ANALYSIS OF SOLID AND LIQUID SAMPLES IN THE CONTEXT OF SWIM USING LDI FT-ICR MS

EU_FT-ICR_MS – 2nd Advanced User School

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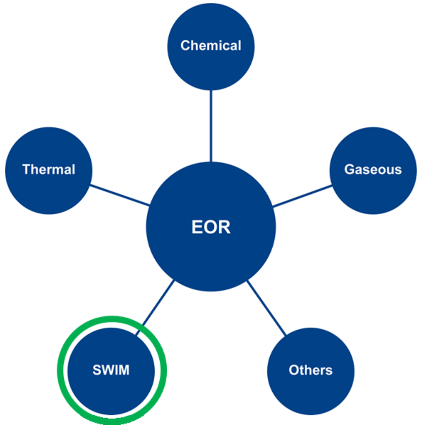
Introduction

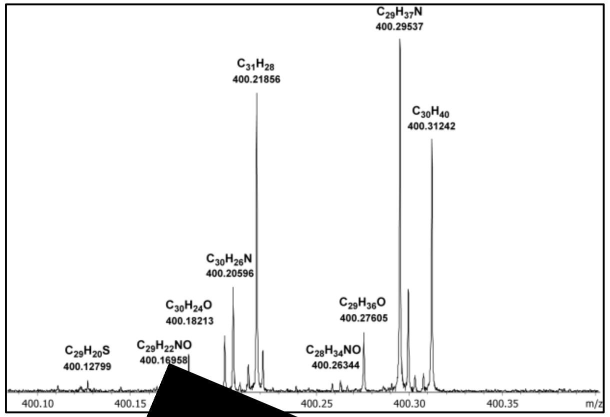
SMART water = low salinity water
(or water with a controlled composition)

SWIM effects: wettability changes and increase in oil recovery rate

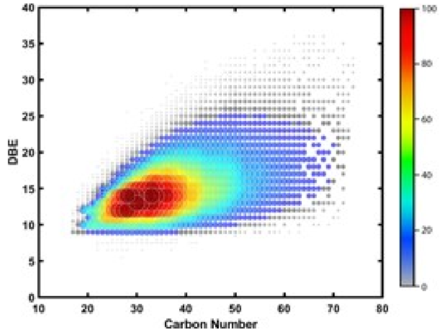
Determining mechanism: unknown, despite the several proposed mechanisms found in literature

Need of a better characterization of organic species adsorbed onto the rock surface and their influence on wettability changes during SMA[redacted] waterflooding

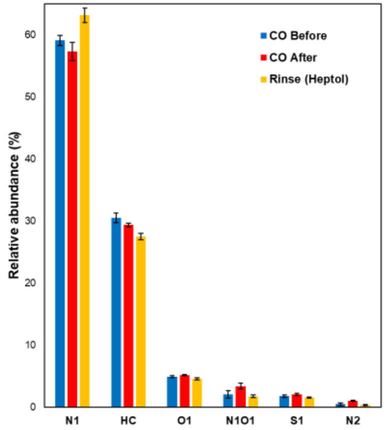




Intensity	m/z	Error (ppm)	Formula
2686100	400.12799	0.092	$C_{29}H_{20}S$
3966114	400.16958	0.022	$C_{29}H_{22}NO$
8365222	400.18213	0.083	$C_{30}H_{24}O$
23188654	400.20596	0.035	$C_{30}H_{26}N$
66491568	400.21856	0.019	$C_{31}H_{28}$



