Tasting "Weird and Wild" Jelly Bean Flavors Using HS SPME Gas Chromatography Mass Spectrometry

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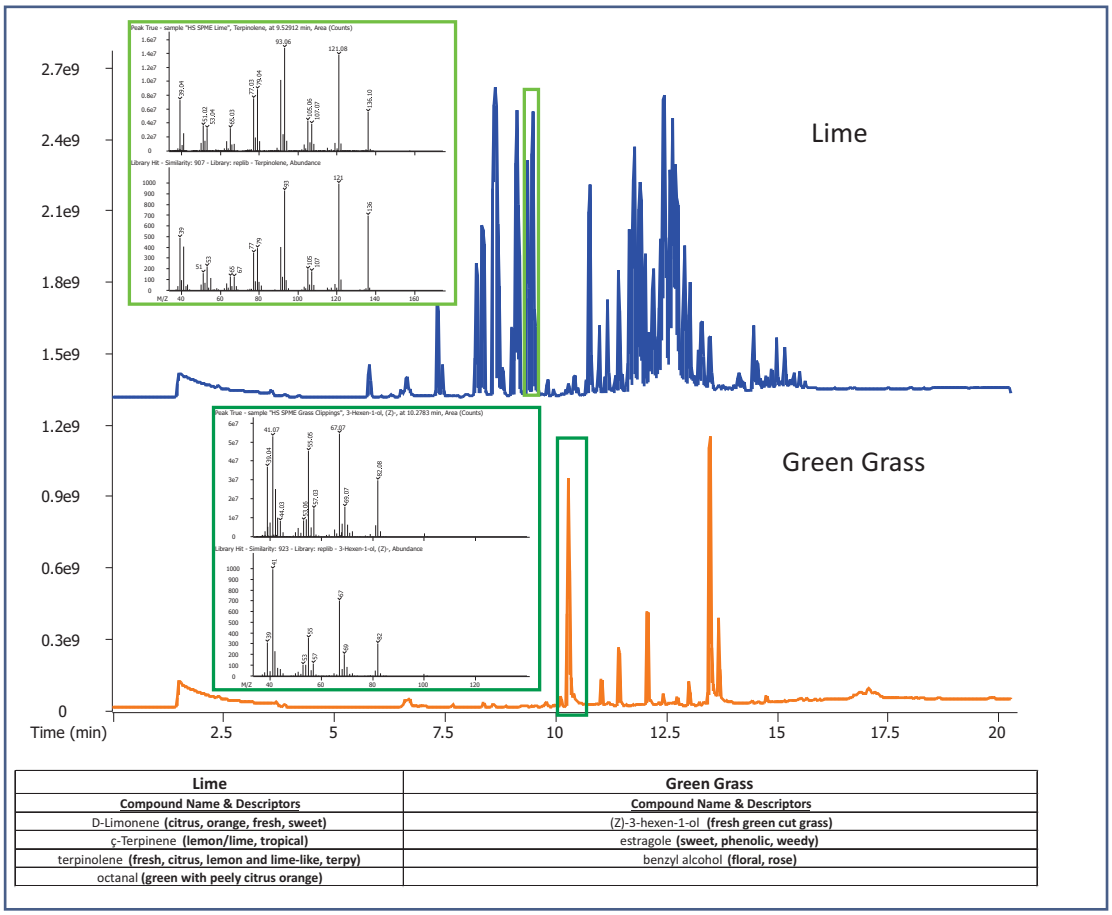
Key Words: GC-TOFMS, GC-MS, Pegasus® BT, Flavor

1. Introduction

Bring Your Child to Work Day is a national event in the United States, which is often difficult for children of scientists to celebrate due to lab safety protocols. This application note details a safe experiment designed to stimulate interest in the sciences for all ages while demonstrating the ease-of-use and capabilities of a new benchtop Time-of-Flight GC-MS to effectively differentiate exotic flavor profiles in store-purchased jelly beans.

