

YOUR DATA.

### **NFDI4Chem Terminology Service - News & Updates** Fostering the Community Curation of Chemical Ontologies

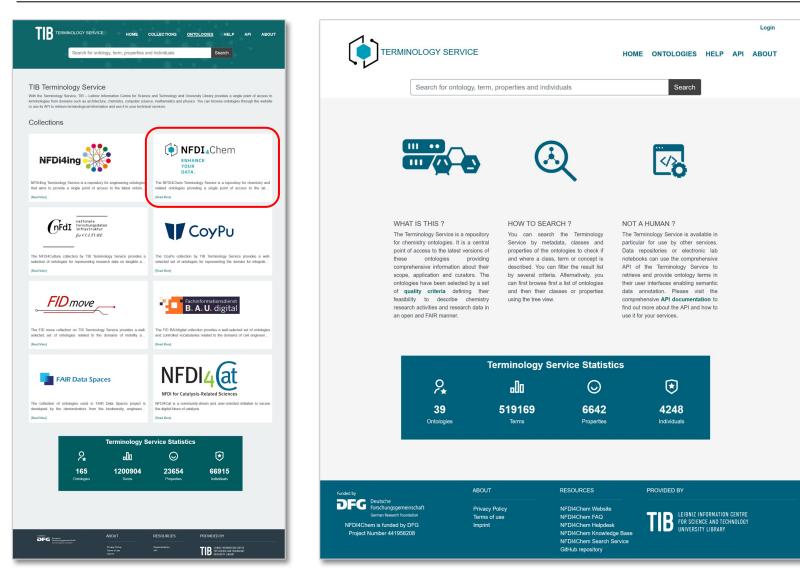
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2nd Ontologies4Chem Workshop 2023 - Day 1, October 11th - 12th 2023

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#### A part of TIB TS general





- based on EBI's OLS
  - added new features
- part of TIB TS
  - NFDI4Chem collection
  - project based frontend
- 39 ontologies
  - 15 chemistry specific
  - SKOS ready
- A point of entry for exploration and curation

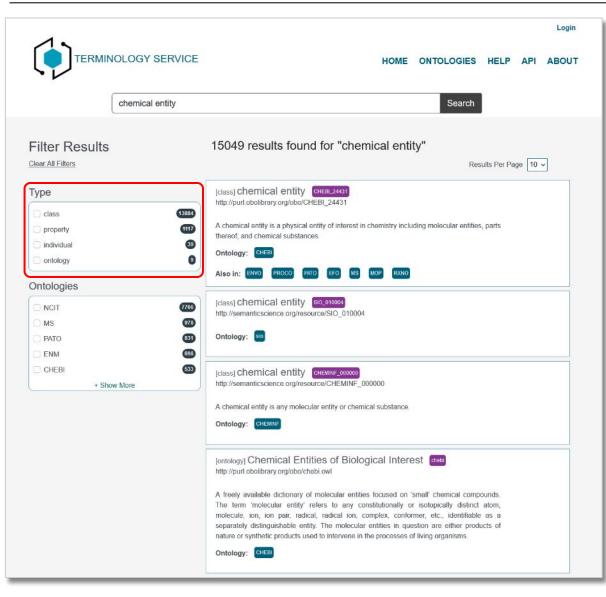
#### **Exploring Ontologies: General Search**

	Login VICE HOME ONTOLOGIES HELP API ABOUT
Chemical entity	Search
Filter Results Clear All Filters	15049 results found for "chemical entity" Results Per Page 10 ~
Type class property individual ontology Ontologies NCIT MS PATO	Image: Signature of the second sec
CHEBI + Show More	Class] Chemical entity CHEMNE_000000     http://semanticscience.org/resource/CHEMINF_000000     A chemical entity is any molecular entity or chemical substance.     Ontology: CHEMNE
	[ontology] Chemical Entities of Biological Interest (Interest Interval) (Interval) (Inte



- search in all indexed fields
  - e.g. ontology description & title, term label, definition, ...

