

QSAR Toolbox 3.1

Release Notes

Document history

Version	Comment
Version 1.0	12.01.2013

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Language: English

If you have questions or comments that relate to this document, please send them to ehscont@oecd.org or visit the QSAR Toolbox discussion forum at: https://community.oecd.org/community/toolbox_forum

Overview

The Toolbox 3.1 installation is a minor update distributed as a standalone installation as well as a patch to Toolbox 3.0. When applying patch, upon first start of the application, an update procedure will be performed on the database. It is a onetime operation that should not be canceled.

System Requirements

Minimum system requirements

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OS: Windows 2000, Windows XP, Windows Vista, Windows 7
CPU: Pentium 4 1GHz
RAM: At least 1GB of RAM
HDD: 10 GB free hard drive space
File system: NTFS

Recommended system requirements

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OS: Windows XP or newer
CPU: Pentium 4 2GHz or faster processor
RAM: 4GB of RAM
HDD: 12 GB free hard drive space
File system: NTFS

Change log

I. Observed databases:

1. Observed Rat In vitro metabolism database – one new chemical is added to current database
2. Observed Rat In vivo metabolism – new database

II. Simulators:

1. Autoxidation simulator – changes in transformation table are applied regarding polycyclic aromatic fragments
2. Autoxidation simulator (alkaline medium) - changes in transformation table are applied regarding polycyclic aromatic fragments
3. Rat liver metabolism – changes in transformation table are implemented regarding polycyclic aromatic fragments
4. Skin metabolism simulator - changes in transformation table are implemented regarding polycyclic aromatic fragments
5. Microbial metabolism simulator - changes in transformation table are implemented regarding polycyclic aromatic fragments

III. Profilers

1. DNA binding by OASIS v.1.1. - One additional structural boundary has been added to category "Haloalkanes with electron-withdrawing group at beta-position"

IV. General

1. Feature: Study pad rewritten to accommodate different multiplications for a single chemical
2. Updated EPI suite reports for some of the database chemicals
3. Added list of last entered target chemicals (Input>Select or F7)
4. Added list of last open files (Input>List)
5. In subcategorization window long category names are shown in hint window
6. About widow of databases/inventories uses common about form of other Toolbox objects
7. Added option user to control showing of different warning messages (Options>Main\Warning messages)
8. Query tool is activated by F3 key; Query in data matrix by Ctrl+F3
9. Implemented additional ways of input of quantity for mixtures (fraction, mass concentration, volume concentration)
10. Domain of prediction in Gap Filling can be viewed before saving the model or accepting the prediction
11. Default Gap Filling calculation options are available on Toolbox options form
12. Different modes for marking of chemical sets in Gap Filling based on X descriptor values are implemented; they are available on Toolbox options form
13. Some improvements in the content of "Summary" section of TPRF were made:
 - Information for belonging of target chemical to model domain is added to Summary page
 - Phrase "degradation product" is changed to "metabolite/trans.products"
 - Information for test "duration" used for obtaining the prediction is added
14. Efficiency improving of query tool searching: new functionality is implemented allowing to search structures by :
 - aromatic forms – searching structures with conjugated double bonds
 - as it is – searching structures as entered into the system
 - any – searching structures by their skeleton structure
15. Visualization of quantities of hydrolyzing products on datamatrix
16. New functionality allowing to calculate 2D and 3D parameters separately
17. Additional help information for "Independent" and "Similar" mode of action is added to F1 help.
18. BUGFIX: Gather data - with "from tautomers" also gathered data from structures with same CAS which are not tautomer.
19. BUGFIX: Query tool - search by name is now case insensitive.
20. BUGFIX: Query tool - reduced list with most used metadata fields.
21. BUGFIX: Query tool - added different structural modes sub-fragment search.
22. BUGFIX: Query tool - fixed an access violation when searching an empty metadata field
23. BUGFIX: Import - Fixed a case where polymer structure where incorrectly marked as mixtures.
24. BUGFIX: 2DEditor - SMILES pasted in 2DEditor with defined quantities in mol or weight % where not parsed correctly.

25. BUGFIX: Server - log was reporting same message multiple times.
26. BUGFIX: Server - changed library compared to Toolbox installation for core features.
27. BUGFIX: Statistic for recalculated QSAR models was incorrect
28. BUGFIX: When displaying the training set of newly created model the endpoint tree path appeared; now it changed to the endpoint
29. BUGFIX: When deleting predictions from QSAR some other predictions were also deleted
30. BUGFIX: When applying a QSAR containing clauses for filtering of tautomers, the applicability domain for the target chemical was not calculated correctly
31. BUGFIX: Action "Create new QSAR" didn't work
32. BUGFIX: Chart title of Gap Filling window in QSAR mode reported incorrect number for visible/invisible points
33. BUGFIX: When filtering by WS and no descriptor was selected, the system crashes
34. BUGFIX: When changing the Gap Filling approach (RA to TA, or vice versa) the descriptors on "Adequacy" chart disappeared
35. BUGFIX: After positioning the mouse over Gap Filling actions list (right panel), help tip appears/disappears very quickly
36. BUGFIX: Report creation failed if domain explanation contains square brackets
37. BUGFIX: In TPRF, "Summary" section, some of table headers were partially hidden
38. BUGFIX: In TPRF "degradation product" was changed to "metabolite/transformation product"
39. BUGFIX: The species in TPRF sometimes were not reported correctly
40. BUGFIX: The picture of Gap Filling chart, which appears in TPRF sometimes contained selected points
41. BUGFIX: Uncertainty of prediction was missing in the report (TPRF 4.4)
42. BUGFIX: When reporting a prediction from QSAR the value of prediction in TPRF was reported in original dimension of QSAR, but not in the default dimension of data matrix
43. BUGFIX: When reporting a prediction of mixture based on predictions from two different QSARs, some of sections of TPRF contained incorrect information
44. BUGFIX: incorrect save of similarity subcategorization threshold in model domain
45. BUGFIX: calculating of similarity as 2D calculator
46. BUGFIX: wrong conversion of temperature in F
47. BUGFIX: bug when resize chart in profiling report window
48. BUGFIX: flashing of "Save as" button in reporting

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