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Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

Minutes for E13.15 Subcommittee Working Group

10:40 am – 12:30 pm EDT

June 30, 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 | David Martinsen, ACS |
| Maren Fiege, Waters | Alex Mutin, Shimadzu |
| Steve Hoffman, BMS | Dale O'Neill, Agilent |
| Joe Koury, ASTM | Alexander Roth, NIST |
| Gary Kramer, NIST | Burkhard Schäfer, BSSN |
- III Next virtual meeting:** The next virtual working group meeting will be held on July 28, 10:30 am - 12:30 pm EDT.
- IV Approval of minutes:** Minutes from the May 26 meeting were posted. The draft minutes were created using the session recording, which did not indicate the participants. The following changes were recommended:
- **Additions:** Alex Mutin, Shimadzu and Michael Boruta, ACD
 - **Deletions:** Stuart Chalk
- A motion was made and seconded to approve the minutes as amended. The motion carried.
- V Web Site Postings.** It was noted that recent presentations could were not available on the web. Burkhard said that the presentations were there, but links to the presentations were not reliable. He offered to enable the links, but there was a discussion about several issues:
- PDF was recommended instead of, or in addition to, ppt format
 - Permission of presenters should be granted before making the presentations public. All presenters that were present granted permission, and Gary Kramer granted permission for all of the NIST presentations. The presentation lacking permission was that of Mark Mullins. Dale O'Neill said the thought it was ok, but would check with Mark to be sure.
 - AnIML graphics and slides are beginning to appear in other presentations, and there was some concern that people were using these without attribution. The consensus was that there was no objection, as long as attribution was made. Burkhard will remove the ppt files until a copyright notice can be created so that people need to see the copyright notice before they can load the files. The PDFs will be available now, and the ppt files added when the copyright form is in place.
- VI AnIML PR.**
- A tentative schedule, including names and emails of speakers, promotional text, and application and methodology codes, is needed by July 3 for PittCon 2007. The group selected the codes for the session. There was some discussion about the goal of the session, and the presentations needed to meet that goal. Some of the items discussed included whether or not we could include presentations about the documents up for ballot; whether or not we would have items ready for ballot at that time; presentations on various technique-specific files; generic viewers; whether we needed commitments to speak on specific topics now, or if the need was less specific at this time. The group agreed to the following proposed session:
 - Burkhard Schäfer, General overview on how AnIML works
 - Maren Fiege, UV/Vis
 - To-be-determined, IR
 - Dale O'Neill, Chromatography

- Mark Bean, LCMS
- Suggested: Robert Lancashire or Stuart Chalk, Generic viewers (Gary will make contact to ask for participation)
- Alex Mutin, Limitations at Shimadzu

The group also agreed that PittCon would be an ideal venue to present the two standards documents (the core and technique schemas), but that the status for having those ready was unclear at this time.

VII Core Developer Meetings. The core group had two meetings since our last working group meeting, with progress in the following areas:

- Discussion on how comments and descriptions, such as those used in JCAMP, could be added to the schemas. Questions on the developer mailing list, as well as the motion from the 26 May meeting, were considered.
- Both schemas were changed to follow the NDR rules. The group asked for feedback on whether anything was missing, or if there were better alternatives for implementing these changes.
- Auxiliary techniques were discussed.
- It was noted that the NDR document is complete, and should be moved into the “Documentation” part of the site. This would finally allow the “Coming soon” text to be removed from that area, to be replaced by a real file.
- A major discussion in the core group centered on the relationship between spectra and chromatograms. The current AnIML model is hierarchical, with the chromatogram at the top, with spectral children. Chromatograms are created out of a set of spectra, with some sort of link between the chromatograms and the spectra. For LCMS, something other than a direct parent-child relationship is needed. A spectrum may result from the summation/subtraction of multiple spectra, so there is not always a 1:1 correspondence between a chromatographic point and a spectrum. As there can be many chromatograms (vectors) per detector, if we want a relationship between spectrum and a parent chromatogram point, we must know which chromatogram to refer to. It was noted that this problem is not unique to LCMS, but could also be seen with other multi-dimensional techniques. The problem in this case is that the parent chromatogram may not actually exist; it may simply be derived from one or more spectra. Reference was made to an earlier AnIML presentation, which outlined the generation of a spectrum by summing spectra over a 20-30 second time period, which could include sample spectra, and background spectra. The core group will consider this model, and determine whether or not it could solve this case.
- Another problem concerns peak lists. Under the chromatogram hierarchy, at the same level as the vectors, one could have peak tables. The question was raised as to how the peak tables could be associated with the appropriate chromatogram. It was noted that this relationship is resolved through the implementation of references to vectors, which are now part of the AnIML schema.

VIII Standards Documents: Gary Kramer will draft an outline for the documents describing the two AnIML schemas. Mark Bean and Burkhard Schäfer will send Gary existing material to use as a starting point for this new draft, for a discussion at the next virtual meeting. Once we agree on the outline, different parts of the documents will be assigned to different members of the working group.

IX Miscellaneous:

- **UnitsML:** The OASIS technical committee has had a preliminary meeting, and is in the process of scheduling the first real meeting. Gary Kramer will send out a notice once the time is set. Preliminary NDRs and schemas are available for UnitsML, and may be on the web site, or are coming soon. The announcement of UnitsML within the OASIS community has resulted in comment from other groups who feel that UnitsML may really belong within an existing group.
- **AnIML “Contact us” link:** Joe Koury requested that the “Contact us” link be changed from “morrissey” to “koury”.
- **AnIML at EAS:** Joe Koury will schedule both a business meeting and a working group meeting at EAS in November. The working group meeting will be scheduled for Sunday, November 12, 3-5pm. It was suggested that we try to get some technique experts to review the available technique documents at that meeting.
- **JCAMP/IR Group:** Gary noted that the IR group of JCAMP has been working on XML. He will contact Robert Lancashire to find out the status.

X Adjournment: The meeting was adjourned at 12:33 pm EDT.

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