Supplementary Information: Exploring the link between molecular cloud ices and chondritic organic matter in laboratory

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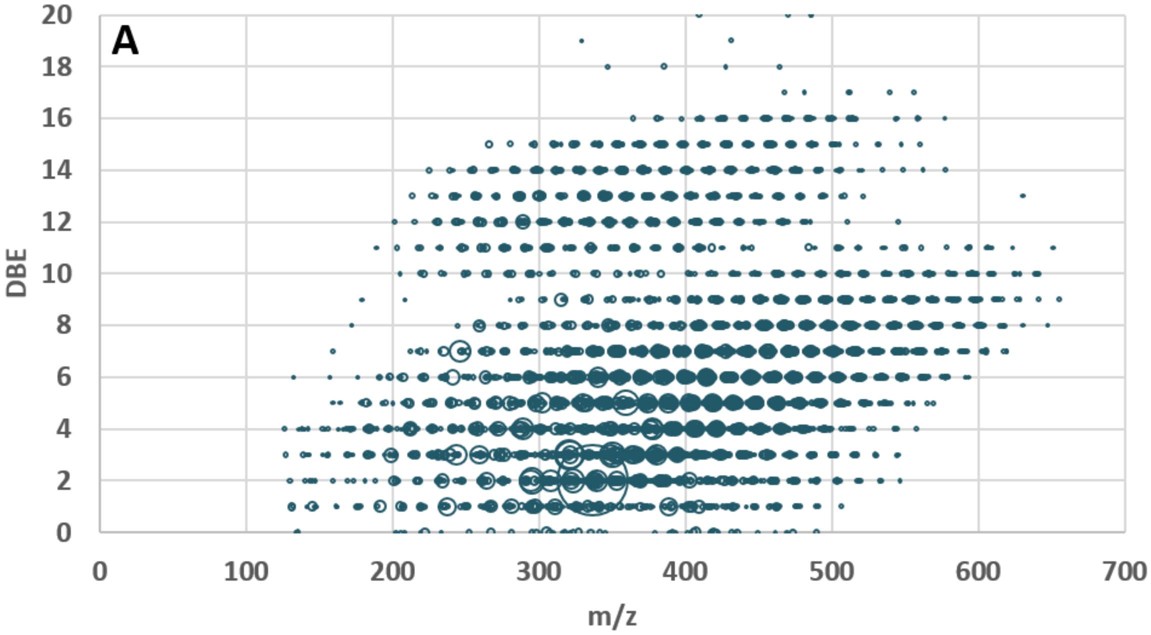
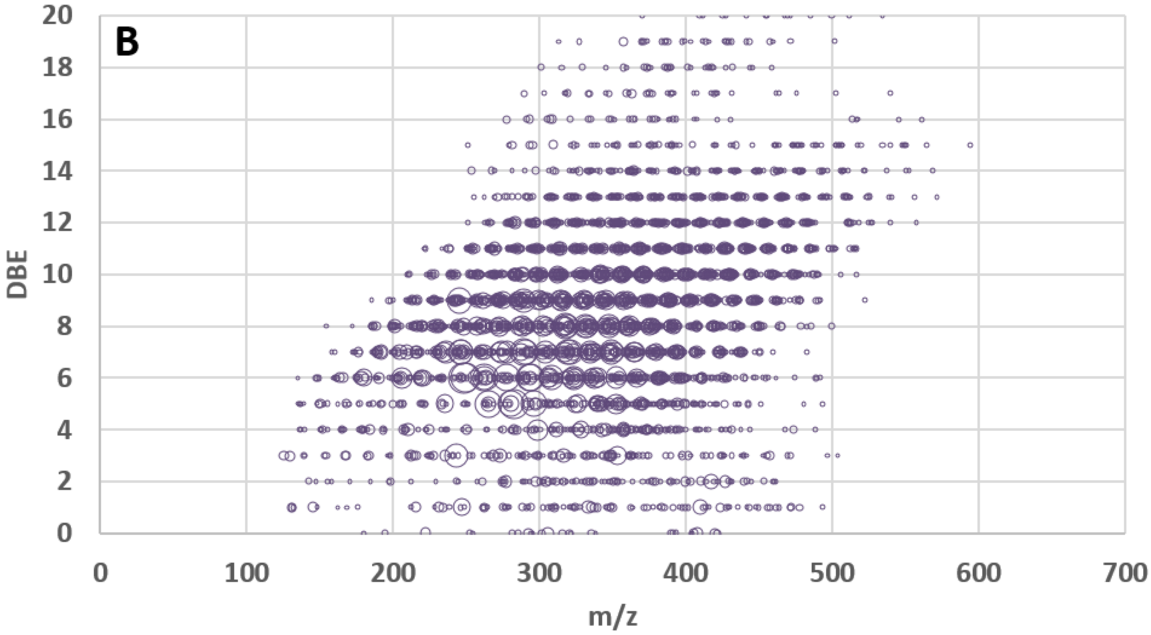
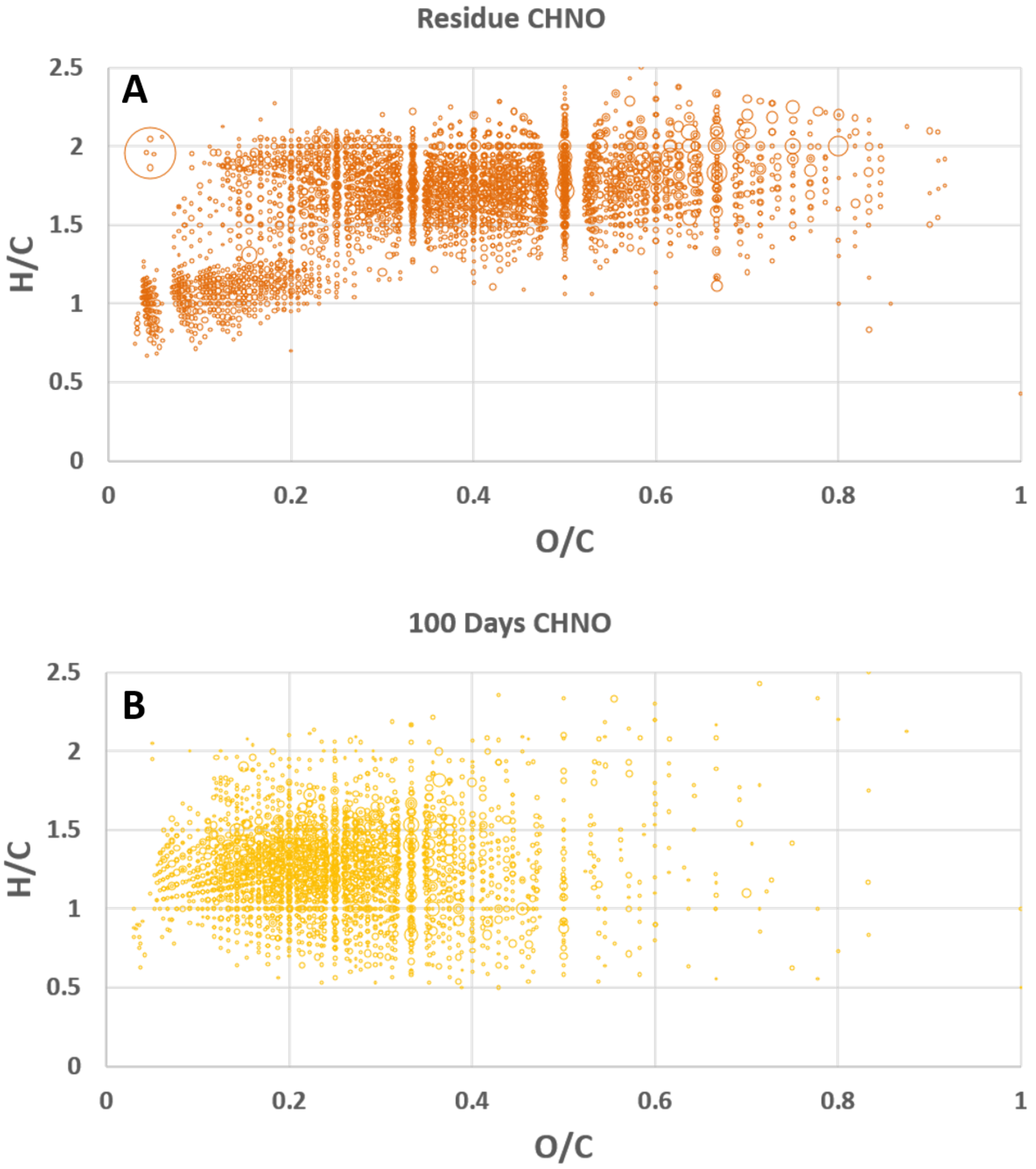
Evolution of DBE as a function of m/z for pre-accretional organic residue and post-aqueous organic products





