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Gas Chromatography and Mass Spectroscopy (GC/MS)

An understanding of available chemical analyses provides insight into the types of questions that chemical investigations can address. One such combination of analytical instruments is gas chromatography (GC) and mass spectroscopy (MS). Gas chromatography analysis separates compounds in complex mixtures, while mass spectroscopy analysis determines the molecular weight and ionic fragments of individual components, aiding in the identification of those compounds. GC/MS is an excellent way for experts to identify substances in a sample because it is a specific test. A specific test when coupled with expert interpretation can positively identify the actual presence of a particular substance in a given sample.

How a Gas Chromatography Mass Spectrometer Works

The GC analytical process provides a representative chromatographic output. The analyst or a computer controlled auto-sampler injects the sample into the injection port of the GC instrument. The GC vaporizes the injected sample and separates the various components. Each of the components in the sample generates a specific peak which is recorded electronically. GC measures the retention time, which is the elapsed and recorded time between the injection of the sample and the process of elution (separating one material from another). The retention time helps the scientist to differentiate between some compounds. The peaks that are recorded are generally proportional to the quantity of the corresponding substances in the sample analyzed.

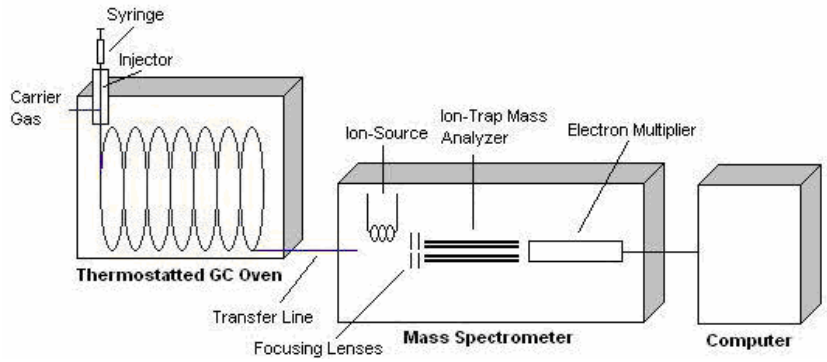
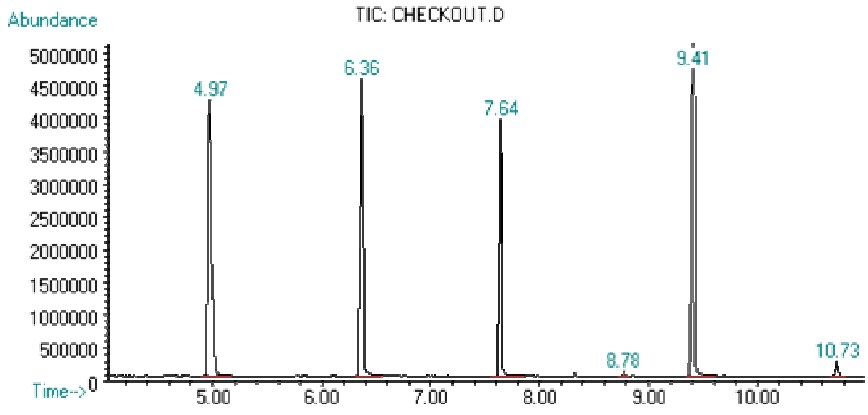
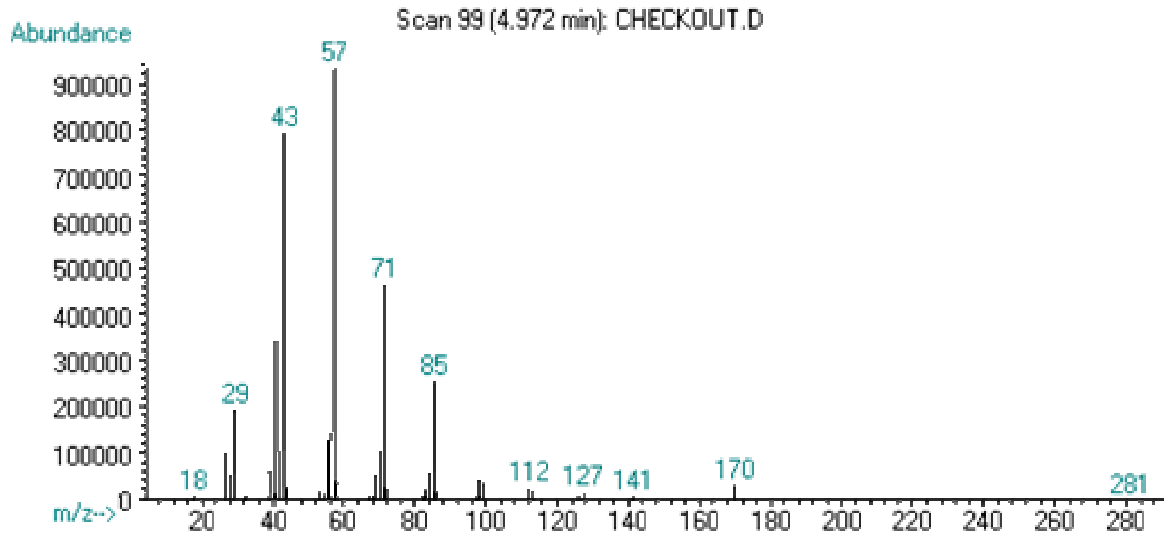


Diagram of a Gas Chromatography Mass Spectrometer



Example of a Chromatogram from a Gas Chromatograph

The MS analytical process identifies substances by electrically charging (or ionizing) the sample's molecules, breaking the molecules into charged fragments, accelerating them through a magnetic field, and detecting the different fragments. The results of this process provide the analyst with a plot which displays the mass and relative amount of each fragment from the compound. The analyst can utilize the compound's mass spectrum for qualitative identification. By determining the molecular mass and the mass of the fragments, the analyst is able to utilize and compare reference data to determine the identity of the specimen sample.



Example of a Mass Spectrum from a Mass Spectrometer

The National Institute of Standards and Technology (NIST) Mass Spectral Library and Standard Reference Database is available for determinations. Numerous American Society for Testing and Materials (ASTM) standards that cover GC/MS are also utilized for routine determinations. The mass spectrum is relatively unique for each substance, particularly compounds with different molecular weights and/or elemental constituents. When the analyst uses the GC instrument to separate compounds before analysis with an MS instrument, a complementary relationship exists. This combination gives the analyst information on both the retention times and mass spectral data. Scientists consider GC/MS analysis as a tool for conclusive proof of identity and it is therefore widely used.

It should be noted that laboratories often merely use NIST database best statistical fit without performing confirmation testing or evaluating other factors in the case. In reality, the top statistical options must be evaluated by the qualified forensic investigator using specific knowledge of the actual event in order to identify the correct compound(s). Reports generated by opposing experts are especially vulnerable to refutation if the report does not demonstrate a personal confirmation assessment by the expert.

Conclusion

A case can often hinge on the presence or absence of compounds identified using GC/MS. The use of GC/MS in legal proceedings can be a two-edged sword. Properly performed, interpreted and documented GC/MS analysis can provide a robust determination of chemicals present in an incident. It is especially important to use an experienced investigator since lack of proper quality control, insufficient documentation, or reliance only on computer generated spectrum matching, can provide opportunities to challenge GC/MS identification by opposition counsel's experts.

Forensic Science Insights is a publication by Gossman Forensics, a division of ChemRight Laboratories, Inc. Please contact David Gossman, Chief Investigator, at 563-652-2822, by email at dgossman@gossmanforensics.com or visit us on the web at GossmanForensics.com.