AN EFFECTIVE LC-MS STRATEGY OF NON-TARGET ANALYSIS USING THE DATABASE STOFF-IDENT[1]

GROSSE S. and LETZEL T.[1]

[1] Analytical Research Group, Chair of Urban Water Systems and Engineering, Technische Universität München, Am Coulombwall 8, 85748 Garching, Germany
E-mail: s.grosse@tum.de

The identification of unknown organic compounds via LC-MS moves increasingly into the focus of different research projects. The so called 'non-target' analysis is currently extremely time-consuming and costly as well as complex in instrumentation.

For identifying purposes there is a need of compound and mass spectrometric databases. Unfortunately, the databases often contain thousands of entries of different origin.

Based on that drawback, a database (STOFF-IDENT) was developed, which contains exclusively potential water relevant molecules, like pharmaceuticals, pesticides, herbicides, drugs as well as known transformation products and metabolites. Besides, a retention time factor was established and integrated into this database. The factor is based on normalization of retention time and the physicochemical parameter logD value of apolar molecules. The mostly used chromatographic technique is the reversed-phase chromatography for mid and apolar compounds. Thereby there is a loss of polar compound information. The polar analytes are well separated by hydrophilic liquid interaction chromatography, shortly known as HILIC. A combination of these two techniques gives the possibility of screening polar and apolar compounds in water matrices in just one single run. The poster will show a strategy of 'non-target' screening to identify polar and apolar compounds with the aid of the newly developed database STOFF-IDENT and by using the integrated tool retention time index (RTI).

Keywords: HILIC-RP, non-target, RTI, STOFF-IDENT

REFERENCES

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