

# NFDI4Chem Consortium Meeting 2.0

14/15 October 2021 (Zoom)

## General Discussion with the Advisory Boards

14 October: 16:15 – 17:15

Topics that have been discussed with the Advisory Boards:

### Output formats of Analytical instruments

- NFDI4Chem is in contact with vendors
- For most devices readable data file types are available
- Big files (e.g. raw data from mass spectrometers) are uploaded on servers, use selection in ELN

### Terminology and Ontology

- Make sure guidelines, data model and implementation are in sync
- The IUPAC non-ontology Terminology (Gold book) <https://goldbook.iupac.org/>
- Include industry partners into development that have similar challenges (ontologies/ data formats), bring together producers and community (users)
- Allotrope Foundation and OntoCommons are initiatives with industry participation

### Metadata

- Friction between communities
- IUPAC gold book includes lots of concepts worked on over the past years and can be re-used
- Necessity of training, many people at different levels have to be convinced
- Chemotion implementations, discussion about front-end for creating chemical structures

### The NFDI and Cultural change

- Adoption from analogue to digital systems: roll out to leading groups first
- Competition in ELN and LIMS; NFDI4Chem pledged to open API
- Standardization of data important for interoperability

### International Cooperations

- IUPAC important collaborator for outreach
- Active participation in InChI
- European level: GAIA-X
- Data sharing in trans-university collaborations not solved yet; NFDI section 'Legal Aspects' will deal with IP questions