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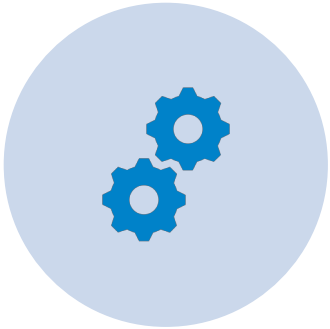
A PROPOSED DATA STANDARD FOR BREATH SAMPLE DATA AND METADATA

BO ZHAO

BACKGROUND

Metabolomics data standards



Reproducibility

Quality assurance

POPULAR METABOLOMICS DATA STANDARDS

ISA Tools

ISA-Tab
ISA JSON

Metabolomics Workbench

mwTab

HUPO Proteomics Standards Initiative

mzTab
mzTab-M

A GOOD DATA STANDARD

Readability

- Human readable
- Machine processable

Usability

- Ease of use

Extendibility

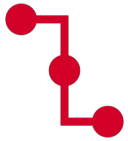
- Configurable design

EXTENDING ISA

ISA data model

Diverse data support

Rich metadata



Enhanced relationship

Chain of processes

Quality control

Validated results

ENHANCED RELATIONSHIP

Ontology based

- Ontology annotations in ISA data model

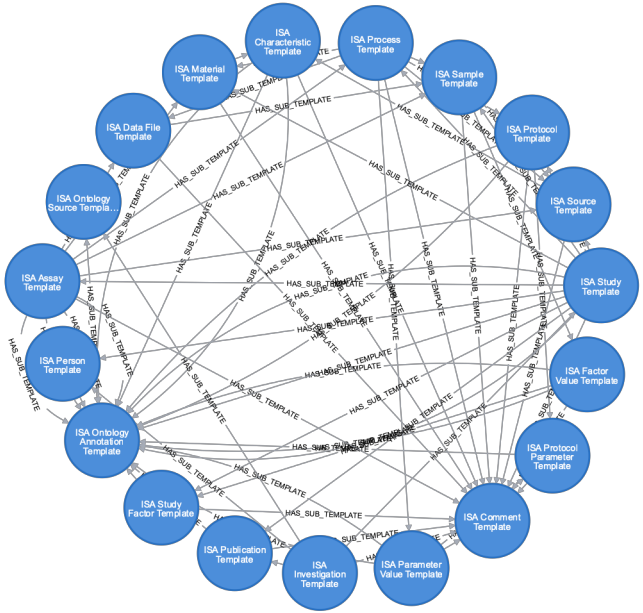
Pre-defined

- Model-based built-in relationship definitions

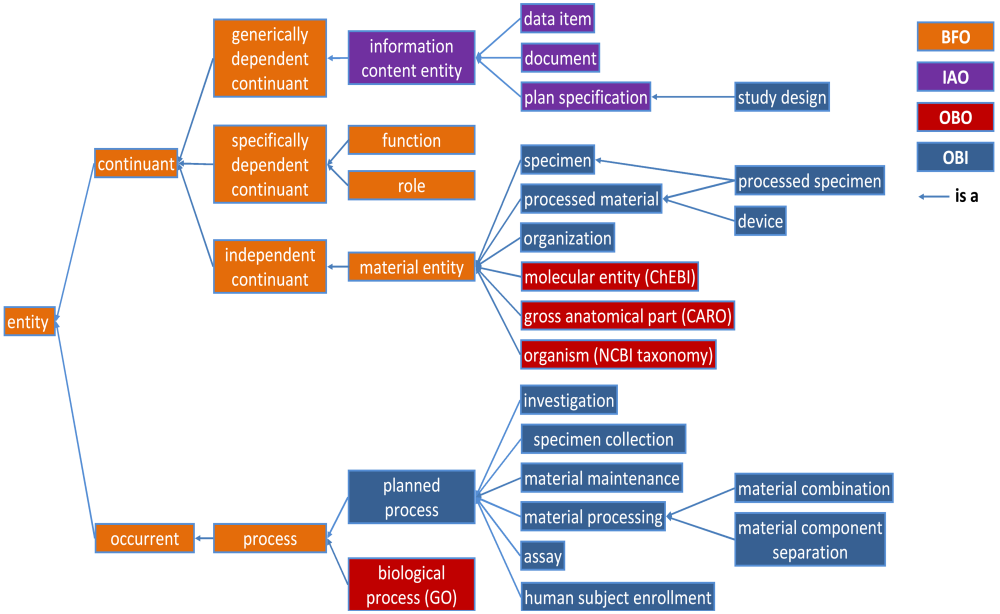
User defined

- Study-specific configurations

ENHANCED RELATIONSHIP



Low-level ISA components relationships



Partial high-level structure of OBI classes (*Bandrowski et al. 2016*)