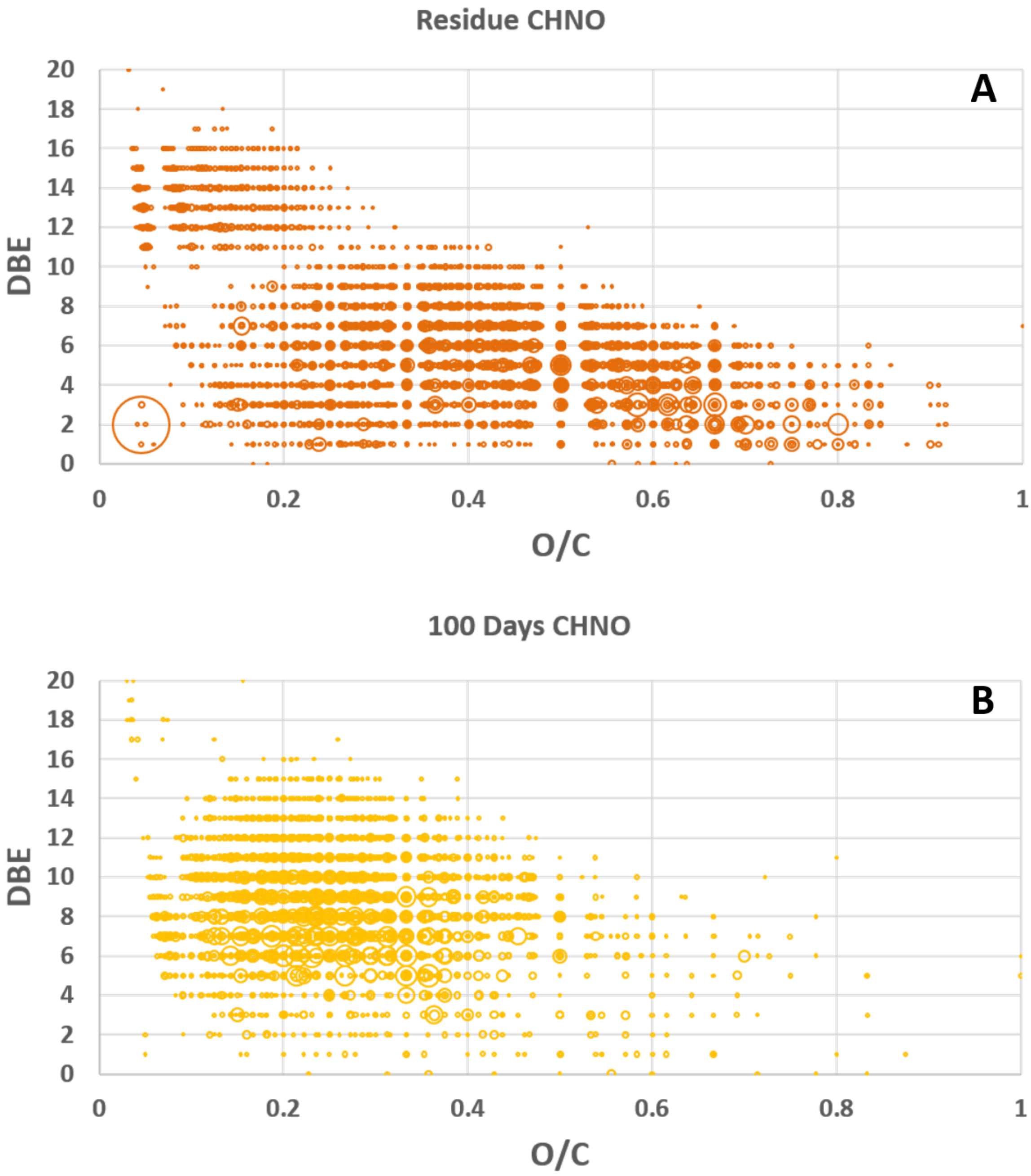
Supplementary Figure 1 – Evolution of Double Bound Equivalent (DBE) as a function of the experimental mass (m/z) for the pre-accretional organic residue (3964 molecular attributions) (A), and of post-aqueous organic product after 100 days (3424 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

Complementary data regarding the Van Krevelen diagrams for H/C vs O/C of the CHNO family for pre-accretional and post-aqueous organic residues after 100 days of reaction



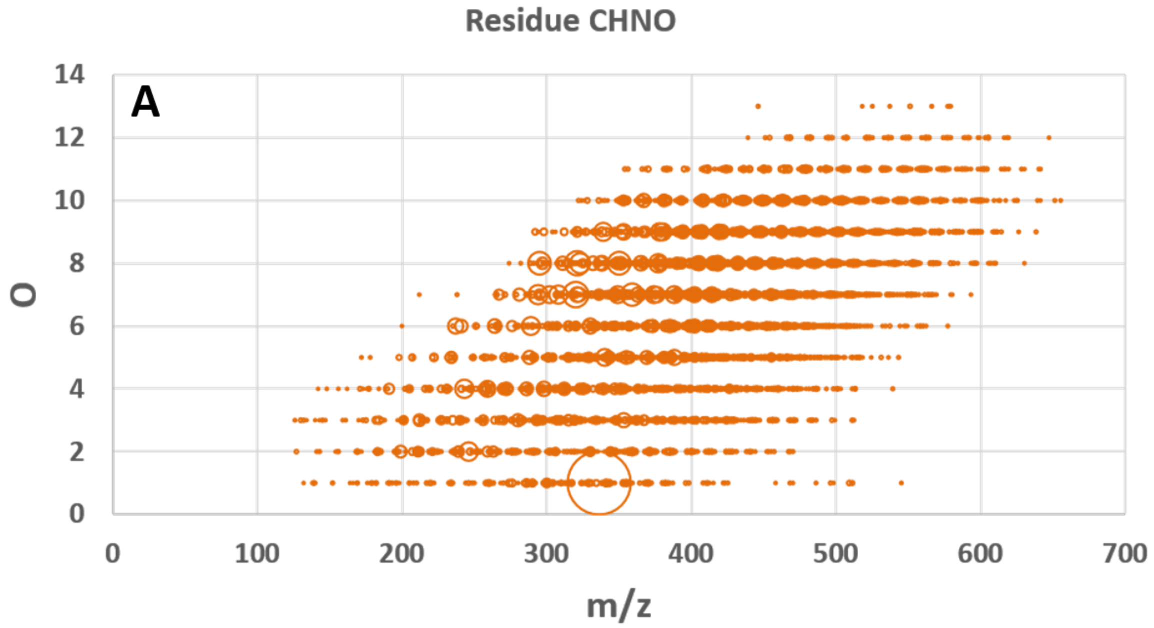
Supplementary Figure 2– Van Krevelen diagrams are displayed for H/C vs O/C relative to the CHNO family for pre-accretional (3512 molecular attributions) (A) and post-aqueous organic products after 100 days (2591 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

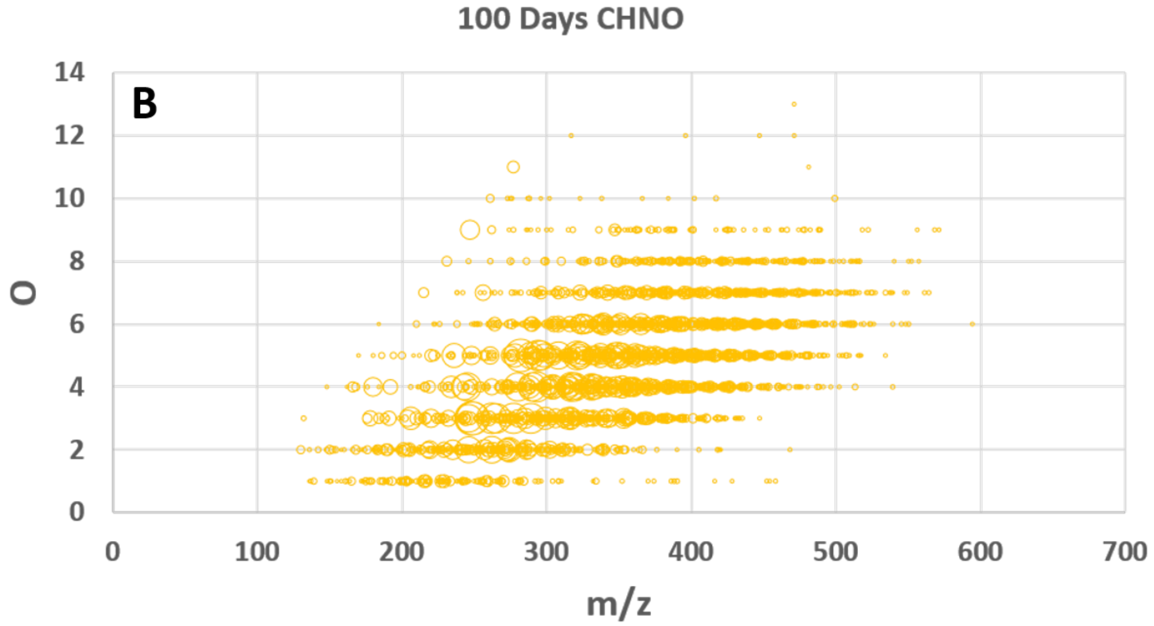
Complementary data regarding the DBE vs O/C of the CHNO family for pre-accretional and post-aqueous organic residues after 100 days of reaction



Supplementary Figure 3– – DBE vs O/C relative to the CHNO family for pre-accretional (3512 molecular attributions) (A) and post-aqueous organic products after 100 days (2591 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

