Comparison of Aroma and Flavor Profiles of Strawberry-Flavored Candy and Fresh Strawberries

LECO Corporation; Saint Joseph, Michigan USA

Key Words: GC-TOFMS, GC-MS, Pegasus® BT, HS-SPME, Deconvolution, Produce, Strawberry

1. Introduction

Characterizing and differentiating samples based on similarities and differences of individual analytes can be important for many food and flavor applications. Gaining this type of understanding about a sample can lead to better quality control or process optimization. GC-TOFMS is a powerful analytical tool for making these comparisons, as individual analytes are separated chromatographically and full m/z range data are provided for identification and quantification. This tool allows the analyst to see more analytes and uncover what they might be missing. In this application, we demonstrate a comparison of compounds in a strawberry-flavored candy and a fresh strawberry to determine similarities and differences that may contribute to the taste and aroma.

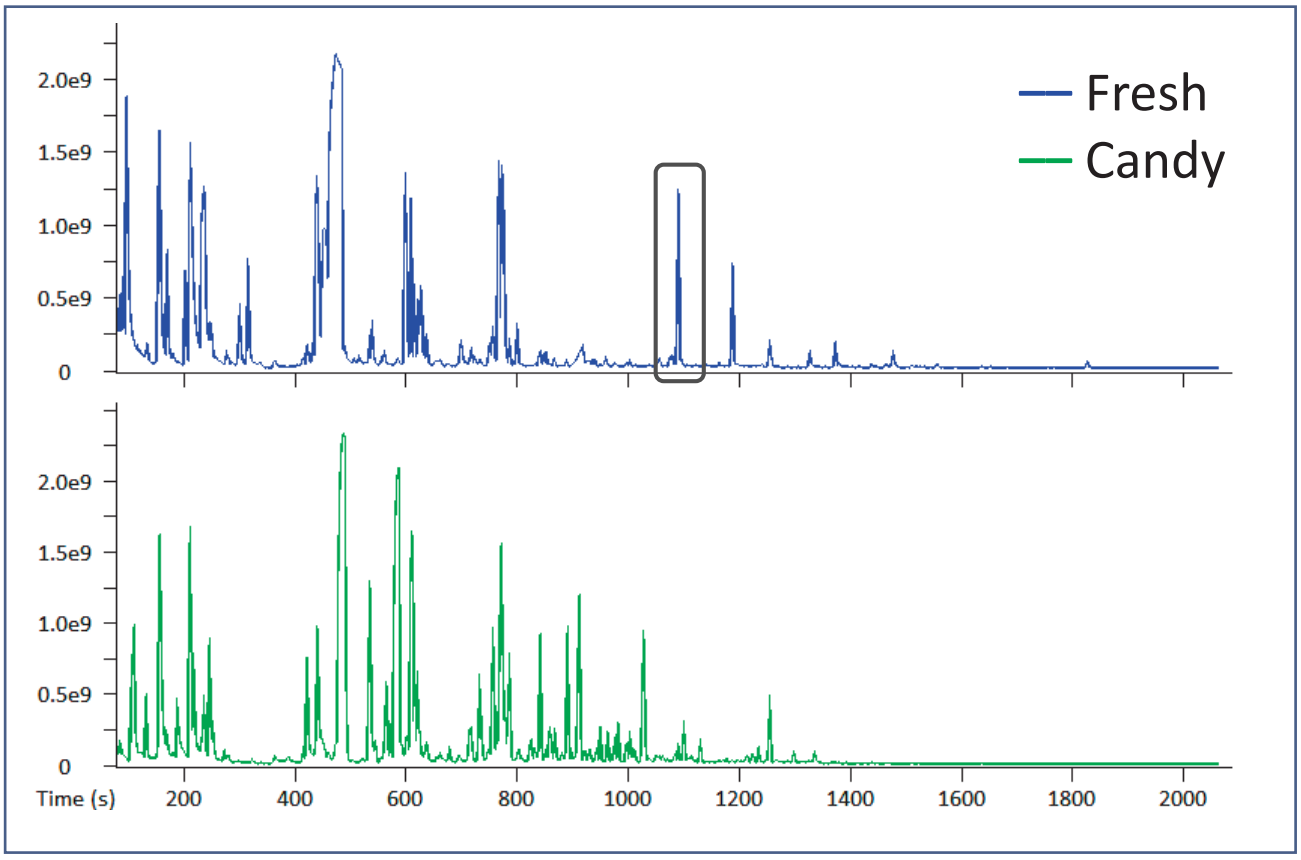


Figure 1. Total ion chromatograms (TICs) for a strawberry-flavored candy and a fresh strawberry are shown. These samples have dramatic differences with hundreds of analytes observed in each.

