

Dear friends and collaborators,

It's been almost a year since our last newsletter and there's plenty to tell you about! After the management buy-out in August last year, Carole, the team and I have been focussing on the most critical issues: consolidation of the business and investments, enlarging and clarifying our offer and strengthening our partnerships and network.

It's been intense, with major advances on our 2D and 3D "docking models" for EATS endocrine modalities and our inclusion in the French Endocrine Disruptor platform "PEPPER"; We've been working hard on the new iSafeRat® Desktop update that has come out this Summer; We've had 2 toxicology articles published in Regulatory Toxicology and Pharmacology and a third article on ecotoxicology explaining our method for predicting mixture toxicity, in Environmental Science & Technology. We also presented a bunch of posters and oral presentations or chaired sessions at the SETAC, OpenTox, EUROTOX and WC11 congresses which were all well received; Our MechoA profiler has now been included in the latest version of OECD Toolbox (v4.5); we have recruited a postdoc with expertise in physical chemistry and machine learning and a PhD student working in collaboration with University of Lorraine on ecotoxicology of mixtures; and we have launched our new website on www.kreatis.eu which is in both English and French versions and we feel is far more ergonomic, aesthetically appealing and easier to read than the previous site. We even took advantage of the lock-down situation to spruce up our offices to make them a more appealing place to work.

We hope you enjoy reading about all these updates in this November issue of our newsletter.

VISIT US AT WWW.KREATIS.EU



Come and visit our brand new website (and yes, I admit that we're quite proud of it) on: www.kreatis.eu. Now available in both English and French versions. We've packed it with all the latest information on what we do, how we do it (even why we do it!). You can find all our most critical publications, peer reviewed articles, exhibited posters, videos and magazine articles, ongoing research projects and news. We'll make much more effort now to drop useful information about technological progress, events, impactful regulatory changes etc to keep you wanting to visit our site again and again. The red door of KREATiS is now wide open!

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KREATiS "MechoA" PROFILER ACCEPTED BY OECD



In the last issue of the Newsletter, we reported that the KREATiS MechoA (Mechanisms of toxic Action) profiler has been accepted for inclusion in the OECD toolbox. Next came the hard work of beta testing the model and then getting the interface into shape for inclusion into the OECD QSAR Toolbox's complex framework. It's been a long haul but we're at last ready with a downloadable addition to the available profilers. Here's the link: <https://repository.qsartoolbox.org/>

OECD has changed policy and from now on new profilers will need to be downloaded separately. It's not so simple as you may think to install the new profilers available as you will need installation rights in your company to do it. So, we provide a link [here](#) to help you out with that phase. We can also provide training on the last version of the OECD Toolbox (v4.5).

We also recently announced [here](#) our partnership with Liverpool John Moore's University and Unilever to update the MechoA system. Stay tuned!

NEW RECRUITS: 3 brilliant individuals join the team



Introducing Emel Ay-Albrecht, PhD in organic chemistry (2012) and postdoctoral fellow at the Nakamura group at the University of Tokyo, Japan working on OLED/organic dye development. Afterwards she worked for 3 years at the Mulhouse Material Science Institute (IS2M) in Prof. Jacques Lalevée's photochemistry group as a research engineer. Recently she completed a 6-month internship in Deep Learning as part of her master's degree in Mathematics and Data Sciences. Emel joined our team in September and will integrate the most positive aspects of machine learning.



Meet Ludovic FARAVEL, who received his master's degree in Environment Management in University of Lorraine (UL), Metz in 2020, developing skills in ecotoxicology and ecosystems analysis. In 2021 he joined KREATiS in collaboration with the Laboratoire Interdisciplinaire des Environnement Continentaux (LIEC) as a PhD student to investigate the ecotoxicity of cosmetic products continuing efforts to develop iSafeRat® to predict toxicity of even more complex mixtures of chemicals in the aquatic environment.

