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# Partitioning taste from aromatic flavor notes of fresh tomato (*Lycopersicon esculentum*, Mill) to develop predictive models as a function of volatile and nonvolatile components

E.G. Abegaz<sup>a</sup>, K.S. Tandon<sup>b</sup>, J.W. Scott<sup>c</sup>, E.A. Baldwin<sup>d</sup>, R.L. Shewfelt<sup>a,\*</sup>

<sup>a</sup> Department of Food Science and Technology, University of Georgia, Athens GA 30602, USA

<sup>b</sup> Food Science Department, Cornell University, NYSAES, Geneva, NY, USA

<sup>c</sup> University of Florida, Gulf Coast Research and Education Center, Bradenton, FL, USA

<sup>d</sup> USDA/ARS Citrus & Subtropical Products Lab., Winter Haven, FL, USA

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## Abstract

Sensory descriptive measures of six breeding lines and four supermarket items of tomatoes were determined using the 150 mm unstructured line scales with and without partitioning of taste from aromatic flavor notes using nose clips. Chemical/instrumental analysis measurements of pH, titratable acid, soluble solids, glucose, fructose, total sugars, sucrose equivalents and gas chromatographic analysis of flavor volatiles was also conducted. Taste descriptors were significantly correlated to nonvolatile components when partitioned from flavor perception. Aroma descriptors were more pronounced when following taste perception than when evaluated simultaneously with taste descriptors. Regression models were more effective at predicting sensory descriptors when taste descriptors were partitioned than when they were not partitioned.

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## 1. Introduction

A complex mixture of sugars, acids, amino acids, minerals and volatile compounds contribute to the characteristic flavor of tomato fruits (Baldwin et al., 1991a, 1991b). Although over 400 volatile compounds have been identified in tomato fruits, less than 20 compounds are considered to be important for flavor based on their odor thresholds. The esters, aldehydes, alcohols and ketones present in

tomatoes include acetaldehyde, acetone, methanol, ethanol, 1-penten-3-one, hexanal, *cis*-3-hexenal, 2 + 3 methylbutanol, *trans*-2-hexenal, *trans*-2-heptenal, 6-methyl-5-hepten-2-one, *cis*-3-hexenol, geranylacetone, 2-isobutylthiazole, and  $\beta$ -ionone. These compounds have been reported to be important contributors to characteristic flavor (Buttery et al., 1987; Tandon et al., 2000).

The major sugar substances that contribute to sweetness are glucose and fructose with fructose playing a major role (Stevens et al., 1977). The sour taste in tomatoes is attributed mainly to citric and malic acids (Petro-Turza, 1987). Free amino acids may play the role of taste-enhancement or buffering effect

\* Corresponding author. Tel.: +1 706 542-5136; fax: +1 706 542 1050.

E-mail address: [shewfelt@uga.edu](mailto:shewfelt@uga.edu) (R.L. Shewfelt).

(Bucheli et al., 1999) with glutamic acid the major free amino acid present in tomatoes (Kader et al., 1978). Potassium and phosphates affect pH, titratable acidity and buffering capacity which in turn influence the is taste (Petro-Turza, 1987). A strong positive correlation is observed between trained panel response of sweetness and reducing sugar or total soluble solids content (Malundo et al., 1995; Bucheli et al., 1999; Tandon et al., 2003). ‘Sourness’ closely correlates with titratable acidity (Stevens et al., 1977; Malundo et al., 1995; Bucheli et al., 1999; Tandon et al., 2003).

‘Fruitiness’ (Bucheli et al., 1999) and ‘sweetness’ (Kamal et al., 2001) have been identified as two critical contributors to flavor of fresh tomatoes. Higher concentrations of hexanal present in pericarp tissue contribute to the perception of the ‘green/grassy’ descriptor by trained panels (Petro-Turza, 1987). Several recent studies have developed mathematical relationships between sensory descriptors and instrumental measures of fresh tomato flavor (Baldwin et al., 1998; Krumbein and Auerswald, 1998; Auerswald et al., 1999; Gajc-Wolska et al., 2000; Krumbien et al., 2000; Maul et al., 2000; Tandon et al., 2003). Since flavor is so complex, several investigators have suggested that taste be partitioned from other sensory sensations by the use of nose clips to block the nasal passage and thus retronasal perception of aroma (Murphy et al., 1977; Murphy and Cain, 1980; O’Mahony, 1991; Lawless and Heymann, 1999).

