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

A Data Management Plan created using DMPonline

Creators: Matthew Cliff, Robert Field

Affiliation: University of Manchester

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ORCID iD: 0000-0002-0287-5594

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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 broad-spectrum 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 high-affinity, 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.

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0. Proposal name

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1. Description of the data

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

NMR FIDS and spectra, and associated metadata

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

2. 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

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

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.

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

Standard for UoM IT research data storage

4. Data security and confidentiality of potentially disclosive information

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.

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

5. Data sharing and access

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.

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 Mendeley data archives associated with them.

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

Data will be available on publication

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

External users will not be bound by formal data sharing agreements

6. Responsibilities

Researchers are responsible 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

Policy	URL or Reference
Data Management Policy & Procedures	http://documents.manchester.ac.uk/DocuInfo.aspx?DocID=33802%20
Data Security Policy	http://documents.manchester.ac.uk/display.aspx?DocID=14914
Data Sharing Policy	http://documents.manchester.ac.uk/DocuInfo.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

Matthew Cliff
matthew.cliff@manchester.ac.uk
0161 3065179

