# SCREENING OF VOLATILE COMPOUNDS IN BEVERAGE CANS USING PURGE AND TRAP (P&T) TECHNIQUE COUPLED TO GC-MS

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## INTRODUCTION

It is well known that packaging materials can be a potential source of contaminants. The migration of chemicals from packaging to food and beverages is one of the main concerns for food safety authorities [1].

In the present study, a screening method was performed to investigate potential volatile migrants from ten polymeric can coatings of beverages. The sample was directly analyzed using a purge and trap (P&T) system coupled to gas chromatography with mass spectrometry detection (GC-MS). This technique allows to concentrate the volatiles in a sorbent material.

It is important to consider that, in this study, the samples analyzed were already in contact with the food, since the material was not available prior to contact. Therefore, the mass transfer could take place in both directions, migration from the packaging to the food and sorption from the food into the packaging. Moreover, it should be taken into account that the analysis of the material includes both sides, internal and external

## MATERIALS AND METHODS

### SAMPLES OF BEVERAGES

| CODE | DESCRIPTION | ORIGIN |
|---|---|---|
| BC01 | Traditional Beer | Spain |
| BC02 | Vodka mixed drink | Italy |
| BC03 | Mixed lemon flavour | Spain |
| BC04 | Energy drink zero | Ireland |
| BC05 | Star wars space punch | Germany |
| BC06 | Green cola | Spain |
| BC07 | Tonic original | Spain |
| BC08 | Tonic water original | Spain |
| BC09 | Premium tonic water | Germany |
| BC10 | Natural mineral water drink | Spain |

**Table 1:** Information about the samples included in the study.

### IDENTIFICATION OF POTENTIAL VOLATILE MIGRANTS FROM POLYMERIC CAN COATINGS

For the analysis of potential volatiles from polymeric can coatings a previous step of concentration was performed using a Teledyne Tekmar Stratum Purge and Trap (P&T) system. The GC-MS analysis was carried out using a Finnigan Trace Gas Chromatograph Ultra with a Finnigan Trace DSQ mass detector.

| | |
|---|---|
| Sample T$^a$ | 90 ºC |
| Purge flow | 40 mL/min |
| Purge time | 20 min |
| Desorb time | 2 min |
| Desorb T$^a$ | 250 ºC |
| Desorb flow | 400 mL/min |

**Table 2:** Experimental conditions of P&T.

| | |
|---|---|
| Carrier gas | Helium 1mL/min |
| Column | Rxi-624Sil MS (30m x 0.25mm x 1.40 µm) |
| Gradient T$^a$ | 45-250ºC |
| Ionization source | Electron impact |
| Transfer line T$^a$ | 250 ºC |
| Source T$^a$ | 250 ºC |
| Data acquisition | Full scan (range m/z 20-500) |
| Spectrum library | NIST/EPA/NIH 11 v. 2.0 & Wiley 8th |

