DISCRIMINATION OF PBPS IN WEATHERED SAMPLES.

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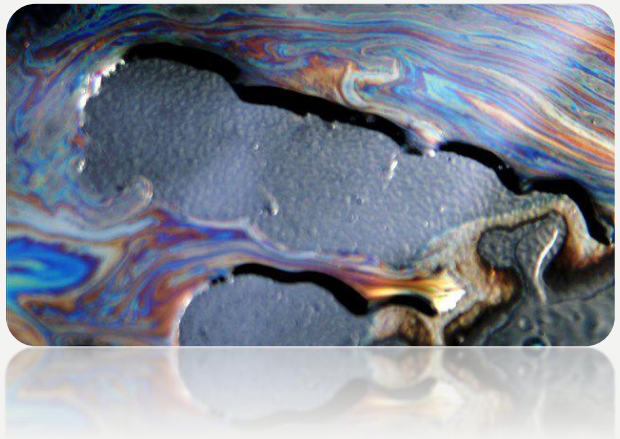
DOCTORADO EN AGROALIMENTACIÓN

INDEX

Big development in the petroleum industry

Increase of the number of petroleum based products



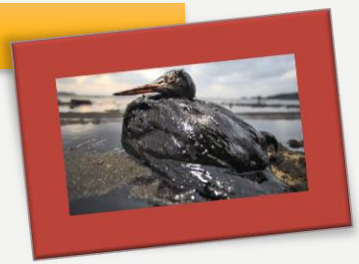
ACCIDENTS OCCUR!

Dramatic consequences

High risk of uncontrollable fires

Water contamination

Damage of animal life



WEATHERING PROCESS

MAIN PROBLEMS OF ANALYSTS

- Destructive nature of the fire
- High temperature reached
- Firefighting efforts
- Time of the evidence remaining at the scene
  - Evaporation
  - Pyrolysis
  - Microbial degradation
  - **Weathering**

Faster evaporation of the most volatile compounds (VOCs) of a mixture: affects the relative distribution of chemical residues. This distribution has been used to estimate the age of ignitable liquids and predict the effect of them in the nature.

OBJETIVES

- Petroleum based products (PBPs) detection in weathered samples
- Petroleum based products (PBPs) discrimination in weathered samples
  - Important m/z in the discrimination → Elaboration of fingerprints
- Influence of the support used

METHOD AND MATERIALS

PBPs

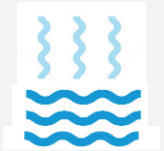
Commercial materials

Weathering simulated samples

0.5 x 0.5 cm material

Add to HS-MS vial

Add 40uL** of PBPs



Open vials laboratory hood

Control temperature: 25ºC

Flow zero: Natural conditions

Different times: 0 h, 6 h, 12 h, 24 h, 72 h... 7, 15, 21 and 30 days

HS-MS system

Non separative method

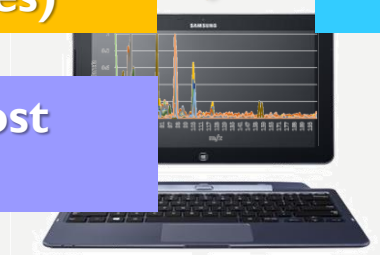
Green technique

Fast analysis (minutes)

