



NFDI₄Chem

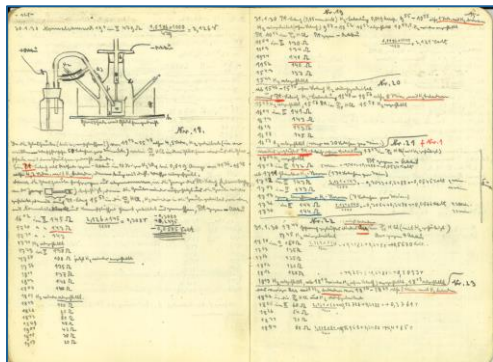
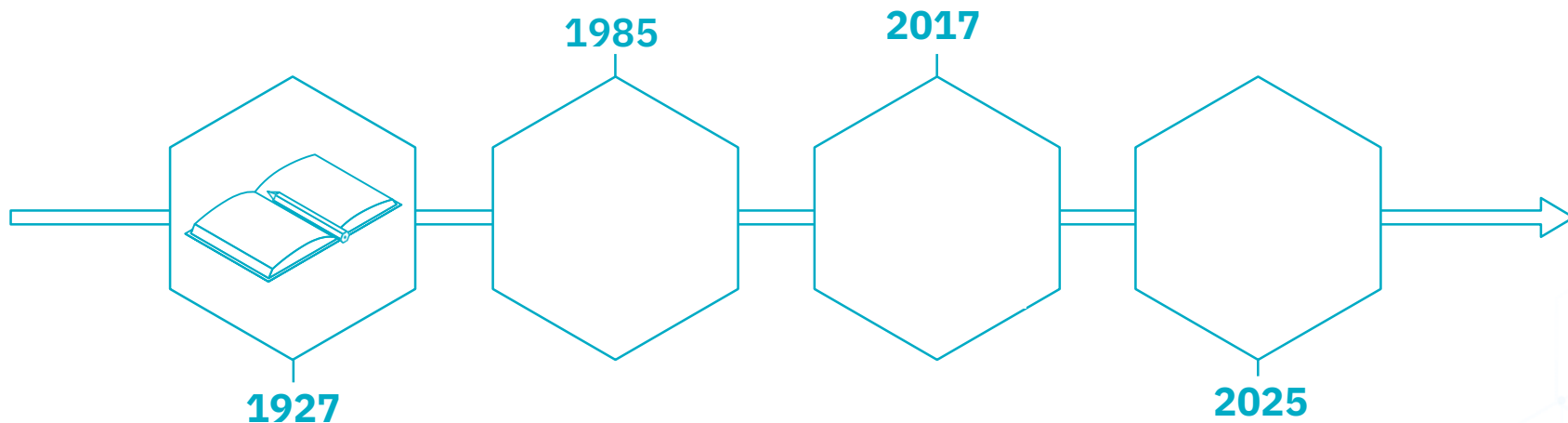
ENHANCE
YOUR
DATA.

Unlocking Chemical Research Data - The NFDI4Chem Service & Infrastructure Federation

Oliver Koepler, TIB, RSC Webinar „Data Management“, 18 Nov 2025

NFDI4Chem is supported by DFG
under project number 441958208

Speed of Evolution vs. Digitisation in Chemistry



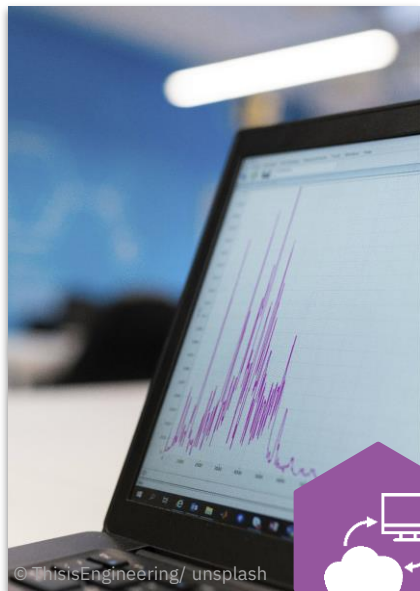
Supporting Users from Data Creation to Re-use



© F. Garg/ NFDI4Chem



Create Data
Smart Lab



© ThisIsEngineering/ unsplash



Publish & Access Data
Repositories



© F. Garg/ NFDI4Chem

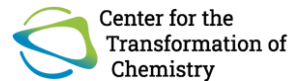
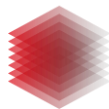


