Environmental regulations focus on monitoring a limited number of well-known compounds which represent only a small fraction of the anthropogenic chemicals found in the environment. Theoretical prediction tools can help to identify new degradation pathways and thus increase the number of targetable compounds. However, merely using computational methods to detect contaminants is not sufficient. In this work we show the use of commercial and open-source libraries as a complementary tool to detect contaminants in environmental samples. A combination of a commercial software platform (MassHunter) and public libraries (MassBank) was used to screen water samples from different wastewater treatment plants (WWTPs) in Germany. In addition, the open-source software library known as NORMAN was utilized as an alternative solution.

The MassHunter software platform is a powerful tool for analyzing complex matrices and allows detection of known compounds and simultaneous profiling. However, the detection of new compounds is not within its capabilities. The MassBank database, on the other hand, is specifically designed for identification of novel compounds. Its novelty database provides a unique set of libraries for detecting and identifying new contaminants in water matrices.

By combining these two approaches, we were able to detect a variety of compounds, including those that are not present in the MassHunter database. This is a significant advantage as it allows for the detection of emerging pollutants and compounds that are not yet regulated or recognized.

In conclusion, the combination of commercial software platforms and open-source databases is a powerful tool for environmental monitoring. It allows for the detection of both known and novel compounds, providing a more comprehensive picture of the chemical environment. This approach is essential for meeting the increasing demand for environmental monitoring and ensuring the safety of our water resources.