The objective of this study was to determine the effect of partitioning taste components from flavor during descriptive analysis on prediction of sensory descriptors as a function of volatile and nonvolatile components.

## 2. Materials and methods

### 2.1. Fall 1999 tomatoes

Three tomato inbreds and three hybrids (‘Solar Set’, ‘Florida 47’, and Fla. 7859) were grown using standard agricultural practices at Bradenton, Florida and were harvested at two stages of maturity, red and breaker stages. The tomatoes were transported to the University of Georgia for sensory evaluation. Red tomatoes were stored in boxes overnight at 10 °C until they were evaluated by trained descriptive panelists.

Breaker tomatoes were ripened at 22 °C for 1 week when they were evaluated.

### 2.2. Spring 2000 tomatoes

Four tomato items—nonrefrigerated, ‘vine-ripe’, cherry clusters and ‘organic’ tomatoes were purchased from local supermarkets. The tomatoes were transported to the University of Georgia for sensory evaluation. They were evaluated by trained descriptive panelists on the day of purchase.

### 2.3. Chemical analysis

When the tomatoes reached the table-ripe stage of maturity as determined visually (USDA, 1975), they were halved. One half was further divided into wedges for sensory analysis. The remaining halves for each treatment were blended for 30 s in an Oster blender (Oster Corporation, Milwaukee, WI) held 180 s and 25 g removed and combined with 10 mL saturated (at room temperature) calcium chloride and homogenized an additional 10 s, to denature and salt our enzymes (Buttery et al., 1987). A 100 mL homogenate was placed in a plastic ziplock bag and frozen for subsequent sugar, acid and soluble solids analysis. An aliquot of the homogenized samples (2 mL) were then placed in 6 mL GC vials with crimp top and Teflon-silicone septa, flash frozen in liquid nitrogen and stored at –80 °C (comparison to a cryofocusing method where samples were not heated showed that the heating did not create artifacts). Tomato volatile compounds were identified and quantified by gas chromatography (GC) using a headspace analysis technique (Baldwin et al., 1991b, 1998). Samples were thawed, and vials rapidly heated and incubated at 80 °C for 15 min before injection using a Perkin Elmer HS-6 headspace-sampler (Perkin Elmer, Norwalk, CO, USA). The analysis was carried out using a Perkin Elmer Model 8500 gas chromatograph equipped with a 0.53 mm × 30 m polar stabilwax capillary column (1.0 m film thickness, Restek Corp., Bellefonte, PA, USA) and a flame ionization detector. Initial column temperature was held at 40 °C for 6 min, then raised to 180 °C at a rate of 6 °C/min where it was held constant for an additional 8 min. The GC peaks for the aroma volatile compounds were quantified in mL/L using standard curves as deter-

mined by enrichment of bland tomato homogenate, obtained after roto-evaporating tomato volatiles for 4 h at 50 °C, then mixed with known concentrations of authentic volatile compounds standards for GC analysis (Baldwin et al., 1991b).

#### 2.4. Sensory method

Flavor attributes of tomato wedges were evaluated using a the Spectrum™ technique for descriptive analysis (Meilgaard et al., 1991) modified such that panelists were calibrated based on reference standards using 150 mm line scale (Malundo et al., 1995) instead of using the 15-point scale in the original protocol.

#### 2.5. Sensory panel

Nine panelists were recruited for the Fall samples of whom seven had previously participated in descriptive analysis test on tomato flavor at the Food Process Research and Development Laboratory in the Department of Food Science and Technology at the University of Georgia. The Spring panel consisted of eleven panelists of whom three had participated in the Fall descriptive analysis test. The recruitment criteria included that the panelists were (1) between the ages of 18 and 50, (2) not allergic to tomatoes, (3) consumers of fresh tomatoes at least twice a month, (4) able to pass a flavor acuity test and (5) available and willing to participate during training and testing sessions. Fall panelists were trained for 10 sessions, 60 min per session; while Spring panelists were trained for seven sessions, 90 min per session. During the training, panelists were presented with different kinds of commercially available tomatoes in order to acquaint them with different flavor attributes of tomatoes. Definitions of tomato flavor descriptors previously developed (Meilgaard et al., 1991; Civille and Lyon, 1996) were provided as a guide during terminology expansion. A final list of tomato flavor attributes definitions was retained after consensus by panel members. Panelists were trained using reference standards for sweet, sour, salty bitter and astringency (Meilgaard et al., 1991), plus fruity, earthy/musty, green/grassy and bite (Civille and Lyon, 1996). We also used the term tomato-like defined as “a general term that combines those characteristics commonly associated

with tomato” using fresh cut tomatoes in training. The panel was calibrated to a maximum difference in response of  $\pm 10$  mm on the 150 mm scale for each descriptor.