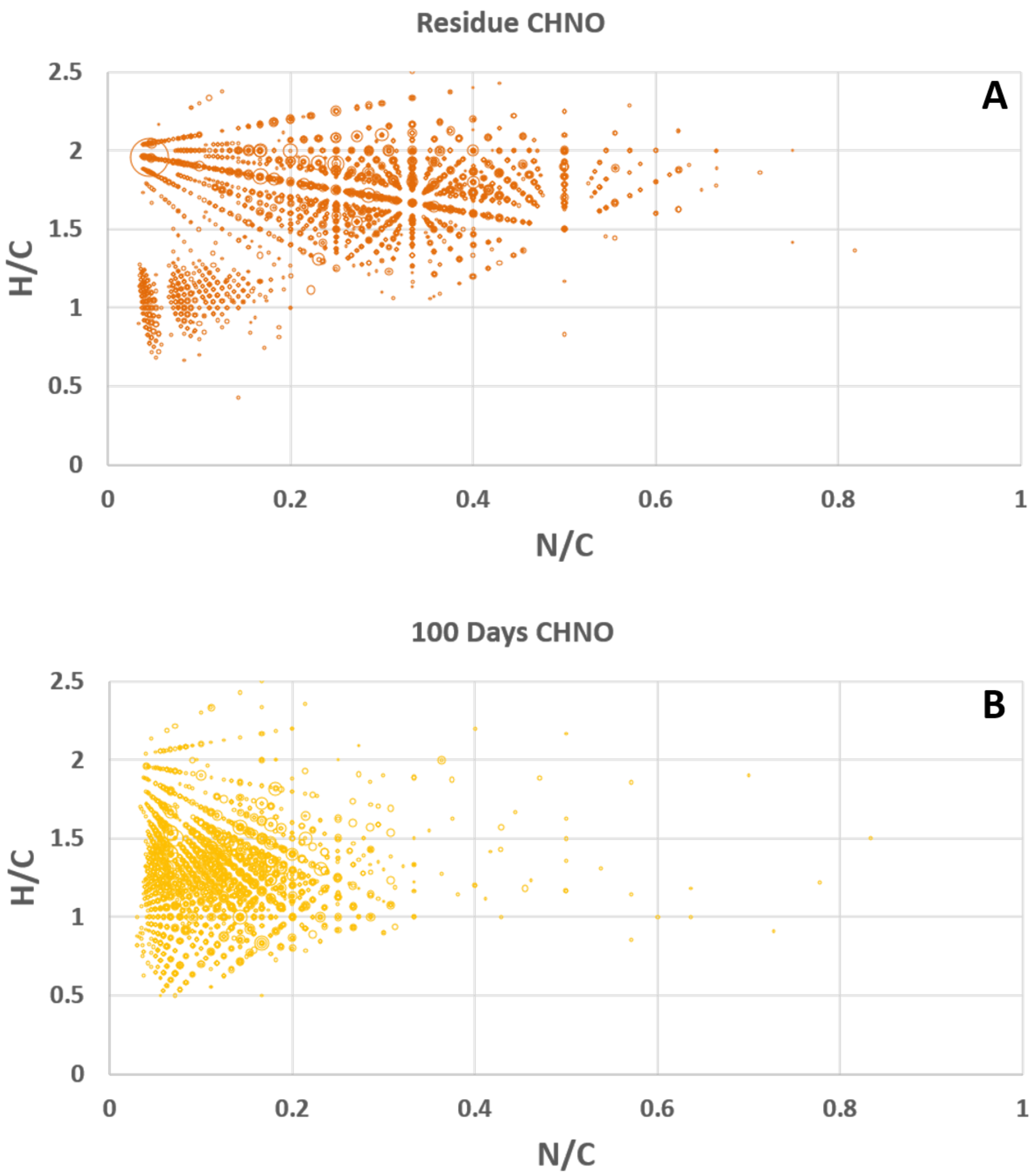
Complementary data regarding the O vs m/z of the CHNO family for pre-accretional and post-aqueous organic residues after 100 days of reaction





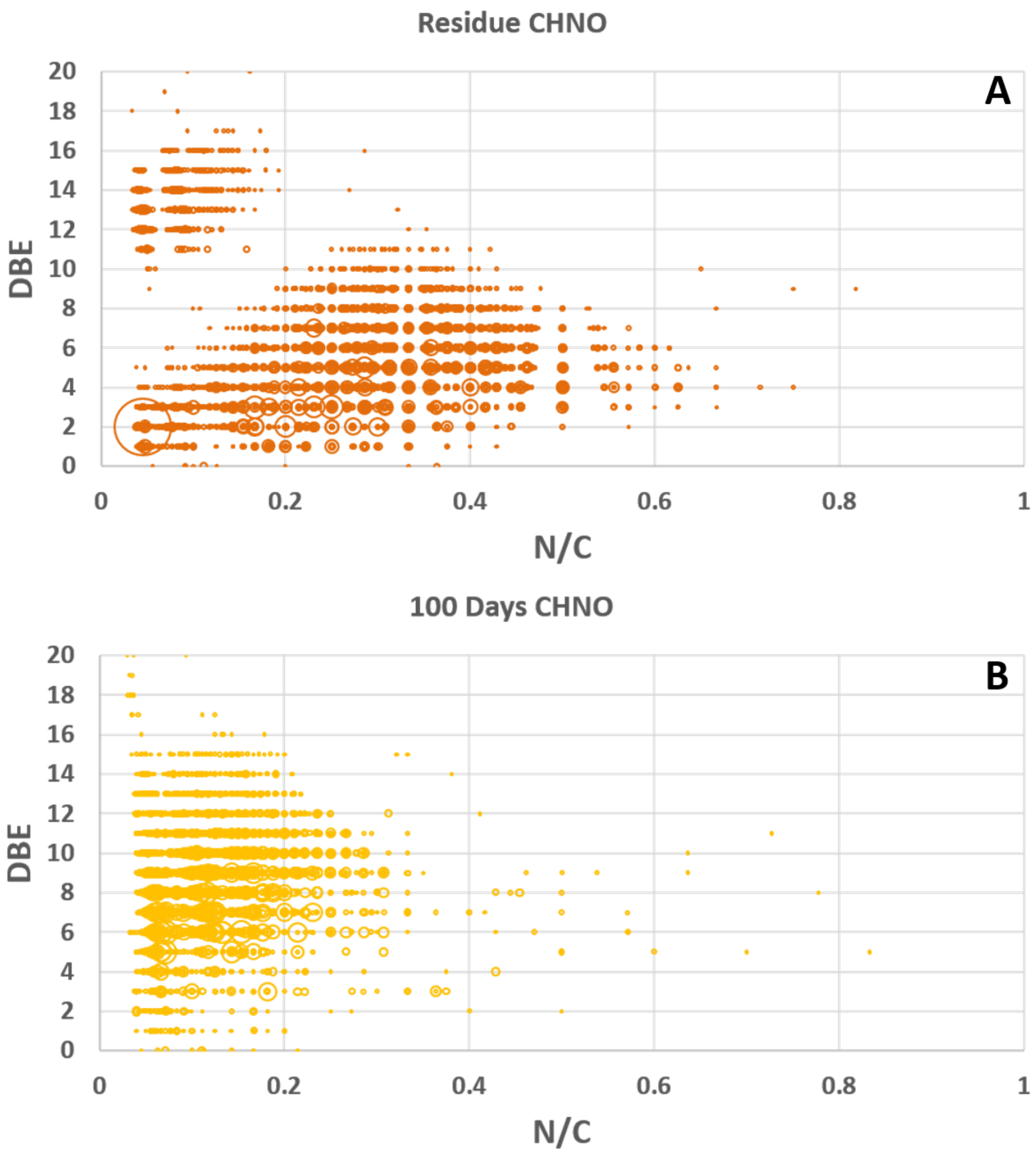
Supplementary Figure 4– – O vs m/z relative to the CHNO family for pre-accretional (3512 molecular attributions) (A) and post-aqueous organic products after 100 days (2591 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

Complementary data regarding the Van Krevelen diagrams for H/C vs N/C of the CHNO family for pre-accretional and post-aqueous organic residues after 100 days of reaction



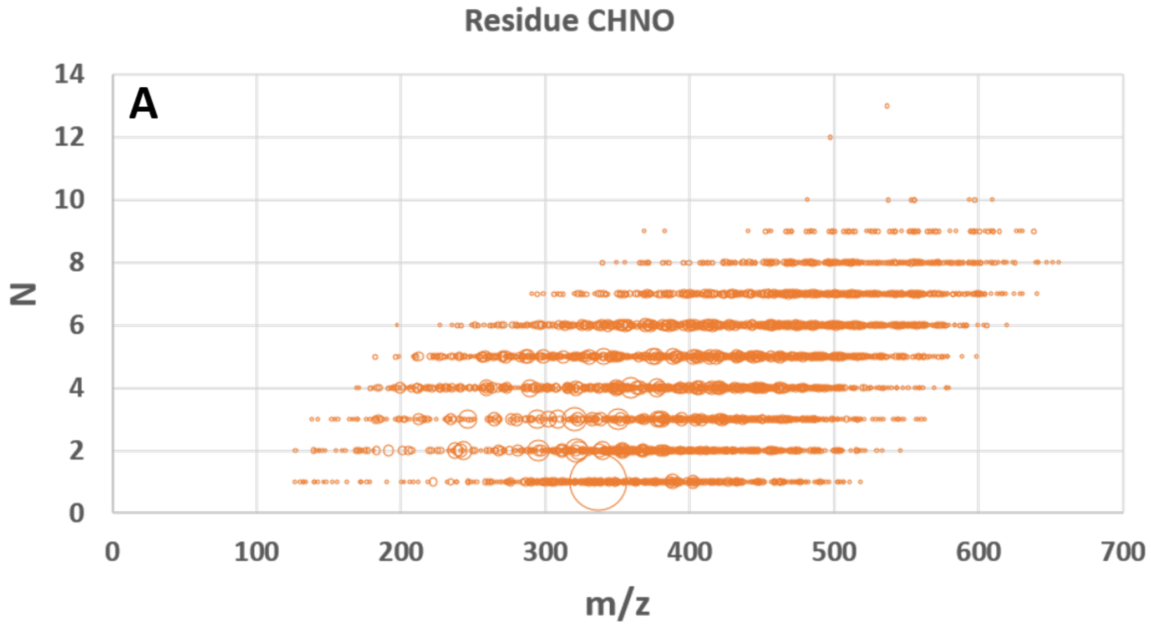
Supplementary Figure 5– Van Krevelen diagrams are displayed for H/C vs N/C relative to the CHNO family for pre-accretional (3512 molecular attributions) (A) and post-aqueous organic products after 100 days (2591 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

