

A Proposed Standard for Describing NMR-Based Metabolomics Experiments

Helen Jenkins

University of Wales, Aberystwyth

Denis Rubtsov

Cambridge University

The Group

- Cambridge:
 - Jules Griffen
 - Denis Rubtsov
- Aberystwyth:
 - Nigel Hardy
 - Helen Jenkins
- Birmingham:
 - Mark Viant
 - Christian Ludwig
 - John Easton
 - Ulrich Guenther

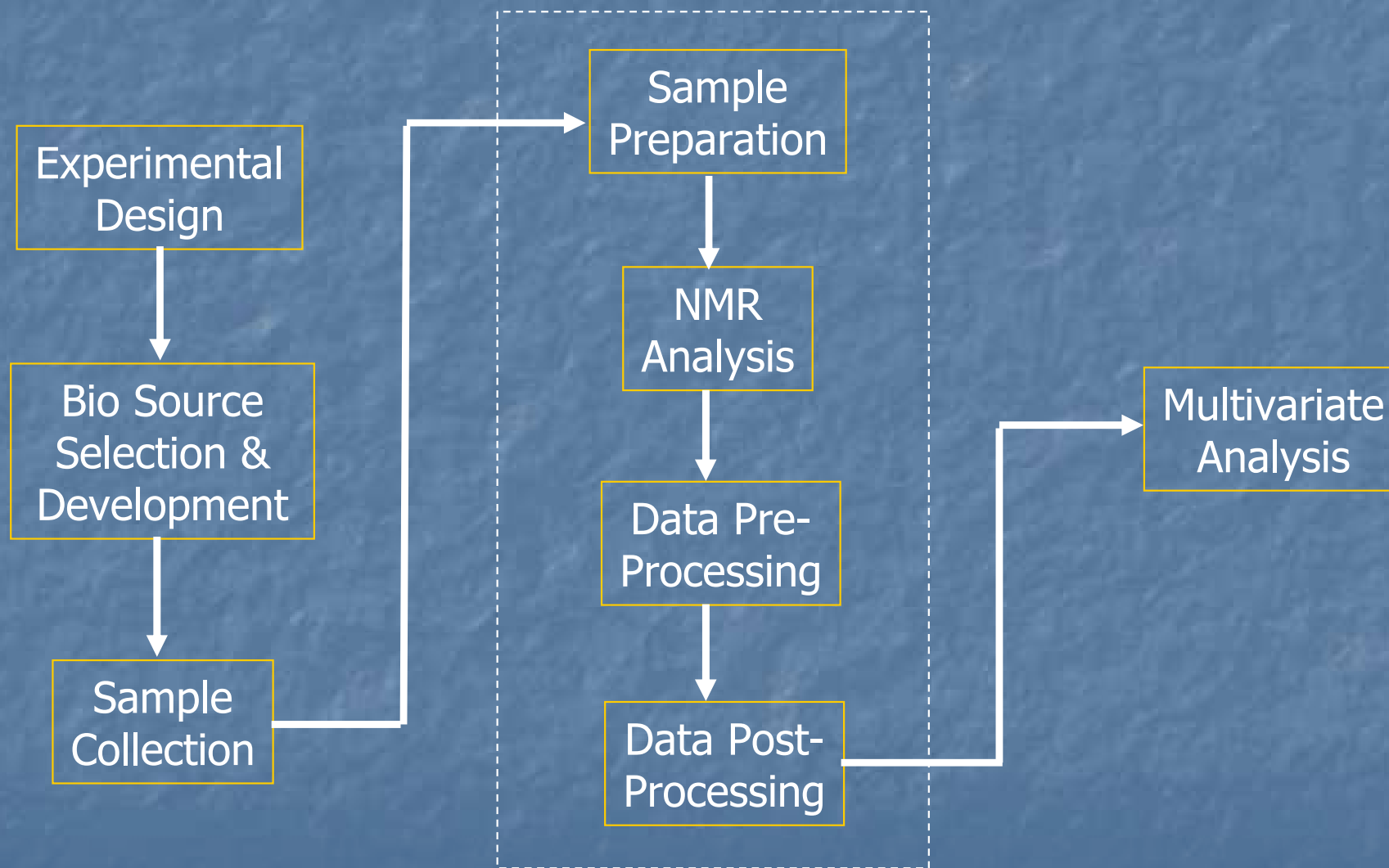
Our Aim

- To specify reporting requirements for NMR-based metabolomics experiments that provide datasets that are sufficient for third party interpretation.

