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**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

**Minutes for E13.15 Subcommittee Working Group**

10:30 am – 12:30 pm EDT

July 28, 2006

Virtual Meeting

- I. Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 10:40 am EST. The ASTM release form for recording the session was displayed on the screen. There being no objections, the meeting was recorded.
- II. Attendees:**
- |                                      |                        |
|--------------------------------------|------------------------|
| Mark Bean, GSK                       | Ronny Jopp, NIST       |
| Michael Boruta, ACD                  | Joe Koury, ASTM        |
| Stuart Chalk, Univ. of North Florida | Gary Kramer, NIST      |
| Rajesh Doda, GSK                     | Peter Linstrom, NIST   |
| Maren Fiege, Waters                  | Alexander Roth, NIST   |
| Francois Gilardoni, Topcombi         | Burkhard Schäfer, BSSN |
| Steve Hoffman, BMS                   | Danny Tsang, GSK       |
- III. Next Meeting:** Schedule for next meeting: August 15, 10:30 - 12:30
- IV. Other meetings:**
- Monday: Discussion of technique NDRs
  - Tuesday: UV Group, discussion of UV technique definition
  - Friday: Core Group. Since Alex is leaving on August 18, the core group has been requested to review the technique NDRs before presentation to the next working group meeting on August 15.
- V. Welcome:** to Danny Tsang and Rajesh Doda from GSK. They are working for Tony Davies on a lab data preservation project, involving the AnIML Chromatography Technique.
- VI. Minutes:** The June 30 minutes were sent out with the agenda, and had also been sent previously to those attending the meeting. Joe noted that the minutes need to include a statement that the meeting form was posted, and no objections were made to recording the meeting. Mark Bean didn't see the alterations he had suggested, so the approval of the minutes will be deferred until Dave returns.
- VII. Collaboration:** The news article on AnIML appeared in Standardization News. Ron Bird, who is involved on the A01 Committee, from stainlessfoundry.com provided some feedback. He was concerned that AnIML will only work for analytical techniques, and felt that the standard should be broader. He suggested that we establish liaisons with other committees. Gary will reply to his comment, noting that we have always tried to reach out to other groups, and the

standard will be able to supports a broad range of techniques. He will also be invited to join the discussions. However, we will continue to focus on the analytical instrument domain.

Along similar lines, Francois noted that Topcombi's interest was to use AnIML in the consortium, report problems back to the committee to improve the standard. That's how they view their contribution.

**VIII. PittCon 2007:** Gary has coordinated the PittCon 2007 session with the PittCon committee. The only change is that Peter Linstrom has been added. The current lineup is:

1. Gary Kramer: Introduction
2. Burkhard Schafer: How AnIML works
3. Maren Fiege: Appying Animl to UV data
4. Dale O'Neill: Crhomatography
5. Mark Bean: AnIML and LCMS data
6. Robert Lancashire: Experiences implementing viewers and converters.
7. Peter Linstrom: Using Animl to publish data on the internet.
8. Alex Mutin: Animl and XML at Shimadzu
9. Gary Kramer: Closing Remarks

Abstracts are due Aug 25 to Pittcon. Abstracts should also be sent to Gary for posting on the AnIML web site.

Stuart Chalk noted that he has submitted a short course on XML and metadata. He doesn't know yet if and when it will occur. Burkhard will also be doing a short course. Gary will ask PittCon to try to avoid overlap, if possible.

**IX. Core developers:** There has been fruitful discussions on different approaches to resolving relationship between chromatography and spectroscopy. A number of options put been identified, and the advantages and disadvantages of each one have been listed, providing a chance to record what was good and bad about each one. This has lead to the conclusion that the current structure could be used to store LCMS data. There are some aspects which would be awkward, but not impossible. The discussion will continue next time.

The differences stem from the fact that we don't have a fixed frame of reference for the multidimensional techniques. The AnIML schema tries to use concept of chromatograms to provide that frame of reference. This can sometime be artificial, since the chromatogram my not actually exist. There may not even be a fixed time base in multidimensional techniques, since samples may get to detectors at different time because of flow rates. It is an AnIML problem, but comes about due to the context of multidimensional experiments. With respect to LCMS, the assumption that spectra would go under chromatograms, when in fact there is no relationship, leads to the difficulty. Chromatography doesn't produce any data at all.

