FWO DMP Template - Flemish Standard Data Management Plan

Version KU Leuven

Project supervisors (from application round 2018 onwards) and fellows (from application round 2020 onwards) will, upon being awarded their project or fellowship, be invited to develop their answers to the data management related questions into a DMP. The FWO expects a **completed DMP no later than 6 months after the official start date** of the project or fellowship. The DMP should not be submitted to FWO but to the research co-ordination office of the host institute; FWO may request the DMP in a random check.

At the end of the project, the **final version of the DMP** has to be added to the final report of the project; this should be submitted to FWO by the supervisor-spokesperson through FWO's e-portal. This DMP may of course have been updated since its first version. The DMP is an element in the final evaluation of the project by the relevant expert panel. Both the DMP submitted within the first 6 months after the start date and the final DMP may use this template.

The DMP template used by the Research Foundation Flanders (FWO) corresponds with the Flemish Standard Data Management Plan. This Flemish Standard DMP was developed by the Flemish Research Data Network (FRDN) Task Force DMP which comprises representatives of all Flemish funders and research institutions. This is a standardized DMP template based on the previous FWO template that contains the core requirements for data management planning. To increase understanding and facilitate completion of the DMP, a standardized **glossary** of definitions and abbreviations is available via the following link.

1. General Project Information	
Name Grant Holder & ORCID	**Linde Achten 0000-0001-8992-9729**
Contributor name(s) (+ ORCID) & roles	**Wim Dehaen 0000-0002-9597-0629 promotor**
Project number [1] & title	Oxapillar[n]arene[m]quinones (OPAQs): a novel class of promising macrocyclic hosts
Funder(s) GrantID [2]	11P8824N
Affiliation(s)	x KU Leuven ☐ Universiteit Antwerpen ☐ Universiteit Gent ☐ Universiteit Hasselt ☐ Vrije Universiteit Brussel ☐ Other: ROR identifier KU Leuven: 05f950310

[1] "Project number" refers to the institutional project number. This question is optional. Applicants can only provide one project number.

[2] Funder(s) GrantID refers to the number of the DMP at the funder(s), here one can specify multiple GrantIDs if multiple funding sources were used.

Please provide a short project description	Pillar[n]arenes hold a prominent position within supramolecular chemistry. Their importance is directly related to their facile synthesis, rigid cavity, tunable solubility, and ease of functionalization. However, the latter stands in stark contrast to their challenging selective desymmetrization. Additionally, functionalization of the 3,6-aryl and lateral positions is significantly underexplored. Larger ring sizes of pillar[n]arenes have, moreover, only scarcely been reported due to the low yield and difficult reproducibility of their synthesis. Despite these drawbacks, such macrocycles have proven crucial for influential applications. Therefore, a new class of macrocyclic rings facilitating desymmetrization, extensive functionalization, and the synthesis of large rings would be attractive. This project tackles these limitations through the synthesis and functionalization of novel oxygen-containing members of the pillar[n]arene family, the oxapillar[n]arene[m]quinones (OPAQs). These macrocycles, having a robust synthesis, were obtained in preliminary work. As their qualities are promising to counter the mentioned drawbacks, this project will build on these results and focus on four principal goals. The first goals are developing a synthetic method for OPAQs of different substitution patterns and ring sizes, and establishing suitable postfunctionalization routes. Then, extensive structural characterization will be performed. Lastly, the host properties will be evaluated.

2. 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 [3].

				ONLY FOR DIGITAL DATA	*ONLY FOR DIGITAL DATA*	*ONLY FOR DIGITAL DATA*	*ONLY FOR PHYSICAL DATA*
Dataset Name	Description	New or Reused	Digital or Physical	Digital Data Type	Digital Data Format	Digital Data Volume (MB, GB, TB)	Physical Volume
Observational data and procedures on chemical synthesis	Detailed notes on the used amounts of reagents, procedure, observations, and the obtained amount of product, written down in analog lab notebooks or the ELN.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☒ Physical	☐ Audiovisual ☒ Images ☐ Sound ☒ Numerical ☒ Textual ☐ Model ☐ Software ☐ Other:	.pdf, .docx, .cdx	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	Several analog lab notebooks will be generated.
Chemical compounds	Vials containing several mg of compounds.	☒ Generate new data ☐ Reuse existing data	☐ Digital ☒ Physical	NA	NA	NA	Several boxes of compounds stored in KU Leuven Chem&Tech in stock room 01.186 under a universal and clear filing system.
NMR	Data folders generated by the spectrometer containing raw and processed data.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☐ Physical	☐ Audiovisual ☒ Images ☐ Sound ☐ Numerical ☐ Textual ☐ Model ☐ Software ☒ Other: Experimental	.pdf, .txt, .exec, .png, .docx, .mnova	☐ < 1 GB ☒ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	NA

[3] Add rows for each dataset you want to describe.

