AN004N – Determination of Sensory Scores
Application to Vegetable Oils Assessed by a Panel

Results obtained at Alpha MOS Laboratory (Toulouse, France) with oil samples supplied by Bunge (Hungary), a leading agribusiness and food company.

BUNGE NEW PRODUCTS & TECHNOLOGY EMEA

Introduction

The sensory quality of vegetable oils is dependent upon several parameters such as the origin and quality of vegetable raw materials, the extraction and refining process. Consumed in seasonings or entering the composition of many processed foods as a base ingredient, the sensory features of vegetable oils must be of high and constant quality. Sensory evaluation following recommended methods is often employed to evaluate the organoleptic properties of these oils.
This application note describes the analysis of sunflower oil with an electronic nose and the correlation of the instrumental measurements with those of a sensory panel.

Equipment
HERACLES Flash GC Electronic Nose

HERACLES Electronic Nose (Alpha MOS, France – Fig. 1) is based on ultra fast chromatography. It features 2 metal columns of different polarities (non polar RXT-5 and slightly polar RXT-1701, length = 10m, diameter = 180µm, *Restek*) in parallel and coupled to 2 Flame Ionization Detectors (FID). Two chromatograms are obtained simultaneously, allowing a sharper identification of the chemical compounds. It allows headspace or liquid injection modes.
The integrated solid adsorbent trap thermo-regulated by Peltier cooler (0-260°C) achieves an efficient pre-concentration of light volatiles and shows a great sensitivity (in the pg range).
With fast column heating rates (up to 600°C/min), results are delivered within seconds and the analysis cycle time is around 5 to 9 minutes.

Fig. 1: Ultra Fast GC based HERACLES Electronic Nose

The electronic nose is coupled to an autosampler (HS 100, CTC Analytics) to automate sampling and injection.
The instrument is operated through Alpha Soft software. In addition to classical chromatography functionalities, it provides chemometrics data processing tools such as sample fingerprint analysis and comparison, qualitative and quantitative models, quality control charts.

AroChemBase: Kovats Index library for chemical & sensory characterization

HERACLES e-nose was additionally equipped with AroChemBase module (Alpha MOS, France) that can be used within AlphaSoft E-Nose software. It consists of a library of chemical compounds with name, formula, CAS number, molecular weight, Kovats retention Index, sensory attributes and related bibliography. It allows pre-screening the chemical compounds and giving sensory features by directly clicking on the chromatograms' peaks.

Samples & Analytical Conditions

Eight batches (labeled FVF_01 to FVF_08) of refined sunflower oil were analyzed by:

- ✓ HERACLES electronic nose,
- ✓ Sensory evaluation.

HERACLES analytical conditions

Parameter	Value
Sample quantity	10 g ± 0.01 in a 50mL vial
Headspace generation	20 min at 60°C
Syringe temperature	70°C
Injected volume	5000 µL
Injection speed	100 µL/s
Injector temperature	200°C
Injector carrier pressure	10 kPa
Injector vent	30 mL/min
Trap temperature	20°C
Trap pressure	40 kPa
Split	5 mL/min
Trapping time	60 s
Trap desorption	240°C
Columns temperature program	40°C (2) to 80°C by 1°C/s then to 280°C (11s) by 3°C/s
FID temperature	280°C
Acquisition duration	120 s
Time between 2 analyses	9 min

Sensory evaluation conditions

Parameter	Value
Method	AOCS recommended practice Cg 2-83
Number of assessors	8
Oil scoring scale	1 (bad quality) to 10 (good quality). Average score considered
Duration	2.5 to 3 hours

Chromatograms

The comparison of the chromatograms (fig. 3) run with HERACLES e-nose shows important differences in terms of VOCs concentration between different batches of sunflower oil. This may indicate differences in sensory attributes.

Chemical characterization

Using the AroChemBase and Kovats indices on MXT-5 & MXT-1701 columns, indications about the chemical composition could be determined.
The main volatile compounds are listed in table 1, the ones in bold being mainly responsible for the differences between batches (see the proportions of these compounds in figure 4).

