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Relating Descriptive Sensory Analysis to Gas Chromatography/Mass Spectrometry of Palm Sugars Using Partial Least Squares Regression

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Abstract: Sensory attributes of four different palm sugars were related to gas chromatography/mass spectrometry (GC/MS) analysis using partial least squares regression (PLS). The sweet caramel and burnt-like sensory attributes were strongly associated with 2-furfural and 2-furan methanol volatile compounds. The sensory scores for roasty and nutty were also associated with the GC/MS ratings for roasty and nutty-like aroma by its highest scores obtained from 2-ethyl-5-methyl pyrazine, 2,5-dimethyl pyrazine and 2,3-dimethyl pyrazine volatile compounds along the PC1 dimension. PLS analysis did not show correlation for the character impact compound furaneol, 2-ethyl-3,5-dimethyl pyrazine (EDMP) and 2,3-diethyl-5-methyl pyrazine (DEMP), which are perceived to be responsible for the sweet caramel-like and roasty/nutty attributes of palm sugars, respectively. This lack of relationship could partially be explained by covariance among the sensory ratings for the samples.

Keywords: Palm sugar (*Arenga pinnata*), partial least squares, sensory evaluation, gas chromatography/mass spectrometry, chemometrics

INTRODUCTION

Palm sugar, traditionally produced by heating a palm sap (*Arenga pinnata*) in a big wok is a thermally processed food. The aroma in most thermally processed foods such as bread, cereal products, roasted peanuts and roasted coffee, are largely due to the Maillard reaction. Among these Maillard type flavours, the N-, O- and S- heterocyclic compounds with desirable aromas and low odour thresholds make the most significant contributions (Vernin and Parkanyi, 1982). Hence, comparisons between human sensory response and gas chromatography mass spectrometry (GC-MS) data are of paramount importance to obtain a better understanding of flavour or aroma differences among food products or processing treatments (Foster *et al.*, 2002). However, obtaining a representative sample for GC-MS analysis is crucial to obtain an accurate aroma profile.

The study of food flavour has been, and still is, one of the greatest challenges in the flavour industry. Food that are more complex in flavour especially those resulting from the Maillard reaction such as coffee, meat or chocolate may involve 800 or more volatile constituents (Nijssen *et al.*, 1996). Of these volatiles, a limited number which may be adequate to characterise the aroma of a food were heat-labile compounds or may be too low to be recognizable. According to Pawliszyn (1997), headspace solid phase micro-extraction (HS-SPME) has become the method of choice in aroma analysis offering

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non-destructive and non-invasive methods, solvent-free, rapid sampling with low cost, ease of operation, sensitive, selective and also compatible with low detection limits. In addition, because of low extraction temperature used, SPME could give a better estimation of the aroma profile as perceived by the human nose.

While the analytical chemists may concentrate their efforts on a potent chemical or limited number of character impact compounds, the food scientists, on the other hand have to deal with the flavour perception. Hence, it is important to obtain an accurate sensory data. Quantitative descriptive analysis (QDA) is one of many sensory descriptive techniques that have been developed (Stampanoni, 1993). This method employs a group of experienced panellists to generate because the panellists do not have any preconceived ideas or biases because they are not involved in the development of the descriptors (Stampanoni, 1993). The results of sensory analysis, is then evaluated against the GC-MS data. The sensory characteristics of a product generally result from many activities of the chemical compounds concerned (Chien and Peppard, 1993). The sensory impact of some compounds may be masked by other compounds (Grosch, 2001), enhanced by other compounds (McBridge, 1990), or the combination of compounds may produce a sensory response entirely different from the sensory character of the constituents (Kendall and Neilson, 1966). Multivariate multiple regression (MMR) models may provide one method for evaluating the relationship between sensory response and chemical analysis of a food.

Partial least squares (PLS) regression analysis has been widely used to estimate the MMR models that illustrate the relationships between sensory analysis and instrumental data sets (Noble and Ebeler, 2002). This statistical method was designed to handle data sets in cases where the number of variables is much greater than the number of samples, when there is a high degree of co-linearity among response variables (sensory) and among predictor variables (GC-MS), and when there is a significant amount of random error in the data (Chien and Peppard, 1993). Partial least squares analysis provides an indicator of how well the variables in one data set explain the variation among variables in another set, and this is the reason why the method is used here. No attempt is made to "test the level of significance" of the final model of confirm if compounds associated with a particular aroma are actually responsible for that aroma. The primary objective of this study was to evaluate GC-MS as a chemical analysis technique to aid in identifying the compounds responsible for the individual sensory attributes that make up the characteristic palm sugar flavour.

