

What's new in Toolbox 4.x (compared with Toolbox 3.4)

A. Core modules features:

1. Expanded chemical identification
2. SMART language and 2D Editor (overview)
3. Structural similarity expanded with PubChem features
4. Expanded species taxonomy
5. New format of the Report
6. New database management server-PostgreSQL

B. New functionalities:

1. Added target endpoint concept for workflow streamlining
2. Reliability scores for Databases and data
3. Relevancy of profilers to the target endpoint
4. Alert performance calculation for:
 - a. alert identified in the target
 - b. alert identified after AU or SM activation
5. Automated/Standardized workflows for:
 - a. Skin sensitization
 - b. Ecotox endpoints
6. Quantitative metabolic information and related functionalities
7. Pilot predefined prioritization scheme

C. New Profiling schemes:

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

D. New databases

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

E. User interface modifications:

1. Document tree manipulation
2. Filtering/Sorting/Coloring of resources (profilers and databases)
3. Helpers
4. Display active and background working actions status
5. Calculating parameters for mixtures – parameters are calculated for each of the multiconstituent component
6. Define target endpoint was improved by adjusting the number of fields
7. Panel was improved by more compact organization of buttons (Filter, Sort, Grouping buttons are smaller)
8. Description of the queries with using metabolism in the profiling schemes was improved
9. The coordinates of the nodes in dendroid schemes are saved
10. "Explain" option of the profiling results is improved
11. Protein binding alerts for Skin sensitization according to GHS classification (for predicting GHS classification)
12. "Alert performance" functionality is improved
13. Category definition by "Define with metabolism" is improved
14. 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
15. Data matrix – possibility to report the data matrix