

From Ontologies to Knowledge Graphs

with the ELN Herbie

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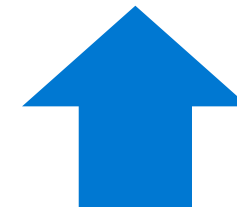
Knowledge Graph¹



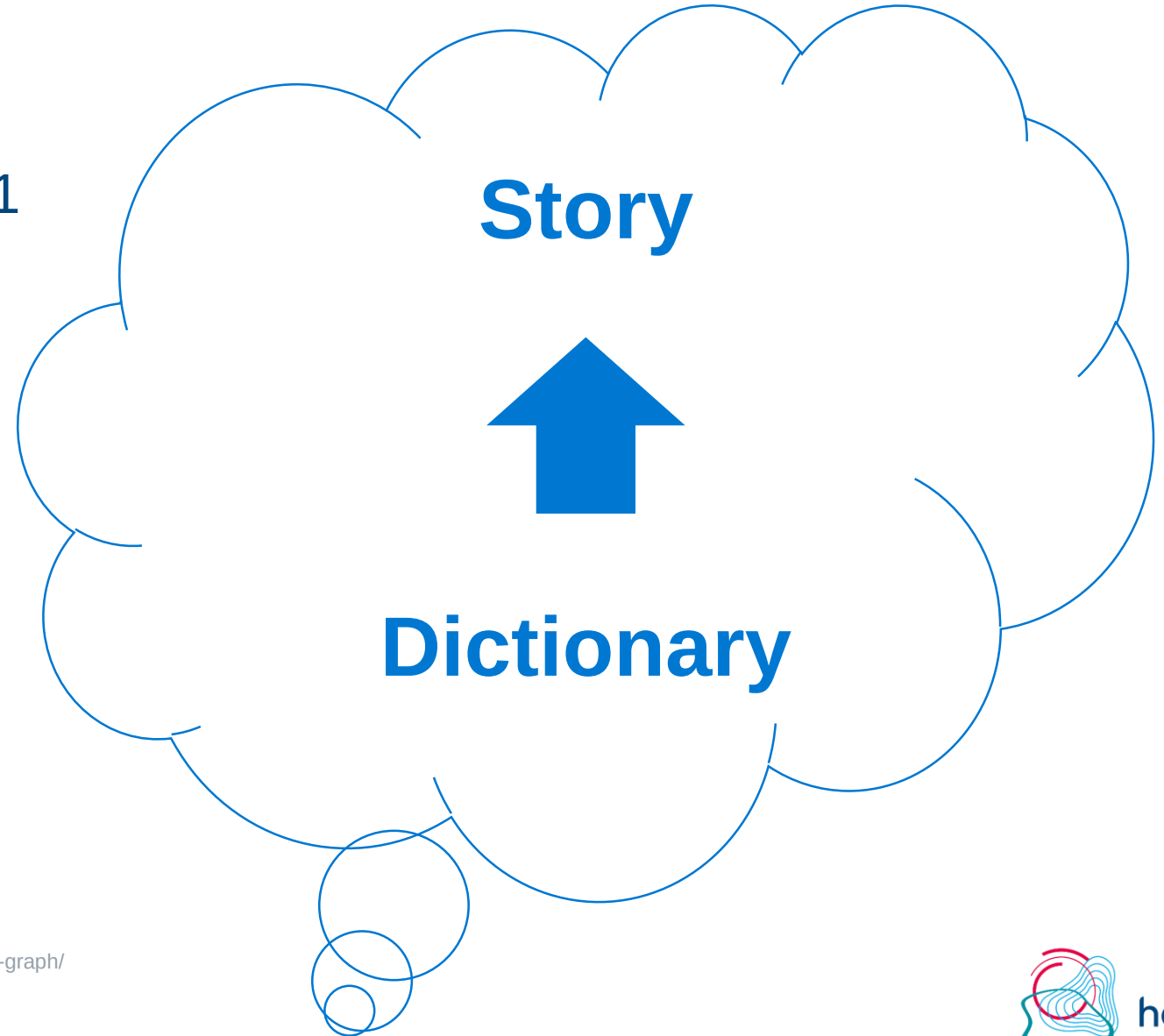
Ontology

Mental model

Story



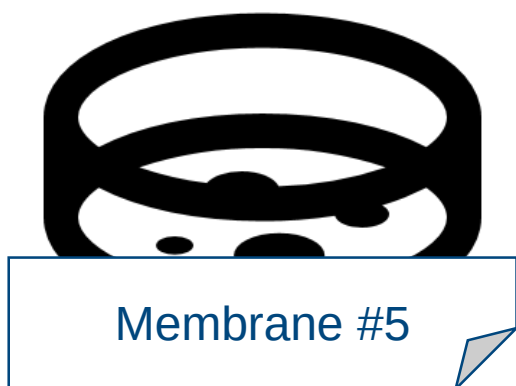
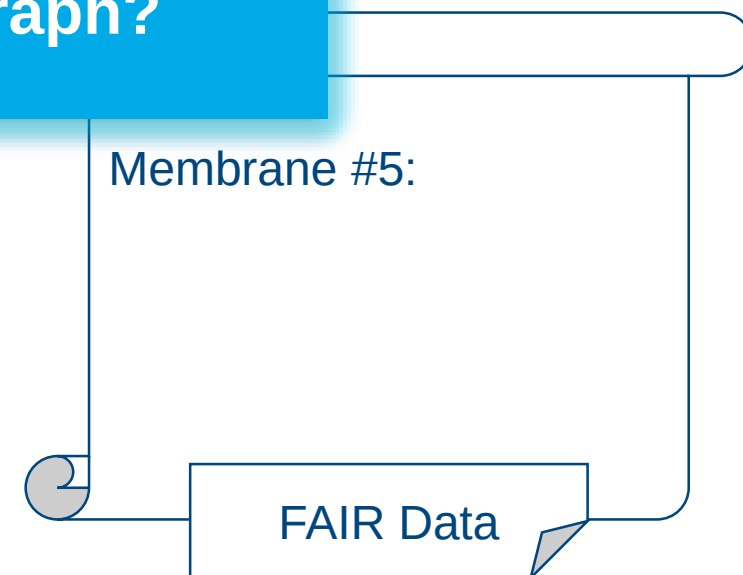
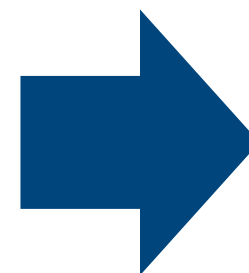
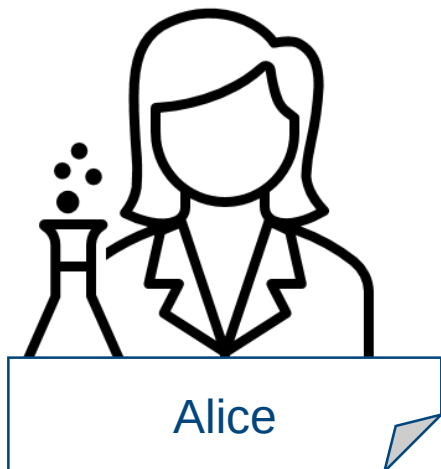
Dictionary



[1] <https://www.ontotext.com/knowledgehub/fundamentals/what-is-a-knowledge-graph/>

