

- Simple format (preferred): `template_name vX.Y.Z`
- Key=value format: `NT=template_name;VV=vX.Y.Z`

```
source name ... comment[sdrf template] comment[sdrf template]
sample_1     ... human v1.1.0      crosslinking v1.0.0
```

Common examples:

| Experiment Type | Template Columns |
|---------------------|---|
| Human MS proteomics | <code>comment[sdrf template] = human v1.1.0</code> |
| Mouse MS proteomics | <code>comment[sdrf template] = vertebrates v1.1.0</code> |
| Human crosslinking | Two columns: <code>human v1.1.0</code> + <code>crosslinking v1.0.0</code> |
| Human Olink | Two columns: <code>human v1.1.0</code> + <code>olink v1.0.0</code> |

10.3. Available Templates

Sample templates (organism-specific):

| Template | Use For | Key Columns |
|-------------------------------|------------------------|---|
| Human | Human clinical samples | disease, age, sex, ancestry |
| Vertebrates | Mouse, rat, zebrafish | disease, developmental stage, strain |
| Invertebrates | Drosophila, C. elegans | disease, developmental stage, genotype |
| Plants | Arabidopsis, crops | disease, developmental stage, growth conditions |

Experiment-type templates:

- [DDA Acquisition](#) - dissociation method, collision energy, modifications
- [DIA Acquisition](#) - scan windows, isolation width, spectral library
- [Cell Lines](#) - Cellosaurus integration
- [Single-Cell](#) - cell isolation, carrier proteome
- [Immunopeptidomics](#) - MHC class, HLA typing
- [Crosslinking MS](#) - crosslinker reagents
- [Metaproteomics](#) - environmental sample type

Download templates from the [templates folder](#).

10.4. Extending Templates

You can add custom columns beyond template requirements for study-specific metadata. Rules:

- Use `characteristics[...]` for sample metadata, `comment[...]` for technical metadata
- Column names MUST be valid ontology terms (search [OLS](#))
- Use controlled vocabularies for values when available

See [Common Additional Columns](#) and [SDRF Terms Reference](#) for commonly used columns.

10.5. Contributing New Templates

To propose a new template, open an [issue on GitHub](#) and submit a pull request.

Chapter 11. 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.

11.1. Column Format

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

11.2. When to Use Factor Values

Use factor values to indicate:

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

NOTE

Use `normal` (not "control") in the disease field for healthy samples. "Control" is an experimental design concept, not a disease state. See [Disease Annotation Guidelines](#) for details.

11.3. 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

11.4. Example

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

| source name | ... | characteristics[disease] | characteristics[disease staging] | ... | factor value[disease] | factor value[disease staging] |
|-----------------|-----|--------------------------|----------------------------------|-----|-----------------------|-------------------------------|
| 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 staging` are factor values because the experiment aims to compare expression differences between disease states and across cancer stages.

Chapter 12. 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 | |
| General | NCI Thesaurus (NCIT) | Biomedical terminology | |
| General | PRIDE Controlled Vocabulary | Proteomics-specific terms | |
| Organism and Taxonomy | | | |
| Taxonomy | NCBI Taxonomy (NCBITaxon) | Organism classification | |
| 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 (see Disease Annotation Guidelines) | | | |
| Disease | Mondo Disease Ontology (MONDO) | Unified disease ontology | RECOMMENDED |
| Disease | Experimental Factor Ontology (EFO) | Disease terms from EFO | |
| Healthy samples | Phenotype And Trait Ontology (PATO) | Use normal (PATO:0000461) for healthy samples | |
| Cell Lines | | | |
| Cell Lines | Cellosaurus | Cell line knowledge resource | RECOMMENDED |

| Category | Ontology/CV | Description | Notes |
|---|---|--|--------------------|
| Cell Lines | Cell Line Ontology (CLO) | Cell line ontology | |
| Mass Spectrometry and Proteomics | | | |
| MS/Proteomics | PSI Mass Spectrometry CV (PSI-MS) | Instruments, methods, parameters | |
| 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 13. Examples of Annotated Datasets

The following table provides links to example SDRF files for different experiment types. Click "View in Explorer" to open the SDRF file in the interactive viewer.

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

TIP

Use the [SDRF Explorer](#) to browse all {total_datasets}+ annotated datasets with filtering, statistics, and interactive viewing.

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

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