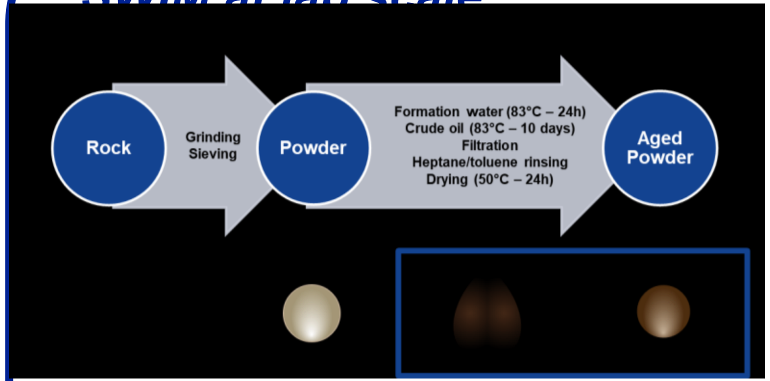
$$DBE = c - \frac{h}{2} + \frac{n}{2} + 1$$



TotalEnergies

Experimental Methods

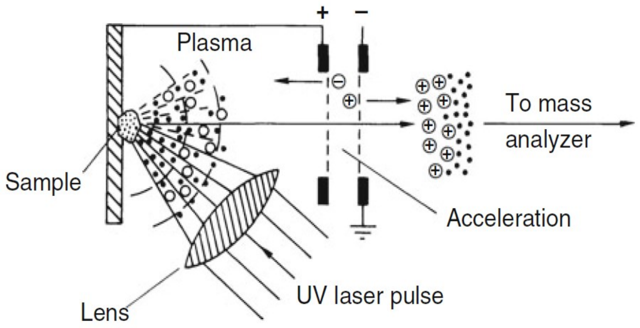
SWIM at lab scale



How to analyze (and to compare) crude oil and aged powder samples?

Laser Desorption Ionization (LDI)

Frequency-tripled Nd:YAG laser (355 nm)

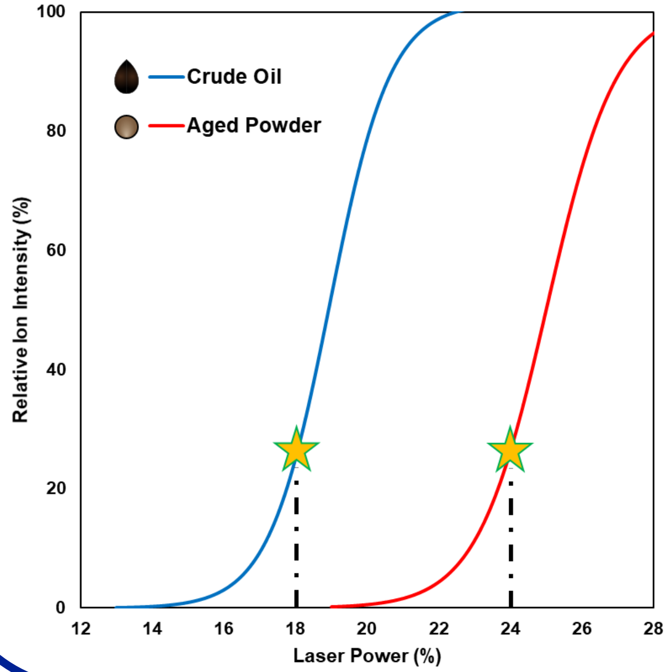


Mamyrin BA (1994) Laser Assisted Reflectron Time-of-Flight Mass Spectrometry. Int J Mass Spectrom Ion Proc 131:1–19. doi:10.1016/0168-1176(93)03891-O

Laser Power Optimization

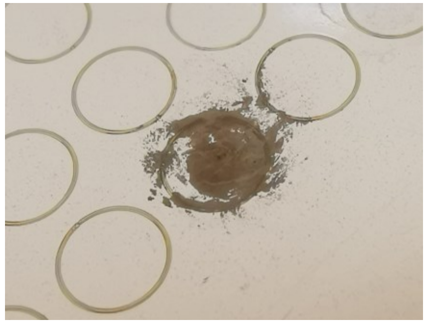
- Ion production threshold
- Artifact formation and fragmentation

