

DRAFTAGENDA

26.011.2015

Workshop on CEFIC LRI Project EEM9.3

Linking LRI AMBIT Chemoinformatic system with the IUCLID Substance database to Support Read across of Substance endpoint data and Category formation

Venue: CEFIC Offices in Brussels

Date: January 21, 2016, 10.30 – 16.00 h

Topics

- 1. 10.30 – 10.15 Welcome to the CEFIC LRI Workshop**
(Bruno Hubesch)
- 2. 10.30 – 11.00 Project Overview**(Volker Koch, Clariant)
 - Accessibility of IUCLID substance data
 - Extracting relevant substance data from IUCLID using data filters
 - Use of the LRI Chemoinformatic System AMBIT to assign structures to substance constituents, impurities and additives
 - Implement workflows for Read across of Substance endpoint data and Category formation
- 3. 11.00 – 11.30 IUCLID Substance Data**(Joachim Schneider-Reigl, Clariant)
 - IUCLID Substance Identity Concept: Characterisation of a substance using constituents, impurities and additives
 - Extracting data from IUCLID using filters which can be fine tuned
- 4. 11.30 – 12.00 AMBIT Chemoinformatic System**(Nina Jeliaskova, Ideaconconsult Ltd)
 - Enhancing AMBIT Version 2.1 to allow import of IUCLID substance data
 - Implementation of different search functionalities related to structures, substances and endpoint data
 - AMBIT user management system to grant access rights via roles
 - IT Technique necessary to run AMBIT
- 5. 12.00 – 13.00 Lunch**

6. 13.00 – 13.30 Assessment Workflows for Read across and Substance Category formation (UdoJensch, Clariant)

- General aspects on non-testing approaches
- How to support an assessor in establishing a justification for a read across / category formation
- Elements of the read across / category formation workflow
 - Steps in the workflow
 - Reporting

7. 13.30 – 14.00 Demonstration of the Use of AMBIT (Qiang Li, Clariant)

8. 14.00 – 14.15 Technical Implementation of AMBIT (Nina Jeliaskova, Ideaconsult Ltd)

9. 14.15 – 16.00 Hands on AMBIT functionality using the own notebook (all interested)