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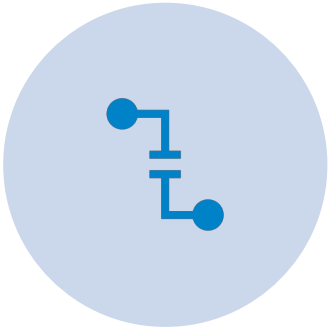
ENHANCED QUALITY CONTROL



Extensively applied

Customisable approaches

(in development)

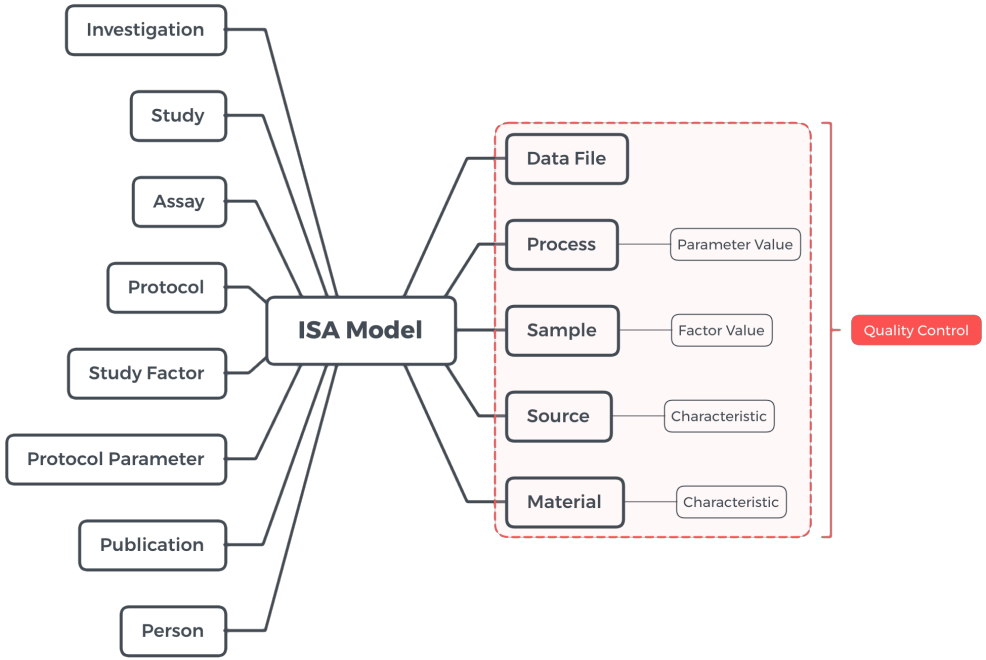
Built-in support for basic statistical validations

