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Knowledge Management of Historical Data: Ontology Development for Chemical Reactions

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Materials Data Science for Stockpile Stewardship

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Knowledge Management of Historical Data: Ontology Development for Chemical Reactions

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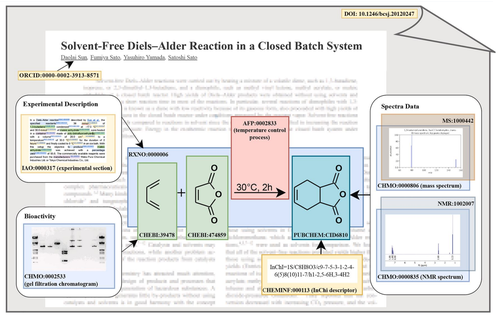
1. INTRODUCTION

LITERATURE KNOWLEDGE

- **Figures**:
  - Chemical structures and equations
  - Results (NMR, FTIR, UV-Vis, DSC, mechanical, etc.)
- Detailed reaction conditions and setup in **written text**
- Raw data aren't available
- Analyses and data transformations aren't available
- Articles saved in **arbitrary folders** on local laptops



Knowledge is scattered in articles on the web/local computer. How to integrate and manage knowledge efficiently?

EXPERIMENTAL DATA

Samples prepared with user-defined sample IDs → Instrument parameters (recipes) setup & sample analyzed → Metadata saved in notebooks or computer software → Raw data saved as .txt or .xls on local computer/software → Data analyzed containing user-defined variable names → Results published & stacked away

METADATA

- User-defined:
  - Sample & experiment IDs
  - Variable names
  - File names + Folder structures
- Not all metadata needed to reproduce experiments is recorded
- Metadata cannot be found by computers

DATA

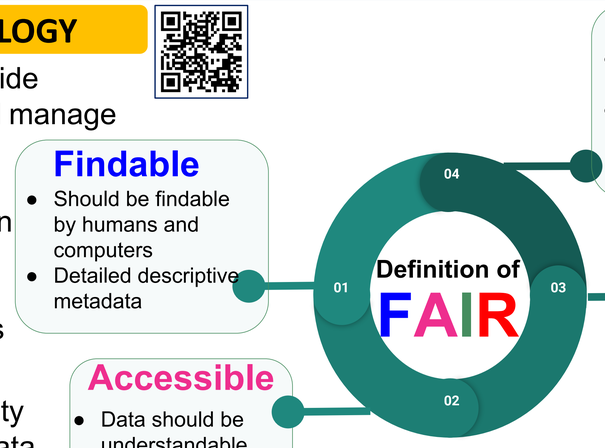
- Data get lost over time
- "Everything" is saved in arbitrary folders on local or instrument computers
- **Integration with other labs/fields is challenging because user-defined variables**
  - Only make sense to the working researcher(s)
- Data and/or required licenses cannot be found by computers

Metadata and data in various formats sources. How to integrate and manage data efficiently?

2. METHOD

FAIR AND ONTOLOGY

- **FAIR principles**[2] provide guidelines to collect and manage metadata.
- **Ontology**
  - a formal representation of knowledge;
  - composes of a set of standardized concepts and definitions;
  - Increase interoperability
  - Organize metadata, data, and knowledge in a meaningful and efficient manner.



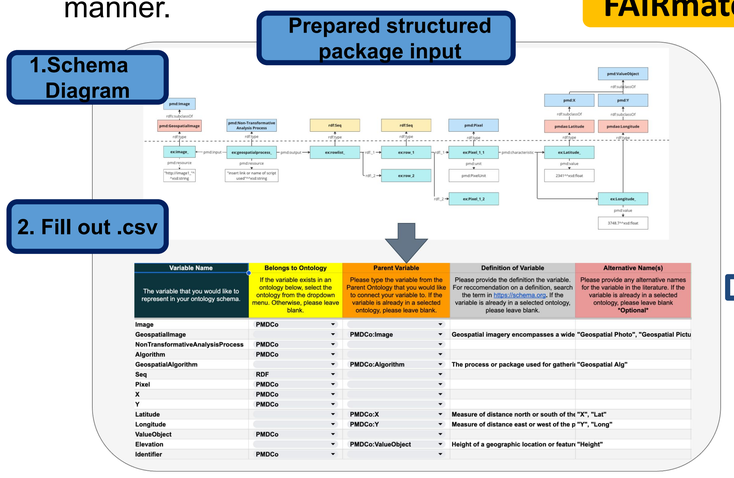
Findable
- Should be findable by humans and computers
- Detailed descriptive metadata