Example scenario

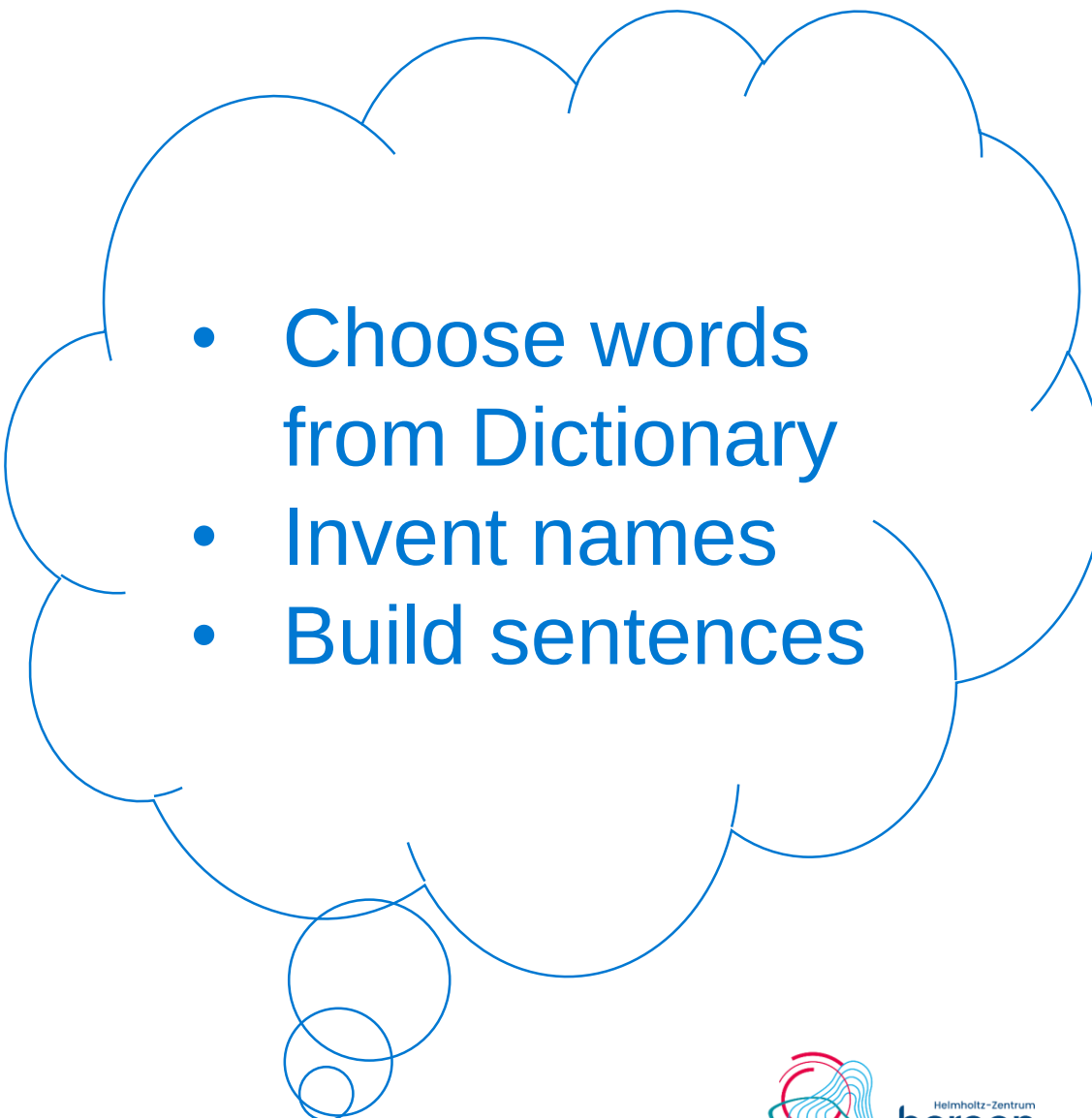
How do we turn this into a
Knowledge Graph?



Alice performed an **SEM** measurement of the **PTFE Membrane #5**. She prepared the sample by applying a **coating** of **500 nm thickness**. She then used the **SEM Leo 1550 VP** to perform an imaging analysis and determined a **mean pore diameter** of **20 nm** of the sample.

Formalize all information into a Knowledge Graph

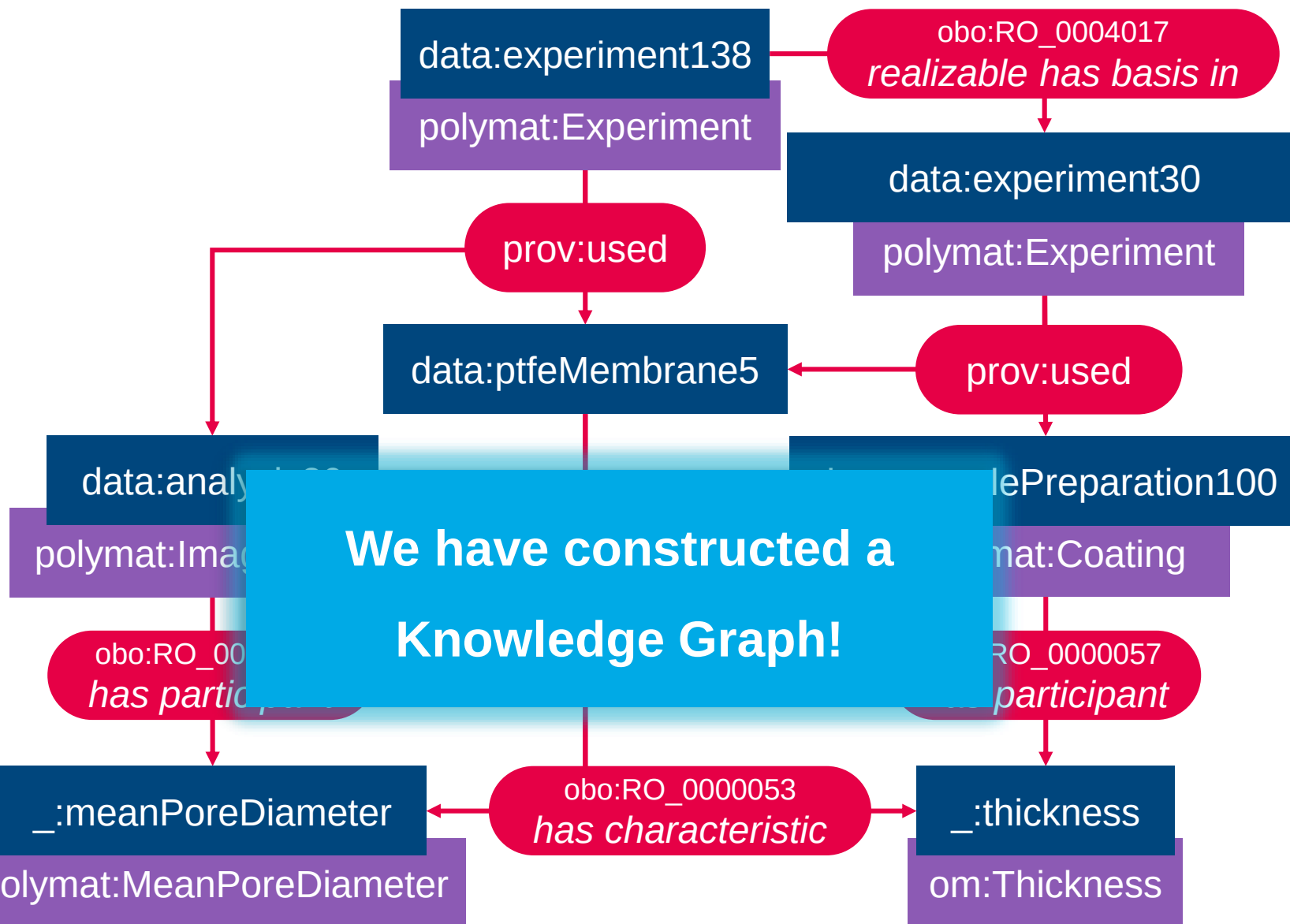
- Choose classes and properties from Ontology
- Invent identifiers (IRIs²)
- Build RDF triples³

- 
- Choose words from Dictionary
 - Invent names
 - Build sentences

[2] <https://datatracker.ietf.org/doc/html/rfc3987>

[3] <https://www.w3.org/TR/rdf11-concepts/>

Knowledge Graph



Alice performed an **SEM** measurement of the **PTFE Membrane #5**.

