The Compare Feature of ChromaTOF®—Its Use in Forensic Chemistry to Assist with the Determination of the Cause of Death

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1. Introduction

Purpose of Analysis

The LECO ChromaTOF® software package contains a Sample Comparison algorithm, which can be used to compare samples and identify differences between, for example, good and bad batches of product after their analysis with Gas Chromatography—Time-of-Flight Mass Spectrometry (GC-TOFMS). Whole chromatograms for two samples can be quickly compared on a peak-by-peak and mass spectrum-by-mass spectrum basis. For some samples, by adjusting the initial Reference Table to contain a smaller number of search compounds, the Compare process can be further simplified. An example taken from a recent Forensic Chemistry investigation is shown below.

Background

In cases of accidental death or suicide, the determination of the cause of death is of extreme importance. During a recent investigation into such a death in South Africa, it was suspected that the deceased had died as a result of the ingestion of an industrial cleaning solution. By comparing the stomach extract of the deceased with a sample of the industrial cleaner, it was possible to determine if this had indeed occurred.

This note describes this analysis using GC-TOFMS. The samples submitted for analysis in this study were obtained from the Forensic Chemistry Laboratory, Department of Health in Johannesburg, South Africa.

2. Experimental Conditions

GC: Agilent 6890N
Column:
30 m x 0.25 mm x 0.25 µm Rtx-CLPesticides
Oven Program:
60°C (2 minutes), 12°/minute to 300° (2 minutes)
Inlet Temp: 200°C
Injection Volume: 1 µL, splitless
Carrier Gas:
He at a constant flow of 1 mL/minute
Transfer Line Temp: 220°C
Total Run Time: 24 minutes

MS: LECO Pegasus® III GC-TOFMS
Ionization: Electron ionization at 70 eV
Mass Range (u): 45 to 450
Acquisition Rate: 20 spectra/second
Source Temp: 200°C

Data Processing

LECO ChromaTOF software was used to for Automated Peak Find, spectral deconvolution, and Compare.

3. Results

The industrial cleaner sample and the stomach extract were analyzed using the conditions described above. The Total Ion Chromatograms (TICs) for these samples are shown in Figures 1 and 2.

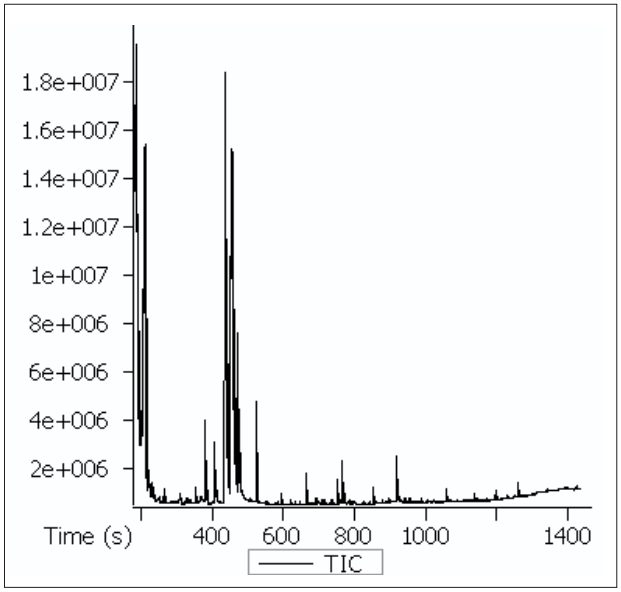

Figure 1. TIC for the industrial cleaner sample.

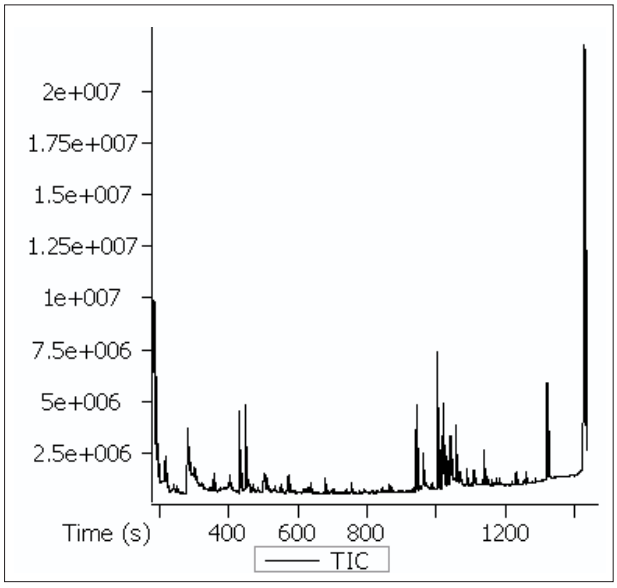

Figure 2. TIC for the stomach extract sample.

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An overlay of the chromatograms for the two samples is shown in Figure 3.

