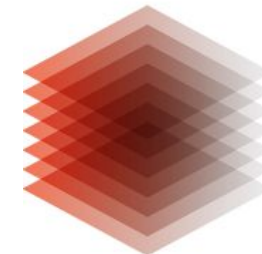




**NFDI<sub>4</sub>Chem**

ENHANCE  
YOUR  
DATA.



**TIB**

dct:title

## Ontologies4Chem:

Current chemical ontologies 4 research data management

dct:identifier

[DOI:10.5281/zenodo.7049724](https://doi.org/10.5281/zenodo.7049724)

dct:references

[DOI:10.1515/pac-2021-2007](https://doi.org/10.1515/pac-2021-2007)

dct:creator

[ORCID:0000-0002-1595-3213](https://orcid.org/0000-0002-1595-3213)

ro:'participates in' Ontologies4Chem Workshop (day 1, talk 2)

dct:identifier

[DOI:10.25798/frnp-sn04](https://doi.org/10.25798/frnp-sn04)

sdo:duration

2022-09-08T14:40:00+02:00/PT10M

# Finding ontologies to describe chemical research data

DOI: 10.1246/bcsj.20120247

## Solvent-Free Diels–Alder Reaction in a Closed Batch System

Daolai Sun, Fumiya Sato, Yasuhiro Yamada, Satoshi Sato

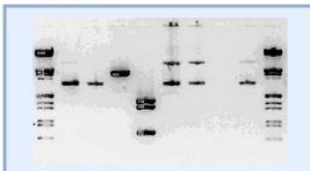
ORCID:0000-0002-3913-8571

### Experimental Description

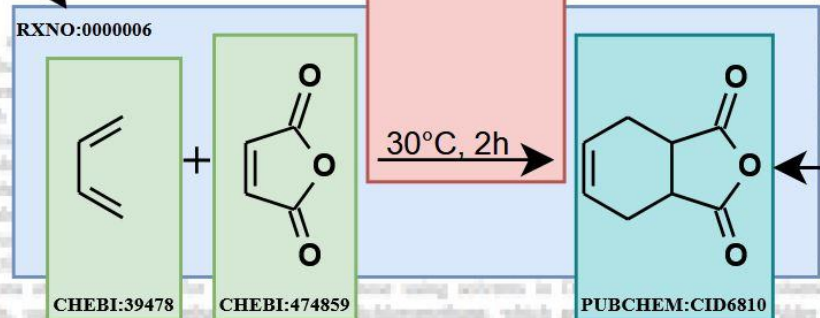
In a Diels-Alder reaction described by Sun et al., the specified reactants, 26 mmol of 3,3,4,4-tetrahydrophthalic anhydride and 30 mmol of maleic anhydride, were heated in a container made of poly(tetrafluoroethylene) with a volume of 20.0 mL to a temperature of 30.0 °C for the duration of 2 hours and finally cooled to 0 °C in an ice bath. With this setup the objective to produce maleic anhydride was achieved with a percentage yield of 95.8. The commercially available reagents were purchased from the manufacturers Wako Pure Chemical Industries Ltd. or Tokyo Chemical Industries Co., Ltd.

IAO:0000317 (experimental section)

### Bioactivity



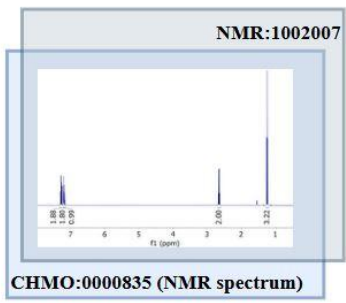
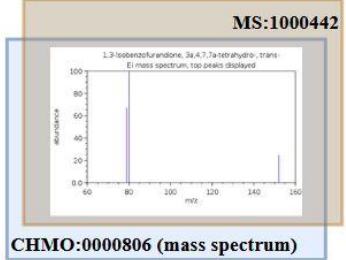
CHMO:0002533 (gel filtration chromatogram)



AFP:0002833 (temperature control process)

InChI=1S/C8H8O3 /c9-7-5-3-1-2-4-6(5)8(10)11-7 /h1-2,5-6H,3-4H2  
CHEMINF:000113 (InChi descriptor)

### Spectra Data



FAIR annotations → FAIR data

- based on ontologies
  - But which ones to use?
- [see our overview in PAC](#)
  - not an exhaustive list
  - starting point for NFDI4Chem
  - found in OLS, OBO Foundry, BioPortal & references in publications