ENHANCED QUALITY CONTROL

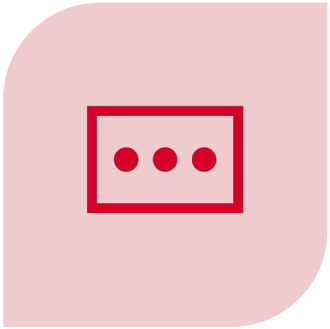
Component level verification

Configurable in study design

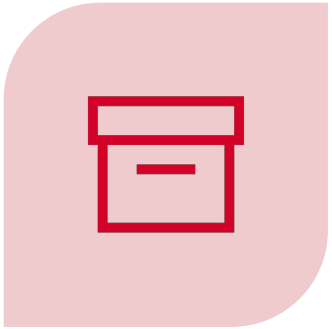
Quality control result file



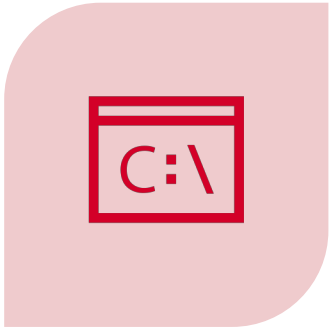
DATA MANAGEMENT TOOL



Local installation or on a server

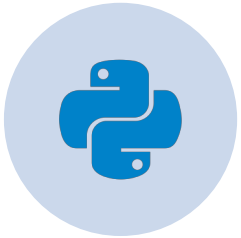


Compatible with original ISA archives



Command line and user-friendly interfaces

TOOL FEATURES



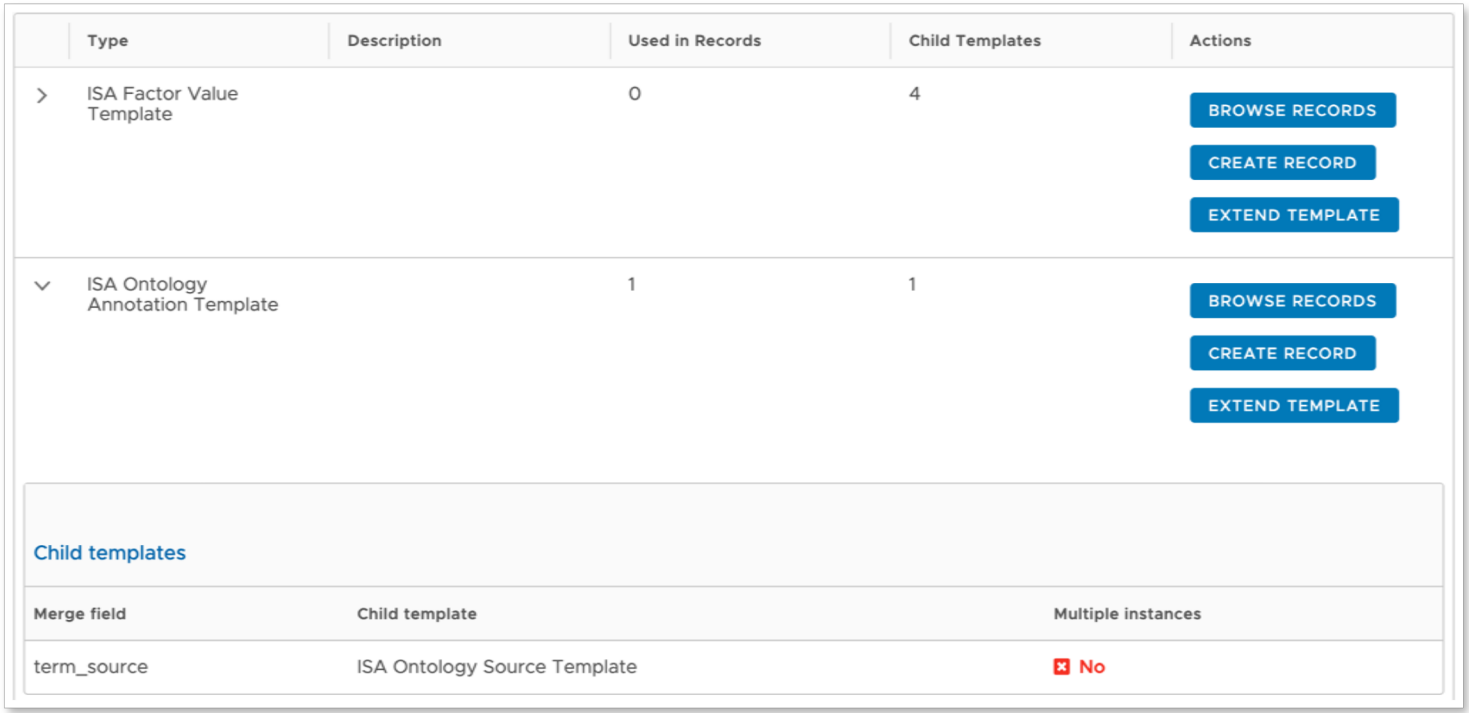
Written in python

Easy to install

Easy to embed

Guided access

USER INTERFACE – TEMPLATE BROWSER