IR	Data folders generated by the spectrometer containing raw and processed data.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☐ Physical	☐ Audiovisual ☒ Images ☐ Sound ☐ Numerical ☐ Textual ☐ Model ☐ Software ☒ Other: Experimental	.pdf, .png, .docx, .mnova, .dpt	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	NA
UV-Vis-NIR	Data folders generated by the spectrometer containing raw and processed data.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☐ Physical	☐ Audiovisual ☒ Images ☐ Sound ☐ Numerical ☐ Textual ☐ Model ☐ Software ☒ Other: Experimental	.pdf, .dsw, .sl, .png,.docx	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	NA
MS related chromatography	Data folders generated by the spectrometer containing raw and processed data.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☐ Physical	☐ Audiovisual ☒ Images ☐ Sound ☐ Numerical ☐ Textual ☐ Model ☐ Software ☒ Other: Experimental	.pdf, .png, .docx	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	NA
MPLC	Data folders generated by the spectrometer	☒ Generate new data	☒ Digital ☐ Physical	☐ Audiovisual ☒ Images ☐ Sound	.pdf, .txt	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB	NA

	containing raw and processed data.	☐ Reuse existing data		☐ Numerical ☐ Textual ☐ Model ☐ Software ☒ Other: Experimental		☐ < 5 TB ☐ > 5 TB ☐ NA	
X-ray data (single crystal)	Data folders generated by the spectrometer containing raw and processed data.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☐ Physical	☐ Audiovisual ☒ Images ☐ Sound ☐ Numerical ☐ Textual ☐ Model ☐ Software ☒ Other: Experimental	.png, .cif	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	NA
Elemental analysis	Data folders generated by the spectrometer containing raw and processed data.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☐ Physical	☐ Audiovisual ☐ Images ☐ Sound ☒ Numerical ☒ Textual ☐ Model ☐ Software ☒ Other: Experimental	.pdf, .txt, .dat	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	NA
HPLC	Data folders generated by the spectrometer containing raw and processed data.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☐ Physical	☐ Audiovisual ☒ Images ☐ Sound ☒ Numerical ☐ Textual ☐ Model	.pdf,.txt, .png	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	NA

				☐ Software ☒ Other: Experimental			
Cyclic voltammetry	Data folders generated by the apparatus containing raw and processed data.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☐ Physical	☐ Audiovisual ☒ Images ☐ Sound ☐ Numerical ☐ Textual ☐ Model ☐ Software ☒ Other: Experimental	.cif, .pdf	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	NA
Isothermal calorimetry	Data folders generated by the spectrometer containing raw and processed data.	☒ Generate new data ☐ Reuse existing data	☒ Digital ☐ Physical	☐ Audiovisual ☒ Images ☐ Sound ☐ Numerical ☐ Textual ☐ Model ☐ Software ☒ Other: Experimental	.pdf, .png, .ict, .csv, .opj	☒ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	NA

GUIDANCE:
The data description forms the basis of your entire DMP, so make sure it is detailed and complete. It includes digital and physical data and encompasses the whole spectrum ranging from raw data to processed and analysed data including analysis scripts and code. Physical data are all materials that need proper management because they are valuable, difficult to replace and/or ethical issues are associated. Materials that are not considered data in an RDM context include your own manuscripts, theses and presentations; documentation is an integral part of your datasets and should described under documentation/metadata.
RDM Guidance on data

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.	NA
Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.	☐ Yes, human subject data; provide SMEC or EC approval number: ☐ Yes, animal data; provide ECD reference number: ☐ Yes, dual use; provide approval number: ☒ No Additional information:
Will you process personal data[4]? If so, please refer to specific datasets or data types when appropriate and provide the KU Leuven or UZ Leuven privacy register number (G or S number).	☐ Yes (provide PRET G-number or EC S-number below) ☒ No Additional information:
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 ☐ No If yes, please comment: Should the synthesized compounds proof to be highly applicable, it could be that commercial valorization is within reach. However, this would definitely be in a far of future. -Procedures on chemical synthesis: synthetic procedures towards the potent compounds. -Characterization data: all the data proving the structure of compounds (NMR, MS, IR, X-ray data, etc.) that are essential for the development of further application. -Binding studies: the synthesized compounds will be evaluated in binding studies testing their host behavior towards various guests. Therefore, the valorization potential of this work is highly dependent on the data of the binding studies.