#### 2.6. Sample evaluation

In Fall, six tomato breeding lines harvested at two stages of maturity were evaluated in six sessions (four lines per session) with each panelist evaluating each line at each level of maturity twice. The first three sessions were conducted with tomatoes that were harvested and evaluated at table-ripe stage. The next three sessions were conducted one week later for tomatoes harvested at breaker stage, but they were evaluated at table-ripe stage. In Spring, four tomato types were evaluated in six sessions, morning and afternoon (four cultivars per session) with each panelist evaluating each type twice.

Tomato lines were removed from the storage an hour before evaluation and were equilibrated at room temperature (22 °C). Four to six tomato samples from each line were cut into wedges and placed in 4oz souffle cups and capped with lids. Each sample was evaluated using two techniques with and without partitioning. The partitioning technique involved separation of the taste from flavor components by blocking the nose for taste components (sweet, sour, salty and bitter) with nose clips followed by evaluation of the aromatic and chemical feeling factors upon removal of nose clips. Panelists rated samples under incandescent light in partitioned booths. Three-digit coded samples were presented to the panelists monadically and the order of presentation to each panelist was randomized. Palates were cleared with unsalted top crackers and bottled water between samples.

#### 2.7. Statistical analyses

Regression analysis was performed to determine the relationship between sensory response with instrumental measurements of volatile and nonvolatile flavor components with multiple linear regression using the SAS procedure, PROC REG backward selection method ( $P = 0.1$ ). Correlations between sensory data and instrumental/chemical analysis were determined using the SAS procedure, PROC CORR (SAS, 1990).

### 3. Results and discussion

Very different patterns of correlation between nonvolatile and volatile components emerged as perceived by panelists depending on whether the nasal passage was blocked to evaluate taste descriptors. A composite of all data collected over the two seasons revealed the 'sweet' note is positively correlated with soluble solids, glucose, fructose, total sugars, and sucrose equivalents with partitioning (taste followed by aroma). No significant correlations were obtained without partitioning (aroma plus taste) (Table 1). In previous studies strong positive correlation has been observed between trained panel response of 'sweetness' and reducing sugar and total soluble solids content (Bucheli et al., 1999; Tandon et al., 2003). The 'bitter' note was positively correlated to acidity and negatively correlated to soluble solids when evaluating taste followed by aroma. Both 'tomato-like' and 'fruity' were positively correlated to acidity and negatively correlated to soluble solids in aroma plus taste trials but not in the taste followed by aroma trials. A possible explanation in the lack of correlations with many of these descriptors is that there was little difference between these treatments in the lines selected. It is clear that evaluating for taste plus aroma was more sensitive than evaluating for aroma plus taste.

The composite results across season and tomato types, when evaluating aroma plus taste, revealed more significant correlation coefficients between aromatic descriptive notes and volatile compounds than when evaluating taste followed by aroma (Table 2). Both techniques resulted in significant relationships between volatile compounds and the 'fruity' descriptor, but only hexanal was significant for both methods. Both techniques showed significantly negative correlation coefficients for specific compounds and 'fruitiness', but the 'green/grassy' note showed a significantly positive correlation with several compounds in aroma plus taste evaluations. Separation of the data by season revealed a greater number of significant correlation coefficients, but the results were not consistent between the Fall and Spring (data not shown). While genotypic differences between Fall and Spring may account for some of this variation, the relationships between chemical components and sensory perception across genotype and season should be consistent.

Table 1  
Pearson correlation coefficients between instrumental nonvolatile components and sensory descriptors when evaluated by taste followed by aroma or aroma plus taste for the combined data from Fall and Spring

Descriptor	Taste followed by aroma						Aroma plus taste					
	Soluble solids	Acidity	Glucose	Fructose	Total sugars	Sucrose equivalents	Soluble solids	Acidity	Glucose	Fructose	Total sugars	Sucrose equivalents
Sweet	0.59	-0.56	0.67	0.67	0.68	0.68	-	-	-	-	-	-
Bitter	-0.52	0.56	-	-	-	-	-	-	-	-	-	-
Tomato-like	-	-	-	-	-	-	-0.66	0.71	-	-	-	-
Green/grassy	0.50	-	-	-	-	-	-	-	-	-	-	-
Fruity	-	-	-	-	-	-	-0.72	0.73	-	-	-	-

Only significant relationships are shown ( $P \leq 0.10$ ).

