

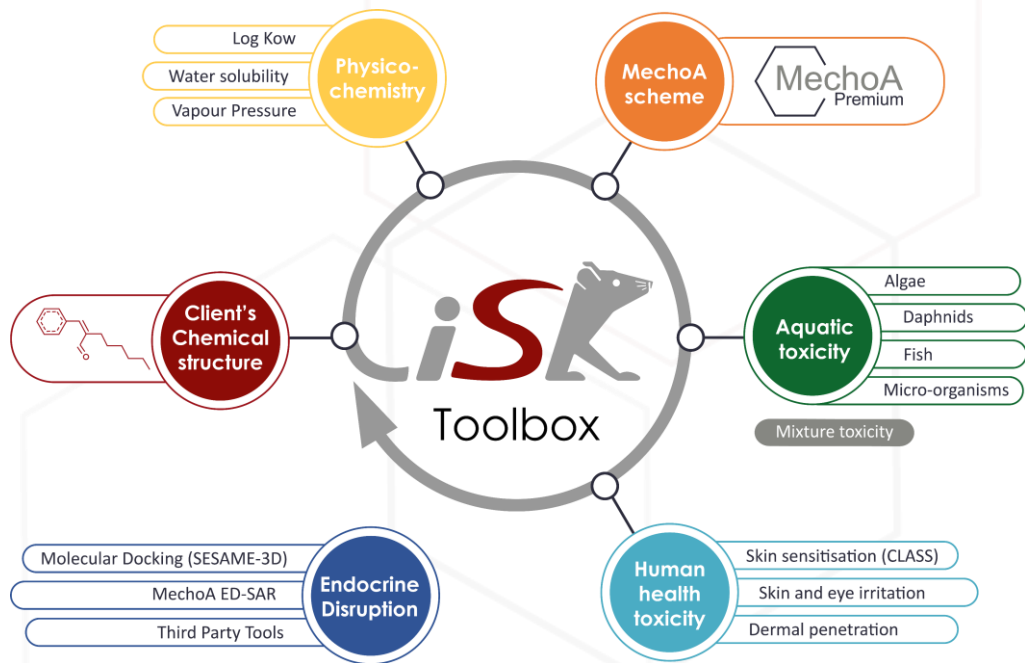
# KREATiS

Re-Thinking Experimentation

**iSafeRat®**  
*In Silico* Consulting  
3D-modelling  
Training

## New Approach Methodologies

In these days of increasing regulatory burden to ensure the safety of your products, it is important to make the right decisions for your dossier rapidly. **iSafeRat<sup>®</sup>** (in silico Algorithms For Environmental Risk And Toxicity) is KREATiS' answer offering High Accuracy QSAR (HA-QSAR) modules. Our aim is to offer the most reliable and accurate *in silico* approach to replace all kinds of experimental studies related to human health and the environment.



## iSafeRat<sup>®</sup> Platform

Our endpoint values obtain an accuracy at least as good as that from the best experimental technique available following OECD Guideline methods for a fraction of the price of a laboratory study. And in a fraction of the time. **iSafeRat<sup>®</sup>** is available in desktop version and is a valuable addition to any regulatory scientist's substance assessment tools.

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## How hazardous is my substance ?

Often one expert is not enough to evaluate the complex properties of organic molecules, even with modern third-party tools at your disposal. This is why KREATiS offers a multi-disciplinary team of expert organic chemists, (eco)toxicologists, who work together to provide the most accurate chemical profiling using a consensus approach across a host of *in silico* tools.

## *In silico* experts for faultless profiling

Our team offers expert advice and constructs solid, regulatory ready profiles based on our in-house software **iSafeRat**<sup>®</sup> and third-party softwares to predict toxicology (e.g., OECD QSAR Toolbox, Leadscope and Derek), ecotoxicology and physical chemistry endpoints for all kinds of regulatory and R&D needs.

Our substance profiles (including QMRF and QPRFs in compliance with QAF) can save you months of work and massively reduce the cost of your regulatory dossiers and time to market.



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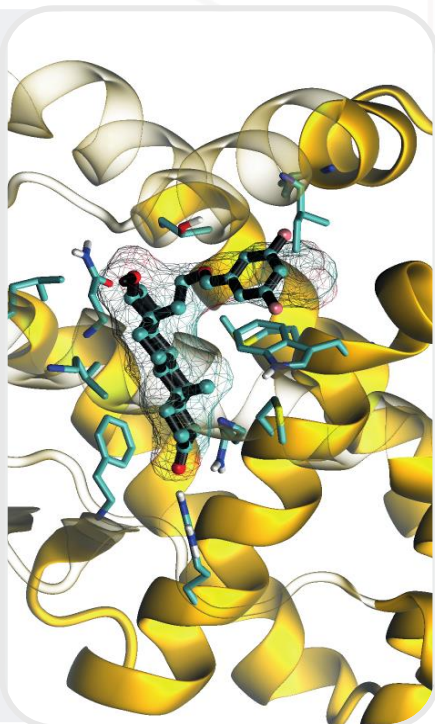
## *In silico* New Approach Methodologies

The need for mechanistic understanding of substance-biological matrix interactions in human and environmental science is increasing. Modern Computational Biophysics integrates 3D-modelling tools, a step in the direction of predicting specific molecular impacts induced by chemical substances, not just for Endocrine Disruption, but for a host of other proteins.

## SESAME-3D

The KREATiS model, **SESAME-3D**, offers computational evaluation of protein-ligand interactions, where any organic molecule can be tested against customized biological applicability domains. Currently, many EATS receptors are covered as mentioned in the ECHA/EFSA guidance (2018).

Extra biological targets can be included in a study depending upon the availability of experimentally derived structural models for the requested proteins. Consult us now to see whether we can derive a complete 3D-structure for your needs.



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## Struggling to get a grip on *in silico* modelling ?

There are a host of *in silico* tools around that you can use to fill your regulatory dossiers or to screen your substance portfolio. However, many of those tools are not so easy to use or interpret without a huge boost in hands-on experience (notably the vast **OECD QSAR Toolbox** software). A specific training on **iSafeRat®** platform can also be included.

## Let KREATiS help you hone your *in silico* skills

All KREATiS training courses are intensive and hands-on. You will get to use the software and will have ample time to work through practical examples and really get to understand how to use the tool efficiently and interpret the results correctly.

The courses can be provided in English or in French and face to face or online.

Bespoke training courses can be organised according to your specific needs. Specific training for chemistry, regulatory toxicology or ecotoxicology are also available provided by regulatory expert from KREATiS.



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