She prepared the sample by applying a **coating** of **500 nm** thickness.

She then used the **SEM Leo 1550 VP** to perform an imaging analysis and determined a **mean pore diameter** of **20 nm** of the sample.

Legend

Instance

Class

Property

Knowledge Graph

RDF Turtle⁴

[4] <https://www.w3.org/TR/turtle/>

data:experiment138

Publish file to Gitlab/Zenodo/...
including Ontology files

FAIR

data:analysis30

polymat:Imaging

obo:RO_0000057
has participant

_:meanPoreDiameter

polymat:MeanPoreDiameter

obo:RO_0000053
has characteristic



*sem_experiment_data.ttl - Notepad

File Edit Format View Help

```
data:experiment138 a polymat:Experiment ;
  prov:used data:ptfeMembrane5 ;
  obo:RO_0004017 data:experiment30 ; # "realizable has basis in"
  prov:used data:analysis30 .

data:experiment30 a polymat:experiment138 ;
  prov:used data:samplePreparation100 ;
  prov:used data:ptfeMembrane5 .

data:samplePreparation100 a polymat:Coating ;
  obo:RO_0000057 _:thickness . # "has participant"

_:thickness a om:Thickness ;
  om:hasValue [
    om:hasNumericalValue 500 ;
    om:hasUnit om:nanometre ] .

data:analysis30 a polymat:ImagingSEM ;
  obo:RO_0000057 _:meanPoreDiameter . # "has participant"

_:meanPoreDiameter a polymat:MeanPoreDiameter ;
  om:hasValue [
    om:hasNumericalValue 20 ;
    om:hasUnit om:nanometre ] .

data:ptfeMembrane5
  obo:RO_0000053 _:thickness ; # "has characteristic"
  obo:RO_0000053 _:meanPoreDiameter . # "has characteristic"
```

Ln 37, Col 1

100%

Windows (CRLF)

UTF-8

Pros

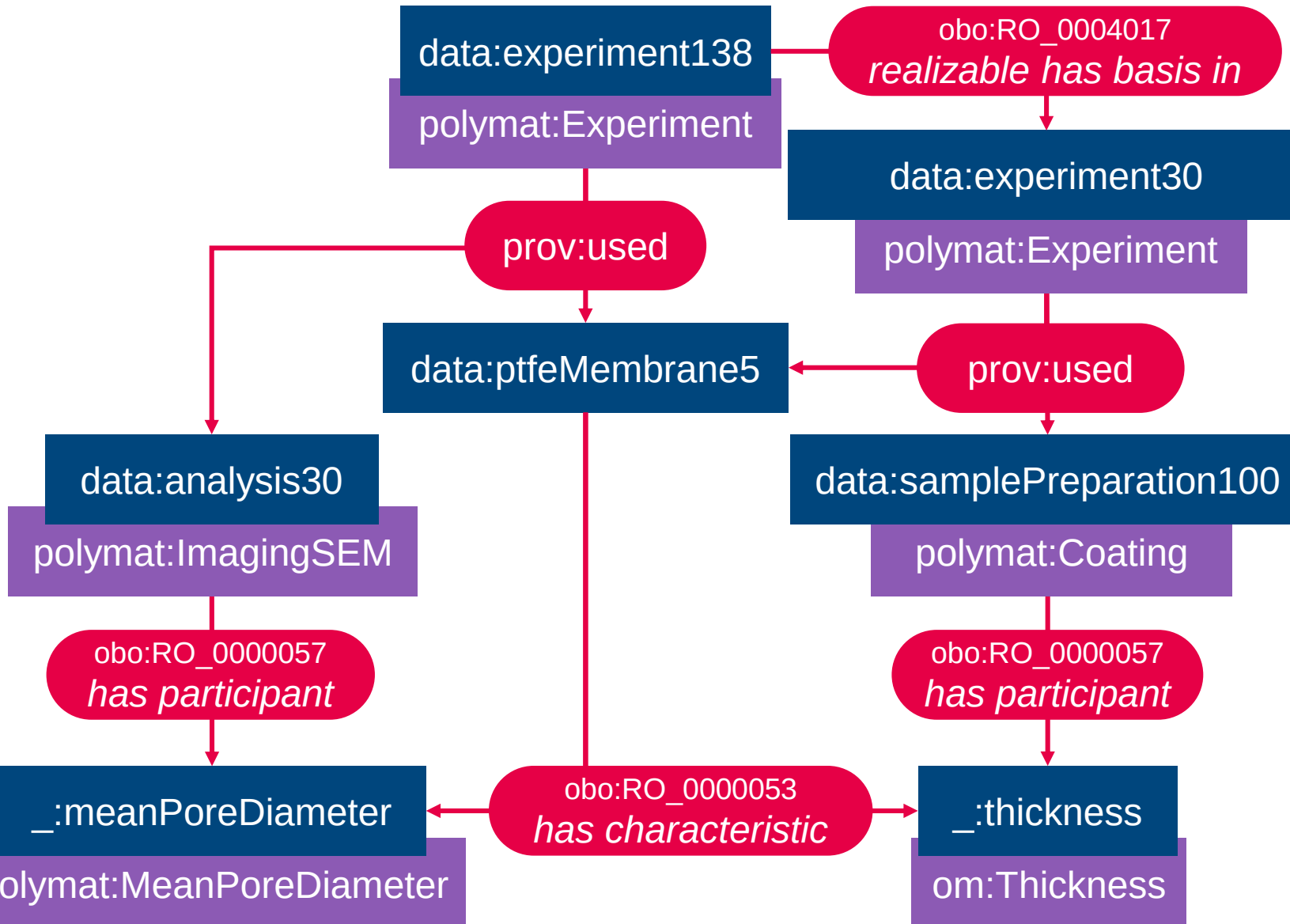
- Structured knowledge
- No extra tools required
- Very flexible