*RT MXT-5 (±0.1s)	*RT MXT-1701 (±0.1s)	**RI MXT-5 (±20)	**RI MXT-1701 (±20)	Possible compounds	Sensory attributes	Presence in batches
24.8	22.2	431	448	Undetermined	/	3 - 4
24.8	23.8	431	483	Acetaldehyde	Ethereal, fresh, fruity	4-5 < 3-6-7-8 < 1-2
28.9	24.8	500	502	Pentane	Alkane	5-6 < 8 < 1-2 << 7 < 4 < 3
28.9	29.2	500	580	Propan-2-ol	Alcoholic, ethereal,	7 < 4 < 3
36.5	30.4	601	599	Hexane	Alkane	5 < 1-2-4-6 < 3-7-8
44.5	37.8	669	675	Undetermined	/	5
48.2	40.1	700	700	Heptane	Alkane	7 < 4 < 3
60.7	63.1	801	894	Hexanal	Fatty, green	1-2-3-4-8

Table 1: Possible volatile compounds identified by their Kovats indices in the headspace of sunflower oils
*Retention Time
**Retention Index (Kovats Index)

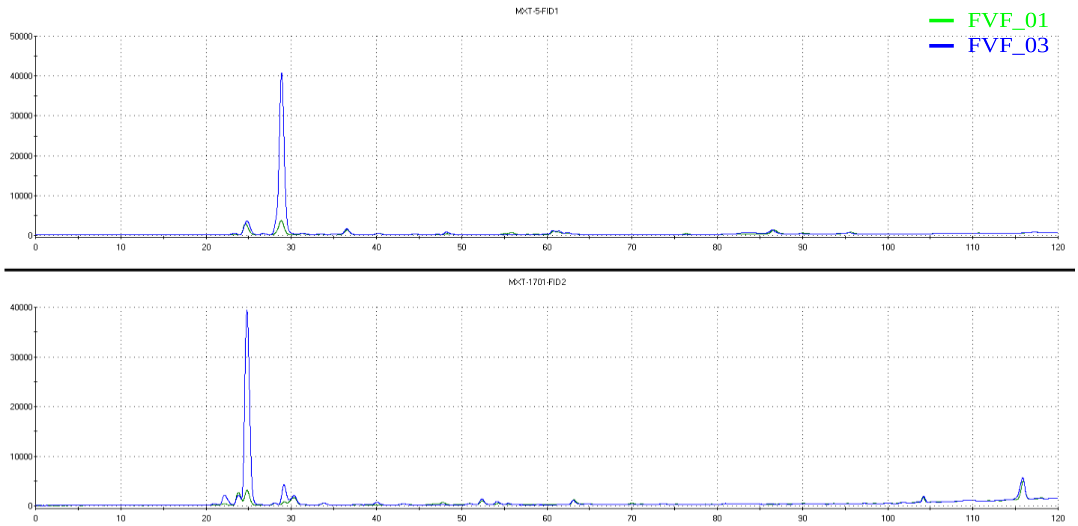

Fig.3: Chromatograms of 2 batches of sunflower oil (FVF_01 & FVF_03) on the 2 columns of HERACLES