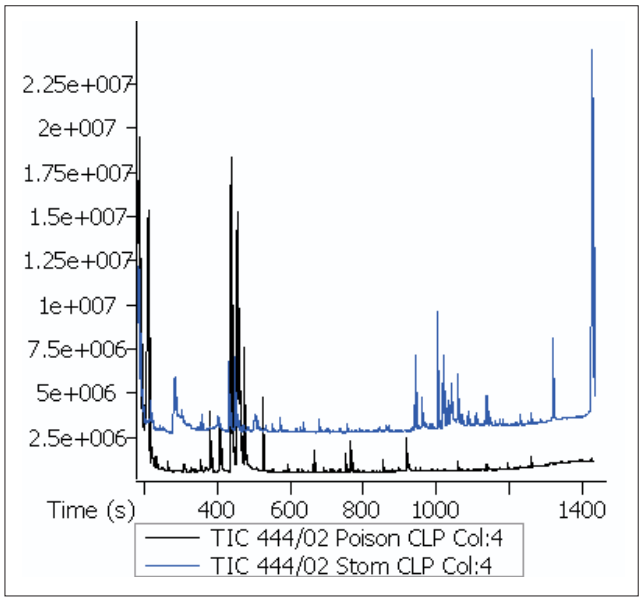

Figure 3. Overlay of the TICs for the industrial cleaner (Poison, black) and the stomach extract (Stom, blue).

As can be seen, the two samples are both complex. It is difficult to determine from their chromatograms alone whether components of the industrial cleaner (labeled as Poison in Figure 3) are in the stomach extract. This may be because of dilution and metabolism of components of the cleaner in the stomach. Rather than try to match all of the cleaner sample compounds with stomach components, 12 compounds were chosen that were considered to be characteristic of the cleaner. Subsequently, a Reference Table was created using the Peak Table created from the automated peak find and spectral deconvolution for the GC-TOFMS of the industrial cleaner sample, which contained only those 12 compounds (Table 1).

Table 1. Marker compounds in Reference Table for industrial cleaner sample.

Peak #	Name	R.T. (sec.)	Similarity	Unique Mass	CAS
44	Benzaldehyde	379.95	969	106	100-52-7
47	Benzyl Alcohol	406.70	929	108	100-51-6
48	2-Propanol, 1,1'-oxybis-	437.75	863	72	110-98-5
57	Dipropylene glycol	472.80	957	57	25265-71-8
60	Naphthalene	517.95	834	128	91-20-3
61	Acetic acid, phenylmethyl ester	524.30	958	108	140-11-4
71	Piperonal	664.15	969	149	120-57-0
81	à Isomethyl ionone	751.45	911	135	127-51-5
84	Lilial	765.45	929	189	80-54-6
85	2H-1-Benzopyran-2-one	768.80	962	118	91-64-5
101	Isopropyl Myristate	895.45	910	228	110-27-0
126	Trans-Farnesol	1260.50	857	69	106-28-5

Using this Reference Table in a ChromaTOF Data Processing Method called Compare, the stomach sample was automatically processed (including peak find and spectral deconvolution), and searched for these 12 compounds. The results are shown in Table 2.

Table 2. Data processing results from Compare.

Peak	Name	R.T. (sec.)	Similarity	Unique Mass	Type
41	Benzaldehyde	378.05	730	106	Match
46	Benzyl Alcohol	402.35	859	108	Match
50	2-Propanol, 1,1'-oxybis-	431.35	934	89	Match
58	Dipropylene glycol	469.20	793	59	Match
65	Naphthalene	517.40	880	128	Out of Tolerance
66	Acetic acid, phenylmethyl ester	522.75	773	108	Match
87	Piperonal	663.35	591	149	Match
100	à Isomethyl ionone	751.00	653	135	Match
103	Lilial	765.00	781	189	Match
104	2H-1-Benzopyran-2-one	768.20	842	118	Match
122	Isopropyl Myristate	895.10	769	228	Match
178	Trans-Farnesol	1260.20	854	69	Match

Table 2 indicates that all 12 marker compounds for the industrial cleaner were present in the stomach extract, and provides strong confirmatory evidence that the death did indeed occur after ingestion of the industrial cleaner. The software was set to allow a large concentration discrepancy, (i.e. a Match was indicated if the components in the stomach extract were present at levels of at least 1% of those in the neat cleaner). In spite of this, one component, naphthalene, was designated as being Out of Tolerance. This means that the compound was present in the stomach sample, but at a level <1% of the neat cleaner.

4. Conclusions

Compare, an integral feature of ChromaTOF software, provides an extremely fast and simple method for searching through a set of results for a limited basket of components. This type of process is extremely convenient for an analysis such as the above in the forensic field. Similarly it could easily be used to identify a pesticide cocktail in agricultural produce, or indeed any limited compound set in a complex matrix.

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