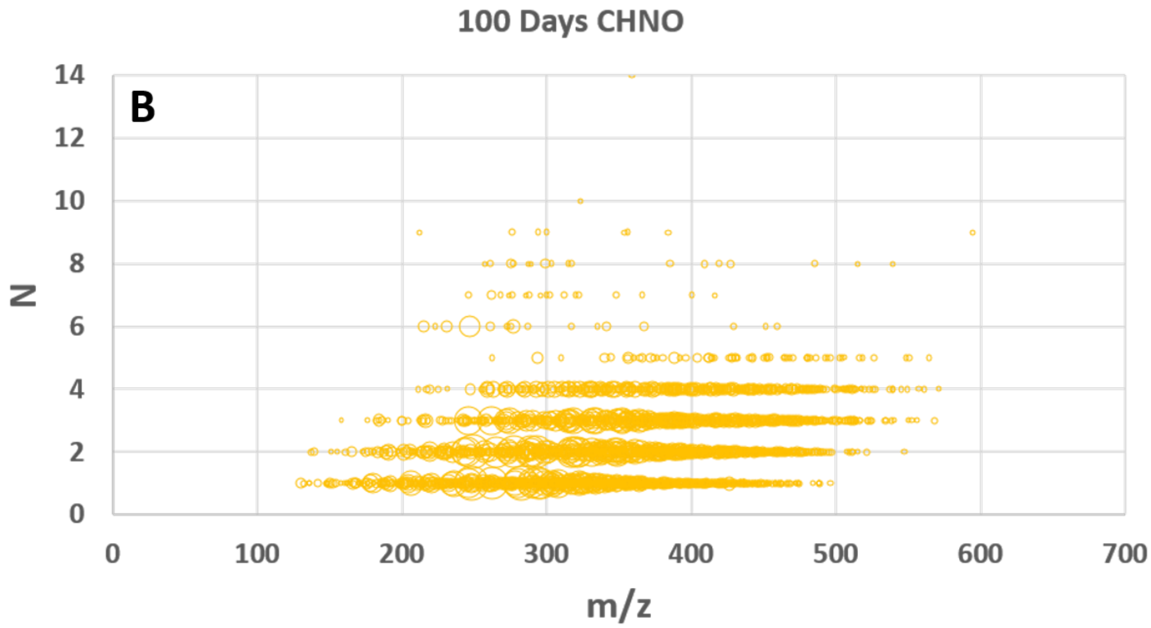
Complementary data regarding the DBE vs N/C of the CHNO family for pre-accretional and post-aqueous organic residues after 100 days of reaction



Supplementary Figure 6– – DBE vs N/C relative to the CHNO family for pre-accretional (3512 molecular attributions) (A) and post-aqueous organic products after 100 days (2591 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

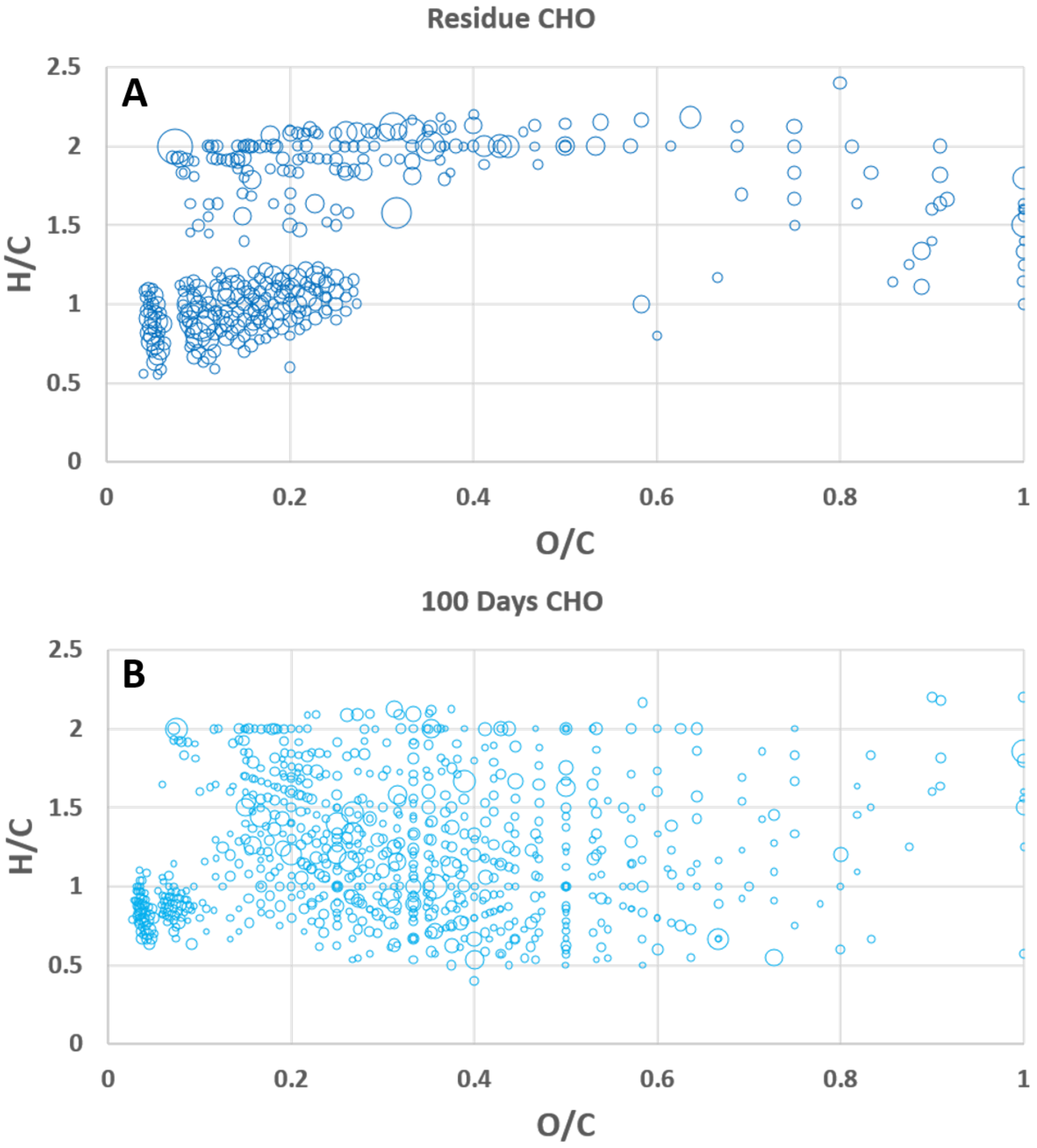
Complementary data regarding the O vs m/z of the CHNO family for pre-accretional and post-aqueous organic residues after 100 days of reaction





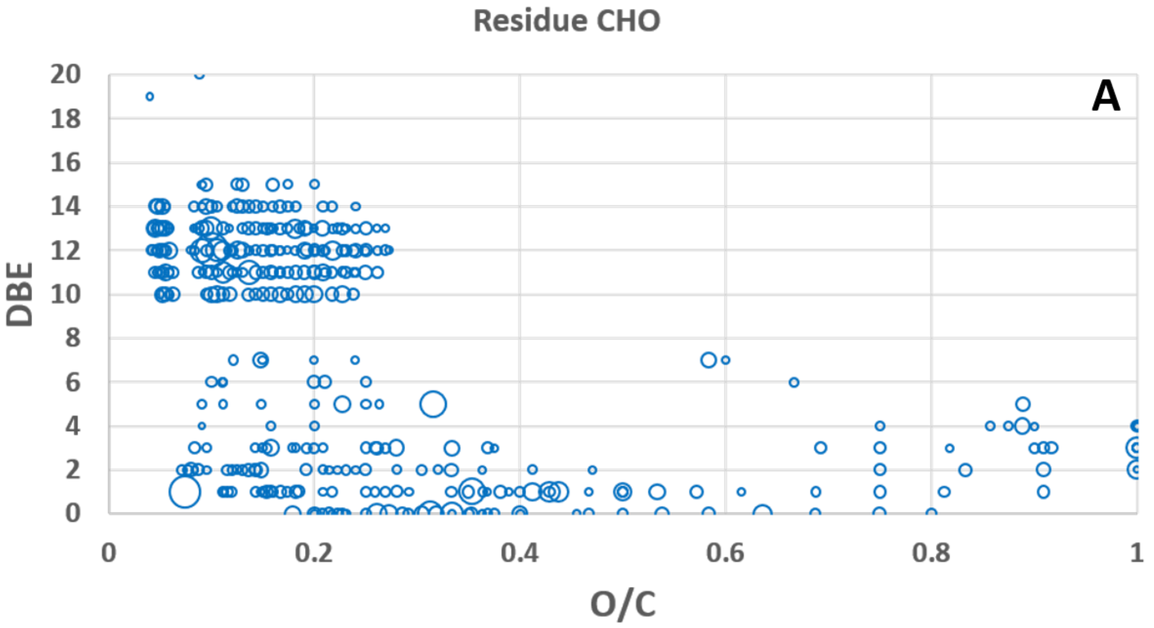
Supplementary Figure 7 – N vs m/z relative to the CHNO family for pre-accretional (3512 molecular attributions) (A) and post-aqueous organic products after 100 days (2591 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

