Departamento de Química Analítica
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Universidad de Zaragoza

UNIVERSIDADE CATÓLICA PORTUGUESA

AARHUS UNIVERSITY

TRAINING SCHOOL PLANNED BY THE COST ACTION CIRCUL-A-BILITY (CA13124)

Advanced mass spectrometry for food packaging safety

1. Date and length:

- **3 days**:
  - Start date: Tuesday 7th May – morning (09:00).
  - End date: Thursday 9th May (17:00).

Workflow:
That included in the publication of Food Additives and Contaminants (see Figures 1 and 2 below) and we also agreed:

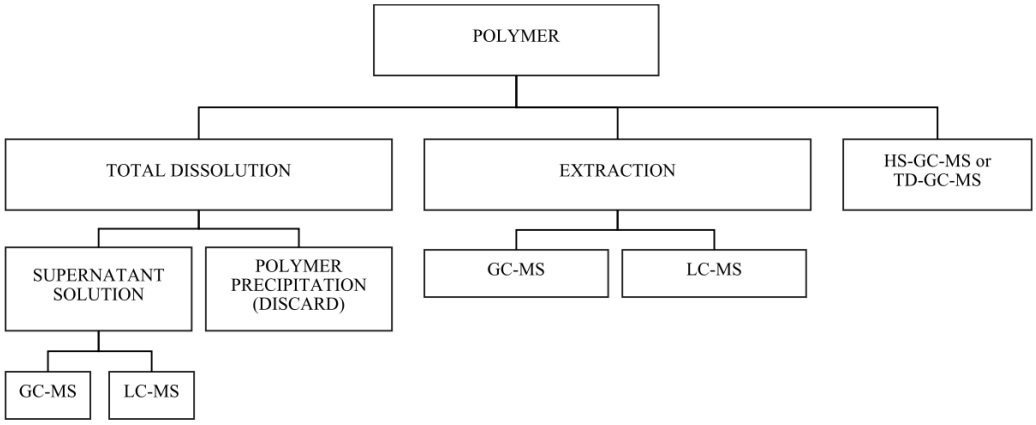

Figure 1. Screening procedure for sample preparation and analytical techniques for identification of NIAS in polymers.

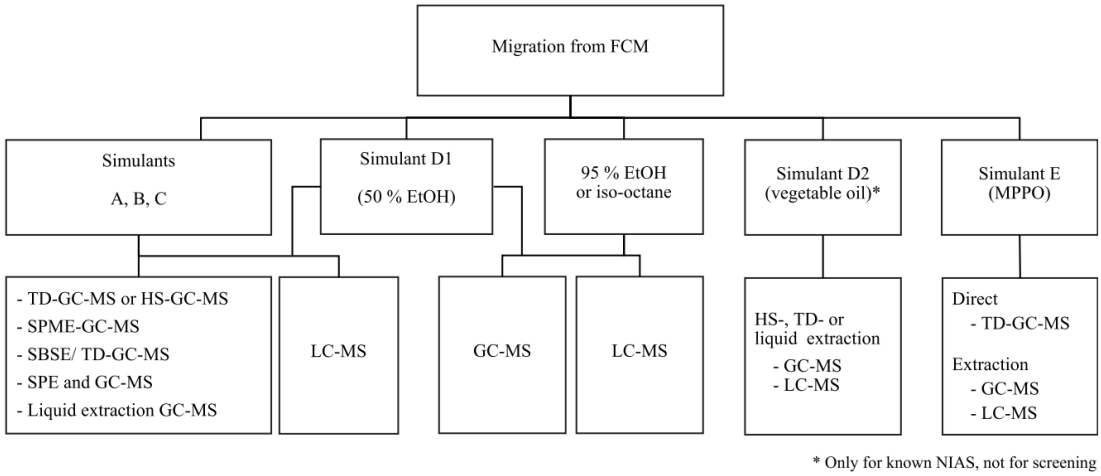

Figure 2. Screening procedure for identification of NIAS in simulants.

Samples:

- Solution of a few standards gravimetrically prepared and hand out to all participants.
- Sample preparation (depending on the selected samples; flakes or pellets).
  - Cryogenic milling (demonstration → application).
  - Dissolution/extraction (depending on the analytical technique).
- Several real samples given to each group, one sample /each group. The following have been suggested (one sample pre group applying the comprehensive workflow):

A. Evaluation of material

- **Group 1:** Flakes of rPET (contain oligomers and volatile and non-volatile contaminants
- **Group 2:** Pellets of rPP (contain bisphenols, volatile and non-volatile contaminants)

B. Evaluation of migration

- **Group 3:** Capsules made of rHDPE with cap for migration studies. Contain volatile and non-volatile contaminants. Migration tests could be done with D1 simulant or with real milk.
- **Group 4:** Printed board for migration study using Tenax® (one side test) containing volatile and non-volatile substances.
- **Group 5:** PA ladels/spatulas (kitchenware utensils; PA oligomers can be identified and quantified).

- In all cases the students will do the sample preparation, the screening of volatile and non-volatile substances and also the target analysis/quantification of a few compounds. Then, the objective is that all of them work with all instruments/techniques.

- The sample preparation in case of flakes and pellets start with the cryo-milling. To facilitate and accelerate the work, one flakes sample will be cryo-milled to show them the system and importance of the sample size, homogeneity and representativeness, but later, the powdered samples will be given to them for the experimental work.

- All the mentioned samples have been already analyzed in depth and we know what they have and what they release to 10% ethanol, 3% acetic acid, Simulant D1, 95% ethanol and Tenax® (accelerated migration at **70ºC for 2h**).

Available equipment

- 2 GC-MS equipped with HS and SPME
- 2 UPLC-MS-TQ
- 1 UPLC-QTOF MS
- 1 UPLC-IMS-QTOF (just to confirm the identification with the library containing more than 10,000 substances from packaging)
- 1 cryo-mill
- Devices required for sample treatment and the work on FCM.