

# SUSTAINABLE PRODUCTION OF BIO-BASED MULTI-REACTIVE ISOCYANATES

*A Data Management Plan created using DMPonline.be*

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**Project abstract:**

The main objective of PROMIS is to provide the chemical and materials industry with new biomass-based renewable aromatic and cyclic aliphatic base structures, which can result in 'lookalike' or new amine structures, to produce the most important isocyanates for polyurethane (PU) production, i.e. to replace MDI, TDI and IPDI. A second goal of PROMIS is the development of a phosgene-free route to convert renewable amines into 'blocked' isocyanates. A final objective of PROMIS is the sustainability evaluation of the synthesis procedures and resulting end products.

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VLAIO DMP (Flemish Standard DMP)

## 1. RESEARCH DATA SUMMARY

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

Dataset Name	Description	New or reused	Digital or Physical	Only for digital data			Physical volume
				Digital Data Type	Digital Data format	Digital data volume (MB/GB/TB)	
Analytical measurements	Analysis of reaction products (GC, GC-MS, NMR, HPLC, IR, DSC)	Generate new data	Digital	Experimental	.txt .csv .xls	<100GB	/
Stored product samples	Product samples.	Generate new data	Physical	/	/	/	1/2 shelf cupboard
Experimental data (generated) quantitative	Processing of measured, experimental, data	Generate new data	Digital	Compiled/aggregated data	.xls .ppt	<100 GB	/
Reference data	Literature summary and organization of literature	Reuse existing data	Digital	Compiled/aggregated data	.pdf .docx	<100 GB	/

If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type:

The literature study for this project will be compiled from existing data as DOI, URL or PDF files, and summarized in a review document (.docx, .xls).

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? Describe these issues in the comment section. Please refer to specific datasets or data types when appropriate.

- No

Will you process personal data? If so, briefly describe the kind of personal data you will use in the comment section. Please refer to specific datasets or data types when appropriate.

- No

**Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, ...)? If so, please comment per dataset or data type where appropriate.**

- Yes

This work might have potential for tech transfer and valorization. Therefore, there will be restrictions for data disclosure as it may contain IP-sensitive information. All data will be subjected for their patentability prior to any publication. If applicable, patent applications will be filled. IP management will be conducted as described in the collaboration agreement SWOK: Patent applications will be made for relevant innovative procedures/products and the costs will be shared according to ownership percentage that shall be subject to negotiation on a pro rata basis. The IP can be filled by one partner on exclusive project results or by multiple partners to protect common project results (joined IP). Following the SWOK, the intention to file a patent application should be reported to the consortium at least two weeks prior to the filing date. Furthermore, to avoid publication of IPR sensitive results, all partners will be responsible for transfer of anticipated publications.

**Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material/Data transfer agreements/ research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.**

- Yes

For this cSBO Cluster project a research collaboration agreement is drawn up (i.e. SWOK). Furthermore, material product samples will be transferred between partners. Common project results and data will be shared in (bilateral) technical meetings (.ppt). Future (joined) anticipated publications or patent applications will be discussed in consortium meetings. The agreements concerning IPR are, briefly, reported in the previous question and described in the SWOK.

**Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.**

- No

## 2. DOCUMENTATION AND METADATA

**Clearly describe what approach will be followed to capture the accompanying information necessary to keep data understandable and usable, for yourself and others, now and in the future (e.g., in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, Codebook.tsv etc. where this information is recorded).**

1. Regular set of raw experimental data will be collected per every experiment. Experiments will be classified based on date and type of experiment.
2. Additional document (a living document, as .xls or .ppt) will contain a detailed summary of every experiment to keep track of experimental details.
3. Another overview file (ppt) explains the organization of data storage (raw files, processed files, progress report files).

**Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify (where appropriate per dataset or data type) which metadata standard will be used. If not, please specify (where appropriate per dataset or data type) which metadata will be created to make the data easier to find and reuse.**

- Yes

The metadata for the data in this project entails:

- Creator of the dataset
- Name of the dataset
- File type of the dataset (depending on the employed software different file formats will be generated).
- Date of generation
- Data type (experimental or modelled)
- Software employed to generate the data (in case of modelled)

### **3. DATA STORAGE & BACK-UP DURING THE RESEARCH PROJECT**

#### **Where will the data be stored?**

All data will be stored in a cloud service offered by the university: KULeuven-One drive.  
This storage is regularly backed up by IT-service of KUL. Copies will be made and kept on personal drives (I:).

#### **How will the data be backed up?**

The data will be stored on the university's central servers with automatic daily back-up procedures.

**Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely.  
If no or insufficient storage or backup capacities are available, then explain how this will be taken care of.**

- Yes

Yes, there is currently sufficient storage and backup capacity

#### **How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?**

In the cloud service offered by the university (One drive) the access to the data can be strictly authorized. Furthermore, we made the arrangement with the KU Leuven ICTS department that we can use the K-Drive for long-term data storage. Here, one folder will have read-only rights for certain users to check data collected by the team (and which they can see, copy to their local storage space, but can't modify) and another folder with "edit" rights for users as "input" folder. Furthermore a third folder will be made with authorization limited to the data managers (i.e. Bert Sels, Bert Lagrain, Laura Trullemans) of this project to back-up the data of the two working folders. The data managers need to copy manually data from input to other 2 folders, which will be done every month. Note, separated folders will be created to share information with partners in this project. Hence, partners have no access to internal file exchange.

#### **What are the expected costs for data storage and backup during the research project? How will these costs be covered?**

There are no additional costs related to the data storage and backup.

#### 4. DATA PRESERVATION AFTER THE END OF THE RESEARCH PROJECT

**Which data will be retained for at least five years (or longer, in agreement with other retention policies that are applicable) after the end of the project? In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).**

Retained data:

- Publications (experimental manuscripts, review papers, PhD) stored in Lirias.
- Regular progress and final reports (as ppt and doc files)
- Processed experimental data (as xls files)

Not retained data:

- Raw experimental data (as csv, txt, xls,... format) - easy and low cost reproducibility

**Where will these data be archived (stored and curated for the long-term)?**

The data will be stored on the university's central servers (K-drive of CSCE, [K:\SET-CSCE-Archive-Data-D0771](#)) with automatic back-up procedures for at least 10 years, conform the KU Leuven RDM policy

**What are the expected costs for data preservation during the expected retention period? How will these costs be covered?**

K-drive long-term storage costs covered by project budget

## 5. DATA SHARING AND REUSE

**Will the data (or part of the data) be made available for reuse after/during the project? In the comment section please explain per dataset or data type which data will be made available.**

- Yes, in a restricted access repository (after approval, institutional access only, ...)

Data will be available only in a format of publications (PhD, IP, master thesis) or strictly for internal use within research group internally

**If access is restricted, please specify who will be able to access the data and under what conditions.**

1. In a restricted access repository
2. Upon request by mail and approval by responsible PI (main data owner)
3. Via publications, patents

**Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)? Please explain in the comment section per dataset or data type where appropriate.**

- Yes, Intellectual Property Rights

Like reported in question 1.5, this work might have potential for tech transfer and valorization. Therefore, there will be restrictions for data disclosure as it may contain IP-sensitive information. Note, this will not be applicable on the reference dataset, however it might be applicable on the experimental, analytical and sample storage dataset. In the section 'article 6 Publication' of the collaboration agreement, the procedure of publication of results generated in this project covers the following requirements:

- In all forms of dissemination the collaboration of the consortium should be mentioned.
- A partner can not publish results which he/she does not own.
- The type of dissemination of results will be discussed in the steering group, taking into account the valorization potential of these results.
- A publication should be shared with the collaborating partners at least 30 days before submission, to allow them to register objection within 15 days after reception.
- If there is any objection, the involved partners will discuss this a meeting and try to find, as soon as possible, a solution, or tackle this problem by adapting the manuscript. If there is no objection, the publication can be submitted.

**Where will the data be made available? If already known, please provide a repository per dataset or data type.**

The experimental and analytical data will be stored in a restricted access repository. This data and insights will be, later, made available via publications or patents, which are accessible via LIMO (KU Leuven) and search engines like patentscope. More detailed information and data can be shared upon request by mail and approval by responsible PI (main data owner)

**When will the data be made available?**

Upon publication of the research results

**Which data usage licenses are you going to provide? If none, please explain why.**

The usage of licenses is not applicable to the data generated in this project.

**Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, you have the option to provide it in the comment section.**

- Yes

Once the research results will be published, the DOI will be linked to the dataset including the project results.

**What are the expected costs for data sharing? How will these costs be covered?**

Publications in specific sources might be a subject of additional costs that will be paid from running projects.



## **6. RESPONSIBILITIES**

### **Who will manage data documentation and metadata during the research project?**

The postdocs and PhD students will manage their own data and data documentation during the project based on mutual agreements about data sets (see part 2). They will be assisted by professor and project manager.

### **Who will manage data storage and backup during the research project?**

Project manager will take responsibility to organize data collection (set-up One-drive), coordinate of data management activity (incl. manual back-ups) and assist people involved in the project in proper handling of collected data (documentation of data, sharing data etc.). Professor will take a helicopter view on data management (assign roles, specify access permissions etc.). Project manager of current project (Laura Trullemans) will be always backed-up by other group members involved in project management (research manager Ekaterina Makshina, IOF valorization manager Bert Lagrain, PI Bert Sels)

### **Who will manage data preservation and sharing?**

Research manager (Ekaterina Makshina), main PI/professor (Bert Sels)

### **Who will update and implement this DMP?**

The end responsibility for updating and implementing the DMP is with the supervisor (promotor) and project managers.