Find & Use Data
**Metadata, Semantics
& Standards**

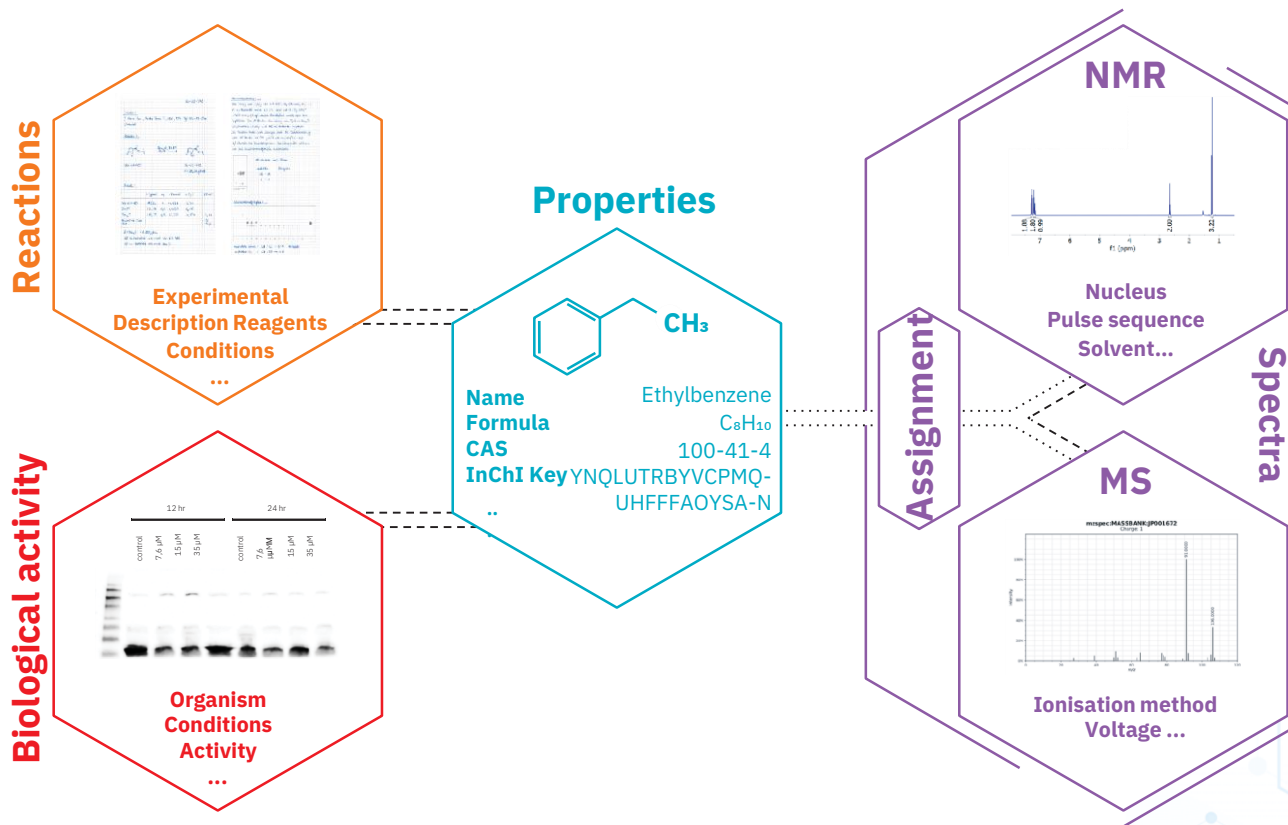


Data Discovery & Reuse
Semantic Data Hub

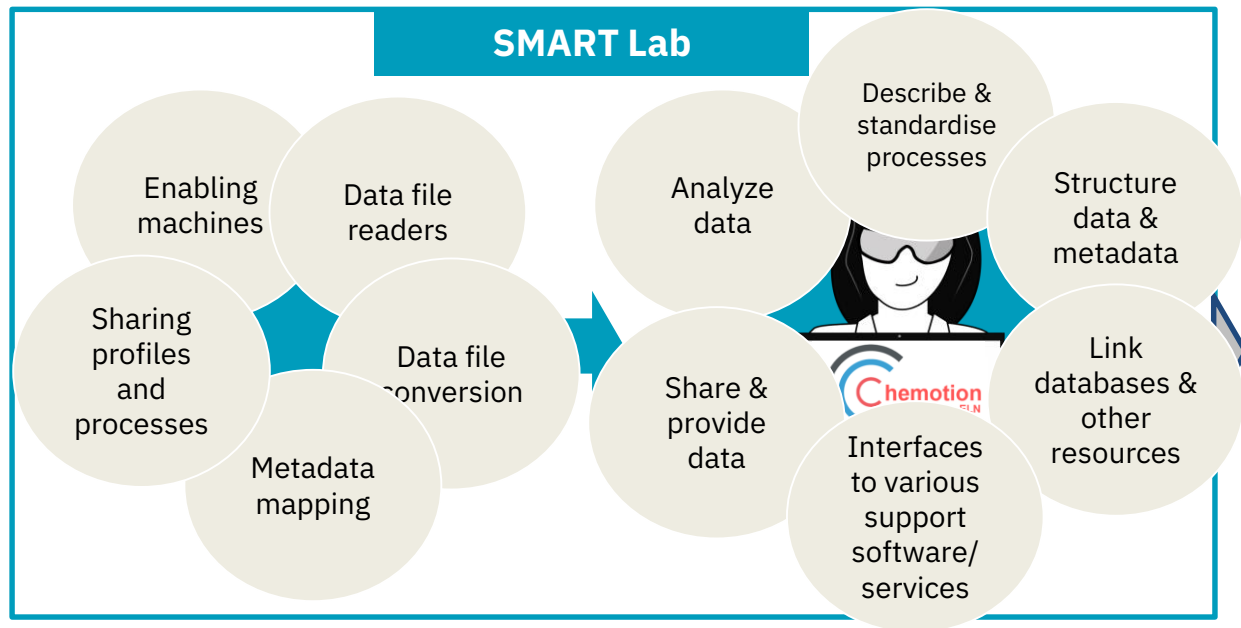
NFDI4Chem is community-driven



Data we cover - Molecules and related meta(data)



Smart Lab - Enabling Digitisation and Seamless Data Flows



Trusted Federation of Repositories



Core Repositories

Process & Analytics



Spectroscopy



Subdomain specific



Multidisciplinary



VibSpec DB



Associated Repositories

CSD



Harmonisation across resources - MICH



Chemists, RDM Experts & Computer Scientists develop Minimum Information for Chemical Investigations

Guideline Article



Checklist

- Separation column and pre/guard column
 - Manufacturer, model number/name, stationary media composition (support and coating, e.g. silica, C18, etc.) and physical parameters (i.e. coating thickness for GC/MS, particle size and pore size for LC/MS), internal diameter, and length.
- Technique-specific sample preparation
 - Resuspension of sample (e.g. in mobile phase), amount injected.
 - Derivatization reaction conditions if relevant, (e.g. OMS/trimethylsilyl; chemical manufacturer, temperatures, and duration).
 - Sample spiking e.g. internal standards, retention-index standards.