Cons

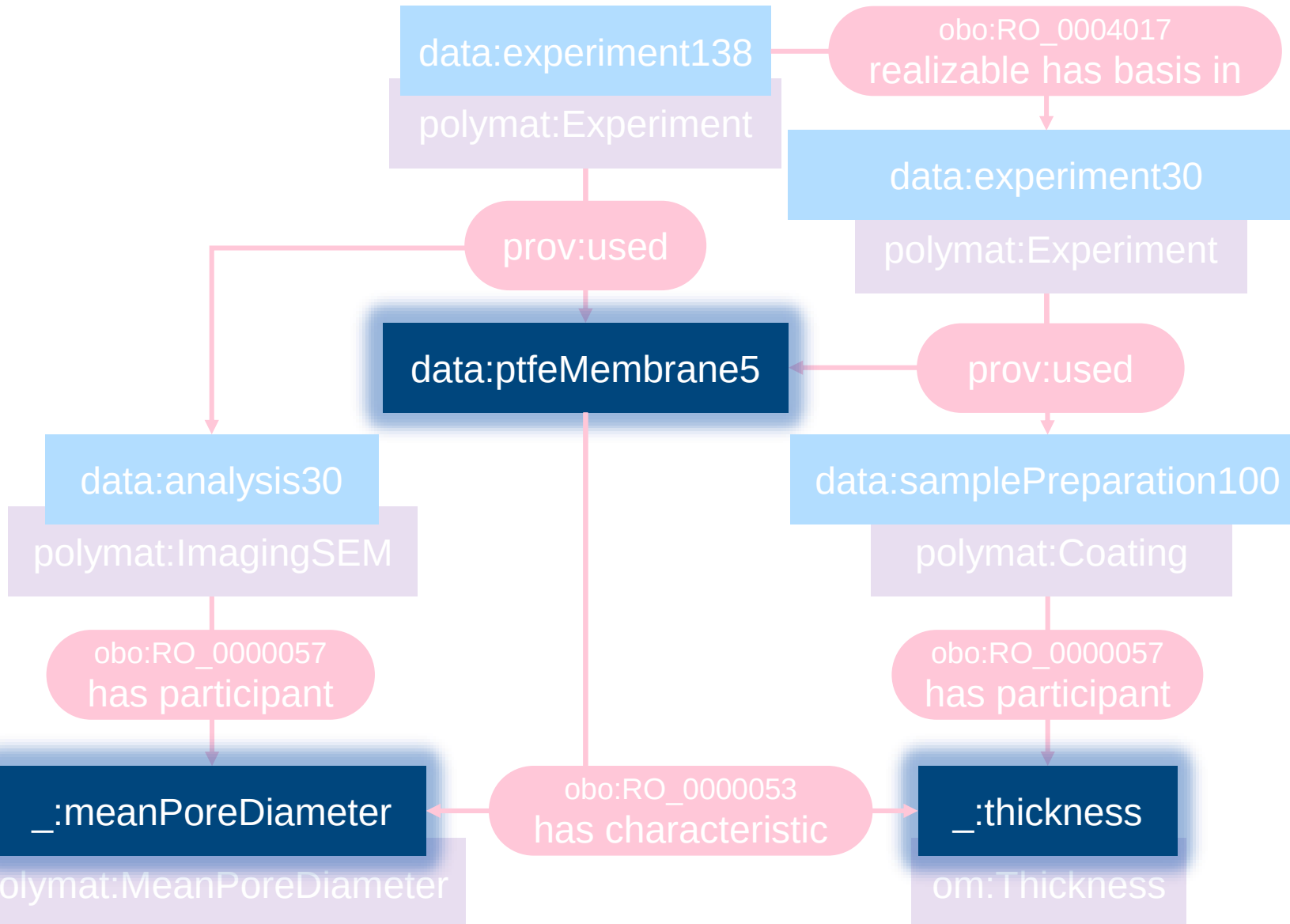
- Text editor
- Very flexible
- No validation
- FAIRness not guaranteed
- Complicated
- Tedious
- Repetitive

Can we do better?

