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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

August 15, 2006

Virtual Meeting

- I. Introductions and welcome:** Gary Kramer called the meeting to order at 10:30 am EDT. The release form was displayed. There being no objections, the meeting was recorded.
- II. Attendees:**
- | | |
|---------------------|--------------------------|
| Mark Bean, GSK | Gary Kramer, NIST |
| Michael Boruta, ACD | Peter Linstrom, NIST |
| Tony Davies, GSK | Alex Roth, NIST |
| Rajesh Doda, GSK | Burkhard Schäfer, BSSN |
| Maren Fiege, Waters | Danny Tsang, GSK |
| Joe Koury, ASTM | Wolfgang Winter, Agilent |
- III. Pittcon:** The deadline for submission of abstracts for each presentation is August 25. Those making presentations should submit their abstracts.
- IV. Next meeting:** September 15, 2006, 10:30 am - 12:30 pm EDT.
- V. Core Group:**
- The Core Group has continued discussion of the chromatography/spectroscopy problem. The different models are converging. Discussions will continue.
 - The UV/Vis group requested that the Core Group consider whether some parameters, such as sampleName and sampleDescription should be moved into the core. If these are generic enough, then every technique will use them, or will come up with different names for the same concepts. There is a benefit of putting more things into the core, since common elements are handled in a standard way. If each technique defined its own elements for these generic parameters, applications will be unnecessarily complex. However, there is also a problem with the core becoming overloaded with elements which only a few techniques actually use.
 - The Core Group also looked at methods for annotating how events happen in time. They are considering a timer application technique to handle this need. There are also a couple of other areas where such a lightweight

techniques, such as subsampling and a topology map. These would give a standard mechanism for attaching time/coordinate data to a sample.

VI. UV/Vis technique:

- a. There was a lengthy discussion on how to handle custom parameters in JCAMP-DX files. One of the initial requirements of AnIML was that it be rich enough to allow complete conversion of legacy JCAMP-DX files in a 21CFR11-compliant manner. However, JCAMP-DX files can contain a number of vendor-specific data in “#\$” fields. The problem with these fields is that there is often little documentation as to their meaning. In addition, the vendor sometimes used these fields to encode data which was required in other JCAMP fields. This happened as the vendors developed ways to handle data elements which were not defined in earlier JCAMP definitions, and then perhaps continued using their custom fields, even when JCAMP was updated. Since vendors may know the details of their custom fields, the best solution would be for the vendor to create a vendor layer, and convert the custom fields to the tags defined in that layer. However, the general user who wishes to convert legacy files might run into a problem. It was noted that there is also a problem in that JCAMP uses 7-bit ASCII, while AnIML uses Unicode. Simply enclosing the JCAMP custom fields with a special AnIML tag wouldn't necessarily solve the problem. The discussion finally led to a consensus that if a container for these JCAMP custom fields was created, using CDATA tags to handle the character coding question, that the user would be no worse of a position with respect to the content in those fields.

Note that this same discussion also applies to ANDI, as well as other legacy data formats.

The following proposal was made there was consensus agreement: **We will not do anything to the technique definitions as we've defined them now. We will create an example in the documentation to show how to create a JCAMP extension in which to put these custom parameters as a single extension. We won't implement that, but will tell people how to do it. At the same time, we will suggest that they use the extension mechanisms that we've created for vendor, user and enterprise extensions to do the job properly if they have the sufficient documentation and knowledge.**

- b. Another issue centered on the method used for naming of tags. For example, in the UV technique definitions, there are many multiple names, such as sampleName, sampleBoilingPoint, sampleDensity, etc. If the context made it clear that all of these belonged in the sample hierarchy, then removing the redundant text “sample” would make the data more human readable. Because the ability to see the terms in context depends on

the application, the behavior of IE, as well as Dominik's viewer were discussed. In both cases, the presentation of the hierarchy is very clear. This principle can also apply to other parameters. For example, an instrument may have instrumentDetails, instrumentVendor, instrumentModel, instrumentSerialNumber, etc. The text "instrument" could be left out.

The following proposal was made and there was consensus agreement: **Do not repeat the container name in the element name.**

It was noted that a rule could be written to check this. If was added to the NDRs, NIST has a framework already present to make the check

VII. Other Business:

- a. Mark Bean reported that another major pharmaceutical company is requiring Sciex to provide AnIML support. Because of this, Sciex wants to provide expertise from their software group. This could be of benefit to resolving the chromatography/spectroscopy problem.
- b. The Lab Automation conference will be held from 27-31 January 2007. Abstracts are due very soon. Gary will have two new students submit posters. Burkhard will contact track chair for informatics to submit a paper.
- c. Tony Davies raised a question about experimentStepSet and measurementData from Mark Bean's documentation. It turns out that the documentation being used was an old version, and no longer corresponds to the current schema. At this time, the schema itself is the authoritative document. This led to a discussion on the way to handle recursive experiments, where an experimentStepSet might contain multiple experimentSteps. Mark Bean suggested that the other developers from the GSK group should join the core group discussion on 25 August to bring raise their concerns.
- d. The UV/Vis group will meet tomorrow at 10. Invitations will be issued later today.
- e. Burkhard raised a question for people to think about for a future discussion. Up to now, we have had an element subPage, nested under other pages. However, there has never been an instance where there has been a need for subPage. This is a core group question. It was agreed that simplification would be good, but perhaps after the AnIML structure has been finalized.
- f. Tony Davies requested technique committees share minutes. It was noted that there are not formal minutes. Rather, changes are made within the documents during the meeting. The resulting documents represent the minutes of the meeting.