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Probing the Molecular Composition of Humic Substances Extracted from Green Composts and Used for Soil Remediation

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Humic Substances (HS) consist of supramolecular associations of heterogeneous small molecules with amphiphilic properties which are organized in pseudo-micellar domains in aqueous solutions. When recalcitrant hydrophobic organic compounds adsorbed on the surfaces of solid soil particles come into contact with humic solutions, they preferentially partition into the humic hydrophobic domains, thus being removed from the soil. At the same time, the acidic functional groups of humic substances can complex heavy metals present in the soil and thus extract them. Hence, a sustainable and eco-friendly method for effectively removing pollutants from soil involves using HSs extracted from composted waste biomass. However, the molecular composition of HSs may vary greatly between different types of compost and within a compost type, based on its maturation stage, which in turn may affect their behaviour. Indeed, extent of metals removal depends of the molecular composition of the humic matter employed in the soil washing. It is then essential to investigate their molecular characteristics before using them for soil remediation strategies. Besides, use of soft ionization techniques combined with ultrahigh resolution mass spectrometry may help us better understand the individual compounds within the complex HS architecture involved in chelation of heavy metals / partitioning of recalcitrant hydrophobic organic compounds.

In this study, we assessed and compared the molecular composition of HSs extracted from different green composts prepared from agricultural residues and coffee waste before and after “soil washing” experiments of soils heavily contaminated with various heavy metals. We combined (i) electrospray and photoionization with ultrahigh resolution Orbitrap Lumos 1M mass spectrometry with nuclear magnetic resonance (NMR) spectroscopy to capture the molecular heterogeneity of HS used as raw material for soil remediation studies. Our results show that the HSs extracted from the different composts actually displayed relative similar molecular space across samples. Lignin derived compounds and carboxylic-rich alicyclic molecules (CRAM) ranged from 42 to 50 % of the molecular composition of all samples, followed by an almost equal relative amount of lipids and unsaturated hydrocarbons (approximately 20% each).