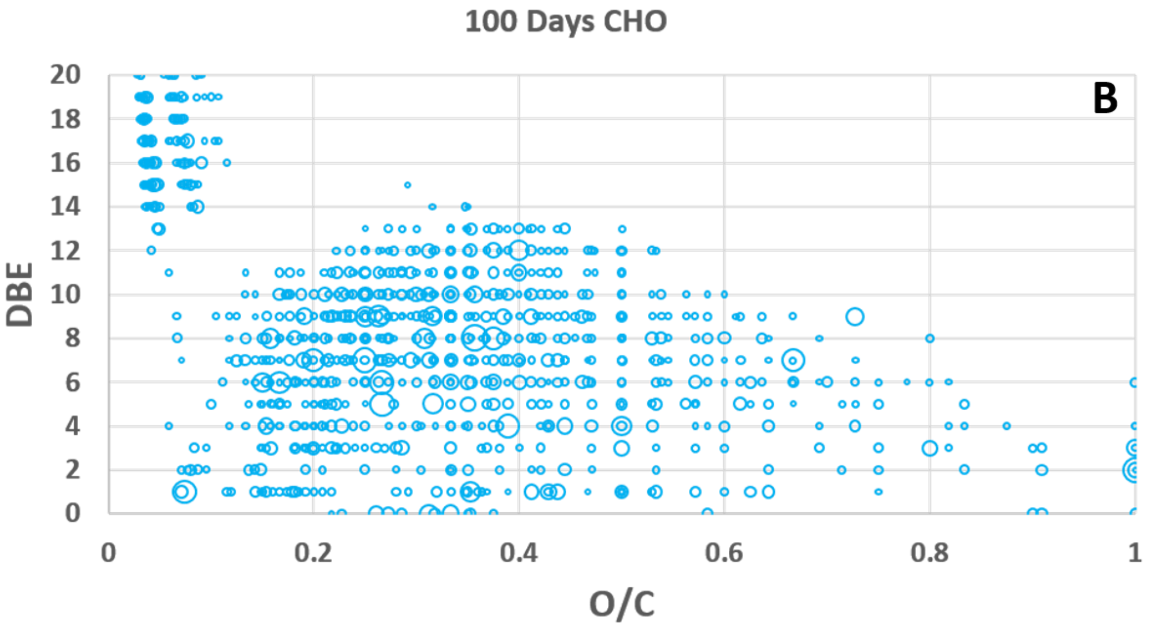
Complementary data regarding the Van Krevelen diagrams for H/C vs O/C of the CHNO family for pre-accretional and post-aqueous organic residues after 100 days of reaction



Supplementary Figure 8 – Van Krevelen diagrams are displayed for H/C vs O/C relative to the CHO family for pre-accretional (351 molecular attributions) (A) and post-aqueous organic products after 100 days (711 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

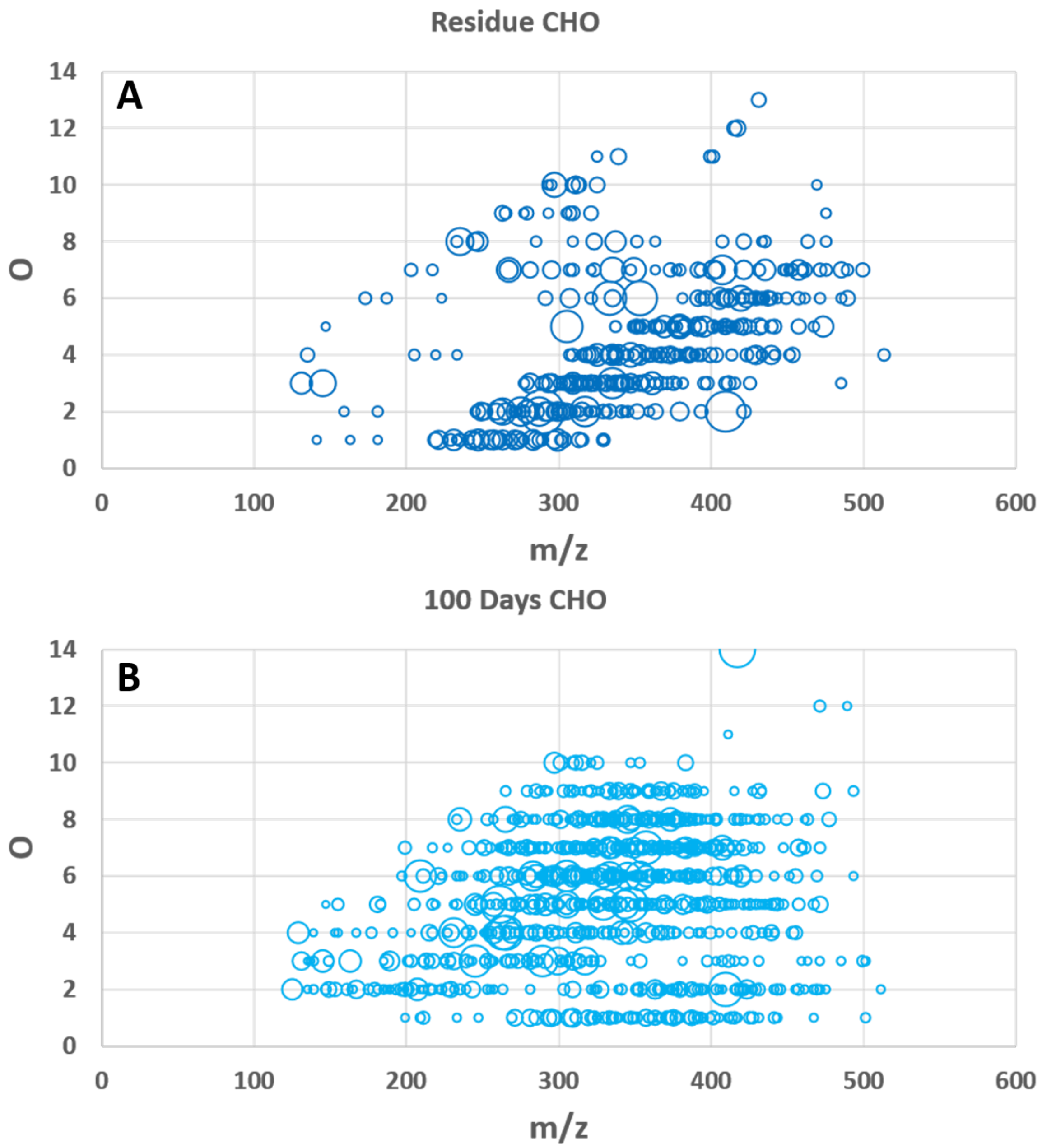
Complementary data regarding the DBE vs O/C of the CHO family for pre-accretional and post-aqueous organic residues after 100 days of reaction





