

FWO STRUCTURAL, MOLECULAR, AND CELLULAR BIOLOGY OF PKD2 ALLOSTERIC MODULATORS AS NOVEL THERAPEUTICS FOR CANCER

DMP TITLE

ADMIN DETAILS

Project Name:FWO Structural, molecular, and cellular biology of PKD2 allosteric modulators as novel therapeutics for cancer

Project Identifier: u0047937

Grant Title: G095522N

Principal Investigator / Researcher: Arnout Voet

Description: In this project we will characterise a novel class of allosteric PKD2 kinase inhibitors using molecular biology methods and experimental structural biology methods with the aim of rationally design improved derivatives as cancer therapeutics

Institution: KU Leuven

1. GENERAL INFORMATION

Name applicant

Arnout Voet

FWO Project Number & Title

G095522N FWO Structural, molecular, and cellular biology of PKD2 allosteric modulators as novel therapeutics for cancer

Affiliation

- KU Leuven

2. DATA DESCRIPTION

Will you generate/collect new data and/or make use of existing data?

- Generate new data

Describe in detail the origin, type and format of the data (per dataset) and its (estimated) volume. This may be easiest in a table (see example) or as a data flow and per WP or objective of the

project. If you reuse existing data, specify the source of these data. Distinguish data types (the kind of content) from data formats (the technical format).

Type of data	format	volume	how created
expression constructs	sample	20 microliter	custom gene synthesis by biotech company
protein purification data	docx	100MB	experimental reports documenting every step of the process
raw diffraction data	.cbf, h5	1TB	diffraction at synchrotron
protein crystal structures	.pdb,mtz	4-10GB	solving diffraction at synchrotron radiation facilities
interacion assays	.csv	25GB	BLI measurements,
virtual screening	.mdb, .pdb, .sdf	250GB	using the MOE software
Protein kinase assays	.pzf, .xlsx	25GB	ADP Glo kinase assay on plate reader
Western blots	.tif	6GB	Transfer of proteins to membrane, followed by ECL which is visualised in a blot imager ImageQuant LAS4000
Cell proliferation assays	.xlsx	20MB	MTT assay, with readout on a plate reader
Cell migration assays	Xlsx, .pzf	4GB	Scratch wound assay in Incucyte toestel
RNA seq	.bam, .bai	3 GB per group (containing 5 biol replicates) (max 24 GB in total)	Will be performed by genomics core KU Leuven

3. LEGAL AND ETHICAL ISSUES

Will you use personal data? If so, shortly describe the kind of personal data you will use. Add the reference to your file in KU Leuven's Register of Data Processing for Research and Public Service Purposes (PRET application). Be aware that registering the fact that you process personal data is a legal obligation.

- No

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, add the reference to the formal approval by the relevant ethical review committee(s)

- No

NA

Does your work possibly result in research data with potential for tech transfer and valorisation? Will IP restrictions be claimed for the data you created? If so, for what data and which restrictions will be asserted?

- Yes

compounds with potential to be developed into drugs will be protected as supported by LRD

Do existing 3rd party agreements restrict dissemination or exploitation of the data you (re)use? If so, to what data do they relate and what restrictions are in place?

- No

NA

4. DOCUMENTATION AND METADATA

What documentation will be provided to enable reuse of the data collected/generated in this project?

1. For every protein construct, The genetic code, vector map and ORF will be stored into the benchling digital lab book. Using Altec label printer and QR barcoding system the sample will be labeled and linked to the digital data indicating storage location.
2. For every protein the full purification details will be written down in the digital lab notebook.
3. Crystallisation of relevant proteins, followed by diffraction and data solving will be performed. For every protein a folder will be created which contains all crystallographic data and meta data indicating the steps of processing. This progress will also be included into the digital lab book.
6. For every biophysical characterisation of protein interaction and inhibition a separate folder will be created per method (BLI ADPGLO, ...) which contains the raw observations (saved as .csv files) with meta data describing the experiments. The experimental details and analysis will also be included into the digital lab book.
7. For every 3D model a PDB file will be created stored within its own folder with a README file detailing the modelling procedure, as well as noted into a digital lab book
8. for every virtual screening. Docking or pharmacophore modelling experiment all results will be saved as mdb, pdb and sdf file formats in separate folders each containing README files detailing the modelling procedure, as well as noted into a digital lab book.
9. For every cell based assay a separate folder will be created per method (proliferation, migration, ...) which contains the raw observations (saved as .xlsx files) with meta data describing the experiments. The experimental details and analysis will also be included into the digital lab book.

