AnIML Requirements Document

Agreed Principles

- AnIML files will be XML
- ANDI and JCAMP-DX files must be able to migrate to AnIML files with no loss of information
- Technique Phase 1
  - Infrared Spectroscopy
  - Nuclear Magnetic resonance Spectrometry
  - UV/Vis
  - Mass Spectrometry
  - Chromatography
  - Ion Mobility Spectrometry
- Techniques Phase 2
  - Electron Magnetic Resonance
  - Near Infrared Spectrometry
  - Crystallography
- Techniques Phase 3
  - Chemometrics
- Support for Hyphenated Techniques
- Support for Rack/High Throughput Experiments
- Extensible
- Technique Definitions are independent from one-another

Archiving

- Core information to be agreed as applicable to all instruments of a particular technique
- Agreed Data Dictionaries for Core Techniques - all that is required to allow compete interpretation of data sets
- Agreed method of adding vendor/instrument specific content not covered by Core.
- Hardware/Software/Operating System Independent
- Migration for a Vendor Specific format to AnIML must be possible without loss of information
- Long-term stable
- Human Readable

Reprocessing

- Agreed Data Dictionaries for metadata that are required to allow complete interpretation and re-processing of data sets
- Mechanism to identify Raw and processed data
- AnIML must allow software which only recognizes certain techniques to read and process those technique sections.

Compliance

- e.g. 21CFRpart11 Compliance Ready
  - Digital Signatures
  - Audit Trails