MATERIALS AND METHODS

Materials

Palm sugar samples labelled K1, K2, K3 and K4 were obtained from four different manufacturers in Kuala Pilah, Negeri Sembilan, Malaysia. Samples labelled K1 and K2 were traditionally produced while samples K3 and K4 were bought from a grocery shop. Standard solutions used as reference were 2,3-dimethyl pyrazine, 2-ethyl-5-methyl pyrazine, 4-hydroxy-2,5-dimethyl-3(2H)-furanone (Furaneol) and furfuryl alcohol and all were purchased from Sigma Aldrich (> 98% purity).

Sample Preparation

Approximately 100 g of each palm sugar was manually cut into smaller sizes. All the standards were prepared to give 0.1% solution propylene glycol solvent. All samples and reference standards were kept at -18°C in a freezer prior to analysis.

Headspace Solid Phase Microextracion (HS-SPME)

Approximately 1 g of palm sugar was placed in 10 ml headspace glass vials sealed tightly with crimp cap and PTFE/silicone septum. An internal standard (1 ppm tridecane solution) was added to the palm sugar and the vial was

vigorously shaken for 1 min using a vortex mixer. The vial was placed in a 50°C water bath for 10 min. A manual SPME holder containing a PDMS/DVB/CAR fiber (Supelco, Bellefonte, Pa., U.S.A.) was inserted into the vial and exposed for 10 min. The fiber was then transferred to the injector of the GC and desorbed for 10 min. Thermal desorption of the analytes from the fiber inside the GC injector port with a SPME inlet liner (0.75 mm i.d., Supelco) was carried out in the splitless mode at a desorption temperature of 240°C for 5 min. The SPME fibre was left in the injection port for re-conditioning during the complete run of the GC before it was exposed to the headspace of the next sample. All samples were run in triplicate.

Gas Chromatography – Mass Spectrometry Analysis Conditions

All samples were analyzed with a HP 6890 gas chromatography coupled to a 5973 mass selective detector (HP) equipped with an electronic pressure controller. Separation was with a a HP-5MS capillary column (30 m x 0.25 mm i.d., 0.25 mm film thickness) purchased from J and W Scientific. The injector and detector temperature were 240°C and 280°C, respectively. Carrier gas helium was used at a flow rate of 2 ml min^{-1} and at a pressure of 117.5KPa. The column temperature was programmed from 50°C (held for 2 min), at 20°C/min to 80°C (held for 1 min), at 20°C min^{-1} to 100°C (held for 1 min), then at 30°C min^{-1} to 230°C (held for 2 min). Other conditions were as follows: scanning range (m/z) 50-550 a.m.u at a rate of 1.5 scan sec^{-1}; electron ionization energy, 70eV. Semi-quantitative evaluation of the concentration of volatiles was based on comparison of peak area to the peak area of the internal standard, tridecane.

The samples were analyzed by using GC-MS. The measured mass spectra were compared with those obtained from reference compounds if available, as well as with data found in the literature (the respective references are given in Table 1) and from a commercially available mass spectra database (Wiley 275.1). Additionally, the volatile compounds were identified by matching retention indices (RI), calculated according to the equation of van den Dool and Kratz (1963) and based on a series of alkanes (C7-C22). The retention indices for the compounds of interest are given in Table 1. The relative concentrations of the investigated compounds were calculated by relating the areas of the internal standard tridecane to the areas of the compounds of interest. Integration of all of the chromatographic peaks was performed by choosing the three masses among those specific for each compound, with the highest matching index so as to discriminate them from the nearest neighbours.

