### 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	Cuilian Liu ORCID: 0000-0002-5353-0094
Contributor name(s) (+ ORCID) & roles	Tatjana Parac-Vogt ORCID: 0000-0002-6188-3957, promoter
Project number <sup>1</sup> & title	1273724N  Polygyamatalata hasad Matal Organia Assamblias Tayyards Synramalasydar Catalysis
Funder(s) GrantID <sup>2</sup>	Polyoxometalate-based Metal-Organic Assemblies Towards Supramolecular Catalysis FWO
Affiliation(s)	⊠ KU Leuven
	☐ Universiteit Antwerpen
	☐ Universiteit Gent
	☐ Universiteit Hasselt
	☐ Vrije Universiteit Brussel
	☐ Other:
	ROR identifier KU Leuven: 05f950310
Please provide a short project description	Polyoxometalates (POMs) represent a unique class of anionic metal-oxygen clusters with special
	characteristics that have been extensively investigated for various applications. Most POMs are
	characterized by high stability in solid-state, however, understanding their solution chemistry and
	extending their functions in solution are challenging tasks. This research proposal addresses the
	current challenges in POM chemistry by developing supramolecular approaches to stabilize and
	solubilize POMs is an interesting alternative to overcome these drawbacks. We will bridge this
	knowledge gap by exploring the key design strategies for integrating POMs into supramolecular
	assembles through host-guest encapsulation, in situ POMs formation, and using POMs as building
	blocks for the self-assembly of cages. Thus, enabling the diversity of a new family of POMs-based
	metal-organic assembles and exploring their potential as supramolecular catalysts in solution.

<sup>&</sup>lt;sup>1</sup> "Project number" refers to the institutional project number. This question is optional. Applicants can only provide one project number.

<sup>&</sup>lt;sup>2</sup> 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.

### 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 <sup>3</sup>.

				ONLY FOR DIGITAL DATA	ONLY FOR DIGITAL DATA	ONLY FOR DIGITAL DATA	ONLY FOR PHYSICAL DATA
Dataset	Description	New or Reused	Digital or	Digital Data Type	Digital Data	Digital Data	Physical Volume
Name			Physical		Format	Volume (MB, GB,	
						TB)	
NMR	Chemical	□ Generate new	□ Digital	☐ Audiovisual	TXT, PAR, XWP,	□ < 1 GB	
	composition by	data	☐ Physical		JPG, PDF	⊠ < 100 GB	
	NMR	☐ Reuse existing		☐ Sound		□ < 1 TB	
		data		⋈ Numerical		□ < 5 TB	
						□ > 5 TB	
				☐ Model		□NA	
				☐ Software			
			⊠ Other:				
Mass	Chemical	⊠ Generate new	□ Digital		RAW, JPG, PDF	⊠ < 100 GB	
	composition ESI-	data	_	⊠ Other:			
	MS date						
XRD	Single crystal	□ Generate new	□ Digital		CIF, JPG, PDF,	⊠ < 100 GB	
diffraction	diffraction	data			HKL, INS		
			⊠ Other:				
UV-VIS	UV-VIS date	☑ Generate new	□ Digital		TXT	⊠ < 1 GB	
		data					
CV	cyclic	⊠ Generate new	□ Digital		TXT	⊠ < 1 GB	
	voltammetry	data					
	date						

<sup>&</sup>lt;sup>3</sup> Add rows for each dataset you want to describe.

ranging from raw data to processed and analysed data valuable, difficult to replace and/or ethical issues are a	IP, so make sure it is detailed and complete. It includes digital and physical data and encompasses the whole spectrum a including analysis scripts and code. Physical data are all materials that need proper management because they are associated. Materials that are not considered data in an RDM context include your own manuscripts, theses and ur datasets and should described under documentation/metadata.
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.	Not Applicable
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.	<ul> <li>Yes, human subject data; provide SMEC or EC approval number:</li> <li>Yes, animal data; provide ECD reference number:</li> <li>Yes, dual use; provide approval number:</li> <li>No</li> <li>Additional information:</li> </ul>
Will you process personal data <sup>4</sup> ? 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).	<ul> <li>☐ Yes (provide PRET G-number or EC S-number below)</li> <li>☑ No</li> <li>Additional information:</li> </ul>
Does your work have potential for commercial valorization (e.g. tech transfer, for example spinoffs, commercial exploitation,)? If so, please comment per dataset or data type where appropriate.	☐ Yes ☑ No If yes, please comment:

<sup>&</sup>lt;sup>4</sup> See Glossary Flemish Standard Data Management Plan

Do existing 3rd party agreements restrict	☐ Yes
exploitation or dissemination of the data you	⊠ No
(re)use (e.g. Material/Data transfer agreements,	If yes, please explain:
research collaboration agreements)?	
If so, please explain to what data they relate and	
what restrictions are in place.	
Are there any other legal issues, such as	☐ Yes
intellectual property rights and ownership, to be	⊠ No
managed related to the data you (re)use?	If yes, please explain:
If so, please explain to what data they relate and	
which restrictions will be asserted.	

#### 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.

All experimental details will be thoroughly recorded in personal lab books, and a standardized template will be consistently used for lab notes to promote uniformity among coworkers. Each experiment's specifics, including labels, numbers, dates, conditions, outcomes, and characterizations, will be documented comprehensively. The labels of both experimental raw data and processed data will strictly correspond to the original records in personal lab books. The researcher will be responsible for day-to-day data storage and backup during the project. These data will be stored on OneDrive or KU Leuven servers for long-term storage, with raw and processed data organized in separate folders. Experiments related to a subproject or a single publication will be consolidated into one folder for easy retrieval. Additionally, an accompanying extensive README.txt file will provide an overview of experiment details, compound structure, lab book location, sample physical location, and digital storage locations.

