

**ANALYSIS OF PRODUCTS OBTAINED FROM SLOW PYROLYSIS OF
POLYETHYLENE TEREPHTHALATE BY FOURIER TRANSFORM ION
CYCLOTRON RESONANCE MASS SPECTROMETRY COUPLED TO
ELECTROSPRAY IONIZATION (ESI) AND LASER DESORPTION IONIZATION
(LDI)**

Asma DHAHAK[†], Vincent CARRE[‡], Frédéric AUBRIET[‡], Guillaïn MAUVIEL[†], Valérie
BURKLE-VITZTHUM^{†*}

[†] Laboratoire Réactions et Génie des Procédés (LRGP-CNRS UMR 7274), 1 rue Grandville, BP 20451, 54001
Nancy, Cedex, France

[‡] LCP-A2MC, FR 2843 Institut Jean Barriol de Chimie et Physique Moléculaires et Biomoléculaires, FR 3624
Réseau National de Spectrométrie de Masse FT-ICR à très haut champ, Université de Lorraine, ICPM, 1 boulevard
Arago, 57078 Metz Cedex 03, France

* Corresponding author: valerie.vitzthum@univ-lorraine.fr

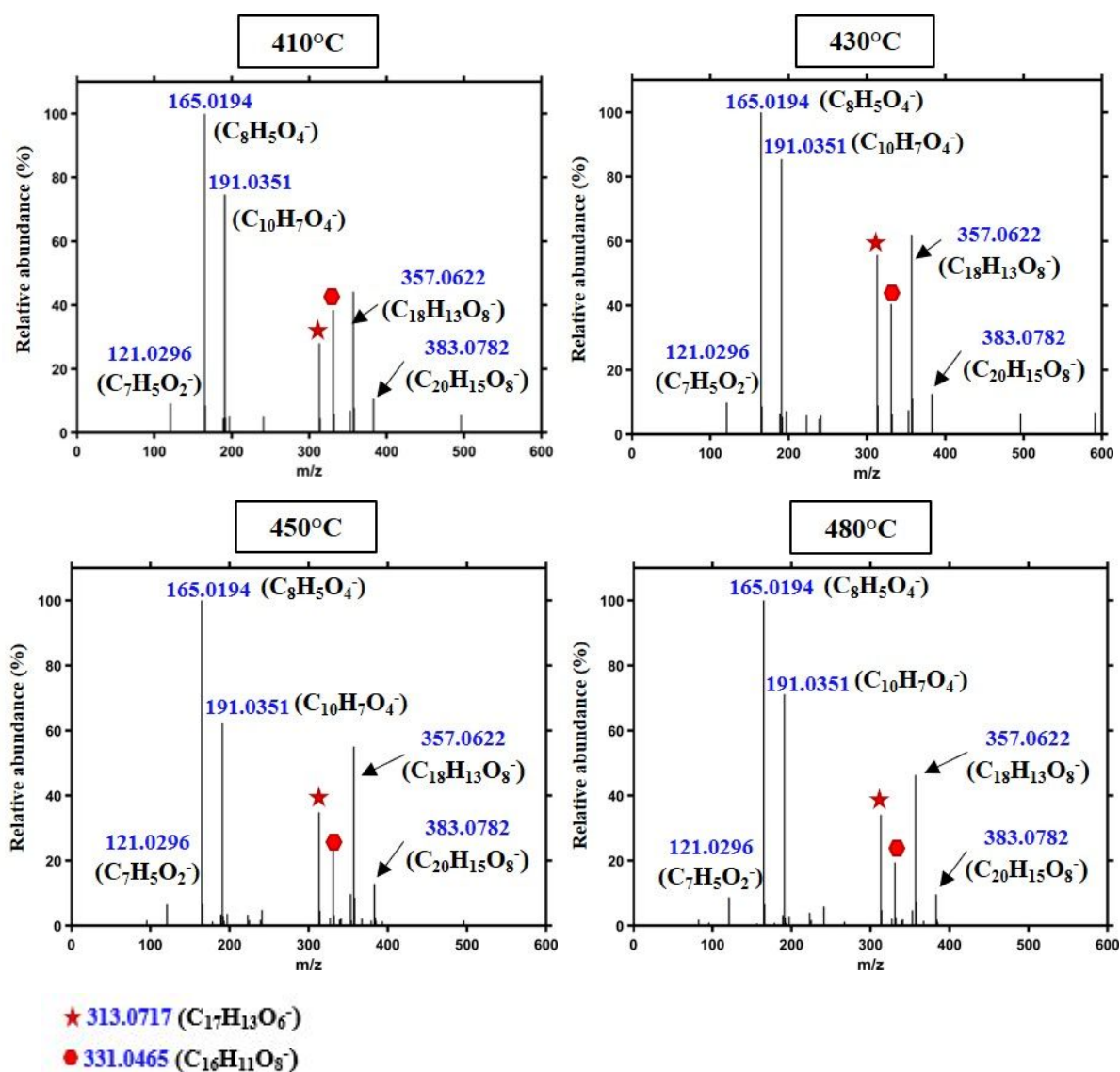


Figure S-1: Mass spectrum of the waxy products ($m/z < 400$) obtained by (–) ESI FT-ICR MS in respect with the final pyrolysis temperature. The detected ions are relative to the deprotonated $[M-H]^-$ of $C_xH_yO_z$ PET pyrolysis products.

Note: After the ionization, the ions passed through a hexapole Q1 (to focus the ions) and the quadrupole Q2 (to select a given mass range). The ions are then transferred to the ICR cell by an ion guide (hexapole). For higher values of RF (radiofrequency), we favor mass ranges over higher m/z values. So:

Q1 / Q2 = 60.5 V means that they are both at the same amplitude of RF and this is favoring the high masses.

Q1/Q2= 26.6 V for lower masses.

