

Abstract

Application for Validation of Compound Identification in GC×GC Based on Retention Index [†]

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[†] Presented at the 3rd International Electronic Conference on Processes—Green and Sustainable Process Engineering and Process Systems Engineering (ECP 2024), 29–31 May 2024; Available online: <https://sciforum.net/event/ECP2024>.**Keywords:** GC×GC; MS; computational method; volatile compound

Comprehensive two-dimensional gas chromatography (GC×GC) is a powerful technique for separating, identifying, and quantifying volatile and semi-volatile compounds in complex samples. Typically, mass spectrometry (MS) is used for peak identification in GC×GC, but relying solely on MS library comparison can have limitations, especially for isomers with similar mass spectra. Additionally, optimizing the separation conditions to achieve improved resolution in GC×GC can be challenging.

This research presents a computational approach to simulate GC×GC results using a calculation method based on first- and second-dimensional retention indices (¹I and ²I). The simulation includes the prediction of the retention times (¹t_R and ²t_R) and contour plots of samples from GC×GC-MS data. For cases where ¹t_R and ²t_R data of alkane references (¹t_{R(n)} and ²t_{R(n)}) are not available, the following steps are applied: curve fitting based on the van den Dool and Kratz relationship to simulate ¹t_{R(n)} using a training set of volatile compounds with their experimental ¹t_R data; or simulation of ²t_{R(n)} at different ¹t_{R(n)} values to construct isovolatility curves based on a nonlinear equation with six constants, obtained through curve fitting using the experimental ²t_R data of the training set.

The approach was applied to simulate results for 622 compounds in various samples, including saffron, *Boswellia papyrifera*, acacia honey, incense powder/smoke, and perfume. The simulated results were compared with experimental data, showing good correlation with R² values, ranging from 0.975 to 0.999 for ¹t_R and 0.449 to 0.992 for ²t_R. The approach was then applied to propose 10 compounds that may have been incorrectly identified in the literature based on significant differences between the simulated and experimental ²t_R values

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/proceedings2024105053/s1>. Conference presentation.

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