#### **Exploring Ontologies: General Search**





- search in all indexed fields
  - e.g. abstract, label, definition
- filter by type of term
  - class, property, individual or ontology

#### **Exploring Ontologies: General Search**



1.	Login
	HOME ONTOLOGIES HELP API ABOUT
chemical entity	Search
Filter Results Clear All Filters	15049 results found for "chemical entity" Results Per Page 10 -
Type class (388) property (517) individual (3) ontology (3) Ontologies	[class] Chemical entity CHEBL 24431         http://purl.obolibrary.org/obo/CHEBI_24431         A chemical entity is a physical entity of interest in chemistry including molecular entities, parts thereof, and chemical substances.         Ontology: CHEBI         Also in: ENVO PROCO PATO EFO MS MOP RXNO         [class] Chemical entity (Sic.01000)
MS     979       PATO     639       ENM     699       CHEBI     639       + Show More	http://semanticscience.org/resource/SIO_010004         Ontology:         Iclass] Chemical entity         OHEMINE_000000         http://semanticscience.org/resource/CHEMINF_000000         A chemical entity is any molecular entity or chemical substance.
	Ontology: CHEMNE         [ontology] Chemical Entities of Biological Interest (the product of biological interest of biological interest (the product of biological interest (the product of biological interest of biological intervention of biology (the product of biology)         Ontology:       CHEBI

- search in all indexed fields
- filter by type of term
- filter by ontology
  - sorted by number of hits

#### **Exploring Ontologies: General Search**

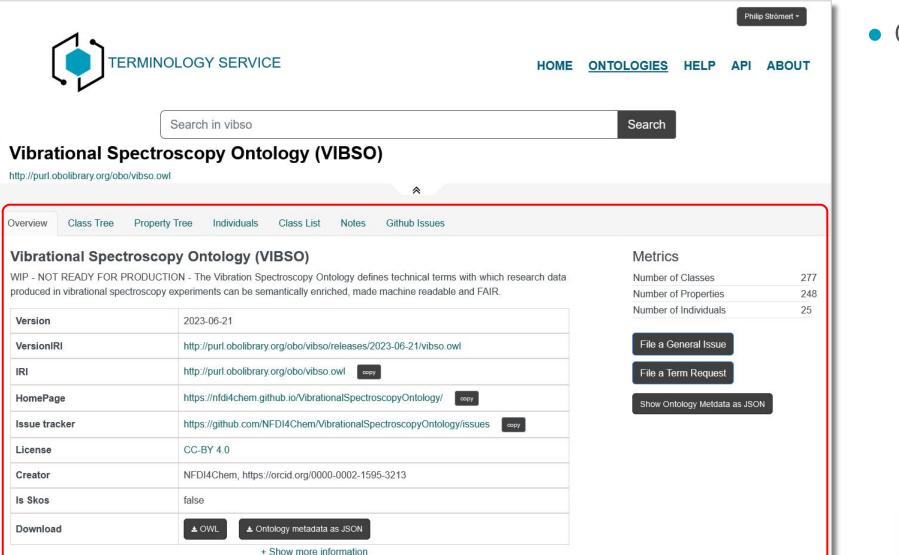


15	Login
	HOME ONTOLOGIES HELP API ABOUT
chemical entity	Search
Filter Results	15049 results found for "chemical entity" Results Per Page 10 v
Туре	[class] Chemical entity CHEBI_24431 http://purl.obolibrary.org/obo/CHEBI_24431
class     (1883)       property     (117)       individual     (39)       ontology     (9)	A chemical entity is a physical entity of interest in chemistry including molecular entities, parts thereof, and chemical substances. Ontology: CHEM
Ontologies	Also in: ENVO PROCO FATO EFO MS MOP RXND
NCIT         7769           MS         979           PATO         633           ENM         669	[class] Chemical entity       SO_010004         http://semanticscience.org/resource/SIO_010004         Ontology:       BD
CHEBI	[class] Chemical entity CHEMINF_000000 http://semanticscience.org/resource/CHEMINF_000000 A chemical entity is any molecular entity or chemical substance.
	A chemical emity is any indecular emity of chemical substance. Ontology: CHEMNE
	[ontology] Chemical Entities of Biological Interest
	A freely available dictionary of molecular entities focused on 'small' chemical compounds. The term 'molecular entity' refers to any constitutionally or isotopically distinct atom, molecule, ion, ion pair, radical, radical ion, complex, conformer, etc., identifiable as a separately distinguishable entity. The molecular entities in question are either products of nature or synthetic products used to intervene in the processes of living organisms. Ontology:

