

IDENTIFICATION OF NON-VOLATILE COMPOUNDS IN **BIO-BASED** AND/OR **BIODEGRADABLE PACKAGING MATERIALS** USING A NON-TARGETED **LC-HRMS** METHOD

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INTRODUCTION

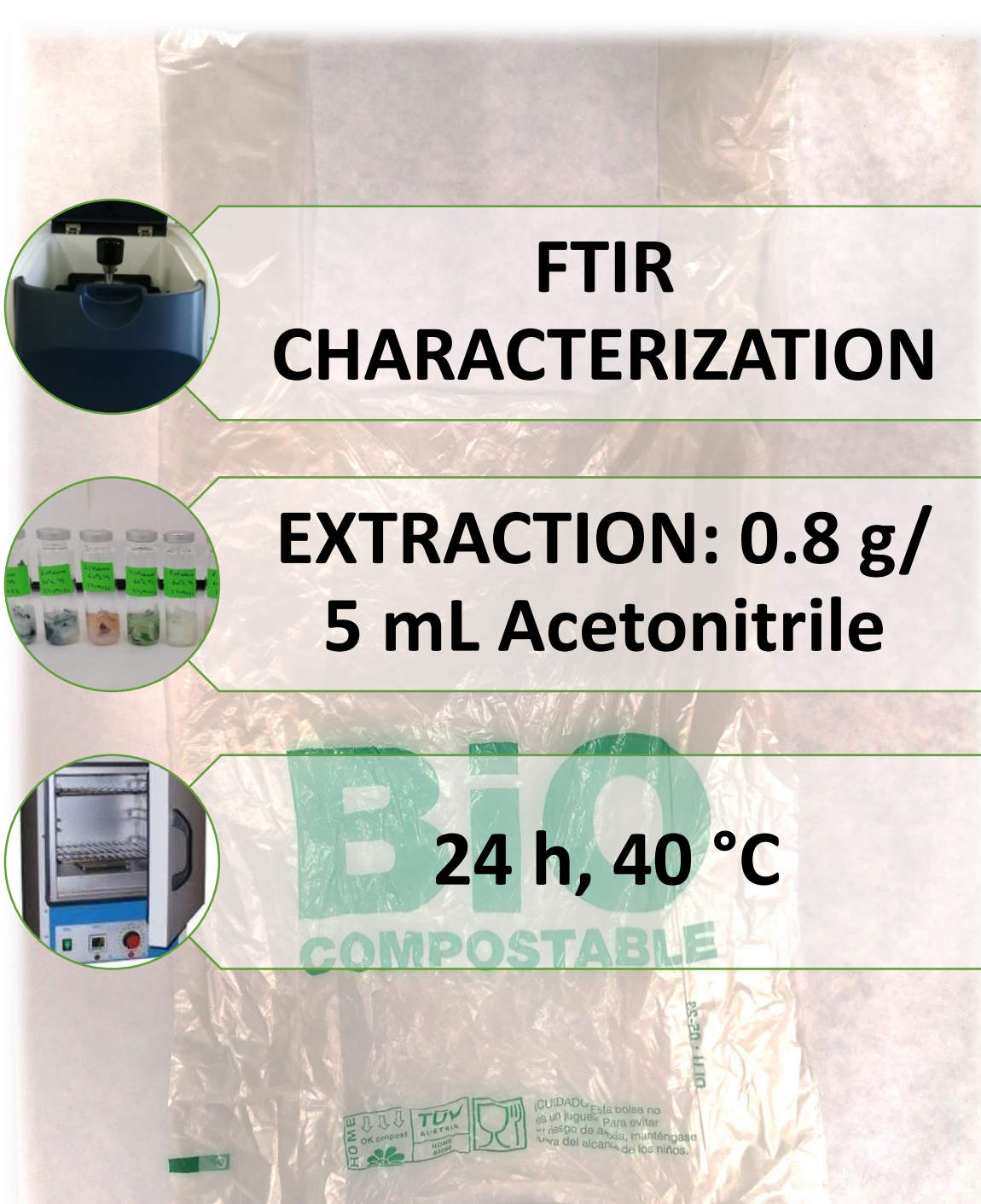
The development of sustainable packaging is increasing, and the use of environmentally friendly materials are being more demanded to replace conventional petroleum-based plastics. Bio-based and biodegradable polymers are being increasingly used for food packaging applications. However, the **knowledge on** chemical safety of these biopolymers is scarce.

In this work, potential migrants including monomers and additives, as well as reaction, degradation products and impurities known as NIAS were studied. For that purpose, samples characterized by FTIR as polyester based materials, polylactic acid (PLA), and polypropylene (PP) were extracted and analyzed by LC-HRMS using a non-targeted analysis to investigate non-volatile compounds extracted from these packaging materials labeled as bio-based and/or biodegradable and intended to be in contact with food. Data were acquired in full scan mode and processed using an interface under the open-source programming R environment [1].

