



(SCDS) Subcommittee on Cheminformatics Data Standards

Subcommittee on Cheminformatics Data Standards (SCDS)
(Subcommittee of the Committee on Publications and Cheminformatics Data Standards)
December 20, 2016, 9am - 10am US-EST
(Web conference)
Minutes

SCDS Members Present: Leah McEwen, Dave Martinsen, Ron Weir, Greg Banik, Ian Bruno, Robert Lancashire, Stuart Chalk, Tony Davies

1. *Welcome new members*
 - a. **Gregory Banik**, General Manager of the Informatics Division at Bio-Rad Laboratories
 - b. **Ron Weir**, Current Chair of the IUPAC Interdivisional Committee on Nomenclature, Terminology and Symbols
2. *Approved Minutes of October 25, 2016*

Approved
3. *Process for developing digital standards (continued from previous meeting)*
 - a. Ron gave an overview of process and ICTNS role, Tony gave an overview of process for JCAMP-DX
 - b. When IUPAC took over, industry stakeholders / instrument vendors need to be brought along, beyond academic exercise, instrument vendors need to test, outreach workshops at their meetings to check the concept
 - c. Review process across IUPAC happen within/as part of the process, not just wait until the end as some stakeholders have already tested and later reviewers not familiar
 - d. Feedback was that industry needs the opportunity to discuss and come to agreements as a community
 - e. ICTNS was supportive of this parallel process, RDA works on this process for input along the way to make the 18mos target, process determined primarily by project group, has a technical advisory board, deliverables are guidelines,
 - f. Concerns about developing digital standards
 - i. Representing scientific aspect of the standard, with expression and units
 - ii. Technical format, how does this age? Critical longevity
 - iii. Data storage within stds is problematic as this changes in the industry
 - iv. Generation of files to meet the "standard"
 1. Industry implementers have to do cleanup on "standard" files that people write to
 2. Consider a machine process for file generation (e.g., software)
 - v. Key to manage deployment of standard, look to process used in InChI Trust, Allotrope



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- g. SCDS discussed the possibility formulating a Handbook for Digital Standard Development. Key issues raised:
- Scientific aspect
 - Technical constructs (e.g., prototypes, validation software, etc.)
 - Management of generation and maintenance
 - Reviewing examples from other organizations
 - Timeline for release

ACTION: *Dave Martinsen* and *Leah McEwen* will consider next steps to discuss with SCDS.

4. Update on the status of the Gold Book

- Please see migration project proposal previously circulated to SCDS, now submitted
- Stuart gave an update
 - had to use the WayBackMachine to retrieve some files
 - overview of the migration of data to stable storage and structure
 - next focus on digital access (incls simple API) and mechanism for updating terms (goal from previous project)
 - code files and documentation will go up in GitHub repository

ACTION: *Stuart Chalk* will periodically update SCDS on the Gold Book progress.

5. 2017 conferences and workshops

- EBI, UK March - InChI / Open structures workshop
- ACS San Francisco, April - CRDIG discussion session: chemistry publishers forum on data publishing, managing identifiers for researchers, use cases for chemical identifiers
- RDA Barcelona, April, CRDIG open session, use cases for chemistry data/information
- Beilstein Institute: Chemistry Data Management symposium, May
- IUPAC World Congress, Chemistry Data / Big Data, July
***Special Issue of Chemistry International**
- InChI User Meeting (cheminformatics and beyond), DC, Aug
- ACS DC, Aug - symposia on: Open Structures, Data Publishing, Safety information/data exchange as a global concern
- RDA Montreal, September

Respectfully submitted,

Leah McEwen, Co-Chair, Subcommittee on Cheminformatics Data Standards

February 11, 2017