

## ToxML Project Advisory Board

### **Minutes of the Meeting held on 22<sup>nd</sup> July 2014 at 16.00 BST**

Attendees: Ash Ali, Kirk Arvidson, Dan Benz, Dave Bower, Bertrand Dagallier, Philip Judson, Shree Nath, Igor Tetko and Joerg Wichard.

#### 1. Minutes of the meeting held on 28<sup>th</sup> April 2014 and actions from them

No errors were detected/reported and the minutes were circulated.

#### 2. Report on Progress

Joerg was unable to discuss ToxML during the eTox consortium meeting (held in Paris, May 2014) but confirmed that a postdoc who is working on SEND (and is also on the eTox project) has joined Bayer. Philip said she would be welcome to join the ToxML group.

Philip – PhUSE collaboration. Gitte Frausing and colleagues are looking at data not currently in SEND and perhaps looking at an extension to SEND that would cover the data. They are also looking at alternative formats. Philip and Ash had a teleconference with Gitte and agreed to pilot a study where data from a micronucleus study assay could be represented in the ToxML environment. Some discussion with Dave has taken place and a teleconference meeting with the PhUSE group has been scheduled for 12<sup>th</sup> September 2014.

Shree – How data gets formatted in various standards is one issue, another is how to model custom domains. SEND looks at exchanging and modelling data from an individual subject level. It has a general comments field but no layered structure to encompass additional study findings, summary findings etc. ToxML on the other hand can deal with additional study findings in a more structured way. SEND reflects the needs of the FDA reviewers who want unbiased data and perform independent analyses.

Dave – We need a more formalised schedule for ToxML specification updates and reviews. Philip agreed that Dave, Ash, and he should decide on a schedule with the aim of ensuring that updates take place at least as often as that but still allowing earlier updates if the need arises.

Philip - During conversation, Gitte Frausing suggested that we need to have immediately accessible information on the website telling visitors to the site ‘what can ToxML do for me’. Dave and Kirk indicated their willingness to help with this. Dave mentioned that some of the FDA SOP guideline might be a useful source of ideas.

Action: Ash/Philip to draw up draft wording for the website. Dave/Kirk to supply suggested source material for this to Ash/Philip.

Ash mentioned the RDF version of SEND that has been developed by the PhUSE group and proposed it could be a component in ToxML – Dave confirmed that this could be a possibility but pointed out that CDISC is also working on an RDF representation of SEND. Shree explained that an XML CDISC dataset is being piloted by FDA for clinical studies and some

sponsor companies are testing it out. However there are problems with using XML for large datasets because it is so verbose. E.g. the XML representation of a two year carcinogenicity study resulted in over ninety pages.

Dave said that although XML is verbose, they find that it compresses very well into a zip file, with a compression ratio of about 95:1.

Dave has been working on ToxML specification and has added new tag values for analytical methods such as HPLC.

Bertrand reported that the OECD has finalised the revision of twelve Harmonised Templates. He will circulate details to the TSO advisory board via Ash. The OECD is also working with ECHA (on IUCLID) and they have identified revisions or amendments to some templates. They are about to launch a consultation on two new templates that collate information on 'Use and Exposure'. A draft template for intermediate effects is being prepared by EC Joint Research Centre.

Dave said he is working with Kirk on result findings for longer term studies and how these results are reported. This update can be added to the online specification. Shree said the Inhand working group of the Society of Toxicologic Pathology are doing something similar and it might make sense to collaborate. Dave agreed.

#### 4. Publicity/promotion: any new opportunities

OpenTox Euro 2014: 22-24, September 2014, Athens, Greece.

Philip will be hosting a session on metabolism at this event. He will be networking with delegates and will promote ToxML.

#### 5. AOB

Shree recommended having more communication between the quarterly meetings and that perhaps updates could be provided via email as to what progress is being made etc. Philip agreed and thanked Shree for pointing this out. He will liaise with Ash to initiate regular discussions and progress updates. Ash mentioned this could perhaps be via a page on the website.

Relating back to his comment earlier in the minutes, Dave said that we need to review procedures for releasing new versions of the specification. E.g. how will his additions for HPLC data are rolled out.

#### 6. Date of next meeting

The next meeting will be held in November 2014 to coincide with the AGM.

Ash will set up a Doodle poll to find a suitable date.