



Analyzing Tomato Essence To Identify Key Markers

Sensus Technical Note (SEN-TN-00024)

04/03/2009

Kevin L. Goodner, Ph.D.

ABSTRACT

Sensus produces essences for both red and green tomatoes. Determining if an essence is red or green tomato and its relative strength (weak, normal, strong) is currently accomplished by sensory analysis. In order to develop a more analytical approach, eighty lots of tomato essences were assessed for its tomato character, analyzed by GC-MS, and analyzed by multivariate statistics to determine which compounds most influence panelists in their classifications. One sensory assessor focused on 6-methyl-5-hepten-2-one, benzaldehyde, and 2-isobutylthiazole to determine if a sample was red or green. The same assessor keyed in on acetone, dimethyl sulfide, benzaldehyde and ethyl acetate to determine the strength of the sample (weak, normal, strong).

INTRODUCTION

Sensus, in partnership with a tomato producer, produces tomato essences for both red and green tomatoes. Due to natural variations, the red or green character varies in both quality and intensity. Therefore the batches of tomato essence are characterized as red or green essence, and then by their relative strength (i.e. weak, normal, strong). Then by blending select batches, standardized tomato essences for red and green are produced. The samples are classified by a sensory assessment of generally a single employee. This is a point in the process that could be improved since an assessor could be sick, distracted, or even leave the company. In addition, in a single shipment from the processing plant, there might be 80 or more batches to analyze. This takes a considerable amount of time and introduces other errors such as sensory fatigue and other errors. In order to improve this process, a more analytical approach has been undertaken. By using multivariate statistics, it is possible to identify key markers that an assessor is keying in on for their classifications. Using these key markers, it might be possible to develop a model that would be more consistent and minimize the possible sources of error in the current method.

MATERIALS AND METHODS

A Gerstel MultiPurposeSampler (MPS-2) (Baltimore, MD) was used with a 2-cm 3-phase (divinylbenene, Carboxen, Polydimethylsiloxane) for sample preparation. A 10-min incubation followed by a 40-min exposure was used to capture the volatiles on the fiber for injection into the GC. The sample was stirred using a 3x12mm stirbar in the 20mL vial. The fiber was desorbed for 5-min in the GC injector for 5 min. An Agilent 7890A gas chromatograph (Palo Alto, CA) was used for the analysis. Analysis was performed in the splitless mode with a helium flow rate of 1.25mL/min through a 60mx0.25mmx0.25µm RTX-5ms column. The initial oven temperature was

Copyright by SENSUS, LLC.

1

50°C immediately followed by a 4°C/min temperature ramp to 170°C which was followed by a 100°C/min ramp to 250°C and held for 5min in order to ensure no sample to sample contamination. The transfer line to the Leco TruTOF MS (St. Joseph, MN) was held at 240°C. Data was collected for 30-250 m/z at an acquisition rate of 10 spectra per sec. Identification was based on a combination of MS library matching along with reported retention indices. The samples were then prepared for analysis by pipetting 50 μ L into 4.9mL of water along with 50 μ L of internal standard (phenol-D6, 100 ppm).

80 tomato essences were sampled and odor assessed by 5 panelists for classification as either red or green tomato and normal, weak, or strong intensity. Red tomato was assigned a 1, 2, or 3 for weak, normal, and strong, while green tomato was assigned a value of 104, 105, or 106. This scheme was chosen to exaggerate the difference between red and green. Statistica version 8 was used for all multivariate statistical analyses. Sensory analysis was checked for outliers using the GOOD Method (Goodner, 2008).

RESULTS AND DISCUSSION

Table 1 contains the sensory results for the 80 lots that were received from the California processing facility. Rows highlighted in yellow have a questionable sensory response from one of the panelists. Thirty-one (38.8%) of the samples had a statistical outlier. This belies the problem of sensory assessment. There are many possible reasons for such a high number of outliers. Assessing 80 samples in approximately 1-2 hours can cause sensory fatigue, reference samples might not be representative enough, differences in experience in assessing tomato essence, assessing the samples by aroma alone (e.g. no tasting), memory affects (nose isn't cleared before next sample), and transcription errors are some of the possible sources of error.

