Plan Overview

A Data Management Plan created using DMPonline

Title: GLYCOVID-19: Heparin as a versatile intervention for COVID-19 disease management

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Funder: UKRI Future Leaders Fellowships

Template: UKRI Template

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Project abstract:

Heparin, the second most widely-used drug by weight globally, is formulated as a polydisperse, heterogenous natural product. Unfractionated heparin, low molecular weight heparins and heparinoids are clinically approved as anticoagulants/thrombotics with excellent safety, stability, bioavailability and pharmacokinetic profiles alongside possessing broadspectrum activity against a multitude of distinct viruses, including previous SARS-associated coronavirus and SARS-CoV-2 alongside a significant anti-inflammatory property. Furthermore, our research has demonstrated the heparins bind to Spike 1 RBD of SARS-CoV-2 with highaffinity, inducing conformational changes and stabilizing it. Crucially, heparin possesses key pharmacological activities which are relevant to treatment of COVID-19, and growing evidence shows that coagulopathy and the 'cytokine storm' are associated with high mortality rates in COVID-19 patients. Consequently, repurposing heparins as a rapid emergency medicine is an attractive, feasible and timely strategy. Additionally, these useful activities are present in different components of the complex mixture that constitutes heparin, which allows fractionation and identification components with the activities required at different stages of COVID-19 disease, so allowing better-focussed treatments and minimising off-target effects.

ID: 57679

Last modified: 28-05-2020

Grant number / URL: N/A

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GLYCOVID-19: Heparin as a versatile intervention for COVID-19 disease management

0. Proposal name

0. Enter the proposal name

GLYCOVID-19: Heparin as a versatile intervention for COVID-19 disease management

1. Description of the data

1.1 Type of study

NMR study of natural and synthetic heparins and their interactions with Spike 1 protein receptor binding domain from SARS-CoV-2

1.2 Types of data

NMR FIDS and spectra, and associated metadata

1.3 Format and scale of the data

Bruker format NMR data (directories), processed in Topspin.

2. Data collection / generation

2.1 Methodologies for data collection / generation

1H and 13C NMR spectra will be collected using the MIB NMR spectrometers on samples, identified in the directory naming, and with meta data recorded in the title file

2.2 Data quality and standards

Referencing will be to recognised standards, i.e TSP, TMS or DSS depending on interactions with compounds. Quantitation is not standard, but can be done with reference to Malate standards. NMR

spectrometers are checked for consistency regularly

3. Data management, documentation and curation

3.1 Managing, storing and curating data

Data are stored initially on the spectrometer PC, and then mirrored onto UoM Research Data Storage (hourly). Metadata are collected into searchable database. Published data will be converted to NEF format where appropriate.

3.2 Metadata standards and data documentation

Sample components, concentration, solvent, referencing, temperature, originator.

3.3 Data preservation strategy and standards

Standard for UoM IT research data storage

4. Data security and confidentiality of potentially disclosive information

4.1 Formal information/data security standards

Data will be stored on UoM research data storage and backed-up according to UoM policy (snapped and replicated). Original data is recorded on disks with internal IPs only and firewalled so that only a handful of computers have access.

4.2 Main risks to data security

Unauthorised access, loss of back-up (although snapped and replicated). UoM IT services manage this risk

5. Data sharing and access

5.1 Suitability for sharing

Although suitable for sharing, NMR data is not currently shared by a formal mechanism. Only standard methods will be applied. Samples may be shared, but managed by University of Keele for this project.

5.2 Discovery by potential users of the research/innovation data

NMR data can be discovered through the literature and by request to the authors. Carbohydrate NMR does not yet have a sharing standard, but the community is working to address this to approach the standards of protein and metabolomics NMR Databases. Frequently publications will have Menderley data archives associated with them.

5.3 Governance of access

PI and/or NMR facility manager will decide on access to data, and continuity of access will be managed by the University of Keele.

5.4 The study team's exclusive use of the data

Data will be available on publication

5.5 Restrictions or delays to sharing, with planned actions to limit such restrictions

There is no restriction on data sharing except that imposed by publication in scientific journals, which often require exclusivity.

5.6 Regulation of responsibilities of users

External users will not be bound by formal data sharing agreements

6. Responsibilities

6. Responsibilities

Researchers are responible for metadata creation and quality assurance data. Research Facility Manager is responsible for quality assurance, and data security (along with UoM RDS)

7. Relevant policies

7. Relevant institutional, departmental or study policies on data sharing and data security

Policy	URL or Reference
Data Management Policy & Procedures	http://documents.manchester.ac.uk/Doculnfo.aspx? DocID=33802%20
Data Security Policy	http://documents.manchester.ac.uk/display.aspx?DocID=14914
Data Sharing Policy	http://documents.manchester.ac.uk/Doculnfo.aspx? DocID=33802%20
Institutional Information Policy	http://documents.manchester.ac.uk/display.aspx?DocID=24420
Other	http://www.itservices.manchester.ac.uk/our- services/security/policy/
Other	http://documents.manchester.ac.uk/display.aspx?DocID=14916
	http://documents.manchester.ac.uk/display.aspx?DocID=28526
	http://documents.manchester.ac.uk/display.aspx?DocID=24420

8. Author and contact details

8. Author of this Data Management Plan (Name) and, if different to that of the Principal Investigator, their telephone & email contact details

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Created using DMPonline. Last modified 28 May 2020