As part of the experiment, children participated in a game, taking turns selecting jelly beans from one of several visually-identical pairs. Each jelly bean pair had either an appealing or appalling taste. After tasting their selections, each child quickly realized there was no way to successfully predict which jelly bean was the appealing taste. In the second part of the experiment, the children were allowed to prepare and analyze a portion of their jelly beans using the *Pegasus* BT GC-MS, and use the data to assist them in making their selection. When using the GC-MS data, the children were consistently successful at selecting their preferred flavor.



Lime	Green Grass
Compound Name & Descriptors	Compound Name & Descriptors
D-Limonene **(citrus, orange, fresh, sweet)**	(Z)-3-hexen-1-ol **(fresh green cut grass)**
ç-Terpinene **(lemon/lime, tropical)**	estragole **(sweet, phenolic, weedy)**
terpinolene **(fresh, citrus, lemon and lime-like, terpy)**	benzyl alcohol **(floral, rose)**
octanal **(green with peely citrus orange)**	

Figure 1. The figure above shows GC-MS total ion chromatograms (TIC) for a good-flavored jelly bean (Top, lime) vs. a bad-flavored one (Bottom, green grass) along with Peak True (deconvoluted) and NIST library spectra for a key flavor-contributing compound from each jelly bean. The table contains additional flavor-contributing compounds and their flavor descriptors, which each child used to successfully choose good-flavored jelly beans.

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2. Experimental

As part of the experiment, children participated in a game in which they took turns selecting a jelly bean from one of the matching pairs shown in Table I below.

Table I. Description of Jelly Bean Pairs

Good	Bad
Fruity	Smelly Socks
Popcorn	Spoiled Eggs
Peach	Vomit
Lime	Green Grass
Blueberry	Minty Toothpaste
Chocolate	Dog Food

They were then asked to taste their selection to see if they had "won" or "lost" by selecting an appealing vs. appalling flavor. It was evident that selections based on visual appearance of the jelly beans alone led to random results during the taste tests. Example responses from our willing participants are shown in the photos below.

A second round of the game was started, and each child was given an option to have LECO's *Pegasus* BT GC-MS system "taste" the jelly beans first, prior to the children making a selection. The components identified by the GC-MS, and their respective taste and odor descriptors, were used to aid in selecting jelly beans in this round.

The children participated in safely preparing the jelly beans for a HS-SPME GC-MS experiment that would provide the data used to influence their selections. A portion of a single jelly bean was placed into a 20 mL HS vial along with 5 mL of HPLC grade H_2O, and 1g of NaCl.

The children were then able to load the samples into the autosampler of the GC-MS system and start the sample queue on their own.

A 1 cm PDMS/Carboxen/DVB SPME fiber was used to extract aroma compounds from the headspace of each jelly bean and deliver them to the GC–MS for analysis. An Rtx-200 MS column was used for the chromatographic separation. The TOFMS data were acquired from 30 to 500 m/z at 20 spectra/second. The jelly beans were analyzed on the *Pegasus* BT under the conditions shown below in Table II.

