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Enhanced pesticide screening with GCxGC-Q-ToF-MS

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Pesticides play a critical role in agricultural developments and success, therefore it is no surprise that new pesticides are constantly being developed. Several pesticides are also used in the domestic setting to protect flowers and plants from attack. Unfortunately some pesticides are harmful to the wider environment and to humans consuming exposed produce. In order to safeguard both humans and the environment it is of utmost importance that analytical methods are constantly developed and improved to monitor these pesticides in various matrices e.g. soil, food products and wastewater. By analysing these samples it should be possible to build up a comprehensive picture of what pesticides humans and the environment are exposed to. With this in mind a GCxGC-Q-ToF MS analysis method to analyse incoming and outgoing wastewater samples has been developed, using an Agilent Technologies 7200B GC-EI-Q-ToF MS with GCxGC coupling. This is used in conjunction with SPE as a sample concentration step. By harnessing the superior separation power of the GCxGC it is possible to resolve matrix interferences from the analyte peaks, even in such complex matrices as wastewater. When coupled with the high resolution and high mass accuracy of the Q-ToF MS, it is possible not only to conduct targeted library searches with high levels of confidence, but also to retrospectively mine the data for newly determined key analytes. In combination this facilitates both a targeted and non-targeted approach to identify as many analytes of interest as possible. To show the power of this technique spiked samples in a wastewater matrix were analysed using a 74 min GC temperature gradient, with a second GC dimension separation included. A range of pesticide and non-pesticide analytes (a total of 30 compounds) were successfully separated and detected in a targeted screening mode. The identities of these compounds were confirmed by accurate mass and isotope pattern information as well as being searched against the NIST library. Further non-targeted data mining (deconvolution of spectra and matching of unknowns to NIST library) showed the presence of several unexpected pesticides. The detection of these unexpected compounds was only possible because of the enhanced separation, away from the matrix, through GCxGC. Unambiguous formula confirmation was established through accurate mass and isotope pattern investigation.