# WheelOscent: Presentation of an innovative GC-Olfactometry-dedicated software using intuitive aroma wheel interface

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## Abstract

GC-Olfactometry is a valuable methodology commonly used to investigate odor active compounds in complex food aroma profiles. Considering the number of studies using this technique, little is done to improve olfactometric data acquisition although it is essential for quality results. Efforts were mainly done to automate recording of moments of perception but intensity and description of perception are still often communicated orally, which disrupts the judge's breathing rhythm during analysis. Solutions that integrate all recording parameters result in a multiple steps acquisition procedure, scarcely compatible with the transience of the perceptions evaluated during olfactometry. The objective of this work was to develop a new olfactometric software that include olfactometric data acquisition and processing capabilities. The WheelOscent software was designed to improve the users' task and overcome constraints and bias of existing systems. More specifically the software, coded with Java technologies, implements innovative components:

- a data acquisition interface based on intuitive aroma wheels, adaptable to each product studied, which enables judges to characterize all parameters related to odors perceived in a simple and intuitive move,
- a data store, for collected data,
- a data analysis interface, which provides easy and direct analysis of data displayed into interactive and graphical visualization.

Providing good usability, this software enables a precise characterization that allows to point out special features of products even with close and complicated aroma profiles. This disposal is now used for wine analysis, where judges take advantage of the wheel aroma presentation, currently used for wine sensory characterization.

## Introduction

GC-Olfactometry is a valuable methodology commonly used to investigate odor active compounds in the aroma of food products. Considering the number of studies using this technique, small number of papers deals with the improvement of olfactometric data acquisition although it is essential for the quality of the results. Despite many drawbacks, some olfactometric studies are still conducted with an oral transmission of judges' sensory impressions. This practice leads to perturbation of breathing rhythm, breakdown of sensorial perceptions and complicates the recording of the judge's perception. Besides, it mobilizes an operator to capture judges' comments and restricts olfactometry sessions to a single judge. To avoid these bias, instrumental devices were developed to automate the acquisition of judges' perceptions. A pushing button was first employed to record time and duration of odor events and finger-span system was developed to record the intensity perceived by using the distance between the thumb and the major finger of the judge to represent the odor intensity score. [1,2] However, when recorded, descriptors

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were independently captured. Tape and digital recorders could be used to overcome the presence of an operator and devices can merge vocal information into numerical data through a voice recognition system, but these appliances don't prevent perturbations associated with speaking. Besides, when descriptors are freely chosen by judges, a consensus can be complicated to obtain for a same odor event. Even if training of judges strongly reduces these difficulties linked to individualities, this lack of consensus can persist due to the difficulty for human brain to link the olfactory and semantic memories and thus, to clearly associate a word to an odor. [3] To come through this problem, an acquisition software proposed to constrain judges to first choose an odor category and then a more precise term. [4] Despite the intuitiveness of this software using pictures, the odor description is made in several steps which delayed data recording and could fail to characterize closely eluted odorants. Currently, and according to literature, there was no device that, all at once, prevents judges from speaking, enables to record simultaneously all odor event parameters, and permits data processing.

The objective of this work was to introduce an innovative olfactometric software based on an intuitive wheel interface that allows a simultaneous and automatic recording of moment, duration, intensity and description of the perceived sensations (patented). [5,6] This approach was conceived to respect the breathing rhythm and the continuity of sensorial judge's perceptions while offering direct data processing possibilities. This original integrative system named WheelOscent is herein presented through a wine aroma analysis.

## Experimental

### *Material*

The wine used for the study was a red wine, 13% alcohol, from appellation Bourgueil, elaborated in 2010 from a Cabernet Franc vineyard. Chemical standards and n-alkanes were purchased from Sigma Aldrich (St Quentin Fallavier, France) with purity > 97%.

