

**PROCEEDINGS
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INTERNATIONAL
SYMPOSIUM
ON THE FORENSIC
ASPECTS OF
ARSON INVESTIGATIONS** (1995)



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An Improved Method of Obtaining Ion Profiles from Ignitable Liquid Residue Samples

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This study was undertaken to improve the collection of extracted ion profiles from mass spectral data. Using the full scan method of collecting data frequently results in a higher detection limit relative to GC/FID and ion profiles with a noisy baseline or a baseline which is off the bottom of the scale. One goal of this study was to produce ion profiles with a more chromatographic appearance and another goal was to decrease the lower limit of detection. Ion profiling is also known as mass chromatography and has been used for fire debris analysis since it was first described by Smith (1982) and has been codified in ASTM E-1618, *Standard Guide for Ignitable Liquid Residues in Extracts of Fire Debris Samples by Gas Chromatography/Mass Spectrometry*.

MATERIALS AND METHODS

All samples were run on a Hewlett-Packard (HP) 5890 Series II gas chromatograph connected to a HP Model 5971A mass selective detector. Data analysis was accomplished using HP ChemStation software. The column was a 25 meter HP-1 0.2 mm I. D., 0.5 μ m film thickness, operated at an initial temperature of 60°C for 6 minutes, ramped at 20°C/min to 280°, and held at 280°C for 4 minutes. A 50:1 split ratio was used on 0.5 μ l samples injected with an HP Model 7671 automatic liquid sampling system.

Comparisons were made between data collected using the scan method (33-300 amu) and the selected ion monitoring method, using the 15 ions collected as shown in Table 1. The effect of varying the dwell time

for this group of ions was also studied. Dwell times of 10, 20, 50, 100, and 200 milliseconds were used. In addition, a special program looking only at Ion 57 was examined.

Weathered gasoline and kerosene, ranging in concentration from 1% down to 1 ppm dissolved in diethyl ether, were examined.

RESULTS

The use of the SIM mode of collecting data resulted in a significant decrease in the lower limit of detection. Identifiable ion profiles of the most important groups of gasoline compounds could be collected from samples containing 10 ppm gasoline, while it was necessary to have a concentration of 100 ppm of gasoline in order to obtain useful ion profiles when the data was collected using the full scan. When a special program designed to look strictly at Ion 57 was applied to kerosene, a concentration of 1 ppm could be detected as opposed to a concentration of 100 ppm required for the full scan method.

A dwell time of 50 milliseconds was found to be sufficiently low to allow for the resolution of the p-ethyltoluene shoulder on the m-ethyltoluene peak. Decreasing the dwell time resulted in slightly improved resolution, but slightly increased noise.

Use of the SIM method precludes obtaining individual mass spectra from a given peak, but in almost all cases, analysts are attempting to recognize a pattern of peaks; this can be accomplished at

concentrations equal to or less than those required for pattern production by GC/FID.

The SIM method of collecting data does not result in significantly larger signals, but there is a reduction in the background noise of between 1 and 2 orders of magnitude. The SIM ions selected result in a total ion chromatogram which very closely resembles that produced by the full scan. The reduction in the background noise provides selected

ion profiles with a much cleaner and more chromatographic appearance than ion profiles extracted from full scans. A comparison of two profiles is presented in Figure 1.

REFERENCES

Smith, R. M. Arson analysis by mass chromatography. *Analytical Chemistry* (1982) 54:1399A-1409A.

amu	Ion
31	Alcohols
45	Alcohols
55	Alkenes
57	Alkanes
71	Alkanes
78	Benzene
83	Cycloalkanes
91	Xylenes, Styrenes
105	Cumenes
117	Indenes
119	Heavier Aromatics
128	Naphthalenes
131	Methylindenes
142	Methylnaphthalenes
156	Dimethylnaphthalenes

