

# Non-targeted screening for volatile compounds in food contact bioplastics using Purge and Trap coupled to Gas chromatography-Mass Spectrometry

P. Vázquez Loureiro<sup>1</sup>, A. Lestido-Cardama<sup>1</sup>, R. Sendón<sup>1</sup>, L. Barbosa-Pereira<sup>1</sup>, J. Bustos<sup>2</sup>, A. Gasco<sup>2</sup>,  
P. Paseiro Losada<sup>1</sup>, A. Rodríguez Bernaldo de Quirós<sup>1\*</sup>

<sup>1</sup>Dept. Analytical Chemistry, Nutrition and Food Science, Faculty of Pharmacy, University of Santiago de Compostela, 15782, Santiago de Compostela, Spain.

<sup>2</sup>National Food Centre, Spanish Agency of Food Safety and Nutrition, E-28220 Majadahonda, Spain.

\*Presenting author: ana.rodriguez.bernaldo@usc.es

## 1. INTRODUCTION

Bio-based and/or biodegradable plastics are being developed as sustainable packaging solutions. Similarly to petrochemically based polymers bioplastics are subject to the regulatory requirements of food contact materials in terms of inertness and safety of the material. Both intentionally (IAS) and non-intentionally added substances (NIAS) should be evaluated to protect the consumers' health. Sample preparation is the first step in the analysis of potential migrants and usually it is a laborious and time-consuming procedure. The Purge & Trap system coupled to Gas chromatography-Mass Spectrometry (P&T-GC-MS) has demonstrated to be an efficient analytical tool for the extraction and subsequent analysis of volatile compounds. In this work, a P&T-GC-MS method was optimized for the analysis of volatile compounds in food packaging samples labeled as bio-based and/or biodegradable and based on polypropylene (PP), polyester and Polylactide (PLA).

## 2. EXPERIMENTAL

### 2.1. Samples

Polymer type	Plastic product	Type
Polyester base	Bag for foodstuff	FP
PP	Bag for foodstuff	FP
PLA	Bag for foodstuff	FP
PLA	Film	FP
PLA	Pellets	RM

FP: Final product; RM: Raw material

Table 1.- Samples description

### 2.2. Extraction and Analysis



Fig.1.- Purge & Trap system coupled to Gas chromatography-Mass Spectrometry (P&T-GC-MS)

### 2.3. Analytical conditions

Purge and Trap (P&T)	
Purge Time	30 min
Purge Flow	40 mL/min
Trap	Vocarb 3000
Desorb t & T	2 min, 250°C

Table 2.- P&T conditions

Chromatography	
Column	Rxi-624Sil MS (30 m × 0.25 mm i.d., 1.40 µm film thickness)
Oven T (°C)	From 35°C to 300°C
Injection Port (T)	200°C
Carrier gas	Helium (1 mL/min)

Table 3.- Chromatographic conditions

Mass Spectrometry	
Acquisition mode	Full scan
Mass range	m/z 35-500
Mass spectral libraries	-NIST/EPA/NIH 11 (version 2.0) -Wiley Registry TM 8th edition

Table 4.- Mass spectrometry conditions

### Optimized sample extraction conditions



## 3. RESULTS

t <sub>R</sub> (min)	Compound	Polyester base	PP	PLA	Remarks
5.48	Chloroform	✓		✓ (b)	Solvent residue
7.13	2,3-Pentanedione			✓ (f, p)	PLA degradation product (1)
8.59	Toluene	✓	✓	✓ (b, f, p)	Solvent residue
9.81	Propylene Glycol	✓			Monomer
14.91	Undecane	✓	✓	✓ (f, p)	Alkane
16.63	Dodecane	✓	✓	✓ (b)	Alkane
16.79	1,4-Dioxane-2,5-dione,3,6- dimethyl-			✓ (f, p)	Cyclic lactide dimer
21.86	Butylated hydroxytoluene	✓			Antioxidant
23.35	Phthalic acid	✓			Monomer
24.16	Benzophenone	✓			Photoinitiator
26.49	Phthalic acid, diisobutyl ester	✓			Plasticizer

b: bag; f: film; p: pellet  
Table 5.- Table extract with some of the compounds tentatively identified in the samples