### *Wine aroma extraction and chromatographic conditions*

Volatiles from a 5 mL sample of wine were extracted by solid phase micro-extraction with a Car/PDMS fiber (10mm length, 85µm film thickness; Supelco, Bellefonte, PA, USA) placed in the headspace of the vial for 10 minutes at 34°C after 1 hour of incubation. The fiber was then directly introduced into the injection port of the gas chromatograph (T=260 °C). Besides the analyses of the samples, a solution of C5 to C32 n-alkanes was injected under the same chromatographic conditions. Analyses were carried out with a gas chromatograph (GC 7890A, Agilent Wilmington, DE, USA) equipped with a DB-Wax column (Agilent, 30m length, 0.25mm internal diameter, 0.5µm film thickness). Hydrogen was used as the carrier gas and the oven temperature was programmed as follows: 50°C (0min) to 80 °C at 5 $°C\cdot min^{-1}$, then 80 to 200 °C at 10 $°C\cdot min^{-1}$, and 200°C to 240 °C (4min) at 20 $°C\cdot min^{-1}$. GC was coupled to a mass spectrometer (MS 5975, electron impact mode 70 eV, scan m/z 33-300, 2.7 $scan.s^{-1}$, Agilent) and a dual olfactometric port (transfer line T= 200°C, Gerstel ODP 3, Mülheim an der Ruhr, Germany). The olfactometric ports were equipped with nose glass funnels and supplied with humidified air to prevent dehydration of the nasal mucosa.

### *Olfactometric analysis*

The eluate was analyzed by 8 judges throughout successive runs. Judges were trained to aroma recognition and the use of an intensity scale. Judges' perceptions (time, intensity and description) were recorded in real time *via* the WheelOscent software coded with Java technologies, described above (Figure ). Descriptors were presented on a dedicated aroma wheel especially designed for wine aroma. The wheel is structured in 23 poles associated to general odor families written in capital letters. These poles can be divided into sections associated to more precise descriptors.

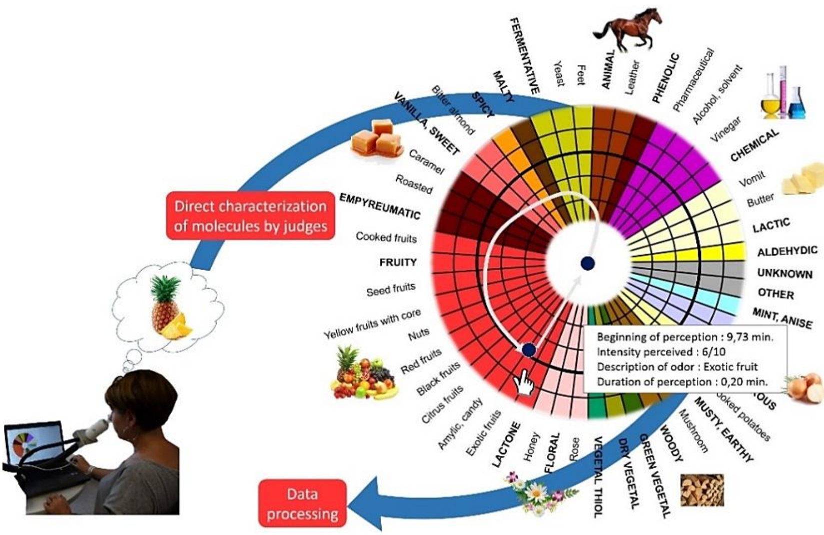


**Figure 1:** Schematic functioning of the WheelOscent olfactometric software presenting the aroma wheel interface (patent pending) [5,6]

Colors were also associated to poles to help the judges to rapidly find terms corresponding to the perceived odors. During the GC-Olfactometric run, judges were asked to signal the perception of an odor by directing the mouse pointer outside the central zone and then to direct it to the section of the wheel corresponding to the adequate odor term. They were also asked to score the intensity of the odor by clicking on the 0-10 intensity scale represented by the radius of the wheel (center of the wheel= 0, edge of the wheel=10). When an odor was no longer perceived, judges were asked to direct the pointer of the mouse back to the center of the wheel. Judges were encouraged to describe each odor perceived using terms proposed on the wheel. If the odor perceived did not correspond to any descriptor, judges were invited to describe the odor by the name of the pole corresponding to the general odor family or failing that, by the "Unknown" or "Other" sections.

