

Use of classifications and mass spectral filtering to process GC×GC–TOFMS data for brominated flame retardants

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Nowadays comprehensive two-dimensional gas chromatography (GC×GC) is more and more the method of choice to solve separation problems for complex environmental samples. GC×GC increases peak capacity by applying two independent separations to a sample in one analysis separated by a thermal modulator.

Due to modulation, most GC×GC peaks are on the order of 50 to 250 ms wide, requiring a fast detector, where in case of MS, only Time-of-Flight (TOF) has the necessary acquisition rates (hundreds of full spectra/second). The ability of the thermal modulator to narrow peaks and thereby increasing their height, also affords the ability to increase TOFMS sensitivity.

GC×GC–TOFMS offers the possibility of handling complex samples, but the data generated is itself complex. This makes data processing routines very important to realize the full potential of GC×GC–TOFMS. One of the ways that data can be processed is by taking advantage of the structured GC×GC chromatograms. This as certain compounds elute in certain geographic areas (Classes) of the contour plot, and can be grouped. Another way is to employ mass spectral filtering (Scripts) which can be done in conjunction geographic classification of compounds.

In this contribution, classifications and scripts software is employed to process brominated flame retardants data generated using GC×GC–TOFMS.