Solid samples require higher laser power



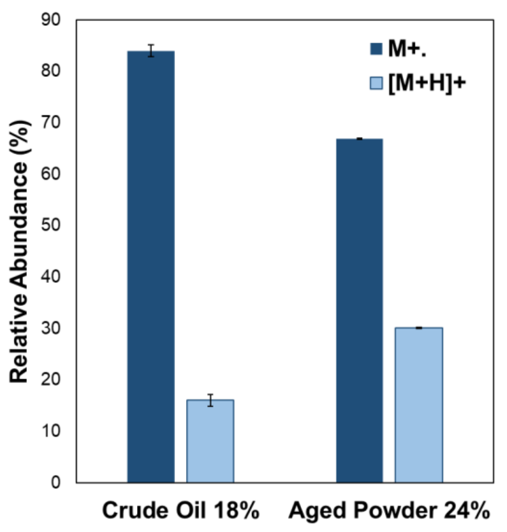
Sample deposit on the target

- Dry droplet method for crude oil samples
- Powder samples deposited with the help of a pestle

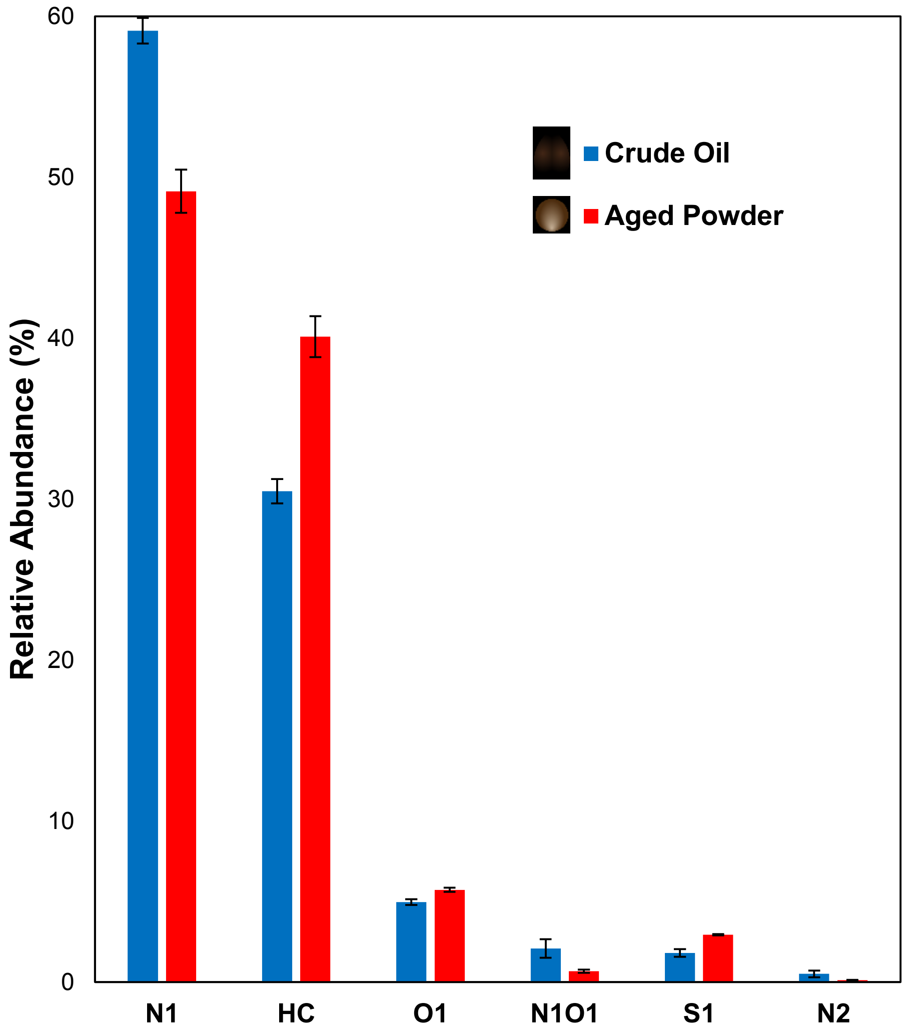


TotalEnergies