Table 2

Pearson correlation coefficients between instrumental volatile components and sensory descriptors evaluated by taste followed by aroma or aroma plus taste for the combined data from Fall and Spring evaluations

Volatile compound	Taste followed by aroma				Aroma plus taste			
	Tomato-like	Over-ripe	Green/grassy	Fruity	Tomato-like	Over-ripe	Green/grassy	Fruity
Acetaldehyde	–	–	–	–	–	–	–	–0.55
Ethanol	–0.51	–	–	–	–	–	–	–
Geranylacetone	–	–	–	–	–	–	0.61	–
Hexanal	–	–	–	–0.63	–	–	0.56	–0.54
<i>cis</i> -3-hexenal	–	–	–	–	–	–	–	–0.64
<i>cis</i> -3-hexenol	–	–	–	–	–	–	0.59	–
Methanol	–	–	–	–	–	–0.60	–	–
2 + 3 methylbutanol	–	–	–	–0.63	–	–	0.46	–
6-Methyl-5-heptene-2-one	–	–	–	–0.66	–	–	0.54	–
1-Penten-3-one	–	–	–	–0.71	–	–	0.55	–

Only significant relationships are shown ( $P \leq 0.10$ ).

Linear regression models provide a different view of the relationships between descriptors and composition than simple correlation. Tests of taste followed by aroma generally provided better models (greater  $R^2$  and lower  $P$ ) than those with aroma plus taste (Tables 3 and 4). Both volatile and nonvolatile components contributed to relationships for most descriptors. The compositional factors for the relationships were only similar for both techniques for methanol in the ‘over-ripe’ model as well as for acidity and 6-methyl-5-hepten-2-one in the ‘bite’ model. In this

study, more volatile components were related to aromatic sensory descriptors when evaluating taste followed by aroma. It appears that removal of the nose clips heightened sensitivity of the panelists. The lack of consistency observed between simple correlation and linear regression demonstrates the complexity of the relationships between sensory and instrumental data.

A comparison of the predictive models developed from the Fall crop (Tables 3 and 4) and the actual scores for the following Spring tomatoes is shown

Table 3

Linear regression models of trained panel flavor ratings related to instrumental measurements of Fall 1999 tomatoes evaluated by taste followed by aroma (only significant relationships are shown)

Descriptors	Linear models	$R^2$	$P$
Sweet	8.56 + 1.02 (ethanol)	0.39	0.03
Sour	48.80 – 0.045 (pH) – 148.16 (acetone) + 14.28 (2 + 3 methylbutanol) + 0.69 ( <i>trans</i> -2-hexenal)	0.95	0.06
Salty	22.90 – 0.98 ( <i>trans</i> -2-hexenal) + 4.61 (6-methyl-5-hepten-2-one)	0.84	0.001
Bitter	0.36 + 840.85 (acidity) – 1.72 (2 + 3 methylbutanol)	0.71	0.02
Tomato-like	–57.58 + 2710.81 (acidity) + 8.75 (2 + 3 methylbutanol) – 34.30 (6-methyl-5-hepten-2-one) + 128.47 (geranylacetone)	0.88	0.0004
Over-ripe	13.61 + 11.24 (soluble solids) – 0.14 (methanol)	0.59	0.001
Green/grassy	16.20 + 24.55 (geranylacetone)	0.30	0.07
Fruity	43.79 – 1.18 ( <i>cis</i> -3-hexenal)	0.39	0.03
Astringency	38.48 – 116.22 (acetone) + 1.19 (hexanal) + 7.20 (6-methyl-5-hepten-2-one)	0.72	0.04
Bite	1.42 + 1494.33 (acidity) + 3.21 (6-methyl-5-hepten-2-one)	0.51	0.06

All variables left in the model are significant at  $P = 0.1$  level. All volatile measurements ( $\mu\text{L/L}$ ).  $R^2$ : coefficient of determination. Soluble solids (%). Acidity ( $[\text{H}^+]$  g/g FW).