Life Science and Chemical Analysis Solutions

2. Experimental

A fresh strawberry and a strawberry-flavored candy were analyzed and compared. Approximately 6.5 g of each sample was transferred to a glass vial for HS-SPME analysis. The samples were incubated for 5 minutes at 50 °C and then extracted with a DVB/CAR/PDMS fiber (Supelco) for 30 minues at the same temperature. The samples were subsequently analyzed by GC-TOFMS with instrument conditions listed in Table 1.

Table 1. GC-TOFMS (*Pegasus* BT) Conditions

Gas Chromatograph	**Agilent 7890 with LECO L-PAL3 Autosampler**
Injection	SPME, 2 min desorption in 250 °C inlet, splitless
Carrier Gas	He @ 1.0 mL/min
Column	Rxi-5ms, 30 m x 0.25 mm i.d. x 0.25 µm coating (Restek)
Oven Program	2 min at 40 °C, ramp 5 °C/min to 200 °C, ramp 10 °C/min to 300 °C hold 1 min
Transfer Line	250 °C
Mass Spectrometer	**LECO *Pegasus* BT**
Ion Source Temperature	250 °C
Mass Range	35-650 m/z
Acquisition Rate	10 spectra/s

3. Results and Discussion

Representative TIC chromatograms for the complex strawberry-flavored candy and fresh strawberry samples are shown in Figure 1. Hundreds of analytes were determined and deconvolution provided the ability to further separate chromatographic coelutions to get more information on more analytes and to better characterize the sample. An example of deconvolution from the strawberry-flavored candy is highlighted in Figure 2, where two analytes that coelute were mathematically separated. The lactone adds coconut and fruity flavor notes, and glycerol triacetate is a common food additive, sometimes used as a solvent for flavoring.

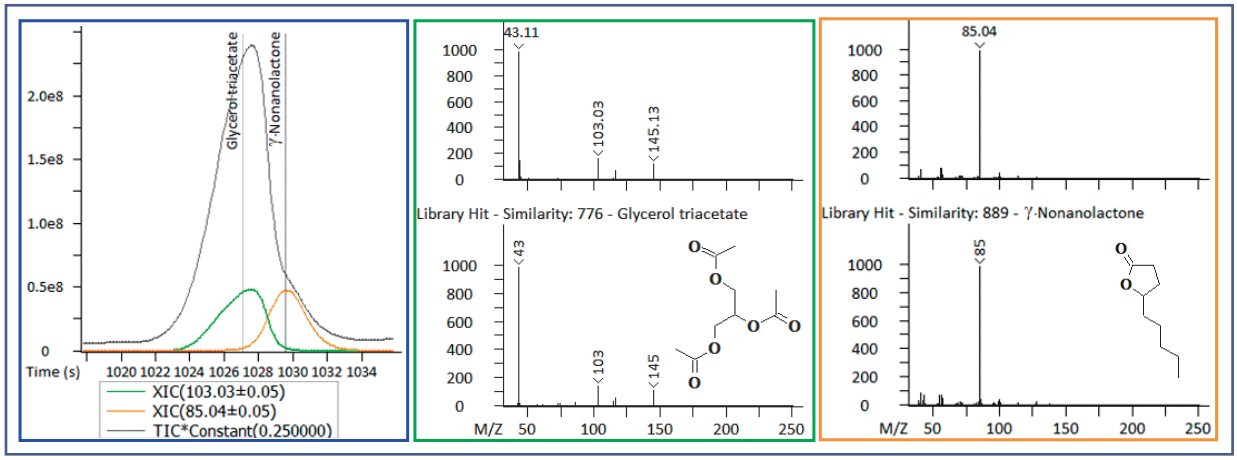


Figure 2.Hundreds of analytes were observed and a deconvolution example from the Strawberry candy is highlighted where the additive, glycerol triacetate chromatographically coelutes with the lactone, τ -nonalactone. Deconvolution mathematically separated these analytes and provided pure peak profiles and spectral information for library searching which led to these tentative identifications.

