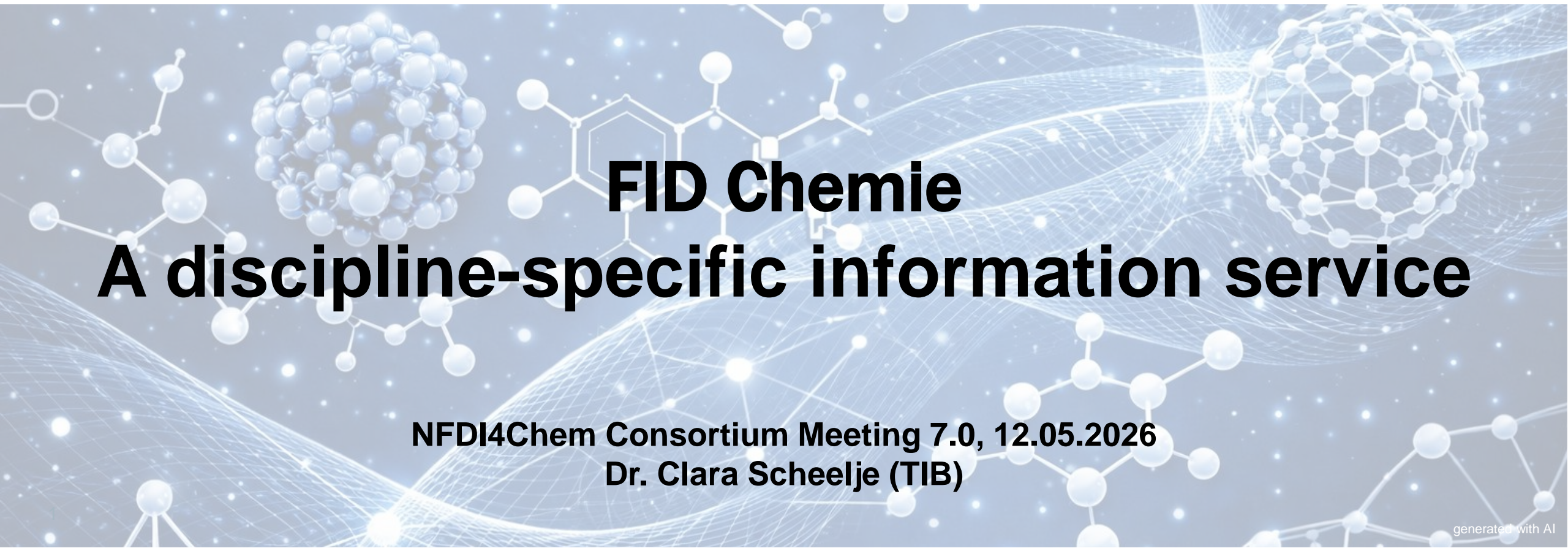


TIB LEIBNIZ INFORMATION CENTRE
FOR SCIENCE AND TECHNOLOGY
UNIVERSITY LIBRARY



Karlsruhe Institute of Technology



FID Chemie

A discipline-specific information service

NFDI4Chem Consortium Meeting 7.0, 12.05.2026
Dr. Clara Scheelje (TIB)

Overview

Funding programme: Fachinformationsdienste (FID)




- project duration: **three years**, possible extensions
 - nationwide provision of (primarily) digital information
 - services for cutting-edge research

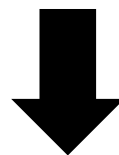
FID Chemie

- joint project between TIB, the KIT Library, and KIT-IBCS
- funded: 02/2026 – 01/2029
- first funding period: focus on **molecular chemistry**
- currently 10 people involved, 2.5 funded positions



FID Chemie: Challenges

-  scattered chemistry-relevant **information** and **overviews**
-  **open science** not widely established in all areas of the chemistry community
-  diverse set of regional chemistry **initiatives**



FID Chemie

a central infrastructure for chemistry information

web portal: **ChemPortal**

FID Chemie: Central access to information and licenses

 scattered chemistry-relevant **information** and **overviews**:

→ local **licences** and access to literature, software, and databases

Central access to information



- search function based on the TIB library search
- overviews: databases, software, etc.
- information on patent search, training tutorials, etc.
- needs-based continuous expansion

Database and API licences

- specialised subject databases
- single-user licences for Science of Synthesis (Thieme)
- further needs assessment and negotiations planned
- overview of APIs, licensing models

FID Chemie: Open Science

 **open science** not widely established in all areas of the chemistry community:

→ scattered initiatives; limited **machine-readability** of research findings

Open Science

- collaboration with the open-access.network, creation of subject-specific pages
- training courses, self-study courses
- collaboration with the libraries' subject specialists and OS initiatives
- presentation of best practices
- overview of open educational resources



