Internship for a 5 to 6 month period (beginning early 2023)

Understanding anthraquinones: Creating a new building block in mechanistic based ecotoxicological and physicochemical *in silico* predictions

Synthetic organic dyes are organic chemicals that are widely used in industrial activities such as textile, printing, food and cosmetics industries and represent a yearly production volume amounting to 1000s of tons per year. And yet their potential to pollute the environment and their effects on the environment are largely unknown. To place such compounds on the European market, the Registration, Evaluation and Authorization of Chemicals (REACH) regulation requires the characterization of various features belonging to environmental hazard assessment (e.g. ecotoxicity towards aquatic organisms, physico-chemistry, fate in the environment) that are usually assessed *via* laboratory experimentation. However, for animal welfare purposes, recent regulatory texts propose guidelines for avoiding the tests performed on vertebrate animals (e.g. fish). The use of New Approach Methodologies (NAMs) like Quantitative Structure-Activity Relationship (QSAR) to predict these features represent a promising alternative to standard studies. Among the diversity of existing dyes, this internship will focus on the anthraquinone family which is especially used in textile activities. The aims will be to i) estimate the stability of anthraquinone compounds in water media as well as in the organisms of interest for regulatory purposes, ii) identify potential transformation products, iii) characterize the physicochemical and ecotoxicological (e.g. organism sensitivity, mechanisms of action) features of parent compounds and transformation products and ideally iv) build anthraquinone dedicated QSAR models to estimate their physicochemical and ecotoxicological properties.

This internship will rely on information obtained from literature and regulatory dossiers as well as investigating various modeling tools (e.g. OECD Toolbox). However, the project will not include laboratory experimental activities for the trainee. Thus the applicant must be motivated by secondary scientific research (i.e. daily work using a desktop computer to compile and analyze data and thereby discover new mechanisms) to cover the requirements for this project. We are looking for an enthusiastic, autonomous and rigorous master or engineer school student with basic knowledge and a strong interest in ecotoxicology, organic chemistry and computer modelling. Notions of programming (e.g. Python, R) are an asset.

The internship will take place at KREATiS, situated at L'Isle-d'Abeau (France) and will be supervised by a multidisciplinary team (organic chemists and ecotoxicologists). Two days of work from home per week are possible.

If you are interested in joining our team and getting experience of working in an R&D environment, send a CV and a motivation letter to Floriane Larras (floriane.larras@kreatis.eu) and Gaspard Levet (gaspard.levet@kreatis.eu) before the 30th of November.

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