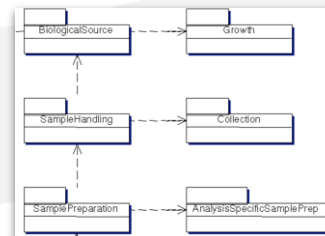


MICH

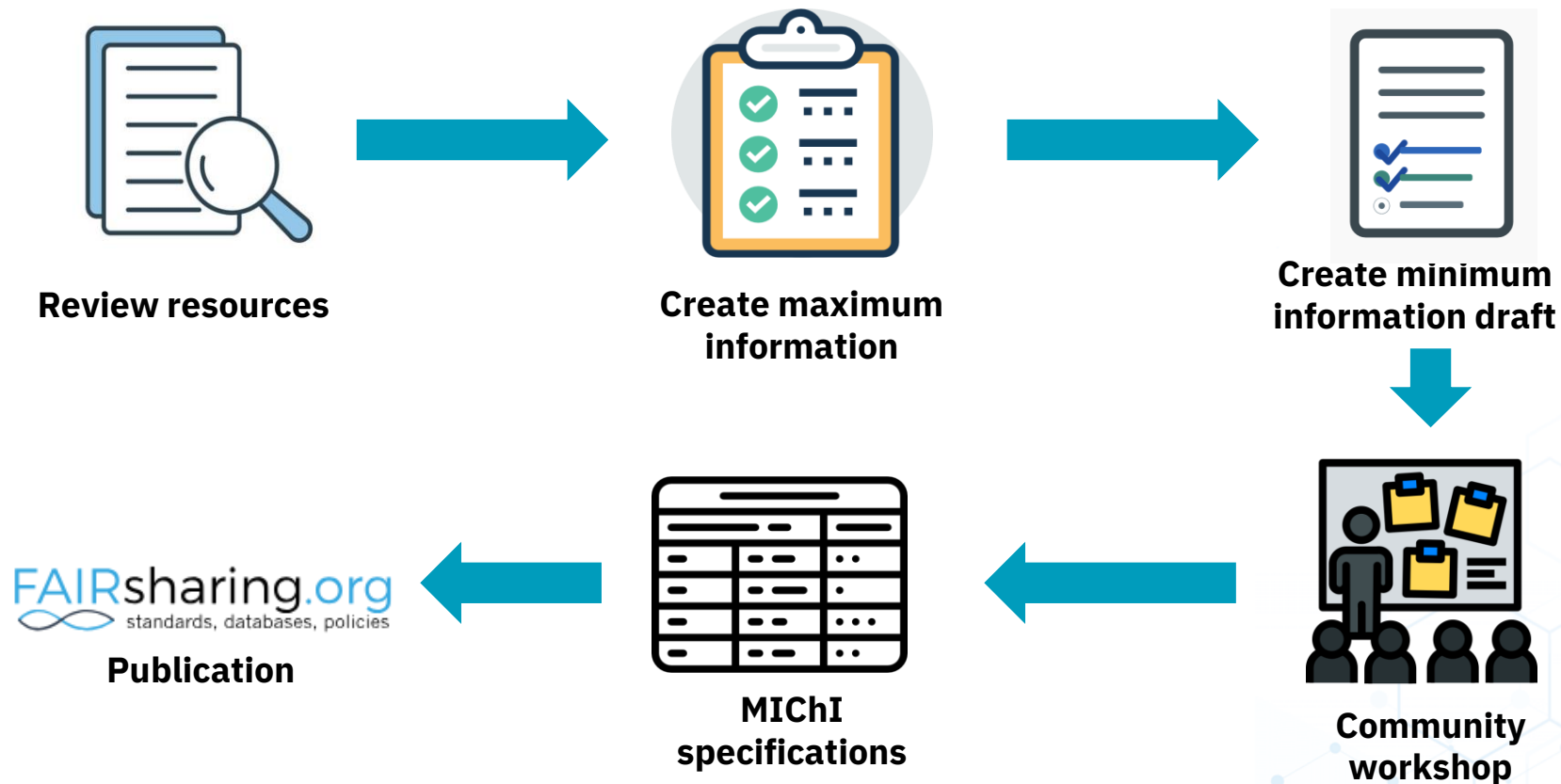
Implementation

Type of Polymer	Homopolymer
Molecular Mass Distribution	
Number average MW (Mn)	g/mol
GPC standard	
Molecular Properties	

Data Model



MIChI Development Workflow



MIChI in NFDI4Chem



NMR MICHIs: on FAIRSharing
doi.org/10.25504/FAIRsharing.c29400

MIChI Standard for Reporting Liquid-State NMR Experiments of Small Molecules (MARGARITAS)

DOI: 10.25504/FAIRsharing.c29400

Type: Reporting guideline

Registry: Standard

Description: MARGARITAS stands for 'Michi stAndard foR reportinG liquid-state nmr experimenTs of smAll molecules'. This MIChI standard is a proposal from NFDI4Chem to outline essential metadata required for documenting liquid-state NMR experiments of small molecules. We aim to make it suitable for NMR repositories and the supplementary materials of publications. The standard consists of two parts: tabular recommendations that include the actual checklist of properties and textual guidelines explaining the meaning and use of the checklist. We actively maintain and optimise our MIChI, which results in new versions.

Homepage: <https://nfdi4chem.github.io/workshops/docs/category/margaritas-michi-standard-for-reporting-liquid-state-nmr-experiments-of-small-molecules/>

No.	Property	Definition
0	Differential optical absorption spectrophotometry	
0.1	UV-Vis Differential Optical Absorption Sample	
0.1.1	Chemical structure	Chemical structure identifier in the form of an alphanumeric text string
0.1.2	Solvent	
0.1.3	Concentration	
0.1.4	Optical path length	
0.1.5	Sample ID	Identifier for the sample which is unique within the project

UV-Vis MIChI:
Community workshop

No.	Property	Definition
1	Chemical Entity	Chemical Entity (CHEBI:24431)
1.1	Identification	
1.1.1	Primary Identifier	A globally unique, persistent value assigned to an entity that distinguishes it from all other entities in a dataset or system. It is a dcterm Identifier
1.1.2	Title/ name/ label	dcterm Title
1.1.3	Alternative identifier	An identifier that refers to the same entity as the primary identifier but comes from a different identification system, source, or context. Not the main reference. It is a dcterm Identifier
1.1.4	Alternative Title name/ label	

