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**Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY**

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

10:35 am – 12:25 pm EST

Wednesday March 3, 2006

Virtual Meeting

**I Introductions and Welcome:** Gary Kramer, E13.15 Chair called the meeting to order at 10:35 am EST.

**II Attendees:**

Mark Bean, GSK

Maren Fiege, Waters

Steve Hoffman, Bristol Myers Squibb

Ronny Jopp, NIST

Joe Koury, ASTM

Gary Kramer, NIST

Richard Larsen, JASCO

Peter Linstrom, NIST

David Martinsen, ACS

Mark Mullins, Agilent

Dale O'Neill, Agilent

Alexander Roth, NIST

Burkhard Schäfer, BSSN

**III Schedule for next virtual meeting:** The next working group meeting will be held on March 15, at PittCon. The next virtual meeting will be scheduled at that time.

**IV Approval of minutes:** Two corrections were suggested for the Minutes of the February 10 meeting.

- The following corrections were given for the draft minutes of the February 10 meeting: 1) Section VI, bullet 2: BM should be BMS – for Bristol Myers Squibb; 2) Section VII, paragraph 2: “there” in sentence 1 should be deleted; 3) the url for the CVS directory on [animl.sourceforge.net](http://animl.sourceforge.net) should be provided: [https://sourceforge.net/cvs/?group\\_id=76803](https://sourceforge.net/cvs/?group_id=76803); 4) Section VIII, “Naming and Design Requirements” should be “Naming and Design Rules”.
- A motion was made and seconded to approve the minutes as amended. The minutes were approved as amended.
- It was noted that the recording of the last virtual meeting was quite helpful to those who couldn't attend at the time of the meeting. It was suggested that we look at recording these in the future. The recorded meetings are retained for one or two weeks after the meeting.

**V AnIML at PittCon.**

- The Business Meeting is scheduled for 5:30 – 7:30 pm on Monday, March 13, 2006 in room West 230-C.
- The Working Group meeting is scheduled for 5:15 – 7:30 pm Wednesday, March 15, 2006 in room West 230-C, followed by dinner.
- The AnIML Workshop is scheduled for Thursday, March 16, 2006, in room 202-A. The session is from 1:30 – 5:30 pm, but Gary Kramer requested that speakers arrive early to address any technical problems. If possible, speakers should bring slides on a USB-drive, or a CD-ROM, to transfer to Gary's laptop. This is not a requirement, but might reduce the chance of difficulties when switching laptops.
- Each of the speakers present gave either a presentation of their slides, or an outline of their talk. The purpose of this exercise was to determine if there were any problems with overlap between the talks, and also to see if there was anything missing which could be assigned to one of the talks. Note that Tony Davies talk will be presented by Maren Fiege.
- Under topics for the business meeting, it was suggested that the structure of the technique task groups be re-evaluated. There has been little activity on the part of these committees. It was noted that there are a number of problems here – including the lack of documentation on the core, the lack of information in the format they need, as well as the extra work for already busy people.

**VI JCAMP to AnIML Converter.** There was some discussion about the JCAMP to AnIML converter posted by Stuart Chalk. The Core Group looked at it, and found that it can create valid AnIML files from IR and UV data, within certain size limits. While it has limitations, it is encouraging to see that it was possible for this to be done.

**VII Generic Viewers.** There was a discussion regarding generic viewers, following up on a discussion from the previous meeting. There was some question as to whether a generic viewer is possible, and if it was, what it could do. It was noted that a generic viewer could not handle processing of data – integrating data or applying Fourier transforms, for instance. That would require a technique-specific viewer. In addition, a generic viewer would not be able to handle data from the vendor layer. Vendors would still be allowed to write extensions for their environments.

It was noted that we are not writing a generic viewer, but rather providing the data which a generic viewer could understand. A generic viewer might need to know something about different types of techniques. However, at the simplest level, it would simply need to understand the page structure and the relationships between the vectors containing the data. The development of generic viewers doesn't preclude technique-specific viewers from being developed. Those viewers would need to know something about the details of the technique.

There was some discussion about whether the committee should add a generic viewer to our requirements. It was noted that the requirements document, November version, includes a requirement for a format which could allow data to be viewed using generic viewers. This requirement will need further discussion.

**VIII Adjournment:** The meeting was adjourned at 12:32 pm EST.

Minutes taken by David Martinsen