As observed in Figure 1, there are dramatic differences between the candy and the fresh strawberry. To better understand these differences, the coeluting analytes from Figure 2 were compared in Figure 3. In the TIC, it appears that there is only one peak and that it is only present in the candy. When extracted ion chromatograms (XICs) are plot for each analyte, however, it becomes apparent that while the additive is only in the candy, the lactone is present in both, though at a much lower level in the fresh strawberry. Deconvolution along with full mass range data made it possible to make this observation.

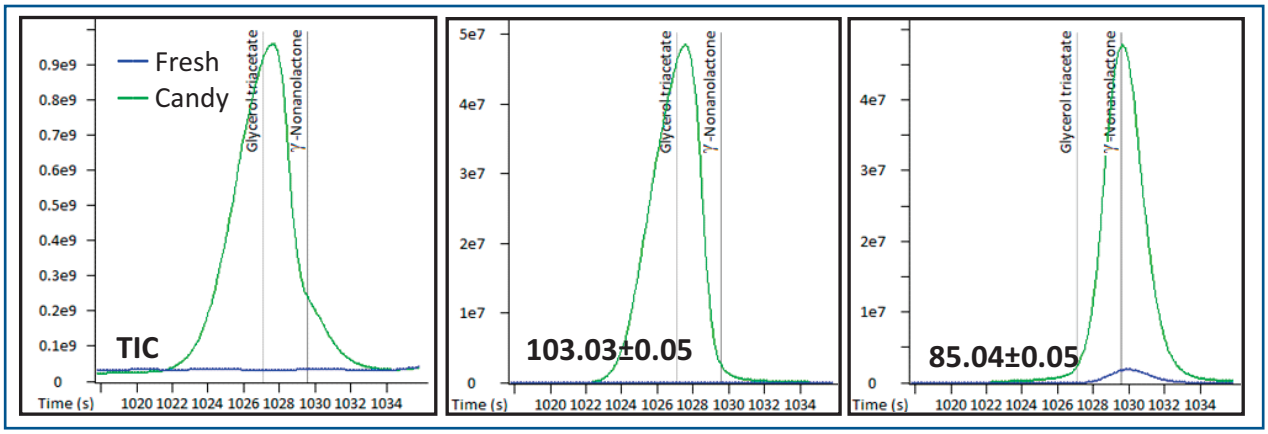
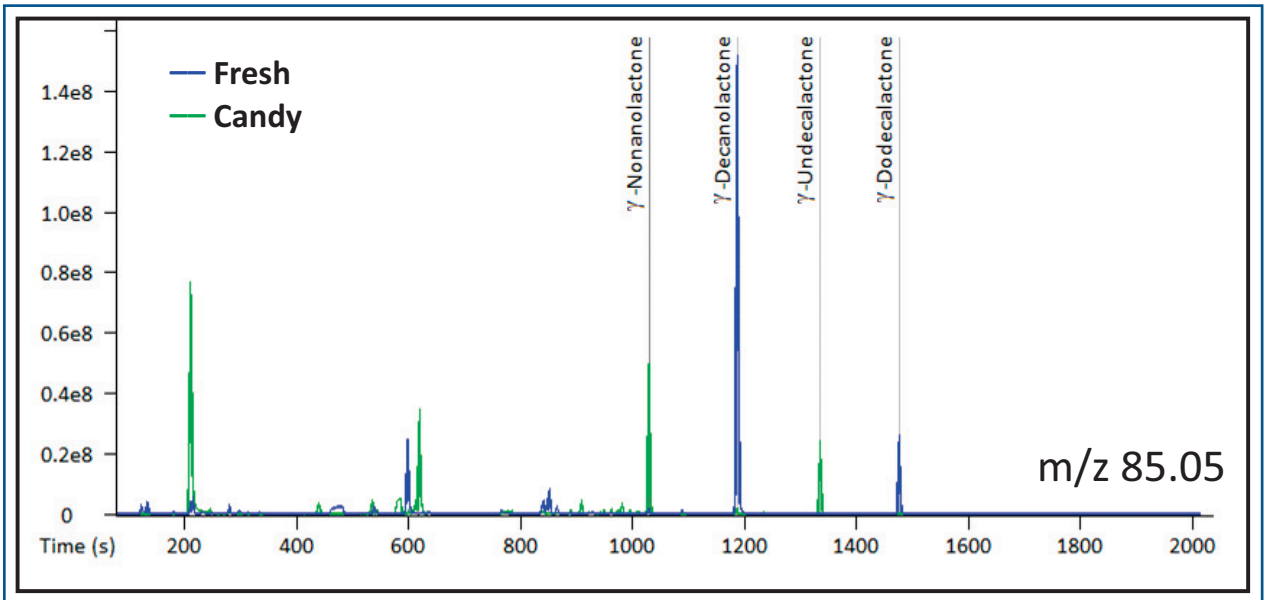


Figure 3. The strawberry candy was compared to a fresh strawberry. The additive was observed only in the candy, while the lactone was observed in both, but at a much lower level in the fresh strawberry. In the TIC, there was no evidence of either peak in the fresh strawberry.