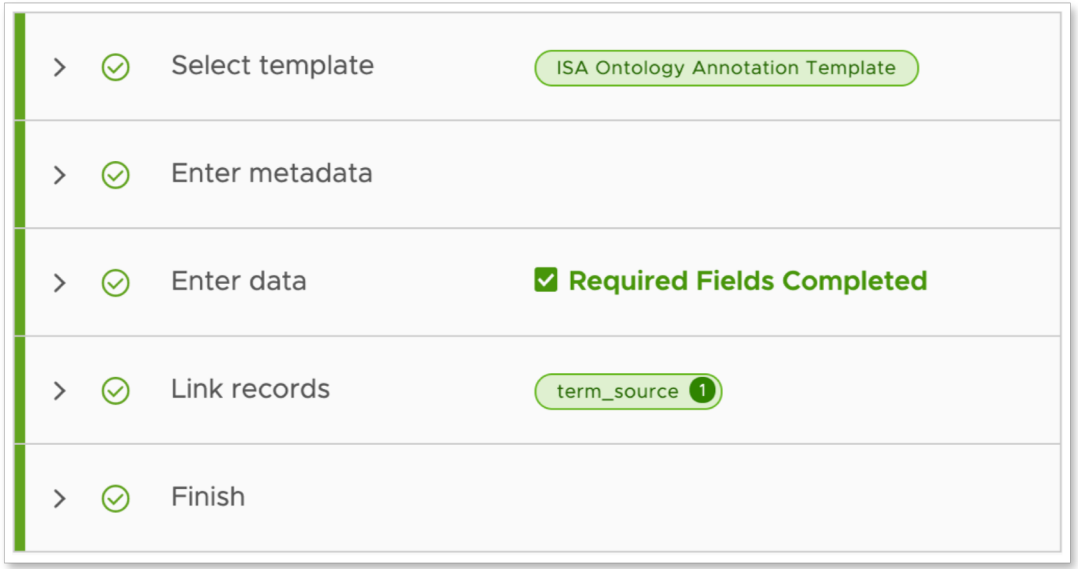
Type	Description	Used in Records	Child Templates	Actions
ISA Factor Value Template		0	4	BROWSE RECORDS CREATE RECORD EXTEND TEMPLATE
ISA Ontology Annotation Template		1	1	BROWSE RECORDS CREATE RECORD EXTEND TEMPLATE

Child templates

Merge field	Child template	Multiple instances
term_source	ISA Ontology Source Template	No

USER INTERFACE – GUIDED RECORD CREATION

1. Template
2. Metadata
3. Data
4. Link
5. Review



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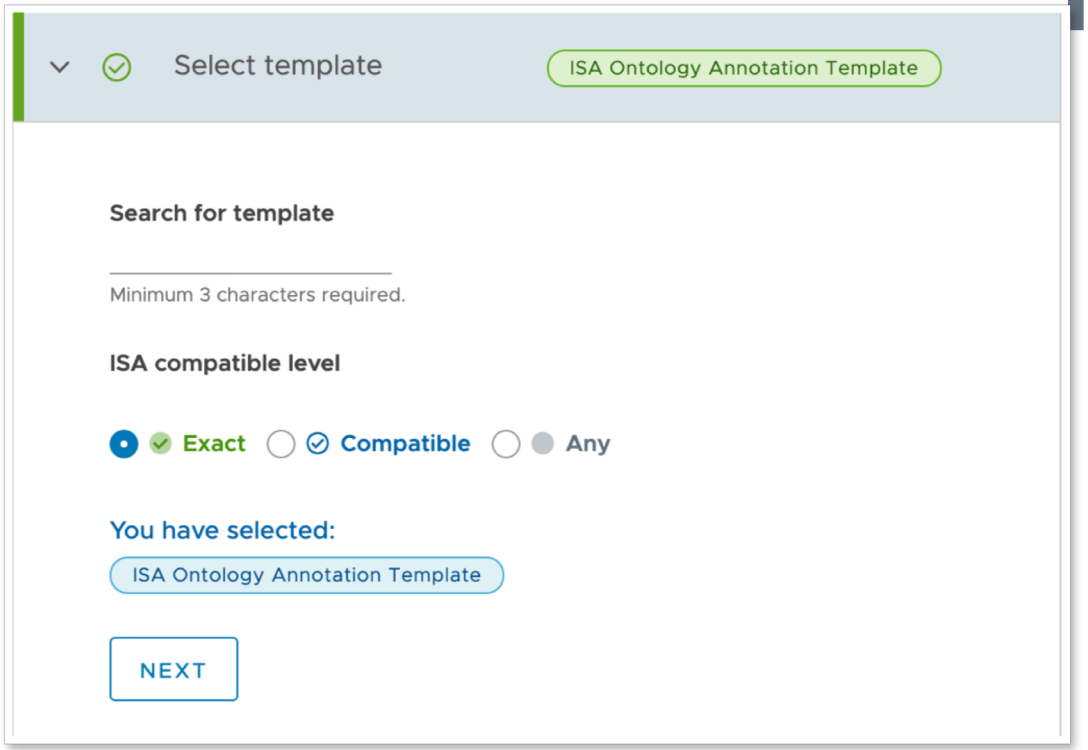

