

ToxML Project Advisory Board

Minutes of the Meeting held on 15th January 2013

Attendees: Philip Judson, Ash Ali, Dave Bower, Dan Benz, Bertrand Dagalier, Ahmed Abdelaziz, Igor Tetko, Joerg Wichard, Rupert Kellner, Liz Covey-Crump and Mukesh Patel. Apologies for absence were subsequently added by Philip for Nina Jeliaskova. She had not received connection details and Philip did not pick up an email from her requesting them until after the meeting.

1. Minutes of the meeting held on 1st October 2012 and actions from them:
 - a) No errors were detected/reported in the minutes circulated from October 2012 and they were approved.
 - b) Philip and Ash have written a short summary/introduction about ToxML. This document is available from the Publications section of the website:
<http://toxml.org/posters/A%20Brief%20Introduction%20to%20ToxML.pdf>
 - c) Compatibility with SEND: Shree Nath has not been able to attend any meetings to discuss this. Dan was unable to find any contacts relating to SEND other than the ones we already know about.
 - d) Approaching data/software suppliers – contacts who registered for the vICGM (webinar) were sent details of this meeting.
 - e) Publicity/promotion – Ash has submitted an abstract for the SOT 2013 conference.
2. Report on presentation to OECD IUCLID Users' Group at ECHA on 3rd December 2012:
 - a) Both Ash and Philip attended this meeting and found the event very useful. Encouraging feedback was received from ECHA and it was agreed that a follow up meeting would be organised.
 - b) Bertrand also commented that there was a high level interest in ToxML during the meeting and reiterated that it would be good to build a relationship with Templates/IUCLID Users' Group.
 - c) An internal Lhasa report had been written and the parts relevant to the ToxML project will be circulated to the TSO Advisory Board.
3. Discussion on how to increase contact with the SEND community:
 - a) It has not been possible to meet with Shree Nath (despite a number of attempts) and hence there has been no progress.
 - b) Philip asked if anyone knew any other person or organisation we could work with.
 - c) Dan stated that SEND is likely to become mandatory for submitting reports to FDA (in US). The general consensus is that SEND is not satisfactory for QSAR work. This potentially limits the usefulness of submitted data to, for example, CDER, but since SEND is sufficient for its original purpose of

making regulatory submissions it is difficult to make a case for FDA to support a different format.

4. Approaching data producers and software suppliers:

- a) A number of suggestions were made. These included scientific software developers and suppliers and CROs. Joerg commented that he and Andreas Sutter are keen to see ToxML used in the eTox project. Philip stated that he is encouraging Lhasa to push this forward but he is aware that the timeframes are such that it may not be possible to implement ToxML in the eTox project before the current project comes to an end.
- b) Ahmed from eADMET is interested in ToxML for QSAR work. Igor agreed and mentioned that he would forward to Philip information on another data sharing project proposal where ToxML may be relevant.
- c) Dan stated that CROs are the obvious target. He said that many of them will be at the SOT and it would be wise to organise meetings with them there.

Action Item: Ash and Philip: arrange for someone to visit the CRO exhibition stands at SOT.

Action Item: Igor: forward information on the data sharing project.

5. Discussion on long-term funding:

- a) Philip made the case that we were not looking for large amounts of funding but we need a small amount to keep the project running. Currently Lhasa and Leadscope are facilitating the project at no charge. One approach might be for people who use the standard to pay a small membership fee.
- b) Dan commented that if ToxML was backed by a recognised scientific society/company/organisation (e.g. SOT, ACS or RSC) it would give it more credibility. Perhaps such an organisation might provide some modest funding.
- c) Philip wondered how the UNICODE standard is funded, Joerg explained that it is maintained by a consortium of software companies who pay a small membership fee.

Outstanding Action Item: (from the previous AB meeting) Philip/Ash to deliver a discussion document on options for long-term funding.

6. Publicity/promotion: any new opportunities:

- a) SOT 2013: The draft for a poster has been prepared and this will be exhibited by Mukesh Patel from Lhasa on behalf of Ash, who cannot attend due to other commitments.
- b) Board members were invited to comment on the poster and also asked to take any opportunity to present ToxML in meetings that they might be attending this year.
- c) Igor pointed out that if data was available in ToxML format publically, this would make it more aware to everyone. Philip wondered if OpenTox data

could be made available in ToxML format and, if so, whether we could have a link to OpenTox. He said he would also find out if Lhasa and/or Leadscope had any data they were willing to make public in ToxML format on their websites.

- d) Dan also mentioned potential opportunities at the American College of Toxicology (ACT) and Genetic Toxicology Association (GTA) meetings in 2013
- e) Mukesh identified the International Conference on Chemical Structures (ICCS) meeting series as another potential opportunity for publicity. URL: <http://bulletin.acscinf.org/node/258>

7. AOB:

- a) Philip promised to send minutes/information to Rupert Kellner who attended on behalf of Inge Mangelsdor (Fraunhofer Institute for Toxicology and Experimental Medicine) but joined the meeting as it was coming to an end because of a misunderstanding about the start time.

8. Date of next meeting:

- a) Dave Bower was asked to set up a doodle poll for a meeting during April 2013. We should avoid the second week, as it would clash with OECD and ACS meetings.