# Finding ontologies to describe chemical research data

DOI: 10.1246/bcsj.20120247

## Solvent-Free Diels–Alder Reaction in a Closed Batch System

Daolai Sun, Fumiya Sato, Yasuhiro Yamada, Satoshi Sato

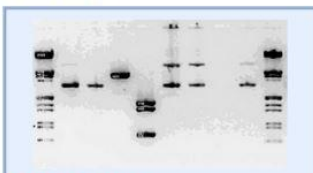
ORCID:0000-0002-3913-8571

### Experimental Description

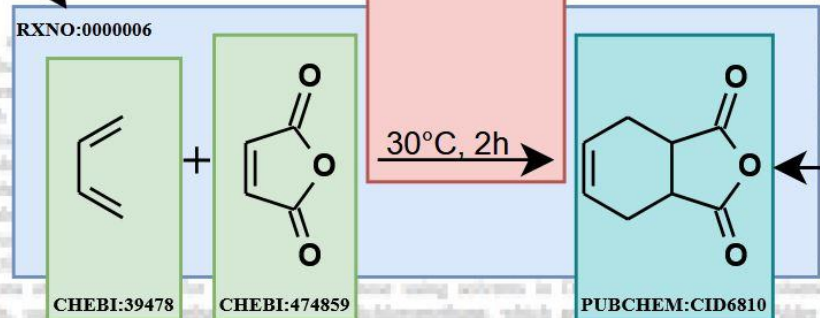
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IAO:0000317 (experimental section)

### Bioactivity



CHMO:0002533 (gel filtration chromatogram)



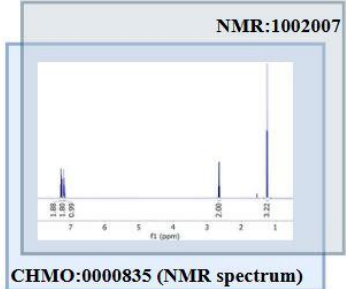
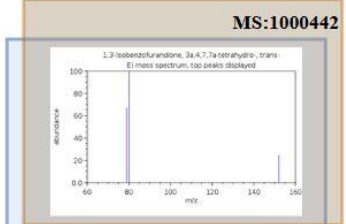
AFP:0002833 (temperature control process)

30°C, 2h

InChI=1S/C8H8O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-2,5-6H,3-4H2

CHEMINF:000113 (InChi descriptor)

### Spectra Data



FAIR annotations → FAIR data

- based on ontologies that are
  - within NFDI4Chem scope
    - organic, inorganic, physical, analytical, macromolecular, pharmaceutical chemistry & biochemistry

# Finding ontologies to describe chemical research data



DOI: 10.1246/bcsj.20120247

## Solvent-Free Diels–Alder Reaction in a Closed Batch System

Daolai Sun, Fumiya Sato, Yasuhiro Yamada, Satoshi Sato

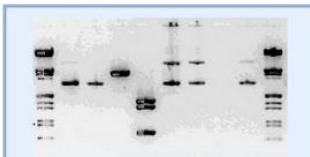
ORCID:0000-0002-3913-8571

### Experimental Description

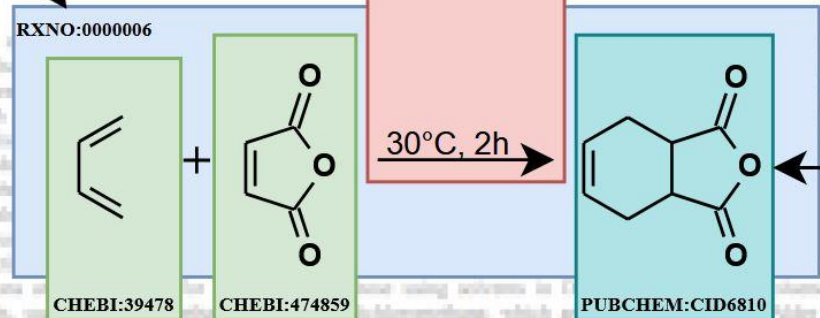
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IAO:0000317 (experimental section)

### Bioactivity



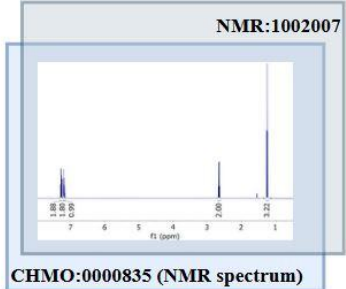
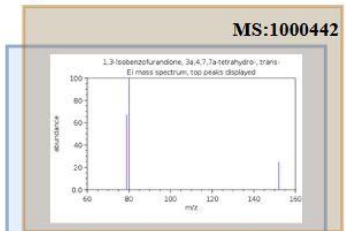
CHMO:0002533 (gel filtration chromatogram)