Will a metadata standard be used to make it	☐ Yes
easier to <b>find and reuse the data</b> ?	⊠ No
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.	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:
REPOSITORIES COULD ASK TO DELIVER METADATA IN A CERTAIN FORMAT, WITH SPECIFIED ONTOLOGIES AND VOCABULARIES, I.E. STANDARD LISTS WITH UNIQUE IDENTIFIERS.	

4. Data Storage & Back-up during the Research Project			
□ Shared network drive (J-drive)			
☑ Personal network drive (I-drive)			
☐ OneDrive (KU Leuven)			
☐ Sharepoint online			
☐ Sharepoint on-premis			
☐ Large Volume Storage			
☐ Digital Vault			
☐ Other:			
☑ Standard back-up provided by KU Leuven ICTS for my storage solution			
☐ Personal back-ups I make (specify)			
☐ Other (specify)			

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.	<ul> <li>✓ Yes</li> <li>☐ No</li> <li>If no, please specify:</li> </ul>
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	All the data will be stored on the drive provided by KU Leuven ICTS for my storage solution, where strict authorizations are in place, and no external/unauthorized user can access the data. The data processing will take place on a KU Leuven-associated computer that requires a username and password, which must be changed yearly. For projects in collaboration with other researchers/groups, only limited access to that specific portion of the data will be granted.
What are the expected costs for data storage and backup during the research project? How will these costs be covered?	Standard backup drive and Microsoft OneDrive provided by KU Leuven ICTS are free of charge if the capacity of 2 TB is not exceeded.

## 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	<ul> <li>✓ All data will be preserved for 10 years according to KU Leuven RDM policy</li> <li>☐ 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</li> <li>☐ Certain data cannot be kept for 10 years (explain)</li> </ul>
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.	<ul> <li>□ KU Leuven RDR</li> <li>□ Large Volume Storage (longterm for large volumes)</li> <li>☑ Shared network drive (J-drive)</li> <li>☑ Other (specifiy):</li> <li>The archival network drive of the host group provided by KU Leuven ICTS (K-drive)</li> </ul>
What are the expected costs for data preservation during the expected retention period? How will these costs be covered?	The data will be stored on the standard backup drive of KU Leuven for at least 10 years for free. Extra generated costs will be afforded by the host group.

## 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	<ul> <li>✓ Yes, as open data</li> <li>The data used for research papers, will include as the open data of the paper.</li> <li>☐ Yes, as embargoed data (temporary restriction)</li> <li>☒ Yes, as restricted data (upon approval, or institutional access only)</li> <li>The unpublished results will be restricted data upon approval by the promoter and me.</li> <li>☐ No (closed access)</li> <li>☐ Other, please specify:</li> </ul>
If access is restricted, please specify who will be able to access the data and under what conditions.	The full dataset will be stored on the standard backup drive of KU Leuven, and will also be transferred to my promoter. Most of the valuable data will be used for research papers in peer-reviewed journals and made available to the public, unpublished results will be restricted data upon approval by promoter and me that allows for setting up new projects and the continuation of future works.
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.	<ul> <li>Yes, privacy aspects</li> <li>Yes, intellectual property rights</li> <li>Yes, ethical aspects</li> <li>Yes, aspects of dual use</li> <li>Yes, other</li> <li>No</li> <li>If yes, please specify:</li> </ul>
Where will the data be made available? If already known, please provide a repository per dataset or data type.	<ul> <li>□ KU Leuven RDR</li> <li>□ Other data repository (specify)</li> <li>☑ Other (specify)</li> <li>Not already known</li> </ul>

When will the data be made available?	<ul> <li>☑ Upon publication of research results</li> <li>☐ Specific date (specify)</li> <li>☐ Other (specify)</li> </ul>
Which data usage licenses are you going to	☐ CC-BY 4.0 (data)
provide? If none, please explain why.	☐ Data Transfer Agreement (restricted data)
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.	☐ MIT licence (code) ☐ GNU GPL-3.0 (code) ☑ Other (specify) CC-BY-NC-4.0
Do you intend to add a PID/DOI/accession	☑ Yes, a PID will be added upon deposit in a data repository
number to your dataset(s)? If already available,	☐ My dataset already has a PID
please provide it here.	
INDICATE WHETHER YOU INTEND TO ADD A PERSISTENT AND UNIQUE IDENTIFIER IN ORDER TO IDENTIFY AND RETRIEVE THE DATA.	
What are the expected costs for data sharing? How will these costs be covered?	The data is shared through publications in peer-reviewed journals, normally, it is free except some journals will be charged a fee. The possible publication fee will be covered by the host group or by my FWO bench fee.

# 7. Responsibilities

Who will manage data documentation and	Cuilian Liu (the researcher) will be responsible for day-to-day data documentation and metadata during
metadata during the research project?	the project.
Who will manage data storage and backup	Cuilian Liu (the researcher) will be responsible for day-to-day data storage and backup during the project.
during the research project?	
Who will manage data preservation and	Cuilian Liu (the researcher) will be responsible for data preservation and sharing during the project, and
sharing?	Prof. Parac-Vogt (the promoter) will be responsible for long-term data preservation and sharing after the
	project.
Who will update and implement this DMP?	Cuilian Liu (the researcher) and Prof. Parac-Vogt (the promoter)