

# A Proposed Standard for Describing NMR-Based Metabolomics Experiments

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# The Group

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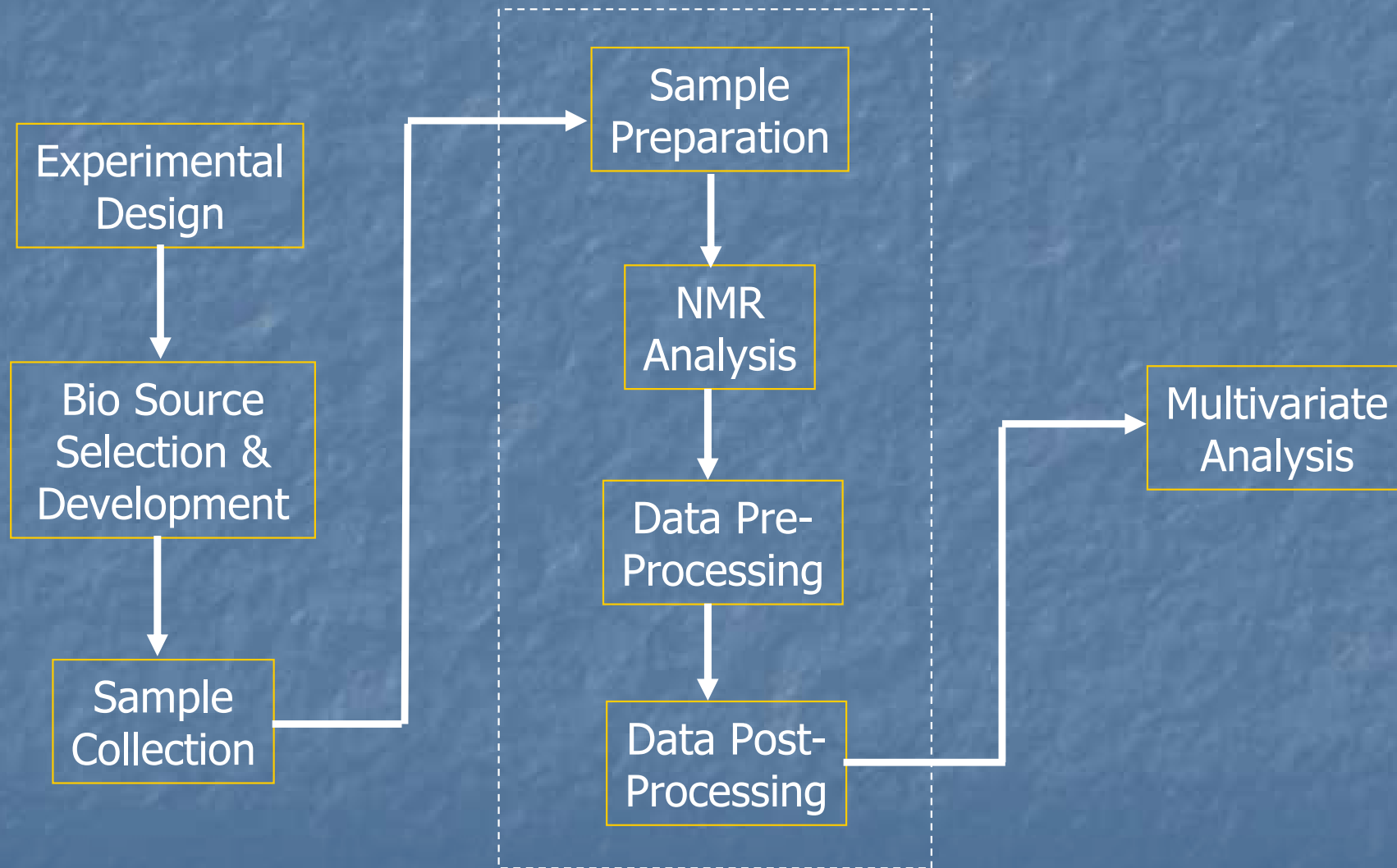
# Our Aim

