

Abstract

J. Chromatogr. B, **789**, 3-7 (2003)

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Systematic toxicological analysis: computer-assisted identification of poisons in biological materials.

A new software was developed to improve the chances for identification of a “general unknown” in complex biological materials.

To achieve this goal, the total ion current chromatogram was simplified by filtering the acquired mass spectra via an automated subtraction procedure, which removed mass spectra originating from the sample matrix, as well as interfering substances from the extraction procedure.

It could be shown that this tool emphasizes mass spectra of exceptional compounds, and therefore provides the forensic toxicologist with further evidence—even in cases where mass spectral data of the unknown compound are not available in “standard” spectral libraries.