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Monitoring London's drug habits by analyzing raw sewage

How the Shimadzu LCMS-8060 helps provide near real-time analysis of the use of illicit drugs and other contaminants

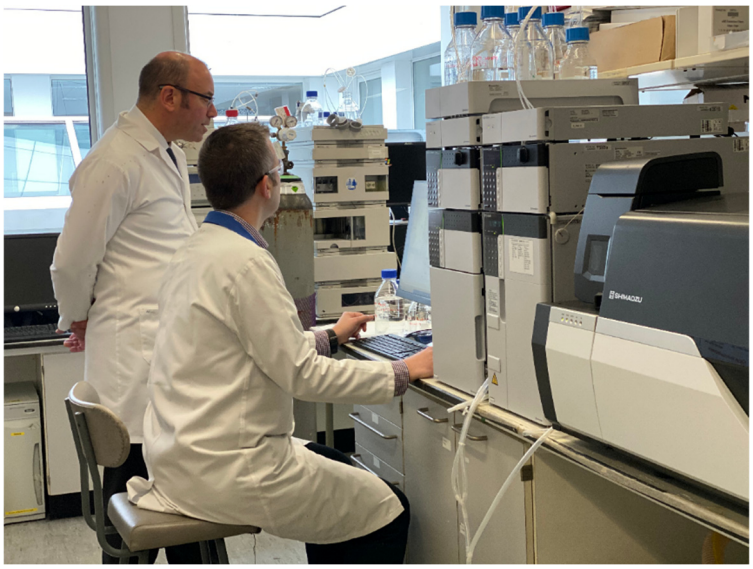
The global issue of chemical pollution can be observed through the rising levels of chemical hazards, termed "contaminants of emerging concern" (CEC), which include pharmaceuticals, personal care products, industrial chemicals, pesticides (legal or illegal) and illicit drugs. As part of efforts to reduce this contamination, specialists in environmental forensics work to determine the source, distribution, final destination and effects of these CECs, including any potential associated risks to human health, wildlife and the environment. By using defensible analytical methods - i.e. high assurance, confirmatory methods that will 'stand up' in cases that go to court – these specialists can support the work of organizations such as the Environment Agency that aim to protect and enhance the environment.

One such specialist is Dr Leon Barron, a well-published researcher and senior lecturer at King's College London (KCL). An expert in forensic science and analytical toxicology with over 70 publications in peer-reviewed journals, Dr Barron has led the Chemical Hazards research group at KCL since 2009. The group's recent work has included wastewater-based epidemiological studies involving the analysis of target residues in London's sewage in order to assess community-scale activities, such as the capital's cocaine and MDMA consumption habits.

For this research, Dr Barron and his team had three essential requirements of their liquid chromatography-mass spectrometry (LC-MS) instrument: high sensitivity at the pg/mL or ng/L concentration level; high speed to handle a large number of samples; and the ability to detect CECs in complex environments (i.e. raw wastewater) without time-consuming sample preparation.

Improving accuracy through direct injection of raw wastewater

The system that met all these requirements was Shimadzu's LCMS-8060 liquid chromatography-mass spectrometer. The team were able to quickly and accurately identify more than 100 different compounds at ng/L concentrations, as Dr Barron explained: "For the first time, we were able to develop a direct injection LC-MS method to determine 166 acidic, basic and neutral organic compounds in filtered wastewater…[and] still achieve very good quantitative reproducibility on our measurements". Since raw wastewater could be directly injected into the LCMS-8060, this mainly removed the need for extensive sample preparation with the result that, as Dr Barron added, "…our precision and accuracy has improved enormously over methods we have used in the past."



The LCMS-8060 features a triple quadruple mass spectrometer allowing high throughput analysis which hugely benefits research labs producing large amounts of data. For example, the team at KCL run over 280 injections per day with a 5-minute run-time. "For us, the speed of the instrument means we can run rapid gradient LC separations and still maintain very high data acquisition frequencies (>20-30 datapoints per peak) for at least two transitions per compound, as well as transitions for its corresponding stable isotope-labelled internal standard [SIS], simultaneously", revealed Dr Barron. SISs are often used in LC-MS to compensate for any sample processing interferences caused by complex biological matrices, such as raw wastewater. "We now routinely monitor over 70 compounds and their corresponding SIS analogues, at any single timepoint in the LC gradient - and the LCMS-8060 can do even more if needed!"

Exceptional customer service supports great research

Working successfully with such complex samples underlines the importance of a close working relationship between instrument manufacturer and scientist. "The Shimadzu UK team have been excellent…they are very open minded to new ideas and commit to helping overcome the associated challenges with our requests", said Dr Barron. "It can't have been easy for them to contemplate working with us when we proposed injecting raw wastewater onto the LCMS-8060! The instrument has been working at this for over a year now; thanks to their help we now deliver really coherent methods to monitor very large numbers of compounds in wastewater which goes a really long way to telling in near real time what a city is doing…so that we're ahead all the time."

Summarizing the contribution of the LCMS-8060 to the group's work, Dr Barron concluded: "It has really underpinned and advanced our research progress, primarily through its speed and sensitivity. The instrument is able to detect ng/L quantities of emerging contaminant residues in environmental samples, actually negating the need for sample preparation using solid phase extraction in many cases. We can develop very, very fast gradient methods for large numbers of compounds, and we can still achieve very good quantitative reproducibility on our measurements, with well over 20 data points per peak."