**Table 3:** Experimental conditions of GC-MS.

## RESULTS AND DISCUSSION

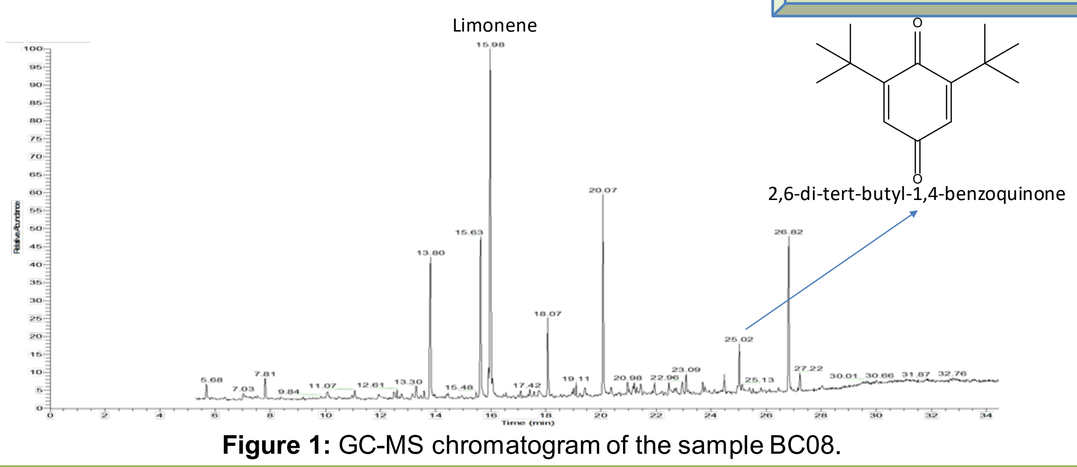


**Figure 1:** GC-MS chromatogram of the sample BC08.

| TR (min) | CAS Number | Compound Name | m/z | BC 01 | BC 02 | BC 03 | BC 04 | BC 05 | BC 06 | BC 07 | BC 08 | BC 09 | BC 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **7.85** | 71-36-3 | Butanol | 56, 41 | X | X | X | X | X | X | X | X | X | X |
| **8.36** | 110-62-3 | Pentanal | 44, 58 | | | | | | | | | X | |
| **9.86** | 108-88-3 | Toluene | 91, 65 | X | X | | X | X | X | | X | X | |
| **13.75** | 80-56-8 | α-pinene | 93, 77 | | | | | X | | | | | |
| **13.79** | 111-76-2 | 2-butoxyethanol | 57, 45 | X | X | X | X | X | X | X | X | X | X |
| **15.92** | 124-13-0 | Octanal | 43, 56 | X | | X | X | | X | | X | | |
| **17.03** | 108-95-2 | Phenol | 94, 66 | X | X | X | X | | X | | X | | X |
| **17.10** | 1120-21-4 | Undecane | 57, 43 | X | | X | | X | X | | X | | |
| **18.09** | 124-19-6 | Nonanal | 57, 70 | X | X | X | X | X | X | X | X | X | X |
| **20.09** | 98-55-5 | α-terpineol | 59, 93 | | | | | X | | | | X | |
| **20.97** | 100-97-0 | Hexamethylenetetramine | 42, 140 | X | | | X | | X | | | | |
| **21.16** | 122-99-6 | 2-phenoxyethanol | 94, 77 | | | | X | | | | | | |
| **22.47** | 105-60-2 | Caprolactam | 56, 113 | | X | X | | | | X | X | | X |
| **22.74** | 629-59-4 | Tetradecane | 57, 71 | | | X | X | X | | | X | X | X |
| **22.94** | 102-76-1 | Triacetin | 43, 145 | | X | X | X | | X | X | | | X |
| **25.03** | 719-22-2 | 2,6-di-tert-butyl-1,4-benzoquinone | 177, 135 | | X | X | | | X | | X | | X |
| **27.23** | 84-66-2 | Diethyl phthalate | 149, 177 | X | X | X | X | X | X | X | X | X | X |
| **28.00** | 119-61-9 | Benzophenone | 105, 77 | | | | | | X | | | | |

**Table 4:** Chemicals selected identified in the polymeric can coatings analyzed.

- A wide variety of compounds including alcohols, ethers, aldehydes and some phthalates such as diethyl phthalate were detected using this screening technique. Only compounds with the best matches found during the library search were considered for the study.
- Figure 1 show the GC-MS chromatogram of the sample BC08. As can be seen, the most intense peak corresponds to limonene, probably it comes from the beverage.
- Eighteen compounds were positively confirmed by injection of the respective standard comparing the retention times and their respective mass spectra (Table 4).
- To the best of our knowledge very limited literature about the application of this technique to analyze polymeric coatings have been reported.
- This study also allows to obtain information on the production of coatings. For example, 2-butoxyethanol was used in the polymerization step and/or as a solvent

## References

(1) [1] Poças, M. F. et al., Trends in Food Science & Technology 18 (2007) 219-230.

## Acknowledgement

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