(+) LDI FT-ICR MS

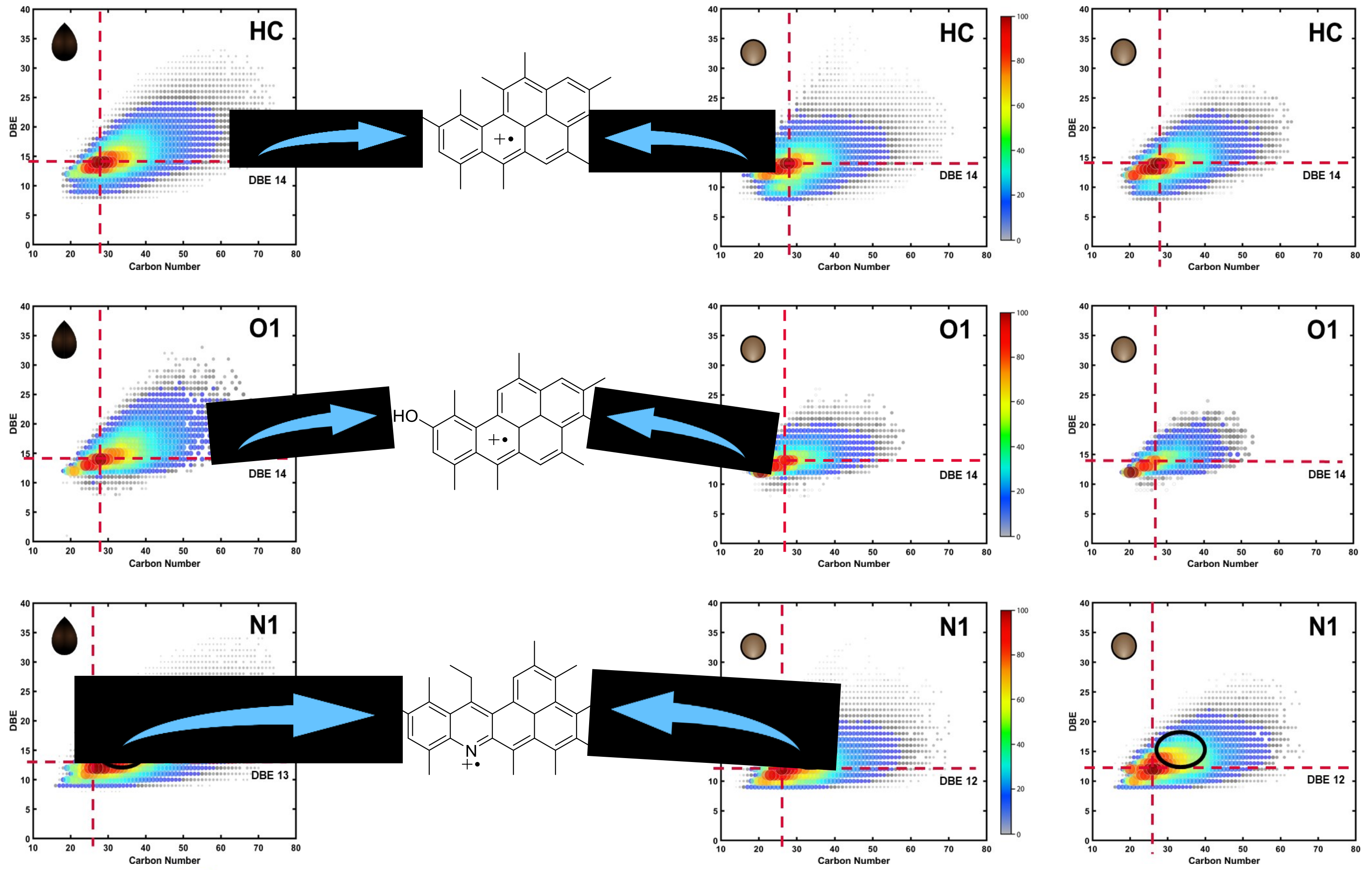


- Odd-electron ions are dominant in positive mode
- Higher laser power (24%) increase the formation of even-electron ions
- N1 and HC classes represent ~ 90% of the detected ions
- Decrease of N1 for aged powder