AFP:0002833 (temperature control process)

InChI=1S/C8H8O3  
/c9-7-5-3-1-2-4-6(5)8(10)11-7  
/h1-2,5-6H,3-4H2  
CHEMINF:000113 (InChi descriptor)

### Spectra Data



FAIR annotations → FAIR data

- based on ontologies that are
  - within NFDI4Chem scope
  - made by domain experts

# Finding ontologies to describe chemical research data



DOI: 10.1246/bcsj.20120247

## Solvent-Free Diels–Alder Reaction in a Closed Batch System

Daolai Sun, Fumiya Sato, Yasuhiro Yamada, Satoshi Sato

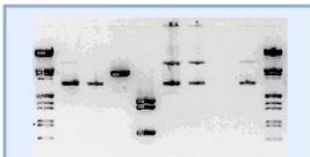
ORCID:0000-0002-3913-8571

### Experimental Description

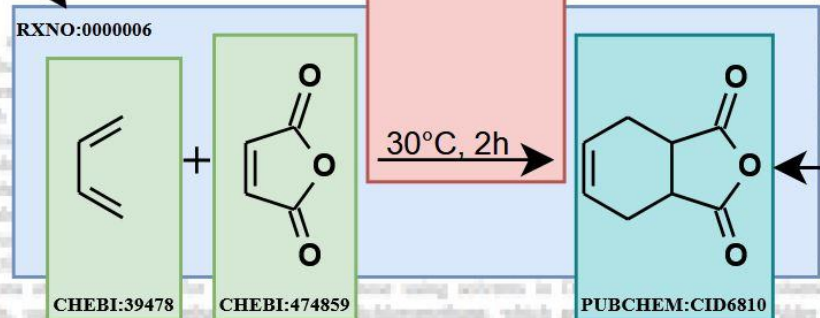
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IAO:0000317 (experimental section)

### Bioactivity



CHMO:0002533 (gel filtration chromatogram)

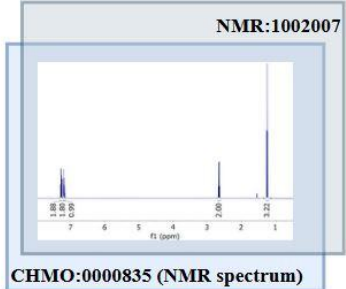
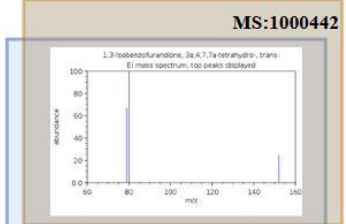


AFP:0002833 (temperature control process)

30°C, 2h

InChI=1S/C8H8O3  
/c9-7-5-3-1-2-4-6(5)8(10)11-7  
/h1-2,5-6H,3-4H2  
CHEMINF:000113 (InChi descriptor)

### Spectra Data



FAIR annotations → FAIR data

- based on ontologies that are
  - within NFDI4Chem scope
  - made by domain experts
  - also FAIR

# Finding ontologies to describe chemical research data



DOI: 10.1246/bcsj.20120247

## Solvent-Free Diels–Alder Reaction in a Closed Batch System

Daolai Sun, Fumiya Sato, Yasuhiro Yamada, Satoshi Sato

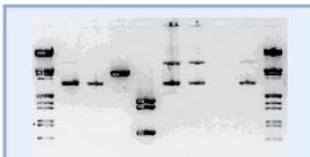
ORCID:0000-0002-3913-8571

### Experimental Description

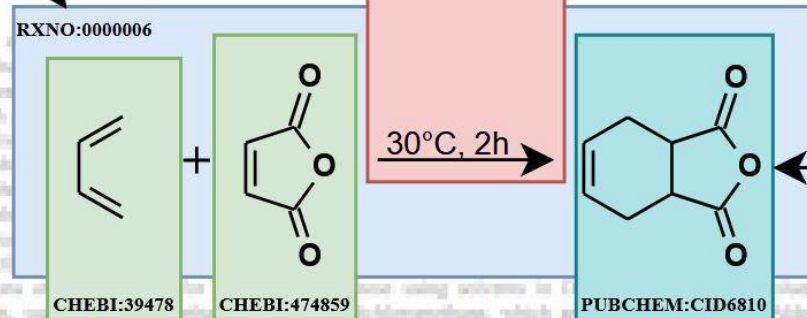
In a Diels-Alder reaction described by Sun et al., the specified reactants, 28 mmol of 3,3,4,4-tetrafluorocyclopentadiene and 30 mmol of maleic anhydride, were heated in a container made of poly(tetrafluoroethylene) with a volume of 20.0 mL to a temperature of 30.0 °C for the duration of 2 hours and finally cooled to 0 °C in an ice bath. With this setup the objective to produce maleic anhydride was achieved with a percentage yield of 95.8. The commercially available reagents were purchased from the manufacturers Wako Pure Chemical Industries Ltd. or Tokyo Chemical Industries Co., Ltd.