Chemoinformatic tool development

- machine-readable, semantic annotation of chemical drawings and structures
- optical character recognition, ML/NLP
- knowledge structuring:
 - Open Chemistry Knowledge Base^[1]
 - Open Research Knowledge Graph^[2]

[1] https://chemwiki.scc.kit.edu/main/mediawiki/Main_Page

[2] <https://orkg.org/>

FID Chemie: Collaboration Opportunities

- diverse set of regional chemistry initiatives:
→ **coordination** of common positions and interests

Networking and pooling of interests



- chemistry research community
- chemical societies/ institutions
- related FID and NFDI
- university libraries, subject specialists
- open access/ open source initiatives
- scientific advisory board



FID Chemie & NFDI4Chem

different focuses – leveraging synergies

- alignment of web portal content: research data search, guidance, events, crosslinks
- joint outreach (conferences, workshops, ...)
- collaboration on shared goals
- sharing expertise, reusing resources

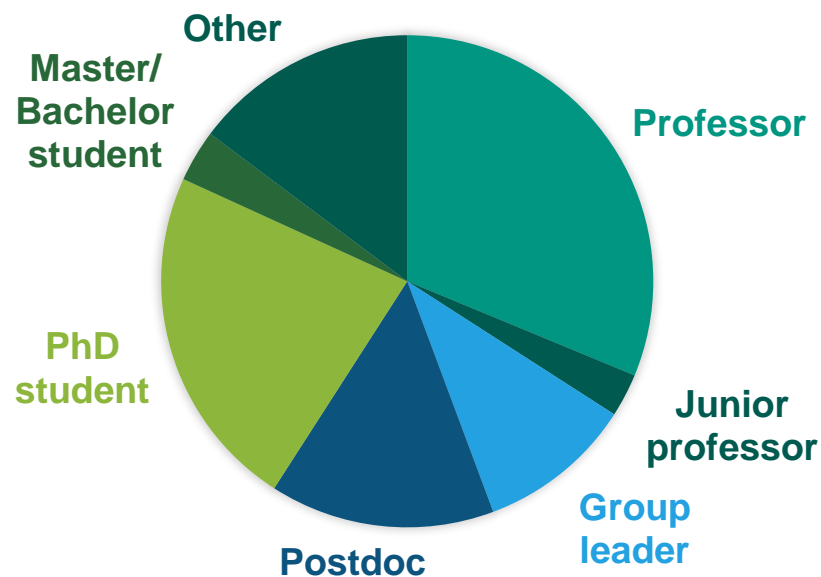


FID Chemie & NFDI4Chem: Joint Survey on Structure Editors

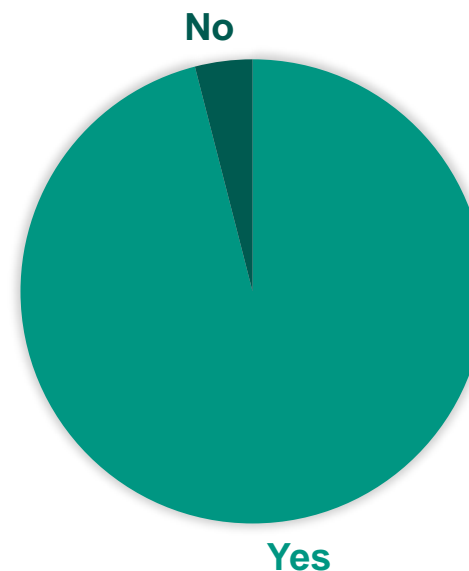
- online survey on open source structure editors
- presented at different conferences
- 176 participants:

~90% use ChemDraw, but:

What is your current position?