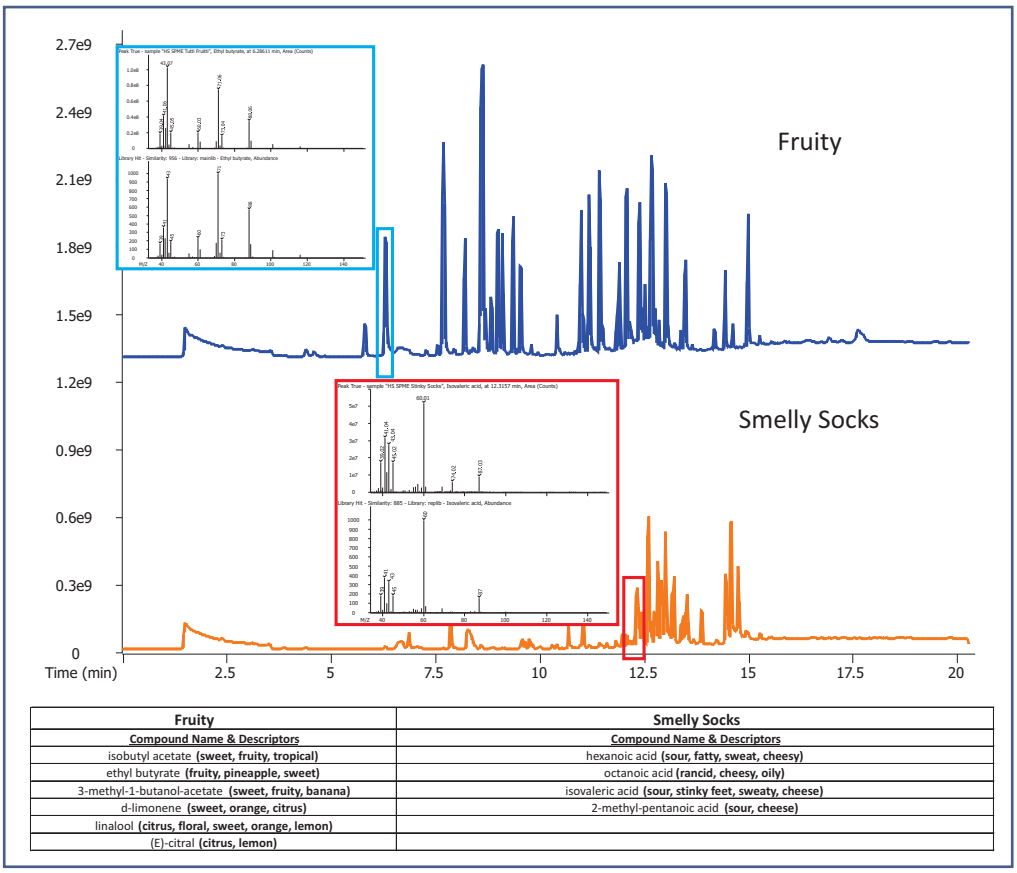
Table II. GC-TOFMS (*Pegasus* BT) Conditions

Gas Chromatograph	**Agilent 7890 with LECO L-PAL 3 Autosampler**
Injection	2 min SPME desorption, Split 10:1 at 250 °C
Carrier Gas	He @ 1.0 mL/min, Constant Flow
Column	Rtx-200 MS, 30 m x 0.25 mm i.d. x 0.25 µm coating (Restek)
Oven Program	5 min at 35 °C, ramp 20 °C/min to 240 °C, hold 5 min
Transfer Line	250 °C
Mass Spectrometer	**LECO *Pegasus* BT**
Ion Source Temperature	250 °C
Mass Range	30-500 m/z
Acquisition Rate	20 spectra/s