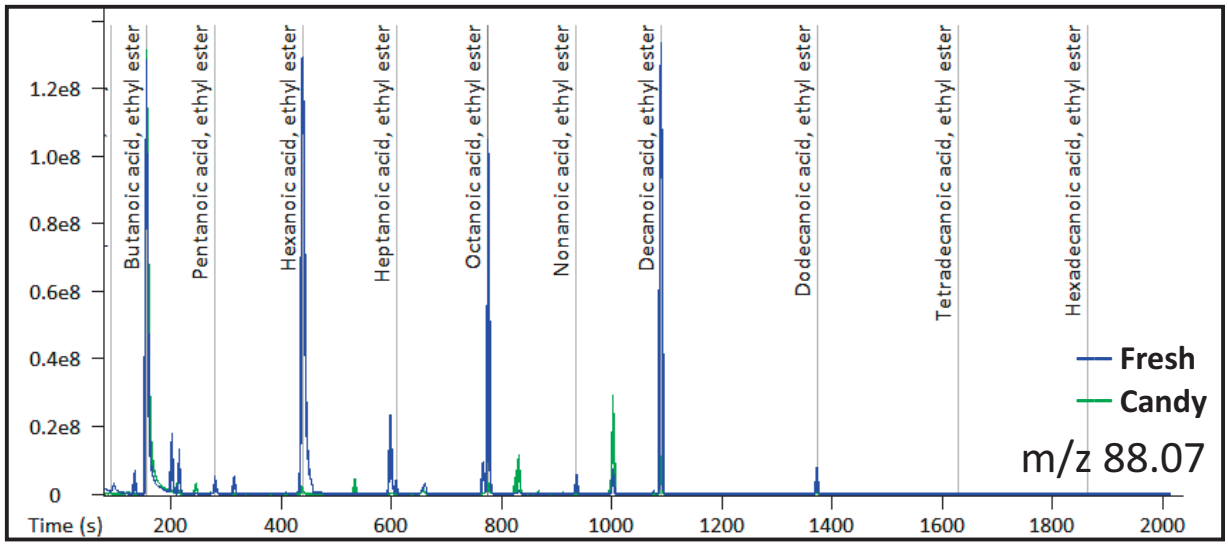
Because lactones tend to be important flavor and odor contributors, this class of compounds was further investigated and compared in Figure 4. Four lactones are highlighted and compared. The candy had much higher levels of γ-nonalactone and γ-undecalactone and the fresh strawberry had much higher levels of γ-decanolactone and γ-dodecanolactone. The odor properties of each of these are slightly different, contributing to the different overall flavor characteristics.



Name	R.T. (s)	Formula	CAS	Similarity	Ratio
γ-Nonanolactone	1029.59	$C_9H_{16}O_2$	104-61-0	889	0.044
γ-Decanolactone	1187.8	$C_{10}H_{18}O_2$	706-14-9	931	154
γ-Undecalactone	1335.45	$C_{11}H_{20}O_2$	104-67-6	940	0.011
γ-Dodecalactone	1476.59	$C_{12}H_{22}O_2$	2305-05-7	880	75.4

Figure 4. Lactones observed in the fresh strawberry and strawberry candy and their relative levels are shown. These important flavor compounds differ between the samples. The ratio is reported as Fresh/Candy.

Other compound classes can also be investigated to better understand the flavor characteristics of each sample. For example, ethyl esters are compared between the samples in Figure 5. Almost all of the ethyl esters were at higher levels in the fresh strawberry compared to the candy. Esters provide many of the flavors and odors for a food product and these differences are important for understanding the samples. More general characterization can also be accomplished with comparison of XIC traces. For example, m/z 204.22 is a common mass in sesquiterpenes and is plot in Figure 6. This class of compounds tends to be higher in the candy compared to the fresh strawberry.