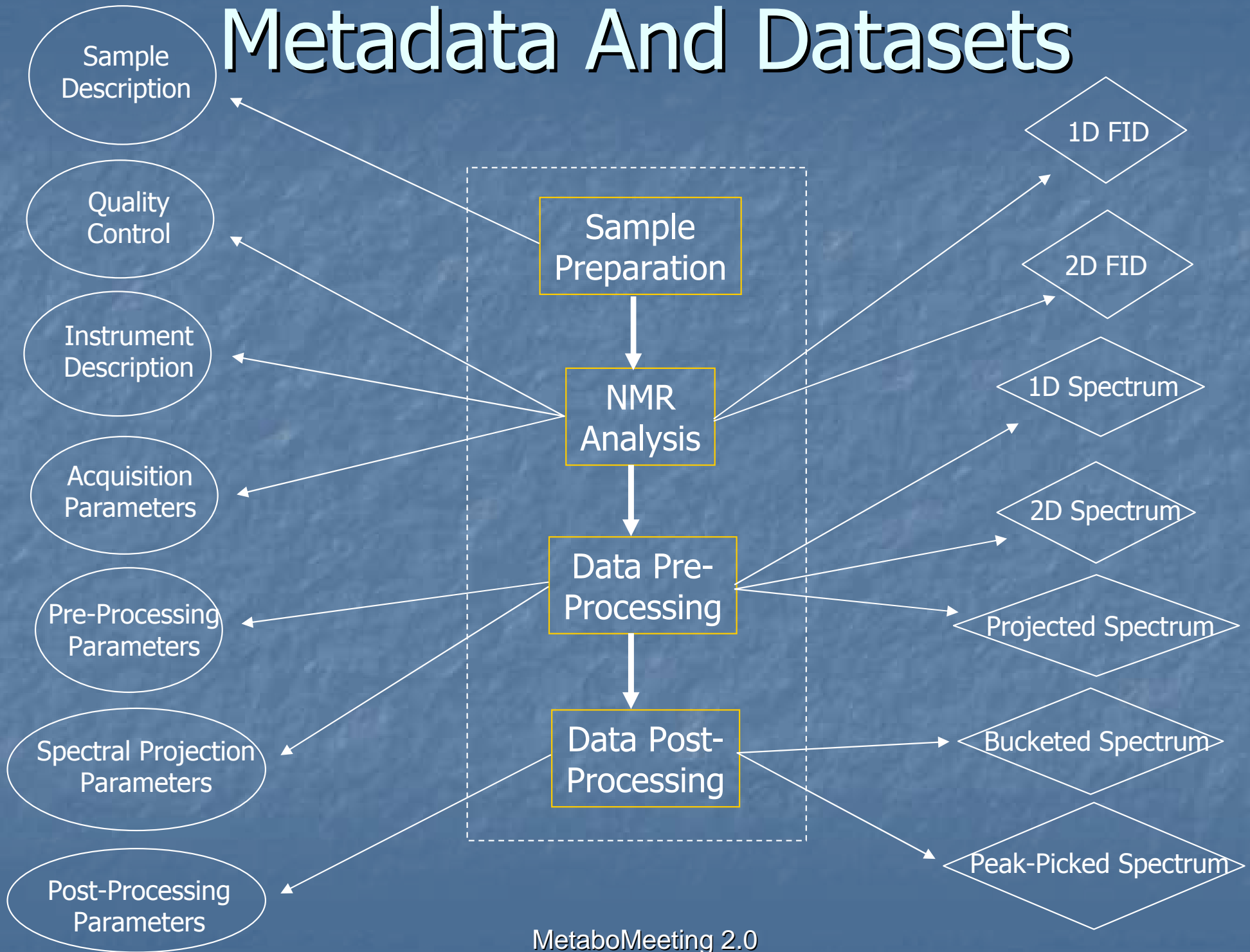
How Far Have We Got?