Quantitative Descriptive Analysis (QDA)

Quantitative evaluation of the palm sugar flavour was performed using descriptive analysis (Wu *et al.*, 2000). Ten panelists, 3 men and 7 women aged between 22 and 50 years, were chosen based on their interest and availability and were given a tokenl non-monetary reward after each test. Training sessions, lasting 1 h, to evaluate a palm sugar, was provided to the panelists once a day for a total of 1 week. Initial training sessions of the panel included introduction to the samples and discussions to develop aroma attributes. The aroma attributes included nutty, roasty, sweet caramel-like and burnt. Familiarity with the 4 aroma attributes was provided by using volatile compounds as references. References and samples were rated using a 15 cm universal Spectrum™ line scale with 0 cm representing "none" and 15 cm representing "strong" (Munoz and Civille, 1998). Panelists were instructed on the proper use of the scale through instructions to rate aroma intensity such that a product receiving a rating of 10 would have an aroma intensity twice as high as a product receiving a rating of 5, independent of aroma characteristics. The panelists discussed individual scores for each of the reference aroma attributes among

Table 1
Comparison of volatile compounds from 4 different types of palm sugars[a]

Peak No	Compounds[b]	RI[d]	K1	K2	K3	K4
	N-Heterocyclic (Pyrazines)		**55708**	**14030**	**4751**	**136**
1	Pyrazine[c]	672	1779	474	99	0
2	2-methyl pyrazine[c]	823	6963	3663	1226	0
3	2,5-dimethyl pyrazine[c]	912	11481	4991	2310	90
4	2-ethyl pyrazine	917	1989	1078	0	0
5	2,3-dimethyl pyrazine[c]	919	8258	1206	579	0
6	2-ethyl-6-methyl pyrazine	992	3138	886	0	0
7	2-ethyl-5-methyl pyrazine[c]	1001	9487	998	471	46
8	2-ethenyl-6-methyl pyrazine	1016	730	196	0	0
9	3-ethyl-2,5-dimethyl pyrazine	1082	3896	222	66	0
10	2-ethyl-3,5-dimethyl pyrazine[c]	1088	1711	0	0	0
11	5-ethyl-2,3-dimethyl pyrazine	1089	1579	145	0	0
12	2,5-diethyl pyrazine	1091	588	34	0	0
13	Dimethyl-2-vinyl pyrazine	1098	764	52	0	0
14	5-methyl-6,7-dihydro-5H-cyclopenta pyrazine	1147	712	29	0	0
15	3,5-diethyl-2-methyl pyrazine	1162	1415	0	0	0
16	2,3-diethyl-5-methyl pyrazine	1171	705	56	0	0
17	3-furfuryl-2,5-dimethyl pyrazine	1413	513	0	0	0
	O-Heterocyclic (Furan derivatives)		**14190**	**9947**	**2353**	**1538**
18	2-methyl furan	599	1015	868	848	707
19	2-methyl tetrahydro furanone	806	854	146	35	57
20	2-furfural[c]	835	3287	5234	984	551
21	2-furan methanol[c]	860	4742	2742	363	145
22	5-methyl furfural[c]	964	2830	861	123	78
23	2,5-dimethyl-4-hydroxy-3(2H)-furanone	1060	817	23	0	0
24	3-fenyl furan	1224	645	73	0	0
	Aldehydes		**2477**	**350**	**240**	**153**
25	Benzeneacetaldehyde	1046	1436	157	35	0
26	Nonanal	1103	461	97	119	68
27	Decanal	1202	580	96	82	85
	Ketones		**1084**	**98**	**74**	**107**
28	6-methyl-5-hepten-2-one	984	1054	70	0	29
29	2-nonanone	1093	0	0	0	23
30	2-undecanone	1238	0	0	46	34
31	Geranyl acetone	1421	30	28	28	21
	Carboxylic Acid		**641**	**315**	**887**	**344**
32	Octanoic acid	1174	0	0	76	0
33	Dodecanoic acid	1499	98	0	42	0
34	Tetradecanoic acid	1625	363	152	283	158
35	Pentadecanoic acid	1690	0	0	48	0
36	9-hexadecenoic acid	1750	31	27	103	38
37	Hexadecanoic acid	1763	149	136	335	148
	Total volatiles		**74100**	**24740**	**8305**	**2270**

[a] Data are expressed as mean (n=3) in part per billion (ppb) concentration
[b] Tentatively identified on the basis of mass spectral data unless otherwise stated
[c] Mass spectra and GC retention indices were consistent with those of authentic standard compounds
[d] RI, retention indices

Table 2
Relative percentage concentration of several classes of volatile compounds in palm sugars

Samples	Chemical Classes of Volatile Compounds (%)				
	Pyrazines	Furan derivatives	Aldehydes	Ketones	Carboxylic acids
K1	75.18	19.15	3.34	1.46	0.09
K2	56.71	40.21	1.41	0.40	1.27
K3	57.21	28.33	2.89	0.89	10.68
K4	6.00	67.75	6.74	4.71	15.15

themselves and decided on the intensity of the attribute by mutual consensus.