- search in all indexed fields
- filter by type of term
- filter by ontology
- most important details at once
  - type, label/title, IRI,

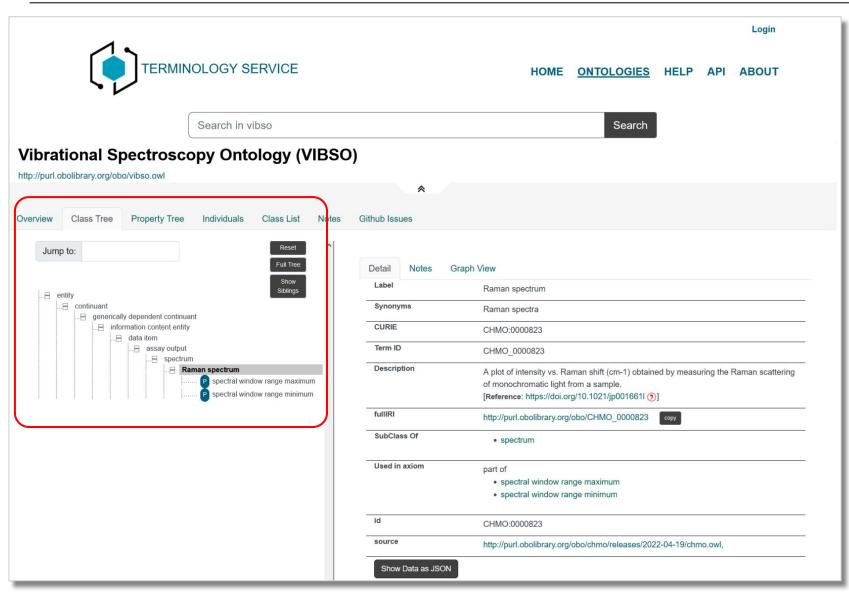
description/definition, source, reusage

#### **Exploring Ontologies: Ontology Overview**



- Ontology overview
  - Important metadata
  - Tree & list views
  - Notes feature
  - GitHub issues

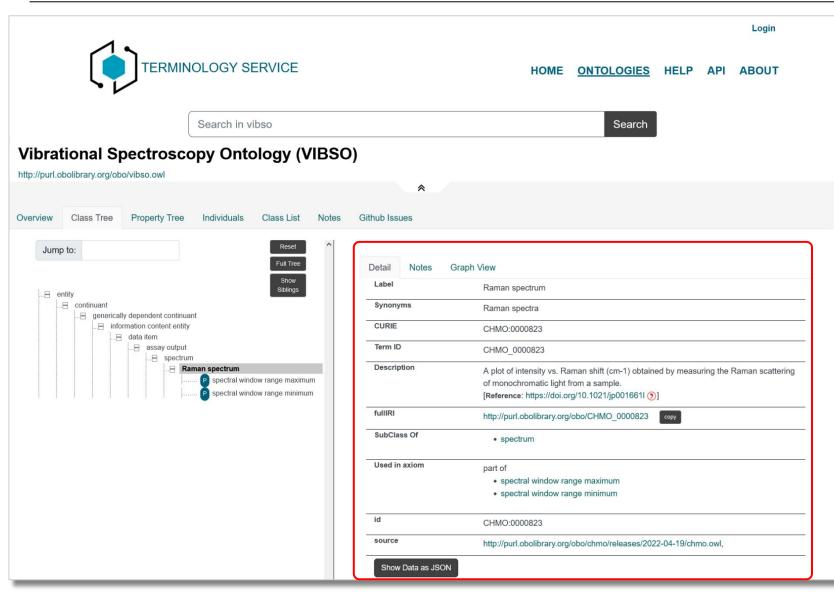
#### **Exploring Ontologies: Class Tree View**





