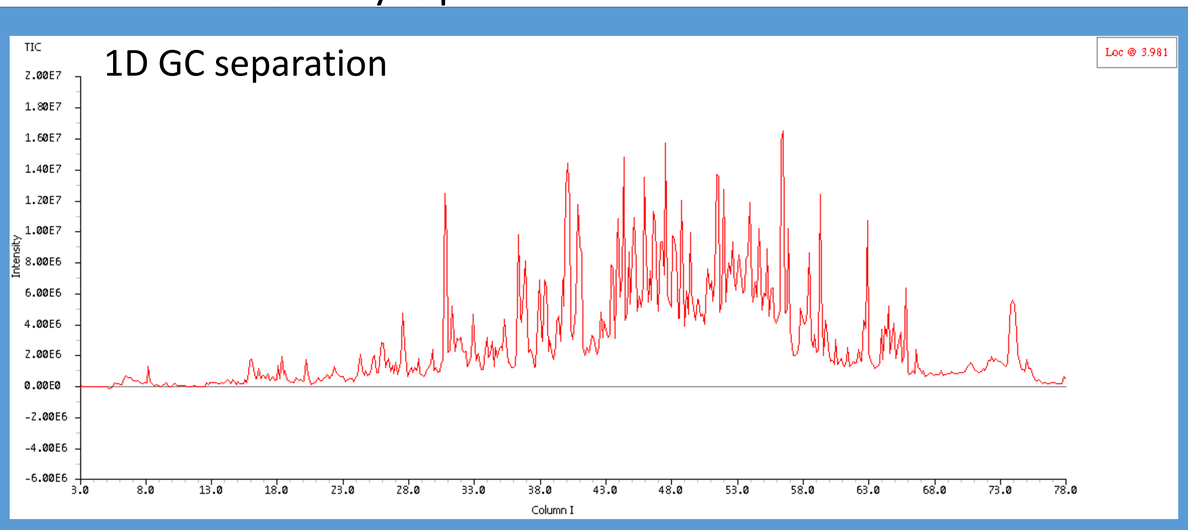
Enhanced pesticide screening with GCxGC-Q-ToF-MS

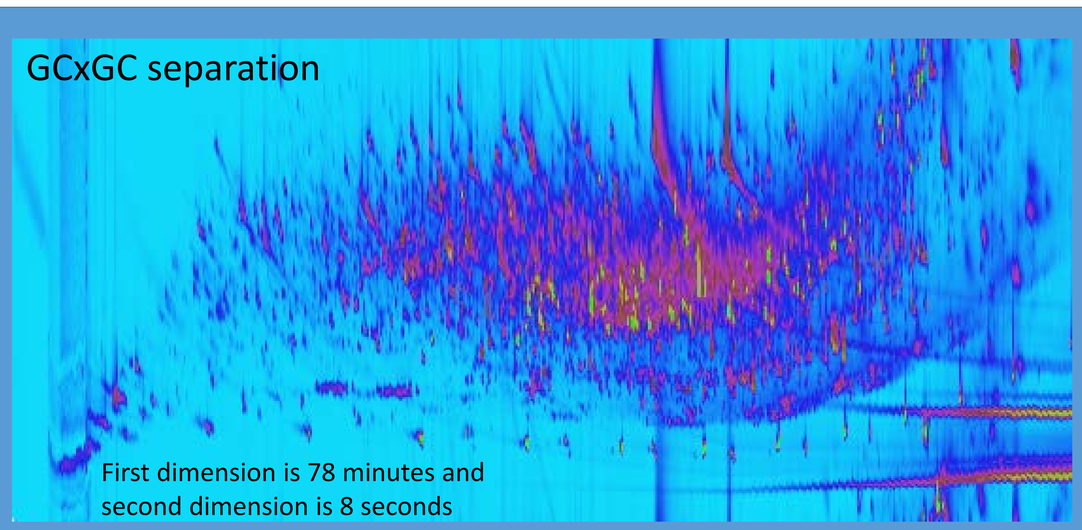
Authors: A. Rydevik[1], L. Lopardo[1], M. Lewis[1], J. Riener[2], A. Lubben[1] and B. Kasprzyk-Hordern[1]
[1] University of Bath, Bath, United Kingdom
[2] Agilent Technologies, Waldbronn, Germany