10. RNAseq datasets will be deposited in the GEO EMBL databank, together with requested metadata.

Will a metadata standard be used? If so, describe in detail which standard will be used. If no, state in detail which metadata will be created to make the data easy/easier to find and reuse.

Yes, where possible otherwise own formats in README format will be made with sufficient explanation

5. DATA STORAGE AND BACKUP DURING THE FWO PROJECT

Where will the data be stored?

The data collected by the voetlab will be saved on the labs NAS

The data collected in the Van Lint lab will be stored as follows. Master copies of the data will be kept purely for archiving on our research unit central storage facility (K-Drive). Additional copies will be kept on J-Drive and on personal devices for data analysis.

How is backup of the data provided?

Double backed up in the cloud and NAS servers

The data of the Van Lint lab will be stored on the university's central servers (K-Drive and J-Drive) 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

Every project gets a dedicated NAS drive at the start of the project, and costs have been budgetted within the project.

Van Lint lab: within the dimensions of our project, the capacity of K-Drive and J-Drive can easily be adjusted according to our needs.

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

they have been budgetted within the awarded project.

Data security: how will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

The NAS drive works with secured directories only accessible to the administrator. Otherwise only the researcher working on this project get access. Others have no reading rights.

Van Lint lab: data will be stored at the university's secure drives until accepted for publication and at least 5 more years after publication. To have access to the data, prof Johan Van Lint will have to give authorisation to the K and J Drive to every member of the laboratory.

6. DATA PRESERVATION AFTER THE FWO PROJECT

Which data will be retained for the expected 5 year period after the end of the project? In case only a selection of the data can/will be preserved, clearly state the reasons for this (legal or contractual restrictions, physical preservation issues, ...).

All data will be retained, with exception of those that will be deposited online in dedicated databases upon publication. Those will no longer be stored at the laboratory

Van Lint lab: all data mentioned will be kept for 5 years on the archive drive of KU Leuven (KDrive). Lab notebooks will be kept for 10 years.

Where will the data be archived (= stored for the longer term)?

NAS drive

Van Lint lab: data will be stored on the university's central servers (K-Drive with automatic back-up procedures) for at least 5 years. If during these 5 years, data would become of interest, this can be prolonged to 10 years.

What are the expected costs for data preservation during the retention period of 5 years? How will the costs be covered?

The hardware has been budgetted as a onetime cost, including cloud based backup at a remote location.

For the cloud based data preservation

Van Lint lab: costs have been budgetted in the project.

7. DATA SHARING AND REUSE

Are there any factors restricting or preventing the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?

NO

Which data will be made available after the end of the project?

All, with the exception of those that are essential to preserve IP rights, for this we will consult LRD

Where/how will the data be made available for reuse?

In an Open Access repository

- 1) The source codes of virtual screening will be released on GitHub.
- 2) Structures will be deposited to the PDB database
- 3) other analysed data will be made available via data repositories. eg mendeley data.
- 4) other raw data is available upon request

When will the data be made available?

Upon publication of the results

Who will be able to access the data and under what conditions?

All data which do not limit our IP position will be made public without restrictions

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

All repositories to be used are free

8. RESPONSIBILITIES

Who will be responsible for data documentation & metadata?

During the course of the project the Phd students and or postdocs working on the project. The PI's will take frequent roles in ensuring correct preservation of the data related tot heir expertise. Following the end of the project, the PI's will be the responsible prerson

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Who bears the end responsibility for updating & implementing this DMP?

The PI's