



APPLICATION NOTE

Gas Chromatography/ Mass Spectrometry

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The Qualitative Characterization of Fruit Juice Flavor using a TurboMatrix HS Trap and a Clarus SQ 8 GC/MS

Introduction

The PerkinElmer® TurboMatrix™ Headspace Trap system coupled with a Clarus® SQ 8 GC/MS is a very convenient means of identifying low concentration volatile organic compounds (VOCs) in foodstuffs. In this application note, the VOCs in various fruit juices were investigated. Sample preparation simply involved dispensing a fixed volume of fruit juice into a sample vial and sealing it. The analysis was fully automated.

Method

The experimental conditions for this analysis are given in Tables 1 to 4.

Table 1. GC Conditions.

Gas Chromatograph/ Mass Spectrometer	Clarus SQ 8
Column	60 m x 0.25 mm x 1.0 μ m Elite-SMS
Oven	35 °C for 5 min, then 6 °C/min to 245°
Injector	Programmable Split Splitless (PSS), 180 °C, Split OFF
Carrier Gas	Helium at 2.0 mL/min (28.6 psig initial pressure), HS Mode ON

Table 2. HS Trap Conditions.

Headspace System	TurboMatrix 110 HS Trap
Vial Equilibration	80 °C for 20 minutes
Needle	120 °C
Transfer Line	140 °C, long, 0.25 mm i.d. fused silica
Carrier Gas	Helium at 31 psig
Dry Purge	7 min
Trap	Air Toxics, 25 °C to 260 °C, hold for 7 min
Extraction Cycles	1 with 40 psig extraction pressure

Table 3. MS Conditions.

Scan Range	35 to 350 Daltons
Scan Time	0.1 s
Interscan Delay	0.06 s
Source Temp	180 °C
Inlet Line Temp	200 °C
Multiplier	1700V

Table 4. Sample Details.

Sample	1 mL of each of the following fruit juices:
	<ul style="list-style-type: none"> • Orange juice • Grapefruit juice • Apple juice • Lemon juice • Lime juice • Cranberry juice
Vial	Standard 22-mL vial with aluminum crimped cap with PTFE lined silicon septum

Results

The total ion chromatograms obtained from the six fruit juice samples are given in Figures 1 to 6. The component identities of the key peaks were established by performing mass spectral library searches. The results of these identifications are annotated in the following figures:

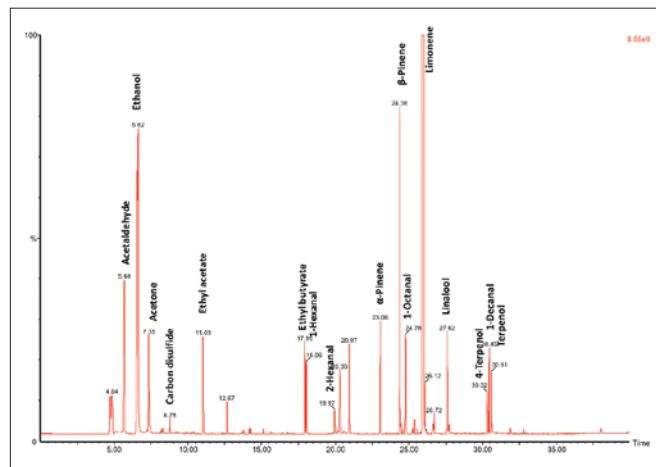


Figure 1. Full Total Ion Chromatogram obtained from orange juice.

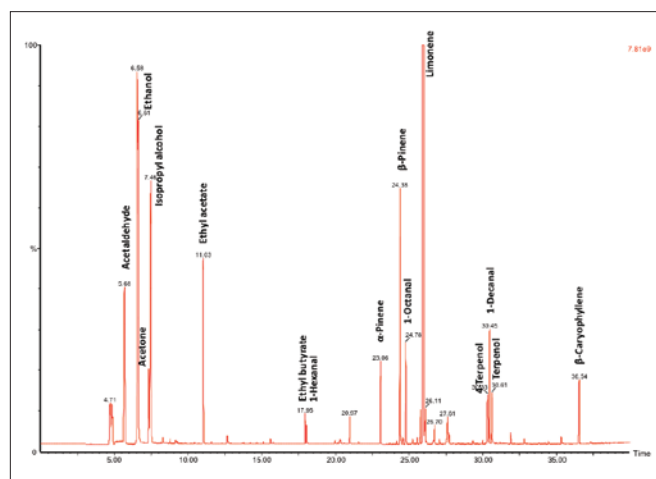


Figure 2. Full Total Ion Chromatogram obtained from grapefruit juice.