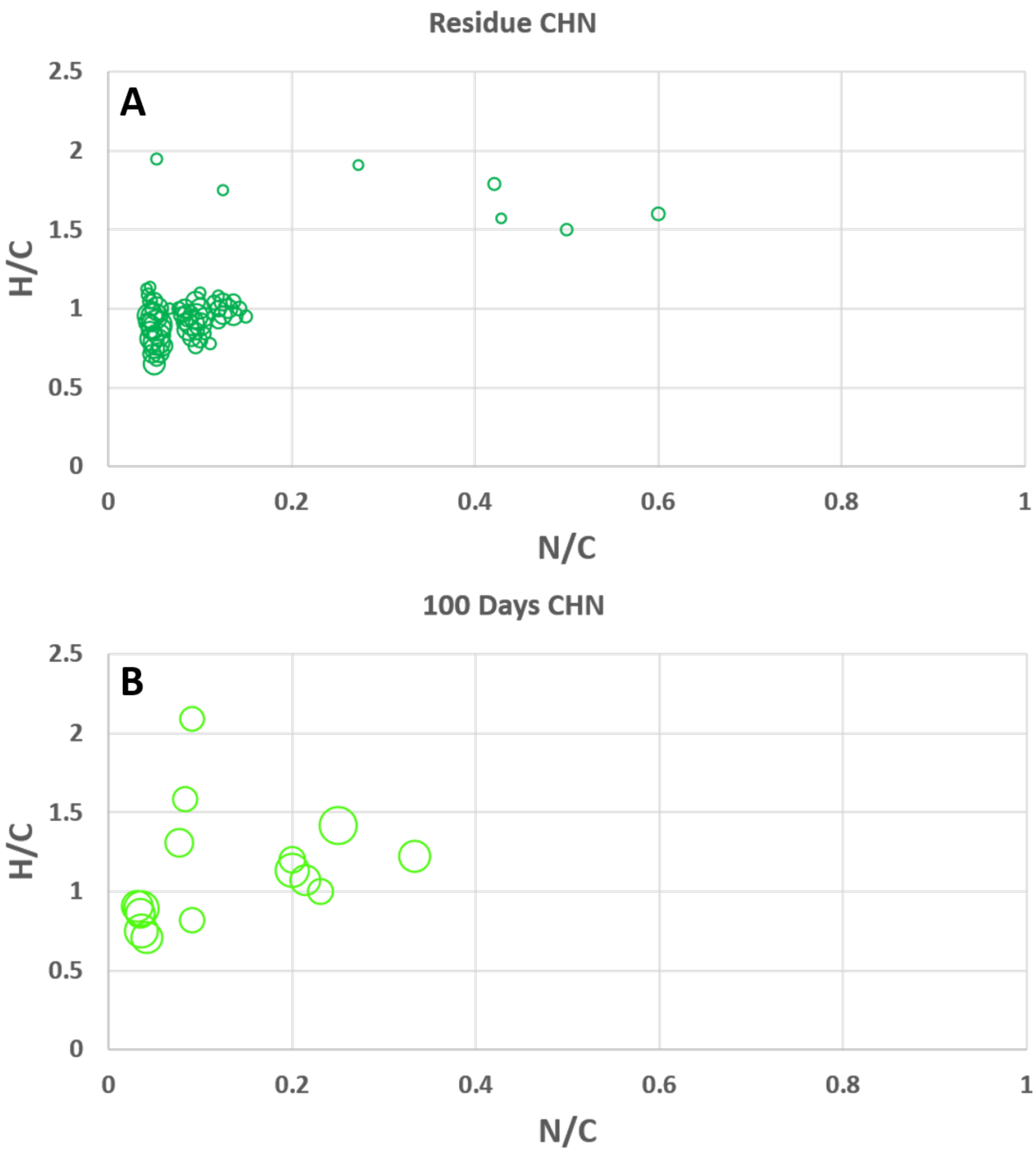
Supplementary Figure 9– DBE vs O/C relative to the CHO family for pre-accretional (351 molecular attributions) (A) and post-aqueous organic products after 100 days (711 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

Complementary data regarding the O vs m/z of the CHO family for pre-accretional and post-aqueous organic residues after 100 days of reaction



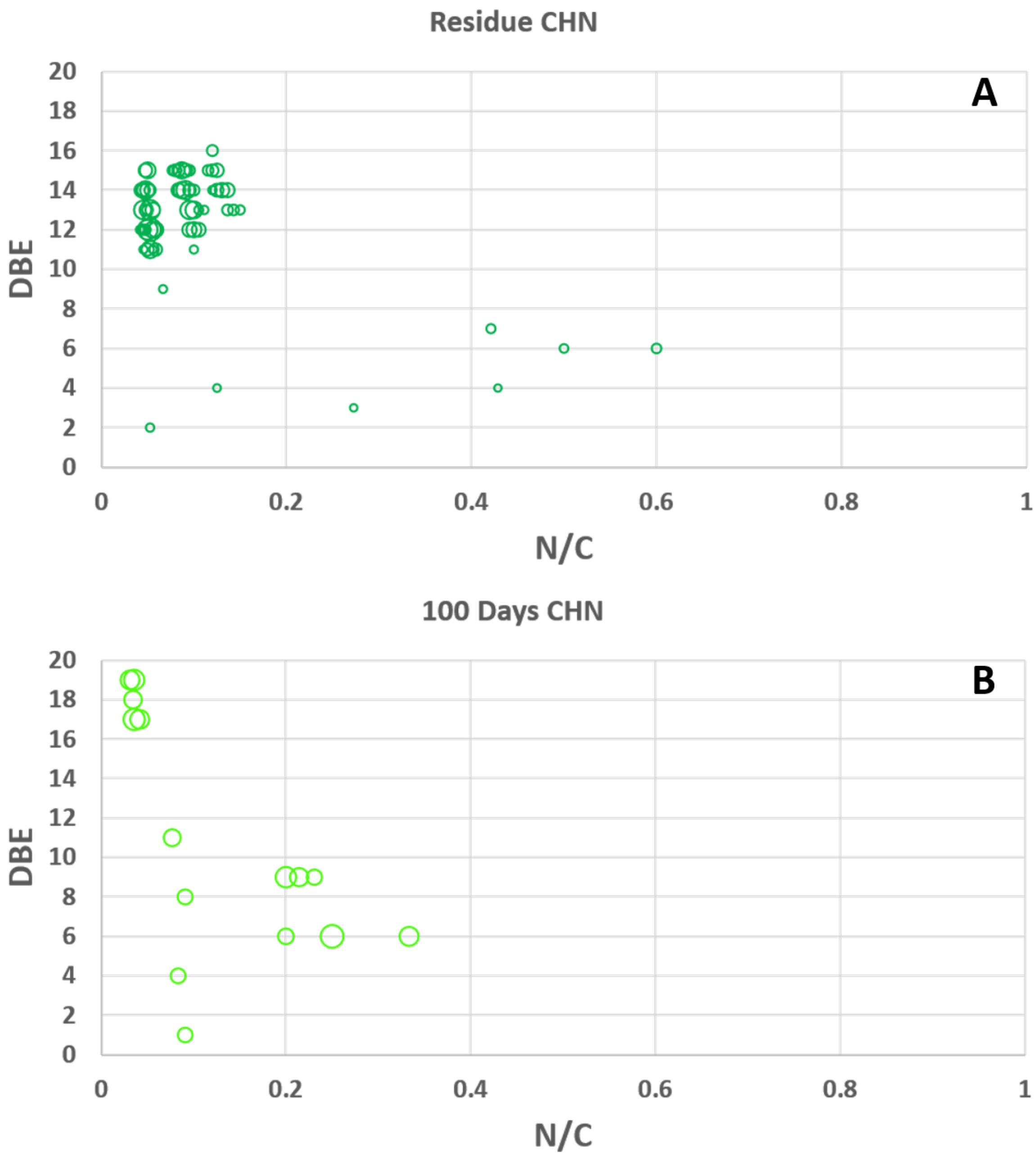
Supplementary Figure 10 – O vs m/z relative to the CHO family for pre-accretional (351 molecular attributions) (A) and post-aqueous organic products after 100 days (711 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

Complementary data regarding the Van Krevelen diagrams for H/C vs N/C of the CHN family for pre-accretional and post-aqueous organic residues after 100 days of reaction



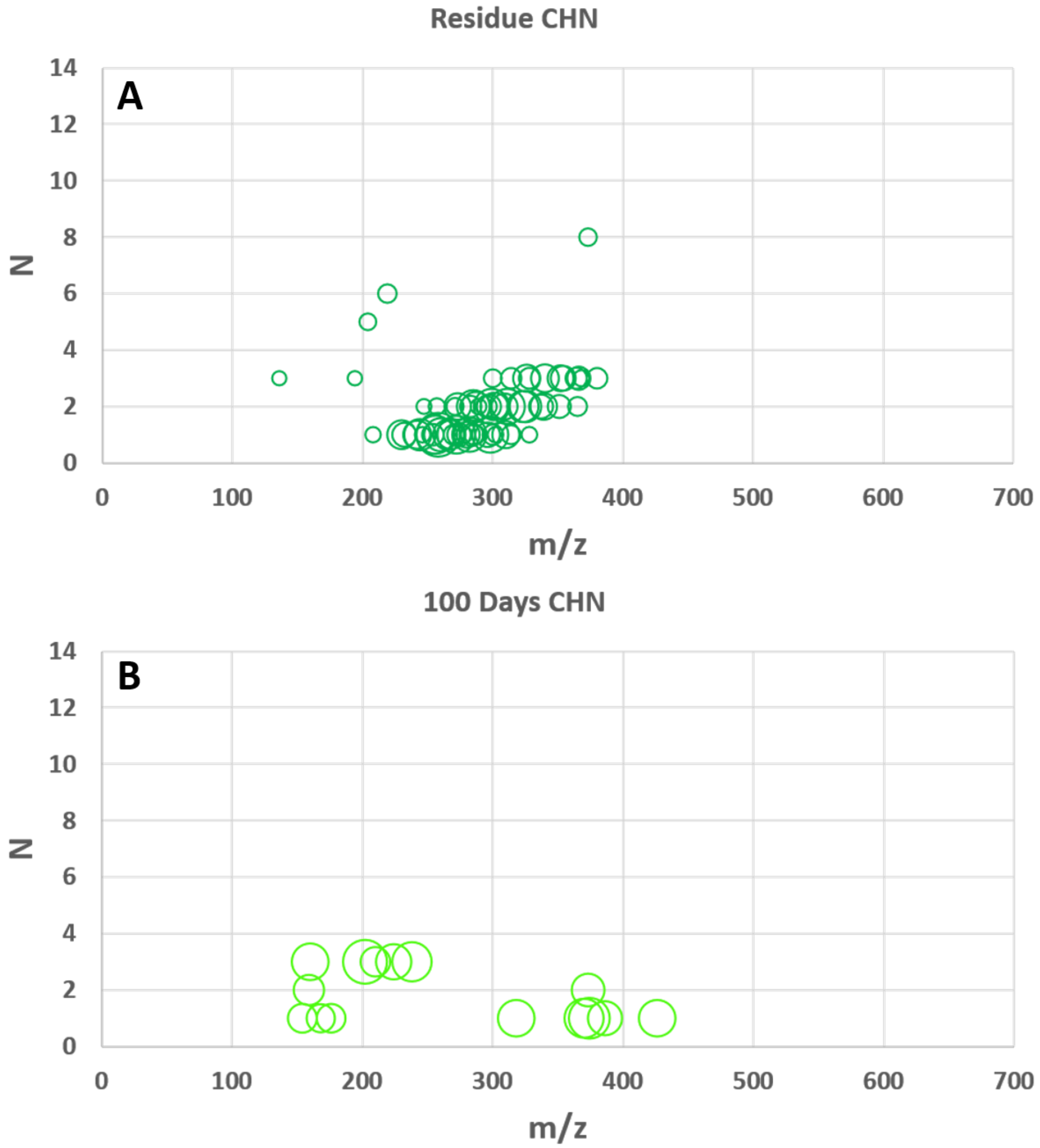
Supplementary Figure 11 – Van Krevelen diagrams are displayed for H/C vs N/C relative to the CHN family for pre-accretional (63 molecular attributions) (A) and post-aqueous organic products after 100 days (15 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

