

What is metadata?

Metadata is the data that describes your data.

For the LIMS, metadata comes in the form of JSON (JavaScript Object Notation) files. These files are collections of key: value pairs that contain the information required in order to incorporate a piece of data into the LIMS system.

Each metadata file captures inputs (from the researcher) about the component(s), polymer(s), and/or composite in the sample; the instrument used in characterization; the type of data captured (i.e. data category); veracity of data (does it describe a sample whose identity & composition is confirmed?); and other parameters.

An example metadata file is shown below:

[metadata.json](#)

```
{
  // acquired_by is the LIMS username of the user
  "acquired_by": "bpm_admin",
  "components": [
    "valine",
    "isoleucine"
  ],
  "component_classes": [
    "Monomer",
    "Monomer"
  ],
  "polymers": [
    "poly-VI"
  ],
  "polymer_props": {
    "polymer_components": [
      "valine",
      "isoleucine"
    ],
    // Component ratios come in the form of a string,
    // where each component is separated by a colon.
    "ratios": [
      "50:50"
    ],
    // Ratio types can be MassRatio or MoleRatio.
    "ratio_types": [
      "MoleRatio"
    ],
    "formulae": [
      "(C11H24N2O4)n"
    ],
    // All molecular weights are expressed as g/mol.
    "molec_weights": [
```

```
    250.0
  ],
  // Tg: glass-phase transition temperature, in C
  "tgs": [],
  // PDI: polydispersity index
  "pdis": [],
  // SMILES string, preferably isomeric SMILES
  "SMILES": [],
  // bigSMILES string, refer to bigSMILES publications @ MIT.
  "bigSMILES": []
},
"polymer_mechs": [
  "StepGrowth"
],
"composite": [],
"composite_props": {
  "ratio": [],
  "ratio_type": [
    "MoleRatio"
  ],
  "pdi": []
},
// Note: synthesis ID and experimental ID are used
// interchangeably in conversation. However, the
// system expects a parameter named synthesis_ID.
"synthesis_ID": [
  "BPM-2023-03-13-46a32bf6-1c89-402e-b214-eb40a30dd45b"
],
"synthesis_date": [
  "2023-03-08 21:12:00"
],
"exp_data_date": [
  "2023-03-07 08:19:00"
],
// Parent synthesis ID. This is the synthesis/experimental ID of
the immediate
// parent experiment from which the current material was derived.
It is an
// optional field and should be used in cases where the material of
interest
// was derived, isolated, extracted, separated, fractionated, etc,
from
// another sample.
"parent_ID": "BPM-2023-05-04-0fc3e959-27bd-451b-b7e2-fa1481b188ea",
// A brief synopsis of the experiment
"synopsis": [
  "The fifth test of the group",
  "Testing the fifth thing."
],
// Synthesis 'platform' where the sample was produced.
// This can be any of the automated capabilities at
```

```
// BioPACIFIC, your PI's lab, a different PI's lab, etc.
"platform": [
  "LBF"
],
"instrument": [
  "ht_rheo_zeiss_axio_obs_7"
],
"data_files": [
  "SRI-PEC_v2_mth_20220912_223358_0GLE9.asc"
],
"data_category": [
  "msd"
],
"is_verified": [
  "unverified"
],
"data_availability": [
  "all"
],
// An optional field, captures files that further
// describe the given data.
"context_files": []
}
```

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