- Ontology overview
- Tree view & navigation
  - is\_a & part\_of relations
  - Autocomplete jump to
  - Adjustable pane
  - Arrow key responsive

### **Exploring Ontologies: Term Details**





- Ontology overview
- Tree view & navigation
- Term details list
  - Sorted by relevance
  - Term annotations
  - Logical axioms
  - Quick API access

#### **Exploring Ontologies: Term Details via API**



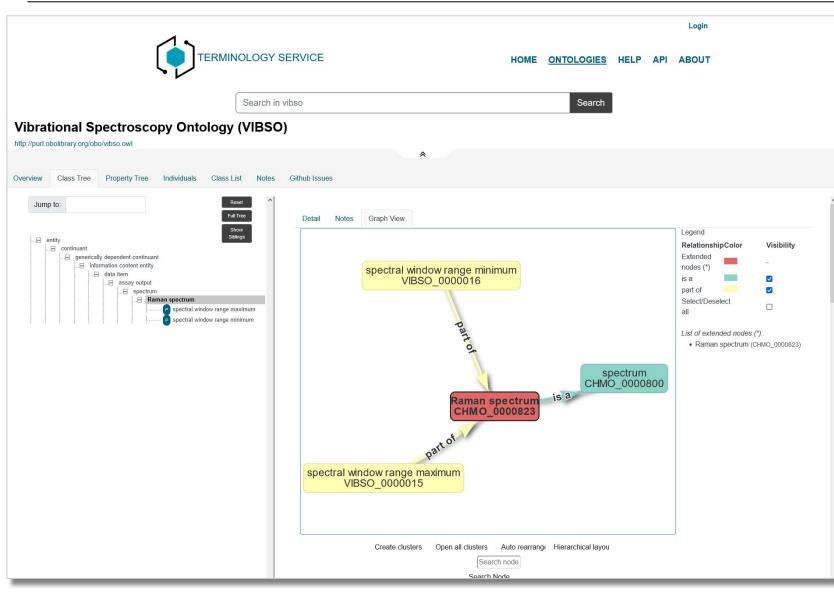
- Ontology overview
- Tree view & navigation
- Term details list
- REST API
  - App & script integration
  - Used in
    - o nmrXiv
    - Ontology Elements
    - Chemotion (WIP)

JSON	Rohdaten Kopfzeilen			
Speichern	Kopieren Alle einklappen	Alle ausklappen 🛛 🖓 JSON durchsuchen		
_embed	ded:			
🔻 term	is:			
▼ 0	8			
	iri:	"http://purl.obolibrary.org/obo/VIBSO_0000010"		
	label:	"groove density setting"		
	description:			
<b>▼</b> 0:		"A setting datum that specifies the number of grooves in a diffraction g		
	annotation:			
	🔻 contributor:			
	0:	" <u>http://orcid.org/0000-0002-1595-3213</u> "		
	▼ editor note:			
	♥ 0:	"This class should better be defined in a more general device ontology o		
	🔻 seeAlso:			
	▼ 0:	" <u>https://github.com/NFDI4Chem/VibrationalSpectroscopyOntology/issues/45</u> "		
	synonyms:	null		
	ontology_name:	"vibso"		
	ontology_prefix:	"VIBSO"		
	ontology_iri:	" <u>http://purl.obolibrary.org/obo/vibso.owl</u> "		
	<pre>is_obsolete:</pre>	false		
	<pre>term_replaced_by:</pre>	null		
	<pre>is_defining_ontology:</pre>	true		