Complementary data regarding the DBE vs N/C of the CHN family for pre-accretional and post-aqueous organic residues after 100 days of reaction



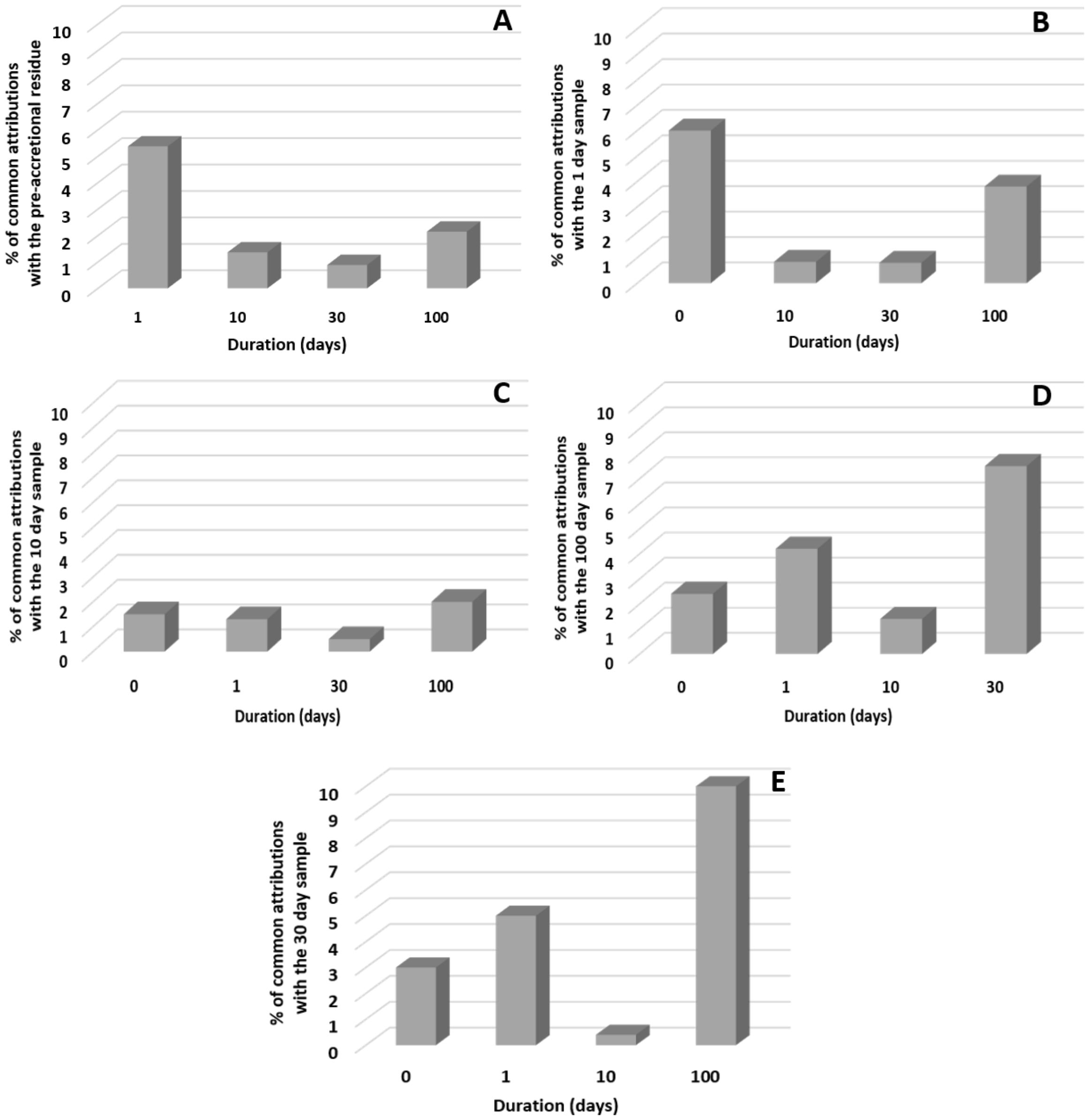
Supplementary Figure 12– DBE vs N/C relative to the CHN family for pre-accretional (63 molecular attributions) (A) and post-aqueous organic products after 100 days (15 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

Complementary data regarding the N vs m/z of the CHN family for pre-accretional and post-aqueous organic residues after 100 days of reaction



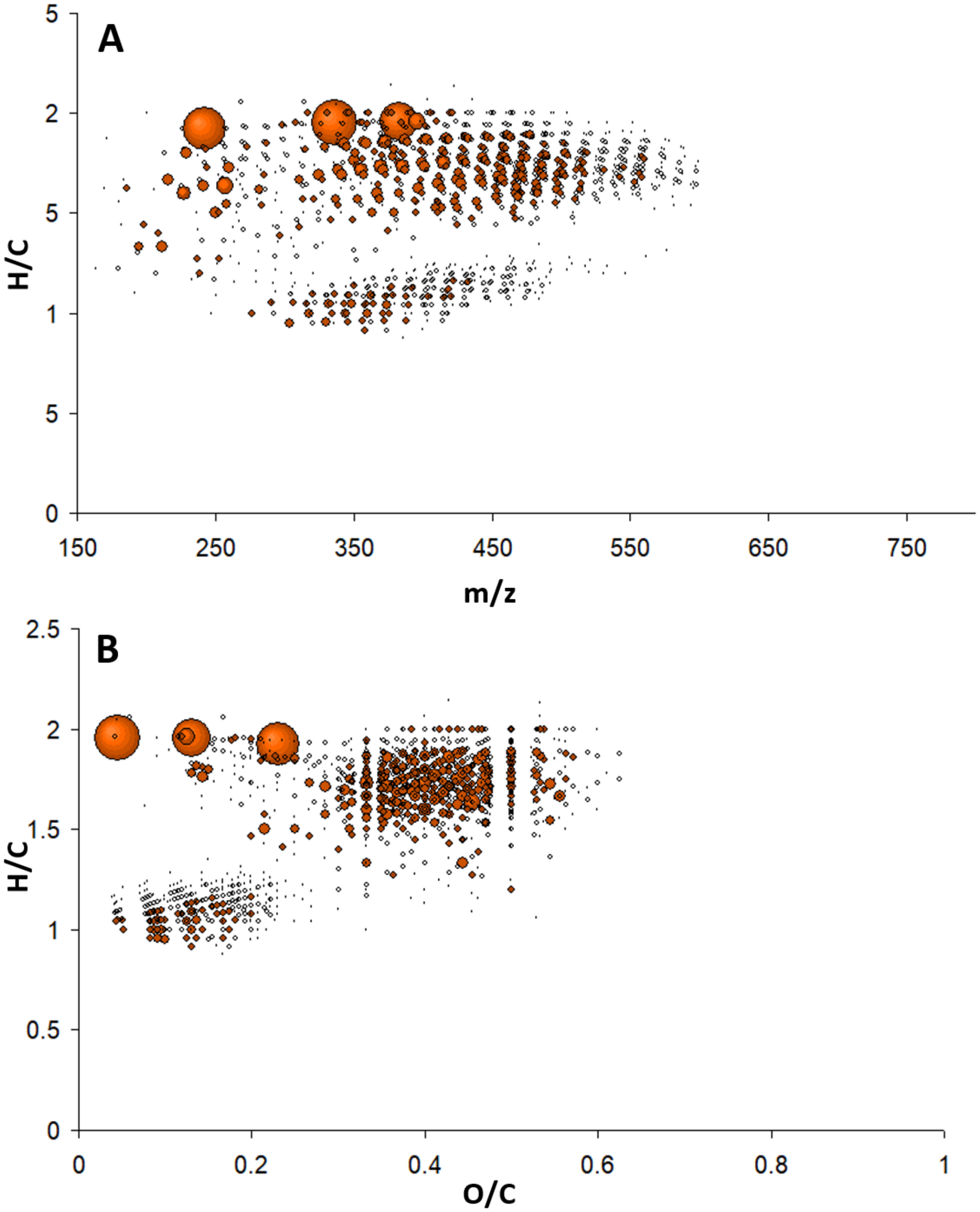
Supplementary Figure 13 – N vs m/z relative to the CHN family for pre-accretional (63 molecular attributions) (A) and post-aqueous organic products after 100 days (15 molecular attributions) at 150°C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

Evolution of common molecular attributions between the different experimental times