Table 4

Linear regression models of trained panel flavor ratings related to instrumental measurements of Fall tomatoes evaluated by aroma plus taste (only significant relationships are shown)

Descriptors	Linear models	R <sup>2</sup>	P
Sweet	0.28 + 1.98 (acetaldehyde)	0.51	0.01
Sour	51.08 – 2.20 (acetaldehyde)	0.57	0.10
Salty	26.99 – 0.242 (sucrose equivalents)	0.52	0.01
Bitter	23.42 – 2.24 (soluble solids) – 0.24 ( <i>cis</i> -3-hexenal)	0.66	0.09
Tomato-like	3.20 + 5.35 (soluble solids) + 0.62 ( <i>trans</i> -2-hexenal)	0.64	0.04
Over-ripe	73.06 – 0.090 (methanol) – 1.05 ( <i>trans</i> -2-hexenal) + 114.79 ( <i>cis</i> -3-hexenol) – 22.55 (geranylacetone)	0.89	0.06
Fruity	27.34 – 3.58 (2 + 3 methylbutanol)	0.39	0.03
Astringency	26.83 – 0.03 (pH) – 0.89 ( <i>trans</i> -2-hexenal)	0.60	0.06
Bite	14.86 + 687.79 (acidity) – 448.24 ( <i>trans</i> -2-heptenal) + 2.09 (6-methyl-5-hepten-2-one) + 66.05 ( <i>cis</i> -3-hexenol)	0.98	0.001

All variables left in the model are significant at  $P = 0.1$  level. All volatile measurements ( $\mu\text{L/L}$ ). R<sup>2</sup>: coefficient of determination. Soluble solids (%). Acidity ( $[\text{H}^+]$  g/g FW). Sucrose equivalents (%).

for taste followed by aroma (Fig. 1) and aroma plus taste (Fig. 2). The models were reasonably effective at predicting the response of taste followed by aroma for all descriptors except for ‘over-ripe’ (for nonrefrigerated and ‘vine-ripe’ tomatoes) and ‘tomato-like’ (for ‘organic’ tomatoes) (Fig. 1). These patterns are distinctive for the four selections in Spring and the models from the taste followed by aroma technique closely mirror those of the actual values. The aroma plus taste technique indicate that the actual ‘sweet’, ‘sour’, ‘over-ripe’ and ‘tomato-like’ notes deviated from the predicted values in most cases (Fig. 2) and the patterns vary from each other. Since evaluation of taste followed by aroma was more effective at providing predictive models for taste and aromatic notes its use should be seriously considered as a systematic approach to reduce interference between volatile and nonvolatile components and thus providing better relationships between sensory descriptors and chemical components.

While different studies provide different relationships between descriptive notes and chemical composition, some patterns are beginning to emerge. Models from taste followed by aroma support previous studies on the contribution of ethanol to the perception of ‘sweetness’ (Tandon et al., 2003); 2 + 3 methylbutanol (Krumbien et al., 2000), 6-methyl-5-hepten-2-one (Baldwin et al., 1998) and geranylacetone (Krumbien et al., 2000; Maul et al., 2000; Tandon et al., 2003) to ‘tomato-like’; and hexenal to ‘astringency’ (Tandon et al., 2003). Negative relationships in the mod-

els from taste followed by aroma are supported for pH (Maul et al., 2000; Tandon et al., 2003), acetone (Tandon et al., 2003) and 2 + 3 methylbutanol (Baldwin et al., 1998) with the ‘sour’ note as well as for 6-methyl-5-hepten-2-one with the ‘tomato-like’ note (Tandon et al., 2003). Results from the models of aroma plus taste support previous studies on the contribution of acetaldehyde to perception of ‘sweetness’ (Tandon et al., 2003) and ‘sourness’ (Baldwin et al., 1998), *trans*-2-hexenal to ‘sweetness’ (Krumbein and Auerswald, 1998; Tandon et al., 2003), and 2 + 3 methylbutanol to ‘fruitiness’ (Tandon et al., 2003).

Use of linear regression data in this and previous (Baldwin et al., 1998; Bucheli et al., 1999; Tandon et al., 2003) articles tends to oversimplify the relationships between sensory descriptors and instrumental measures of flavor. Use of multivariate techniques (Krumbein and Auerswald, 1998; Azodanlou et al., 2003) tends to obscure these relationships for investigators wishing to understand and improve flavor of fresh tomatoes. The lack of consistency between models developed in different studies can be attributed to differences in definition of specific descriptive notes, use of differing cultivars or breeding lines, and the complexity of the task. The use of nose clips to separate the evaluation of taste descriptors from the evaluation of the aromatic descriptors provides models that more effectively predict descriptors in commercially available fruit the following season than if nose clips are not used.