3. Results and Discussion

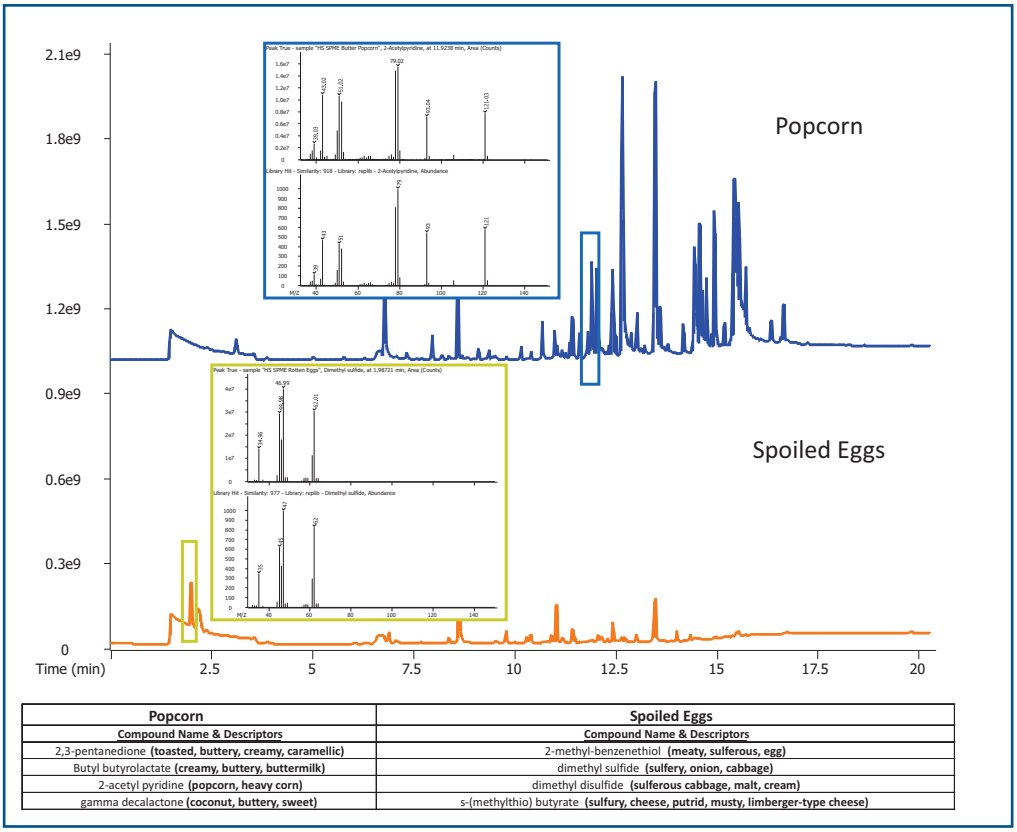
The benchtop time-of-flight GC-MS data was used to differentiate the visually identical jelly beans based on the components detected and identified in their headspace. The data was compiled into tables with key analytes and their taste/odor descriptors so that the kids could use the information to influence their decision when making their second-round jelly bean taste selections.

The Total Ion Chromatograms (TICs) with tables containing the key differentiating ingredients for each Jelly Bean type are shown in Figures 2 through 6. Each chromatogram also includes a Peak True (deconvoluted) mass spectrum from one of the key taste/odor analytes and the NIST library match with similarity score for tentative identification.



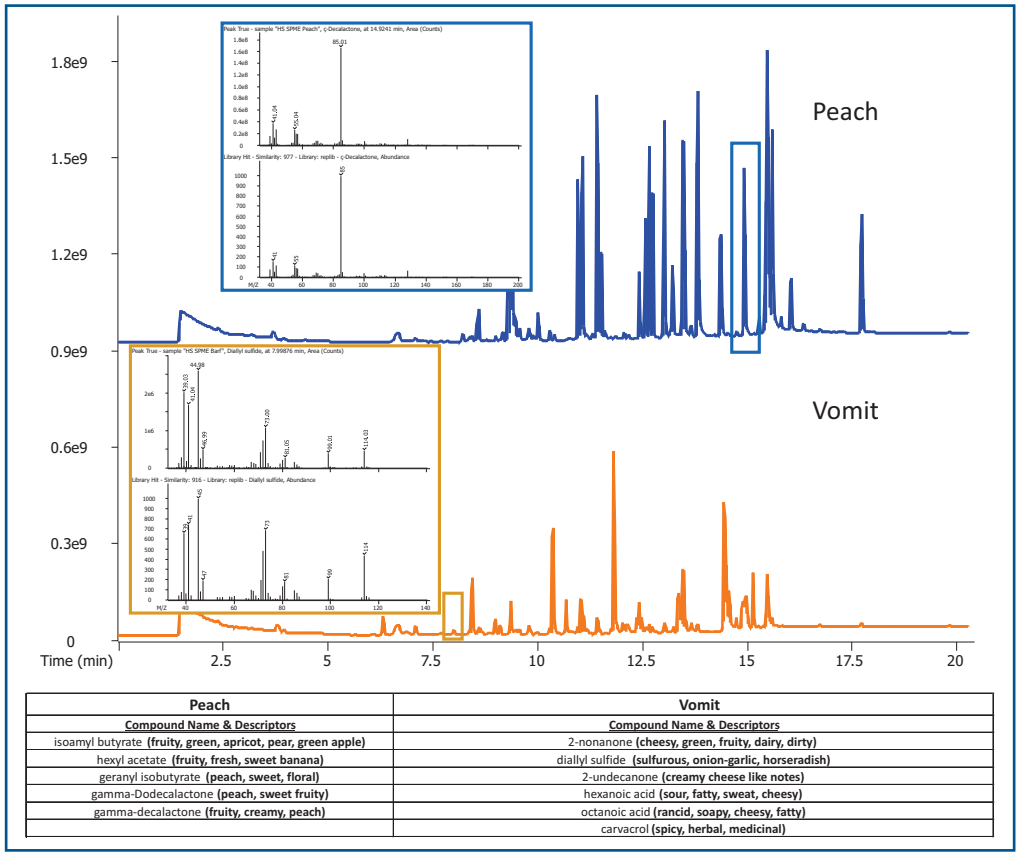
Fruity	Smelly Socks
Compound Name & Descriptors	**Compound Name & Descriptors**
isobutyl acetate **(sweet, fruity, tropical)**	hexanoic acid **(sour, fatty, sweat, cheesy)**
ethyl butyrate **(fruity, pineapple, sweet)**	octanoic acid **(rancid, cheesy, oily)**
3-methyl-1-butanol-acetate **(sweet, fruity, banana)**	isovaleric acid **(sour, stinky feet, sweaty, cheese)**
d-limonene **(sweet, orange, citrus)**	2-methyl-pentanoic acid **(sour, cheese)**
linalool **(citrus, floral, sweet, orange, lemon)**	
(E)-citral **(citrus, lemon)**	