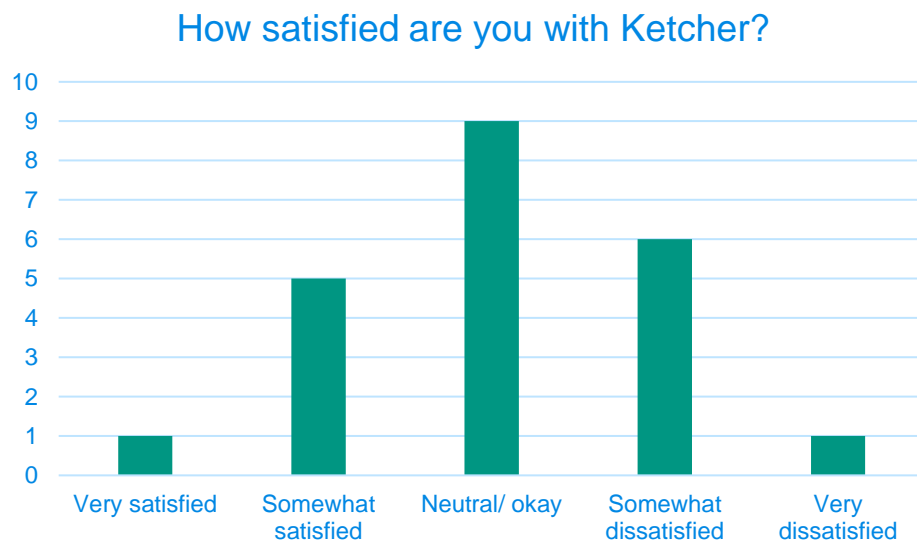


Are you interested in software that does not incur license fees?

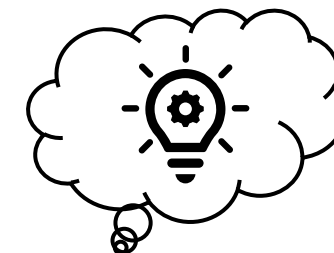


Joint Survey on Structure Editors: Ketcher Editor

- open source, web-based editor for molecules
- used e.g. in Chemotion
- community-driven improvements possible

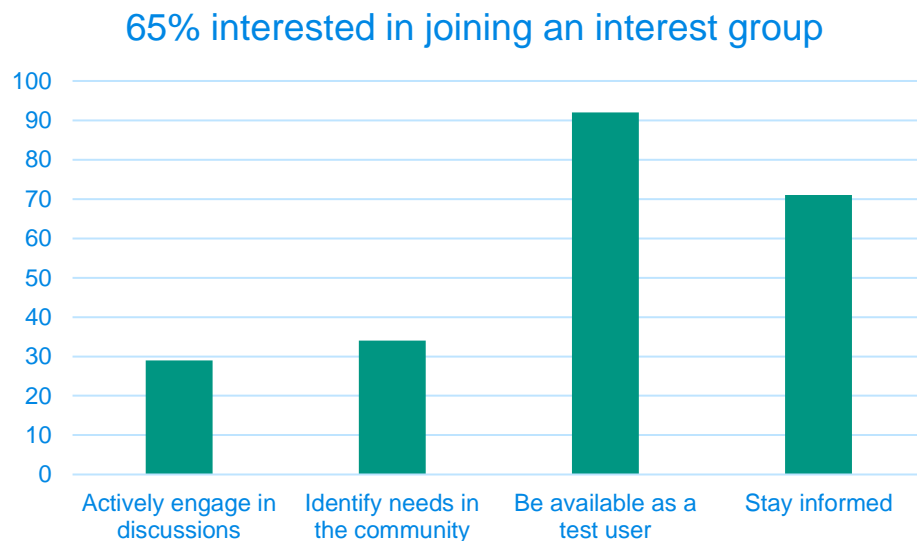


updates, security
range of features
easy to use
Interoperability (e.g. Chemotion)
import options
free, easy access
visually appealing
export options (e.g. vector graphics)
open source
web based

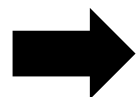
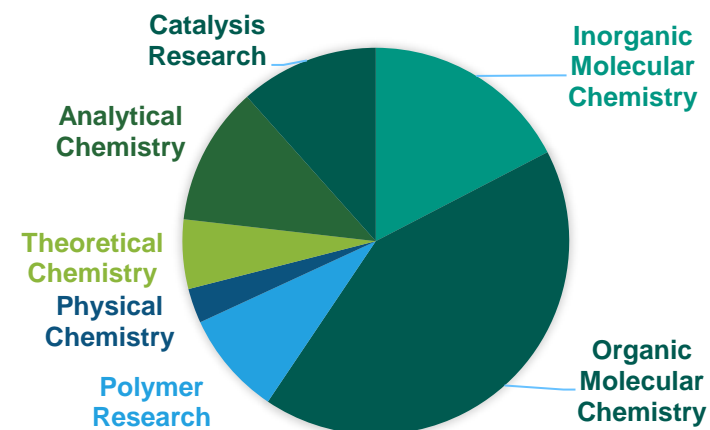


Organometallic functionalities
Interoperability
fast and intuitive use
Conversion to/ from name, identifiers
Calculation of properties
Technical features, visualization tools
style improvements
biology features
import/ export functionalities
extension of functionalities (complex structures)
High quality images for publications
connection to databases

Open Source Structure Editors: Interest group



29 people: Actively engage in discussions



Further plan:

