
Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

Minutes for E13.15 Subcommittee Working Group

10:40 am – 12:33 pm EST

Friday, April 29, 2005

Virtual Meeting

I. Introductions and Welcome: Gary Kramer, NIST, E13.15 Chair at 10:42 am EDT

II. Review of Agenda. The agenda was approved as circulated. The minutes for the April 15 meeting had just been circulated, so no action was taken. People were asked to send comments to Dave Martinsen to incorporate into the draft minutes.

III. Attendees:

Michael Boruta, ACD

Mark Bean, GSK

Tony Davies, Waters

Jamie Duckworth, Thermo

Maren Fiege, Waters

Michael Hardheim, Waters

Gary Kramer, NIST

Peter Linstrom, NIST

Dave Martinsen, ACS

Charlie Manfredi, Agilent

Mark Mullins, SSI

Alex Mutin, Shimadzu

Anh Dao Nguyen, NIST

Burkhard Schäfer,

Carolyn Sheahan, ASTM

Wolfgang Winter, Agilent

IV. AnIML Website Redesign. Gary noted that in the XML files sent out prior to the meeting, the XML referred to paths for the schema which could not be resolved. We need to settle on a path to store the schema, so files of this type can be shared, parsed, and validated by all. Various options were discussed, including W3C and ASTM. The group decided that during this development phase, it was best to store the schema files on the SourceForge site. Mark Bean will propose a path for “permanent” storage of the schemas.

Dave Martinsen and Mark Bean noted that the latest draft of the new AnIML website had been posted at <http://www.candisource.net/animl>. The graphic navigation was removed to make the site easier to modify during development. Once the site design is completed, the graphic elements may be regenerated. Several reported problems accessing the new website. Mark noted that the candisource was unstable, and was sometimes unavailable. In addition, some had an extra period in the URL. People were encouraged to look at the new site and send comments to Mark and Dave.

V. Formal AnIML Requirements Document. There was no activity to report in this area.

VI. Report from the Core Group Virtual Meeting. Mark Bean, Burkhard Schäfer, Maren Fiege, and Mark Mullins had a virtual meeting on April 22, 2005. They studied the hyphenated technique, discussing how peak tables relate to sibling spectra and parent spectra. Mark Mullins and Mark Bean made alternate proposals. UV may define the relationships one way, LC another, MS another. There could be problems if each technique handled these relationships differently. Our job as a committee is to make sure applications and techniques are in sync, across all techniques. The core group will continue to meet on alternate Fridays.

VII. AnIML Example. Anh Dao made a presentation on the UV/Vis technique. Her slides have been loaded on the website, as well as examples of a sample parameters file, a UV technique definition file, a UV technique sample file, and documentation. The presentation included a discussion of the terminology used in the various files, followed by proposed structures for the technique definition, sampleRole, pageBlueprint, parameterCategoryBlueprint, and sampleParameters. Some of the discussion included:

- The difference between sampleMeasurement and Spectrum. Isn't the spectrum the sampleMeasurement? In Anh Dao's example, the sampleMeasurement is metadata about the sample.
- How is the backgroundMeasurement different from the sampleMeasurement? Don't they contain the same information, with the role of the sample being what distinguishes them? The standard must take into account the different ways in which background could be determined and used. In some cases, the instrument dynamically accounts for background, and simply records the background-corrected data. In other cases, one or more background measurements may be made; these are then used as post-measurement corrections to the data. Both instances must be allowed.
- Calibration protocol or measurements present a similar problem. In one sense, they are just another sample measurement, but the sample has a special role. The original idea was not to explicitly define calibration elements, but rather to make a reference to the sample which was used for the calibration.
- How does one determine the techniques to be handled? UV/Vis is a common technique; FT-UV also exists, but is not common. On the other hand, FT-UV is related to FT-IR. Perhaps it should be handled as a way to extend the definitions into the FT-IR world.
- The structure for the sample role in Anh Dao's example may need to be reconsidered. It appears as though this is a module which is UV-specific. The goal is to make the sample parameters usable by all techniques. If there are parts which are UV-specific, then those should be included in the technique definition, not in the sample object. Gary will add to the agenda for next time consideration of how to synchronize the sample object for all techniques.
- The SamplePathLength is an example of a candidate for a UV-only definition. However, it should perhaps be placed above the Page in the parameter set, perhaps in the sampleRole, not the shared object. It was noted that the sampleID is already in the schema itself, and doesn't need to be in this technique definition.
- One question came up regarding the file extension. Earlier, a decision had been made to use the extension ".atid" for AnIML technique instance documents. This example uses ".xml". Burkhard will check the use of instance documents as it applies to these technique documents, to make sure we are using the term properly. Recommendations for changing the approved file extension will be considered based on his assessment.
- INChI was accepted previously as a valid identifier for chemical structures. This needs to be changed to InChI, since the name has been changed.
- In light of the discussion, Anh Dao will add comments and make updates to the xml files for the next meeting.

VIII. Hyphenated Techniques. Mark Bean discussed problems with hyphenated techniques: peak lists related to spectra and chromatograms are not accounted for, conflicts between extensions need to be handled, the concept of upward references from spectra to chromatograms may not be either useful or valid, multiple analyses are not differentiated from hyphenated techniques, and the concept of "sample" is not well defined. There was considerable discussion regarding the definition of a sample, including

the bulk material which exists outside the instrument *vis a vis* the material which might be flying through an instrument at some point in time. The AnIML structure must be clear about what is being defined, and it must be related to some reality which the scientist/analyst also understands.

IX. Agenda Items for Next Virtual Meeting.

- Website comments and redesign
- Review of formal AnIML requirements document
- Reviewing technique files. Re-examination of UV/Vis files
- Synchronizing sample objects across techniques
- Technique document file extensions

X. Action Items:

- Web page redesign
 - All should review, send comments to Dave.
 - subgroup: Dave Martinsen, Mark Bean, Burkhard Schäfer – continue redesign of AnIML web site, add site map, create 3rd draft
- Mark Bean, Alex Mutin – complete formal requirements document, circulate prior to next virtual meeting
- Burkhard Schäfer – check on usage of “instance documents”, make recommendation on the file extension for technique documents.
- Core Group – virtual meeting on May 6, 2005
- Tool developers – post tools and documentation on sourceforge – does anybody have anything to post?

XI. Future Meetings:

- Working Group Meeting
 - May 23, 2005 – Tony and Maren will be in Baltimore week of May 23. A meeting is being planned for May 23 at Shimadzu, in Columbia, MD. Please contact Mark Bean for details.
- Working Group Teleconferences
 - May 13, 2005, 10:30 am – 12:30 pm EDT
 - May 27, 2005, No Virtual Meeting
 - June 17, 2005, 10:30 am – 12:30 pm EDT
- Business Meeting: EAS, November 14-17, 2005, Somerset, NJ
- Business Meeting: PittCon, March 12-17, 2006, Orlando, FL

XII. Miscellaneous.

- UnitsML is nearing completion. It is following a meta-approach; most of the information will be held in a database.
- IQPC Conference on Analytical Informatics is scheduled for December in San Diego.

XIII. Adjournment

Motion. Second. Carried unanimously at 12:33 pm EDT, at which time the virtual meeting evaporated.

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