Agilent Technologies

The issue: Complexity of wastewater samples make analyte screening and identification difficult

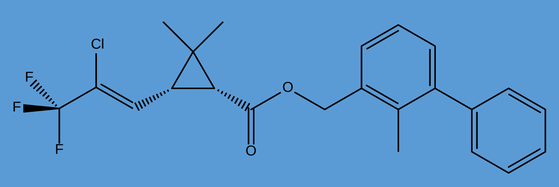
GCxGC reveals more analyte peaks



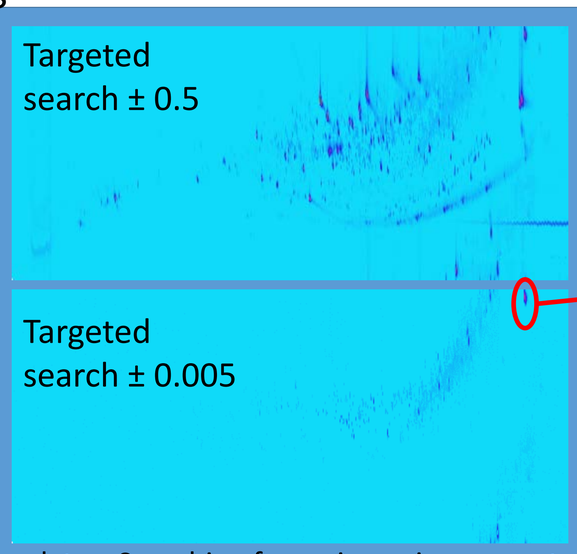


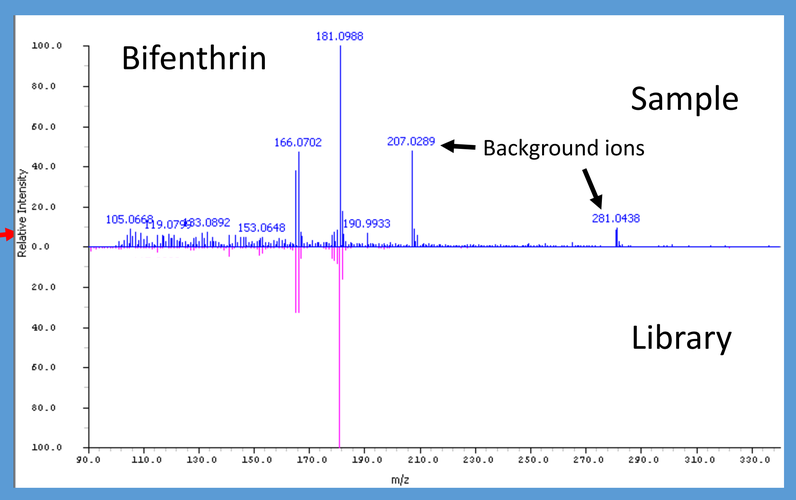
The increased peak capacity in GCxGC results in fewer co-eluting peaks, as can be seen in the analysis of a wastewater sample spiked with 30 analytes above.

