
Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

Minutes for E13.15 Subcommittee Working Group

10:39 am – 12:12 pm EDT

Friday, July 7, 2005

Virtual Meeting

I. Introductions and Welcome: Gary Kramer, NIST, E13.15 Chair at 10:39 am EDT

II. Review of Agenda. The agenda was discussed, and modified as follows: Since Anh Dao is not available for this meeting, her AnIML example will not be discussed. A question arose regarding reports from the technique working groups. Gary will provide an updated list of the technique committee assignments and make it available for posting.

The Minutes for the June 17 meeting, as circulated prior to the meeting, were amended as follows:

- The web seminar referred to as the being organized by the LIMS Institute is actually being organized by John Joyce. The LIMS Institute wants to do a workshop, which is premature, since the standard is not yet finalized. Gary will contact the LIMS Institute to tell them it is still premature for a workshop.
- Carolyn Sheahan corrected some statements in the section on ASTM's requirements for posting the schemas on the ASTM web site.

The minutes were approved as amended. The minutes will be updated to reflect the changes before being posted on the web site.

III. Attendees:

Sven Brehmer, Bruker Daltonics
Tony Davies, Waters
Jamie Duckworth, ThermoElectron
Maren Fiege, Waters
Michael Harzheim, Waters
Gary Kramer, NIST

Peter Linstrom, NIST
Dave Martinsen, ACS
Mark Mullins, SSI
Burkhard Schäfer, Univ. Kaiserslautern
Carolyn Sheahan, ASTM

IV. Location of Schema. Mark Bean was not able to attend this meeting. A proposal for the permanent location of the schema on SourceForge, during the development period, is still forthcoming.

V. AnIML Website Redesign. The new website requires a number of additional changes to simplify the HTML encoding, and to ensure that all existing content is available. Dave Martinsen will follow up with Stuart Chalk, to see if he has had anyone "simplify" the HTML encoding, with the goal of having the new site deployed in the next month.

VI. Formal AnIML Requirements Document. Tony Davies put together a MindMap figure to summarize the requirements for the AnIML format, and discussed the figure point-by-point. A number of comments were made:

- The statement “technique definitions are independent from one another” should be changed to “technique definitions may be different from one another”.
- A key point is that a manufacturer who makes a simple instrument should not have to support other techniques.
- The compliance section needs to be filled out. In addition to 21CFR11, SECD, FERMA (from EPA) and GALP (good automated laboratory practice) need to be considered. If the most stringent compliance standard is met, then we should be all right. In medical devices, 21CFR810 might be significant.
- The right hand side of the figure deals with archiving and reprocessing. There was some discussion on the meaning of “migration must be possible without loss of information”. It might be stated that it is all right to add noise, but not to lose precision.
- It should be stated that there is a compromise between efficiency and readability. If a reasonably educated person with knowledge of XML can read the ASCII-encoded strings, and convert by hand, then the files are readable. However, as a result of this readability, processing the files may be somewhat less efficient.
- The diagram doesn’t capture the assumption that the AnIML group will not create the data dictionaries, but that domain experts, working in conjunction with E13.15, will be needed, especially for those techniques which do not have an existing ontology.
- There is an implication that AnIML is for interchange. Should that be made explicit? Currently, archiving and reprocessing are at the same level. Should interchange be added? Or are archiving and reprocessing simply different examples of interchange? Conclusion: Yes – get rid of reprocessing and replace by interchange.
- The diagram was created by Mind Manager, from Mindjet.

Committee members should review the document and be prepared to comment in the August meeting. Tony will then put the diagram into document form, with input from Alex Mutin and Mark Bean.

VII. Core Developer’s Meeting. Nothing to report.

VIII. AnIML Example. Because Anh Dao is on vacation, there is nothing to report here. However, Jamie Duckworth noted some concerns in reading the minutes from the last meeting, in particular the discussion of what should go in the core, and what should go in the technique layer. He felt that whether or not the technique shares an item with another technique, those objects still go into the separate techniques, not within the core. It was noted that for sample specific objects, the definitions should be in the core. However, concepts like the number of scans, which is appropriate for IR and MS, but not for chromatography, belong in the separate technique definitions. They should not be in the core, even though the discussion of the previous virtual meeting suggested that they should. This creates additional overhead, but the result is greater reusability.

An email from Richard Larsen questioned how data are recorded in an AnIML file. For a given technique, will AnIML enforce a particular unit, or a way of recording data? For example, will UV/Vis or IR, will absorbance be required? The answer is no, AnIML will record as the instrument recorded, or as the user and/or application decides. The AnIML file will record both the data, as well as the method in which the data are stored. In this example, data could be stored as transmittance or absorbance.

It was noted that units are a big problem. The technique definitions include a number of allowed units, encompassing all units that make sense. The definitions can be extended using the vendor extensions.

IX. Miscellaneous.

- A meeting has been scheduled for July 12 at 2:00 pm with ASTM management, for the ASTM management to get a basic understanding of the requirements of the AnIML standard, in terms of files, standards documents, test data, etc. From the subcommittee standpoint, all of the official ASTM standards documents will be balloted, and will be behind the ASTM firewall. However, the name space, the schema files, the technique definition files, and test data and applications need to be outside the firewall and open to all.
- Inquiries:
 - i. Amanda Clair sent an email query to the AnIML developer list. Both Burkhard Schäfer and Maren Fiege indicated that they had replied. Burkhard noted that Clair had drafted a technique definition for a plate reader, which he reviewed and commented on. The question came up as to whether the plate reader is a technique, or just a sample, but Burkhard noted that he was encouraged that she was able to get many things right.
 - ii. Several contacts regarding Process Analytical Technology came up, from Sisler Instruments, and from ASTM E55. Gary Kramer has referred these to the AnIML web site. Also noted was an E13 subcommittee on PAT, and Gary Ritchie.
 - iii. Jamie Duckworth has had contact with SEDD people at EPA. Gary will try to get a presentation from them at a future meeting.

X. Agenda Items for Next Virtual Meeting.

- Review of requirements document

XI. Action Items:

- Web page redesign: Dave Martinsen will deploy new website
- List of technique committee members: Gary Kramer
- Requirements document: Tony Davies (with input from Mark Bean, Alex Mutin)

XII. Future Meetings:

- Working Group Teleconferences
 - August 4, 2005, 10:30 am – 12:30 pm EDT
- IQPC/ALI (January 30 – February 1, 2006, San Diego) and Lab Automation (January 21-25, 2006, Palm Springs, CA)
 - The dates of IQPC/ALI were changed to avoid collision with Lab Automation. A joint symposium/workshop is planned to accommodate attendees of both conferences.
- EAS, November 13-17, 2005, Somerset, NJ, Doubletree Somerset, Room 211
 - Working Group Meeting, November 13, 2005, 3:00 – 5:00 pm
 - Business Meeting, November 14, 2005, 5:00 – 7:00 pm
- PittCon, March 12-17, 2006, Orlando, FL
 - Business Meeting
 - Symposium/Workshop

XIII. Adjournment. Motion to adjourn. Second. Carried unanimously at 12:12 pm EDT.

Submitted by David Martinsen, ACS, ASTM E13.15 Secretary