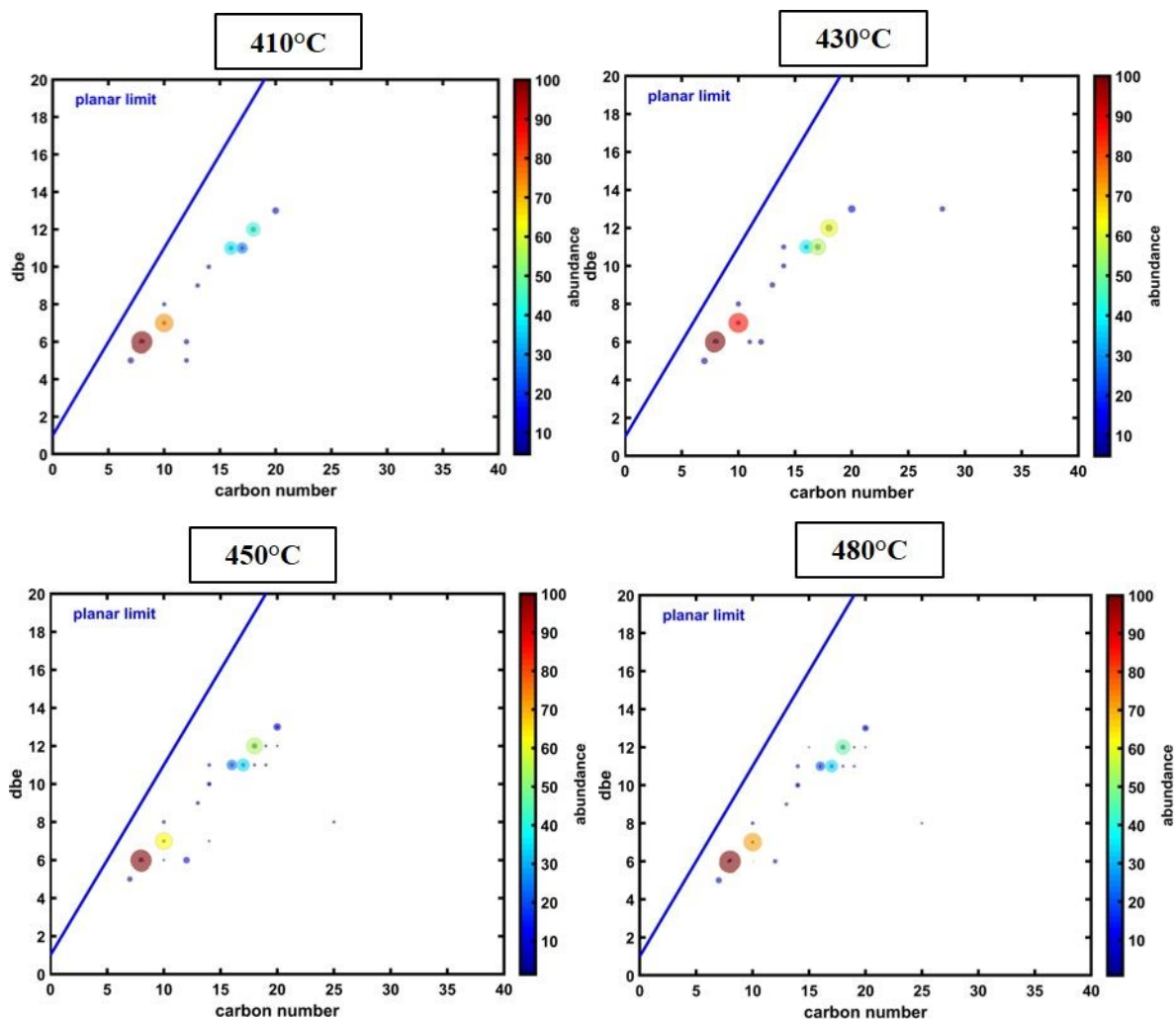


Figure S-2: DBE vs carbon number plots obtained by (–) ESI FT–ICR MS for the different final pyrolysis temperature, for $m/z < 400$. The size of the dots and the color (from dark blue to dark red) are proportional to the relative abundance of the considered compound.