Name	R.T. (s)	Formula	CAS	Similarity	Ratio
Propanoic acid, ethyl ester	91.0622	$C_5H_{10}O_2$	105-37-3	919	fresh
Butanoic acid, ethyl ester	155.819	$C_6H_{12}O_2$	105-54-4	895	0.74
Pentanoic acid, ethyl ester	280.295	$C_7H_{14}O_2$	539-82-2	922	0.99
Hexanoic acid, ethyl ester	438.979	$C_8H_{16}O_2$	123-66-0	922	69.9
Heptanoic acid, ethyl ester	608.983	$C_9H_{18}O_2$	106-30-9	620	fresh
Octanoic acid, ethyl ester	776.22	$C_{10}H_{20}O_2$	106-32-1	919	21.3
Nonanoic acid, ethyl ester	936.411	$C_{11}H_{22}O_2$	123-29-5	915	177
Decanoic acid, ethyl ester	1089.89	$C_{12}H_{24}O_2$	110-38-3	939	15.6
Dodecanoic acid, ethyl ester	1372.74	$C_{14}H_{28}O_2$	106-33-2	773	16.5
Tetradecanoic acid, ethyl ester	1629.43	$C_{16}H_{32}O_2$	124-06-1	671	4.1
Hexadecanoic acid, ethyl ester	1863.42	$C_{18}H_{36}O_2$	628-97-7	752	4.9

Figure 5. Ethyl esters are labeled and compared. The relative levels of each ethyl ester in each sample are shown with the ratio reported as Fresh/Candy. Most of these esters are observed at elevated levels in the fruit compared to the candy.

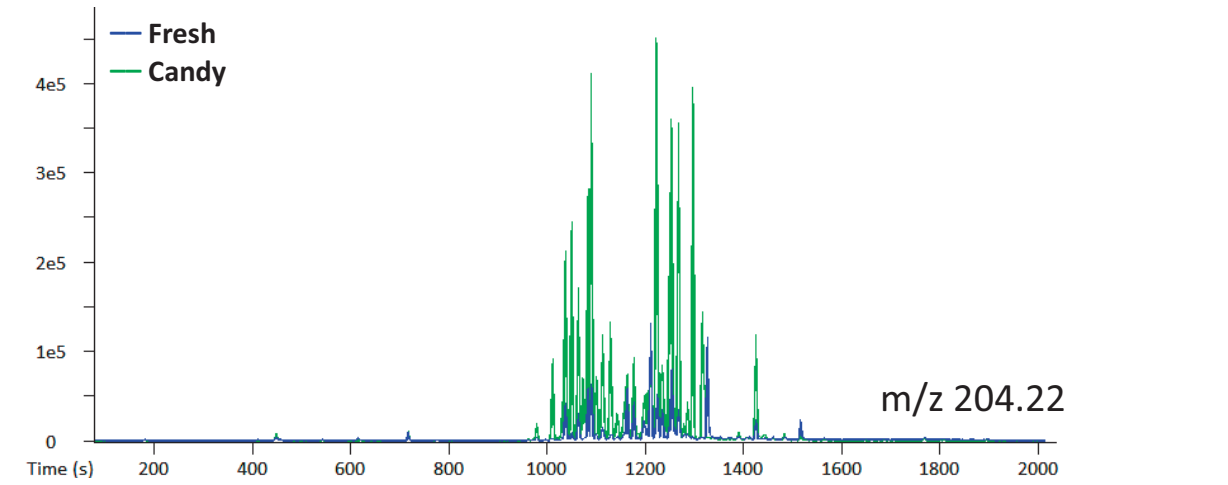


Figure 6. XIC 204.22 for sesquiterpenes is shown. These are present at higher levels in the strawberry candy than they are in the fresh strawberry.

Comparing and contrasting various compound classes as well as individual analytes within those classes between a fresh strawberry and strawberry-flavored candy provides interesting insight to the flavor characteristics of each.

4. Conclusion

The *Pegasus* BT is a powerful tool for gaining a better understanding of your samples. Here, we compared flavor analytes and additives between a strawberry-flavored candy and a fresh strawberry. Deconvolution helped uncover differences that were hidden in the TIC and provided more information on more analytes. Compound classes were investigated with lactones, ethyl esters, and sesquiterpenes compared between each sample. This analytical tool helps you see more in your standard analysis.

Life Science and Chemical Analysis Solutions

LECO Corporation | 3000 Lakeview Avenue | St. Joseph, MI 49085 | Phone: 800-292-6141 | 269-985-5496
info@leco.com • www.leco.com | ISO-9001:2008 | HQ-Q-994 | *LECO is a registered trademark of LECO Corporation.*

Form No. 203-821-533 2/17-REV0