

Laboratory of Mathematical Chemistry

What is new in OASIS CATALOGIC platform?

v. 5.19.1

I. Modifications in the platform

- Removal of Firebird dependency (infrastructure update). The CATALOGIC platform has been fully decoupled from the Firebird database management system. Users no longer need to install or configure Firebird to execute the latest CATALOGIC models. This optimization is driven by upgrades to the OASIS software, which now handles all file operations natively in-process, delivering a more streamlined installation experience.
- Docking with OECD QSAR Toolbox ver.4.9.
- Exporting QSAR predictions to IUCLID 6 (compatible with TETRA v.10) according to the latest QAF (QSAR Assessment Framework) recommendations. Implemented a IUCLID export includes:
 - Bespoke mapping for OASIS models to their respective IUCLID template
 - User Interface (UI) for guiding the export procedure
 - QAF section (with Similar Substances with Experimental Data list). A QAF-related section is integrated within the exported IUCLID dossier. It includes support for handling/exporting the *“SimilarSubstancesWithExperimentalData”* list and representing analogue substances used to support and justify the predictions.
 - Attaching files to the exported datapoint (reports, training sets, reference materials, and other relevant attachments required to provide full traceability and context for the exported data)

II. Modifications in the models

- Biodegradation models
 - OECD 301C model

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Exporting QSAR predictions to IUCLID 6.

- OECD 301F kinetic model

Exporting QSAR predictions to IUCLID 6.

- OECD 301B kinetic model

Exporting QSAR predictions to IUCLID 6.

- Bioaccumulation models

- BCF base-line model

- Exporting QSAR predictions to IUCLID 6.
 - Some changes have been made to the model transformation table related to the improving the simulated metabolism for Okoumal.
 - Theoretical support files for 35 transformations

- BCF base-line D/P model

Exporting QSAR predictions to IUCLID 6.

- BCF base-line model for PFAS

Exporting QSAR predictions to IUCLID 6.

- Hydrolysis models

- Acidic hydrolysis model

- Exporting QSAR predictions to IUCLID 6.
 - Some changes in the transformation table - modification in reaction "Keto-enol tautomerism.

- Hydrolysis model pH5

- Exporting QSAR predictions to IUCLID 6.

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- Some changes in the transformation table.
 - A new applicability domain has been extracted because of the new version of Domain Manager.
- Neutral hydrolysis rate constant model
 - Exporting QSAR predictions to IUCLID 6.
 - Some changes in the transformation table - modification in reactions in “Sulfonyl halides hydrolysis” and “Thioamides hydrolysis”;
- Acute aquatic toxicity models
 - Exporting QSAR predictions to IUCLID 6.