

ToxML Project Advisory Board

Minutes of the Meeting held on 26th March 2015 at 14.00 GMT

Attendees: Ash Ali, Kirk Arvidson, Bertrand Dagallier, Joop Deknecht, Philip Judson and Joerg Wichard.

Apologies for absence were received from Dave Bower.

1. Minutes of the meeting held on 13th November 2015 and actions from them

The minutes were approved with no matters arising.

2. Report on progress

The Chair picked up on the following items which have not been addressed or are still in progress since the last meeting:

i). Wiki website

We need to have accessible information on the website giving practical advice to visitors such as 'what can ToxML do for me'. Dave and Kirk indicated their willingness to help with some material for this. Dave mentioned that some of the FDA SOP guidelines might be a useful source of ideas.

Philip confirmed this has now been prioritised and apologised for the delay.

Action: Ash/Philip to draw up draft wording for the website.

Dave/Kirk to supply suggested source material for this to Ash/Philip – on-going.

ii). New tag values for analytical methods such as HPLC

Dave confirmed (at the last meeting) that this is still in draft format and not yet added to the specification.

Action: Dave to confirm the progress on this.

iii). Addition of results for long term toxicity studies

Dave has been working with Kirk on result findings for longer term studies and how these results are reported.

Kirk confirmed this was in progress, some changes to the schema have been suggested as well as some changes to Leadscope's database builder tool.

Philip commented that if this is a large task we should break it down and have staged deliverables.

Action: Ash/Philip/Kirk/Dave to decide on this following the meeting.

Bertrand provided further details on latest developments at OECD; template updates posted on the public website (see attached pdf). The information was communicated to the members of the advisory board prior to the meeting via email.

Ash commented that it would be useful if Bertrand could indicate which of these templates should be given priority for adding to the ToxML schema. Bertrand said that he would look into this and provide some feedback.

Action: Ash/Philip/Bertrand, prioritise OHTs that need to be added to ToxML.

3. Publicity/promotion: any new opportunities

Ash attended the recent Computational Science Symposium (CSS), organised by the Pharmaceutical Users Software Exchange - PhUSE. The meeting took place in Silver Spring, USA during 15-17 March 2015. Ash presented a poster detailing the work that was done in collaboration with the PhUSE nonclinical roadmap team. The results from this work have been incorporated into the working draft of the specification, details of this are provided below. Ash will be adding this poster to the ToxML website in due course.

Philip mentioned that an important point about this work was that as far as ToxML was concerned we updated the ToxML schema, as a result from this study without any major delay whereas in the case of SEND further agreement/consent would be required before the standard could be updated. Philip reiterated that there is distinction between SEND and ToxML in that ToxML is not a standard for sending data to a regulator; it is a tool for exchanging data more generally.

UK-QSAR 2015: Thursday 21st May 2015, Lhasa Limited, Leeds, UK.

The agenda includes toxicity and metabolism sessions, as well as a panel discussion. This is being hosted by Lhasa and hence there could be an opportunity to present some ToxML work.

SETAC: 3-7 May 2015, Barcelona, Spain

Philip will be attending and will network with people there.

ACS National Meeting & Exposition: August 16-20, 2015, Boston, MA, USA.

Kirk mentioned he may be attending.

Joerg mentioned an iPiE meeting that will take place in Barcelona following the SETAC conference. Although he will not be attending he will mention ToxML (as a way to handle data) to another colleague who will be at the meeting.

Bertrand provided an update on the new templates on 'Use and Exposure'. These have now been officially approved. They will now be translated into a practical template that will be available publically on the OECD website. This job is currently subcontracted to ECHA but may be delayed as ECHA are working on IUCLID 6, but he hopes that it would be complete in a few months.

Philip commented that this is something that we should also talk to ECHA about as it is important to ToxML.

Action: Ash/Philip/Bertrand to consult ECHA.

4. ToxML specification updates schedule

Dave was unable to attend the meeting so could not provide full details of the updates that were due for delivery this quarter. However he was able confirm (after the meeting via email) that the extension to the Results section of the micronucleus assay (work done with the

PhUSE group) has now been added to the Working Draft version of the specification. This can be viewed here:

<https://toxml.lhasalimited.org/working-draft/study?studyTag=InVivoMicronucleusStudies&path=/InVivoMicronucleusStudies/Study/Tests/Test/NegativeTestControls/TestControl/TreatmentGroup/Results/IndividualResults/IndividualResult#/InVivoMicronucleusStudies/Study/Tests/Test/NegativeTestControls/TestControl/TreatmentGroup/Results/IndividualResults/IndividualResult>

I attach a copy of the updated schedule to these minutes (see Appendix 1 below).

5. AOB

Joerg mentioned that the new person working on SEND implementation at Bayer also attended the PhUSE meeting in Silver Spring, last week and it may be appropriate for them to be invited to the next ToxML meeting.

Action: Joerg to provide contact details of his colleague to Ash.

Joop briefly mentioned the Effectopedia project by the OECD (an open-knowledge aggregation and collaboration tool designed to facilitate the interdisciplinary efforts for delineating adverse outcome pathways (AOPs)) and suggested that an update/presentation on this project could be given at the next meeting and collaboration might be possible.

Action: Ash to add this as an agenda item for the next meeting.

Kirk commented that he was developing some SOPs for data entry using the database builder tool. These have been recently updated and efforts are underway to make them generic so that other projects could use them. Ash and Philip both confirmed that this would be useful information to append to the ToxML website.

Action: Kirk to provide details of this when ready to Ash/Philip.

6. Date of next meeting

The dates for the remaining three meetings have now been fixed. The next meeting will take place on Thursday 25th June 2015 at 2pm BST.

Appendix 1: ToxML specification updates schedule

	Details of Update	Delivery Date	Owner	Status
1	In vivo Micronucleus Assay extension to Results to capture individual species results (PhUSE collaboration).	Quarter 1: March 2015	D Bower	Complete
2	New tag values for analytical methods such as HPLC.	Quarter 2: June 2015	D Bower	In Progress
3	Addition of results for long term toxicity studies – Stage 1.	TBC	D Bower/K Arvidson	New