It was suggested that perhaps the difficulty was not in the AnIML core, but could be solved in the technique definition. However, it was noted that to connect spectra to a particular chromatographic trace, when you could have multiple traces for the same detector, you would need complex reference pointers, and this would be defined in the core. The observation was made that complex experiments were going to be the reality. People aren't going to change the

way they conduct experiments in order to conform to the AnIML standard definition. Rather, AnIML needs to handle the complexities of the community.

Mark recommended that Danny should join the discussions because of his responsibilities with Tony. Gary noted that Dale O'Neill will be taking over Mark Mullin's responsibilities, including the chair of the chromatography technique group.

**X. NDRs:** Alex and Ronny have worked on the NDR document for technique definitions. As mentioned earlier, Alex is leaving in a couple of weeks, so there is a need to finish this document. Alex presented an outline of the NDR. Included are the following points:

1. Abstract
2. How to name different elements - guidelines, restrictions
3. How to document the data elements, so people know what information is there.
4. versioning
5. how to create samples/roles - relationships between roles, AnIML documents, and technique documents

Because variety of techniques could be quite large, it may be difficult to find NDRs that are valid for all techniques. Note that in addition to the NDR for technique definitions, Alex also proposed that an additional NDR is needed for the AnIML documents themselves. Gary requested that as the core group works with the NDRs, they should note what is not covered, so we can be sure that these missing items could be addressed in the future.

Before bringing the NDR to the entire group, Alex would like this to be reviewed by the core group, at their next meeting. Then the NDR will be presented to the working group at the August 15 meeting.

**XI. Standards document:** Gary has begun working on the ASTM standard document, using Mark Bean's original document from more than a year ago. He removed the appendix containing the schema itself, since that version of the schema is no longer valid. The group was asked whether they thought the standards document should contain both the Core and Technique Schemas in a single document for balloting, or whether each should be balloted separately. The consensus was that they should be balloted together. If they were balloted separately, and one passed and the other failed, it might be impossible to fix the one which failed without also making changes to the one that passed. Changes to the one that passed would mean it would need to be re-balloted.

There was also some discussion about the nature of the documentation. In some sense, the schema is self-documenting, and the ASTM standard document is a relatively non-useful reformatting of the schema. It was noted, however, that the document is needed in order for AnIML to become an official standard. In addition, the document will contain verbiage to explain the meaning of elements that are used without definition in the schema. A suggestion was made that an introductory section was needed to describe the AnIML model, with the two layers of core and technique, with experiment steps being built by applying an experiment technique to a sample.

There was some question as to whether the ASTM format specification, with its rigid ordering of sections, was the best way to present the standard. Joe offered to arrange for the ASTM editor to attend a future meeting to answer questions from the working group.

An appendix to Mark's document labeled as non-mandatory information contains a series of figures from XMLSpy, describing the schema. A tutorial will be needed to describe the meaning of the different symbols used in the diagrams. This could be done through an external reference, if an explanation exists somewhere in another document, or on the Web. However, in order for people to vote intelligently on the standard, they will need to know what the symbols mean. In general, though, the XMLSpy diagrams are quite useful, and preferable to explaining all of the meaning they convey in prose.

**XII. UnitsML:** The technical committee has been formed. See [www.oasis-open.org](http://www.oasis-open.org) and go to "Committees by Name", select "OASIS UnitsML TC". Bob Dragoset is chair. Some additional material is available at <http://unitsml.nist.gov>. Eventually all material will be moved to the OASIS site. Some NDRs have been done. Ronny did initial draft. The original UnitsML schema have been modified to conform to most of the NDRs, but there are some aspects which are still under discussion. A meeting of the UnitsML committee is scheduled for August 9 at 11 am EDT. If interested, please send email to Bob Dragoset.

**XIII. Other:**

- a. **Recording of sessions:** Joe noted that at the current time, anyone wanting to listen to the recordings needs to sign the standard permission form, even though the form seems to imply that it is for participants granting permission to be recorded. Current practice is to make the recordings available for a limited time. Joe will check to see if they can be stored permanently on the AnIML web site.

Minutes taken by David Martinsen, ACS  
Secretary ASTM E13.15