

Development of QSAR model to predict biodegradation of pharmaceuticals

Level: Bachelor or Master (preferably from Chemistry)

Start: Anytime

Project form: literature review, data analysis and model development

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Over 1900 active pharmaceutical ingredients (APIs) are used to treat and prevent disease in humans. The occurrence of APIs in the aquatic environment is of great concern due to potential risks to the aquatic environment and human health. The main source of APIs in the environment is regarded as treated wastewater because household and hospital sewage is generally discharged into wastewater treatment plants (WWTPs). Many treatment processes in WWTPs (e.g., membrane filtration, biodegradation and ozonation) play a role in removing pharmaceuticals. Among these processes, biodegradation is one of the main steps for removing pharmaceuticals in WWTPs (Figure 1).

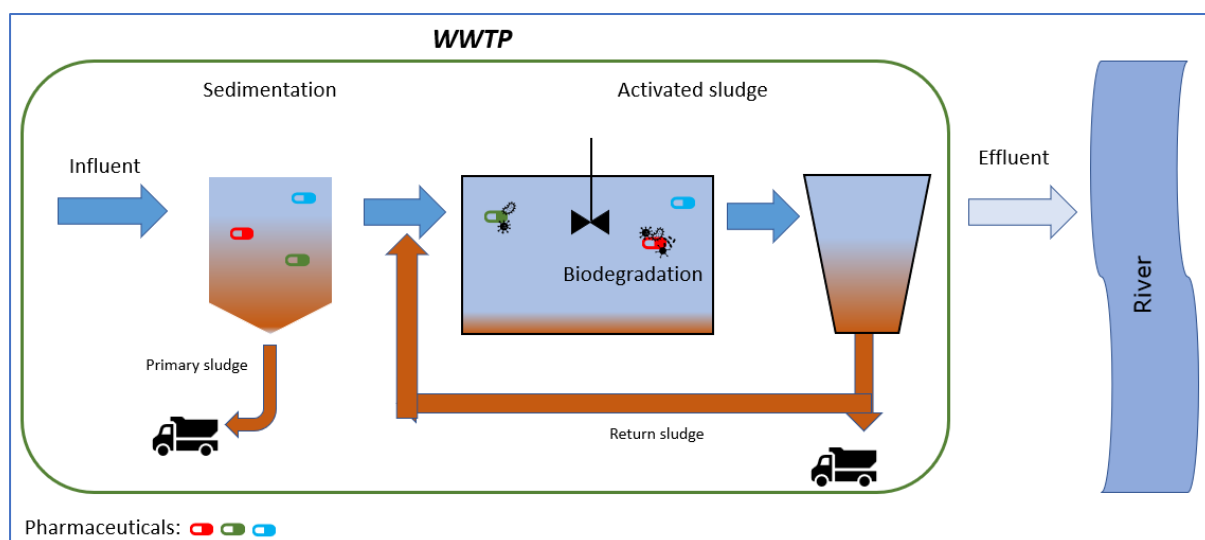


Figure 1. The schematic representation of the biodegradation process in WWTPs.

In the [TransPharm Project](#), we aim to develop more sustainable and greener APIs that simultaneously reduce the environmental footprint together with partners from the public and private sectors. To reach this aim, we will predict the environmental biodegradability of APIs via quantitative structure-activity relationship (QSAR) models that can predict compounds' physicochemical, biological and environmental fate properties from the knowledge of their chemical structure. These mathematical models are useful in silico tools to predict the biodegradability of pharmaceuticals in WWTPs. QSARs could predict the activities of a large number of compounds based on a physicochemical property basis, overcoming the data gaps for pharmaceuticals with little to no prior experimental data on activity such as biodegradation. However, the complexity of pharmaceuticals' removal processes in WWTPs makes the QSAR model development challenging. **Thus, this research aims to develop a QSAR to predict the biodegradation of pharmaceuticals in WWTPs. This new QSAR will help better understand how pharmaceuticals' physicochemical properties are linked with biodegradation in WWTPs.**