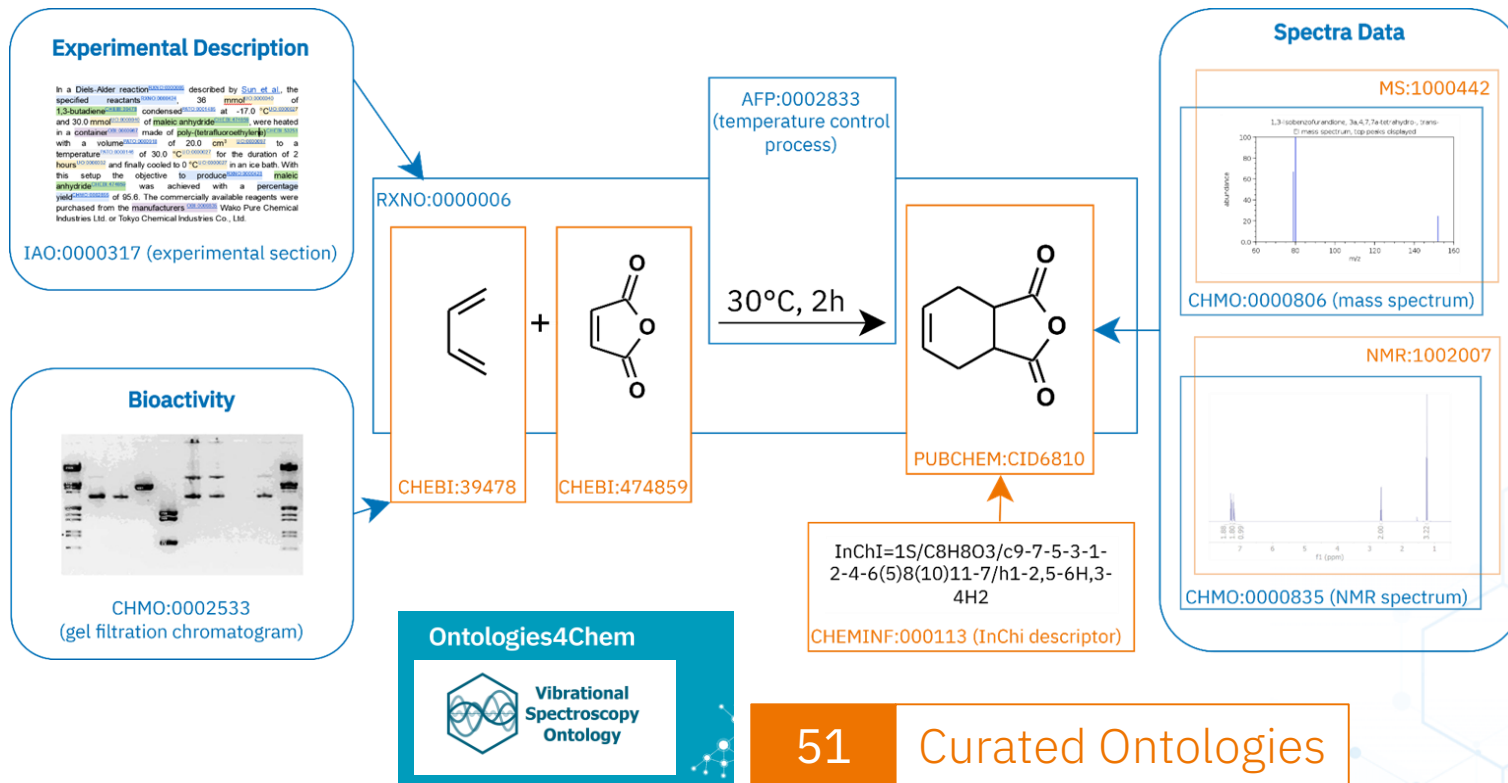
Chemical entity,
MS: Minimum information draft

No.	Property	Definition	Export Format
1	Mass Spectrometry Assay		
1.1	MS Sample		
1.1.1	Analysed Compound and/or Sample ID	A compound analysed in a mass spectrometry (MS) sample using data acquired from a mass spectrometry (MS) analysis	- mol - ChEBI ID or IRI that is a leaf of the ontology term molecular entity (CHEBI:23367) or - Pubchem ID ChEBI ID or IRI that is a leaf of the ontology molecular entity (CHEBI:23367)

Metadata	dx	RRUFF	Prof Bocklitz
Acquisition			
method			
npoints	✓		
sampling procedure	✓		
laser wavelength		✓	✓
instrument settings		✓	
orientation		✓	
laser power			✓
accumulation time			
spectral range			✓
resolution	✓		

Raman: Max Information

Harmonisation across resources - Ontologies





The NFDI4Chem Terminology Service (TS)

TERMINOLOGY SERVICE

HOME ONTOLOGIES HELP API ABOUT

chemical entity Search

Filter Results 14352 results found for "chemical entity" Results Per Page 10

Clear All Filters

Type

- ☐ class 13380
- ☐ property 929
- ☐ individual 20
- ☐ ontology 0

Ontologies

- ☐ NCIT 7760
- ☐ MS 970
- ☐ PATO 840
- ☐ CHEBI 533
- ☐ OBI 502

+ Show More

[class] chemical entity **CHEBI_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: **PROCO ENVO PATO EFO MS RMO MOP**

[class] chemical entity **SIO_010004**
http://semanticscience.org/resource/SIO_010004

Ontology: **SIO**

[class] chemical entity **CHEMINF_000000**
http://semanticscience.org/resource/CHEMINF_000000

A chemical entity is any molecular entity or chemical substance.