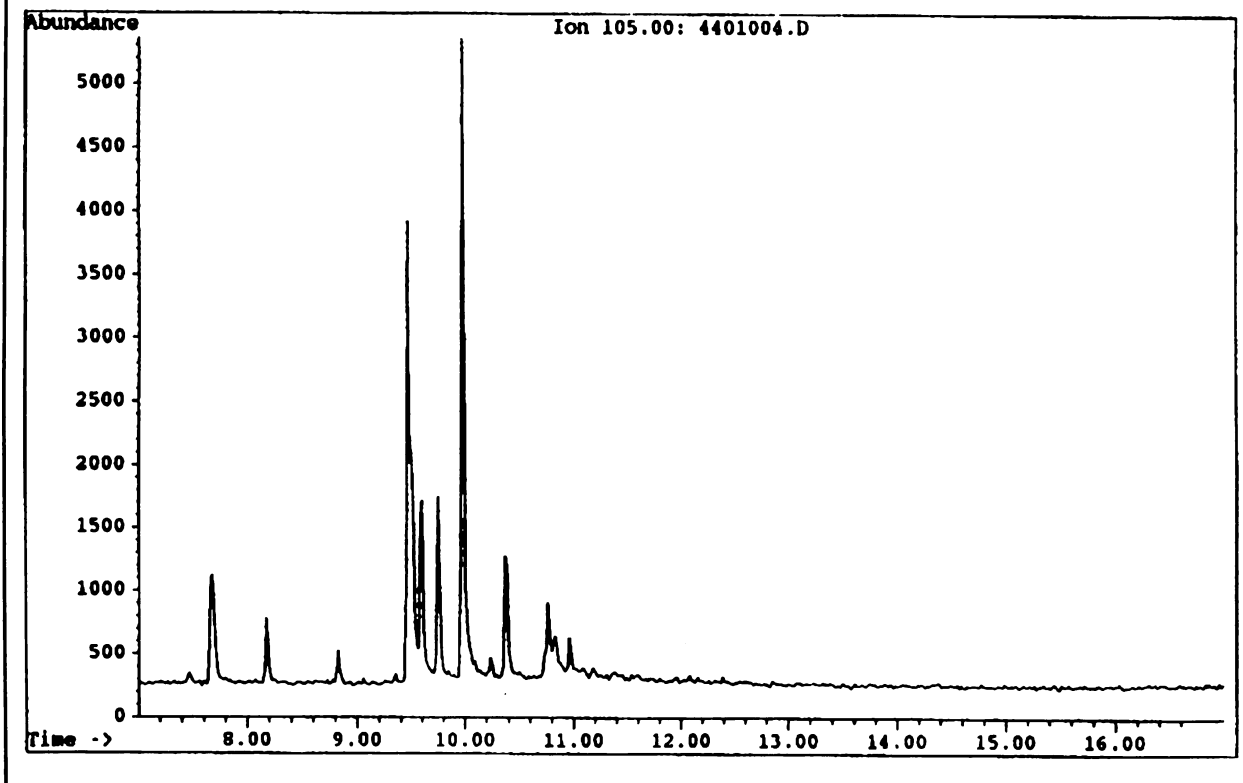
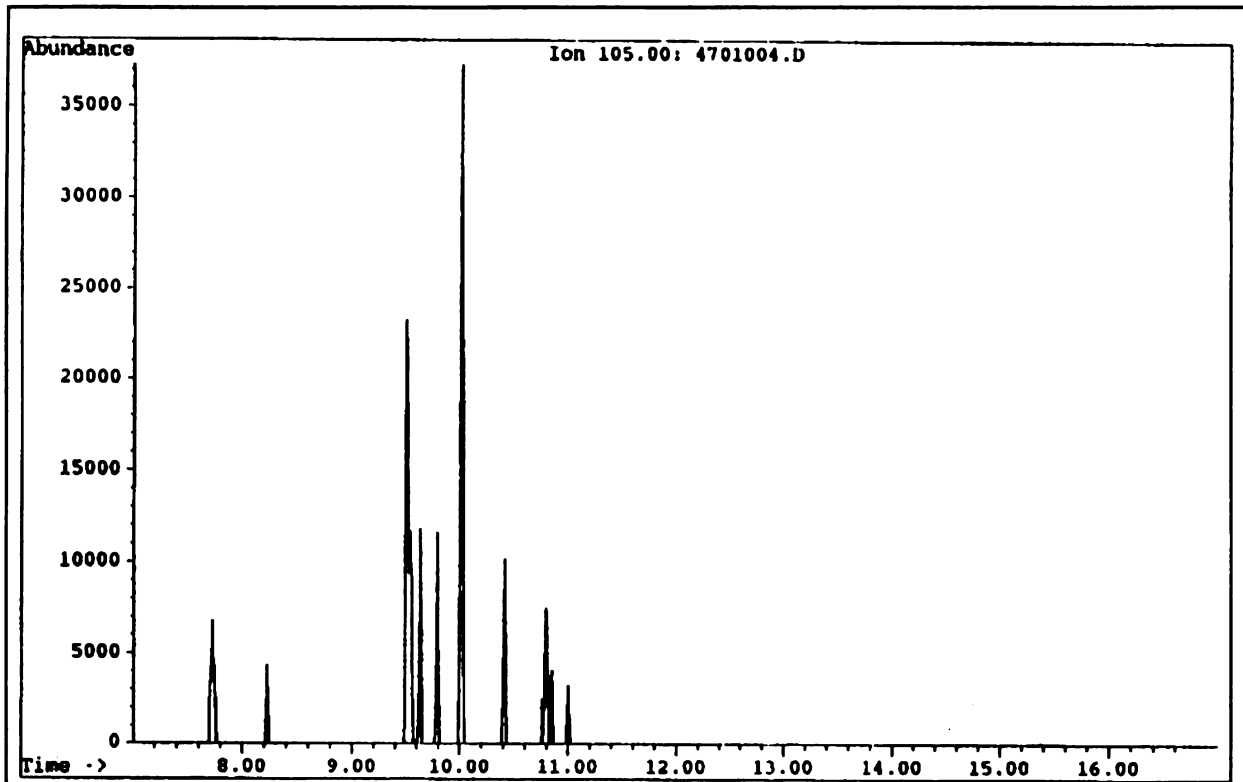


Figure 1. Comparison of cumene profile (Ion 105) from a sample of 100 ppm gasoline run in the full scan mode (top) and 10 ppm gasoline run in the selected ion monitoring mode (bottom).