IAO:0000317 (experimental section)

### Bioactivity



CHMO:0002533 (gel filtration chromatogram)

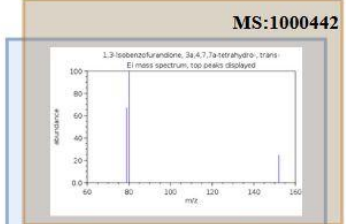


AFP:0002833 (temperature control process)

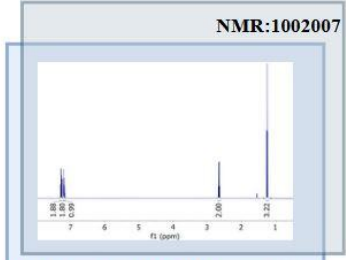
30°C, 2h

InChI=1S/C8H8O3  
/c9-7-5-3-1-2-4-6(5)8(10)11-7  
/h1-2,5-6H,3-4H2  
CHEMINF:000113 (InChi descriptor)

### Spectra Data



CHMO:0000806 (mass spectrum)



CHMO:0000835 (NMR spectrum)

FAIR annotations → FAIR data

- based on ontologies that are
  - within NFDI4Chem scope
  - made by domain experts
  - also FAIR
  - reusable in modules

# Finding ontologies to describe chemical research data

DOI: 10.1246/bcsj.20120247

## Solvent-Free Diels–Alder Reaction in a Closed Batch System

Daolai Sun, Fumiya Sato, Yasuhiro Yamada, Satoshi Sato

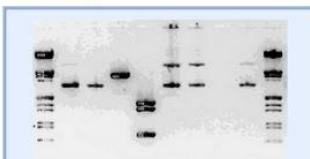
ORCID:0000-0002-3913-8571

### Experimental Description

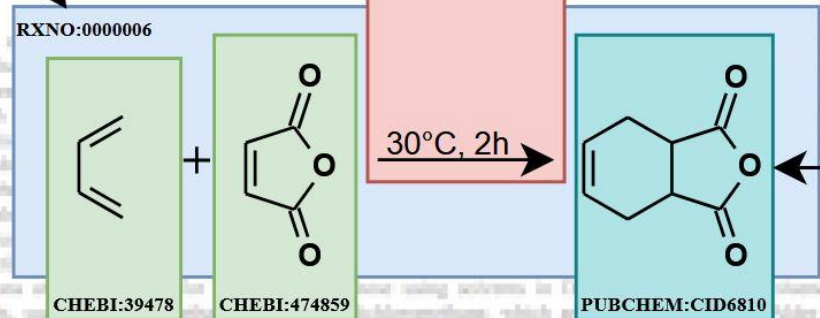
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IAO:0000317 (experimental section)

### Bioactivity



CHMO:0002533 (gel filtration chromatogram)

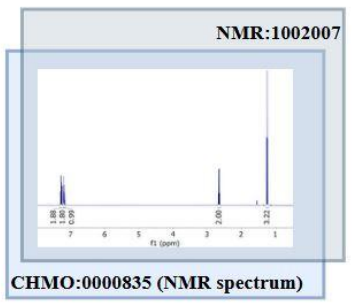
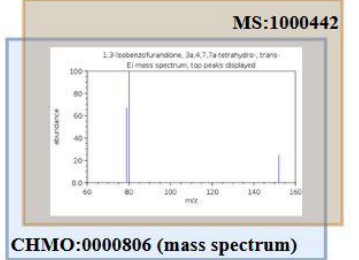


AFP:0002833 (temperature control process)

30°C, 2h

InChI=1S/C8H8O3  
/c9-7-5-3-1-2-4-6(5)8(10)11-7  
/h1-2,5-6H,3-4H2  
CHEMINF:000113 (InChi descriptor)

### Spectra Data



FAIR annotations → FAIR data

- based on ontologies that are
  - within NFDI4Chem scope
  - made by domain experts
  - also FAIR
  - reusable in modules
  - used in known contexts & actively maintained

