

Comprehensive Two-Dimensional Gas Chromatography Coupled with Time-of-Flight Mass Spectrometry for Broad Spectrum Organic Analysis

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The method of Comprehensive Two-Dimensional Gas Chromatography (GC×GC) coupled with Time-of-Flight Mass Spectrometry (TOFMS) is a powerful technique for broad spectrum organic analysis (Liu and Philips, 1991, Dimandja, 2004).

The unique feature of a GC×GC is its ability to separate the sample according to the selectivity of the employed column types. The resulting chromatogram displays the data in a retention plane according to the volatility and polarity of the sample. Qualitative identification of the components can be derived from homologous series standards. By coupling the GC×GC to a TOFMS, quantitative and mass spectrometric information is available for each data point in the chromatogram. The method combines extended peak capacities of up to several thousand peaks per sampling cycle with high sensitivity in the low parts per trillion range, and the ability to access complete mass spectrometric information for each constituent in the sample. We will describe the principle of the technique, instrument configuration, the experimental method, and the preliminary laboratory results achieved with a breadboard prototype.

The team has proven the capabilities of the technique for the analysis of organic compounds with commercially available instrumentation (LECO Corp.). However, this existing commercial instrumentation is not suitable for field applications due to its size, power consumption, and requirements for consumables.

We have developed a modular, bench top, breadboard laboratory prototype, which is capable of performing the desired functions of the commercial instrument. To date, we have achieved miniaturization by approximately a factor of five in size compared to the LECO instrumentation and decreased consumable requirements through innovations in the thermal modulator design and in the integrated packaging of the columns, including the thermal control (RVM Scientific). The thermal modulator is a dual-stage device employing a close gas coolant loop with repetitive resistive heating. The GC detector is a TOFMS with an approximately 0.35 m drift path (Ionwerks Inc.) and uses customized data acquisition software. The system manages the extensive data volume (~1 Gigabyte) generated during a 30 minute sample run time.

Proof of concept with the laboratory prototype has been demonstrated using a four-component sample mixture (hexane, benzene, heptane, and octane) diluted in acetone injected through a split/splitless inlet port. Future iterations for a field portable and consumable-free device will be outlined.

References:

- [1] Liu, Z.; Phillips, J. B. *J. Chromatogr. Sci.* 1991, 29, 227-231.
- [2] Dimandja, J.M. *Anal. Chem.* 2004, 76, 167A-174A.