THE USE OF ARTIFICIAL NEURAL NETWORKS FOR RETENTION TIME PREDICTION IN THE IDENTIFICATION OF METABOLITES AND TRANSFORMATION PRODUCTS IN ENVIRONMENTAL WATERS

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The recent development of wide-scope high resolution mass spectrometry (HRMS) screening methods has resulted in a much improved capability for new compound identification in environmental samples. However, positive identifications at trace levels commonly seen still rely on analytical reference standards for chromatographic retention time and mass spectral comparisons. Chromatographic retention time prediction can play a role in increasing confidence in suspect screening efforts for new compounds, especially when standards are not available.

The current work explores the use of artificial neural networks (ANNs) for retention time prediction in gradient reversed-phase liquid chromatography for this purpose and applied to environmental analysis of waste and surface water samples. From an initial database of more than 500 compounds, 90% of all compounds could be found within a ±2 minute window. Given the increasing concern on the presence of drug metabolites and transformation products (TPs) in the aquatic environment, the model was applied along with HRMS data for the preliminary identification of pharmaceutical-related compounds in real samples.

A total of nine pharmaceutical and illicit drug metabolites and TPs (for four of which standards were available), were able to be tentatively identified in environmental water samples, including 10, 11-dihydroxy carbamazepine, carboxy losartan, 4-desmethoxy omeprazole and O-desmethylvenlafaxine.

Keywords: Retention time prediction, artificial neural networks, metabolites, transformation products, screening of emerging contaminants

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