# Ontologies related to Chemistry

---



## Upper Ontologies

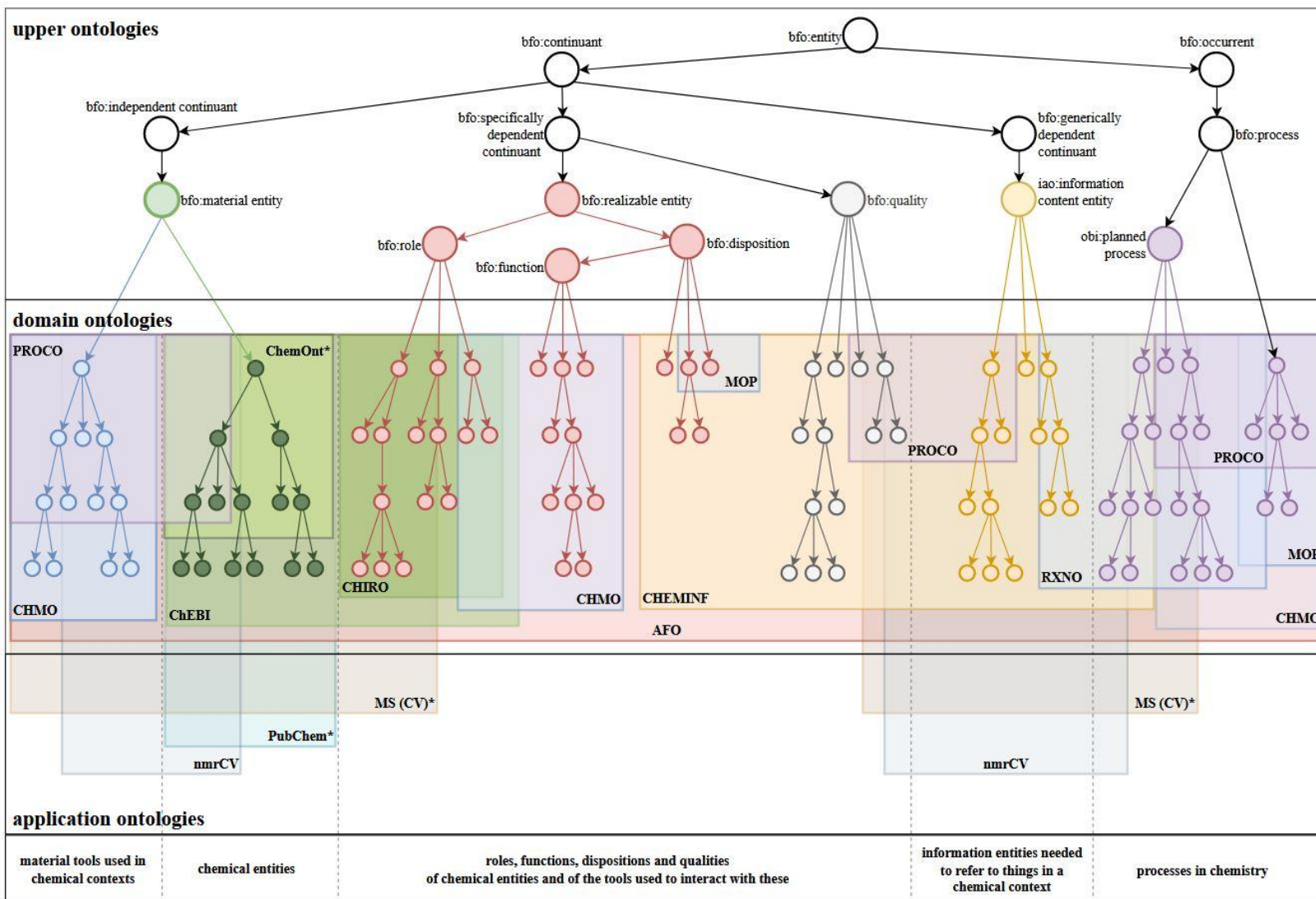
- Basic Formal Ontology ([BFO 2.0](#)) classes only version → abstract basis (continuants & occurents)
- Relation Ontology ([RO](#)) → abstract and general basis for relations & their patterns
- SemanticScience Integrated Ontology ([SIO](#)) → widely used, less complex than BFO & RO (but bridged)
- Ontology for Computer-Aided chemical Process Engineering ([OntoCAPE](#)) → mighty but idiosyncratic