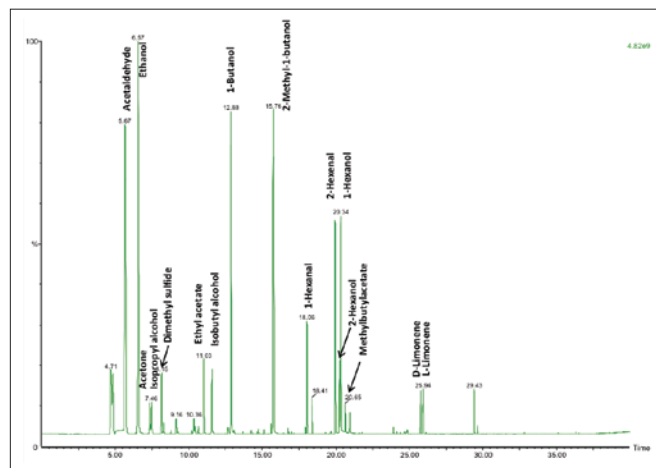


Figure 3. Full Total Ion Chromatogram obtained from apple juice.

Conclusions

This system provides a very simple and convenient way of characterizing the odor and flavor of natural products such as fruit juices. The use of GC/MS enables a very detailed aromatic profile of these fruit juices to be established. The use of a HS Trap system to perform the sample extraction enables low-level components to be visualized without compromising the system with injection of heavier, less volatile, unwanted sample material such as sugars and proteins.

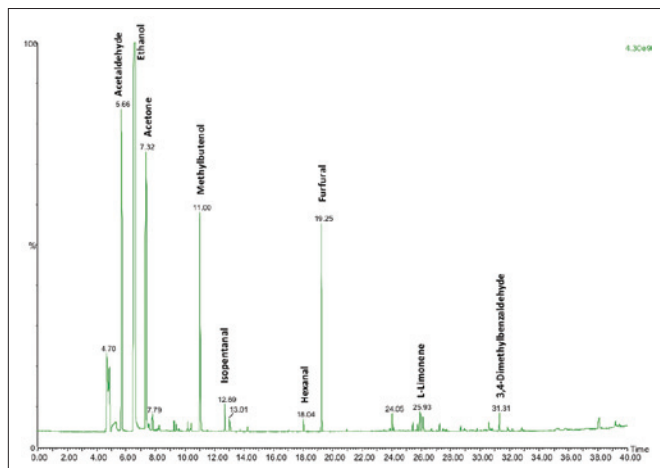


Figure 4. Full Total Ion Chromatogram obtained from lemon juice.

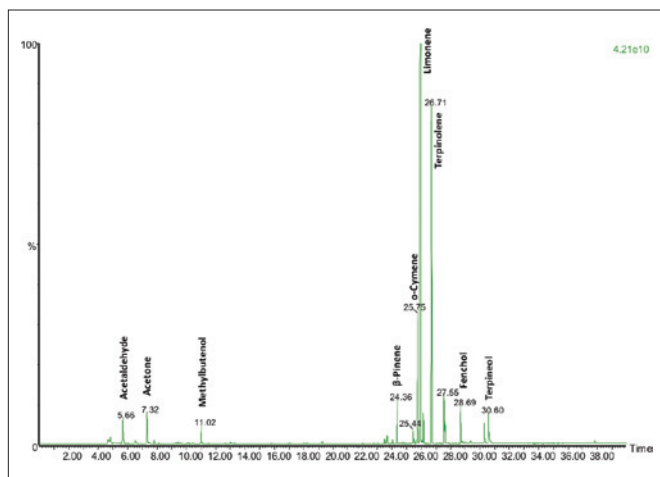


Figure 5. Full Total Ion Chromatogram obtained from lime juice.

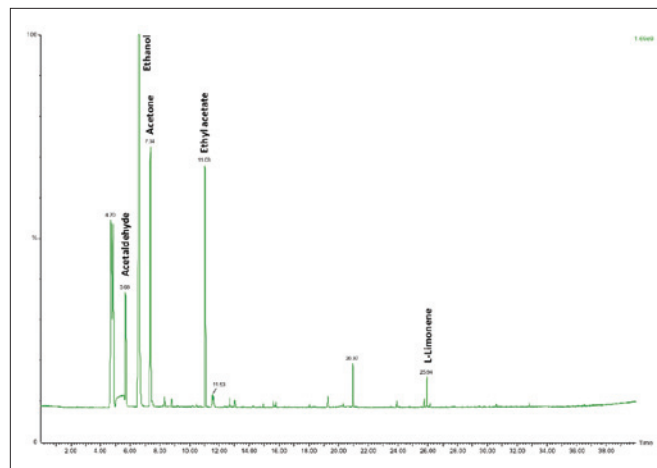


Figure 6. Full Total Ion Chromatogram obtained from raw cranberry juice.