Comparison of “Weird and Wild” Jelly Bean Flavors Using HS SPME Gas Chromatography Mass Spectrometry

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Introduction

Bring Your Children to Work Day is a national event in the United States which often excludes children with parents in the sciences due to lab safety protocols. This poster details a safe experiment which was designed to create interest in the sciences for all ages, while also demonstrating the capabilities of a new benchtop Time-of-Flight GC-MS, to effectively differentiate some very exotic flavor profiles in store-purchased jelly beans.

As part of the experiment, kids 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

Visually Similar Jelly Bean Pairs
Tutti-Fruitti & Stinky Socks
Buttered Popcorn & Rotten Egg
Peach and Barf
Lime & Lawn Clippings
Berry Blue and Toothpaste
Chocolate Pudding & Canned Dog Food

They were then asked to taste their selection to see if they had “won” or “lost” by selecting an appealing vs. appalling jelly bean 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 the kids were given an option to have LECO’s Pegasus® BT GC-MS system “taste” the jelly beans first, prior to the kids 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 kids participated in preparing the jelly beans for a HS-SPME GC-MS experiment that would provide the data used to influence their selections. The details of the sample preparation and subsequent GC-MS analyses are shown in the Methods section.

Figure 1. Pegasus BT

Methods

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. 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 kids were then able to load the samples into the autosampler of the GC-MS system, and start the sample queue on their own. The jelly beans were analyzed on the Pegasus BT under the conditions shown below in Table II.

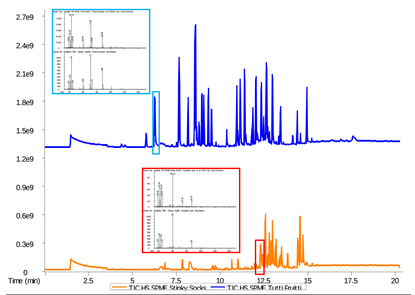
Table II. GC-MS Instrument Conditions

Gas Chromatograph	Agilent 7890 with LECO L-PAL3 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

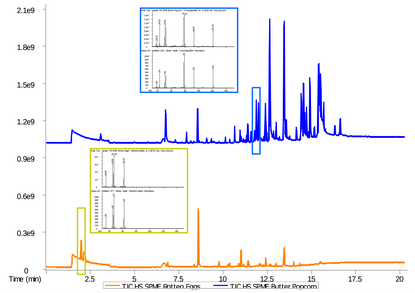
Results

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 selections for tasting.

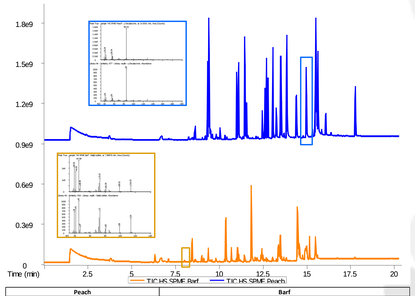
The Total Ion Chromatograms (TICs) with tables containing the key differentiating ingredients for each Jelly Bean type are shown below. Each chromatogram also includes a deconvoluted mass spectrum from one of the key taste/odor analytes, and its NIST library match with similarity score, which were used to tentatively identify them.



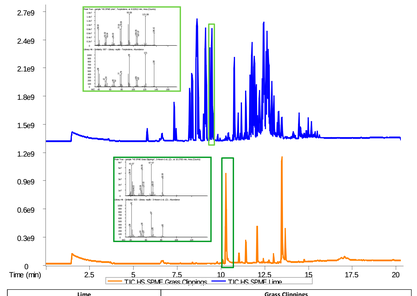
Tutti Fruitti	Stinky Socks
Compound Name & Descriptors	**Compound Name & Descriptors**
isobutyl acetate (sweet, fruity, tropical)	hexanoic acid (sour, fatty, sweat, cheesy)
ethyl butyrate (fruity, pineapple, sweet)	octanoic acid (rancid, cheesy, oily)
3-methyl-1-butanol acetate (sweet, fruity, banana)	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)	



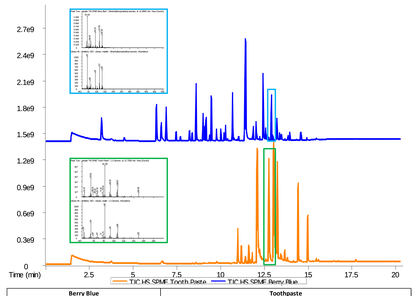
Butter Popcorn	Rotten Egg
Compound Name & Descriptors	**Compound Name & Descriptors**
2,3-pentanedione (toasted, buttery, creamy, caramelly)	2-methyl-benzenethiol (meaty, sulfurous, egg)
butyl butyrolactol (creamy, buttery, butterscotch)	dimethyl sulfide (sulfury, onion, cabbage)
2-acetyl pyridine (popcorn, heavy corn)	dimethyl disulfide (sulfurous cabbage, malt, cream)
gamma-decalactone (coconut, buttery, sweet)	s-(methylthio) butyrate (sulfury, cheese, putrid, musty, limburger-type cheese)



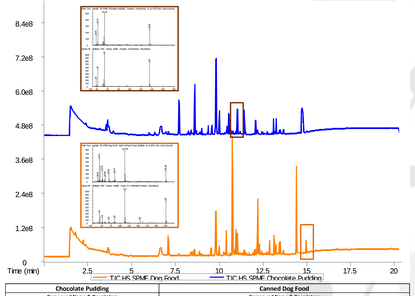
Peach	Barf
Compound Name & Descriptors	**Compound Name & Descriptors**
isoamyl butyrate (fruity, green, apricot, pear, green apple)	2-nonanone (cheesy, green, fruity, dairy, dirty)
hexyl acetate (fruity, fresh, sweet banana)	diallyl sulfide (sulfurous, onion-garlic, horseradish)
geranyl isobutyrate (peach, sweet, floral)	2-undecylidene (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)



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



Berry Blue	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)	

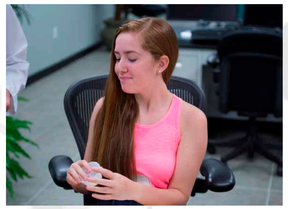


Chocolate Pudding	Canned Dog Food
Compound Name & Descriptors	**Compound Name & Descriptors**
3-methylbutanal (chocolate, peach, fatty)	1-octen-3-ol (mushroom, earthy, raw chicken, oily, fungal)
vanillin (creamy chocolate, sweet vanilla)	2-acetylthiazole (cornchip with musty background, popcorn, roasted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

Conclusions

With the use of the Pegasus BT data, the kids were able to predict the good vs bad flavored jelly beans based on the published sensory descriptors 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 and educational way.



Delivering the Right Results