Data management

The drivers and aims for data management at HWB•NMR are outlined, including responsibilities of users and staff.

Key Drivers

- Scientific data must be recognised as having a potential value that may exceed publications immediately derived from it. Data underpinning a publication are rarely published, yet may increase in value over time, and remain capable of generating further research or be required for re-analysis.
- The quality and availability of administrative data is crucial to the running of all scientific projects.
- It is incumbent upon HWB•NMR and its users to provide adequate Quality Assurance to satisfy funding bodies of our ability to deliver the promised scientific results. Data Management forms an important part of our commitment to Quality Assurance and Risk Management.
- Scientific projects and data, as well as administrative processes and data, are subject to auditing by funding bodies or other external organisations.
- Data may be shared with other organisations or made publicly available.
- The Research Council's Statement on Safeguarding Good Scientific Practice outlines a requirement for data management and the need of users to keep research data for at least 10 years.
- The Research Council's Joint Code of Practice for Research outlines a requirement for adequate and auditable documentation of scientific records and materials.
- Legislation such as the Data Protection Act and the Regulation of Investigatory Powers Act.
- Intellectual property must be protectable.
- Maintaining the excellence of HWB•NMR's science and international reputation.

Broad aims

- To ensure that data management solutions are driven by the needs of HWB•NMR's scientific mission, and support the needs of HWB•NMR staff.
- To ensure that data are appropriately identified, managed, protected and accessible, taking into account HWB•NMR and sponsor requirements, as well as Intellectual Property issues and current legislation.
- To provide and support professional quality data storage and information management systems, keeping pace with evolving requirements and technological change.

Data is categorized as being either scientific (i.e. related to NMR spectra or samples) or administrative (i.e. financial, personnel, management, or computer systems related).

Administrative data is joined-up with the University's administrative services and reporting structures to ensure efficient communication, seamless operation and professional standards.

Administrative Data Aims

1. To encourage "seamless/joined-up" administrative services.
2. To ensure that solutions are cost effective and maximise HWB•NMR's return on investment.
3. To ensure that administrative systems are responsive to the needs of the HWB•NMR user community.
4. To ensure that systems are planned, developed and implemented in a professional and timely manner, and ensuring that risks are understood.
5. To ensure that administrative data is available to all who require it (confidentiality and Data Protection Act permitting).
6. To ensure that administrative systems and data are well managed and supported.
7. To work with and implement the University's Information Services strategy.
8. Plan ahead on a HWB•NMR-wide scale for predicted data storage and management requirements.

Scientific Data Aims (generally refers to the NMR spectra of experimental NMR samples and derived data), **are curated by and are the responsibility of the individual users**:

1. To extract maximum value from the data for scientific benefit.
2. To index/catalogue and annotate such data, as appropriate.
3. To access HWB•NMR data management facilities and storage devices for their own scientific data.
4. To store acquired and processed experimental data for 10 years.
5. To manage risks to their own data, including loss through disaster or corruption, alteration to the data, either intentional or accidental, and to protect their intellectual property.
6. It should be possible to locate spectra relating to samples from a reference in the researcher's laboratory notebook. The data should be referenced to locate the laboratory notebook and page where the sample is described.
7. To ensure that, where possible, the protocols and methods relevant to spectral data collection and processing can be located.
8. To create online databases/catalogues, visible to HWB•NMR and the public where appropriate.
9. Where available, community standards for metadata should be adopted.
10. Stored metadata should include details of sample: originator name, data capture system (including hardware and software versions), sample contents and date, in a standardised searchable data-structure.
11. Where possible data and metadata will be presented in a commonly agreed format that can be accessed from elsewhere in HWB•NMR and, where appropriate, it will be made publicly available.
12. HWB•NMR will provide guidance and mechanisms, where required, to reduce data sets to a form that can be stored online, transferred and/or archived at reasonable cost, e.g. by data compression. It must be possible to adequately reconstruct original data from the compressed form.

Notes

- Handling of samples and materials: **All samples and other experimental materials should be labelled** (clearly, accurately, uniquely and durably), and retained

for a period to be agreed by the Funding Body. The storage and handling of the samples and materials should be as specified in the project plan (or proposal), and must be appropriate to their nature. If the storage conditions are critical, they must be monitored and recorded. Samples must be readily tracked through the stages of analysis or use, and have designated disposal routes and dates.

- Definition of IP: **"Intellectual Property"** means any concept, discovery, invention, process, procedure, development or improvement in process or procedure; and any data, design, formula, model, plans, drawings, documentation, database, computer program or software (including related preparatory and design materials) whether registrable or not and whether or not copyright or design rights subsist in it; and any idea, method, information or know-how which is made, discovered, created or generated by [you/a researcher at HWB•NMR/visiting worker/employee etc] whether alone or with others in the course of your [employment/visit/period at HWB•NMR].