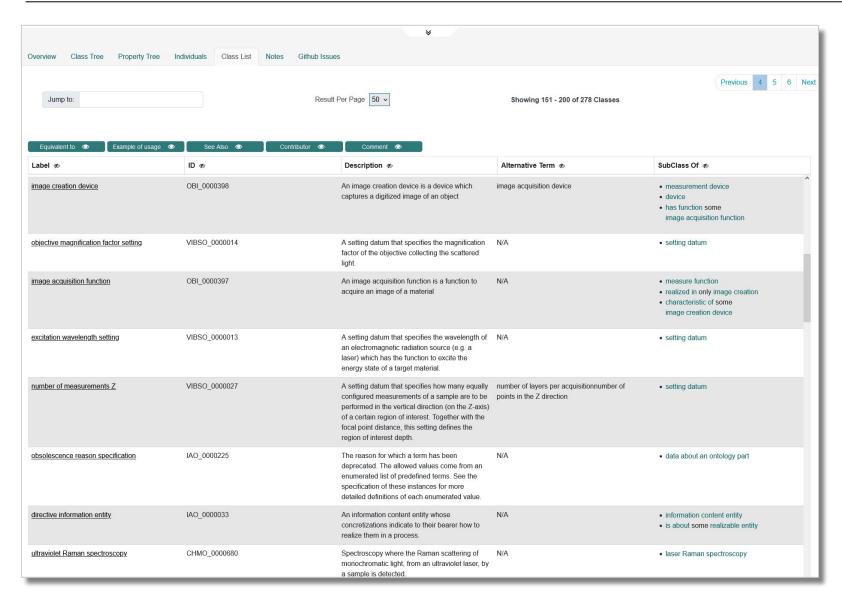
#### **Exploring Ontologies: Graph View**



- Ontology overview
- Tree view & navigation
- Term details list
- REST API
- Graph view (WIP)
  - Visualize relations
  - Traversable Hierarchy



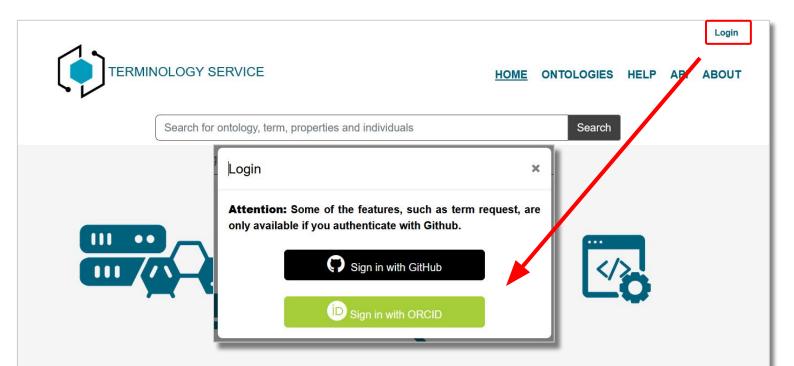
#### **Exploring Ontologies: List View**





- Ontology overview
- Tree view & navigation
- Term details list
- REST API
- Graph view (WIP)
- List view (WIP)
  - Hideable Columns
  - ToDo sorting & filtering
  - Quicker overview of imported & native classes

**Curating Chemical Ontologies Collaboratively** 



#### WHAT IS THIS ?

The Terminology Service is a repository for chemistry ontologies. It is a central point of access to the latest versions of these ontologies providing comprehensive information about their scope, application and curators. The ontologies have been selected by a set of **quality criteria** defining their feasibility to describe chemistry research activities and research data in an open and FAIR manner.

#### HOW TO SEARCH ?

You can search the Terminology Service by metadata, classes and properties of the ontologies to check if and where a class, term or concept is described. You can filter the result list by several criteria. Alternatively, you can first browse first a list of ontologies and then their classes or properties using the tree view.

#### NOT A HUMAN ?

The Terminology Service is available in particular for use by other services. Data repositories or electronic lab notebooks can use the comprehensive API of the Terminology Service to retrieve and provide ontology terms in their user interfaces enabling semantic data annotation. Please visit the comprehensive **API documentation** to find out more about the API and how to use it for your services.