Low cost

MASS

Pattern Recognition Software



Easy to use

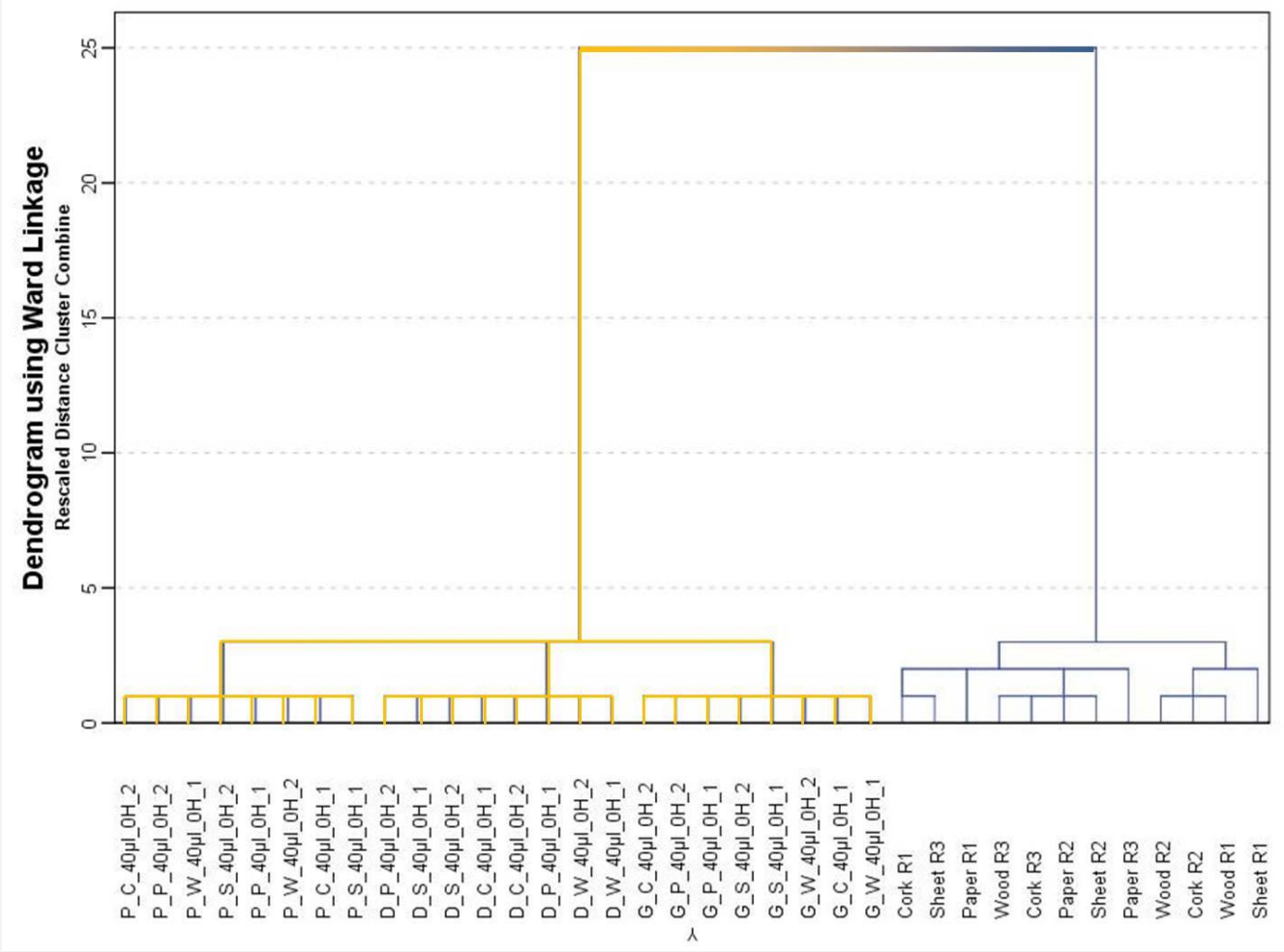
Mass spectra MS

RESULTS AND DISCUSSION

Identification in samples without weathering.

Hierarchical Cluster Analysis (HCA)

39 samples



RESULTS AND DISCUSSION

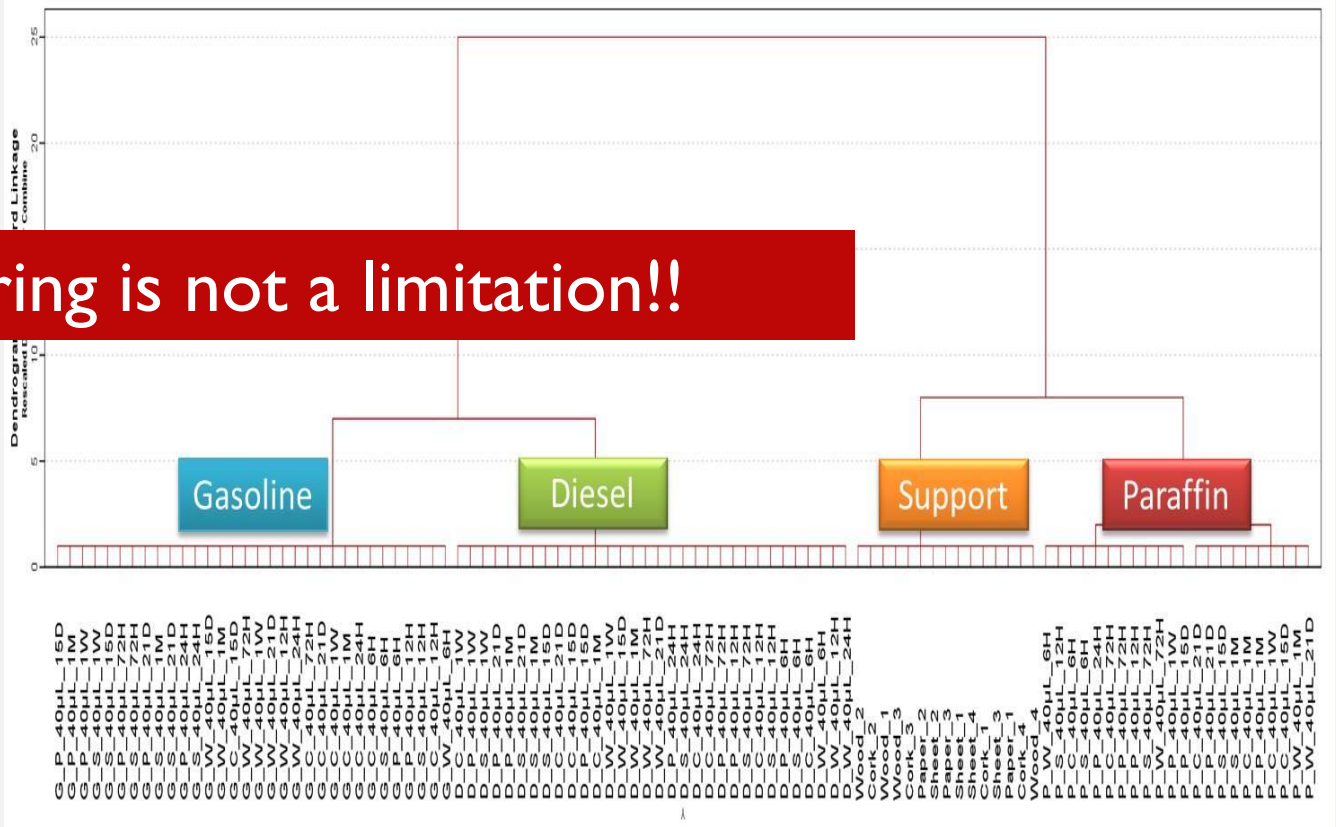
Identification of weathered PBPs..