The 0.1% solution of 2,3-dimethyl pyrazine was labelled "Nutty-like 10", 0.1% solution of 2-ethyl-3,5-dimethyl pyrazine was labelled "Roasty-like 12.5", 0.1% solution of Furaneol was labelled "Sweet caramel-like 12.5" and 0.1% solution of furfuryl alcohol was labelled "Burnt-like 10". Labelled references were presented in 20 ml universal glass bottle during each session to standardize the panel scores and prevent drifting. Several practice sessions (during end of training period) were conducted to ensure all the panelists understood the task, score card and terminology, and to monitor panel performance for repeatability, consistency and discriminating ability. Descriptive sensory evaluations were conducted in a sensory room during the morning (10:00 a.m. to about 12:00 p.m.) and repeated in the afternoon (2:00 p.m. to about 4:00 p.m.), for 2 consecutive days. Experiment samples were prepared 24 h prior to evaluation, kept in a freezer and then warmed to room temperature just before serving to the panelists. References were prepared fresh daily. Samples of 10 g each were placed in 20 ml universal bottle and coded with 3-digit numbers, were served at random to each panel member during each session (Stone and Sidel, 1993). Each panelist evaluated the aroma of each sample by sniffing with a minute break between samples.

Statistical Analysis

Differences in the descriptive ratings for the palm sugar were analyzed using ANOVA (SAS 1990). A Principal Component Analysis (PCA) model was built to analyze the influence of the different types of palm sugars on the instrumental and sensory data of palm sugar. The chemometric package, Unscrambler® 9.0 (CAMO Process AS, Oslo, Norway) was used. The raw data were normalized, with the subtraction of the mean, and auto-scaled, dividing these results by the standard deviation. To explore the relationships between instrumental and sensory variables, PLS Regression was employed. The data was modelled with PLS regression, using instrumental data as the input (X) variables, and a selection of the 4 main sensory variables as the result (Y) variables.

RESULTS AND DISCUSSION

Volatile Compounds

The volatile compounds of the palm sugar are shown in Table 1. The compounds can be classified into pyrazines, furan derivatives, aldehydes, ketones and carboxylic acids. Sample K1 showed the highest concentration of volatile compounds with a total of 74100 ppb ($x10^9$), followed by K2 (24740 ppb), K3 (8305 ppb) and K4 (2270 ppb). The volatiles in sample K1 were mainly from N-Heterocyclic (pyrazines) compounds (75.18%) and followed by O-Heterocyclic (furan derivatives) compounds (19.15%). The relative percentage

contribution of several classes of volatile compounds in each of the palm sugar samples are shown in Table 2.

Both K1 and K2 samples contained 94.33% and 96.92% of the pyrazines (N-Heterocyclic) and furan derivatives (O-Heterocyclic) respectively. Even though both samples (K1 and K2) showed similar percentage of volatile compounds, the ratio between these two chemical classes of volatiles was significantly different. For 94.33% of volatile compositions of compounds in K1, 19.15% was from total volatile compounds of furan derivatives chemical classes, which was only half the percentage of the furan derivatives group in sample K2 (40.21%). Hence, the different ratio among these two chemical classes of volatile compounds in K1 and K2 samples showed a significant difference ($p<0.05$) in the sweet caramel-like attribute. In other words, the combination of several classes of volatile compounds probably provides the distinctive and unique aroma note in K1 and K2 samples.

Pyrazines

Pyrazines classes of volatile compounds are commonly found in roasted and toasted foods (Meynier and Mottram, 1995). Table 1 shows that more than 14 types of pyrazines were detected in K1 and K2 as compared with only 6 and 2 pyrazines in K3 and K4 samples, respectively. Total pyrazines concentration in sample K1 was 55708 ppb, three times higher than in sample K2 (14030 ppb). In terms of quantity, the most abundant pyrazines determined in K1 sample was 2,5-dimethyl pyrazine, followed by 2-ethyl-5-methyl pyrazine, 2,3-dimethyl pyrazine and 2-methyl pyrazine. For the other samples, the pattern of the profile was different, with 2,5-dimethyl pyrazine being the most abundant followed in descending order by 2-methyl pyrazine, 2,3-dimethyl pyrazine and 2-ethyl-5-methyl pyrazine. These patterns of the volatiles indicated that the reaction pathway of generating 2-ethyl-5-methyl pyrazine volatile compound was favourable in sample K1.