## Results and discussion

The results are displayed directly from the software. Concatenated aromagrams can be obtained presenting either the number of detections or the mean intensity of odors perceived *vs* retention time or linear retention index (LRI, Figure). For the investigated wine, 33 odorant zones were perceived by at least 3 judges. Individual aromagrams are also available for each judge with their associated descriptors. Moreover, a table of results that summarize the recorded data for each odorant zone is accessible from the software.

Identification of odorants was performed by comparing their LRI and mass spectra to those of databases (Wiley, Nist and internal databases) and by injection of standard compounds. Descriptors given for each detected compound were also compared with those found in the literature. Identification of compounds associated to each odorant zone and LRI is systematically recorded in the software database, so that a list of plausible odorants with related descriptors is available for exploration of later samples.

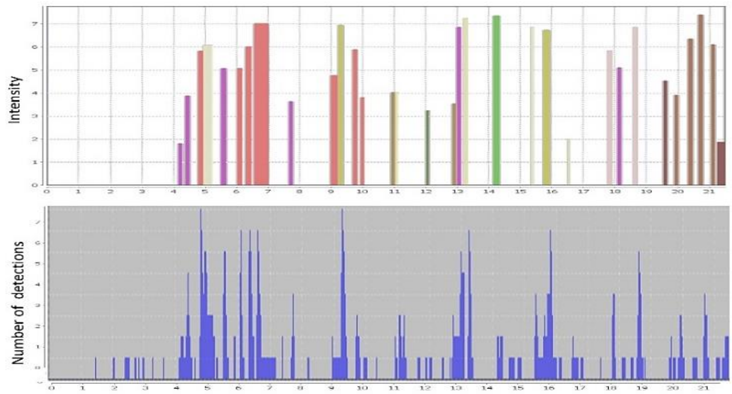


**Figure 2:** Individual and concatenated aromagrams directly obtained from the wheelOscent software after the GCO analysis of the investigated wine

As proved by the excerpt of the table of results obtained after the analysis of the wine sample (Table ), this tool enables to clearly discriminate odorants closely eluted like the 2-ethyl-2-methylpropanoate (4,82min) and the 2,3-butanedione (4,94 min).

**Table 1:** Excerpt of the table of results obtained from the software after olfactometric analysis of the wine

| *LRI apex* | *Retention time* | *Start time* | *End time* | *Judge1* | *Judge2* | *Judge3* | *Judge4* | *Judge5* | *Judge5* | *Judge6* | *Judge7* | *Judge8* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 940 | 4,40 | 4,37 | 4,45 | CHIMIQUE | alcool | CHIMIQUE | | | CHIMIQUE | LACTONE | | |
| 970 | 4,82 | 4,78 | 4,92 | FRUITE | amylique | FRUITE | | VANILLE, DOUX | fruits rouges | amylique | amylique | |
| 978 | 4,94 | 4,92 | 5,18 | INCONNU | beurre | caramel | beurre | beurre | beurre | amylique | beurre | |
| 1018 | 5,57 | 5,52 | 5,62 | INCONNU | alcool | INCONNU | VEGETAL VERT | | CHIMIQUE | | caramel | |

As expected, this software allows a rapid, precise and efficient recording of GC-Olfactometric data, associated with an excellent usability for judges through the intuitive aroma wheel interface. This approach solves bias found in current GC-O data acquisition methods and notably disruption of breathing rhythm inherent to the oral transmission of judges' perceptions. It provides a complete characterization of odor events, and includes data treatment capabilities. The accuracy of the approach makes it a valuable tool to shed light from whatever complex aroma product or compare those with very close aroma profile and point out their significant characteristics. Besides, the wheel presentation of descriptors, consistent with those found in numerous sensory analysis, can facilitate chemometric approaches that attempt to understand the contribution of compounds to a global aroma.

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