Discriminate function analysis (DFA) was performed on the data (semi-quantitative amounts of 12 volatile compounds) using only assessor #1. The graph of the data is shown in Figure 1. In order to make interpretation easier, all the red and all the green samples were labeled the same in Figure 2. Figure 2 makes it clear that the x-axis is the differentiator between red and green. The x-axis is a linear combination of all 12 volatile concentration data. Each compound is weighted and the relative order of importance can be determined by examining these weighting factors. The relative weighting factors for Root 1 and Root 2 are listed in Table 2. As can be seen, 6-methyl-5-hepten-2-one, benzaldehyde, and 2-isobutylthiazole are the 3 largest contributors, while acetone, dimethyl sulfide, benzaldehyde, and ethyl acetate are the 4 major contributors to root 2. By labeling the data points differently, as seen in Figure 3, it can be seen that Root 2 is generally differentiating between "weak" and "normal" intensity red and green tomato.

The analyses in this report are not clear cut, but definitely point to the potential of the technique. It is felt that if the sensory data were better and a broader range of "redness" vs "greenness" were seen along with more variability in the intensity of the aroma, that more meaningful data could be obtained.

Figure 1. Discriminate Function Analysis of Assessor #1

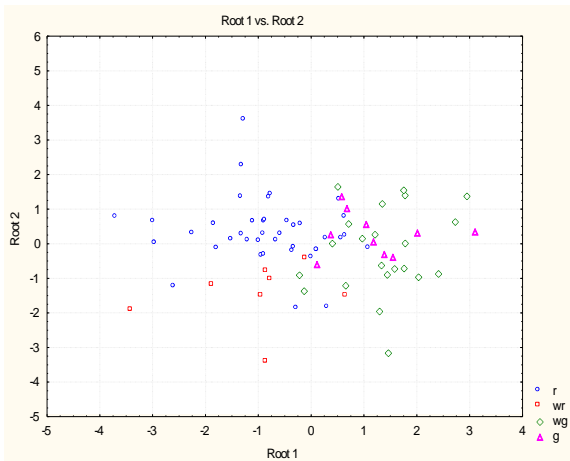


Figure 2. Figure 1 with only red versus green.

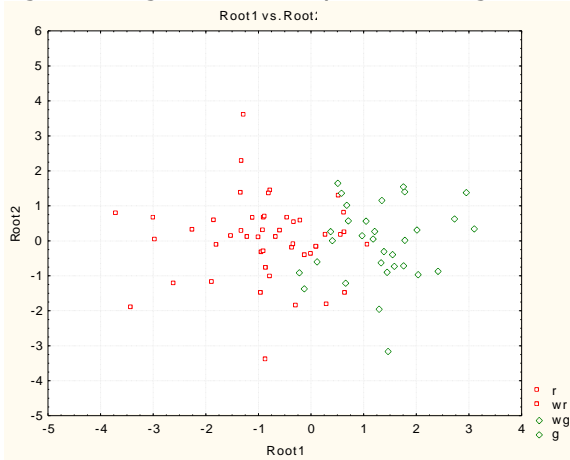


Figure 3. Figure 1 with only weak versus normal.