Accessible
- Data should be understandable
- Data should also be in a repository

Interoperable
- Should be integrable with other data
- **Ontologies** tie data to a standardized vocabulary

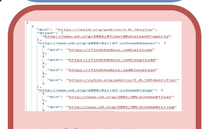
Reusable
- Clear and accessible data usage license
- Data and metadata meet community standards

FAIRmaterials Package[3][4]



An image for users to visualize the ontology schema & ensure its correctness

An OWL File with the ontology schema and populated ontology data



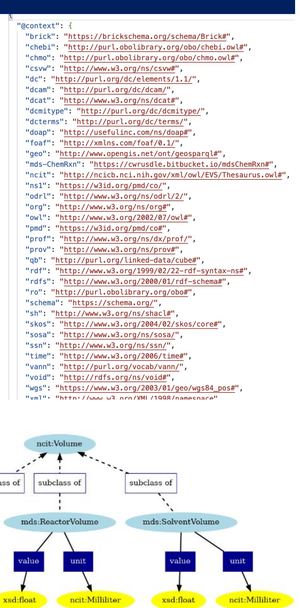
A JSON-LD File with the ontology schema and populated ontology data.

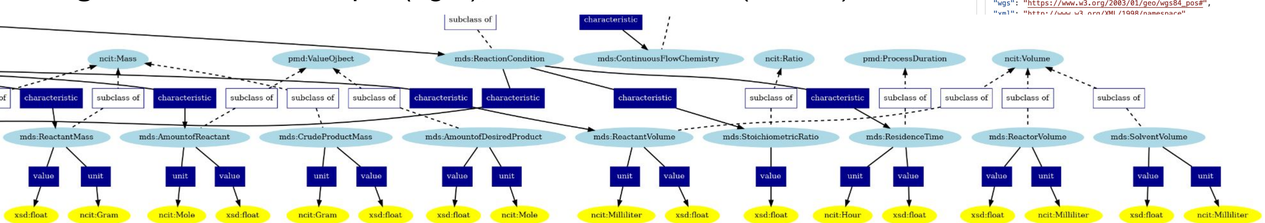
An HTML File with the documentation for the output ontology.

- FAIRmaterials package provides ***an easy to use csv template*** for domain experts to construct their own ontologies mapped from any existing ontologies
- Must connect with a top-level ontology to be interoperable
- Some chemical mid-level ontologies:
  - ***ChEBI, NCIt, CHMO, RXNO***
- The output files (PNG, OWL, JSON-LD, and HTML) allow for better visualization, term definitions and relationships, data population, and documentation, respectively.

3. RESULTS

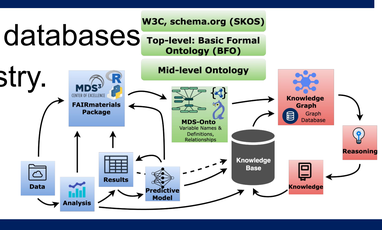
- Investigated mid-level chemical ontologies
  - Must map to Basic Formal Ontology (BFO) as the ISO standard[5]
- Developed an ontology for chemical reaction in nitration of aromatic compounds using continuous flow chemistry
  - A small, concentrated subdomain to ensure the ontology is less overwhelming
  - Specific variable names such as "reactorTemperature" and "reactorFlowRate" instead of just "Temperature" or "flowRate".
- **Figures:** JSON-LD output (right); PNG visualization (bottom).





4. FUTURE WORK

- Build and populate a knowledge base with chemical open-source databases on nitration of aromatic compounds using continuous flow chemistry.
- Equip the knowledge base with a reasoning engine for semantic reasoning.
- Use FAIR and ontology as a backbone of data governance.



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6. ACKNOWLEDGEMENT

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