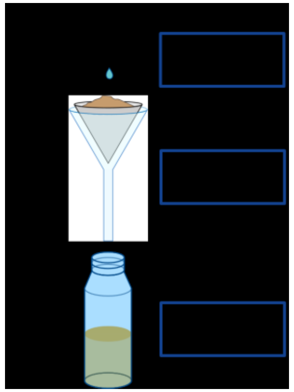


(+) LDI FT-ICR MS – DBE vs C#

CRUDE OIL | AGED POWDER | AGED POWDER EXTRACT



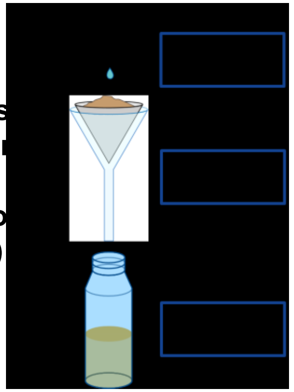
- No significant differences are observed between crude oil and aged powder for HC and O1 species. Same thing happens to even-electron ions
- Depletion of high DBE N1 species is observed in aged powder
- Direct and indirect (solvent extract) analysis of aged powder present similar results

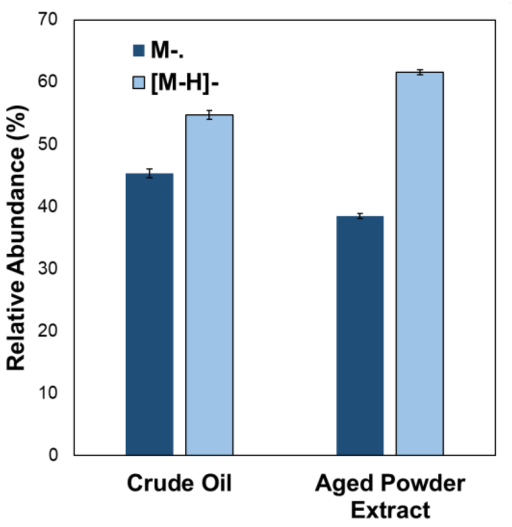


TotalEnergies

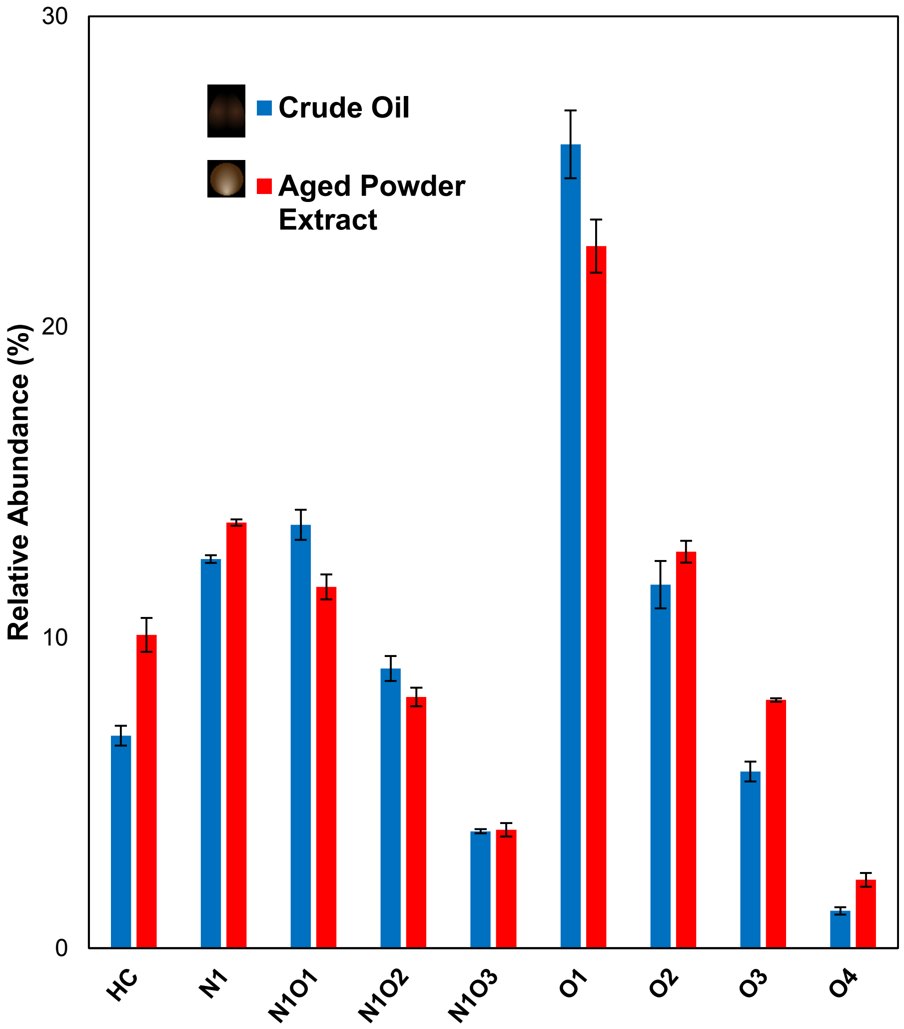