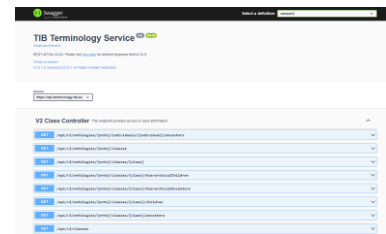
Ontology: **CHEMINF**

[ontology] Chemical Entities of Biological Interest **CHEBI**
http://purl.obolibrary.org/obo/chebi.owl

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: **CHEBI**

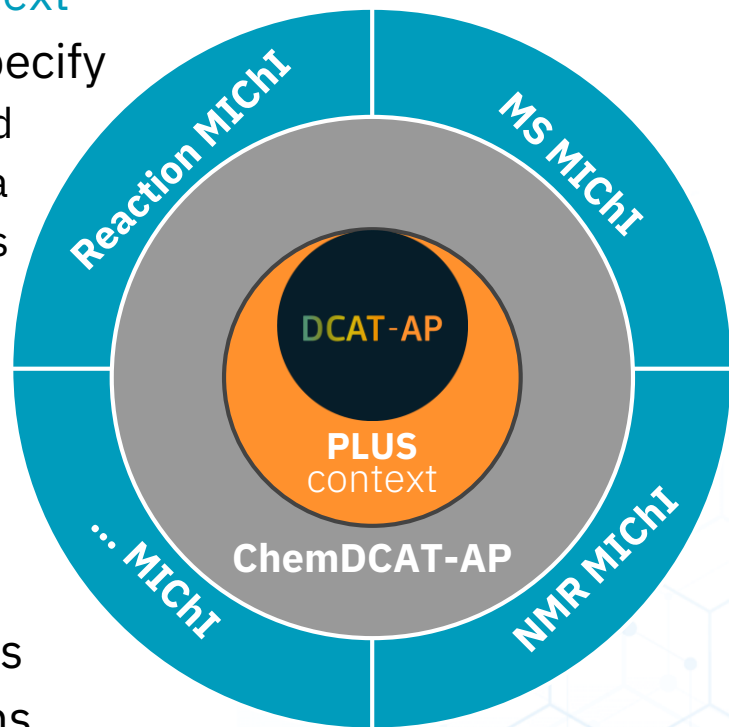
- Search in all indexed fields
 - E.g. abstract, label, definition
- Filter by type of term
 - Class, property, individual or ontology
- Filter by ontology
 - Sorted by number of hits
- API available for service integration



Harmonisation across resources – Metadata



- **DCAT-AP Plus** Links to Use-case Specific context
 - Added classes, properties & constraints to specify
 - The entity or process being evaluated & described
 - The process(es) & tools used to generate the data
 - Entity, process & attribute types via terminologies
- **ChemDCAT-AP**
DCAT-AP PLUS & restrictions shared in all chemistry specific contexts
- **MIChI schemas**
 - ChemDCAT-AP & specific MICHl requirements
 - Developed by domain experts & MICHl admins



- 15





Minimum Information for Chemical Investigations collect ***what*** to report

Metadata Schemas define ***how*** to report data.

Schemas and ontologies form the ***semantic foundation*** and enable harmonisation, metadata harvest & search



Chemotion ELN: Integration of ontologies from TS



Chemotion ELN interface showing a list of reactions on the left and a detailed view of reaction JDJ-R36 on the right.

Reaction List (Left Panel):

- JDJ-R41: Reaction of a pyridine derivative with $\text{H}_2\text{C}=\text{O}$ and H_2O to form a product.
- JDJ-R40: Reaction of a pyridine derivative with H_2O to form a product.
- JDJ-R39: Reaction of a pyridine derivative with H_2O to form a product.
- JDJ-R38: Reaction of a pyridine derivative with H_2O to form a product.
- JDJ-R37: Reaction of a pyridine derivative with H_2O to form a product.
- JDJ-R36 (Selected):** Reaction of a pyridine derivative with H_2O to form a product.
- JDJ-R35: Reaction of a pyridine derivative with H_2O to form a product.

Reaction JDJ-R36 Detail (Right Panel):

Scheme: Reaction of a pyridine derivative with H_2O to form a product.

