CEST 2015

Proceedings of the 14th International Conference on Environmental Science and Technology
Rhodes, Greece, 3-5 September 2015

PEAKTRAMS: AN AUTOMATED COMPUTATIONAL APPROACH FOR THE SIMULTANEOUS DETECTION OF FEATURES IN REVERSE PHASE AND HILIC HRMS SCREENING

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ABSTRACT

Comparison of chromatograms obtained in reserved phase (RP) chromatography and hydrophilic interaction liquid chromatography (HILIC) can provide valuable information for the identification and confirmation of suspect and non-target compounds. The plausibility of the obtained chromatographic retention times (RTs) in both chromatographic modes, as well as the comparison of the MS/MS spectra are strong points to be considered [1]. This work presents the development of a novel automatic approach for the identification of common peaks between RP and HILIC chromatograms. The program is written in R-project and Matlab with a simple and user friendly graphical user interface (GUI).

The first step consists of the introduction of the target chromatograms of the same sample (one obtained by RP and one by HILIC) plus the corresponding blank chromatograms. Blank subtraction was performed first using an algorithm to find in each scan the common m/z features (with a given mass accuracy). This algorithm also considers the RTs (a tolerance interval is applied), so the subtraction takes place even with slight drifts in the RTs between target and blank chromatograms. After blank subtraction, two different lists are obtained with the detected peaks in both RP and HILIC modes. Subsequently, m/z values are compared and matches are listed. Apart from the protonated ions, other adducts such as $[M+Na]^+$, $[M+K]^+$, or $[M+NH_4]^+$ are often detected. Moreover, for intense peaks the isotopic peak M+1 corresponding to ^{13}C is also detected.

The developed workflow was validated with solvent standards and with spiked wastewater samples with a mixture of compounds with a wide range of physicochemical properties. Successful results were obtained for 26 out of the 27 evaluated substances, allowing the recording of the corresponding RTs in both RP and HILIC mode. In addition, the developed program plots the extracted ion chromatograms for all the matched peaks in order to facilitate visual inspection.

Keywords: R-project, Matlab, HILIC, RP, organic pollutants, automated procedure, chromatography

REFERENCES

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CEST2015_00556