### • Personal account

- GitHub or ORCID
- Allows more features



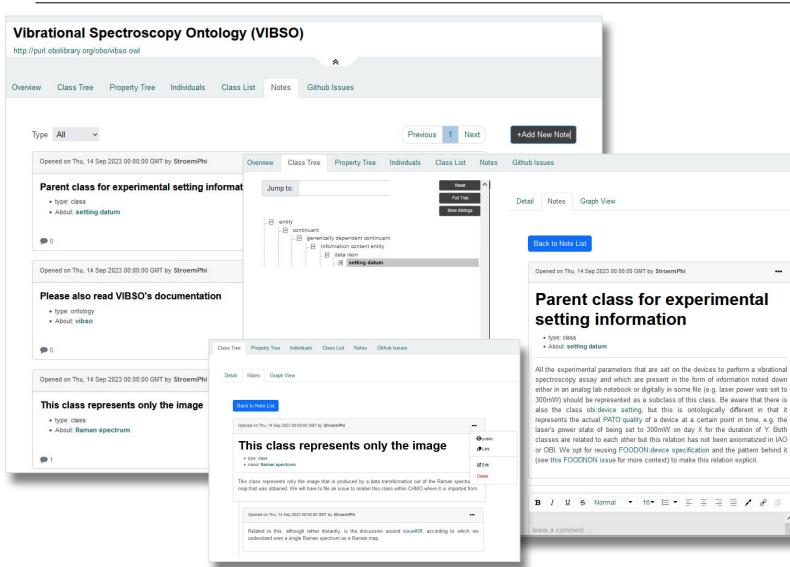
#### **Curating chemical ontologies collaboratively**

State     Open       [NTR] add "Raman scattering" and its subtypes a       #103 opened on 2023-08-11 by StroemPhi	according to ISO	specs New Term Request		
Improve axiomatization of 'groove density' and 'g #102 opened on 2023-08-11 by StroemPhi	proove density se		erty Tree Individuals Class List Notes Github Issues	Metrics
Consider obsoleting VIBSO_0000000 & VIBSO_0000001 #99 opened on 2023-08-04 by StroemPhi Need to import obi:laser #98 opened on 2023-08-04 by StroemPhi		WIP - NOT READY FOR PRODU with which research data produce	Number of Classes Number of Properties	
		wade machine readable and FAIR.       Version     2023-06-21		Number of Individu
Fix missing axioms in CHMO import #97 opened on 2023-08-04 by StroemPhi		VersionIRI	http://purl.obolibrary.org/obo/vibso/releases/2023-06-21/vibso.owl	File a General Issu File a Term Reques
#96 opened on 2023-08-03 by Zack-83 Tabular template for multiple term requests #95 opened on 2023-08-03 by Zack-83 (e)	File a Term Rec Term Request Title* [NTR] add "raw signa Content*			
[NTR] Add concentration and its specialization #90 opened on 2023-06-23 by StroemPhi	B I ⊻ ୫ N			
[NTR] Add Absorbance maximum or Peak po #89 opened on 2023-06-22 by StroemPhi	Preferred term la			
[NTR] Add spectral center (New Term Request) #88 opened on 2023-06-22 by StroemPhi	Synonyms (e.g., acquisition band Textual definition			-
		nal information about the suggested term.	s. Include a DOI or URL to refer to any relevant publication	1
	that provides addition Suggested paren	nal information about the suggested term.		nit



- GitHub integration
  - Listing issues
    - Status overview
  - Writing issues
    - From ontology overview tab
    - Recognizes templates
    - NTR template based on ODK
  - Less context switching
  - Ease external contributions
  - Tighter integration planned

#### **Curating Chemical Ontologies Collaboratively**





### Notes feature

- Ontology or term level
- Private, logged in, public
- Assists curation & use
- Git alternative
- One layered threads
- Linkable

**Curating Chemical Ontologies Collaboratively** 

#### Demo - Adding a note to <u>CHMO:assay output</u>

- Overlap between CHMO and IAO
  - IAO:measurement datum seems to be the same concept
    - If true, the IAO concept should rather be used and the CHMO term be dropped, as IAO coined it first
      - OBO orthogonality principle
      - There are already issues in both ontology trackers for this
  - $\circ$   $\,$  TS as a way to do this detective work



# **Thank You**

# **For Your Attention**