



Factors Affecting Essence Quality: **HDPE vs Glass**

Sensus Technical Note (SEN-TN-0003)

09/04/2008

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ABSTRACT

Once an essence is captured, it is important to ensure proper storage conditions to maintain the highest quality. In this study, a comparison is made between a low headspace, refrigerated essence in a glass container versus a high headspace, room temperature essence in a poly ethylene container. Comparisons after a week show dramatic changes that illustrate the importance of storage conditions to maintaining the highest level of quality.

INTRODUCTION

There are many factors that can affect an essence. For example, temperature, light, acids, bases, storage time, and type of container are known issues. A general rule in chemistry is that a reaction rate will double for every 10°C increase in temperature. This means that reaction rates are approximately four times faster at room temperature than refrigerator temperatures. For long term storage, freezing of essences is preferred for two reasons. First is the lower temperature reduces reaction rates. Secondly reaction rates are greatly reduced in frozen form due to lack of chemical mobility. Ultraviolet (UV) and visible light can initiate reactions and is best to be avoided. This is generally easy to do by using amber colored containers, and since most of the time the essence is in the refrigerator or freezer, there is generally little light. Acids and bases are usually not a problem during storage of essences, but could be a problem in a final beverage. Lastly is storage container. Glass containers are usually best due to the low reactivity and permeability. Plastic bottles are generally not considered optimum due to the permeability. This permeability is a problem in two ways. First is the diffusion of essence volatiles into the plastic which is termed "scalping". Second, is the issue of oxygen permeability. Table 1 is a short table of different plastics and their oxygen permeability. This study was intended to examine the two extreme cases, a refrigerated amber glass container with little headspace and a room temperature HDPE container with a large headspace after one week of storage.

MATERIALS AND METHODS

An Oberk 2 oz container of a Sensus tea essence was stored in the refrigerator (~9°C) for one week. A 1mL aliquot of the tea essence was placed in a 125mL (4oz) HDPE container and stored at room temperature (~27°C). The essences were then prepared for analysis by pipetting 50µL into 4.9mL of water along with 50µL of internal standard (phenol-D6, 100 ppm)

A Gerstel MultiPurposeSampler (MPS-2) (Baltimore, MD) was used with a 1-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

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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 60mx0.25mmx0.25 μ m RTX-5ms column. The initial oven temperature was 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.

RESULTS AND DISCUSSION

The affects of the storage are dramatic and obvious. Figure 1 is a general chromatogram of the “fingerprint region”. It is clear that the HDPE sample (in green) is greatly diminished as compared to the amber glass sample. Figures 2 and 3 are of the internal standards which were added directly before analysis. Figure 4 is a more detailed view of the first part of the chromatograms from Figure 1 where the methyl butanals and hexanal/hexenal are clearly different. Figure 5 is the mid/late region of the chromatogram and once again, the differences are clear. It is clear that storage container and temperature play a fundamental role in product quality. Please see the recommendation section at the end.

Table 1. Oxygen permeability of different polymers.

Polymer	Oxygen permeability ($\times 10^{-13} \text{ cm}^3 \cdot \text{cm cm}^{-2} \text{ s}^{-1} \text{ Pa}^{-1}$)
LDPE-low density poly ethylene	2.0
HDPE-High density poly ethylene	0.4
PET-Polyethylene terephthalate	0.03
PP-Polypropylene	1.7
PC-Polycarbonate	1.0
PS-Polystyrene	2.0
TPX-Polymethylpentene	20
FEP-Fluorinated Ethylene Propylene	3.0
PFA- Tetrafluoroethylene-perfluoro	3.0

Figure 1. “Fingerprint” region of refrigerated amber glass bottle (orange) and the room temp. HDPE sample (green).

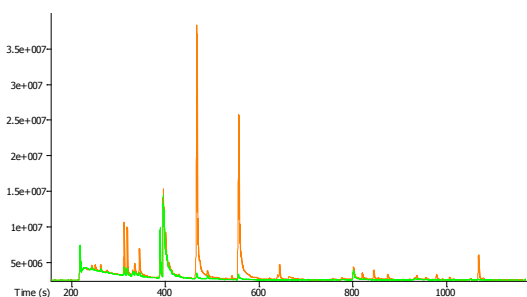


Figure 2. Internal standard #1 (Pyridine-D5) (Orange trace is for glass, green for HDPE)

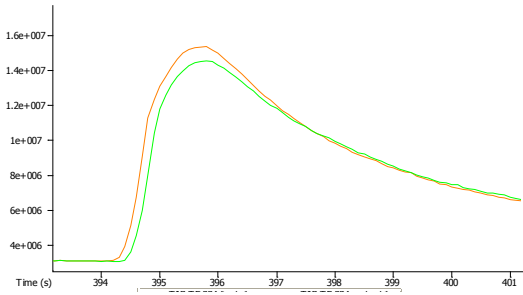


Figure 3. Internal Standard #2 (Phenol-D6) (Orange trace is for glass, green for HDPE)

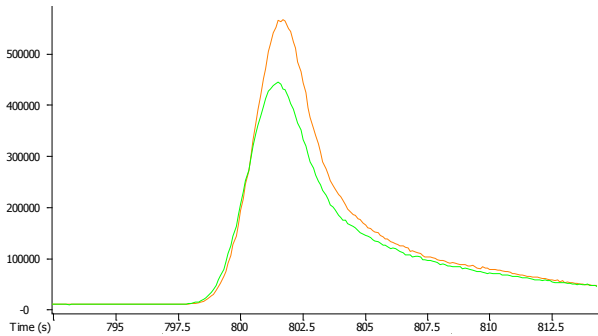


Figure 4. Early eluting region, generally "top notes" (Orange trace is for glass, green for HDPE)

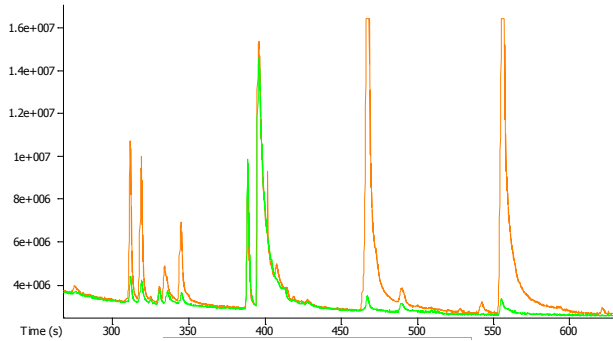
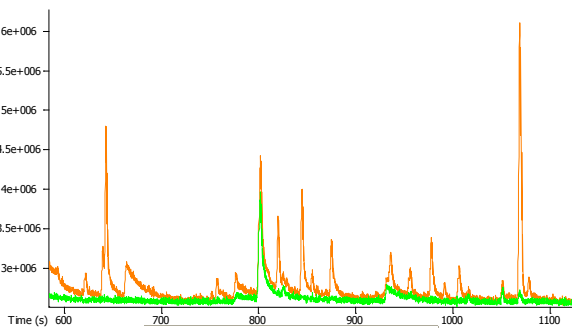


Figure 5. Mid/late eluting region (Orange trace is for glass, green for HDPE)



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