Knowledge Graph



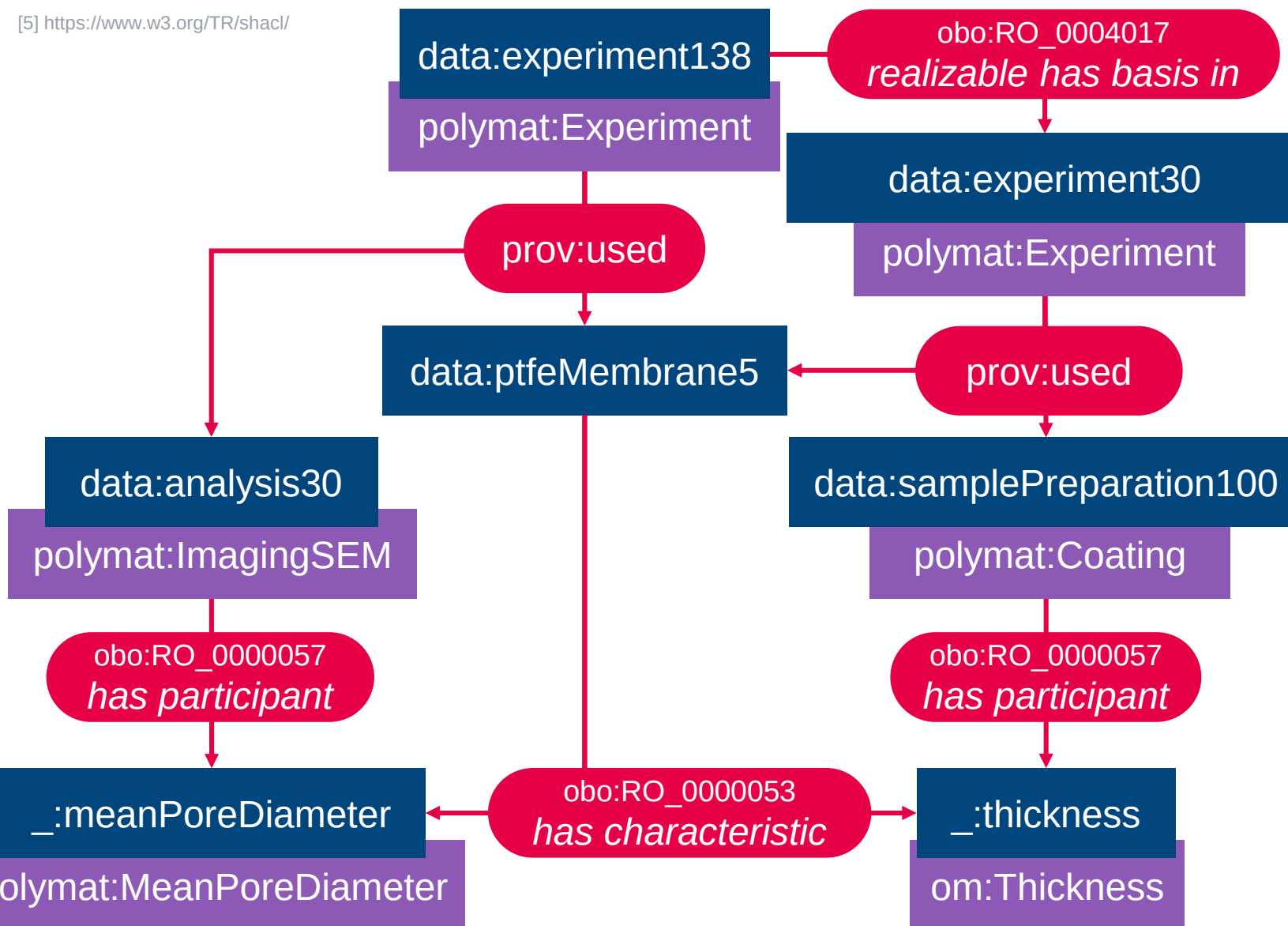
Knowledge Graph



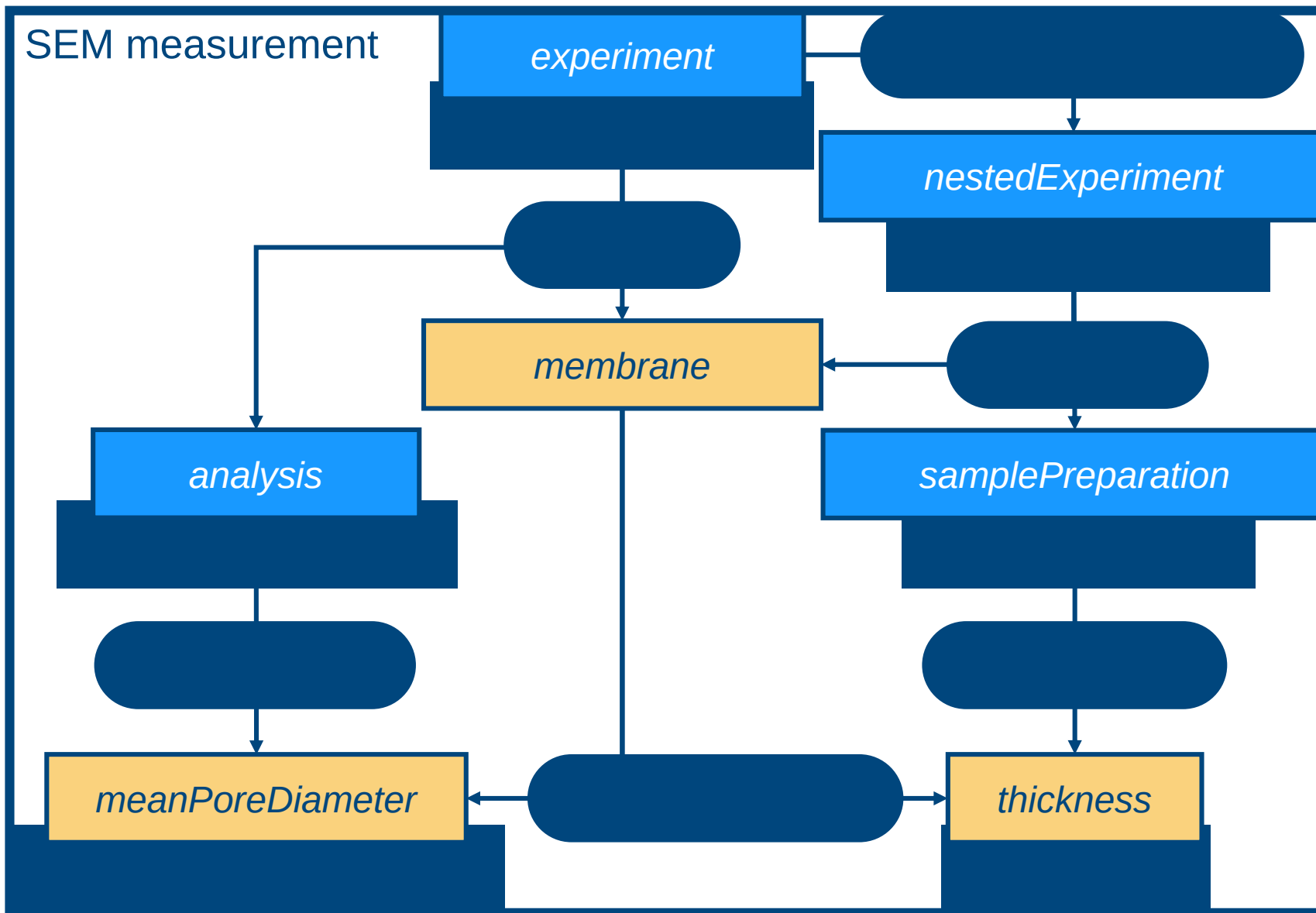
**We only want to enter
these 3 values,
everything else should
be implicit!**

Create a SHACL⁵ shape...

[5] <https://www.w3.org/TR/shacl/>



Create a SHACL⁵ shape...



Fill-in-the-blanks text

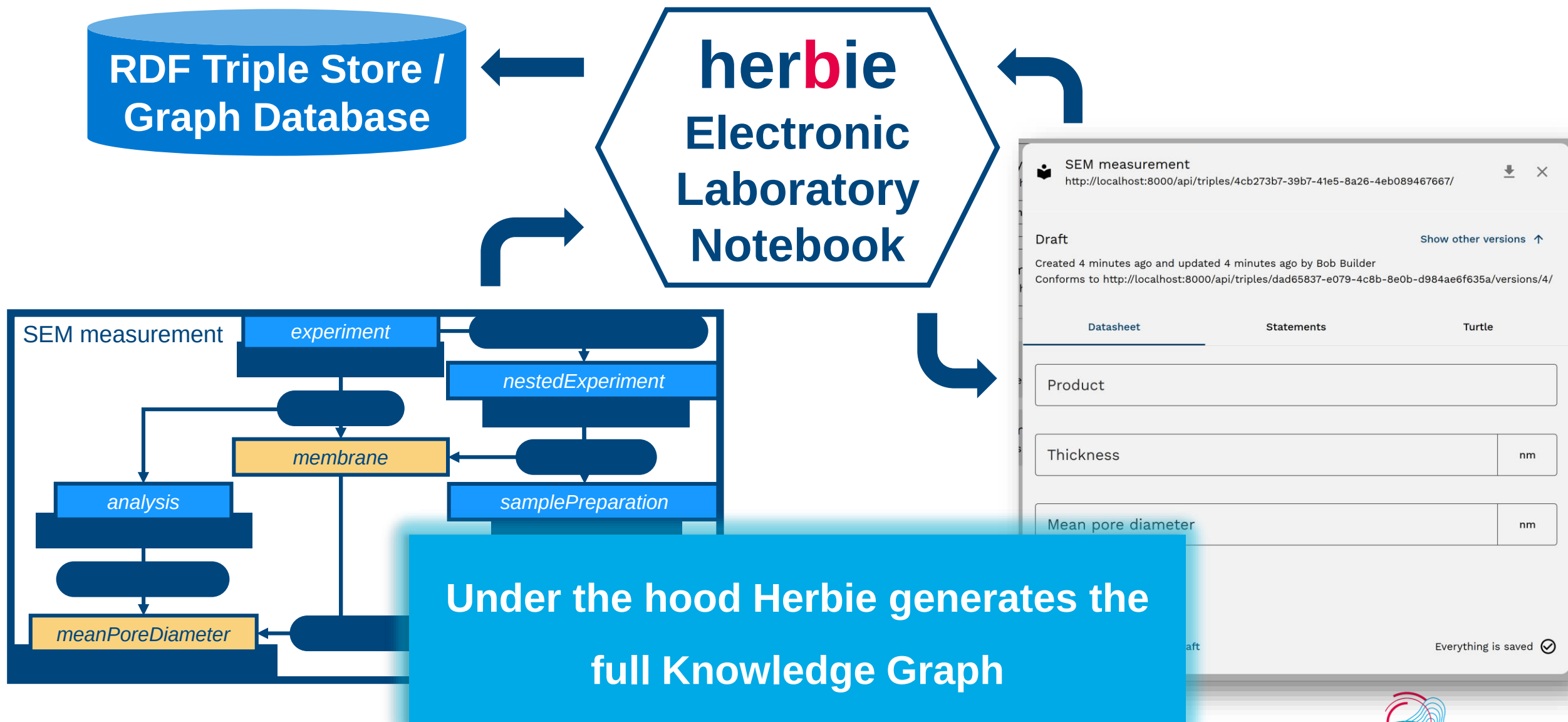
Legend

fixed

will be generated

must be entered

... and Herbie provides an interface for data input



What does Herbie provide?

- **Easy data entry**
- **Flexible interface**
- **Reusability**
- **Customizability**
- **Validation**
- **Guaranteed FAIRness**
- **Versioning**

Planned

- **Access right management**
- **Advanced search and filter**

Summary

Storing data in a Knowledge Graph helps to make it FAIR

Manual approach:

very tedious

prone to error

not reliably FAIR

Using SHACL & Herbie:

Structural work only required once

Data entry fast & easy

Offers a lot of other benefits

Want to learn more?

Find Herbie at
codebase.helmholtz.cloud/hereon-mb/herbie
and reach out to us!

