Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Marco A. Jiménez-González[1], Gonzalo Almendros[1], Ana M. Álvarez[2], and Francisco J. González-Vila[3]

[1] National Museum of Natural Sciences. MNCN-CSIC. Madrid (Spain)

[2] Autonomous University of Madrid (Spain)

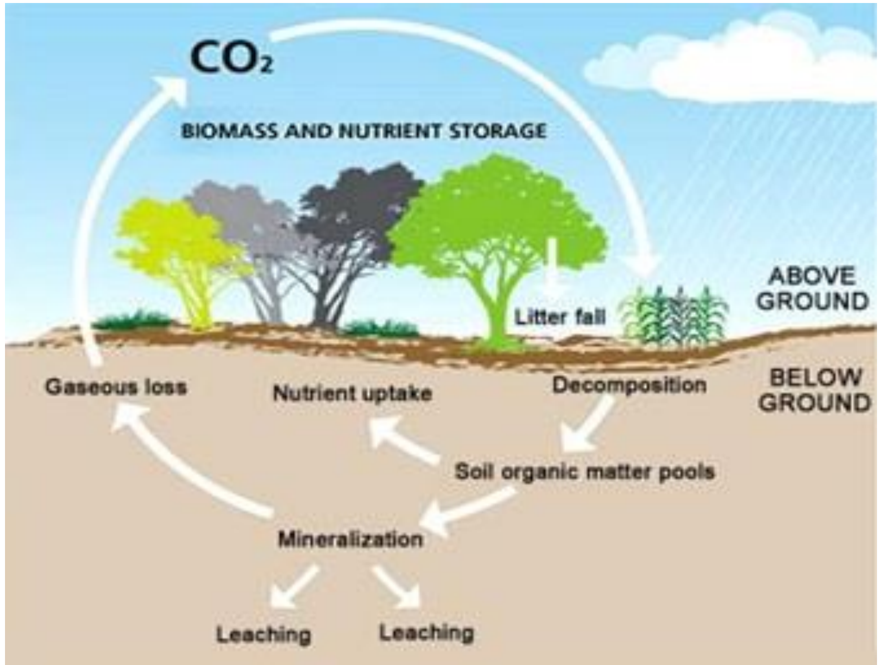
[3] Institute of Natural Resources and Agrobiology of Seville. IRNAS-CSIC. Sevilla (Spain)

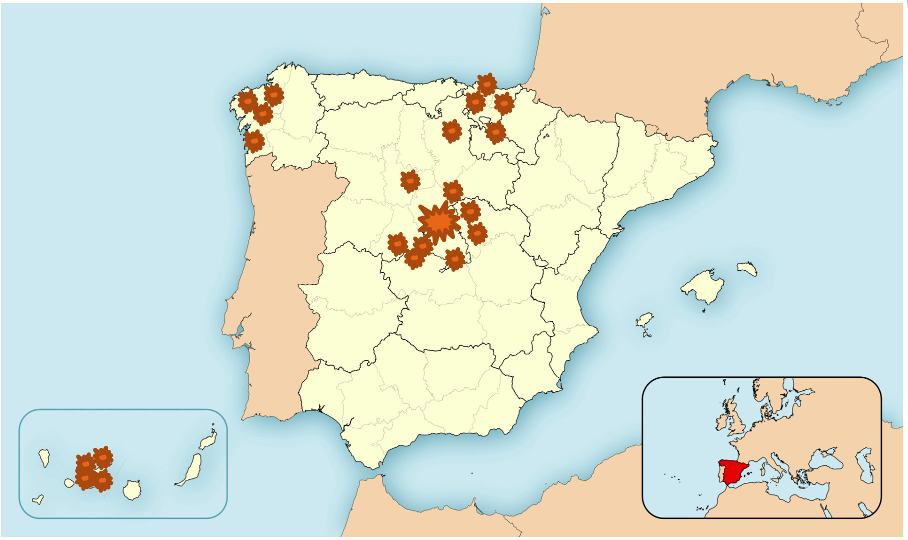
Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Which are the main factors involved in soil C sequestration?

