

State Crime Lab Uses Combined Scan/SIM by GC/MS to Boost Drug Analysis Throughput

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The Mississippi Crime Laboratory (MCL) is using a PerkinElmer® Clarus® 500 Gas Chromatograph/Mass Spectrometer (GC/MS) in selected ion and full ion (SIFI™) mode for their drug analysis. SIFI combines scan and selected ion monitoring (SIM) mode to increase drug analysis throughput by approximately 100%. Doing drug analysis in the past required two separate GC/MS injections to positively identify drugs in samples. The first injection was in the full scan mode to search for a wide range of drugs, the second used the much more sensitive and selective SIM mode to look for specific drugs that were suspected to be present. By utilizing a GC/MS instrument that is capable of acquiring both scan and SIM data in the same injection, the number of GC/MS sample injections required for positive identification has been reduced from two to one (Figure 1). In addition to the decrease in the number of injections

required, the amount of time required for sample preparation and analyzing the results has also been reduced. “We have already achieved substantial time savings and we are planning to achieve even greater gains by establishing a calibration curve for opiates that will allow us to quantify at least that class of drugs on the same scan/SIM run that we use to identify drugs,” said Thomas Pittman, Toxicology Section Chief for the MCL, Jackson, Mississippi.

The MCL, a program of the Mississippi Department of Public Safety, Office of Public Safety Programs, was established by legislative authority granted to the Commissioner of Public Safety in 1956. The MCL’s main laboratory in Jackson is accredited by the American Society of Crime Laboratory Directors/Laboratory Accreditation Board in Biology, Controlled Substance (Drug) Identification, Firearm and Tool

Mark Examinations, Latent Print Examinations, Questioned Document Examinations, Crime Scene Assistance, Toxicology and Trace Evidence Examinations. The Controlled Substance (Drug) Identification Section of the MCL classifies and identifies controlled substances such as cannabis (marijuana), pharmaceuticals and powder material, including cocaine. This section also classifies and identifies miscellaneous substances such as those used in clandestine laboratories for the illegal manufacture of controlled substances. The Controlled Substance Identification Section of the MCL is responsible for just over half of all cases submitted to the laboratory. Increasing productivity has been a major concern of the MCL in recent years because the number of skilled analysts has been reduced due to budget cuts and due to the difficulty in finding replacements for those who have left.

Series of runs required for drug analysis

The toxicology section of the MCL performs two main types of analyses. The first kind of testing is performed under implied consent laws on persons who are suspected of driving under the influence or who are involved in a serious accident. The second type is performed in death investigations. In both types of cases, the laboratory looks for any type of drug that might have a bearing on the case, such as benzodiazepines, opiates, barbiturates, etc. First, forensic scientists screen the samples using two procedures to narrow the scope of possible drugs for identification. Immunoassay

equipment is used to look for several drugs and drug classes. Immunoassay is fast and inexpensive and can be used to detect drugs of abuse. Then, analysts extract samples and run them on a gas chromatograph with nitrogen phosphorus detector (NPD), to look for nitrogen-phosphorus containing drugs at high levels of sensitivity. The NPD, on the other hand, does not detect some drugs or provide positive identification, and its results must be confirmed with a GC/MS as well (Figure 2). Today, many labs skip the NPD step and go directly from the positive immunoassay step to the GC/MS. The next step, in most cases, was to run a GC/MS analysis in scan mode,

which detects the widest possible range of drugs but at a reduced level of sensitivity. Then, another GC/MS analysis was run in SIM mode set up to detect one class of drugs with greater sensitivity than scan mode. The final step, if drugs were detected in the earlier step, was another GC/MS run in scan mode along with internal standard, calibration standards and quality-control samples, which makes it possible to determine the quantity of the drug that is present. This equates to three GC/MS injections for every positive hit.

Section Chief Pittman recognized that the majority of time involved in the drug-analysis process was spent on the highly-accurate but also time-consuming GC/MS runs. Each run takes about 23 minutes and the analyst typically fills the autosampler with somewhere in the neighborhood of 50 samples, which might take 24 hours to run. When the run is completed, an analyst must examine the spectrum for each peak on the chromatogram for identification and prepare the necessary reports, which might take another couple of days. When PerkinElmer mentioned to Pittman that they were developing a GC/MS instrument capable of running in both scan and SIM mode at the same time, he offered to participate in the beta-test program for the software package needed to take advantage of these capabilities. "When I heard about the instruments, I took a trip to Connecticut to look at them that whetted my appetite," Pittman said. "When we first bought the instrument, PerkinElmer was still developing the software needed to take full advantage of it. We worked with them as their primary beta-test site. The software that was developed during this program gives us the ability to generate reports from the