From a qualitative perspective, 2-ethyl-3,5-dimethyl pyrazine (EDMP) (1711 ppb) and 2,3-diethyl-5-methyl pyrazine (DEMP) (705 ppb) which showed a roasty note were found in sample K1. These volatile compounds were reported to demonstrate the highest flavour dilution (FD) factors (>1000) in roasted hazelnut oil (Matsui *et al.*, 1998) and were character impact compounds of roasted beef (Czerny and Grosch, 1992). The latter compound was not detected in K3 and K4 samples, and only DEMP compound was found to be 56 ppb in sample K2. Numerous studies have been done on the effect of thermal treatment on the formation of volatile compound on solid food system such as perilla seed oil (Kim *et al.*, 2000), Arabica coffee (Czerny and Grosch, 2000) and sorghum (Lasekan *et al.*, 1997). These studies indicated that the presence of various pyrazines was a determining factor for the typical nutty, roasty and sweet aroma of this type of product. According to Barbara and Michael (2004), all of those pyrazines were correlated with sensory attributes such as nutty and roasty. Therefore the nutty and roasty aromas of the palm sugar in this study were very much correlated with the presence of pyrazines. From these findings, the desirable nutty and roasty notes of palm sugar were obviously contributed by pyrazines volatile compounds.

Furan Derivatives

Table 1 shows that K1 and K2 samples contained significantly higher level of furan compounds compared to K3 and K4 samples. The compounds of 2-furfural and 2-furan methanol were the most abundant furans, wherein their concentrations exceeded 1 ppm in both K1 and K2 samples. Some furans have been reported to contribute burnt, sweet, bitter, cooked meat and coconut-like flavour in some foods especially nuts and oilseed products (Maga, 1979). Surprisingly, 4-hydroxy-2,5-dimethyl-3(2H)-furanone (Furaneol) detected in K1 and K2 samples at concentrations of 817 ppb and 23 ppb respectively, were the least furan derivatives

Table 3
Mean (n=10) sensory ratings for attributes of the four different palm sugars [a]

Samples	Sensory Attributes			
	Nutty	Roasty	Burnt	Sweet caramel-like
K1	57 [a]	65 [a]	45 [a]	48 [b]
K2	45 [b]	50 [b]	46 [a]	56 [a]
K3	38 [c]	36 [c]	32 [b]	21 [b]
K4	38 [c]	35 [c]	31 [b]	20 [b]

[a]Sensory rating range from Low (0) to High (100). Means of scores for each descriptor followed by the same letter are not significantly different at the 5% level using Duncan' Multiple Range Test

determined even though these compounds were known to be significant flavour compounds and an important aroma constituents of many fruits (e.g. strawberry) (Rychilik and Bosset, 2001; Larson *et al.*, 1992) and processed foods (e.g. Cheddar cheese) (Milo and Reineccius, 1997). Furaneol has also been reported to possess sweet caramel, burnt sugar flavour with appreciable fruitiness and occurs in beer, Arabica coffee and white bread crust (Schieberle, 1995). For this reason, furaneol was the possible compound responsible for sweet caramel-like attributes of palm sugar.

Sensory Analysis

Table 3 shows that K1 has the highest sensory quality compared to other samples for nutty (57%) and roasty (65%) attributes. Meanwhile, sample K2 had the highest score for sweet caramel-like (56%) and burnt (46%) attributes. The other two samples (K3 and K4) had the lowest sensory quality and could not be distinguished from each other due to the lowest scores for all sensory attributes. Analysis of the results from each of the panelists indicated that they were using the rating scale differently, but the relative scores for the sensory descriptors showed very good agreement among all the panelists.