Analyses:

- 1H NMR**
Type: 1H nuclear magnetic resonance spectroscopy (1H NMR)
Status: Confirmed ✓ Instrument: 1/1
Content: ^1H NMR (400 MHz, Acetone- d_6 [2.05 ppm], ppm) δ = 8.53–8.51 (m, 1H), 8.18 (dd, J = 1.3 Hz, J = 8.2 Hz, 1H), 8.05 (d, J = 8.3 Hz, 1H), 8.01–7.98 (m, 1H), 7.89 (s, 1H), 7.76 (dd, J = 1.1 Hz, J = 7.0 Hz, 1H), 7.65 (d, J = 8.3 Hz, 2H), 7.60–7.48 (m, 4H), 7.43 (d, J = 8.1 Hz, 2H), 7.36–7.28 (m, 2H), 5.65 (s, 2H). Impurities: This spectrum contains cyclohexane at 1.43 ppm and water at...
- ^{13}C NMR**
Type: ^{13}C nuclear magnetic resonance spectroscopy (^{13}C NMR)
Status: Confirmed ✓ Instrument: 1/1
Content: ^{13}C NMR (100 MHz, Acetone- d_6 [29.9 ppm], ppm) δ = 192.1, 142.7, 140.1, 140.0, 138.2, 134.9, 131.7, 130.8, 130.3 (q, J = 32.1 Hz), 129.2, 128.6 (3C), 128.3, 127.5, 127.2, 126.9, 126.7, 126.6 (q, J = 3.9 Hz), 125.7, 125.3 (q, J = 271.3 Hz), 124.6, 123.6, 123.5, 118.7, 111.8, 50.6.
- ^{19}F NMR**
Type: ^{19}F nuclear magnetic resonance spectroscopy (^{19}F NMR)

RADAR4Chem: Integration of Ontologies from TS



- Metadata editor: [Suggestion lists of chemistry specific terms](#) (e. g. NFDI4Chem ontology collection) are provided via type ahead.
- Landing page: [Clear presentation of standardized terms / ontologies](#) incl. links to further information.
- Findability of data: [Additional filter options](#) “Keywords” and “Ontology” on publication list.
- MD for “Keywords”: Fosters [semantic interoperability](#) using chemistry-relevant vocabularies.

Keywords ⓘ

Standardised Terminologies (via TS4NFDI)

chemical shift

chemical shift **AFO** > AFR_0002366 ⓘ
A chemical shift is a quality quantification facet quantifying the fractional variation of the resonance frequency of a nucleus in nuclear magnetic resonan...

chemical shift (molecular quality) **AFO** > AFQ_0000319 ⓘ
The fractional variation of the resonance frequency of a nucleus in nuclear magnetic resonance (NMR) spectroscopy in consequence of its magnetic env...

chemical shift **NMRCV2025** > NMR_1000223 ⓘ
Chemical shift is the resonance frequency of a nucleus related to a chemical shift standard. in ppm along x-axis

chemical shift **NMRCV** > NMR_1000223 ⓘ
Chemical shift is the resonance frequency of a nucleus related to a chemical shift standard. in ppm along x-axis, http://en.wikipedia.org/wiki/Chemical_S...

AFO chemical shift (molecular quality) · Weniger anzeigen

chemical shift (molecular quality)

AFO > AFQ_0000319

http://purl.allotrope.org/ontologies/quality#AFQ_0000319

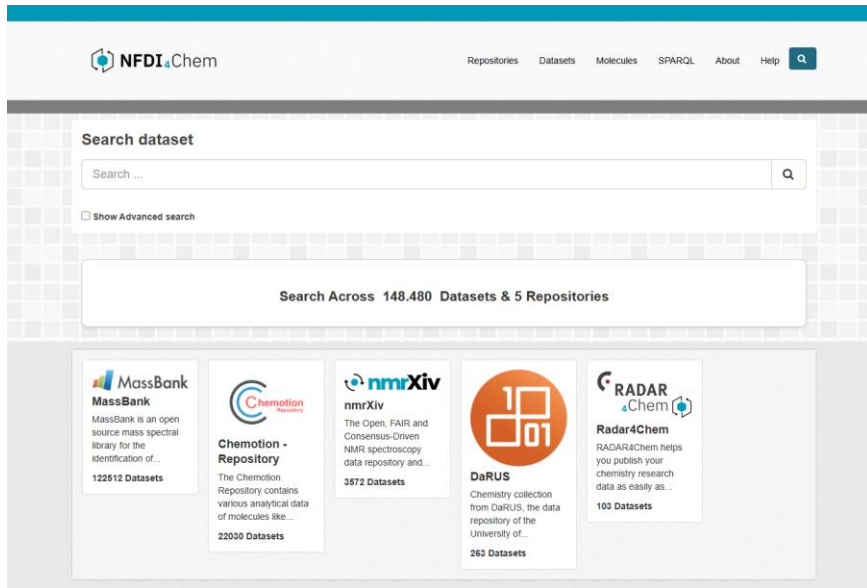
The fractional variation of the resonance frequency of a nucleus in nuclear magnetic resonance (NMR) spectroscopy in consequence of its magnetic environment. [IUPAC]