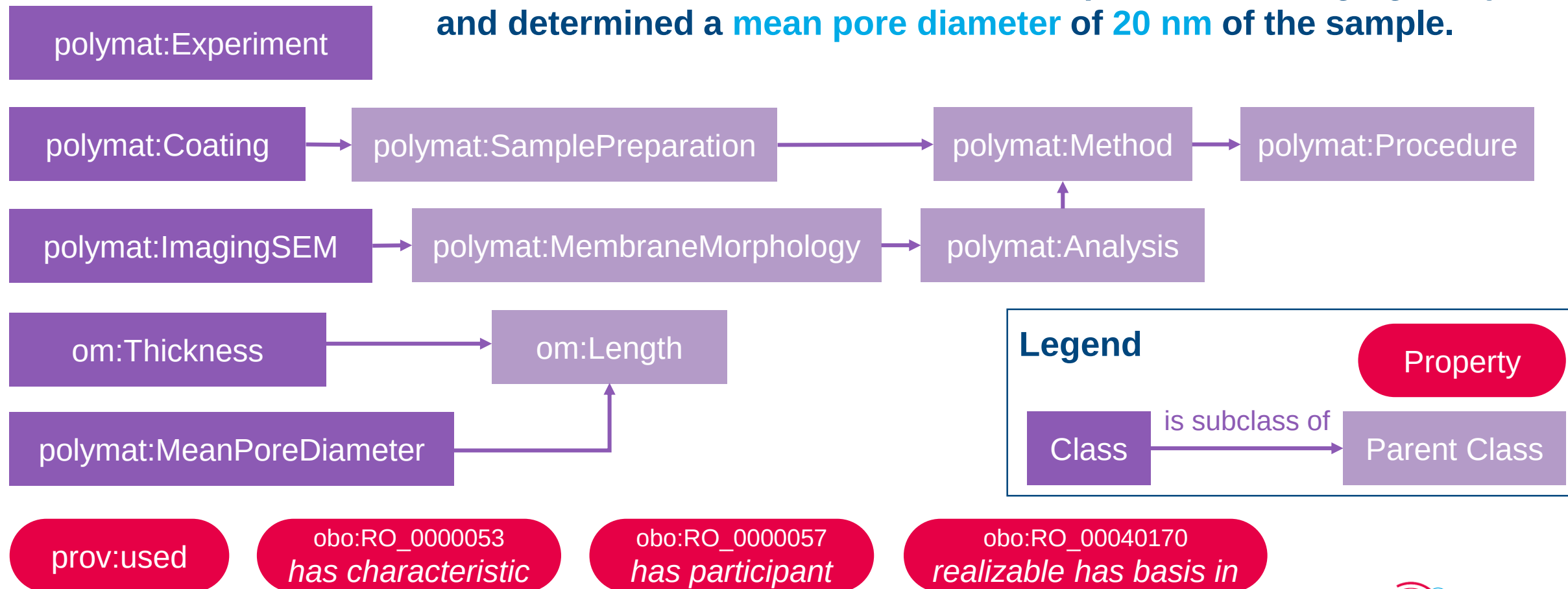
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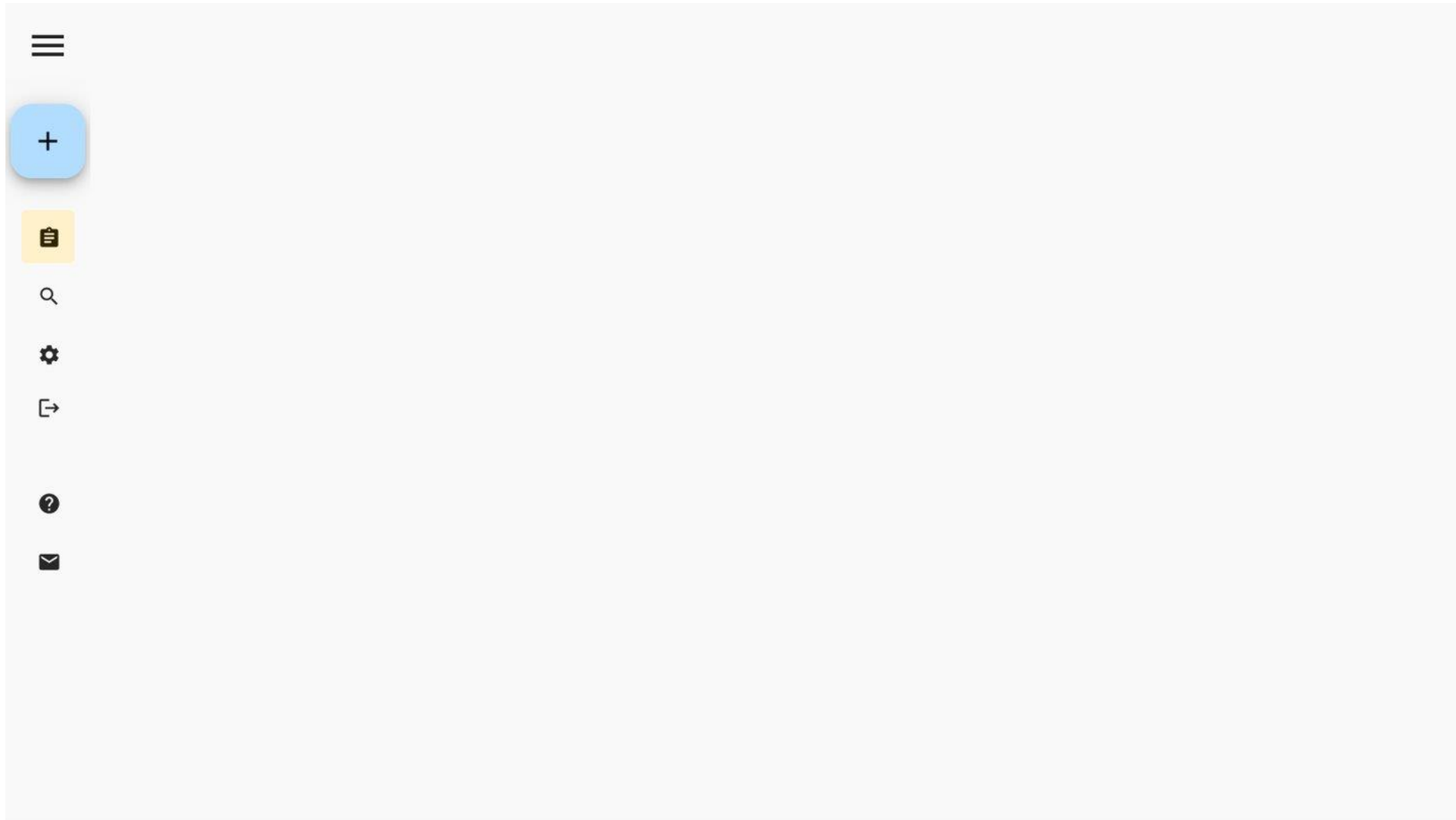


Choose classes and properties

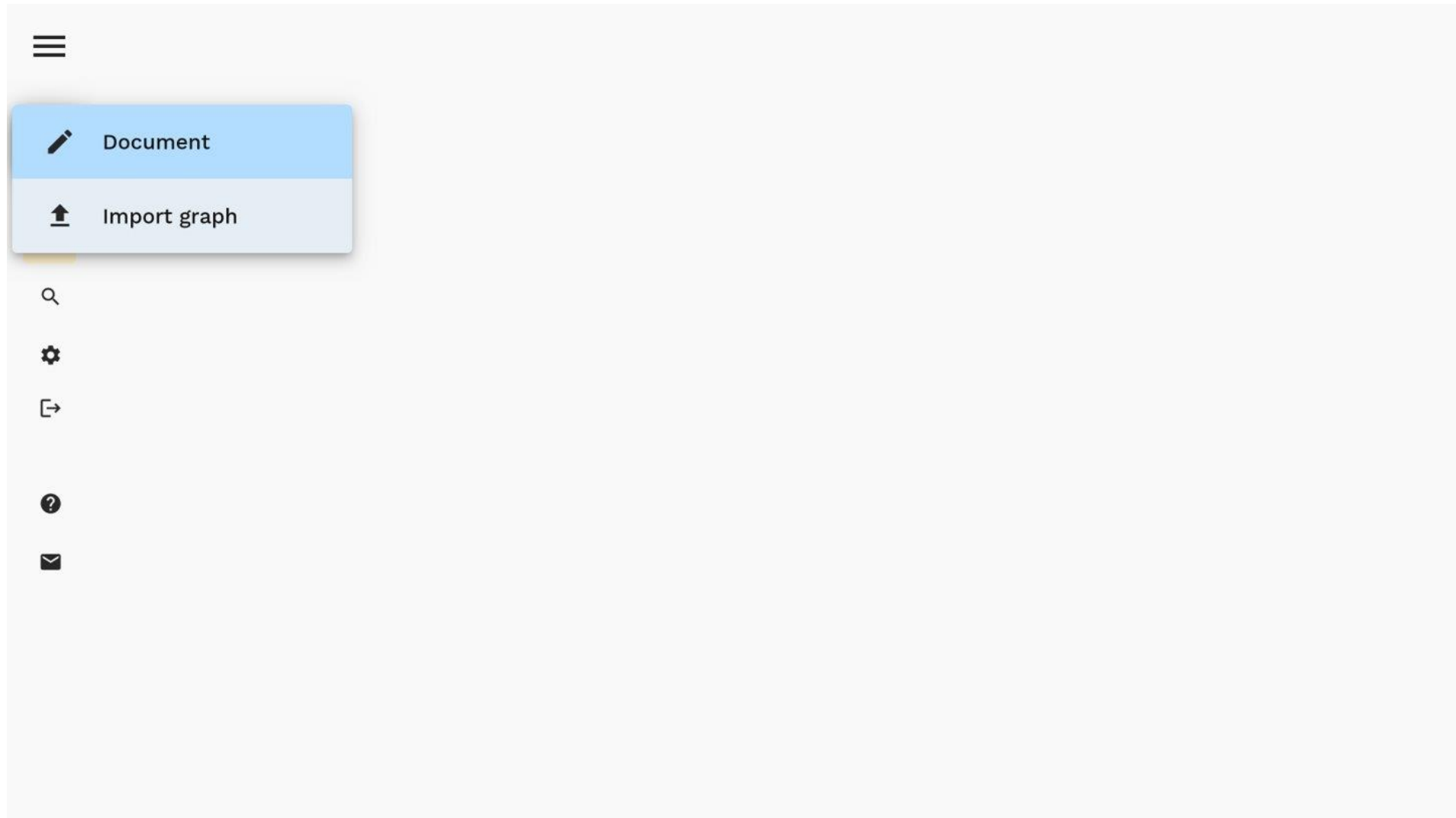
Alice performed an SEM measurement of the PTFE Membrane #5. She prepared the sample by applying a coating of 500 nm thickness. She then used the SEM Leo 1550 VP to perform an imaging analysis and determined a mean pore diameter of 20 nm of the sample.