Hierarchical Cluster Analysis (HCA)

Samples wi[illegible]weathering

Average samples (n=111)

Weathering is not a limitation!!



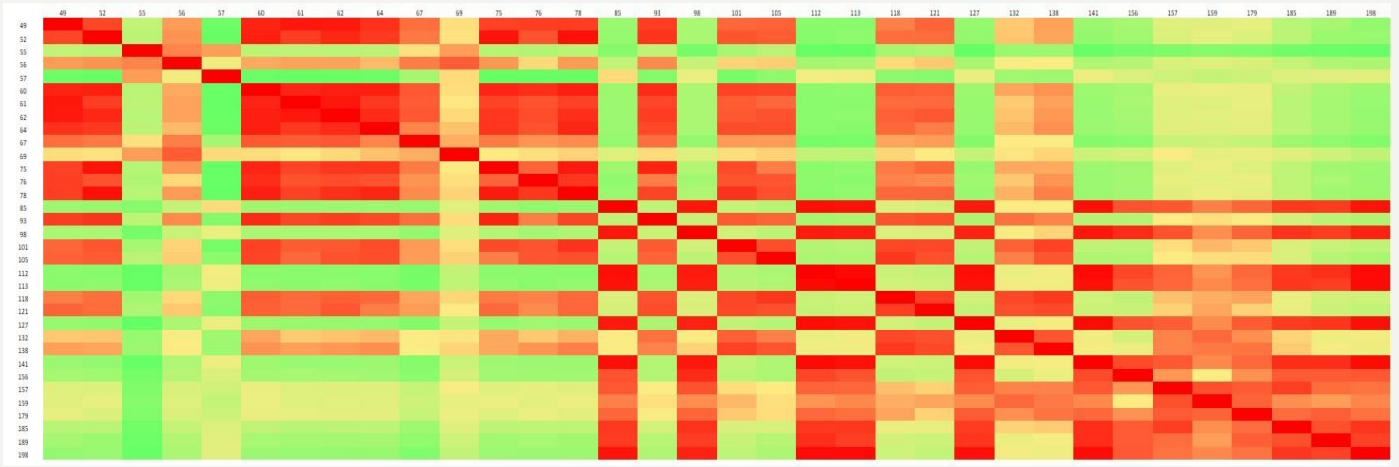
RESULTS AND DISCUSSION

Identification of weathered PBPs..

