What's new in Toolbox 4.1 (compared with Toolbox 4.0)

Document tree:

1. Filtering by test conditions is specified in the document tree

Data matrix:

1. Sorting/ Filtering by mathematical functions (e.g. average, all)
2. Predefined substance type - "Unspecified" is replaced by "Mono constituent"
3. Calculating parameters for mixtures – parameters are calculated for each of the multiconstituent component
4. Possibility to add structure in current list loaded on data matrix (right click "Add in category")
5. Expand on one click data matrix cell when there are more than one result in it

Input:

1. Save/Load – save and load the whole work in the document
2. Define target endpoint was improved by adjusting the number of fields
3. Custom parameters can be defined, e.g. using external values for logKow
4. QueryTool search in ECHA Chem can be implemented
5. QueryTool: possibility to search by structural similarity is available
6. Chemical structures are identified by list with CAS numbers
7. CAS numbers are identified by a list with smiles respectively
8. Loading *.mol files is possible

Profiling:

1. Panel was improved by more compact organization of buttons (Filter, Sort, Grouping buttons are smaller)
2. Description of the queries with using metabolism in the profiling schemes was improved
3. The coordinates of the nodes in dendroid schemes are saved
4. "Explain" option of the profiling results is improved

5. The table with toxicological relations effect-organ for RDT profiler is added
6. Profile statistics for a list of chemicals with metabolism is available

A. New profilers

1. Protein binding alerts for Skin sensitization according to GHS classification (for predicting GHS classification)

B. Updated profilers or profilers not implemented in 4.0

1. OECD HPV Chemical Categories
2. Protein binding alerts by OASIS (general mechanistic)
3. Protein binding alerts for chromosomal aberration by OASIS
4. Biodeg BioHC half-life (Biowin) is available, now
5. Hydrolysis half-life (pH 6.5-7.4) is available, now

C. Updated Metabolism simulators:

1. Autoxidation simulator
2. Hydrolysis simulator (acidic)
3. Hydrolysis simulator (basic)
4. Hydrolysis simulator (neutral)
5. in vivo Rat metabolism simulator
6. Microbial metabolism simulator
7. Rat liver S9 metabolism simulator
8. Skin metabolism simulator

<u>Data:</u>

A. New databases

1. REACH Skin sensitisation database (normalized) – containing curated LLNA (EC3) data as extracted from the REACH dossiers

B. Import/Export

1. Import to IUCLID 6 via web services

Category definition:

1. "Alert performance" functionality is improved
2. Category definition by "Define with metabolism" is improved

Data Gap Filling

1. Domain of prediction is visualized and can be saved as a custom profile or SAR
2. Endpoint vs. Endpoint – the relationship between categorical endpoints is visualized by chart
3. Notification is provided for the chemicals that are not able to be visualized in data gap filling graph due to no value of required x-descriptor
4. TIMES and Catalogic models are docked

Report

1. Data matrix – possibility to report the data matrix
2. QMRF and CCRF – templates for preparing QMRF and CCRF are provided