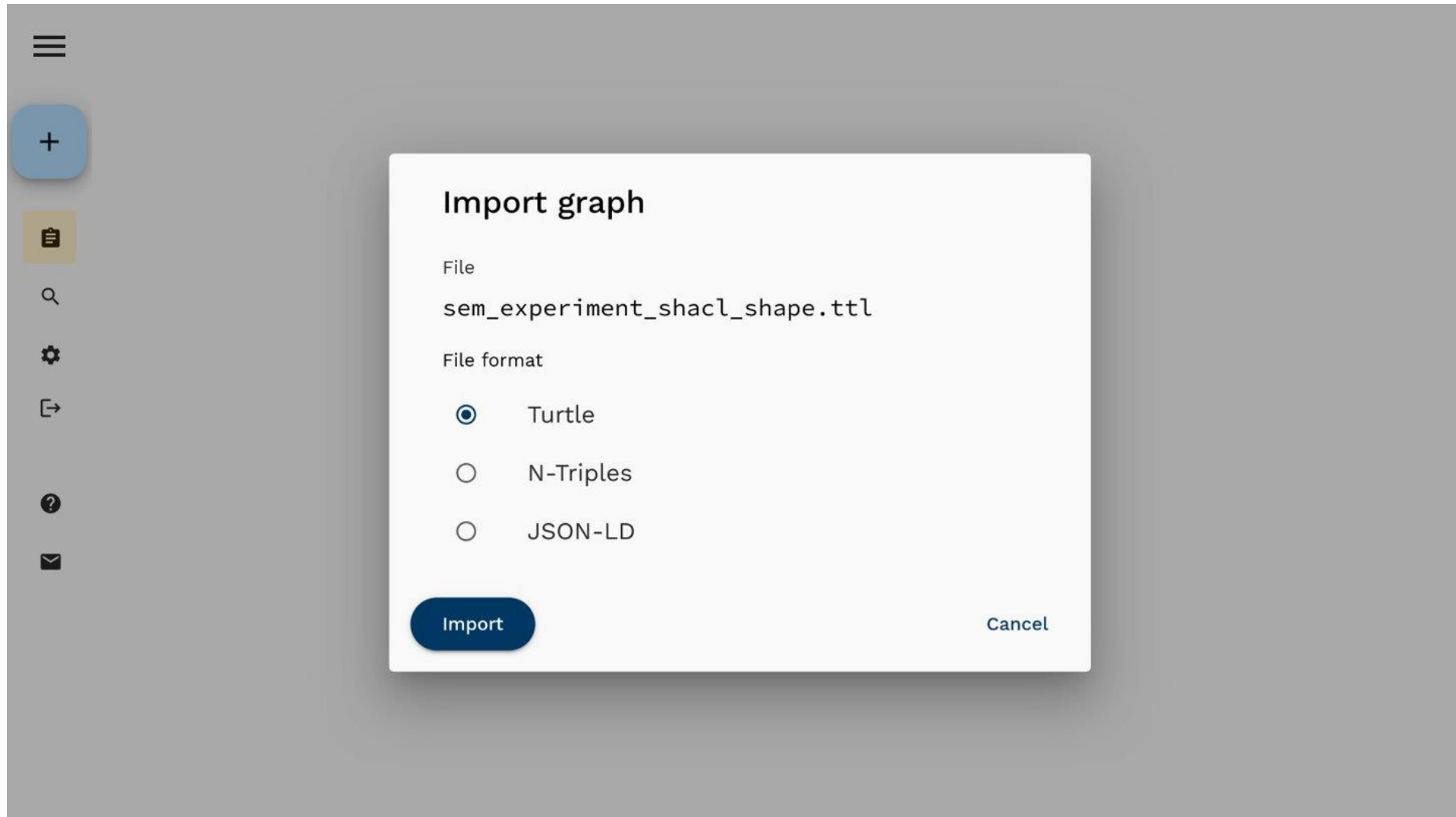
Upload a SHACL Shape to Herbie



Upload a SHACL Shape to Herbie



Upload a SHACL Shape to Herbie



Upload a SHACL Shape to Herbie

The screenshot shows the Herbie web interface. On the left is a sidebar with icons for menu, add, drafts, search, settings, share, help, and notifications. The main area displays a draft titled "The vocabulary for adding a SEM measurement" with the URL `http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/`. A "Create SEM measurement" button is visible. Below the title, it says "Draft" and "Created half a minute ago and updated half a minute ago by Alice Wonderland". There is a link to "Show other versions". The interface has two tabs: "Statements" (active) and "Turtle". Under "Statements", there is a section "Classes (1)" containing "SEM measurement" with a link icon. At the bottom, there are "Submit" and "Delete draft" buttons, and a status message "Everything is saved" with a checkmark icon.

Upload a SHACL Shape to Herbie

The vocabulary for adding a SEM measurement
`http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/`

Create SEM measurement

Draft

Created half a minute ago and updated half a minute ago by Alice Wonderland

Show other versions ↑

Statements Turtle

Classes (1)

SEM measurement

Submit Delete draft

Everything is saved ✓

Upload a SHACL Shape to Herbie

The screenshot displays the Herbie web interface. On the left is a sidebar with icons for menu, add, clipboard, search, settings, share, help, and mail. The main content area shows a modal window titled "The vocabulary for adding a SEM measurement" with the URL `http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/`. The modal includes a "Create SEM measurement" button, a "Current version" section with details "Created at 11/8/2023, 1:19:59 PM • Published at 11/8/2023, 1:20:47 PM • Alice Wonderland", and buttons for "Edit" and "Upload new version".