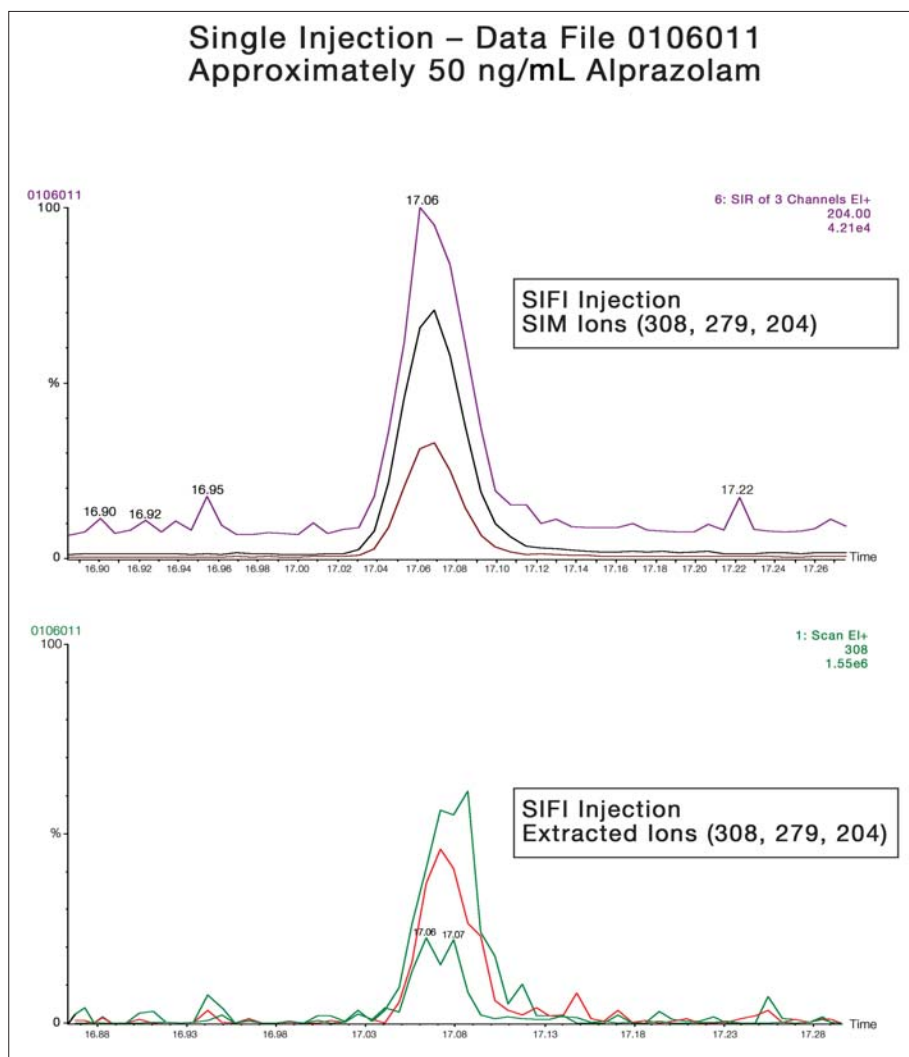


Figure 1. Blood extract positive for benzodiazepines by immunoassay (0.5 μ L injection, 10:1 split ratio, 2 mL extract, 100 mL ethylacetate).

instruments any way we want. The software comes with many templates and can be configured to generate custom reports in nearly any format.”

The Clarus 500 GC/MS runs in scan and SIM mode simultaneously

The PerkinElmer Clarus 500 GC/MS provides SIFI scanning capabilities, where SIM and full scan data are acquired in the same injection. The SIM increases sensitivity by selectively scanning for individual masses, while full scan provides you with a large mass range to identify other components that may be present. The Clarus 500 GC/MS has sensitivity of approximately 1 picogram

per microliter, while SIM extends detection limits into the femptogram range. The full scan mode provides library searchable spectra. In scan mode, the instrument can detect many drugs that are typically found in high concentrations, such as muscle relaxants, barbiturates, anticonvulsants, cold medications, caffeine and nicotine.

“The time savings from running in full scan and SIM mode simultaneously can be quite large,” Pittman said. “For example, consider the case where we run 40 samples in an older-generation GC/MS in full scan mode and 10 of those samples turn out to contain benzodiazepines that may not be seen in the scan mode of operation. We have to immediately

turn around and run those 10 samples on the same instrument in SIM mode to obtain a positive analysis, which might take an analyst a few hours to prepare the samples, 23 minutes for each run on the instrument and 60 minutes to analyze the results. In the past, the lab typically set up the GC/MS to run all the scans one day and then the next day set the same instrument up to run the SIM cases. Now, both runs can be performed simultaneously, which, in essence, saves a day. The exact amount of savings naturally depends on the specific workload mix, which varies from day to day. But, essentially, we have improved our productivity, not taking into account the need to perform quantitative analysis on some of the runs.”

