ATP13A2 agonists for Parkinson’s disease therapy

A Data Management Plan created using DMPonline.be

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Template: KU Leuven BOF-IOF

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Project abstract:

ATP13A2, an emerging drug target for Parkinson’s disease (PD) is the second most common and fastest growing neurodegenerative disorder affecting over 6 million people worldwide. Our compelling insights into the ATP13A2-dependent disease mechanism illustrate that a low polyamine availability and disturbed intracellular polyamine distribution may drive PD pathology. we hypothesize that ATP13A2 agonists will slow down or halt PD progression by restoring tissue and intracellular polyamine levels, thereby rescuing lysosomal and mitochondrial dysfunction. Via a small molecule drug screening program, we here aim to identify, characterize and optimize ATP13A2 agonists to select a minimum of two independent early lead series for further (pre-)clinical development.

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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 / ID	Description	New or reuse	Digital or Physical data	Data Type	File format	Data volume	Physical volume
		Indicate: ***N****(ew data) or* ***E****(xisting data)*	Indicate: **D**(igital) or **P**(hysical)	Indicate: **A**udiovisual **I**mages **S**ound **N**umerical **T**extual **M**odel **SO**ftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
experimental	Protein gel pictures	N	D	I	tiff, jpg, png	<1GB	
experimental	Western blotting pictures	N	D	I	.scn	<100GB	
experimental	Flow cytometry	N	D	SO	.fcs, .pdf	<100GB	
experimental	Plate reader	N	D	T	.xlsx	<1GB	
experimental	Sequencing	N	D	T, SO	.txt, .api	<1GB	
experimental	Plasmid and protein data	N	D, P	T, SO	dna, .prot, .praln	<1GB	20˚C: 2 boxs -80˚C: 2 racks
experimental	Cell lines	N	P				<50 cell lines
experimental & compiled	Structures	N	D	I, SO	pdb, .cif.gz, .pdf, .jpg, .png	<100GB	
experimental	Data from CRO	N	D	I, N,T	.pdf, .pptx, .xlsx	<100GB	
Experimental, observational	Notebook	N	D	SO	.one	<1GB	
experimental	Image data	N	D	I, SO	.czi, .tiff	<100GB	
	Existing data	O	D, P			<100GB	

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:

Data generated from previous work with grant number ZL3A400500-101, including DNA plasmids, protein, cell line and experimental data

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.

- No

Will you process personal data? 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).

- 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

● The aim of the project is to identify novel ATP13A2 small molecule activators which can be further advanced in pre-clinical and clinical development for the treatment of Parkinson's disease. Exploitable results (via patenting, exclusive licensing or transfer) include all experimental data including:

● Detailed assay protocols
● Results of the HTS campaign(s) and validation assays
● Chemical structures of the hit compounds and derived active analogs

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material or 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.

- No

There are no third party agreements that restrict exploitation of the data which is the primary aim of this project.

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.

- Yes

Exploitable results of this project i.e. all data related to the identification and validation of activators of ATP13A2 will be protected by a patent application and/or exclusively licensed or transferred to a third party for further (co) development. Hence these project results will be kept confidential and will only be disclosed under a NDA to an interested third party during advanced licensing/transfer negotiations.

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).

Question not answered.

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.

- No

At LCTS, the researchers use a shared OneNote (e-notebook) dedicated for this project. It contains a list of tabs indicating type of experiments.

Within each tab, the notes are organized by date of experiments and contain detailed information of each experiments, including date, title, experiment temperature, concentration of reagents, timing, adjustments from a previous protocol if there is any, and the exact protocol if a new experiment has been initiated.The raw data and analysis files are stored in personal J-drive folders under this project. Organized in the same manner as in the notebook. It contains subfolders per type of experiment, and within the subfolder, the data from individual experiments organized by date of conduction. Common information including SOP, cell line information, protein sequences is stored in a common J-drive folder of the lab. Each member has access to their own personal folder, the common lab folder and OneNote. The PI and the lab manager have access to all folders.

At Cistim:

Data and metadata will be collected in line with current standards for comparable medicinal chemistry / biomedical research (publication standards, activity databases such as ChEMBL) and recorded within the Dotmatics platform. All procedures such as data analysis are linked to protocols which explain the experiment. Dotmatics support or dedicated persons are responsible for providing naming conventions to define steps, to allow quick data retrieval and analysis calculation.

For chemical substances:

Information will be collected on multiple levels including compound (overall structure), batch or sample level. Batch information captures data associated with individual purchases and registrations of a chemical substance, including (non-limiting) registration date, registered quantity, salt form, supplier and supplier reference (for purchased items) or links to individual laboratory notebooks and analytical data (for substances produced within CISTIM). Sample information captures data associated with the preparation samples (weighted from a specific batch) for the purpose of one or more experiments, including registration date, weighted quantity, unique vial barcode and sample recipient.

