



## **Patterns of nitrogen-containing pyrolytic compounds reflecting soil organic matter quality and carbon storage**

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Recent investigations are paying special attention to soil organic matter (SOM) storage in relation to global change. The assessment of factors involved in soil carbon sequestration is crucial for developing the scientific bases of Earth's biogeochemical cycles. In particular, most current research is focusing mainly on organo-mineral interactions, with less interest in the chemical composition of SOM. Nevertheless, several investigations have suggested significant correlations and possible cause-to-effect relationships between molecular-level descriptors and the quality and quantity of the SOM. In this study we focus on N-bearing SOM constituents. Using gas chromatography/mass spectrometry, we identify and quantify N-compounds released by analytical pyrolysis from whole soil samples. The interest of analyzing the patterns of N-compounds is manifold: i) they amount to a reduced number of diagnostic molecules in pyrograms with more than a hundred of major compounds, which is useful for chemotaxonomic purposes, ii) indices such as the C/N ratio is classically used to describe SOM quality, then changes in the N-containing moiety of the SOM should parallel important biogeochemical processes, iii) progressive accumulation of recalcitrant "unknown" N-fractions is a general diagenetic trend in terrestrial soils, suggesting that SOM maturity could be reflected by the proportions of N-compounds not derived from protein. Assuming these considerations, this research explores the relationships between pyrolytic assemblages of N-compounds and different soil properties with special emphasis on indicators of the quality of the SOM, such as the selective accumulation of aromatic structures as reflected by C-13 NMR and UV-Vis spectroscopy.

In this study a total of 35 samples were collected from different Spanish soils with large variability in the concentration of soil organic carbon (SOC) and ecological properties. The pyrolytic N-compounds identified were classified into seven major groups: indoles, pyridines, pyrazoles, benzonitriles, imidazoles, pyrroles and quinolines. All these compounds are classically considered as useful source indicators derived from pyrolysis of amino acids, amino sugars, nucleotides and chlorophylls. A series of statistical treatments were applied to unravel possible relationships with SOC content and the SOM quality, mainly principal component analysis (PCA), partial least squares regression (PLS) and multidimensional scaling (MDS). The PCA was carried out using the N-compounds as descriptors, but introducing different soil properties as supplementary variables. The results from PCA and MDS suggested that specific compounds viz. pyridine, pyrazole and benzonitriles behaved as surrogates of SOM quality, whereas quinoline, methylindole, indole, dimethylpyridine and methylbenzotrile were closely correlated with the total SOC content. Finally, significant forecasting models for soil carbon storage were obtained by PLS, exclusively using the abundances of N-compounds as descriptors. As a whole, the results suggest that there is a correlation between the qualitative and quantitative performance of soil C storage and the pattern of pyrolytic N-compounds, which requires an interpretation.