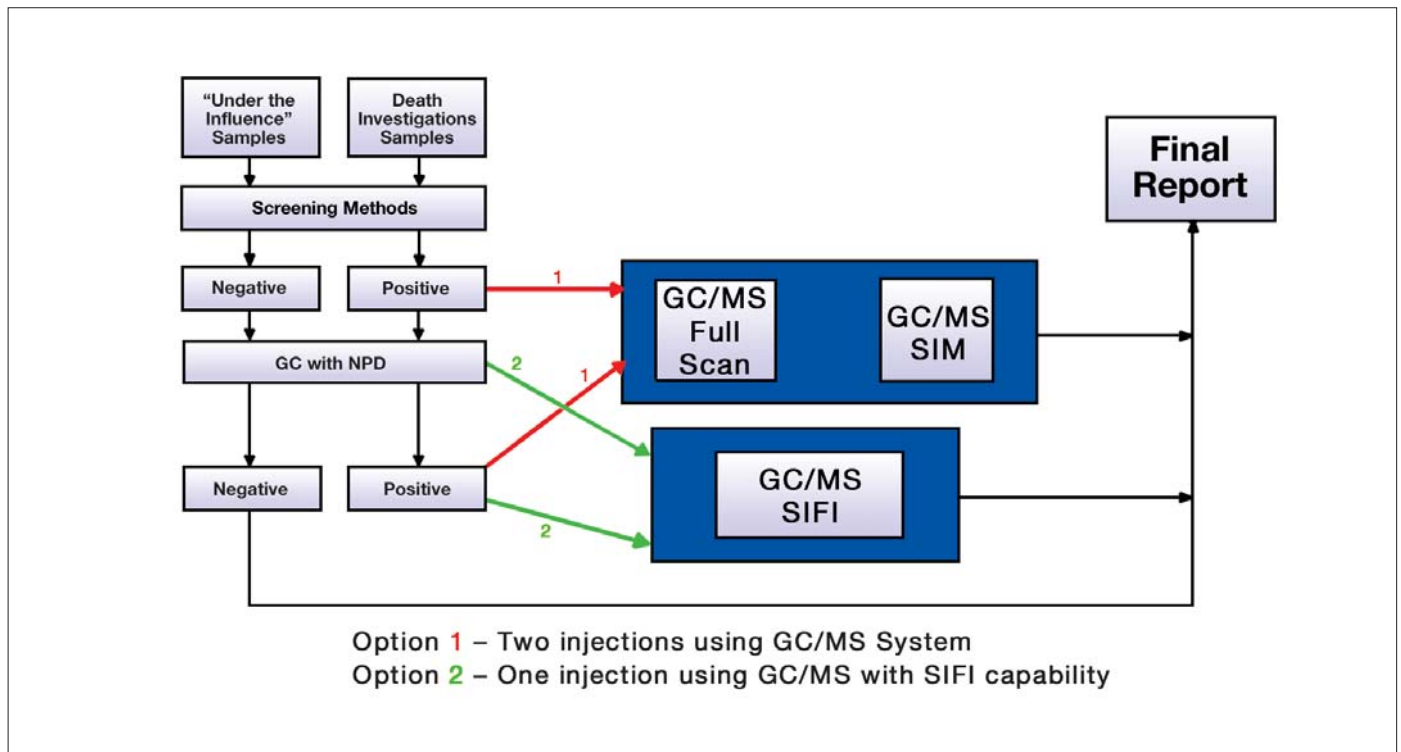


Figure 2. Typical laboratory toxicology sample flow.

Even higher productivity gains are in the offing because Pittman is working on the ability to identify and quantify several drugs in a single GC/MS run. He is developing a set of standards that can be injected into the instrument to establish a calibration curve as part of the batch of samples that would make it possible to quantify the entire batch. The instrument will run in scan mode and also SIM mode with a window configured to identify and quantify opiates. The TurboMass™ software will confirm the presence of opiates and quantify them by measuring the ratio of three ion fragments. “The only hurdle that needs to be overcome is improving

sample-preparation methods,” Pittman said. “Blood samples represent a very complex mixture and the samples that are obtained in death investigations are often degraded or even putrefied. The challenge is coming up with the right extraction to purify the sample to the highest possible degree.”

Pittman said the Clarus 500 GC/MS has other new and helpful features such as updated reporting features and unique injection sizes to assist forensics labs. PerkinElmer TurboMass software provides customizable report templates needed to meet the specific needs of users conducting forensic, clinical

and toxicological diagnostics, as well as general chemical analysis. “Another nice feature of the instrument is that it makes it possible to inject half microliters: 0.5, 1.0, 1.5, 2.0, 2.5, etc., while most of the other instruments on the market will only inject whole numbers of microliters,” Pittman said. “This provides greater control over the amount of drug that you put onto the column, which avoids the risk of overloading and helps extend column life, thus minimizing operating costs. All in all, the productivity gains that we have achieved with the help of the Clarus 500 GC/MS have more than compensated for personnel reductions at the MCL.”

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