Project Name: Synthetic Chemistry / EPSRC example

Description: This research project involves the development of a new chemical reaction for incorporating [your atom of choice] into [your molecule / compound of interest]. An experimental procedure will be developed that will allow the preparation of a range of compounds.

Funder: Engineering and Physical Sciences Research Council

Institution: University of Glasgow

Data Collection

What data will you collect or create?
The data produced from this work will fall into two categories:

1. The various reaction parameters required for optimisation of the chemical transformation.
2. The spectroscopic and general characterisation data of all compounds produced during the work.

I anticipate that the data produced in category 1 will amount to approximately Z MB and the data produced in category 2 will be in the range of X - Y GB.

How will the data be collected or created?
The reaction conditions will be recorded and collated using Excel spreadsheets and named according to each generation of reaction.
The various experimental procedures and associated compound characterisation will be written up using the Royal Society of Chemistry standard formatting in a Word document. The associated NMR spectra will be collated in chronological order in a .pdf document.

These are standard practices for synthetic methodology projects.

Documentation and Metadata

What documentation and metadata will accompany the data?
The data will be accompanied by the following contextual documentation, according to standard practice for synthetic methodology projects:

1. spreadsheet documents which detail the reaction conditions.
2. text files which detail the experimental procedures and compound characterisation.

Files and folders will be named according to a pre-agreed convention.
The final dataset as deposited in the institutional data repository will also be accompanied by a README file listing the contents of the other files and outlining the file-naming convention used.

Ethics and Legal Compliance

How will you manage any ethical issues?
There are no ethical issues in the generation of results from a synthetic methodology project. There are no human subject or samples involved.

**How will you manage copyright and Intellectual Property Rights (IPR) issues?**

This project is being carried out in collaboration with an industrial partner. The intellectual property rights are set out in the collaboration agreement. The intellectual property generated from this project will be fully exploited with help from the University of Glasgow’s IP and Commercialisation Office. The aim is to patent the final procedure and then publish the work in a research journal.

**Storage and Backup**

**How will the data be stored and backed up during the research?**

The data will be stored on hard-drives belonging to the researchers involved in the work. These hard-drives are backed up onto the School of Chemistry’s local servers.

**How will you manage access and security?**

Files created during this project will be encrypted so that only the PI and researcher will be able to access them. Data will be transferred between the PI and researcher on memory storage devices rather than by email.

**Selection and Preservation**

**Which data are of long-term value and should be retained, shared, and/or preserved?**

Any data from this research which underpin or contribute to our patent application or subsequent research publications will be considered to be of long-term value and will be retained and preserved. These data would be suitable for sharing only once the intellectual property is protected by a patent.

**What is the long-term preservation plan for the dataset?**

Data which underpin our patent application and research publications will be stored on the School of Chemistry’s server.

The dataset will also be deposited in Enlighten: Research Data, the University of Glasgow’s institutional data repository. Data in the repository will be stored in accordance with funder and University data policies. Files deposited in Enlighten: Research Data will be given a Digital Object Identifier (DOI) and the associated metadata will be listed in the University of Glasgow Research Data Registry and the DataCite metadata store. The retention schedule for data in Enlighten: Research Data will be 10 years from date of deposition in the first instance, with extensions applied to datasets which are subsequently accessed. This complies with both University of Glasgow guidance and EPSRC policy.

Enlighten: Research Data is backed by commercial digital storage with is audited on a twice-yearly basis for compliance with the ISO27001 Information Security Management standard.

**Data Sharing**
How will you share the data?

If the research is successful, the research will be protected by the filing of a patent. Following this, the research will be disseminated by the publication of an open-access manuscript in a chemical journal. The manuscript will be deposited in our institutional publication repository, Enlighten: Publications. The manuscript will contain a data citation indicating where and on what terms the data can be accessed.

The data which underpins the publication and patent will be made available for sharing via Enlighten: Research Data, the University of Glasgow's Data Repository. This will be available at the time of publication of the corresponding manuscript.

Data in the repository will be issued with a Digital Object Identifier (DOI). This can be included as part of a data citation in publications, allowing the datasets underpinning a publication to be identified and accessed. DOIs will also be linked with appropriate records in Enlighten: Publications, the University's publication repository, to enhance visibility of datasets.

Metadata about datasets held in the Institutional repository will be publicly searchable and discoverable and will indicate how and on what terms the dataset can be accessed.

Information about datasets from the repository will be displayed on researcher profile pages on the University of Glasgow webpages which will also increase the visibility of the datasets.

Are any restrictions on data sharing required?

After the patent is filed to protect the intellectual property, there will be no restrictions on data sharing. The PI will actively disseminate the results as widely as possible.

Responsibilities and Resources

Who will be responsible for data management?

The PI will be ultimately responsible for data management of this project. The researcher will be responsible for organisation and storage of the data as it is produced during the project. The School of Chemistry's IT staff will manage the school's server, where the data will be stored. The University's library staff will be responsible for management of the institutional repositories, Enlighten: Publications and Enlighten: Research Data.

What resources will you require to deliver your plan?

The researcher already has the required software to implement the data collection plan. Funds to cover final deposit of the dataset in the institutional repository have been costed into the grant application as advised by the Research Data Management Service. Funds to support open access publication of the research are available from the institutional RCUK fund for this purpose.