Project title: Exploring the impact of pharmaceuticals on the aquatic environment

Level: Bachelor or Master

Start: Anytime

Project duration: 12 weeks to 6 months **Project form**: Data analysis (R and/or Excel)

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Description of the project

There are more than 1500 pharmaceuticals on the European market. Residues of these active pharmaceutical ingredients (APIs) can eventually reach the environment and pose a risk to the aquatic ecosystem. Assessing the risk of all pharmaceuticals is not feasible as it would require an unacceptable number of animal studies as well as a considerable amount of time and financial resources. Thus, we need to develop computational tools and models to quickly screen pharmaceuticals on the market and assess their potential environmental risk.

The <u>PREMIER</u> project brings together a multi-disciplinary consortium composed of 25 partners from the public and private sectors. Academic partners, regulators and pharmaceutical companies work together for a more sustainable future, by proactively managing the environmental impact of medicines. Considering the ethical, technical and financial constraints, the PREMIER project aims to develop tools that address environmental risks of medicines. In this context, different internship possibilities are possible. Examples follow below.

- 1. Quantification of uncertainty in the environmental risk assessment (ERA) of human active pharmaceutical ingredients. The student will access relevant data sources for human pharmaceuticals data, including the reports published by the European Medicines Agency. Environmental data will be collected and sensitivity analysis will be performed in order to identify the parameters with the highest uncertainties/impact on the risk estimation.
- 2. Linking available in vitro data in mammals with effect concentrations in freshwater species. To this purpose, the student will access the ToxCast database, developed by the United States Environmental Protection Agency. The relationship between in vitro data in mammals and in vivo/in vitro endpoints in freshwater species will be explored. Results of these analysis will be explored to derive an in vivo-in vitro extrapolation factor.
- 3. **Development of a QSAR model to predict ecotoxicity effects of pharmaceuticals in aquatic species**. The model should combine chemical properties (i.e., molecular descriptors), genomics information and consideration on the mechanism of action. The student will perform a literature search to identify the state-of-art and to define the methodology of the study. This step will be followed by collection of relevant data, development and validation of the model.