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

Version 1.1.0-dev, 2026-02-02

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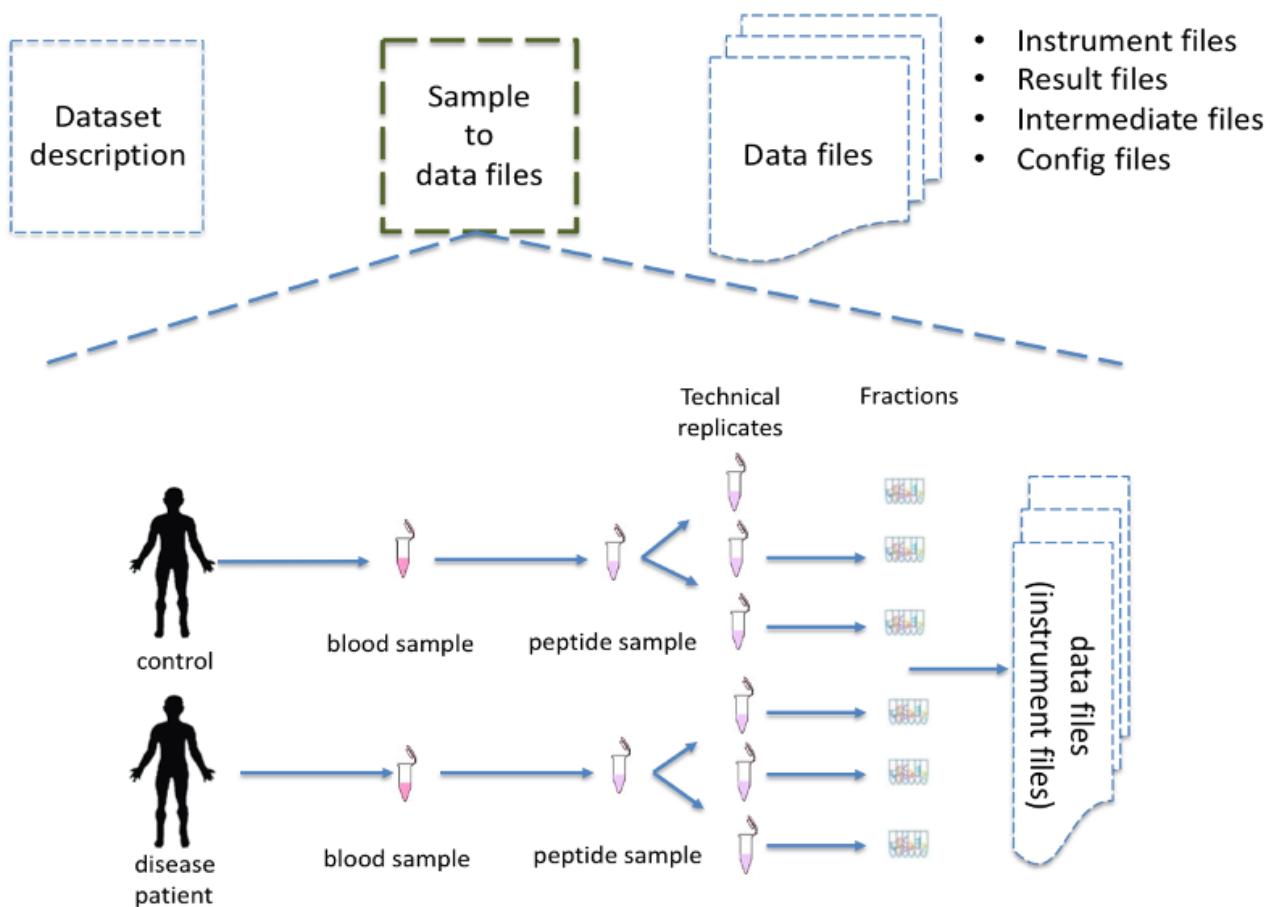
Figure 1: SDRF-Proteomics captures sample information and its relationship to data files.

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[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_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 ¬ 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	characteristics[age] = not available	Patient age was not recorded in the study
not applicable	Value or concept does not apply to this sample	characteristics[age] = not applicable	Synthetic peptide library has no age
anonymized	Value exists but is redacted for privacy protection	characteristics[age] = anonymized	Clinical study with de-identified patient data
pooled	Value represents a mixture of multiple samples	characteristics[biological replicate] = pooled	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
`comment[sdrf version]`	SDRF-Proteomics specification version used. Should follow semantic versioning format (vMAJOR.MINOR.PATCH)	v1.1.0	RECOMMENDED	PRIDE:0000839
`comment[sdrf template]`	Template name and version used for annotation. Two formats are supported: simple format (`name vX.Y.Z`) or key=value format (`NT=name;VV=vX.Y.Z`). Multiple templates can be specified using multiple columns.	human v1.1.0 or NT=human;VV=v1.1.0	OPTIONAL	PRIDE:0000832
`comment[sdrf annotation tool]`	Software tool, script, or method used to generate or annotate the SDRF file. Two formats are supported: simple format (`name vX.Y.Z`) or key=value format (`NT=name;VV=vX.Y.Z`).	lesSDRF v0.1.0 or NT=lesSDRF;VV=v0.1.0	OPTIONAL	PRIDE:0000840
`comment[sdrf validation hash]`	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
`assay name`	REQUIRED	Unique identifier for an MS run/data file	Free text
`technology type`	REQUIRED	Technology used to capture the data	Fixed values
`comment[proteomics data acquisition method]`	REQUIRED	DDA, DIA, PRM, SRM	PRIDE:0000659
`comment[label]`	REQUIRED	Label applied to sample (or "label free sample")	PRIDE - Labels
`comment[instrument]`	REQUIRED	Mass spectrometer model	PSI-MS - Instruments
`comment[cleavage agent details]`	REQUIRED	Enzyme information (use "not applicable" for top-down/undigested samples)	PSI-MS - Cleavage agents
`comment[fraction identifier]`	REQUIRED	Fraction number (1 if not fractionated)	Integer
`comment[technical replicate]`	REQUIRED	Technical replicate number (1 if none)	Integer
`comment[data file]`	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	`comment[sdrf template]` = `human v1.1.0`
Mouse MS proteomics	`comment[sdrf template]` = `vertebrates v1.1.0`
Human crosslinking	Two columns: `human v1.1.0` + `crosslinking v1.0.0`
Human Olink	Two columns: `human v1.1.0` + `olink v1.0.0`

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

Chapter 14. Intellectual Property Statement

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