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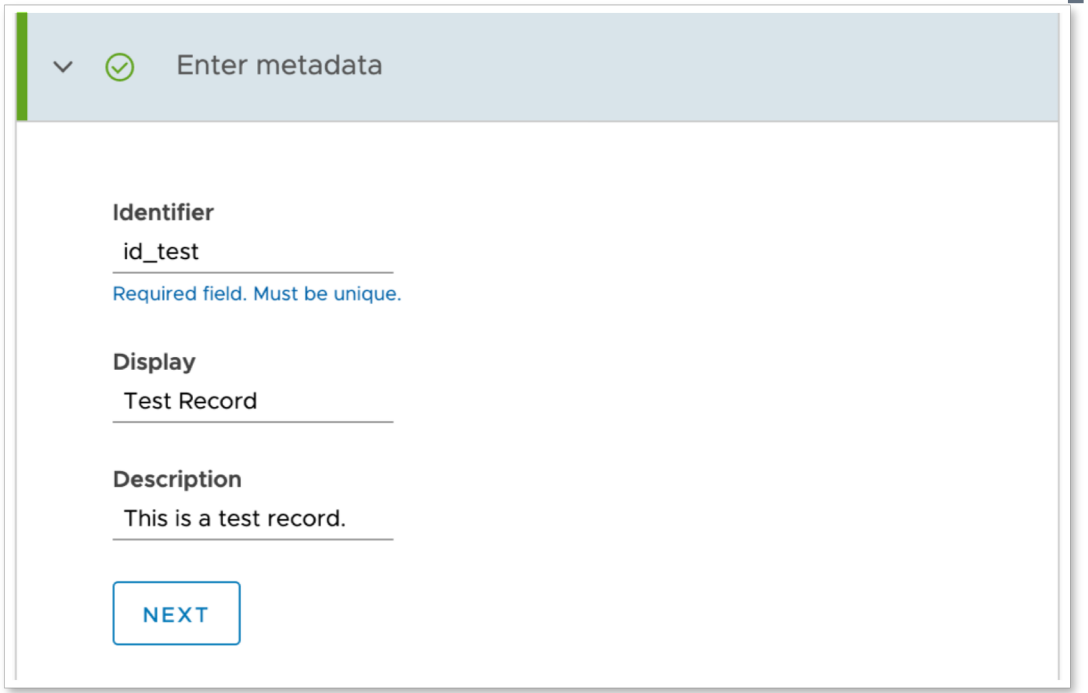

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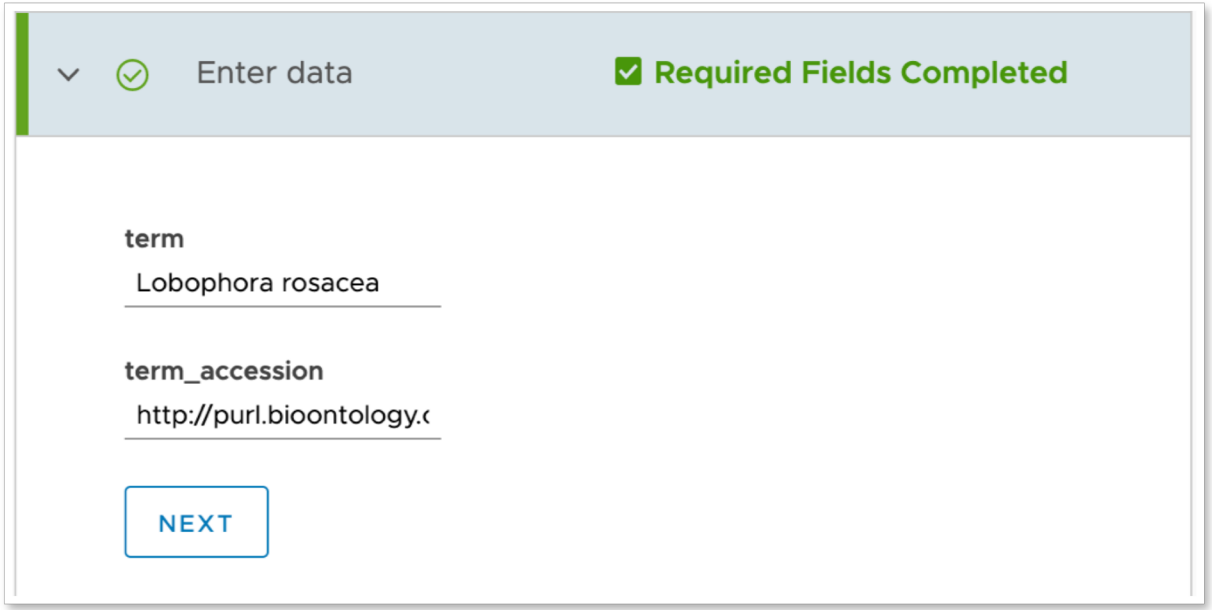

