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**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

**DRAFT Minutes for E13.15 Subcommittee Business/Working Group DRAFT**

1:30 pm – 3:50 pm CEST

August 5, 2007

Lingotto Conference Center, Room M30.1

Turin, Italy

Business Meeting/Working Group Meeting

joint with the

IUPAC/CPEP Subcommittee on Electronic Data Standards (SEDS)

**I. Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 1:30 pm CEST.

**II. Attendees:**

Mohan Cashyap, GSK

Tony Davies, ALIS GmbH

Maren Fiege, Waters

Gary Kramer, NIST

Peter Lampen, ISAS

Robert Lancashire, UWI

David Martinsen, ACS

**III. Next Virtual Meeting:** August 29, 2007, 10:30 - 12:30 EDT

- Chromatography VM: August 8, 2007

**IV. Minutes:**

- The minutes from the February 27, 2007 were displayed. A question was raised about whether or not the proposal to adopt JCAMP data definitions into AnIML techniques had been approved or not. The answer was yes, but at a subsequent meeting. A motion was made and seconded to adopt the minutes as distributed. The motion carried unanimously.

**V. Work Items:**

- **AnIML:** This work item is in progress, and the subject of this meeting.
- **LIMS Validation Guide (E 2066-00):** This will continue without revisions. Revisions are needed by 2012. Jim Powers authored the LIMS Guide, but will not be able to do the LIMS Validation Guide. Gary Kramer is trying to find someone to lead this effort. Tony Davies noted that the FDA is reviewing all

of its standards for industry, and this should be taken into account for the LIMS validation guide. There could be significant change in what validation means in a regulated environment. Mohan Cashyap noted that in many areas, companies are moving away from LIMS and to ELNs. He suggested that it might be time for a standard in the ELN area.

- **NMR Standard (E386-90):** This standard needs to be revised in 2009. There is a project at NIST to adopt NMR standards, and Gary Kramer has talked with several instrument vendors. Suggestions were made to consider mestrec.com, Woody Conover at Acorn, and ACD.

## VI. AnIML

- Gary reported on the current status of AnIML, with a monthly virtual meeting of the working group, and separate meetings, also occurring monthly, of the core group, the UV/Vis group, and the Chromatography group. The meetings have been useful in raising issues, showing areas which are not accounted for in the AnIML model, and also questioning how appropriate the AnIML model is in given situations. The group has had many discussions about how best to represent LCMS, discussions which have general applicability to all hyphenated techniques. There is now an emerging consensus on how to handle some of the complexities related to hyphenated techniques.
- There was some concern over the possible mechanisms for storing data. If a single experiment is stored in multiple files, with indexes in one file pointing to data in another file, there might be a chance for files to get separated. The suggestion was made that each file needs to stand on its own, without losing any data.
- The IUPAC/SEDS group met prior to the E13.15 meeting, and expressed some concern about the progress being made on AnIML, which has diminished AnIML in the eyes of both vendors and vendor customers. IUPAC/SEDS proposed a number of ideas to move forward:
  - The requirements document authored by Mark Bean and Tony Davies be finalized, adopted, and published as a report to the IUPAC/CPEP committee and published in *Pure and Applied Chemistry*.
  - IUPAC/SEDS will be responsible for conversion of the JCAMP data dictionaries for use in AnIML, finding appropriate domain experts from the existing AnIML taskgroups, as well as through vendor contacts.
  - ASTM E13.15 will continue to work on and finalize the schemas, and the procedures to incorporate the data dictionaries into the technique definition files.
  - IUPAC/SEDS will write the first draft of the AnIML document dictionaries as IUPAC Technical Notes.
- There was a consensus that this proposal was a good one, and should be followed. Some time was spent in looking at a possible timeline.

- For 3rd quarter, 2007, SEDS will 1) identify and assemble the domain expert teams; 2) Review the technical notes; and 3) produce “clean” test data. The AnIML working group will confirm the format of the document dictionaries, and will use the data from SEDS as test data in the core and for software development.
- For 4th quarter, 2007, SEDS will revise the draft document dictionaries.
- For 1st quarter, 2008, ASTM E13.15 will prepare draft AnIML technique definitions.
- At Pittcon 2008, the core schema and technique definitions will be delivered to the E13.15 subcommittee for a vote. Following that, ASTM E13 will need to vote on the standard. In order to be on the full ASTM ballot in August, the standards documents need to be to ASTM by the end of June. If rejected, SEDS and ASTM E13.15 will revise the documents and resubmit.
- The documentation of the core schema was also discussed. Support for creating the Technical Documentation for the AnIML Core, the ASTM Guide, and the Technical Documentation for the AnIML Techniques could be channeled through ASTM. A fixed-price proposal with the proposed ToCs of the documents and a time line would be required.

**VII. Additional Notes:** At the CPEP meeting on August 6 and 7, Robert Lancashire presented the report from the SEDS and AnIML meetings. Three members of CPEP indicated interest in AnIML. Miloslav Nič, from the Institute of Chemical Technology in Prague, and knowledgeable about XML, commented that there are some XML details in AnIML which could be modified to better follow best practices in the XML community. René Deplanque from FIZ CHEMIE commented that he is working with a European Union group to develop a repository for data associated with published journal articles. Christoph Steinbeck is also involved in this effort. They have been considering developing an XML definition for their project, but are interested to see if AnIML could meet their needs. They have been informed of the August 29 Virtual Meeting. Mila Nič will not be available, but René and Christoph might attend.

**VIII. Adjourn:** 3:50 pm CEST

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