Linear Discriminant Analysis (LDA)

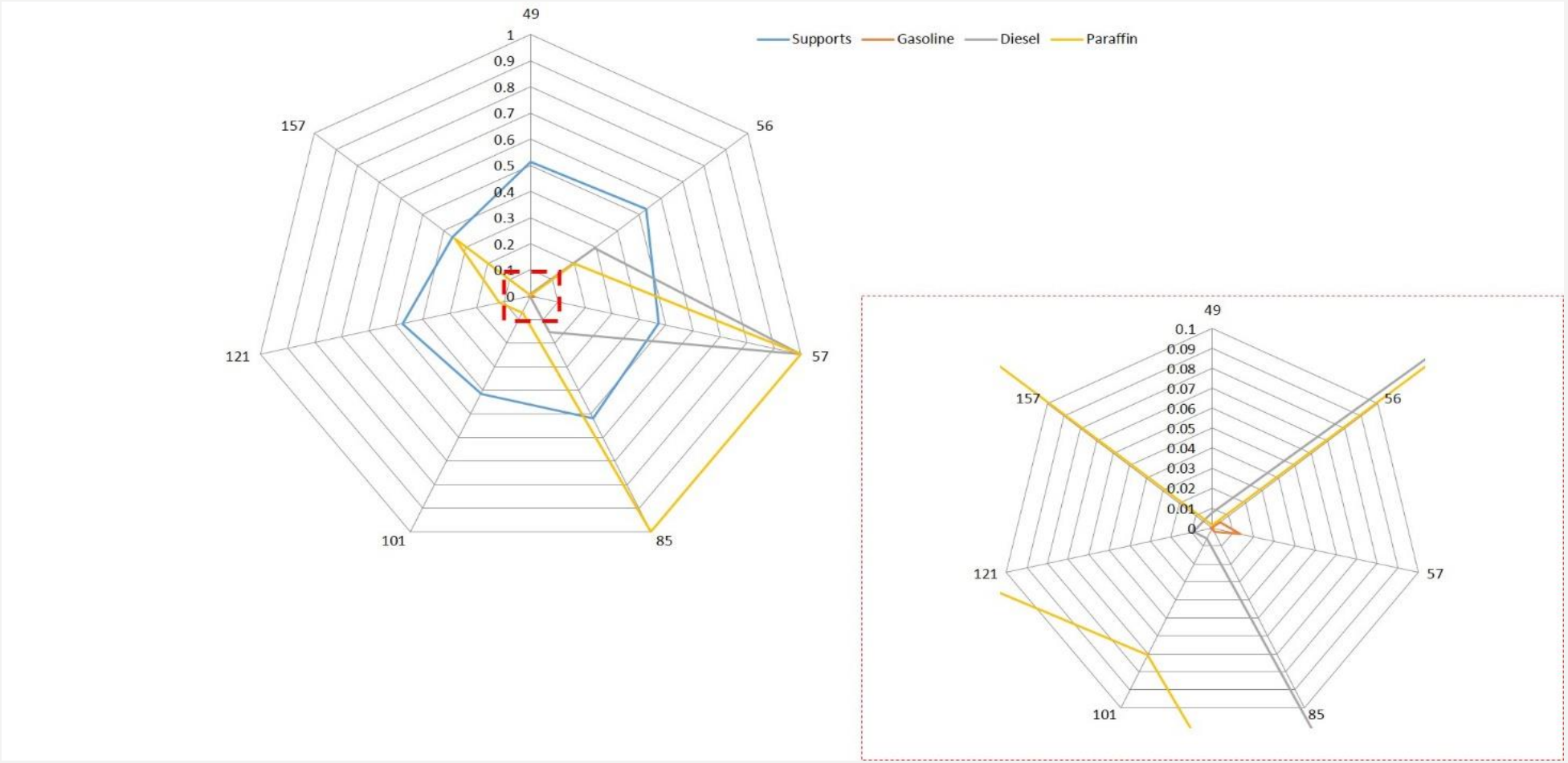
Important m(z in discrimination
34 m/z

Pearson correlation bivariate two-tails.
(Factor 0.75)



m/z 49, 56, 57, 85, 101, 121, 157

RESULTS AND DISCUSSION



FINGERPRINTS

CONCLUSIONS

- HS-MS technique to detect and determine the presence of different petroleum-based product in an unknown sample (even with weathering process started).
- The weathering process is not a disadvantage in the determination and identification.
- Determination of influential m/z in the discrimination of gasoline, diesel and paraffin
- Any influence of the porosity of the support used has been detected.

RESULTS HAVE BEEN PUBLISHED

sensors

MDPI

Article

Study of the Weathering Process of Gasoline by eNose

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Abstract: In a fire investigation the rapid detection of the presence of ignitable liquids like gasoline is of great importance as it allows appropriate treatment of the remains, the identification of prevention methods and detects the possible presence of an arsonist. In some cases, analysts cannot access the fire scene in the first few hours due to the dangers involved in the situation and, as a consequence, phenomena such as weathering start. Ignitable liquid weathering is an evaporation process that results in an increase in the abundance of non-volatile compounds relative to volatile compounds,

Any question?

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