HRMS is vital for efficient and reliable data mining



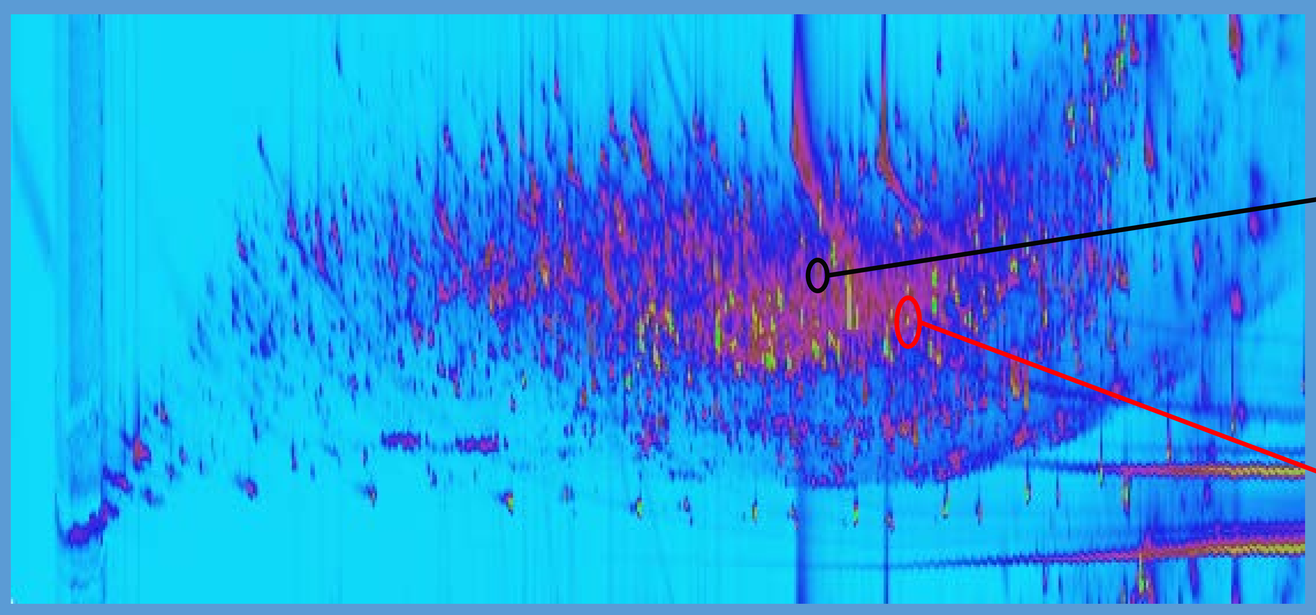
Structure of Bifenthrin
Molecular formula: $C_{23}H_{22}ClF_3O_2$
Nominal mass (main ion) *m/z* 181
Accurate mass (main ion) *m/z* 181.1017