The highest score for nutty and roasty attributes in K1 sample was believed to be contributed by its highest total concentration of pyrazines as compared to other samples. In addition, the character impact compounds of EDMP and DEMP identified in K1 were the indicator for roasty and nutty notes. Surprisingly, the sweet caramel-like and burnt attributes in which K1 showed the highest total concentration of furan derivatives scored lower than K2 sample. It was probably due to the higher ratio of furan derivatives to pyrazines in sample K2 as compared to Kl (K2: 0.71; K1: 0.25). According to Hall and Merwin (1981), each volatile compound may potentially enhance, reduce or mask the sensory attributes in a particular food system as is shown in palm sugar. The highest concentration of total pyrazines in K1 apparently correlated to the highest score for nutty and roasty but on the other hand, it reduced the intensity of sweet caramel-like and burnt attributes.

Principal Component Analysis (PCA)

A comparison of the gas chromatography mass spectrometry (GC/MS) results with sensory data was carried out using principal component analysis (PCA). Figure 1 shows the PCA bi-plot of sensory attributes for palm sugar samples. The PCA model yielded 2 components explaining 100% of the variance of the data set, 80% by PC1 and 20% by PC2. A clear distribution of palm sugar samples into 2 groups was observed along the first component (PC 1), in which K1 and K2 samples grouped on the right side along PC 1

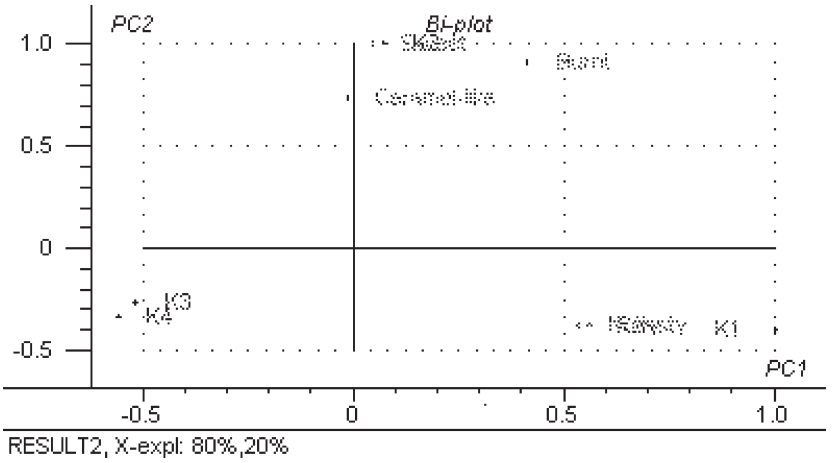

Figure 1: PCA bi-plot of sensory for 4 different palm sugars

while K3 and K4 samples were on the opposite side. The sensory attributes showed high positive magnitude scores along PC 1 which indicates the highest quality was possessed by both K1 and K2 samples.

Figure 1 shows no correlation was observed by increasing all the sensory descriptors along PC 1. Increasing sweet caramel-like and burnt attributes were represented by the PC 2, which also showed decreasing nutty and roasty odour. Therefore, sweet caramel-like and burnt attributes were positively related to each other while nutty and roasty odour gave opposite results. Sample K1 had a higher loading value of roasty and nutty, but less burnt and sweet caramel-like variables. On the other hand, attribute patterns of K2 was shown to have different results. In general, the sensory attributes variable fell into 2 main groups, sweet caramel-like/burnt and nutty/ roasty (Figure 1).

Partial Least Squares (PLS) Analysis

Since the use of sensory descriptive analysis is often expensive and time consuming, the instrumental data (X-variables), which in this case was volatile compounds, analyzed by GC/ MS were used to predict various sensory variables (Y) of palm sugar. To evaluate the relationship between instrumental and sensory variables, partial least squares (PLS) regression was used by plotting the 2-PLS components for each term (Figure 2). The effect of the GC/MS loading value on the sensory score can be evaluated by the magnitude and direction of the principal components (PCs) (Foster *et al.*, 2001). Examples of such evaluation are shown in Figure 2 for 2-furfural (peak 20) which has the highest positive loading value along PC 2, might affect the burnt and sweet caramel-like odour in palm sugar samples.

