The Path to the New ASTM AnIML Standard

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David Martinsen
American Chemical Society

ASTM Committee Structure

ASTM

- ASTM E13: Molecular Spectroscopy and Separation Science
  - ASTM E13.15: Analytical Data

IUPAC: JCAMP-DX

The International Union of Pure and Applied Chemistry

- Committee on Printed and Electronic Publications
  - Subcommittee on Electronic Data Standards (SEDS)
    - Responsible for JCAMP-DX
    - A number of members of SEDS have been involved in the development of AnIML
    - JCAMP-DX: One of the sources for the data dictionary for AnIML

AnIML Timeline

- September 10-11, 2002: exploratory group meeting at Shimadzu, Columbia, MD
- October 15, 2002: Group meeting in Providence, RI
- March 11, 2003: ASTM E13.15 set up at Pittcon/Orlando
- April 23-24, 2003: First meeting of AnIML Working Group at ASTM Headquarters

Precursors to AnIML

- JCAMP-DX
- ANDI – in 2003, the ANDI committee (E01.25) voted to disband, and become part of E13.15
- GAML – ThermoElectron
- SpectroML – NIST

AnIML Committee Structure

- The Working Group
  - Meets at least once per month, usually in virtual meetings
  - Discuss progress on the standard
  - Address questions raised by the other groups
- The Core Group
  - Meets at least once per month
  - Works on development of and modifications to the Schemas
  - Develops examples of AnIML data files for different techniques

AnIML Committee Structure

- The Technique Expert Groups
  - Made up of experts in techniques from other ASTM E13 committees, and others – from vendors, and from the academic, corporate and government communities
  - Develop technique definition files for specific techniques
  - Initial techniques targeted:
    - NMR
    - IR
    - Chromatography
    - UV/VIS
    - MS
    - IMS

The AnIML Standard Specifications

- ASTM Standard Specification for AnIML
  - Specification for AnIML Schema
  - Specification for the Technique Schema
  - General Specification for Technique Documents

The AnIML Standard Guides

- ASTM Standard Guide to Practice for AnIML
  - How to Implement AnIML
  - How to Use AnIML
  - How to Extend AnIML Technique Documents
  - How to Create a Technique Document for an Additional Technique

AnIML Naming and Design Rules

- A new document has recently been added to cover Naming and Design Rules (NDR).
- These rules provide a consistent environment for naming XML tags, version numbering, global vs. local variables, etc.
- The NDRs provide a more readable XML standard.
- The NDRs can be verified algorithmically, providing for an automated mechanism to confirm compliance.

AnIML File Deliverables

- The Core Schema
- The Technique Schema
- Technique Definition Files for the following techniques:
  - NMR
  - UV/Vis
  - IR
  - MS
  - Chromatography
  - IMS
- Examples of AnIML Data Files for each of the techniques
- Tools

The ASTM Standards Process

- The ASTM standards process is quite straightforward:
  - Each standard document is ballotted by the subcommittee (E13.15)
  - Each document is presented to the main committee (E13) and the Society for approval

The ASTM Standards Process: Negative Votes

- The process can become complex when handling negative votes during the subcommittee process, primarily, but also in the main committee process.
- Negative votes can:
  - Result in a change to the standard, making the standard better
  - Be resolved through negotiation with the voter, with the negative vote being withdrawn
  - Be ruled as non-persuasive

Maintenance of the Standard

- Normally, ASTM Standards must be reviewed every 5 years
- We anticipate AnIML require more frequent attention:
  - As the community begins to use AnIML, difficulties may appear in practice which need to be addressed more quickly
  - As AnIML is extended to new techniques, it may be advantageous to incorporate these some new feature, or even the entire new techniques, as standards

Where We Are

- The Core Group is nearing completion of the Core Schema and the Technique Schema
- Initial drafts of Technique Definition Files have been completed for UV/Vis, IR, and Chromatography.
- Some tools have been developed:
  - Encoder/decoder for AnIML data (base64 binary)
  - Generic viewers
  - A technique validator
  - JCAMP-DX to AnIML converter

What We Have Left

- Finalize the core and technique schemas.
- Examine the draft technique definition files with the expert groups, for comment and, most likely, revision.
- Create Standards documents.
- With ASTM, establish permanent locations for the XML files.
  - Unlike other ASTM standards, these files need to be openly available at the time-of-use

Getting Involved in the Process

- It’s not too late: You can help!
- See http://animl.sourceforge.net for details