Figure 2. The figure above shows GC-MS total ion chromatograms (TIC) for a good-flavored jelly bean (Top, Fruity) vs. a bad-flavored one (Bottom, Smelly Socks) along with Peak True (deconvoluted) and NIST library spectra for a key flavor contributing compound from each jelly bean. The table contains additional flavor contributing compounds and their flavor descriptors.



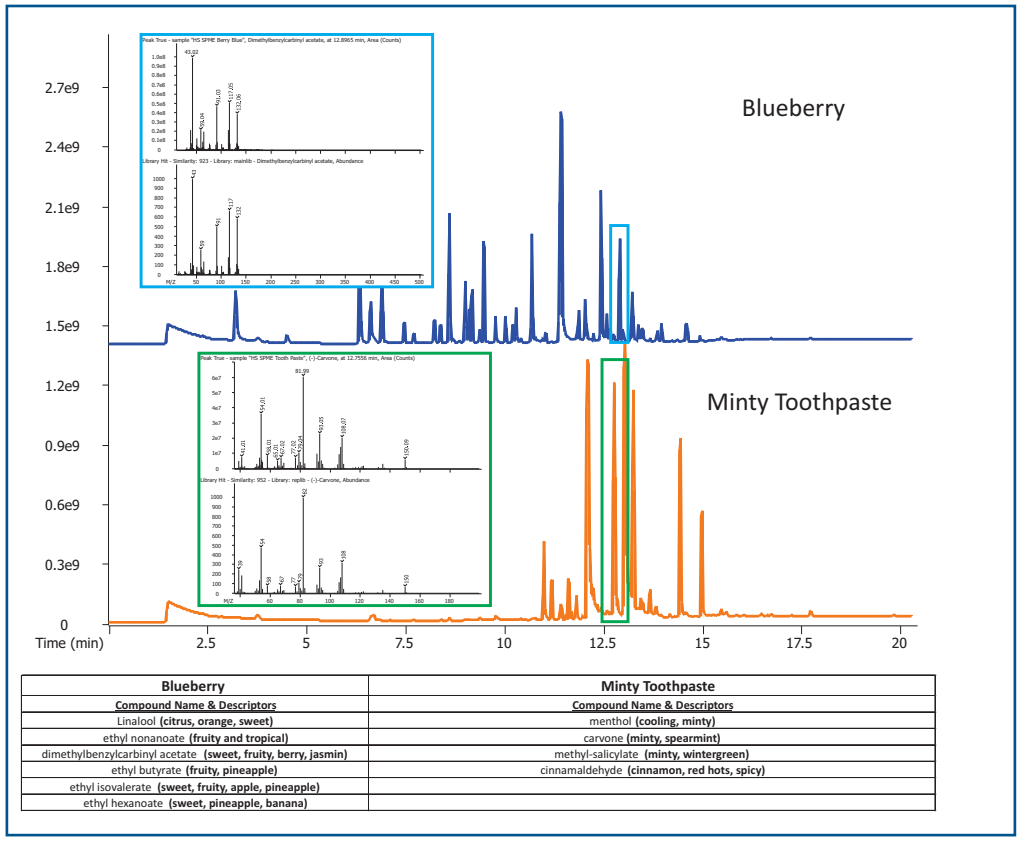
Popcorn	Spoiled Eggs
Compound Name & Descriptors	**Compound Name & Descriptors**
2,3-pentanedione **(toasted, buttery, creamy, caramellic)**	2-methyl-benzenethiol **(meaty, sulferous, egg)**
Butyl butyrolactate **(creamy, buttery, buttermilk)**	dimethyl sulfide **(sulfery, onion, cabbage)**
2-acetyl pyridine **(popcorn, heavy corn)**	dimethyl disulfide **(sulferous cabbage, malt, cream)**
gamma decalactone **(coconut, buttery, sweet)**	s-(methylthio) butyrate **(sulfury, cheese, putrid, musty, limberger-type cheese)**