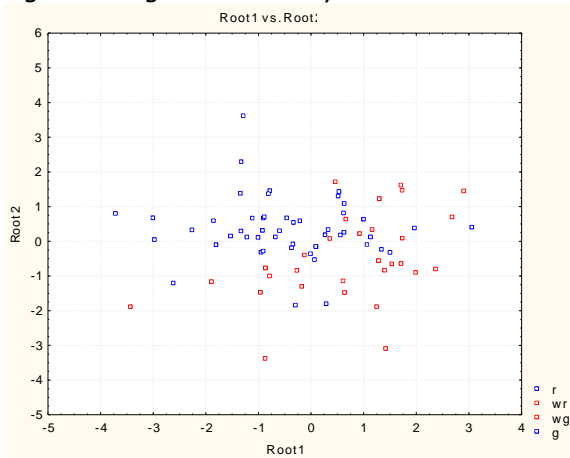


Table 1. Sensory results of tomato batches. Yellow highlighted rows have a statistical outlier.

Batch #	#1	#2	#3	#4	#5
1	2	104	3	104	106
2	3	105	1	105	2
3	2	105	104	105	1
4	1	104	105	106	104
5	1	1	2	2	2
6	2	2	3	2	3
7	2	2	2	2	2
8	2	2	106	2	2
9	2	2	104	106	105
10	2	105	105	105	104
11	1	104	106	106	1
12	2	105	105	105	105
13	2	105	104	106	1
14	2	104	104	104	104
15	2	105	105	105	2
16	2	105	105	106	2
17	3	2	105	106	106
18	2	105	106	106	106
19	2	2	105	105	105
20	2	2	105	104	104
21	2	2	105	104	2
22	2	2	105	105	3
23	1	1	106	106	1
24	1	2	105	104	2
25	1	104	2	104	2
26	1	1	3	106	104
27	2	104	3	106	2
28	2	104	105	105	3
29	2	2	105	106	105
30	2	2	105	105	104
31	2	2	1	105	104
32	2	1	106	104	105
33	1	1	2	105	2
34	2	1	1	106	2
35	2	104	1	105	1
36	2	104	104	104	104
37	2	104	104	105	2
38	2	104	1	106	2
39	2	105	105	105	2
40	2	106	104	106	105

Copyright by SENSUS, LLC.

41	3	105	106	104	2
42	2	2	106	104	105
43	2	105	105	104	2
44	2	1	105	105	2
45	2	104	2	104	2
46	2	105	2	104	2
47	2	105	105	105	104
48	3	105	3	104	105
49	104	1	106	106	104
50	104	1	105	105	105
51	104	105	105	105	104
52	105	1	106	104	104
53	104	3	105	105	105
54	104	105	106	106	105
55	104	2	2	106	104
56	105	105	105	105	104
57	105	104	105	105	1
58	105	2	105	106	1
59	104	105	106	106	2
60	104	105	106	105	104
61	104	104	106	105	1
62	105	105	105	106	2
63	105	105	105	106	105
64	105	106	106	105	2
65	104	2	105	105	104
66	104	2	105	104	1
67	104	2	105	105	2
68	104	105	104	105	1
69	104	2	104	105	104
70	104	2	104	105	1
71	105	1	104	104	2
72	104	104	105	104	1
73	104	105	105	105	1
74	105	2	105	105	105
75	104	2	105	104	105
76	104	2	105	106	105
77	104	2	105	105	104
78	104	105	106	106	2
79	105	104	106	104	104
80	104	105	105	106	2
outliers	8	10	1	2	10

Table 2. Relative contributions to Root 1 and Root 2 by various volatile compounds.

Compound	Relative contribution	
	Root 1	Root 2
Acetone	3	22
Dimethyl sulfide	12	17
2-Butanone	3	1
Ethyl Acetate	3	14
Furan, 3-methyl-	1	9
Butanal, 3-methyl-	5	4
1-Butanol, 3-methyl-	1	6
Hexanal	8	6
1-Hexanol	11	0
Benzaldehyde	17	15
5-Hepten-2-one, 6-methyl-	21	1
2-Isobutylthiazole	16	4

REFERENCE CITED

Goodner, K.L. Practical retention index models of OV-101, DB-1, DB-5, and DB-Wax for flavor and fragrance compounds. LWT 41 (2008) 951–958