Led by the developers:

Organized by:

QSAR APPLICATION TOOLBOX
ADVANCED VIRTUAL TRAINING WORKSHOP – Part I
AGENDA

Day 1

I. **Cramer profiling scheme -** The Cramer classification scheme is widely used for assessing the toxicological profiles of chemicals. In QSAR Toolbox, the latest version goes beyond the original approach, incorporating key expansions and updates developed in collaboration with experts from the EFSA Working Group on Flavourings. Explore the enhanced, comprehensive reporting that provides detailed insights into the structural features of your target chemical, along with a clear, transparent profiling pathway—supporting more informed and reliable decision-making and strengthen regulatory acceptance with confidence.

II. **Building knowledge platform and usage –** You know what a Toolbox profiler is—but do you know how to create your own? Learn how to build custom profilers using your expertise and apply them effectively for (sub)categorization and screening purposes. Explore practical examples, including building a profiler to identify precursors of challenging metabolites like non-degradable or known toxic substances.

III. **(Q)SAR models in QSAR Toolbox –** QSAR Toolbox offers a rich library of ready-to-use well known (Q)SAR models for various properties (such as the ECOSAR and Danish EPA models) —learn how to apply them to predict your target chemicals. Go a step further by discovering how to build and customize your own (Q)SAR models, giving you greater flexibility and control in your assessments.

IV. **Toolbox Repository –** Want to expand your Toolbox capabilities with publicly available modules? Discover the Toolbox repository, explore a wide range of profilers, (Q)SAR models and databases and learn how to easily upload and integrate them into your installation. Unlock new functionalities and make the most of the tools available to you. Strengthen your read-across hypothesis by effectively integrating results from VEGA, KATE, OPERA and other models directly within the Toolbox.

V. **Workflow editor –** a powerful new feature in Toolbox that lets you design and implement your own decision schemes for screening and/or prediction. Learn how to build automated workflows that follow your logic step by step—saving time, increasing consistency, and streamlining your entire analysis process. Practice with a simple example to automatically find chemicals sharing the same mechanisms and organic functional groups.

VI. **Custom calculators –** Learn how to create your own calculator for predicting 2D and 3D properties using experimental data (e.g. for logKow). You'll also discover how to apply it as a descriptor in the data gap filling process—enhancing the accuracy and reliability of your predictions.

VII. **Import/export of data –** Learn how to import your custom databases into QSAR Toolbox, including seamless integration with IUCLID. Take advantage of Toolbox–IUCLID interoperability to transfer your Toolbox predictions directly into your IUCLID database, and strengthen them in line with QAF criteria. You'll also discover how to enrich your assessments by importing additional toxicological and metabolism data from the Toolbox Repository.

Day 2

I. **Handling of mixtures –** Learn how to define your mixtures in QSAR Toolbox and how to specify the exact quantities of each component. Discover how to predict mixture properties based on whether components share a similar mode of action or act independently and generate the relevant specific Toolbox report —helping you to make more accurate and scientifically sound assessments. Examples with acute aquatic toxicity and skin sensitization will be demonstrated.

II. **Toolbox reports: justification documents –** Explore the dedicated justification documents generated alongside the main Toolbox report—designed to support your regulatory submissions with confidence. These documents incorporate the relevant RAAF/QAF criteria, tailored to the specific type of prediction, ensuring your assessments are transparent, consistent, and aligned with regulatory expectations. See practical examples on reporting cases for analogue approaches and (Q)SAR modeling results.

III. **Search in IUCLID databases. Composition search –** Unable to search directly in your IUCLID database? Once your data is transferred to QSAR Toolbox, you can leverage its powerful search capabilities. Easily search for substances, data, and even explore substance compositions for specific impurities and/or additives, e.g. searching of substances with known impurity having isocyanate fragment. Use the simple search engine, organized like IUCLID endpoints, or take advantage of the advanced IUCLID search to define detailed, precise search criteria.

IV. **Query Tool functionality –** The Query tool allow you to perform strategic searches across its databases for chemicals and/or data. Learn all the available search criteria (such as structural, mechenistic, similarity, etc) and how to combine them logically—for example, identify chemicals that are Ames-positive but non-carcinogenic according to experimental data—enabling precise, targeted data mining for your assessments and scientific work.

V. **Endpoint vs. endpoint correlations –** Learn how to correlate different endpoints using chemicals with available experimental data. Apply these correlations to explore whether in vivo endpoints (e.g., EC3 LLNA) can be predicted from in vitro data (e.g., EC3 KeratinoSens), enhancing your ability to fill data gaps efficiently by saving time and reduce the cost associated with animal testing.

VI. **WebClient – searching chemicals and data. -** Access QSAR Toolbox directly from your web browser and explore its WebClient interface. Learn how to efficiently search for chemicals and data, and discover the full range of features and capabilities the WebClient offers for a flexible and streamlined user experience.