## General Domain Ontologies

- Information Artifact Ontology ([IAO](#)) → basis for all things considered information
- Ontology for Biomedical Investigations ([OBI](#)) → basis for terms around scientific investigations
- Phenotype And Trait Ontology ([PATO](#)) → basis for attributes/characteristics of material things
- Units of measurement ontology ([UO](#)) → contains SI units and other units of measure
- Ontology of Quantities, Units, Dimensions and Types ([QUDT](#)) → UO alternative
- Onto. of bioscientific data analysis and data management ([EDAM](#)) → Data, Formats, Processes & Topics



# Chemistry Domain Ontologies



**Covering all domains**

**compounds:** [ChEBI](#), [ChemOnt](#), AFO

**materials:** [CHMO](#), [PROCO](#), [AFO](#)

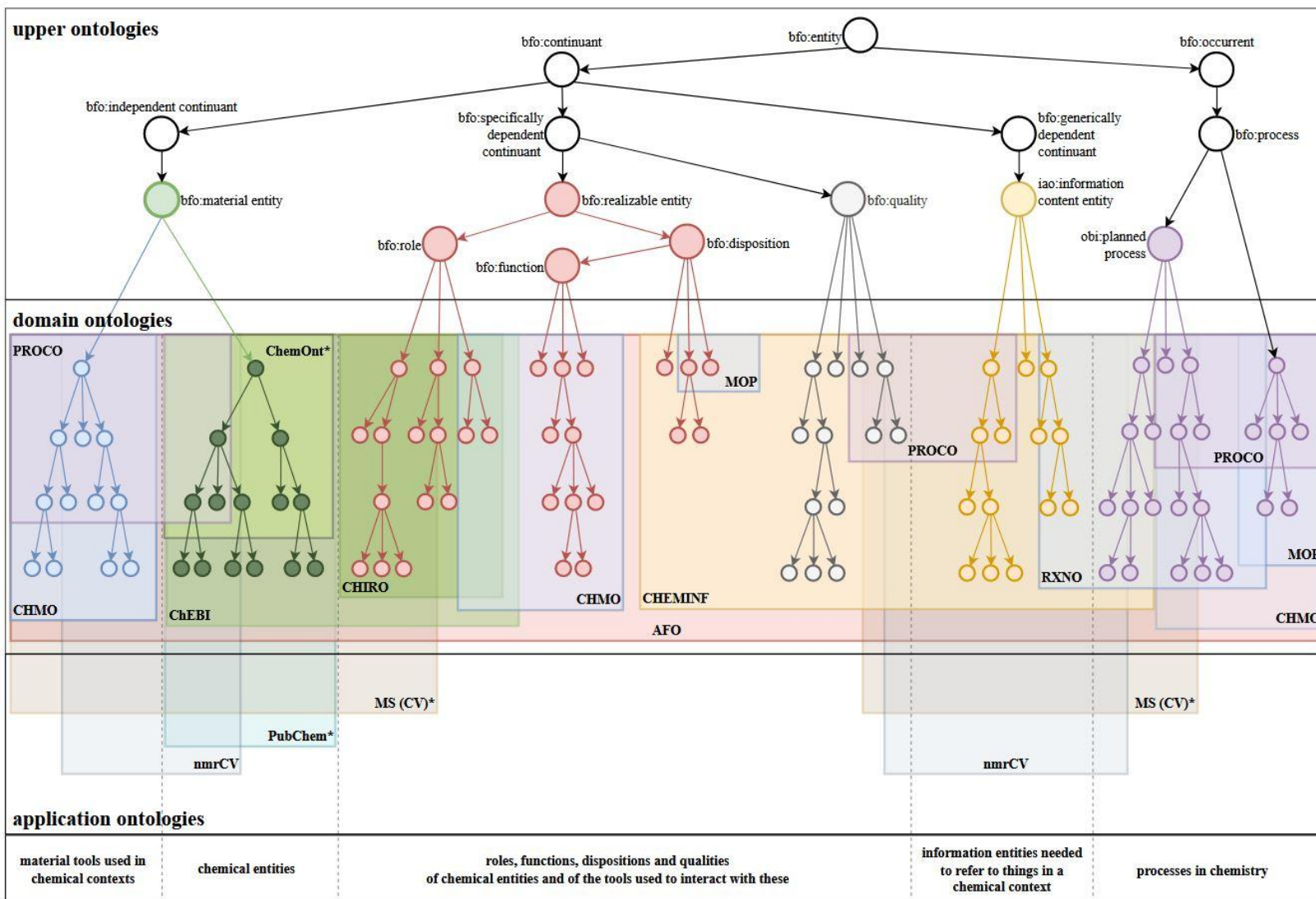
**processes** in: [RXNO](#), [MOP](#), CHMO, AFO, PROCO