[4] See Glossary Flemish Standard Data Management Plan

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 to what data they relate and what restrictions are in place.	☐ Yes ☒ No If yes, please explain:
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 to what data they relate and which restrictions will be asserted.	☐ Yes ☒ No If yes, please explain:

3. 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). *RDM guidance on documentation and metadata.*	Two types of data will be gathered during this project. Chemical data from experiments (reaction conditions, experimental sequence, observations, amount of reagents used) will be stored by the researcher in Microsoft OneDrive (2 TB), MBook ELN(Electronic Lab Notebooks) and analog lab notebooks. Corresponding structural identification data for the obtained compounds (raw and processed) will be uploaded in the ELN and linked to the correct experiment making data traceable. Data from binding studies will be preserved digitally. All project data will be shared with the PI and other collaborators via Microsoft OneDrive and via the ELN.

Will a metadata standard be used to make it easier to **find and reuse the data**? If so, please specify which metadata standard will be used. If not, please specify which metadata will be created to make the data easier to find and reuse. *REPOSITORIES COULD ASK TO DELIVER METADATA IN A CERTAIN FORMAT, WITH SPECIFIED ONTOLOGIES AND VOCABULARIES, I.E. STANDARD LISTS WITH UNIQUE IDENTIFIERS.*	☐ Yes ☒ No If yes, please specify (where appropriate per dataset or data type) which metadata standard will be used: If no, please specify (where appropriate per dataset or data type) which metadata will be created: Metadata will be saved in the OneDrive storage and will be reported in the ELN. Filenames of the data generated (raw and processed) will be annotated in the ELN as well.

4. Data Storage & Back-up during the Research Project	
Where will the data be stored? *Consult the interactive KU Leuven storage guide to find the most suitable storage solution for your data.*	☒ Shared network drive (J-drive) ☒ Personal network drive (I-drive) ☒ OneDrive (KU Leuven) ☐ Sharepoint online ☐ Sharepoint on-premis ☐ Large Volume Storage ☐ Digital Vault ☒ Other: Archive drive (K-drive)

How will the data be backed up? *WHAT STORAGE AND BACKUP PROCEDURES WILL BE IN PLACE TO PREVENT DATA LOSS?*	☒ Standard back-up provided by KU Leuven ICTS for my storage solution ☐ Personal back-ups I make (specify) ☒ Other (specify) The electronic lab book provides a back-up for the analog lab notebooks and is backed-up automatically in the ELN's cloud service. The PI stores the paper copies of the analog lab notebooks and a scanned version in the online archival storage as PDF.
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 ☐ No KU Leuven OneDrive provides space of 2 TB which is regularly backed up and can be extended if needed. If no, please specify:
How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons? *CLEARLY DESCRIBE THE MEASURES (IN TERMS OF PHYSICAL SECURITY, NETWORK SECURITY, AND SECURITY OF COMPUTER SYSTEMS AND FILES) THAT WILL BE TAKEN TO ENSURE THAT STORED AND TRANSFERRED DATA ARE SAFE.* *Guidance on security for research data*	OneDrive is not publicly accessible and password protected. Access needs to be granted by the researcher and will be limited to the PI (and his delegate responsible for data storage). For collaborations, accessibility to the relevant files will be granted if described in a non-disclosure agreement. Archival storage at KU Leuven is not publicly accessible and only people with permission (PI and his delegate responsible for data storage) can access the data.
What are the expected costs for data storage and backup during the research project? How will these costs be covered?	The use of OneDrive is free of charge if the capacity of 2 TB is not exceeded. Archival data storage is centrally offered via KU Leuven at 270 Euro/TB/Year. MBook ELN and the cloud service are offered by Mestrelab at 10 Euro/month for the subscription and a one-time license fee of 120 Euro. These costs are being covered by the general operating budget of the research group, or by the individual bench fee of researchers.

5. 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...). *Guidance on data preservation*	☐ All data will be preserved for 10 years according to KU Leuven RDM policy ☐ All data will be preserved for 25 years according to CTC recommendations for clinical trials with medicinal products for human use and for clinical experiments on humans ☒ Certain data cannot be kept for 10 years (explain) Samples will be stored for 10 years in our depository as long as the long-term stability and quantity of the compound allow it.
Where will these data be archived (stored and curated for the long-term)? *Dedicated data repositories are often the best place to preserve your data. Data not suitable for preservation in a repository can be stored using a KU Leuven storage solution, consult the interactive KU Leuven storage guide.*	☐ KU Leuven RDR ☐ Large Volume Storage (longterm for large volumes) ☒ Shared network drive (J-drive) ☒ Other (specifiy):KU Leuven Archive drive (K-drive)
What are the expected costs for data preservation during the expected retention period? How will these costs be covered?	Data archival at KU Leuven is currently offered at 270 Euro/TB/year. Since no large datasets are generated in this project, one TB of storage will be sufficient and the price for storage for 10 years is 2700 Euro. These costs are covered by the general operating budget of the research group or by the individual bench fee of researchers.