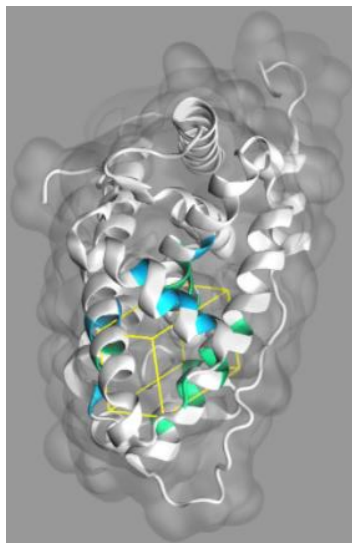


And finally, Elvire NOGUEIRA, our communication and project finance manager who obtained a bachelor's degree in 2008 at the IUT of Lille and then a degree in health in 2010 at the University of Lyon. She worked for nearly 20 years alongside healthcare professionals and as a project manager. In 2018, she created a consulting, training and support company for health and medico-social institutions. Elvire joined KREATiS in May 2021 to assist in administrative tasks, HR and financial management, quality control and communication.

KREATiS CO-MEMBER OF "PEPPER" OPPORTUNITY COMMITTEE

Detection of endocrine disruption modality of molecules, or the lack of it, is one of our highest priorities at this time. EDs have been earmarked by the European Commission and several EU Member States as a major issue but detecting them is no easy matter and furthermore, determining substances as not having endocrine modalities is even more difficult. There are 10s of thousands of substances out there with no ED related testing whatsoever. With that in mind, KREATiS wants to be a driving force in the debate sparking our decision to become a member of AFSSI, the life science association. This membership enables us to wear an AFSSI hat in the Opportunity Committee of "PEPPER", the French ED Platform, together with Watchfrog to keep tabs on future experimental ED methods.

ENDOCRINE DISRUPTORS: A DIGITAL DISRUPTION CHALLENGE



Last year KREATiS rolled out its twin approach using our in-house ED SAR coupled with a carefully selected set of Third-Party Tools and this has already met success on a bunch of different chemical classes, notably from the pesticides and cosmetics industries. After two full years of internal work effort, KREATiS is rolling out its first 3D “docking” tool which we are calling SESAME-3D (acronym for “Sampling of Simulated Structural Ensembles for SAR prediction using Molecular Mechanics”). The docking model requires our supercomputer to function and cannot be run on a normal laptop (unless you’re OK with doing nothing else for 3 days for a single estimation for just one receptor!). The first results came out early this year and we’re now finishing the validation step. Using a test battery of different *in silico* approaches, a consensus of third-party software together with our in-house 2D and 3D “docking” models. This approach can help prioritise or deprioritise organic chemicals for further research.

We are now able to provide our long-awaited triple battery to that we believe can dramatically reduce the need for resorting to experimental testing.

AFTER THE HELLO TOMORROW CHALLENGE WIN, THE BAYER PARTNERSHIP TAKES OFF

Bayer and KREATiS have concluded a partnership agreement initiating a project to create new ecotoxicity QSARs for crop protection products.

Bayer will use the iSafeRat technology in the development of new crop protection chemistries, announcing “Bayer is committed to partnering and working closely with innovative scientists to help meet the expectations of farmers and society”.



Bayer CropScience

AND FINALLY: KREATiS’ RECENT PUBLICATIONS AND SUBMISSIONS

KREATiS is pleased to announce the publication of 3 peer reviewed articles in well recognised journals as follows:

Pascal BICHEREL, Paul THOMAS (2021). Aquatic Toxicity Calculation of Mixtures: A Chemical Activity Approach Incorporating a Bioavailability Reduction Concept. *Environ. Sci. Technol.* 55, 11183. ([link](#))

Carole CHARMEAU-GENEVOIS, Satinder SARANG, Mélissa PEREA, Charles EADSFORTH, Tom AUSTIN, Paul THOMAS (2020). A simplified index to quantify the irritation/corrosion potential of chemicals – Part I: Skin. *Regul. Toxicol. Pharmacol.* 123, 104922. ([link](#))

Carole CHARMEAU-GENEVOIS, Satinder SARANG, Mélissa PEREA, Nathalie MAYER, Charles EADSFORTH, Tom AUSTIN, Paul THOMAS (2020). Simplified index to quantify the irritation/corrosion potential of chemicals – Part II: Eye. *Regul. Toxicol. Pharmacol.* 123, 104935. ([link](#))

Do let us know if you’re interested in receiving a reprint of these publications and we’ll be delighted to send you a copy in pdf format.

We hope you have enjoyed this newsletter. We’ll be back next year with more info on our activities. In the meantime, we would be delighted to receive your feedback. All the best from Paul and the KREATiS team.