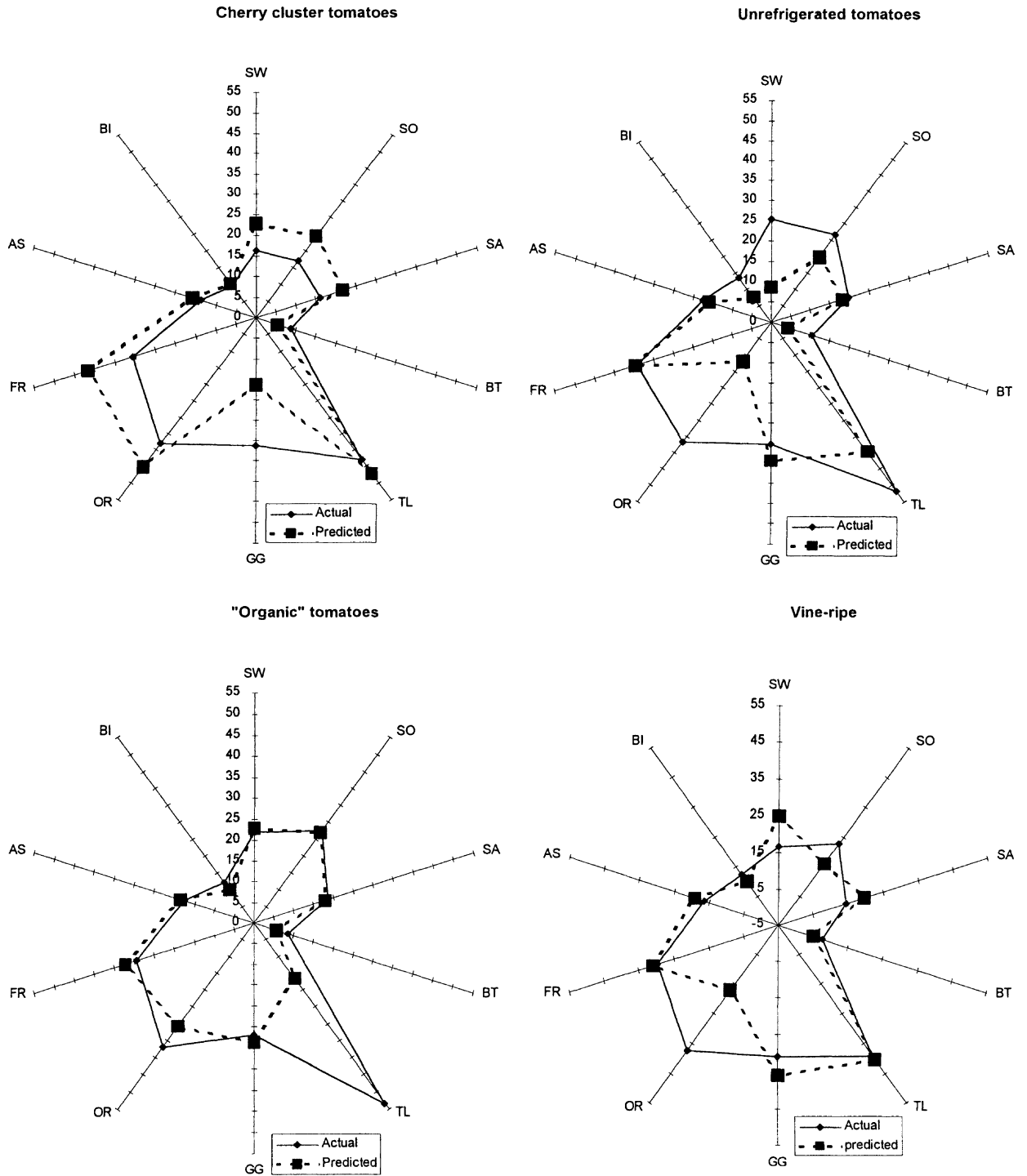


Fig. 1. Actual and predicted trained panel responses as a function of volatile and nonvolatile components with partitioning (taste followed by aroma) technique using four supermarket tomato items. [SW = 'sweet', SO = 'sour', SA = 'salty', BT = 'bitter', TL = 'tomato-like', GG = 'green/grassy', OR = 'over-ripe', FR = 'fruity', AS = 'astringency', BI = 'bite'].