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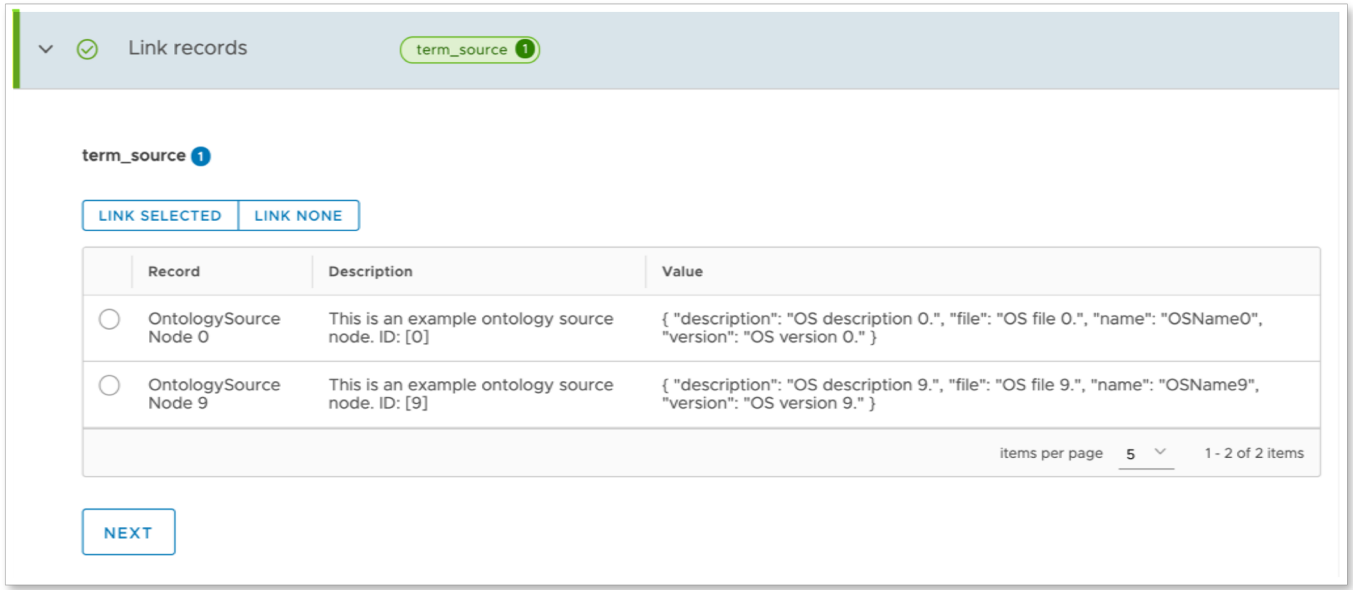