For biological data:

Captured information include the experiment date, individual experiment IDs, individual protocol IDs. Information about the tested substance(s) is recorded on a compound, batch and sample level. Individual data points resulting e.g. from generation of dose-response curves is recorded. The performed analysis, as well as the resulting (alpha)numerical value(s) are recorded. A dedicated field tracks the validation status of the experiment(s). Additional remarks and observations regarding particular experiments can be captured in a dedicated field. Any relevant information that could not be captured within the standard fields from the Dotmatics platform will be associated with (a) dedicated readme file(s). General guidelines regarding the generation of such files can be found on e.g. https://www.library.gatech.edu/repository-metadata or https://www.library.gatech.edu/repository-metadata.

Activities outsourced to 3rd parties:

Procedures, protocols, raw data, processed data, results and reports are shared via online platform (or email) and stored on the J-drive

Data Storage & Back-up during the Research Project

Where will the data be stored?

- OneDrive (KU Leuven)
- Shared network drive (J-drive)

LCTS:

Each researcher will store his/her data on their personal folder on the j-drive. This is our data repository for short term storage which is expandable, fast and the data can be modified by the researcher itself. Only the PI and the lab manager have access to all the folders of the j-drive.

The common data storage concerning cell lines, plasmids, antibodies is in a folder under the j-drive and is under restricted authorization. All members of the lab can read these files, but changes can only be made by the persons with authorization

When data is published, the data will be moved to our k-drive. This is our repository for data archiving, for long term storage. Only the PI and the lab manager can move the data to this drive, but data on this drive cannot be modified or deleted. Only the ICT service can do this.

CISTIM:

All data are stored on secure on premise servers maintained by the KULeuven IT service (KU Leuven Network drive).

How will the data be backed up?

- Standard back-up provided by KU Leuven ICTS for my storage solution

An automatic back-up service is provided by KU Leuven ICT service

Is there currently sufficient storage & backup capacity during the project?

If no or insufficient storage or backup capacities are available, explain how this will be taken care of.

- Yes

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

LCTS:
Data are not saved locally on laptop/desktop but are stored in the KU Leuven secure data center. Only two people have access to all folders: the PI and the lab manager. Changes in the shared OneNote made by another team member will be automatically indicated with the name of the person, and older versions can be restored if needed. Each researcher has access to his own personal folder and the project folder he/she is involved in on the j-drive, and has read only access to the data on the long-term storage (k-drive). Non-authorized persons can't access or modify the data.
CISTIM:
Data are shared via a secure on premise folders under direct control of the KULeuven IT service. Data are stored on secured on-premise servers.

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

Each year €173.40 will be charged from our ICT service for the use of 1 TB on the k-drive (long term storage) and €519.00 will be charged each year for the use of 1 TB of the j-drive (short term storage). Back-up service is included in the price. These costs were foreseen in the application and if more the lab budget will be used to cover these expenses.

Data Preservation after the end of the Research Project

Which data will be retained for 10 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...).

- All data will be preserved for 10 years according to KU Leuven RDM policy

Once the research is completed, all original data and summary/report files will be grouped and collected at the k-drive and will stay there for at least 10 years after the project. The data that are still used in experiments will be stored on the j-drive in shared folder between CD3 and LCTS. Raw data and analysis files will be stored under the folder of the researcher. When the researcher leaves the lab, these data will be moved to the k-drive.

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

- Large Volume Storage (longterm for large volumes)

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

Each year €173.40 will be charged from our ICT service for the use of 1 TB on the k-drive (long term storage), back-up service is included in the price. These costs were foreseen in the budget request of the application and if more, the lab budget will be used to cover these expenses.

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.

- Yes, as restricted data (upon approval, or institutional access only)

A part of the data from this project is under restrictions:
Structures of the drugs are only available to CD3. Only dedicated staff at CD3 (chemists working on the project, PMO, management) has internal access to chemical structures via Dotmatics.
A part of the data about the biology of ATP13A2 generated at LCTS that is not under restricted use will be subject of future publications

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

Structures of the drugs are only available to CD3. Only dedicated staff at CD3 (chemists working on the project, PMO, management) has internal access to chemical structures via Dotmatics.

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, intellectual property rights

The aim is to protect exploitable data via a patent application in the future.

Where will the data be made available?

If already known, please provide a repository per dataset or data type.

- Other (specify below)

Publishable data not related to exploitation will be made available as follows:
DNA plasmids: Addgene
Experimental data sets and associated readme files involved in a publication: zenodo
Experimental protocols: protocols.io

When will the data be made available?

- Upon publication of research results

Which data usage licenses are you going to provide?

If none, please explain why.

- CC-BY 4.0 (data)

Do you intend to add a persistent identifier (PID) to your dataset(s), e.g. a DOI or accession number? If already available, please provide it here.

- Yes, a PID will be added upon deposit in a data repository

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

It will be covered by the current grant

Responsibilities

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

During the research, individual co-workers are responsible to collect and store data on a dedicated personnel j-drive. The data will be reviewed by the principal investigator.

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

Peter Vangheluwe and the ICT service at KU Leuven

Who will manage data preservation and sharing?

LCTS: Marleen Schuermans and Peter Vangheluwe
CISTIM: Michele Curcio and Patrick Chaltin

Who will update and implement this DMP?

Peter Vangheluwe