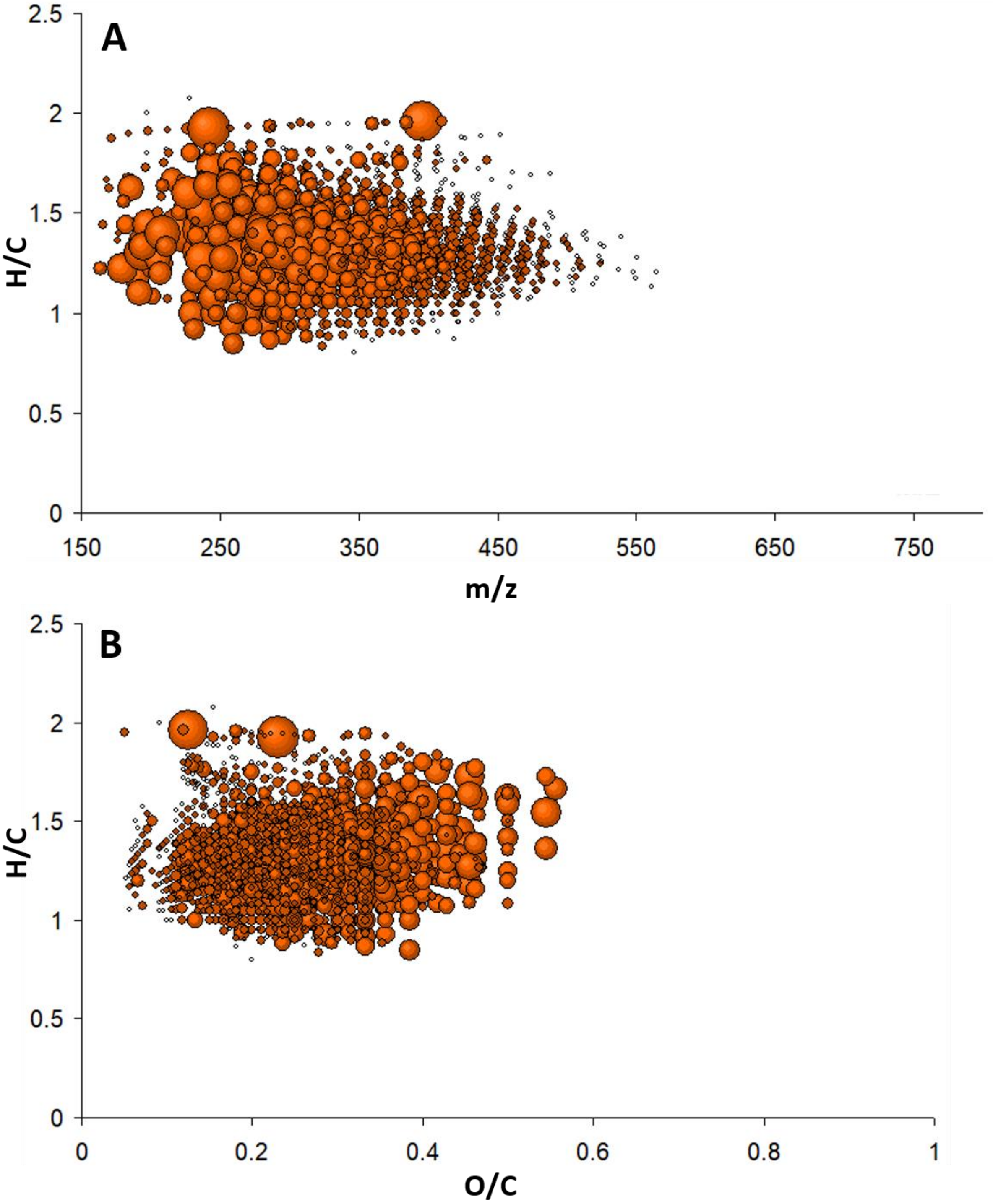
Supplementary Figure 14 – Common molecular attributions between samples of different experimental times. (A) displayed the common attributions of the pre-accretional organic residue with 1, 10, 30 or 100 days of experiments at 150°C. (B) displayed the common attributions of the 1 day sample at 150°C with the pre-accretional organic residue (0), 10, 30 or 100 days of experiments at 150°C. (C) displayed the common attributions of the 10 day sample at 150°C with the pre-accretional organic residue (0), 1, 30 or 100 days of experiments at 150°C. (D) displayed the common attributions of the 100 day sample at 150°C with the pre-accretional organic residue (0), 1, 10 or 30 days of experiments at 150°C. (E) displayed the common attributions of the 30 day sample at 150°C with the pre-accretional organic residue (0), 1, 10 or 100 days of experiments at 150°C.

Common molecular attributions between the pre-accretional organic residue and the Murchison SOM



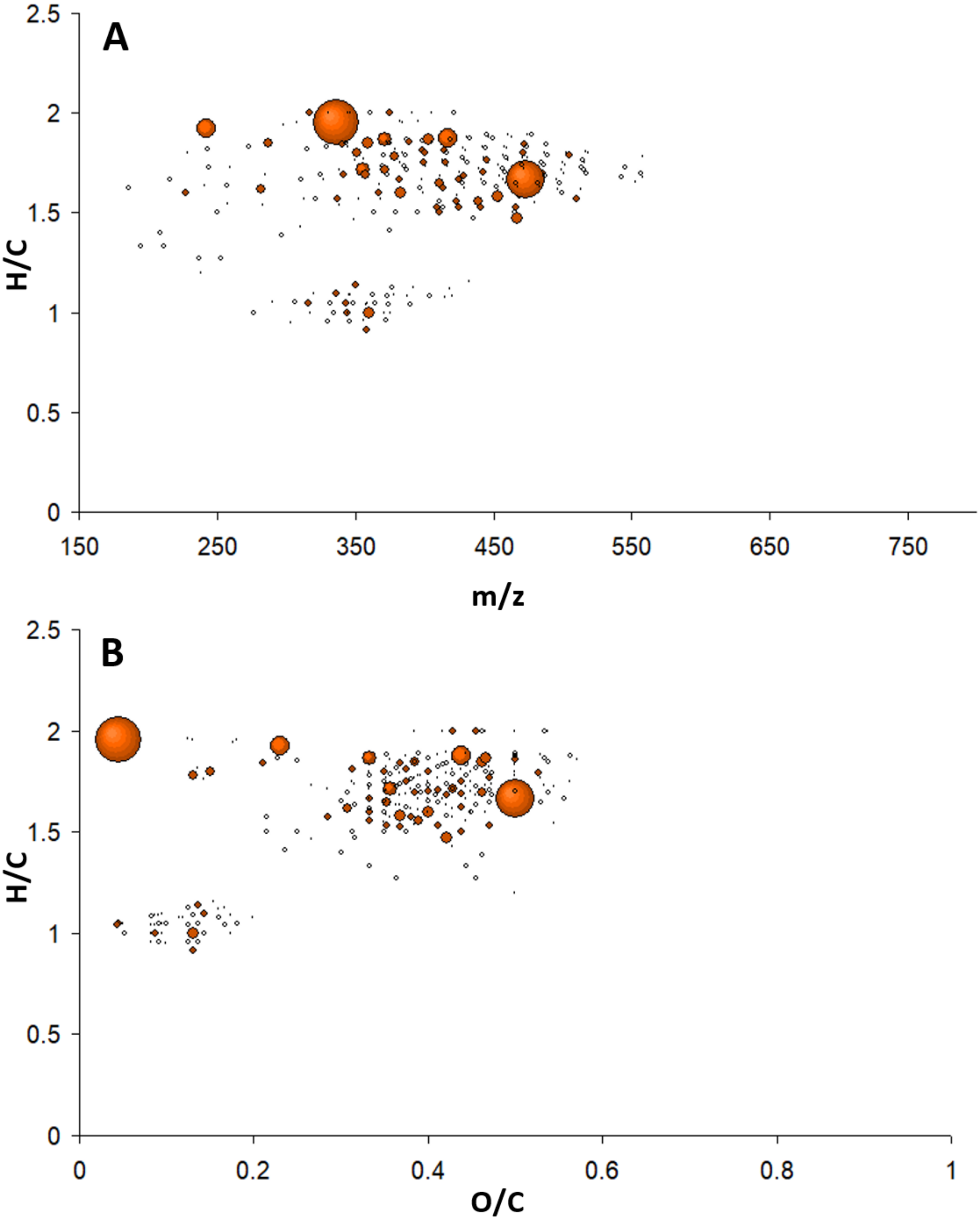
Supplementary Figure 15 – The 1000 molecular attributions in common between the pre-accretional organic residue and the SOM of Murchison represented as H/C vs m/z (A) or with the Van Krevelen diagram H/C vs O/C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

Common molecular attributions between the post-accretional organic products and the Murchison SOM



Supplementary Figure 16 – The 1200 molecular attributions in common between the post-aqueous organic products after 100 days and the SOM of Murchison represented as H/C vs m/z (A) or with the Van Krevelen diagram H/C vs O (B). The size of the circle representing each molecular attribution is proportional to ion intensities.

Common molecular attributions between the pre-accretional organic residue, post-accretional organic products and the Murchison SOM



Supplementary Figure 17 – The 265 molecular attributions in common between pre-accretional residue, post-aqueous organic products after 100 days and the SOM of Murchison represented as H/C vs m/z (A) or with the Van Krevelen diagram H/C vs O/C (B). The size of the circle representing each molecular attribution is proportional to ion intensities.