The sweet caramel-like and burnt attribute were correlated to high positive scores for the 2-furfural volatile compound (peak 20). These volatile compounds might affect the association between sweet caramel-like and burnt odour. As shown in Figure 2, 2-furfural compound has the highest score along component PC 2 among all GC/MS variables. Although its influence on the PLS model is not large (as indicated by the high positive magnitude along PC 2), it is an important factor in separating the sweet caramel-like/ burnt sensory aspect from the other sensory attributes of palm sugar. Stevenson *et al.* (1999) showed that a commercial caramel flavour (not specifically 2-furfural) significantly enhanced sweetness of a sucrose solution. This effect was higher for the caramel flavour than for any

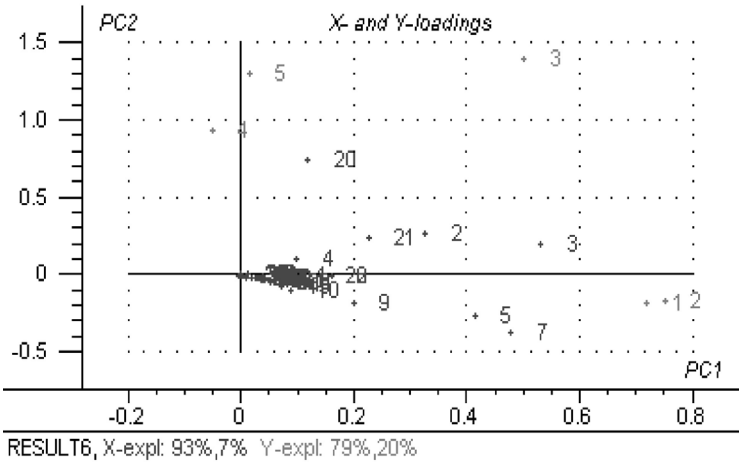

Figure 2: X and Y loading plot of the first two principal components of PCA applied to the data set of sensory scores (Y) compared with GC/MS scores loading. (See Table 1 for GC/MS instrumental variables)

other flavour tested. Another compound, maltol, which has caramel-like attributes, has been reported to increase perceived sweetness (Bingham *et al.*, 1990). Hence, it was thought that a high ratio of total furan derivatives to the pyrazines (K2: 0.71; K1: 0.25) could be used as an indicator to characterize the sweet caramel-like flavour of the palm sugar. For the formation of furan derivatives, two formation pathways are possible: (i) lipid peroxidation and (ii) degradation of carbohydrates. High concentration of 2-furfural (peak 21) and 2-furan methanol (peak 22) which were reported to form by degradation of carbohydrates (Maga, 1979) appeared to be a responsible pathway to produce sweet caramel-like and burnt note of the palm sugar.

The grouping together of nutty and roasty attributes can be explained by a higher loading score of 2,5-dimethyl pyrazine (peak 3), 2,3-dimethyl pyrazine (peak 5) and 2-ethyl-5-methyl pyrazine (peak 7) along PC 1. Matsui *et al.* (1998) reported that those pyrazine compounds were among the most important compounds producing nutty, cocoa and roasty note in the pumpkin seeds. Meanwhile, the higher positive magnitude loading score for burnt odour was also associated with 2-furan methanol (peak 21) and 2-methyl pyrazine (peak 2) compound, in addition to 2,3-dimethyl pyrazine (peak 5), 2,5-dimethyl pyrazine (peak 3) and 2-ethyl-5-methyl pyrazine (peak 7). However, 2,3-dimethyl pyrazine and 2-ethyl-5-methyl pyrazine, which gave nutty and roasty characters respectively and the most positive magnitude loading value along PC 1, may be important in separating the nutty/roasty sensory note. The nutty/roasty sensory position was plotted near the combined pyrazines (peak 3, 5 and 7) loading value, which mainly would give results of the nutty/roasty character. The results showed that character impact compounds such as 2,5-dimethyl-4-hydroxy-3(2H)-furanone (peak 23) and 2-ethyl-3,5-dimethyl pyrazine (peak 11) with higher aroma quality were different from the sensory descriptors, and resulted in the smallest effect on the model system.

CONCLUSIONS

Sample K1 showed the highest aroma quality in terms of total volatile compounds (74100 ppb) and sensory attributes for roasty (65%) and nutty (57%). The use of PCA was successful in categorizing the four different

palm sugars based on sensory attributes scores and produced logical relationships between sensory attributes and the total volatile compounds in the four different palm sugars. PLS analysis however, did not show good correlation for character impact compounds furaneol, EDMP and DEMP, which could be responsible for the perceived sweet caramel-like and roasty/nutty attributes of palm sugars, respectively.

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