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Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

DRAFT Minutes for E13.15 Subcommittee Working Group DRAFT

10:30 am – 12:30 pm EDT

May 15, 2007

Virtual Meeting

I. Introductions and Welcome: Gary Kramer, E13.15 Chair called the meeting to order at 10:35 am EDT. 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
Michael Boruta, ACD
Stuart Chalk, Univ. North Florida
Maren Fiege, Waters
Patrick Gleichmann, NIST
Steve Hoffman, BMS
Joe Koury, ASTM

Gary Kramer, NIST
Robert Lancashire, UWI
Jamie McQuay, Scimatics
Dale O'Neill, Agilent
Kordian Placzek, NIST
Burkhard Schaefer, BSSN

III. Next Virtual Meetings: June 27, 2007, 10:30 - 12:30 EDT

- Core Developers: May 30, 2007, 10:30 - 12:30 EDT
- UV/Vis Technique Group: June 12, 2007, 10:30 am - 12:30 pm EDT.
- Chromatography, May 23, 2007, 10:30 am - 12:30 pm EDT.
- Business Meeting and Working Group, August 4, 2007 (Tentative). The next business meeting will be held in conjunction with the Subcommittee on Electronic Data Standards (SEDS) of the Committee on Printed and Electronic Publications (CPEP) of IUPAC. The meeting will be held at the IUPAC General Assembly in Torino, Italy. The tentative meeting time is August 4, 2007 in the afternoon in Italy. Virtual meeting attendance will be provided. A working group meeting will also be held at this time.
- PittCon 2007: Action item - Burkhard will submit his presentation from PittCon 2007 to Patrick, or to the wiki, for posting.
- PittCon 2008: A session proposal was submitted, but Gary has not received any response.

IV. Minutes:

- March 16, 2007 Minutes:

- o Jamie McQuay’s attribution should be Scimatics
 - o “Welcome to new memers” should read “... members”
 - o Page 7: “Hey” should be “They”
 - o Page 8 “In addition”
 - o A motion was made and seconded to accept the minutes as modified. The motion carried.
- April 13, 2007 Minutes:
 - o Jamie McQuay’s attribution should be Scimatics
 - o Page 8: Peter’s document should read Gary’s document
 - o Last bullet item - splitter, not sampler
 - o Under chromatography working group, the same software should read the same peak finding software
 - o A motion was made and seconded to accept the minutes as modified. The motion carried, with one abstention.

V. Document on indexing variables:

- Kordian and Patrick fleshed out Gary’s document on indexing parameters with graphs, data, and examples of storing data in AnIML. They presented an example of indexing parameters in a kinetics experiment, where the variable is time. An example is given in XML, showing the difference between Mark Bean’s view (implicit experiment steps) and Burkhard’s view (explicit experiment steps. Mark pointed out a problem with the example. In his view, every spectrum goes into a separate experiment step, not hierarchical, but as siblings. Burkhard also corrected the example to more accurately reflect his view:

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<ExpStep “MS”>
  <Page “Spectrum 1”>
  <Page Peak Table>
</ExpStep>
<ExpStep “MS”>
  <Page “Spectrum 2”>
  <Page PeakTable>
</ExpStep>...

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There may be problems with this approach if there are multiple techniques; however, for the purposes of this discussion, we will restrict consideration to a single technique.

There are also complications when considering the details of an experiment over time. If a sample is measured at some point in time for a chromatographic experiment, the sample is actually changing during the course of the experiment. This is caused by the nature of the experiment, and it is the job of AnIML to provide for the storage of the data, and the

characterization of the experiment, not to account for the imperfections in the experiment. The instrument produces a spectrum, AnIML stores the spectrum and records the conditions.

In AnIML, an experiment step is defined as the application of a single technique to a sample. If we apply it twice, we get two experiment steps. This is our choice of granularity. Techniques should always be treated the same way, whether an indexing technique, or even some other technique that we don't know about yet.

Mark Bean pointed out that if we had MS and UV spectra on a chromatogram, the AnIML file could get very complicated. Mass spectra 199 and 200 could occur between UV spectra 2 and 5. It could be difficult to make sense of these. There was some discussion on how to address the ordering. The suggestion was made that whoever was creating the AnIML file would be responsible for ordering the data. If a vendor wanted to put the scramble the data, that would be acceptable. It just means that the software reading the data would require more processing time to unscramble them. Human readability may be more difficult when the data are complex. However, the primary target of the file is computer readability. Human readability is important, but it is not required to be easily readable.

- Another topic for discussion was where to store instrument parameters, whether these belonged in the experimentStep, or the Page. There was some discussion about including requested settings with the experimentStep, but to include measured settings in the page. Not all instruments provide a capability to measure all requested settings, but measured values are data, and properly belong at the Page level. It was noted that for converting legacy data, it is often not known whether the parameters were requested settings or measured settings. In that case, putting them in either the experimentStep or Page introduces a level of ambiguity about that field.
- The discussion concluded with the observation that there is not too much difference between the implied and explicit experiment steps. If we allowed both, the parser could simply interpret a Page-Page sequence as being an implied experiment step. Peak tables could be put in as children of the Page, making it obvious which page they were derived from. In the case where the raw data is not saved, we would need to allow for a void spectrum. Three rules were proposed for storing the parameters:
 - Rule 1: If we don't know where a parameter came from (e.g., a JCAMP file), store it in the experimentStep.
 - Rule 2: Peak tables are children of the spectrum they were derived from. If the spectrum is not there, we have the concept of a null spectrum.

- Rule 3: An ExperimentStep is implied by the sequence Page-Page. You can explicitly include the ExperimentStep, but it is not required.
- Note that these rules provide a resolution of a long-standing difference within the working group regarding how to handle multidimensional data, through use of implicit experiment steps and null spectra.

VI. New Business

- Maren noted that at a user group meeting, a person expressed interest in joining the AnIML effort. She will send the name to Joe Koury, who will add the person to the email list for the main working group virtual meetings.
- Burkhard attended the Combicats conference, and had several good discussions in both a poster session and a talk. After the conference, he joined the topcombi meeting. The TopCombi experiments are very heterogeneous, with custom instrumentation setups. They have decided to support the AnIML standard, are interesting in contributing to the development, and are also willing to serve as a test bed.

VII. Adjourn: 12:30 pm EDT.

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