# livMatS Data Management Plan Template — Chemotion ELN and Chemotion repository

This template for a data management plan (DMP) template implements the *livMatSc RDM policy* by Chemotion ELN and Chemotion repository.

* *Italic entries provide suggestions and are to be adopted per-project.*
* Empty fields are to be filled out with project-specific information.
* Other default text defines unnegotiable content according to the *livMatS RDM Policy*.

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|  | General Information |
|  | Administrative information such as name of applicant, project number, funding programme, and version of DMPThis DMP implements the livMatS research data management (RDM) policy [1]. |
| 1 | Data description and collection or re-use of existing data |
| 1a | How will new data be collected or produced and/or how will existing data be re-used? | * Collaborators will be using the Electronic Lab Notebook (ELN) Chemotion (<https://chemotion.intra.uni-freiburg.de>) to plan and document samples and reactions. Additional data can be uploaded, e.g. experimental data sets and images.

For details see: <https://www.chemotion.net>* Guidelines on how to share data in a working group can be found here <https://chemrxiv.org/engage/chemrxiv/article-details/6231d9dc74104f5f77a6ba20>
* Open access to Chemotion datasets can be achieved by transferring Data to Chemotion Repository (<https://www.chemotion-repository.net>)
* *If you plan on using other third-party repositories (e.g. CSD) – please fill in her*
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| 1b | What data (for example the kind, formats, and volumes), will be collected or produced? | * The ELN data is stored in a PostgreSQL database. Additional experimental data can be uploaded in basically any format. Typically, image files or NMR, IR and MS data are uploded, preferably in open data formats like JCAMP-DX and mz(X)ML.
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| 2 | Documentation and data quality |
| 2a | What metadata and documentation (for example the methodology of data collection and way of organising data) will accompany the data? | * Please refer to the Chemotion ELN Documentation <https://www.chemotion.net/chemotionsaurus/docs/eln/intro> and <https://doi.org/10.1186/s13321-017-0240-0>
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| 2b | What data quality control measures will be used? | * The PI is in charge of ensuring the quality of the data in the ELN. This is done by requesting researchers to send automatically generated reports to the PI.
* Datasets published on Chemotion Repository have to pass an internal review to ensure data quality (<https://www.chemotion-repository.net>)
* *If you plan on using other third-party repositories (e.g. CSD) – please fill in her*
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| 3 | Storage and backup during the research process |
| 3a | How will data and metadata be stored and backed up during the research? | * The virtual machines and storage are provided by the University of Freiburg’s central compute services.
* The Chemotion Database is stored on a virtual machine and dumped to the central storage of the University
* The uploaded data is stored directly on the central Storage of the University
* All stored data are backed-up geo-redundantly
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| 3b | How will data security and protection of sensitive data be taken care of during the research? | * The Chemotion webserver is accessible from within the University of Freiburg network only. ELN entries and uploaded data are readable by the user who created them by default. Sharing with other users is possible.
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| 4 | Legal and ethical requirements, codes of conduct |
| 4a | If personal data are processed, how will compliance with legislation on personal data and on security be ensured? |  |
| 4b | How will other legal issues, such as intellectual property rights and ownership, be managed? What legislation is applicable? | *Achtung Repository! PI fragen vor hochladen.* |
| 4c | What ethical issues and codes of conduct are there, and how will they be taken into account? |  |
| 5 | Data sharing and long-term preservation |
| 5a | How and when will data be shared? Are there possible restrictions to data sharing or embargo reasons? | * Data can be shared with other Chemotion Users within the University of Freiburg
* Open access to Chemotion datasets can be achieved by transferring Data to the Chemotion Repository (<https://www.chemotion-repository.net>)
* *If you plan on using other third-party repositories (e.g. CSD) – please fill in here*
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| 5b | How will data for preservation be selected, and where data will be preserved long-term (for example a data repository or archive)? | * Data will reside on the central university storage system for at least 10 years.
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| 5c | What methods or software tools are needed to access and use data? | * A standard Web Browser (preferably Chrome) is needed to access and use data stored in the ELN.
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| 5d | How will the application of a unique and persistent identifier (such as a Digital Object Identifier (DOI)) to each data set be ensured? | * In Chemotion ELN a UUID is registered parallel to the creation of reaction, samples and analyses.

(c.f. <https://doi.org/10.1186/s13321-017-0240-0>).* Datasets published on Chemotion repository are assigned persistent identifiers (DOI) according to the repository platform’s standards
* *If you plan on using other third-party repositories (e.g. CSD) – please fill in her*
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| 6 | Data management responsibilities and resources |
| 6a | Who (for example role, position, and institution) will be responsible for data management (i.e. the data steward)? | * The data creator (researcher) is responsible for creation and quality of ELN items (Samples, Reaction, etc.) and the creation and quality of uploaded datasets.
* The central compute centre (Rechenzentrum) provides access to the virtual machines and central storage infrastructure.
* livMatS and the IAAC provide access to the chemotion ELN.
* The PI is responsible for implementing, reviewing and revising this DMP. The livMatS data steward may help with this task.
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| 6b | What resources (for example financial and time) will be dedicated to data management and ensuring that data will be FAIR (Findable, Accessible, Interoperable, Re-usable)? | * The livMatS data steward advises researchers on all data management-related topics such as data creation, documentation, storage, curation, publication.
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# References:

[1] <https://www.livmats.uni-freiburg.de/en/members/research-data-management>