

# Data Management Plan for the Focused library comprising bioisosteres of hydrolytic transition state of aspartic protease

Version 0

## Description

This Data Management Plan outlines the processes for collecting, storing, managing, and sharing data generated during the project titled "Focused Library Comprising Bioisosteres of Hydrolytic Transition State of Aspartic Protease – A Study on Novel Selective Antimalarial Drug Development."

The project integrates experimental and computational techniques, including computer-aided drug design (CADD), organic synthesis, and structural biology, to develop new inhibitors of plasmepsin V (plm V) for antimalarial drugs. The DMP will ensure that all research data is handled in accordance with FAIR principles (Findable, Accessible, Interoperable, and Reusable), promoting open access to scientific findings.

Key components of the DMP include:

**Data Collection:** Data generated from computational drug design, organic synthesis, enzymatic assays, and structural studies will be systematically collected and documented.

**Data Storage and Backup:** All data will be securely stored in institutional databases, and backed up regularly on secure servers provided by the Latvian Institute of Organic Synthesis (LIOS) to prevent data loss.

**Data Sharing:** Research data, including structural data (e.g., Protein Data Bank [PDB] entries) and experimental results, will be shared via public repositories such as Zenodo for general data, PDB for structural data, and GitHub for any software/code generated during the project. Open-access publishing will be pursued for scientific publications.

**Metadata and Documentation:** All datasets will be accompanied by comprehensive metadata describing experimental conditions, data formats, and methodologies to ensure reusability.

**Ethics and Intellectual Property:** The project will follow LIOS guidelines for intellectual property management, ensuring proper licensing and ethical considerations in data use.

**Data Retention:** Data will be stored for at least five years after the project's conclusion to allow for further use and validation.

This DMP aims to enhance research transparency, facilitate collaboration, and contribute to advancements in antimalarial drug discovery.

#### Funder

Central Finance and  
Contracting Agency

#### Grant

Focused library comprising  
bioisosteres of hydrolytic  
transition state of aspartic  
protease

#### Researchers

Marija Skvorcova (orcid:0009-0009-0081-426X)

#### Organizations

Latvian Institute of Organic Synthesis

# 1. Main Info

Title of DMP: Data Management Plan for the Focused library comprising bioisosteres of hydrolytic transition state of aspartic protease

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**Researchers:**

[Marija Skvorcova \(orcid:0009-0009-0081-426X\)](#)

**Organizations:**

[Latvian Institute of Organic Synthesis](#)

**Contact:** [Marija Skvorcova](#)

## 2. Funding

**Funding organizations:** [Central Finance and Contracting Agency](#)

Grants: Focused library comprising bioisosteres of hydrolytic transition state of aspartic protease

Project:

### 3. License

License:

Access Rights: [Public](#)

### 4. Templates

#### Descriptions

Focused library comprising bioisosteres of hydrolytic transition state of aspartic protease, supporting information

NMR data, general procedures, biological activity data

Template: [LCS FARP](#)

Type: [Dataset](#)

#### 1.1 Data Summary

##### 1.1.1 What is the purpose of the data collection/generation?

The purpose of the data collection is to identify and optimize inhibitors of plasmepsin V for the development of novel antimalarial drugs. Data will be generated through computational modeling, organic synthesis, and enzymatic assays to evaluate compound efficacy and selectivity. The results aim to contribute to advancements in antimalarial treatment and support future drug development projects.

##### 1.1.2 Type of data generated/collected

Experimental data

##### 1.1.3 Format of data generated/collected

pdf

1.1.4 Expected size of the data – give expected size and choose unit of measurement

18

MB

1.1.5 Are you re-using this data set?

No

## 2.1 Metadata and documentation

2.1.1 Will data be attributed with standard identification mechanism (e.g. persistent and unique identifiers such as Digital Object Identifiers – DOI)?

Yes

doi

2.1.2 Do you plan to provide metadata for your data?

Yes

2.1.3 Will you use any metadata standard?

No

2.1.4 Will search keywords be provided that optimize possibilities for re-use?

Yes

2.1.5 Will you follow any naming conventions for keywords?

Yes

2.1.6 Will you provide clear version numbers?

Yes

## 2.2 Making data openly accessible

2.2.1 What type of access the data generated/produced will have (choose one)?

open (anyone is able to access data without restrictions)

2.2.2 Will you apply embargo period to access for your data?

No

2.2.3 Will data, associated metadata, documentation and code be made accessible with means of a repository?

No

2.2.5 Will documentation about the software needed to access the data included?

No

2.2.6 Is it possible to include the relevant software (e.g. in open source code)?

No

## 2.3 Making data interoperable

2.3.1 Are the formats open to software applications and to recombination with different data sets?

No

2.3.2 Will you use data standard vocabulary/taxonomy to make your data interoperable?

Yes

## 2.4 Increase data re-use

2.4.2 Are the data usable by third parties, in particular after the end of the project?

No

2.4.5 Are data quality assurance processes provided?

Yes

## 3.1 Allocation of resources

3.1.1 How will costs be covered for making data FAIR during project realization?

Euro

3.1.2 Who will be responsible for data management in your project?

Marija Skvorcova (orcid:0009-0009-0081-426X)

3.1.3 How will costs be covered for making data FAIR after project realization?

Euro



## 3.2 Data security

### 3.2.1 What security measures will be used for data security?

Physical access control

## 3.3 Ethical aspects

### 3.3.1 Are there any ethical or legal issues that could have an impact on data collection and sharing?

No

### 3.3.2 Have you got/will you get permission from ethics committee to collect and process data (if applicable)?

No

### 3.3.3 Is informed consent for data sharing and long term preservation included in questionnaires dealing with personal data, if applicable?

No

### 3.3.4 Will data collected/generated include personal data/ sensitive information?

No

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