SAMPLES

LC-HRMS ANALYSIS CONDITIONS

DATA TREATMENT



CHROMATOGRAPHIC CONDITIONS	
Equipment	UltiMate 3000UHPL coupled to an Orbitrap Q Exactive mass spectrometer
Source	ESI
Mode	Positive and negative
Column	C18-like column (100 mm × 2.1 mm, 1.9 μm) guard-column (10 mm × 2.1 mm, 3 μm)
Flow rate	0.4 ml/min
Mobile Phase	10 mM ammonium acetate in both water and acetonitrile/water 99:1 (v/v)
Injection volume	2 μL
Full scan	50-1064 m/z

SPECTROMETRIC CONDITIONS	
Spray Voltage	3500 V
Capillary Temperature	350 °C
Sheath gas	50 AU
Aux Gas	10 AU
S-Lens	70 AU

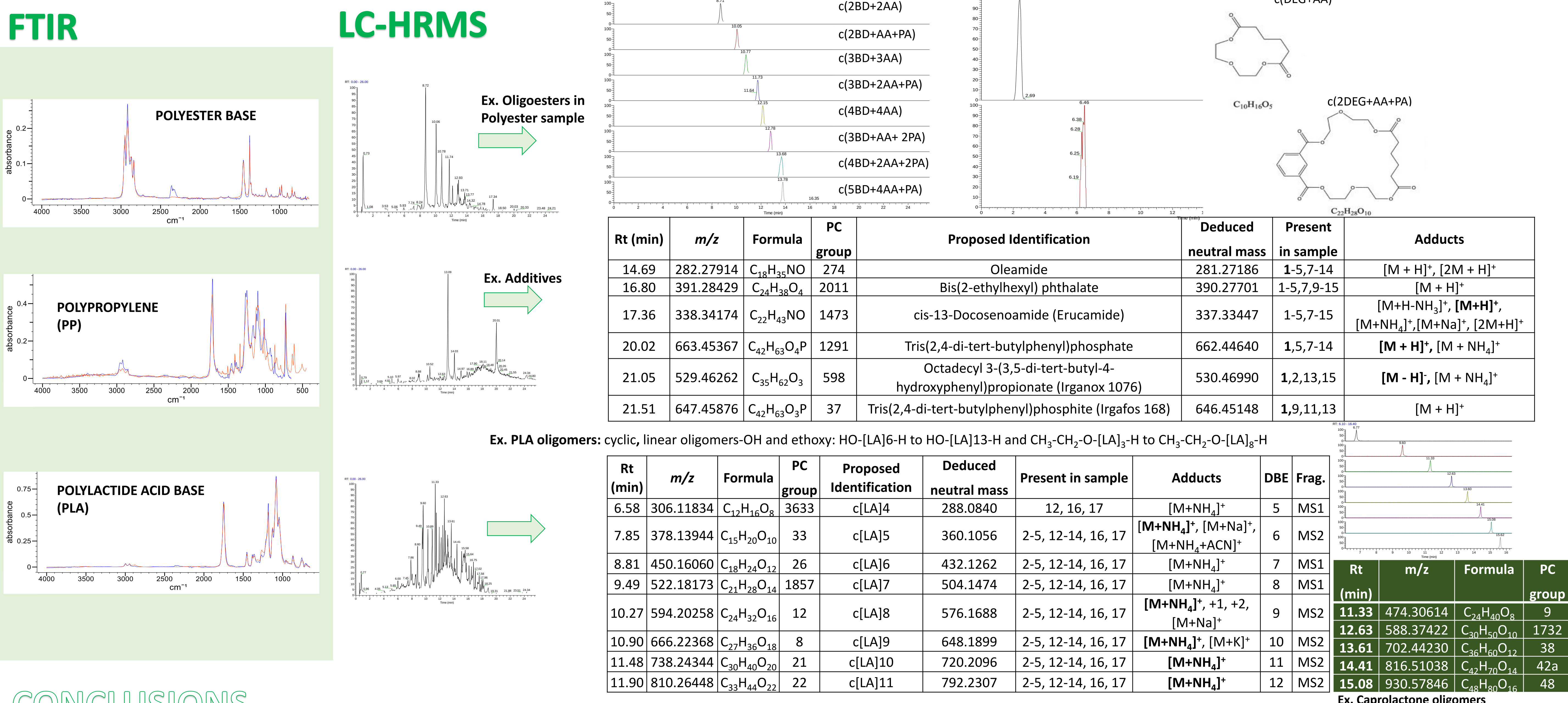


- **PREPROCESSING**
- **MS1: ONE DIMENSIONAL DATA**
- **ADDUCTS:** [M+H]⁺, [M+NH₄]⁺, [M+Na]⁺, [M+K]⁺, [M+NH₄+ACN]⁺
- **ISOTOPS:** 13C contribution
- **MS2: FRAGMENTATION ION (S)**
- **3 COLLISION ENERGIES:** 10, 30, 50 % NCE

IDENTIFICATION

- **In-house libraries**
- **In silico-fragmentation libraries**
- **Bibliography**
- **Tools:** Xcalibur, Envipat, etc.

RESULTS



CONCLUSIONS

High Resolution Mass Spectrometry resulted to be a very powerful technique to provide information about the non-volatile compounds extracted from the bioplastics characterized by FTIR as polyester based materials, PP or PLA. Non target methods were used to identify compounds both IAS and NIAS, present in the food packaging materials. IAS such as the additives antioxidants (e.g., Irgafos 168, Irganox 1076), slip agents (e.g., erucamide) and plasticizers (e.g., DEHP), and NIAS such as oligoesters, formed as a consequence of multiple combinations of diols (ethylene glycol 1,3-butanediol, neopentyl glycol, etc.) and diacids (adipic, phthalic, and sebacic acids) or different caprolactone oligomers were detected in the samples. As in a previous study, most of them presented a cyclic structure [2]. Particular attention should be paid to NIAS, since most of them are unknown compounds and their toxicity has not been evaluated.

REFERENCES

- [1] Omer et al. (2018) Anal. Bioanal. Chem. <https://doi.org/10.1007/s00216-018-0968-z>.
- [2] Lestido-Cardama, et al. (2022) Polymers, 14, 487. <https://doi.org/10.3390/polym14030487>

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