6. Data Sharing and Reuse

Will the data (or part of the data) be made available for reuse after/during the project? Please explain per dataset or data type which data will be made available. *NOTE THAT 'AVAILABLE' DOES NOT NECESSARILY MEAN THAT THE DATA SET BECOMES OPENLY AVAILABLE, CONDITIONS FOR ACCESS AND USE MAY APPLY. AVAILABILITY IN THIS QUESTION THUS ENTAILS BOTH OPEN & RESTRICTED ACCESS. FOR MORE INFORMATION: HTTPS://WIKI.SURFNET.NL/DISPLAY/STANDARDS/INFO-EU-REPO/#INFOEUREPO-ACCESSRIGHTS*	☐ Yes, as open data ☐ Yes, as embargoed data (temporary restriction) ☒ Yes, as restricted data (upon approval, or institutional access only) ☐ No (closed access) ☐ Other, please specify:
If access is restricted, please specify who will be able to access the data and under what conditions.	In general, data generated in projects will be made publicly available at the time of publication. The information that is not publicly available (incomplete datasets, those can be used for the set-up of new projects and the continuation of the group's research), will be stored in the OneDrive account of the individual team members. The group leader Prof. Dehaen will have co-ownership in this folder. Access to data, that is not publicly available, can be provided after signing the non-disclosure agreement.
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 per dataset or data type where appropriate.	☐ Yes, privacy aspects ☐ Yes, intellectual property rights ☐ Yes, ethical aspects ☐ Yes, aspects of dual use ☐ Yes, other ☒ No If yes, please specify:

Where will the data be made available? If already known, please provide a repository per dataset or data type.	☐ KU Leuven RDR ☐ Other data repository (specify) ☒ Other (specify) Data papers describing and promoting the research will be published in peer-reviewed journals. Extra data such as chromatograms or specific spectral data can be made available upon request by email. The final thesis will be stored in the digital repository for KU Leuven Association research (LIRIAS; https://limo.libis.be/).
When will the data be made available?	☒ Upon publication of research results ☐ Specific date (specify) ☐ Other (specify)
Which data usage licenses are you going to provide? If none, please explain why. *A DATA USAGE LICENSE INDICATES WHETHER THE DATA CAN BE REUSED OR NOT AND UNDER WHAT CONDITIONS. IF NO LICENCE IS GRANTED, THE DATA ARE IN A GREY ZONE AND CANNOT BE LEGALLY REUSED. DO NOTE THAT YOU MAY ONLY RELEASE DATA UNDER A LICENCE CHOSEN BY YOURSELF IF IT DOES NOT ALREADY FALL UNDER ANOTHER LICENCE THAT MIGHT PROHIBIT THAT.* *Check the RDR guidance on licences for data and software sources code or consult the License selector tool to help you choose.*	☒ CC-BY 4.0 (data) ☐ Data Transfer Agreement (restricted data) ☐ MIT licence (code) ☐ GNU GPL-3.0 (code) ☐ Other (specify)
Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, please provide it here. *INDICATE WHETHER YOU INTEND TO ADD A PERSISTENT AND UNIQUE IDENTIFIER IN ORDER TO IDENTIFY AND RETRIEVE THE DATA.*	☒ Yes, a PID will be added upon deposit in a data repository ☐ My dataset already has a PID ☐ No

What are the expected costs for data sharing? How will these costs be covered?	No costs are related to depositing data in the LIRIAS repository of KU Leuven. Also depositing data in Mendeley Data is free. No charges apply to the publication of supporting information related to publications. Exceptionally, data will be published at a publication charging a publication fee (around 1500 Euro).

7. Responsibilities	
Who will manage data documentation and metadata during the research project?	The researcher is responsible for collecting all relevant data files and for entering the observational data in the ELN and or analog Lab notebook.
Who will manage data storage and backup during the research project?	The researcher is responsible for storing all relevant data in Microsoft OneDrive (backed up regularly), MBook ELN (backed up regularly) and analog lab notebooks.
Who will manage data preservation and sharing?	The PI (supported by a delegate data manager) is the end responsible for ensuring data preservation and reuse.
Who will update and implement this DMP?	The DMP is updated by the researcher in agreement with the PI