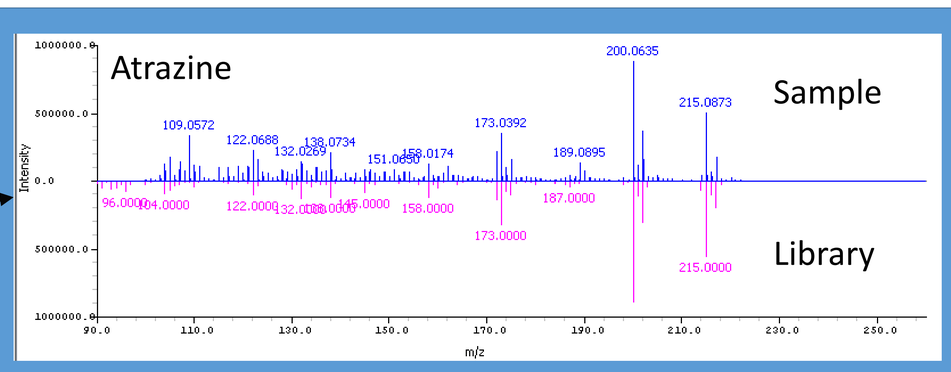


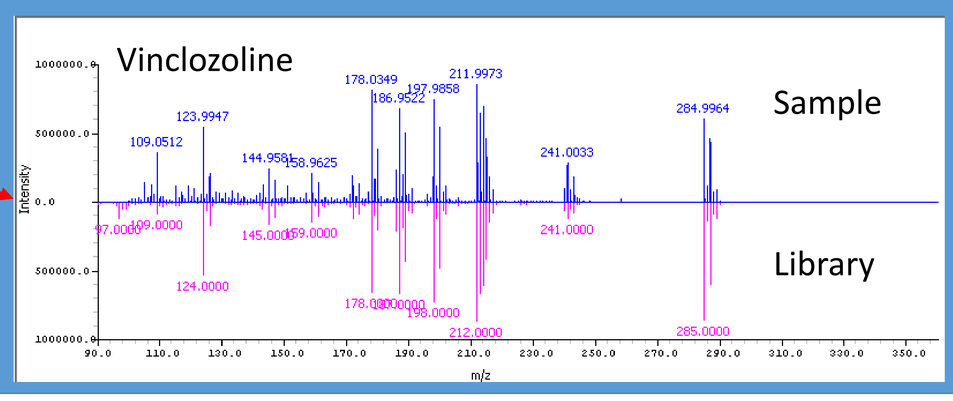


Accurate mass is vital for mining the data when searching for target analytes. Searching for an ion using accurate mass instead of nominal mass gives fewer hits which leads to a quicker identification of the target analyte even in the presence of high intensity background ions (as in the spectra above). Following library matching the accurate mass and isotope pattern can be used for further confirmation.

Fewer spectral interferences even in complex samples

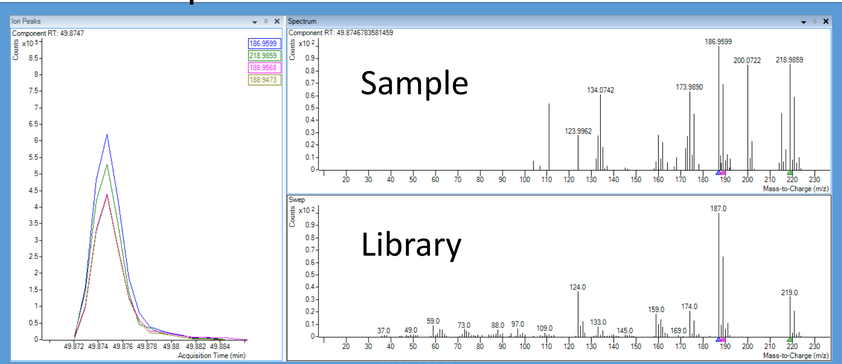


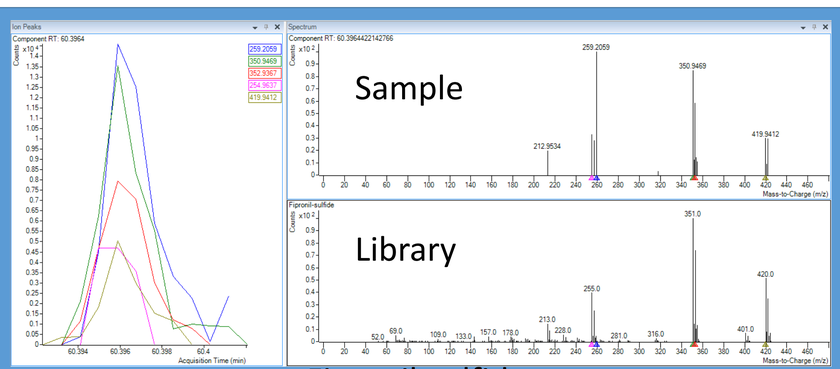




GCxGC enables resolution of components and background even in very complex samples such as wastewater. The top example is Atrazine and the bottom is Vinclozoline, both of which have many other closely eluting compounds in both GC separation dimensions

Deconvolution reveals more pesticides





Deconvolution and library searching reveals the presence of unexpected pesticides in the sample. These are subject to further investigation.

The conclusion: GCxGC-HRMS has the capability to deal with the complexity of wastewater as a sample matrix but more work is needed to fully mine the data for target and unexpected compounds.

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The Leverhulme Trust