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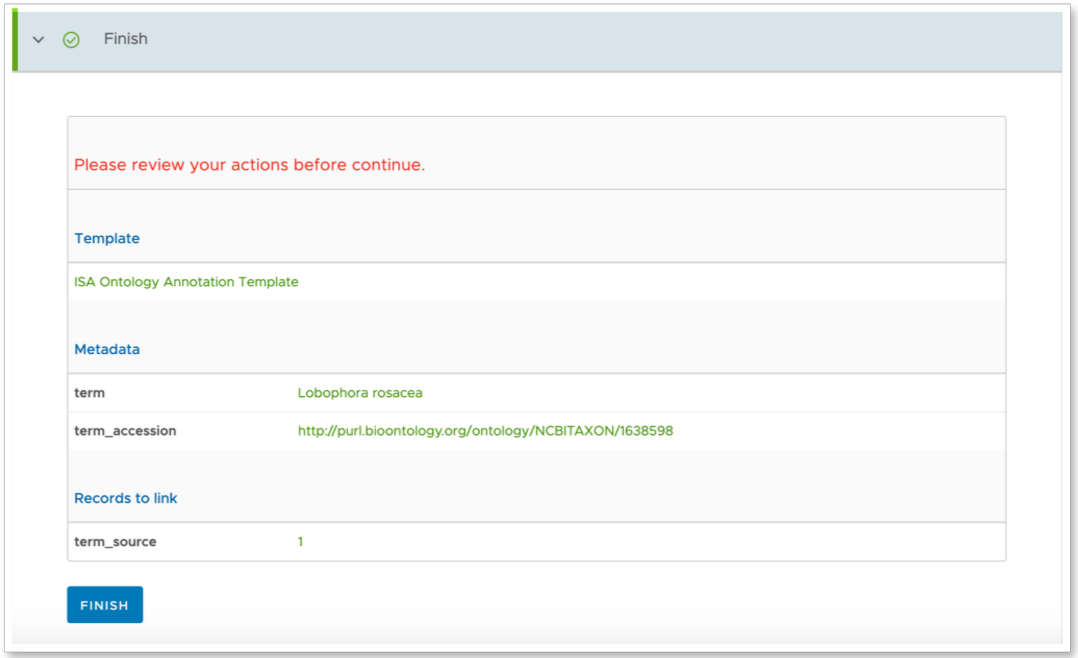
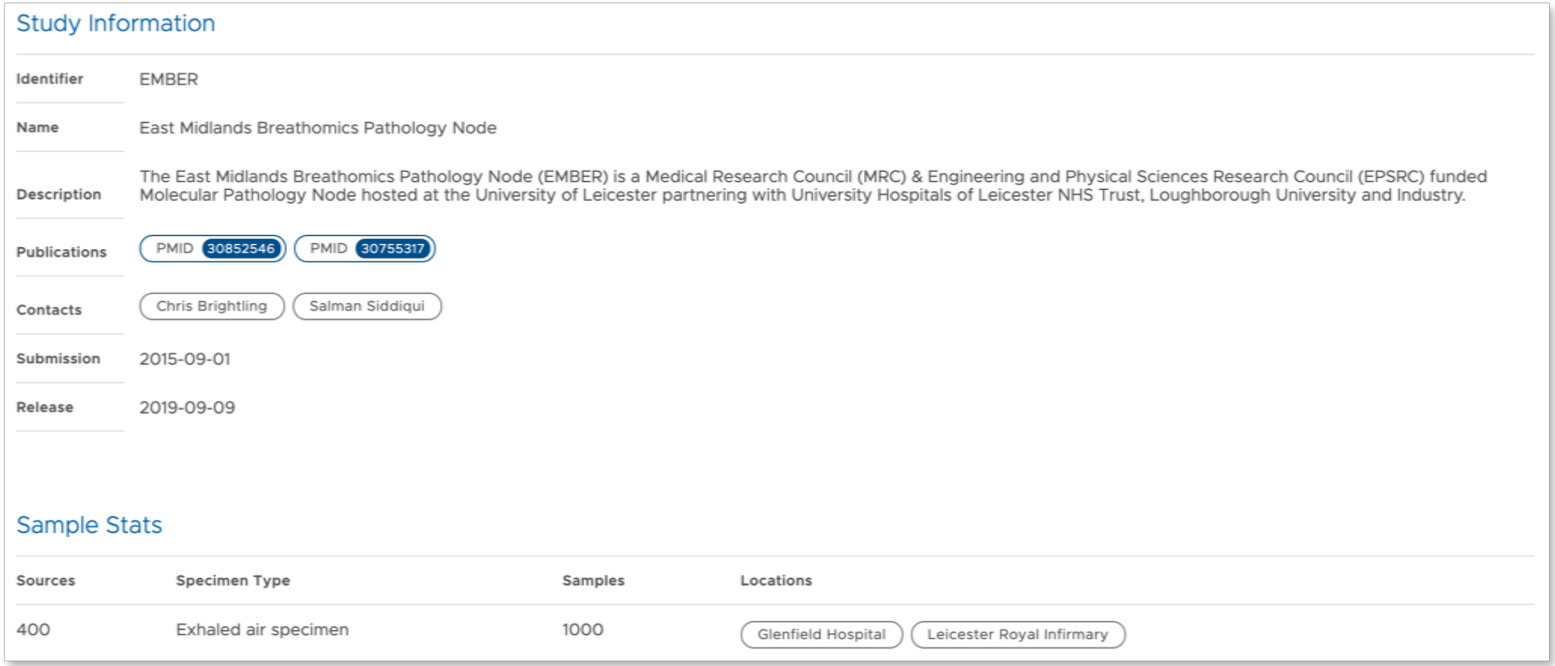


USER INTERFACE - REPORT



Study Information

Identifier	EMBER
Name	East Midlands Breathomics Pathology Node
Description	The East Midlands Breathomics Pathology Node (EMBER) is a Medical Research Council (MRC) & Engineering and Physical Sciences Research Council (EPSRC) funded Molecular Pathology Node hosted at the University of Leicester partnering with University Hospitals of Leicester NHS Trust, Loughborough University and Industry.
Publications	PMID 30852546 PMID 30755317
Contacts	Chris Brightling Salman Siddiqui
Submission	2015-09-01
Release	2019-09-09

Sample Stats

Sources	Specimen Type	Samples	Locations
400	Exhaled air specimen	1000	Glenfield Hospital Leicester Royal Infirmary