Figure 3. The figure above shows GC-MS total ion chromatograms (TIC) for a good-flavored jelly bean (Top, Popcorn) vs. a bad-flavored one (Bottom, Spoiled Eggs) along with Peak True (deconvoluted) and NIST library spectra for a key flavor contributing compound from each jelly bean. The table contains additional flavor contributing compounds and their flavor descriptors.



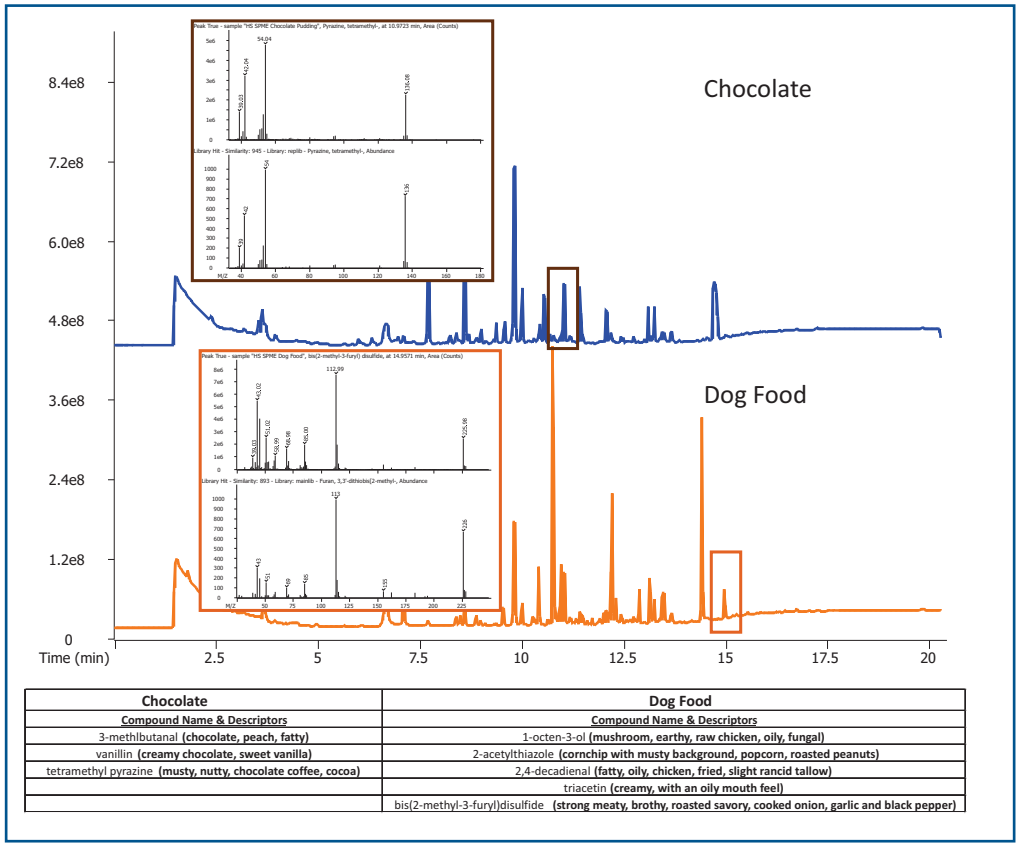
Peach	Vomit
Compound Name & Descriptors	**Compound Name & Descriptors**
isoamyl butyrate **(fruity, green, apricot, pear, green apple)**	2-nonanone **(cheesy, green, fruity, dairy, dirty)**
hexyl acetate **(fruity, fresh, sweet banana)**	diallyl sulfide **(sulfurous, onion-garlic, horseradish)**
geranyl isobutyrate **(peach, sweet, floral)**	2-undecanone **(creamy cheese like notes)**
gamma-Dodecalactone **(peach, sweet fruity)**	hexanoic acid **(sour, fatty, sweat, cheesy)**
gamma-decalactone **(fruity, creamy, peach)**	octanoic acid **(rancid, soapy, cheesy, fatty)**
	carvacrol **(spicy, herbal, medicinal)**