Alternative Names [Hierarchy](#) Cross references About AFO Graph View Depiction

entity
├── continuant
│ ├── specifically dependent continuant
│ │ ├── quality
│ │ │ ├── molecular entity quality
│ │ │ │ └── **chemical shift (molecular quality)**

AFO chemical reaction (molecular) · Mehr anzeigen

Data Discovery with Search Service



- The NFDI4Chem Search Service harvest major repositories of NFDI4Chem Federation
- Currently includes **>148.000 datasets**
- Enables searches **by molecules, analytical methods or chemical structure codes**
- Features are continuously adapted to latest **metadata schema** releases

NFDI4Chem: NFDI4Chem Search Service Available: <https://search.nfdi4chem.de/>

148k

Datasets

Semantic Foundation in Search Service



Metadata Information

Additional

Measurement

Field

Measurement Technique

Measurement Variables

Value

Label: number of data points
Description: None
CURIE: [NMR:1000176](#) DM50-06
defined_in : [NMRCV](#)

[number of data points](#) : 32768 points

[relaxation time measurement](#) : 2 seconds

[NMR spectrum by dimensionality](#) : 1

[NMR probe](#) : 2774

[Temperature](#) : 298.15 K

[magnetic field strength](#) : 9.389766 Tesla

[number of scans](#) : 4096 scans

[nuclear magnetic resonance pulse sequence](#) :
[carbon.jxp](#)

[Spectral Width](#) : 314.0070760448474

MassBank **18,351**

Chemotion - Reposit... **2,470**

nmrXiv **445**

Tags

There are no Tags that match this search

Related Measurements

liquid chromatograp... **18,353**

1H nuclear magnetic... **2,739**

13C nuclear magneti... **2,573**

Infrared absorption... **1,485**

mass spectrometry **1,234**

distortionless enha... **950**

heteronuclear singl... **689**

heteronuclear multi... **606**

1H-13C heteronuclea... **594**

correlation spectro... **565**

Show More Related Measurements

Search molecule



Show Advanced search

21,102 molecules found

Order by: Name Ascending

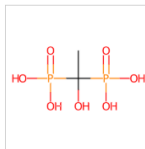
(1-hydroxy-1-phosphonoethyl)phosphonic acid [Molecule](#)

InChIKey

DBVJJBKOTRCVKF-UHFFFAOYSA-N

Molecular Formula

C2H8O7P2



Related Dataset(s)

- Etidronic acid; LC-ESI-QQ; MS2; CE:20 V; [M-H]-
- Etidronic acid; LC-ESI-QQ; MS2; CE:40 V; [M-H]-
- Etidronic acid; LC-ESI-QQ; MS2; CE:30 V; [M-H]-
- 1-Hydroxyethane-1,1-diphosphonic Acid, 1-Hydroxyethylidenediphosphonic acid, Turpinal SL, HEDP, HEDPA, Etidronic acid, EHDP, 1,1,1-Ethanetriol diphosphonate; LC-ESI-QQ; MS2
- Etidronic acid; LC-ESI-QQ; MS2; CE:50 V; [M-H]-
- 1-Hydroxyethane-1,1-diphosphonic Acid, 1-Hydroxyethylidenediphosphonic acid, Turpinal SL, HEDP, HEDPA, Etidronic acid, EHDP, 1,1,1-Ethanetriol diphosphonate; LC-ESI-QQ; MS2
- 1-Hydroxyethane-1,1-diphosphonic Acid, 1-Hydroxyethylidenediphosphonic acid, Turpinal SL, HEDP, HEDPA, Etidronic acid, EHDP, 1,1,1-Ethanetriol diphosphonate; LC-ESI-QQ; MS2
- Etidronic acid; LC-ESI-QQ; MS2; CE:10 V; [M-H]-
- 1-Hydroxyethane-1,1-diphosphonic Acid, 1-Hydroxyethylidenediphosphonic acid, Turpinal SL, HEDP, HEDPA, Etidronic acid, EHDP, 1,1,1-Ethanetriol diphosphonate; LC-ESI-QQ; MS2



NFDI₄Chem

ENHANCE
YOUR
DATA.