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Application of a Shotgun Humeomics Approach by UPLC / Fourier Transform Orbitrap Mass Spectrometry to study the in-depth molecular diversity of green composts

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One third of all food produced worldwide is lost or wasted according to the Food and Agriculture Organization (FAO) of the United Nations (UN). Specifically, green organic wastes are the main urban and agricultural wastes. One possibility would be to recycle green wastes through the production of compost whose humified components are beneficial to the agroecosystem. The objective of this research project is to achieve a deep molecular understanding of the complex chemical composition of humified green compost in regards to its capacity to replenish nutrients in soils and induce plant biostimulation.

To achieve this goal, a Humeomic fractionation procedure was applied to two composts that only differed in maturity. Based on Humeomic fractionation, six aqueous fractions were obtained, which were first characterized by Direct Infusion (DI) ultra-high resolution (ESI and APPI) Orbitrap Lumos 1M mass spectrometry while a second analytical workflow hyphenated size-exclusion chromatography (SEC, using a POLYSEP-GFC-P3000 column) with electrospray ionization Orbitrap tandem mass spectrometry (MS^2). Characterization of aqueous fractions could not be achieved by common dialysis due to subsequent poor solubility of materials prior to the HPSEC-Orbitrap determination. It was found that purification from salts through SPE Bond Elut PPL ensured good solubility in aqueous and organic solutions.

We used the open-source, Python command-line based MetaboDirect pipeline for data exploration and chemodiversity analysis of empirical molecular formulae derived from full scan DI-ESI and APPI Orbitrap spectra. Then, a*b-initio* mass difference transformation networks (MDiNs) were built for each Humeomic fraction's DI-ESI and APPI Orbitrap spectra using Cytoscape in order to gain a better understanding of the biochemical transformations associated with the humification process. On the other hand, SEC- UHR Orbitrap MS allowed to obtain:

1. molecular identification through MS^2 spectral database searchers,
2. diagnostic neutral losses for structural information on unknown neutral loss fragmentations.

This work shows for the first time an in-depth understanding of the molecular constituents of the humified fraction of green compost. The Humeomic procedure and data elaboration of DI- and SEC- Orbitrap results suggest that these combined approaches are essential in solving and understanding the molecular complexity of Humic Matter extracted from compost.