CHEMISTRY

Data Sharing in Chemistry

Chemistry studies the composition, structure, and properties of substances and the transformations that they undergo. Thus, all data generated throughout such a study can be considered chemistry data, and these data can be found in general-purpose repositories/databases, like Zenodo, or in repositories tailored to specific subdomains such as analytical or computational chemistry. Much of the data produced is reported in widely used tabular file formats (e.g. CSV) but molecular structures can be represented by custom formats like InChi or SMILES. Related fields such as biology and materials science may also be good sources for additional resources and tools, and are included in the lists below.

Where can I find resources and tools for...

Data and Processing

- NFDI4Chem knowledge database
- Chemotion
- ChemSpider
- PDB
- AiiDA
- ILL Data Portal

Methods and Documentation

- FAIRsharing Chemistry standards
- Unified Data Model standard format
- InChi
- SMILES

Depositing Data

- Catalysis Hub
- Chemotion
- iochem-bd
- NOMAD
- RADAR4Chem
- HAL
- ICSD
- MassBank
- PubChem

EOSC Portal

The EOSC Portal is a gateway to many of the innovative services, tools, publications and data listed here, and it is constantly growing with additions from the community of Chemistry researchers and research-supporting organisations. Do you have a resource that you want to share with others? Consider onboarding into EOSC.

▶

Community and Professional Supports
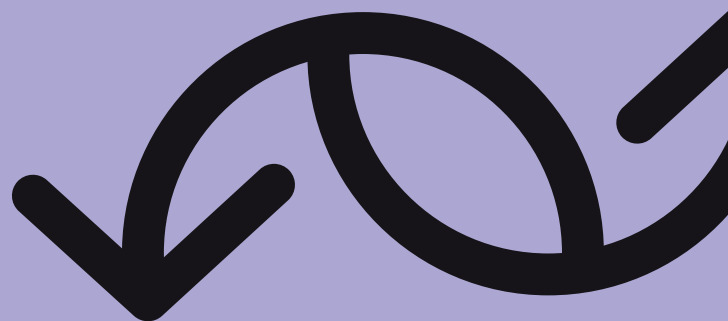
- NFDI4Cat
- NFDI4Chem
- IUPAC
- DECHEMA
- IUCr

Learn more about the Research Data Alliance (RDA)

- RDA Chemistry Research Data Interest Group
- Research Data needs of the Photon and Neutron Science Community Interest Group
- FAIRsharing WG

How to do FAIR and Open Science

- What is FAIR?
- FAIR Community Support
- What is the goal of Open Science?

RDA for Disciplines

What are the challenges for chemistry data in Open Science?

"Work in the lab is still manual, and non-digital data is a huge struggle to make open. Electronic Lab Notebooks will make a big difference to help labs talk the same digital language. As for social supports, the Research Data Alliance is the best place for conversations around open science – with people who are already into Open Science."

How can EOSC help researchers working with chemistry data?

"EOSC provides the workflows and tools that can help to change the manual acquisition process, making it easier to share. I think it will be important to onboard tools and workflows from smaller research projects as well as leading international groups."

— Pedro Mendes
RDA/EOSC Future Domain Ambassador for Catalysis