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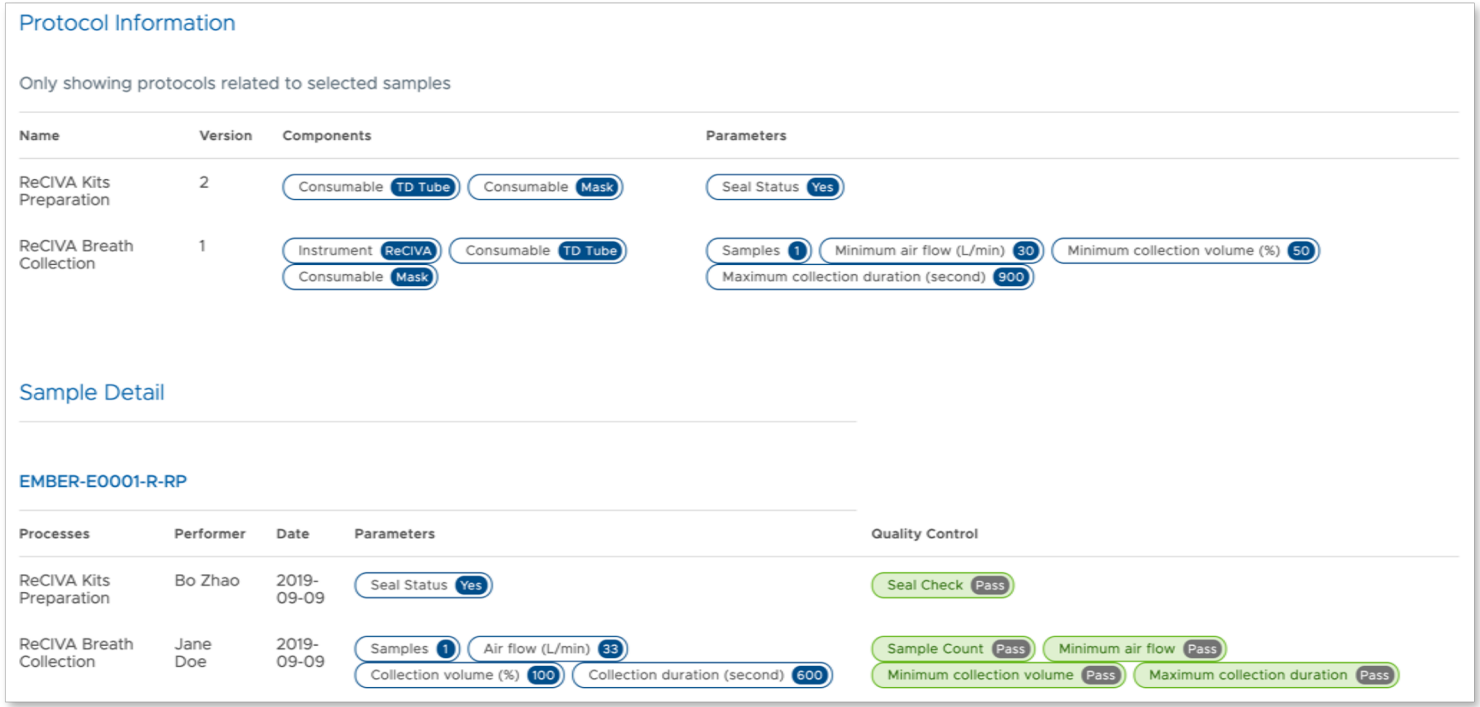
USER INTERFACE - REPORT



Protocol Information

Only showing protocols related to selected samples

Name	Version	Components	Parameters
ReCIVA Kits Preparation	2	Consumable TD Tube; Consumable Mask	Seal Status Yes
ReCIVA Breath Collection	1	Instrument ReCIVA; Consumable TD Tube; Consumable Mask	Samples 1; Minimum air flow (L/min) 30; Minimum collection volume (%) 50; Maximum collection duration (second) 900

Sample Detail

EMBER-E0001-R-RP

Processes	Performer	Date	Parameters	Quality Control
ReCIVA Kits Preparation	Bo Zhao	2019-09-09	Seal Status Yes	Seal Check Pass
ReCIVA Breath Collection	Jane Doe	2019-09-09	Samples 1; Air flow (L/min) 33; Collection volume (%) 100; Collection duration (second) 600	Sample Count Pass; Minimum air flow Pass; Minimum collection volume Pass; Maximum collection duration Pass

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AVAILABILITY

GitHub

https://github.com/rcfgroup

Later this year

OTHER WORKS

- LabPipe
- Ontology for Breath Sample Process

ACKNOWLEDGEMENT

- The research is funded by the EMBER project and NIHR Leicester Biomedical Research Centre – Respiratory.

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