**attributes** in: [CHEMINF](#), CHMO, MOP, AFO & PROCO

**information** in: CHEMINF, CHMO, AFO, PROCO

\* not BFO aligned by default

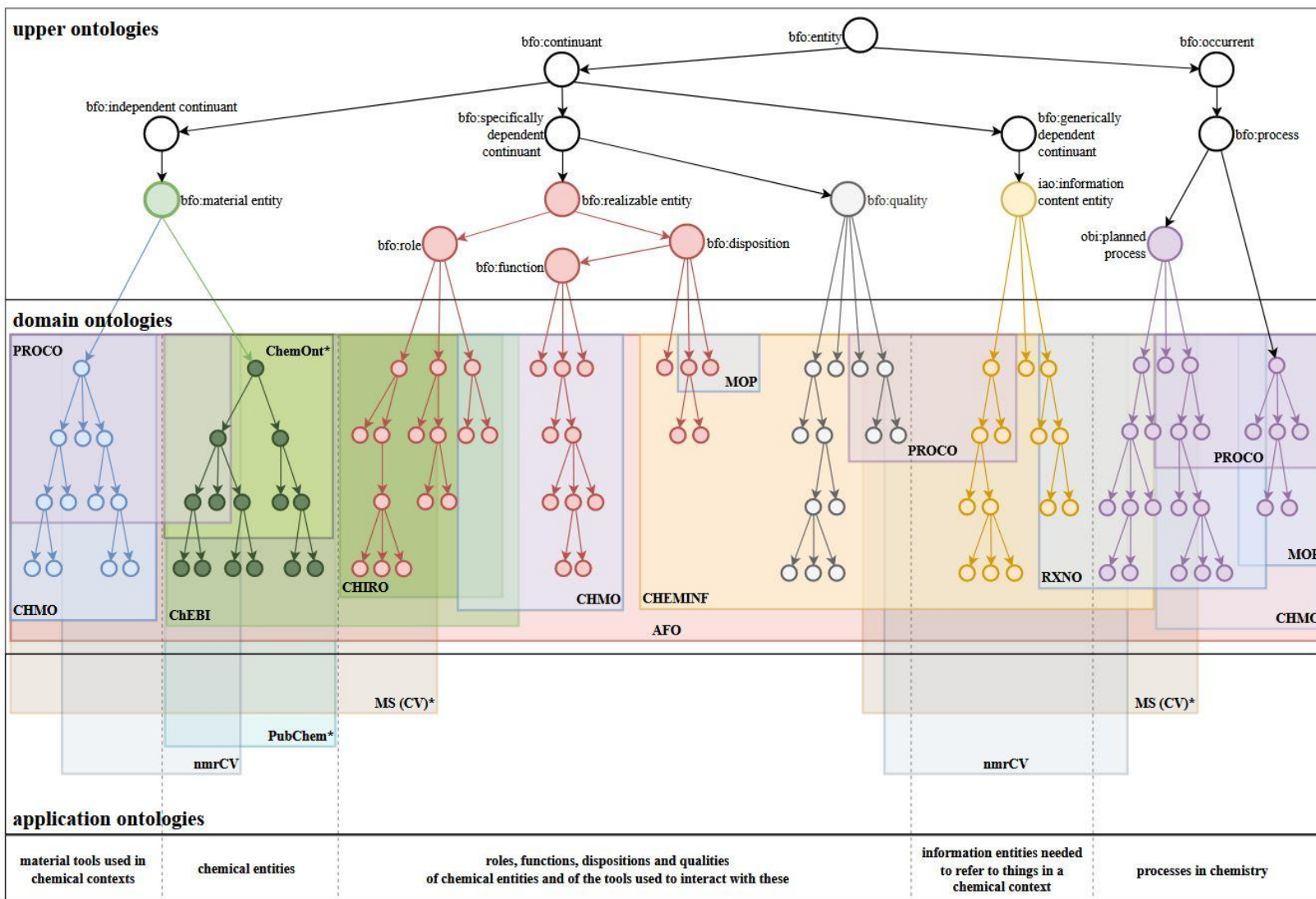
# Chemistry Domain Ontologies



## Issues & Open Questions

- industry & academia differences

# Chemistry Domain Ontologies

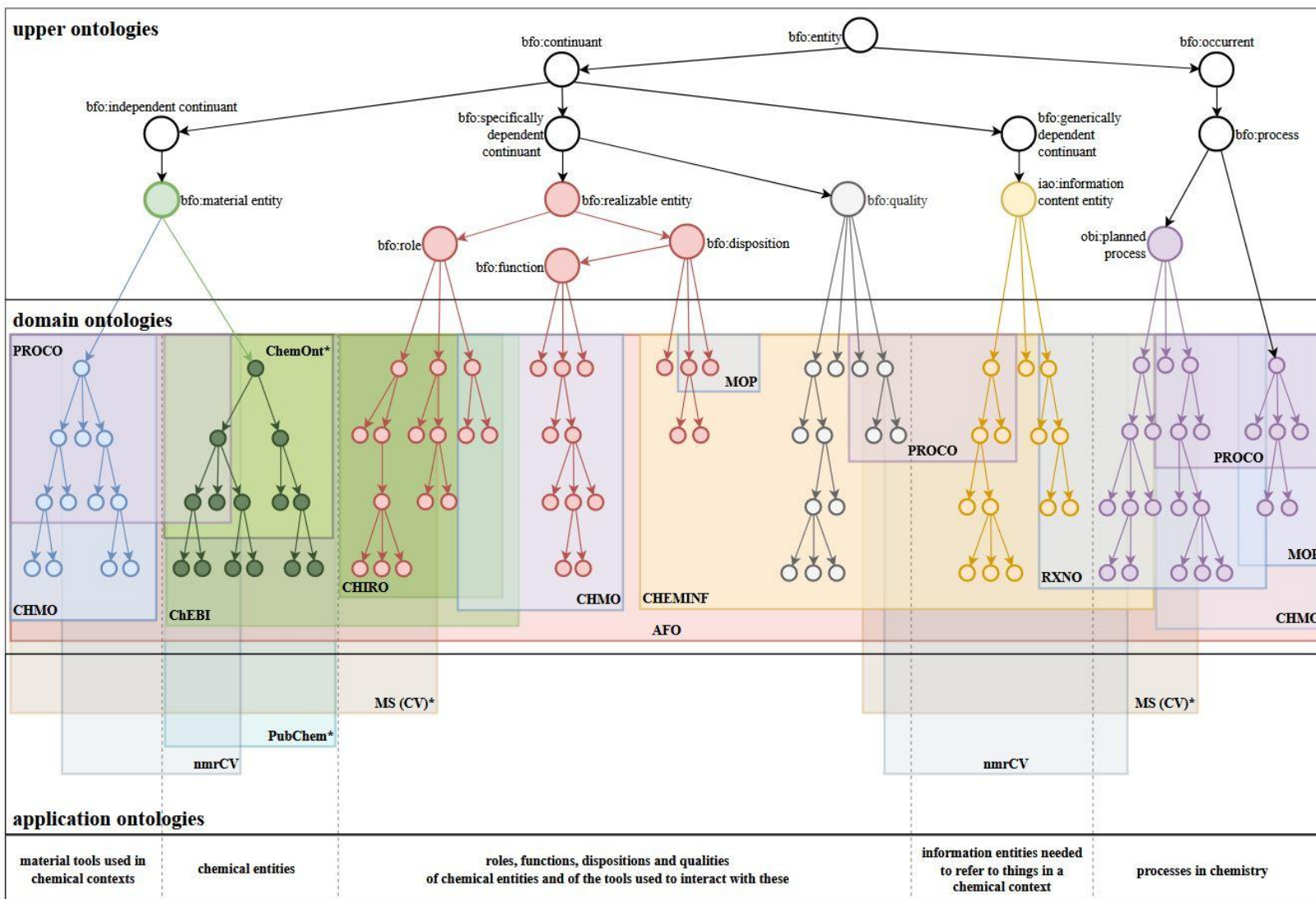


## Issues & Open Questions

- industry & academia differences
- semantic harmonization
- improving orthogonality
- clear division of scopes
- open mappings, bridges & docs

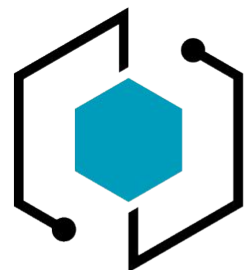
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# Chemistry Domain Ontologies



## Issues & Open Questions

- industry & academia differences
- semantic harmonization
  - improving orthogonality
  - clear division of scopes
  - open mappings, bridges & docs
- more automation → ODK
  - transparent QC & releases
  - better documentation
  - easier to contribute & maintain



**NFDI**<sub>4</sub>Chem

**ENHANCE  
YOUR  
DATA.**