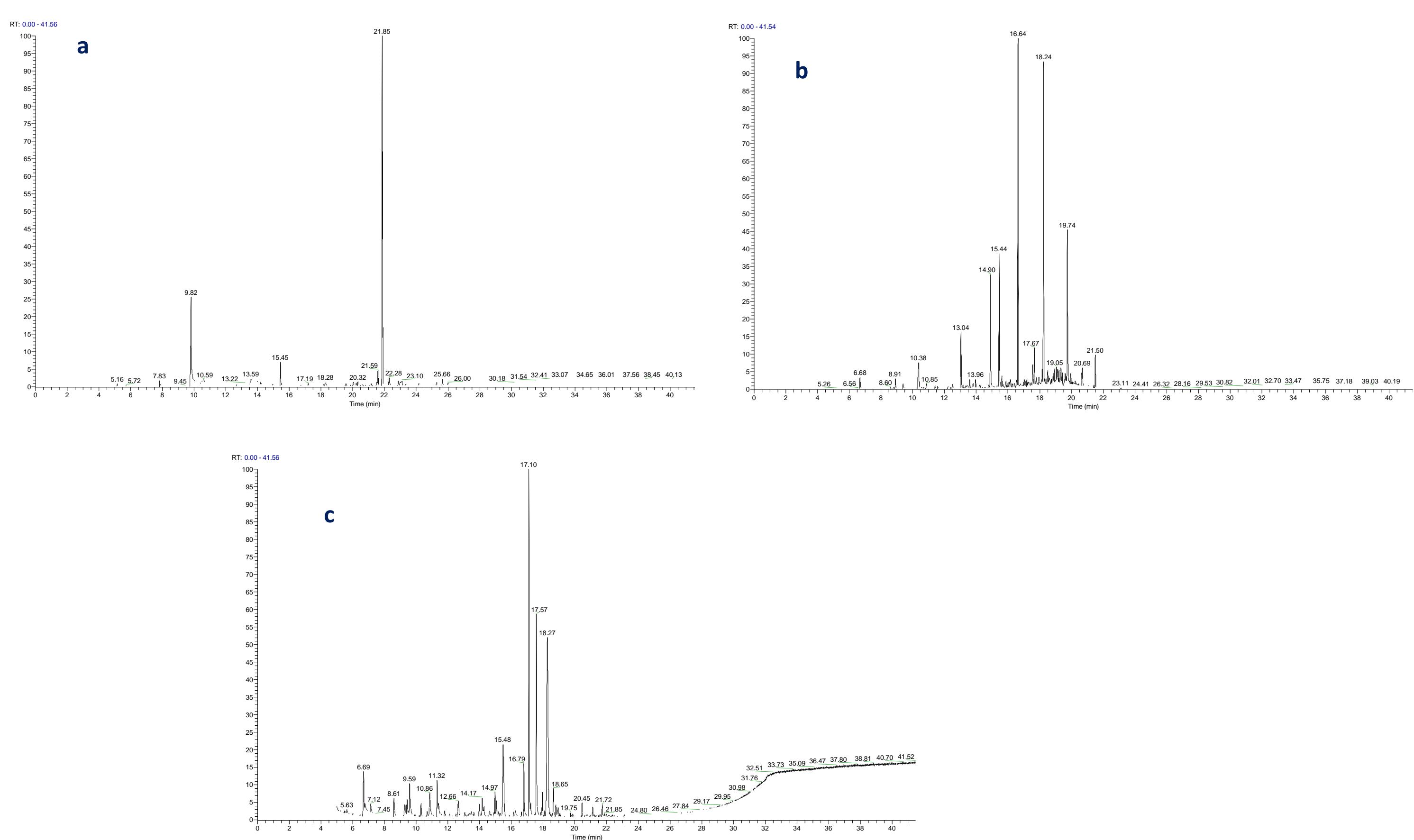


Fig.2.- Chromatograms of a polyester based material (a), PP (b) and PLA (c) samples

## 4. CONCLUDING REMARKS

- P&T coupled to GC-MS has demonstrated to be a powerful analytical tool for the identification of volatile compounds in bioplastics for food contact
- 120 compounds were detected in the samples analysed
- Both IAS and NIAS were detected
- Only 16 of the 120 compounds detected in the samples are listed in the Regulation 10/2011 (2)

## REFERENCES

- (1) Salazar et al. (2017) Polymer Degradation and Stability, 136, 80-88  
(2) European Union. (2011). Regulation (EU) No. 10/2011. Official Journal of the European Union, L12, 1–89.

## ACKNOWLEDGEMENTS

The study was financially supported by the Ministerio de Ciencia e Innovación, Agencia Estatal de Investigación and by Fondo Europeo de Desarrollo Regional (FEDER). Ref.No. PID2021-124729NB-I00 "MIGRABIOQUANT" (MCIN/AEI/ 10.13039/501100011033/FEDER, UE). Authors are grateful to "Ministerio de Ciencia, Innovación y Universidades" for the Predoctoral fellowship (ref. PRE2019-088195) awarded to PVL.