(-) LDI FT-ICR MS

No signal was
obtained duri
the direct
analysis of so
samples in (-)
LDI

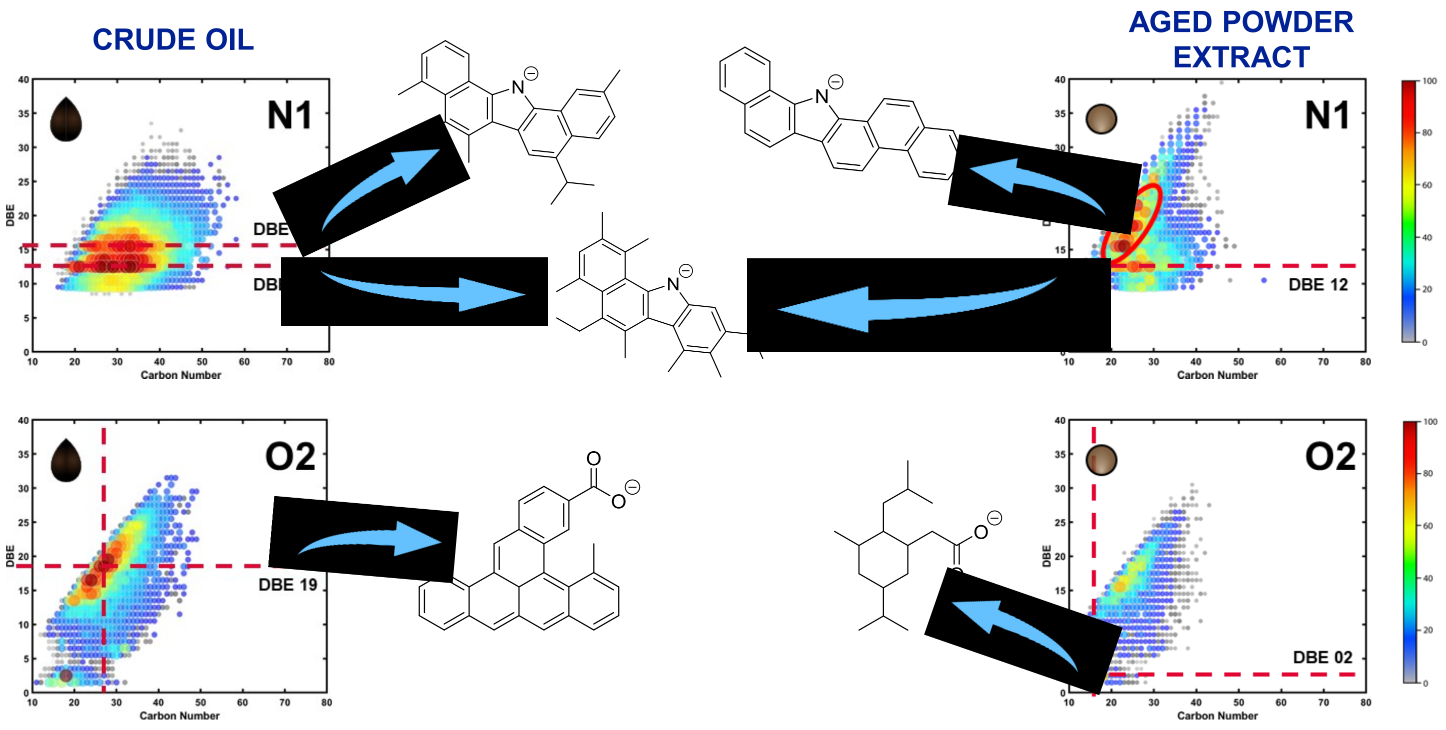


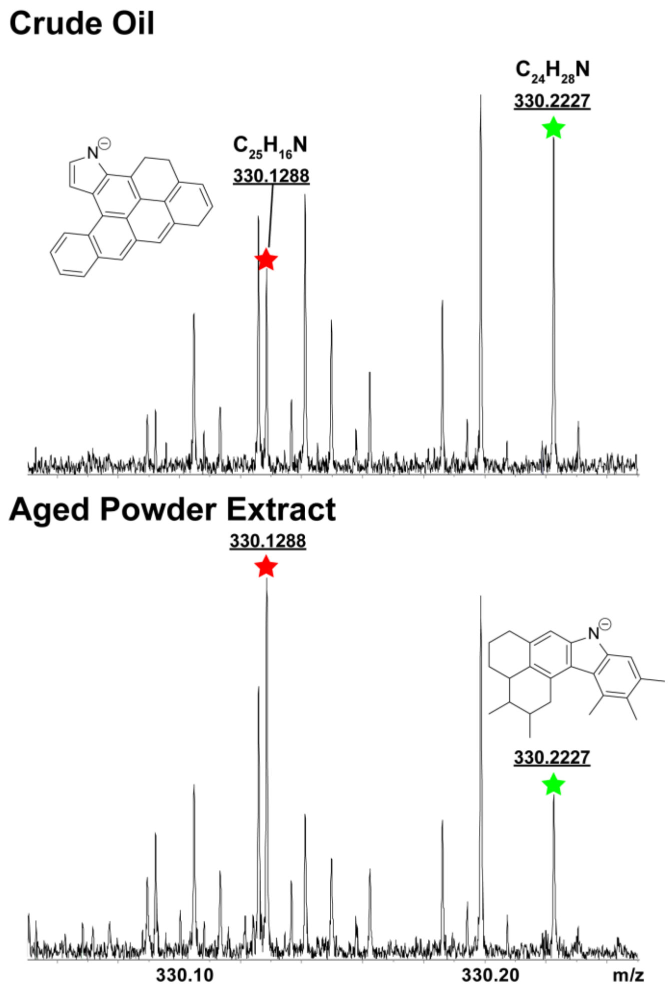


- Even-electron (deprotonated) ions are dominant in negative mode
- Bigger diversity of chemical classes than in positive mode
- Aged powder extract enriched with HC, N1, O3 and O4 compounds



(-) LDI FT-ICR MS – DBE vs C#





- Decrease of bigger N1 ions (bigger C#)
- Decrease of highly aromatic carboxylic acids

Conclusions

- Solid samples demand higher laser power for ionization to happen in positive mode, because the organic species are adsorbed and maybe chemically bound to the powder surface

- Direct and indirect (solvent extract) analysis of aged powder present very similar results in positive mode

- (-) LDI detects a bigger number of chemical classes than (+) LDI

- Aged powder extract is enriched with acidic N1 species with high DBE and small C#. Bigger molecules might remain adsorbed/bound to the powder surface

Thank you

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 731077.