CHEMICAL SPECIATION OF CONSTITUENTS IN PYROLYTIC LIQUID FROM CASSAVA HARVEST RESIDUES BY APPI-Orbitrap MS

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Cassava is the fourth most important crop in the state of Sergipe, Brazil, in terms of tons produced and total planted area [1]. The harvested biomass residue has a high potential as a raw material for the pyrolysis process, which results in high yields of liquid pyrolytic products, as bio-oil and aqueous fraction. These liquid products have been chemically comprehensive characterized by UHRMS using APPI ionization source.
Cassava harvest residue (aerial part of the plant and rhizome) was collected in Sergipe, Brazil's rural area. The material was sun-dried, milled, and pyrolyzed at 500 °C in a rotary kiln reactor, in the same conditions then previously described by Santana et al., 2019 [2]. GC/MS was employed for characterization of volatilizable constituents of bio-oil and APPI-Orbitrap MS was used to characterize the most polar compounds in both, aqueous fraction and pyrolytic cassava oil. Bio-oil and aqueous fraction yields from pyrolysis of cassava harvest residue were 11% and 33%, respectively. 57% of the total area of the TICC was characterized, and the identified compounds were grouped into different classes, of which the majority in the bio-oil were phenolics compounds (33%), carboxylic acids (13%), and alcohols (10%) (Figure 1a). It was noted in the histograms of the classes in Figure 1b that the two liquid products have very distinct chemical compositions. Bio-oil has molecules with 2 to 6 oxygen atoms, whereas the aqueous fraction composition contains more polar compounds, containing 5 to 8 oxygen atoms. The van Krevelen plots (Figure 1c and d) demonstrate that the bio-oil constituents are primarily distributed in the phenolics (O/C ~0.1–0.6 and H/C ~0.6–1.3) and lipidic compounds (O/C ~0.1–0.3 and H/C ≥ 1.2) regions [3], highlighted in green and red, respectively. While the ions of the aqueous fraction are predominantly distributed in the region of phenolic compounds with higher O/C, more oxygenated compounds, and sugar-like compounds and derivatives, which are highlighted in black.

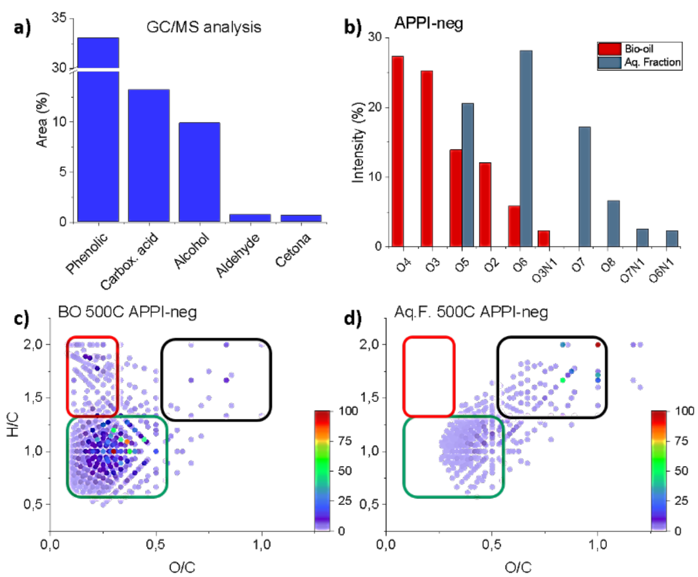

Figure 1 – Characterization by GC/MS (a) and APPI(-) UHRMS Class histograms (b) and van Krevelen diagrams of bio-oil (c) and aqueous phase (d).

As a result of the high content of phenolic compounds, bio-oil has the potential to be used as a raw material source for the fine chemicals industry. Given the difficulty of recovering the compounds in the aqueous phase, this product can be used as a bactericide due to the phenolic compound's antimicrobial activity.

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