31/03/2025

Research Data Management Plan

This Research Data Management Plan (RDMP) is valid for all projects in the Wolf group:

1. Data Summary

New data is generated during research projects by students (Bachelor, student assistants, Master) and PhD, Postdoc or the PI. Data, findings and conclusions are included in research theses and publications as well as in grant proposals. The type and size of data are highly variable (CSV, CIF, PDB, QTOF and GC-MS data, NMR data, IR data, UV-Vis, EPR); below are specifications of best practices to ensure a FAIR (Findable, Accessible, Interoperable, Reusable) data policy in the Wolf Lab.

2. FAIR data

2. 1. Making data (and metadata) findable

Use of Electronic Lab Notebook (ELN) Chemotion for all synthetic projects https://chemotion.net/ or Hardcopy Lab journals. For projects on catalysis other ELN, e.q. Obsidian (https://obsidian.md/) can be used. The letter must be associated with an Excel sheet containing the experiment identifier/Naming and a short description (e.q. the reaction performed) of the experiments.

Everyone uses ELN. New group members (including undergraduate students) are introduced to the ELN on their first day and given access to useful links/information (e.g. tutorial videos). If someone does not have a personal laptop or computer near the bench, the Wolf lab will offer a PC specifically for access to the ELN during the time in our lab.

Requirements for Experiment-Identifiers/Naming conventions:

- Initials (RWO instead of RW when possible, to avoid duplications)
- A clear numbering system (e.g. RWO-1. Others may just number the samples sequentially from 1, 2, 3, do whatever is the best way moving forward with the ELN for chemical reactions)

What to include in the ELN for reactions/experiments?

- Page numbers (not necessary for ELN, but for handwritten lab books if you use one in addition)
- Table of Content (not necessary for ELN, but for handwritten lab book if you use one)
- Chemicals and solvent quality
- Series of addition (e.g. what was added to what, when and how)
- Reaction conditions (in detail)
- Materials, vessels, etc. used (e.g. 50 mL round bottom flask, vial, dropping funnel)
- Note down a standard procedure, refer to it later, but also refer to differences! “overnight” is not acceptable (can vastly differ 8-12 h).

- Colour changes, precipitation, etc. during the experiments.
- Temperature (measured outside in oil bath or inside?) “Room temperature” is not acceptable (can fluctuate)!
- Did everything dissolve or was it a suspension? Habitus of the reaction and product.
- Additional notes for record keeping.
- If you use a handwritten lab book in addition to ELN Chemotion, LABEL EACH EXPERIMENT and MEASUREMENT (NMR, X-ray, UV-vis, etc.)
- Include the experiment identifier in EVERY measurement and the Date of the measurement (name data files AND folders!)
- Please always upload the image of a spectrum and the file of your data to Chemotion. e.g., a .png of the NMR spectrum as well as the .mnova or .fid file. Scan the spectra received from the MS facility and include a picture of your ESI-MS. For UV-Vis use ASCII or CSV. Use a dot for decimal separation! Global English notation for the entire AK Wolf in your data!
- How to structure folders containing data:
  - Initials, experiment number and date (e.q. RWO-001_13-03-2025)
  - Sort by relevance, get rid of trash data etc. regularly (1 year storage time!)
- For all data generated, provide clear version numbers (e.g, raw, reaction solution, reaction monitoring, etc.)

Back up your data!

- Make sure to save your data regularly (use the 3-2-1 rule: Keep at least three copies of your data, and store two backups on different storage media, with one of them located offsite. Use the back-upped “home” partition of the Wolf group (\\Titan-DPS009\DPS009\chemie\anorg2\), hard drives etc.). For tips refer to IT Admin of the group.

2.2. Making data openly accessible

Multiple different types of data are produced for our projects (NMR, MS, X-ray, GC-MS, IR, reaction descriptions with yield and habitus of new compounds etc.). X-ray data will be deposited on the CCSD before the submission of publications

The remaining including NMR, MS, X-ray, GC-MS, IR, EA (elemental analysis), etc. will be deposited in the Radar4Chem repository before publication and included in the supporting information of publications. Data will be converted into easily accessible files or standard file formats where available (CIF, CSV, etc.) and clearly linked to the respective publications.

2.3. Making data interoperable

Where defined, we will adhere to standards for formats compliant with available (open) software applications (e.g. CIF, PDB, ACSII/CSV).

2.4. Increase data re-use

Data will be included as supporting information in an open-access format (BY, ND, NC license). Manuscripts will be deposited to open-access repositories prior to publication.

Once published, the data sets described in the publication will be deposited at Radar4Chem (https://radar4chem.radar-service.eu/radar/de/home)

3. Allocation of resources

Depending on the founding agencies, the costs for open access publications are covered. Project DEAL (with certain publishers, Wiley, Springer) can make publications from UR authors open access.

4. Data security

Short term: 3-2-1- rule. Use our back-upped “home” partition (\\Titan-DPS009\DPS009\chemie\anorg2\) in addition to your computer during your time in the Wolf lab. ELN: transfer the collection with your experiments to PI when you leave the lab. During the Home office: use a VPN tunnel for transferring data.

Long-term: Data safely stored in certified repositories for long-term preservation and curation.

This RDMP, set up by the Wolf lab team (current version April 2025), is continuously updated as needed.