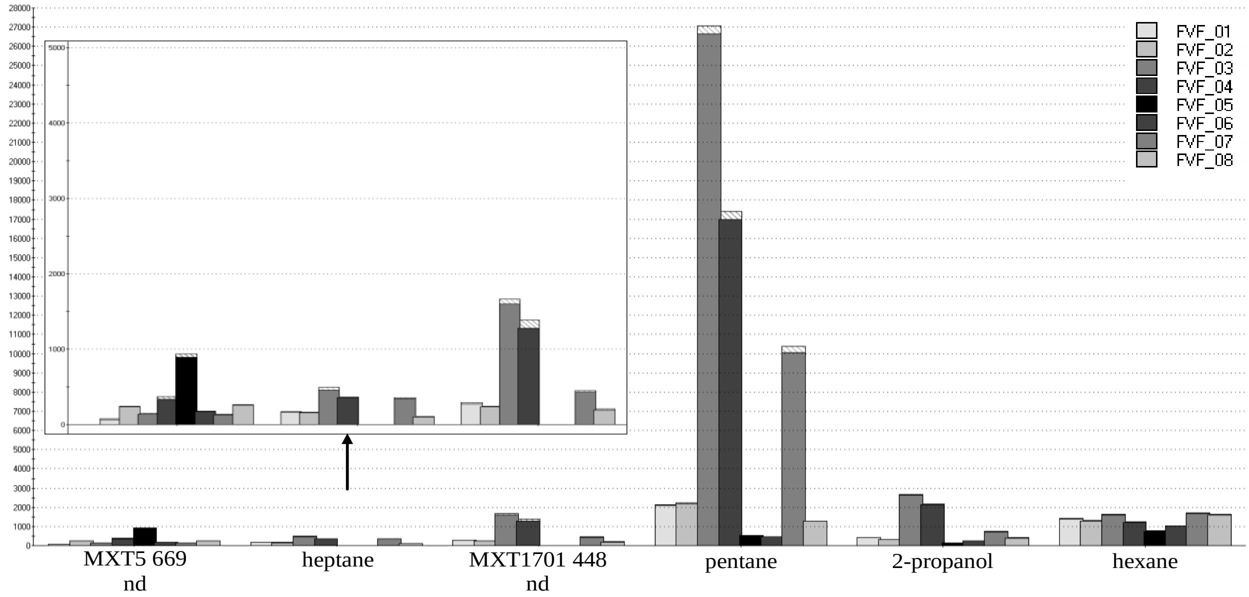

Figure 4: Proportion (peak area) of the most discriminant molecules in refined sunflower oil based on HERACLES e-nose analysis

Odor Characterization

Odor map

A general odor map was established (fig.5) upon selecting the most important chemical compounds on HERACLES e-nose chromatograms. The peaks corresponding to the following retention times were selected:

- On MXT-5 column: 500, 669, 700s
- On MXT-1701 column: 448, 502, 580, 599s.

This odor map, based on Principal Components Analysis (PCA), shows a clear differentiation of the sunflower oils according to their volatile compounds composition.
The distribution of oil samples on the map seems to be related to the sensory note determined by the panel.

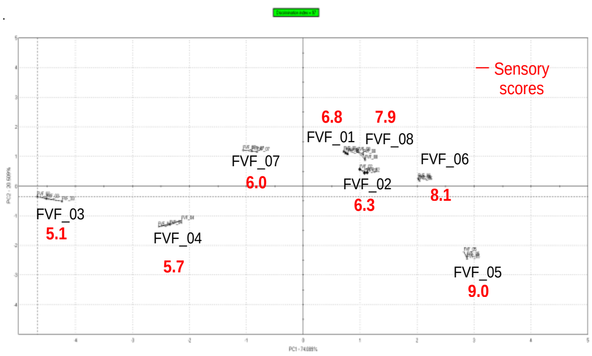

Fig. 5: Principal Components Analysis of sunflower oils obtained with HERACLES e-nose measurements

Sensory evaluation

Table 2 gives the average of all sensory scores attributed by the panelists for each oil sample.

Sample	Average sensory note
FVF_01	6.8
FVF_02	6.3
FVF_03	5.1
FVF_04	5.7
FVF_05	9.0
FVF_06	8.1
FVF_07	6.0
FVF_08	7.9

Table 2: average scores of all panelists' notes for each sunflower oil

Correlation between instrumental and sensory analyses

A qualitative model based on Partial Least Square (PLS) model was set up (fig. 6) between the sensory scores (x axis) and the electronic nose measurement (y axis).
Even if additional samples would be needed in order to obtain a more robust model, this graph shows a high correlation coefficient (0.943). This indicates that the electronic nose can be used to determine the sensory score of new oil samples, based on the same scoring scale as the sensory panel.

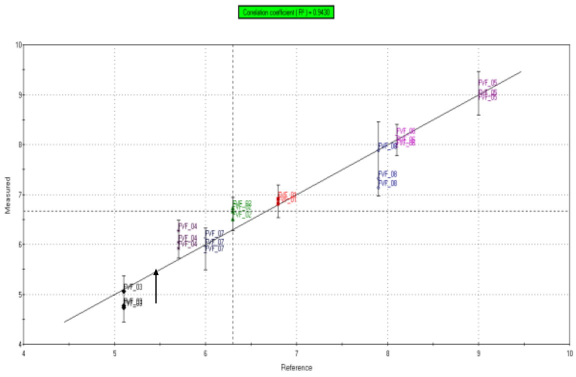

Fig. 6: Correlation model between sensory panel and e-nose measurements based on PLS (Partial Least Square) model

Conclusion

The e-nose can be a very powerful tool to rapidly assess the sensory quality of vegetable oils. By correlating the instrumental measurements to sensory evaluation, the e-nose is capable of determining a sensory note using the same scoring scale.