Figure 4. The figure above shows GC-MS total ion chromatograms (TIC) for a good-flavored jelly bean (Top, Peach) vs. a bad-flavored one (Bottom, Vomit) along with Peak True (deconvoluted) and NIST library spectra for a key flavor contributing compound from each jelly bean. The table contains additional flavor contributing compounds and their flavor descriptors.



Blueberry	Minty Toothpaste
Compound Name & Descriptors	**Compound Name & Descriptors**
Linalool **(citrus, orange, sweet)**	menthol **(cooling, minty)**
ethyl nonanoate **(fruity and tropical)**	carvone **(minty, spearmint)**
dimethylbenzylcarbinyl acetate **(sweet, fruity, berry, jasmin)**	methyl-salicylate **(minty, wintergreen)**
ethyl butyrate **(fruity, pineapple)**	cinnamaldehyde **(cinnamon, red hots, spicy)**
ethyl isovalerate **(sweet, fruity, apple, pineapple)**	
ethyl hexanoate **(sweet, pineapple, banana)**	

Figure 5. The figure above shows GC-MS total ion chromatograms (TIC) for a good-flavored jelly bean (Top, Blueberry) vs. a bad-flavored one (Bottom, Minty Toothpaste) along with Peak True (deconvoluted) and NIST library spectra for a key flavor contributing compound from each jelly bean. The table contains additional flavor contributing compounds and their flavor descriptors.



Chocolate	Dog Food
Compound Name & Descriptors	**Compound Name & Descriptors**
3-methlbutanal **(chocolate, peach, fatty)**	1-octen-3-ol **(mushroom, earthy, raw chicken, oily, fungal)**
vanillin **(creamy chocolate, sweet vanilla)**	2-acetylthiazole **(cornchip with musty background, popcorn, roasted peanuts)**
tetramethyl pyrazine **(musty, nutty, chocolate coffee, cocoa)**	2,4-decadienal **(fatty, oily, chicken, fried, slight rancid tallow)**
	triacetin **(creamy, with an oily mouth feel)**
	bis(2-methyl-3-furyl)disulfide **(strong meaty, brothy, roasted savory, cooked onion, garlic and black pepper)**

Figure 6. The figure above shows GC-MS total ion chromatograms (TIC) for a good-flavored jelly bean (Top, Chocolate) vs. a bad-flavored one (Bottom, Dog Food) along with Peak True (deconvoluted) and NIST library spectra for a key flavor contributing compound from each jelly bean. The table contains additional flavor contributing compounds and their flavor descriptors.

4. Conclusion

With the use of the *Pegasus* BT data, the children were able to predict the appealing and appalling flavored jelly beans based on the taste profile for the analytes which were identified by GC-MS in each of the jelly bean varieties.

The kids found the experiment exciting and were exposed to analytical chemistry in a fun, safe, and educational way.

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