
Committee E13 on MOLECULAR SPECTROSCOPY AND CHROMATOGRAPHY

DRAFT Minutes for E13.15 Subcommittee Working Group DRAFT

3:00 pm – 5:00 pm EDT

November 13, 2005

Eastern Analytical Symposium

Room 211, Doubletree Somerset, Somerset, NJ

- I. Introductions and Welcome:** Gary Kramer, NIST, E13.15 Chair called the meeting to order at 3:05 pm EDT.
- II. Review of Agenda and Minutes.** The agenda was approved without change.

Minutes for the October 14 and October 28, 2005 meeting were not available.

III. Attendees:

Maren Fiege, Waters
Gary Kramer, NIST
Joe Koury, ASTM
Richard Larsen, JASCO
Howard Mark, Mark Electronics
Dave Martinsen, ACS
Alex Mutin, Shimadzu

IV. Requirements Specification Review. The major focus of the meeting was the review of the AnIML Requirements document. The discussion resulted in the following changes:

- a. In Revision History, change “Version” to “Revision”, change the current revision to 2.0.3, and put it onto a separate page.
- b. Remove the graphics on the cover page. They are not necessary, and cause the page to take a long time to print.
- c. A suggestion was made to number each paragraph, in accordance with ASTM format. However, in a subsequent discussion, it was pointed out that this is a specification guide for the developers, and is not intended to be a formal ASTM document. Therefore, adherence to the ASTM format is not required, and the language doesn’t need to be quite as precise. For example, while “reasonable speed” might not be good language for a standards document, it is okay to use in a guide to developers, since it indicates that some attention should be given to performance.
- d. The document refers to ISO 11179 as the specification for use of must, should, will, etc. A comparison should be made with the ASTM recommendations to make sure ASTM specifications are followed.
- e. Where web sites are given as references, the document title, in addition to a url, should be included. This will allow the documents to be found even if the url changes.
- f. In section 2.2, paragraph 2, a period should be added at the end.
- g. In section 2.2, paragraph 6, add “not the subject of these documents”.
- h. At the end of paragraph 6: “AnIML file content defined in the CORE and its standardized technique extension can not be superseded to ensure that”

- i. Section 2.3, paragraph 2: “should” → “shall”
- j. Section 2.3, paragraph 2: “that” → “for”
- k. Section 2.4: “to be capable”
- l. Section 2.5: there was a lot of discussion surrounding the use of the word “speed”, because it is an unmeasurable specification, and is also quite relative. What is adequate speed for one person may not be for another. In light of the comment above, however, it was decided later that these relative terms could be allowed in light of the purpose of the document.
- m. Section 2.6.5 and 2.6.6: no technologies are named above any more. The points should be modified to reflect that fact.
- n. Section 2.7: in a footnote, add the current version number of the software packages mentioned: XMLSpy 2006, Visual Studio XXX, W3C Schema Validator XXX.
- o. Instead of glossary, define at first use, then use abbreviation later.
- p. Section 3.1: remove “all”
- q. Section 3.2, and section 2.3: change to say “AnIML should be simple enough for developers to understand and implement, and for users to write extensions in their own environments”.
- r. In section 3.3: take out “although other ... sacrificed.”
- s. Section 3.4: there was some discussion regarding the 60 year figure, but it was decided to leave it as is, as a guideline.
- t. Section 3.8 heading: change to “Can be viewed”
- u. Section 3.8 paragraph: Viewing of spectra, even from complex hyphenated techniques. Consider 21CFR11 wording: “rate of retrieval to enable accurate and ready retrieval of information”
- v. REQ 17: in “an” extensible manner.
- w. Section 3.12: In Phase 1, specify “hyphenated techniques (such as GCMS, LCMS, etc)” rather than “Hyphenated versions of these”.
- x. Section 3.13: High Priority Requirement: AnIML should work on:
- y. Section 3.14: Remove “allowing viewers” and “(audit trails)”.
- z. Section 3.15: change to “An AnIML file containing data from multiple techniques should be able to be read by software which understands only some of the techniques”.

V. Naming and Design Recommendation Review

- a. Note: in the document, use of the label “Not applicable” means that the AnIML schema does not follow the NDR document.
- b. There are some relatively simple changes which could be made to conform to the standard:
 - i. Datatypes should be in upper camel
 - ii. Singular vs. plural names
 - iii. Order in which words are used – nouns vs. verbs
- c. There are some other recommendations which are not as simple:
 - i. Versioning – how to number major and minor revisions
 - ii. Namespace – distinguish between local and global names, with local names being minimized
- d. It was recommended that the core group look at the NDR, and determine what areas should be implemented what areas are not important. The group should then present their recommendation to the full working group.

VI. Timeline for standard approval.

- a. The following needs to be accomplished:
 - i. Adopt appropriate NDRs
 - ii. Finalize the core
 - iii. Get technique task groups focused on technique definition files, including checking of existing data dictionaries

VII. Adjournment. Motion to adjourn. Second. Carried unanimously at 5:00 pm EDT.

Submitted by David Martinsen, ACS, ASTM E13.15 Secretary