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## Plan Overview

*A Data Management Plan created using DMPonline*

**Title:** Resolving non-equilibrium biomolecular transitions with coherent X-rays

**Creator:** Foivos Perakis

**Affiliation:** Stockholm University

**Funder:** Swedish Research Council

**Template:** Swedish Research Council Template

### Project abstract:

The environment inside a cell is highly crowded, which can alter drastically the behaviour of macromolecular in solution. Such crowding effects can induce the formation of biomolecular condensates, which are liquid-like membrane-less droplets. Despite the general occurrence of biomolecular condensates, the physical mechanism governing the early stages of their formation is still debated. Here, a novel approach is proposed for probing and controlling the early stages of biomolecular condensation using microdroplet reactors. The proposed research aims to provide new exciting experimental insights towards a general framework that predicts and explains the phase behavior of macromolecules. The project's timing is ideal as it utilizes diffraction-limited storage rings (DLSRs) and X-ray free electron lasers (XFELs), which are supported by the Swedish Research Council. The strength of the proposed coherent X-ray techniques is that they allow to capture non-equilibrium structural dynamics at unprecedented resolution, reaching protein molecular level sensitivity and sub-microsecond timescales. The proposed investigations not only train new scientists but also contribute to Sweden's long-term competitiveness in X-ray science. Resolving and controlling the biomolecular condensation mechanism is essential for understanding cellular function, as well as for treating aggregation diseases and facilitate the formulation of future protein-based drugs and materials.

**ID:** 140829

**Start date:** 01-01-2024

**End date:** 31-12-2027

**Last modified:** 12-06-2025

**Grant number / URL:** 2023-05339

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# Resolving non-equilibrium biomolecular transitions with coherent X-rays

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## General Information

### Project Title

Resolving non-equilibrium biomolecular transitions with coherent X-rays

### Project Leader

Foivos Perakis

### Registration number/corresponding

2023-05339

### Version

version 1

### Date

2023-12-20

## Description of data - reuse of existing data and/or production of new data

### How will data be collected, created or reused?

Data from publications will be posted on public repositories like figshare and linked to the papers. Raw data are available by the facilities typically with an associated DOI.

### What types of data will be created and/or collected, in terms of data format and amount/volume of data?

Data at large scale facilities with a standard format that is used in each case. The publication data will be saved in ascii or xvg format.

## **Documentation and data quality**

**How will the material be documented and described, with associated metadata relating to structure, standards and format for descriptions of the content, collection method, etc.?**

For the data analysis we use github repositories and for the metadata are all included in the figshare repositories.

**How will data quality be safeguarded and documented (for example repeated measurements, validation of data input, etc.)?**

Reproducibility is a typical tests performed as part of the initial stages of each measumernt in order to check the systematic sources of error. Procedures are documented at the elogs and data analysis is stored at github where one can track any changes in the history.

## **Storage and backup**

**How is storage and backup of data and metadata safeguarded during the research process?**

Data produced at X-ray facilities are backed up by them. Data generatated at fysikum are backed up at the the fysikum servers.

**How is data security and controlled access to data safeguarded, in relation to the handling of sensitive data and personal data, for example?**

Facilities required user accounts for access and are responsible for the security. For the fysikum data we also required SU accoutns and VPN is also available.

## **Legal and ethical aspects**

**How is data handling according to legal requirements safeguarded, e.g. in terms of handling of personal data, confidentiality and intellectual property rights?**

No ethical issues are raised here.

### **How is correct data handling according to ethical aspects safeguarded?**

No ethical issues are raised here.

### **Accessibility and long-term storage**

#### **How, when and where will research data or information about data (metadata) be made accessible? Are there any conditions, embargoes and limitations on the access to and reuse of data to be considered?**

Data from publications will be posted on public repositories like figshare and linked to the papers. Raw data are available by the facilities typically with an associated DOI.

#### **In what way is long-term storage safeguarded, and by whom? How will the selection of data for long-term storage be made?**

Data from publications will be posted on public repositories like figshare and linked to the papers. Raw data are available by the facilities typically with an associated DOI.

#### **Will specific systems, software, source code or other types of services be necessary in order to understand, partake of or use/analyse data in the long term?**

We use python based code and github repo. The published data are saved in ascii files which can be opened by any text editor.

#### **How will the use of unique and persistent identifiers, such as a Digital Object Identifier (DOI), be safeguarded?**

Data from publications will be posted on public repositories like figshare including DOI and linked to the papers. Raw data are available by the facilities typically with an associated DOI.

### **Responsibility and resources**

#### **Who is responsible for data management and (possibly) supports the work with this while the research project is in progress? Who is responsible for data management, ongoing management and long-term storage after the research project has ended?**

Data from publications will be posted on public repositories like figshare and linked to the papers. Raw data are available by the facilities typically with an associated DOI.

**What resources (costs, labour input or other) will be required for data management (including storage, back-up, provision of access and processing for long-term storage)?  
What resources will be needed to ensure that data fulfil the FAIR principles?**

Data from publications will be posted on public repositories like figshare and linked to the papers. Raw data are available by the facilities typically with an associated DOI.