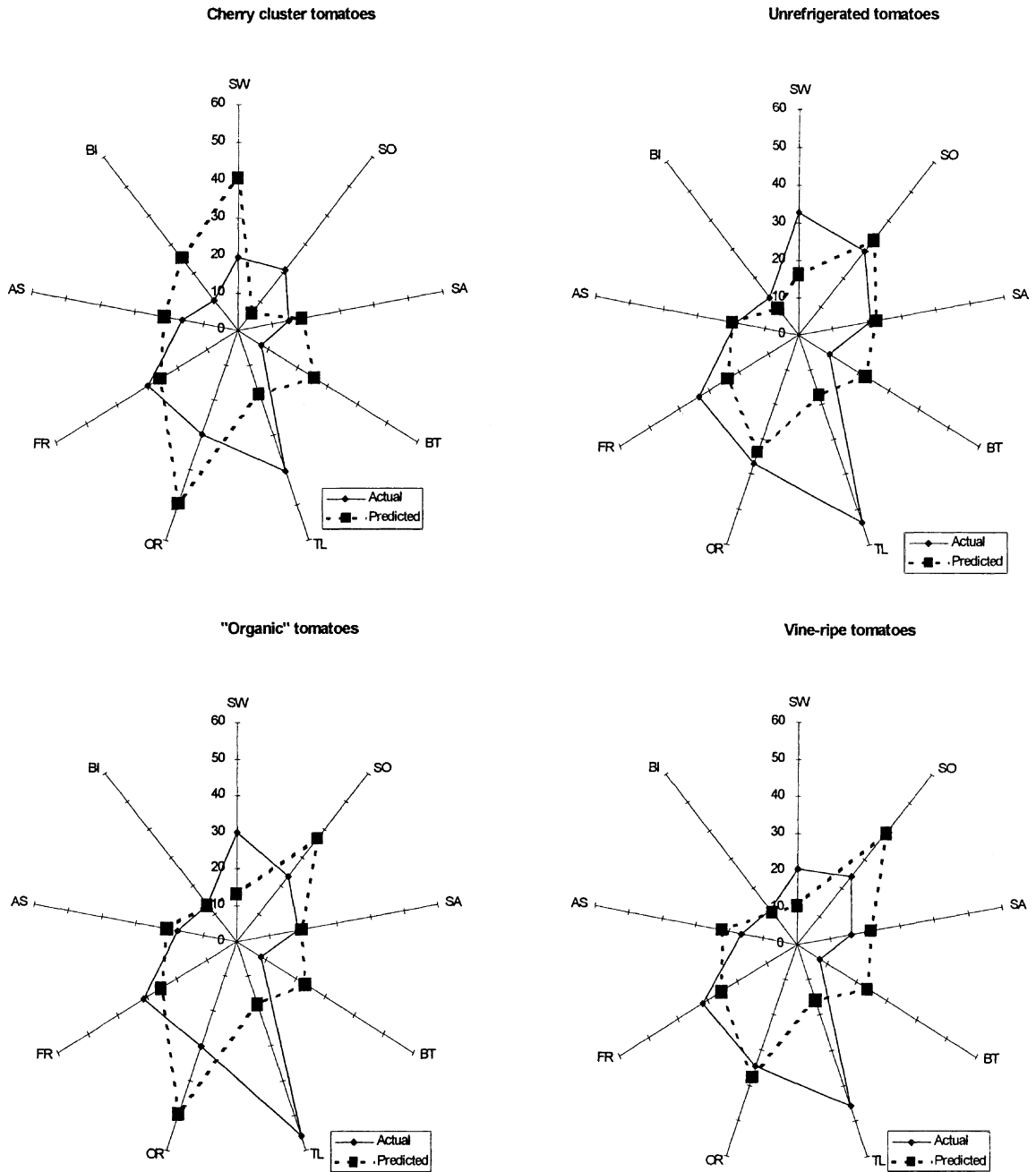


Fig. 2. Actual and predicted trained panel scores as a function of volatile and nonvolatile components without partitioning (aroma plus taste) for four supermarket tomato items. [SW = 'sweet', SO = 'sour', SA = 'salty', BT = 'bitter', TL = 'tomato-like', GG = 'green/grassy', OR = 'over-ripe', FR = 'fruity', AS = 'astringency', BI = 'bite'].



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