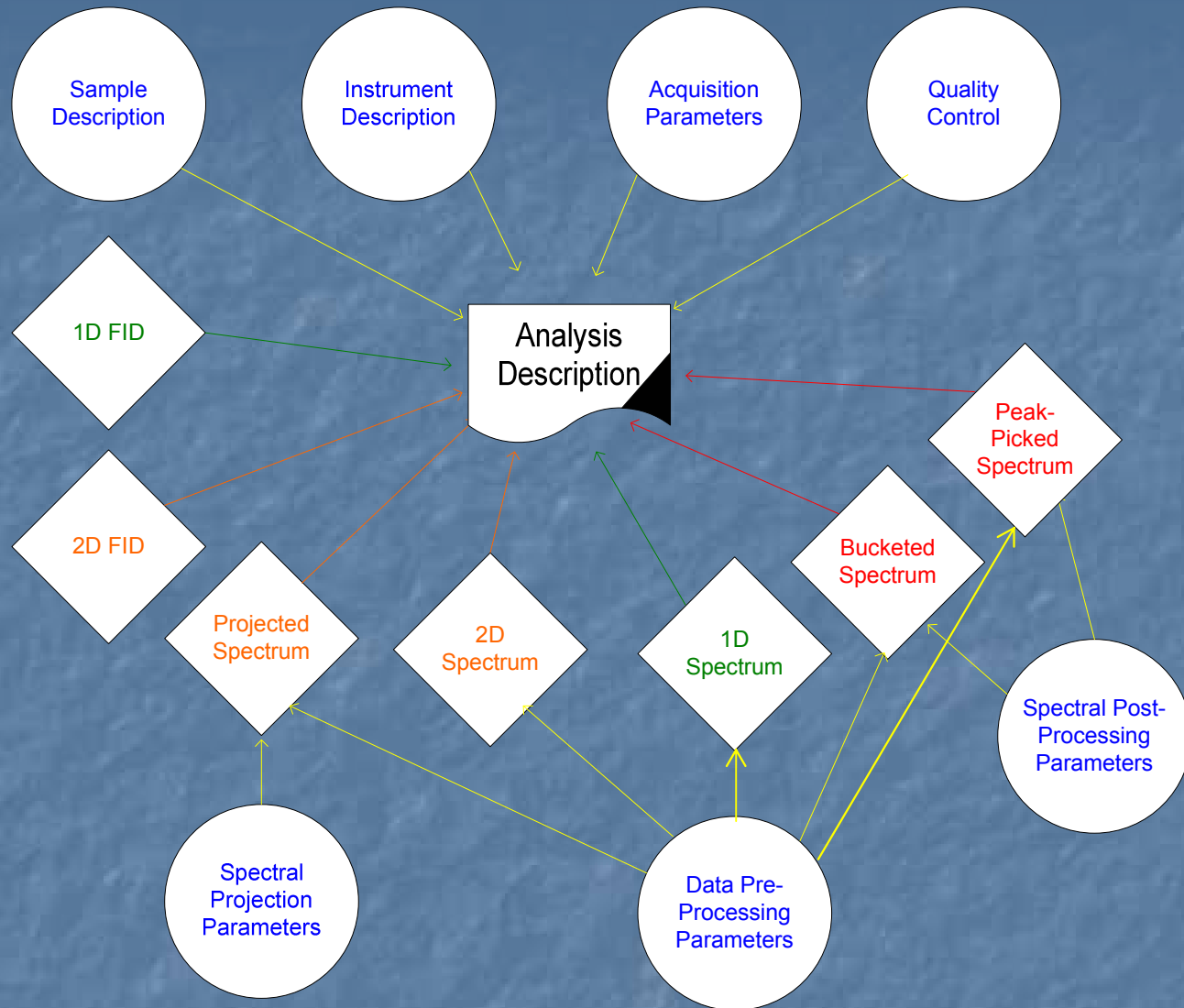
- We have produced:
 - A text document that describes the proposed standard.
 - A draft UML data model.
 - A draft XML implementation of the UML.
 - An almost draft version of an ontology of the terms used in the standard document.

NMR-Based Metabolomics Work Flow



Metadata And Datasets





Controlled Vocabularies

- The standard specifies some initial vocabularies of the valid values for particular fields.
- In the XML we implemented these as separate schemas containing types that enumerate the valid values.
 - Following this approach, no definition or authority information for the terms is available.
 - Possible improvement: The namespaces for these schemas could be Life Science Identifiers that resolve to ontologies/vocabularies containing the extra information.

Where Are We Going?

- Dissemination of the current version of the standard to interested practitioners and others for feedback.
- Comparison with data models from existing initiatives.
- Consultation with the metabolomics society standardisation initiative.