- evaluation of survey
- interest group for improvements and assessment of needs
- software development: cooperation with Beilstein Institute

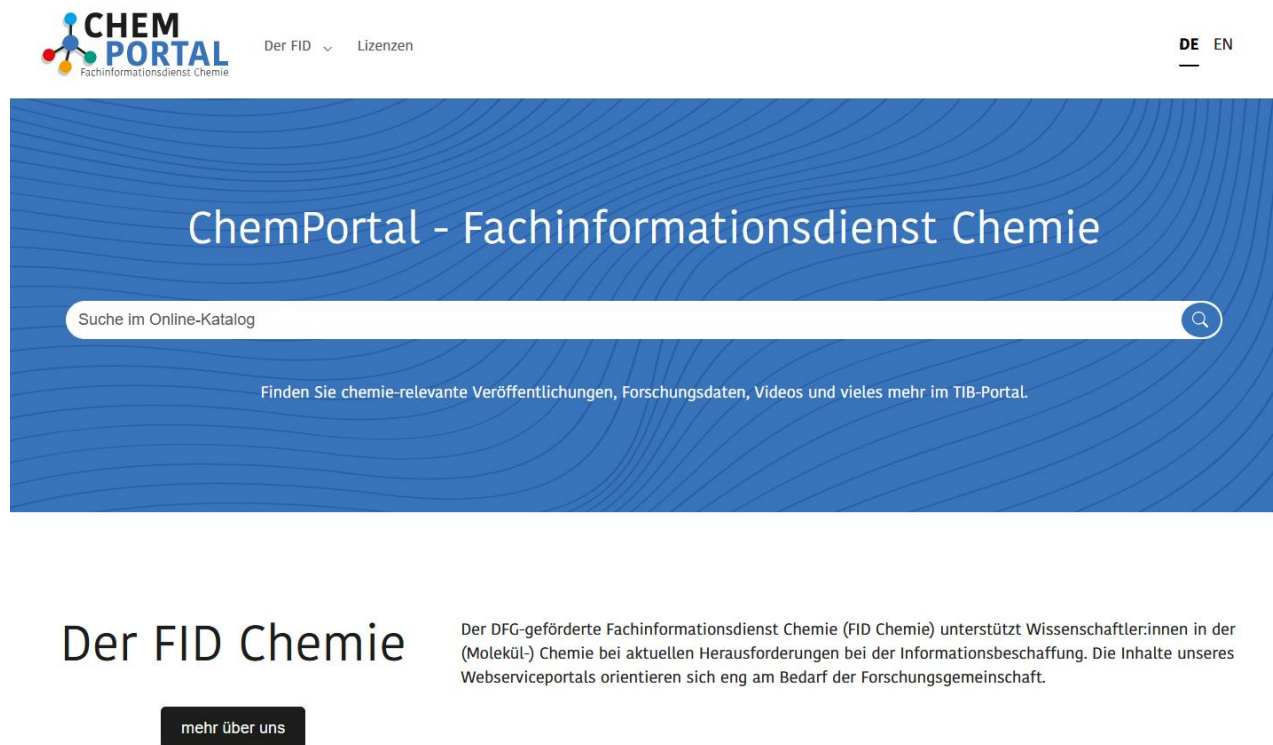
FID Chemie: Next steps

Web portal:

- structure, corporate design, features
- continuous expansion of content:
 - search function
 - open access in chemistry
 - database overview
 - ...

Community building

- coordination with stakeholders (libraries, GDCh, Beilstein, NFDI, other FID)
- scientific advisory board
- attending conferences (BiblioCon, GDCh conferences)



Connect and Stay Tuned

Interests? Ideas? Questions? We are happy to hear from you!

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Mail: fid-chemie@bibliothek.kit.edu



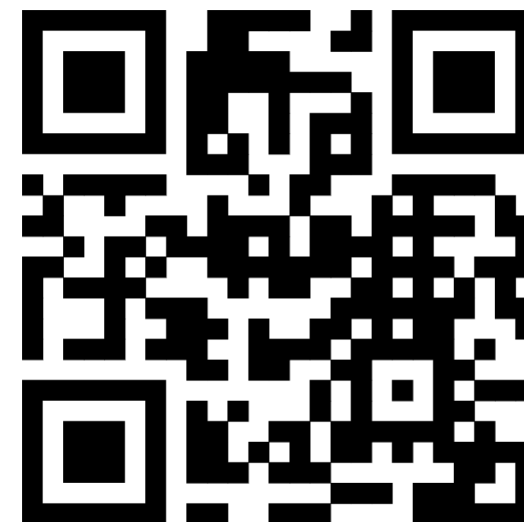
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