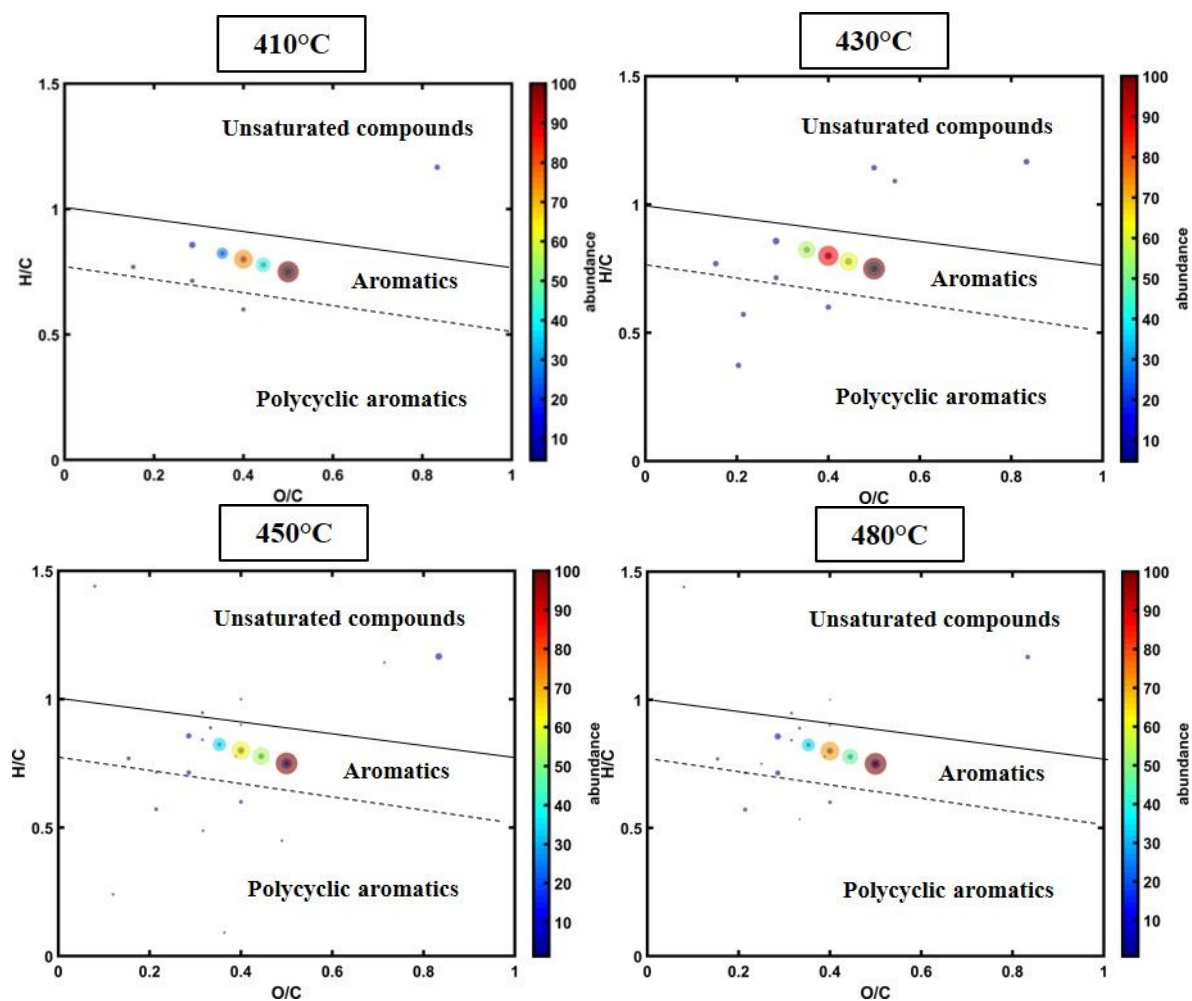


Figure S-3: H/C vs O/C Van-Krevelen plots obtained by (–) ESI FT–ICR MS of waxy products ($m/z < 400$) formed at different PET pyrolysis final temperature. The size of the dots and the color (from dark blue to dark red) are proportional to the relative abundance of the considered compound.

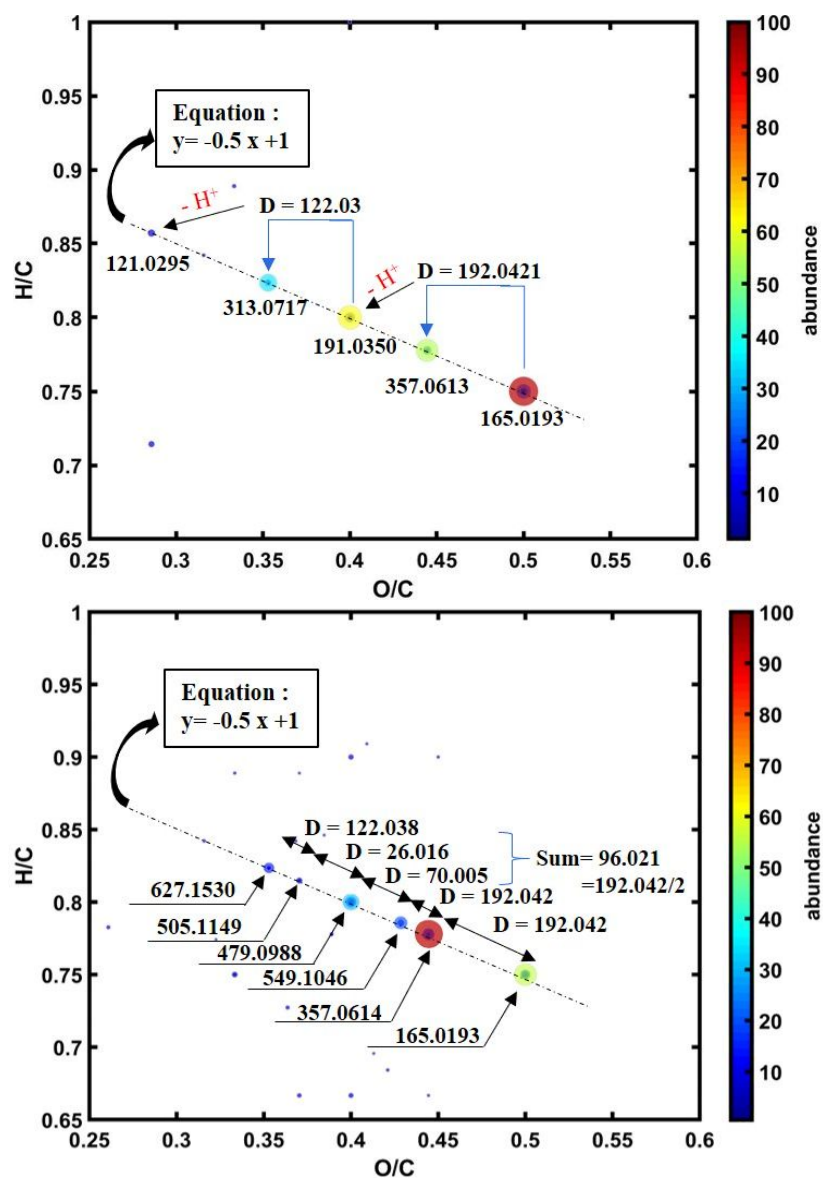


Figure S-4: H/C vs O/C Van-Krevelen plots at 450 °C, for m/z < 400 (up) and m/z < 900 (down).