The vocabulary for adding a SEM measurement
`http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/`

Create SEM measurement

Current version
Created at 11/8/2023, 1:19:59 PM • Published at 11/8/2023, 1:20:47 PM • Alice Wonderland

Edit Upload new version

Upload a SHACL Shape to Herbie





The vocabulary for adding a SEM measurement
Published half a minute ago by Alice Wonderland



Create SEM measurement

Create data from a SHACL Shape





The vocabulary for adding a SEM measurement
Published half a minute ago by Alice Wonderland



Create SEM measurement

Create data from a SHACL Shape

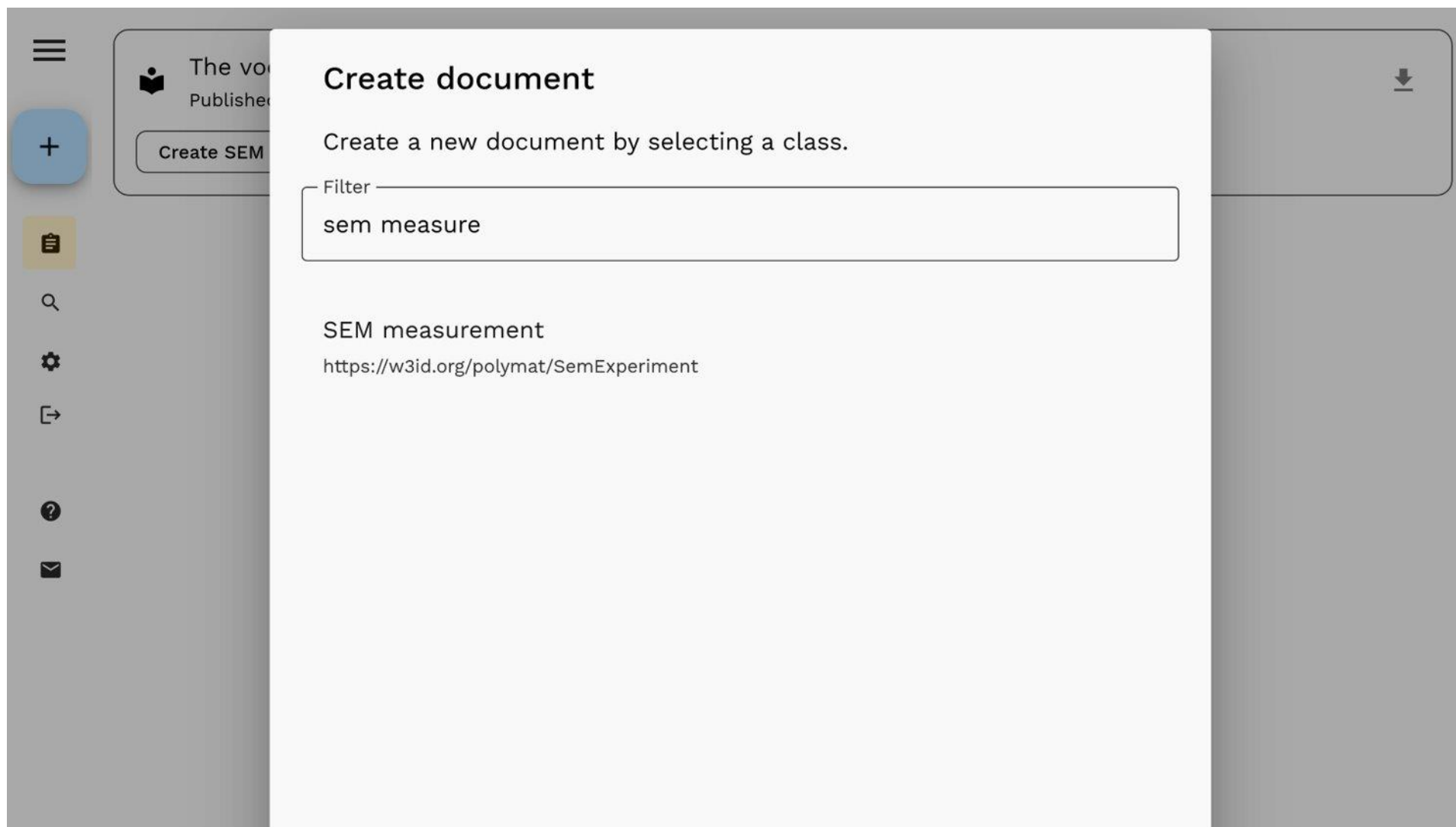
The screenshot shows a web application interface. At the top left is a hamburger menu icon. To its right is a header bar containing a book icon, the text "The vocabulary for adding a SEM measurement", and a download icon. Below the header bar is a dropdown menu with two options: "Document" (highlighted in blue) and "Import graph". Below the dropdown menu is a sidebar with five icons: a magnifying glass, a gear, a square with an arrow, a question mark, and an envelope. The main content area is currently empty.

Create data from a SHACL Shape

The screenshot shows a web application interface with a sidebar on the left containing icons for menu, add, clipboard, search, settings, share, help, and mail. The main content area is partially obscured by a modal dialog titled 'Create document'. The dialog contains the text 'Create a new document by selecting a class.' and a search bar labeled 'Filter'. Below the search bar, there is a list of examples, each with a title and a URL:

- Multi-select combobox example
<http://localhost:8000/api/ont/example/input-dropdown-multiselect/1.0.0/#Root>
- Grid example
<http://localhost:8000/api/ont/example/grid/1.0.0/#Root>
- Extrusion
<http://localhost:8000/api/ont/mb/extrusion/1.0.0/#Extrusion>
- Read-only/generated/persisted field example
<http://localhost:8000/api/ont/example/readonly-generated-persisted/1.0.0/#Root>
- File upload field example
<http://localhost:8000/api/ont/example/file-upload/1.0.0/#Root>
- Single-select combobox example

Create data from a SHACL Shape



Create data from a SHACL Shape

+

🔍

⚙️

🔗

?

✉️

The vocabulary for
Published 2 minutes ago

Create SEM measurement

Drafts

SEM measurement
Modified less than 5 seconds ago

SEM measurement
http://localhost:8000/api/triples/5ab629e8-65f7-4df2-88a7-3d561c5b3a8d/

Download

Close

Draft

Show other versions ↑

Created less than 10 seconds ago and updated less than 5 seconds ago by Alice Wonderland

Conforms to http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/versions/1/

Datasheet

Statements

Turtle

Product

Thickness

nm

Mean pore diameter

nm

Submit

Delete draft

Everything is saved ✓

Create data from a SHACL Shape

+

Q

⚙

↔

?

✉

The vocabulary for
Published 3 minutes ago

Create SEM measurement

Drafts

SEM measurement
Modified one minute ago

SEM measurement
http://localhost:8000/api/triples/5ab629e8-65f7-4df2-88a7-3d561c5b3a8d/

Download

Close

Draft

Show other versions ↑

Created one minute ago and updated one minute ago by Alice Wonderland

Conforms to http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/versions/1/

Datasheet

Statements

Turtle

Product

PTFE Membrane 5

✕

Thickness

3.141

nm

Mean pore diameter

2.718

nm

Submit

Delete draft

Everything is saved ✓

Create data from a SHACL Shape

The screenshot shows a web application interface with a sidebar on the left containing icons for menu, add, clipboard, search, settings, share, help, and mail. The main content area displays a list of items, with one item selected, opening a modal window.

SEM measurement
http://localhost:8000/api/triples/5ab629e8-65f7-4df2-88a7-3d561c5b3a8d/

Current version [Show other versions ↑](#)

Created 2 minutes ago and published less than 10 seconds ago by Alice Wonderland
Conforms to http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/versions/1/

Datasheet	Statements	Turtle
Product PTFE Membrane 5	Thickness 3.141 nm	Mean pore diameter 2.718 nm

[Edit](#) [Upload new version](#)

Create data from a SHACL Shape

≡

+

📋

🔍

⚙️

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✉️

📖

The vocabulary for adding a SEM measurement

Published 4 minutes ago by Alice Wonderland

↓

Create SEM measurement

📋

SEM measurement

Published less than 10 seconds ago by Alice Wonderland

↓

