
Lipid membrane, the missing piece in the puzzle of drug design: Integrated computational/experimental platform

A Data Management Plan created using DMPTuuli

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Project abstract:

The project is focussed on developing, combining and utilizing both computational and experimental techniques and protocols as tools for studying key interactions between lipid membranes, drugs and membrane proteins. Collective analysis of computational and experimental results of the influence of the interaction of the lipid membrane with either potential drug molecules or the protein reaches beyond the current paradigm in drug design to simply studying the "fit" of the drug candidate for the active site of the protein. This provides an entirely new avenue built on biophysical insight to unravel drug molecule selection criteria for the development of therapies for a wide range of diseases.

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Date of the Plan

25.9.2019

1. General Description of Data

The data from the project will consist of raw data files from experiments, experimental analysis data files, microscopy images, videos. Computational simulations will generate new and reuse existing scripts, molecular structures and topologies for performing computational simulations.

Raw measurement data files from experiments will be in ASCII and/or CSV format, experimental analysis data files will be available in ORG, OPJ and/or SPSS format and images will be stored in TIFF format. Digital video data files will be in MPEG-4 format. Scripts, molecular structures and topologies for computational simulations are in ASCII format, and data generated from computational simulations are in machine readable format.

2. Documentation and Quality

Raw measurement data files from experiments will be stored in ASCII and/or CSV format, experimental analysis data files will be available in ORG, OPJ and/or SPSS format and microscopy and other images will be stored in TIFF format. Possible digital video data files will be in MPEG-4 format. Scripts, molecular structures and topologies for computational simulations are stored in ASCII format. Results data from computer simulations will be stored in machine readable format which is generally used by the computer simulation field.

Consistency and quality of data is ensured by applying good laboratory practices in the research. Data will be version controlled and documented. Dates of data retrieval and changes will be recorded, making all data related actions traceable and repeatable.

3. Storage and Backup

All the data and information generated during the project will be regularly stored, collected and backed up on dedicated external hard-disks, as well as deposited on the IDA research data storage service produced by Finnish IT Centre for Science Ltd. (CSC).

Access to data will be controlled through the IDA research data storage service produced by the Finnish IT Centre for Science Ltd. (CSC). All the results in the project will be published according to open science guidelines. Therefore, there will be no sensitive data related to project.

4. Ethics and Legal Compliance

The research project has no ethical issues that concern data collection and research implementation.

Project results will be published according to University of Helsinki open science guidelines. New possible innovations will be first documented in invention disclosures sent to Helsinki Innovation services and then patented where applicable before publication. New innovations are also discussed

with relevant industrial stakeholders.

5. Data Sharing and Long-Term Preservation

All published and relevant data from the project will be openly available for other researchers either from the IDA research data storage, through depositing accepted manuscripts on HELDA - Digital Repository of the University of Helsinki or by request from the authors if results are not subject to patenting issues. When applicable, data generated by the project will also be deposited in various internet based open data repositories.

Long term data archival will be done using the CSC- Finnish IT Centre for Science Ltd IDA data-archival service. CSC is a non-profit, state-owned company administered by the Finnish Ministry of Education and Culture, and is the main provider for computational infrastructure for Finnish universities. Accepted manuscripts will additionally be deposited on HELDA - Digital Repository of the University of Helsinki.

Cost related to the data management for this project is considered to be low and the work and expertise for this will be covered by the Finnish IT Centre for Science Ltd. The typical fees for open access publications are included in the budget of the project.