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

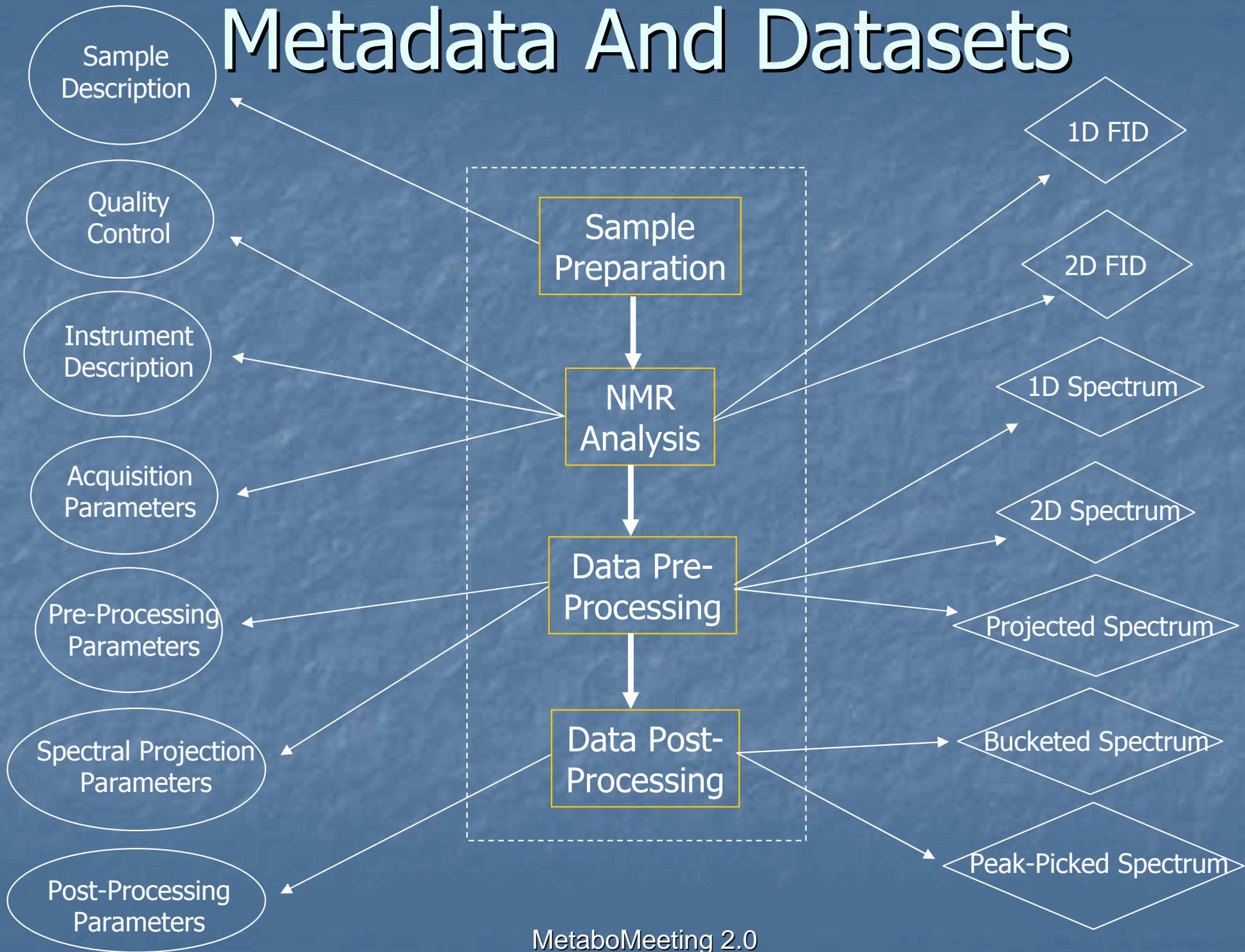
# How Far Have We Got?

- 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.