These factors are manifold and highly dependant on the soil types and environmental conditions





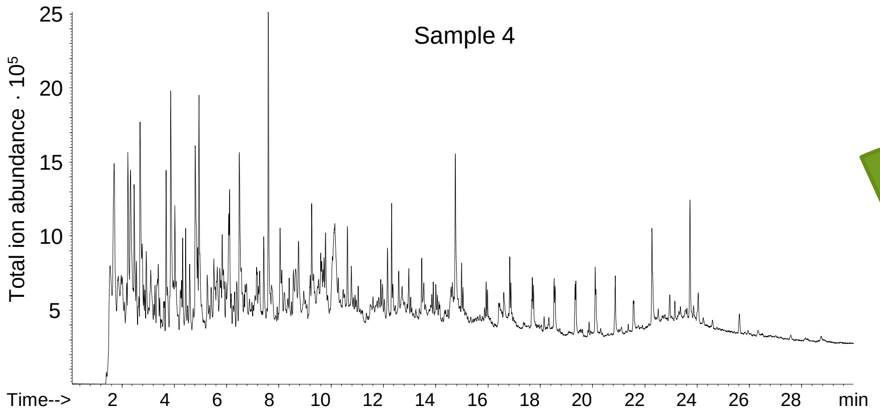
Different soil samples with a wide range of C content are selected for this study

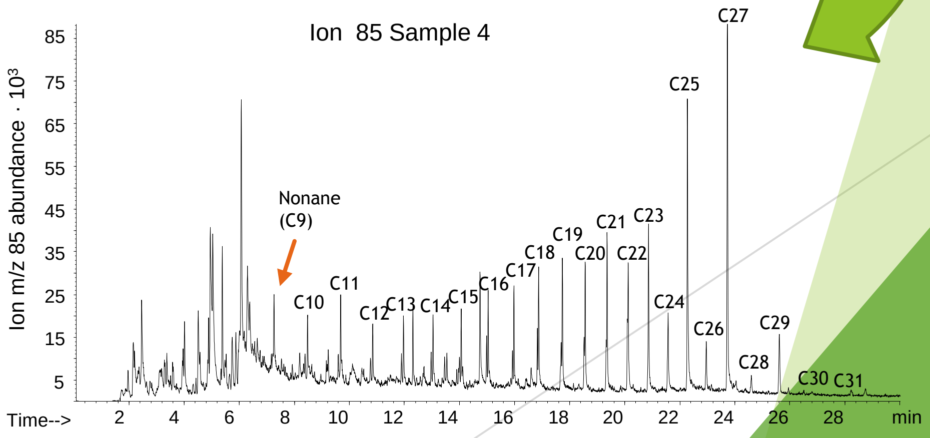
(topsoil samples, ~0—5 cm depth)

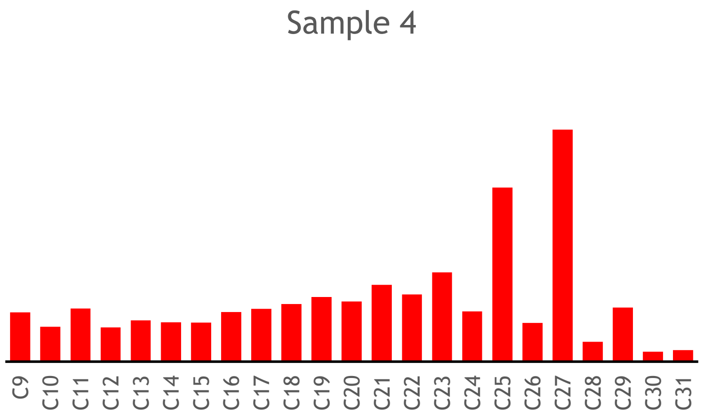
Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Pyrolysis-gas chromatography-mass spectrometry (Py-GC/MS)



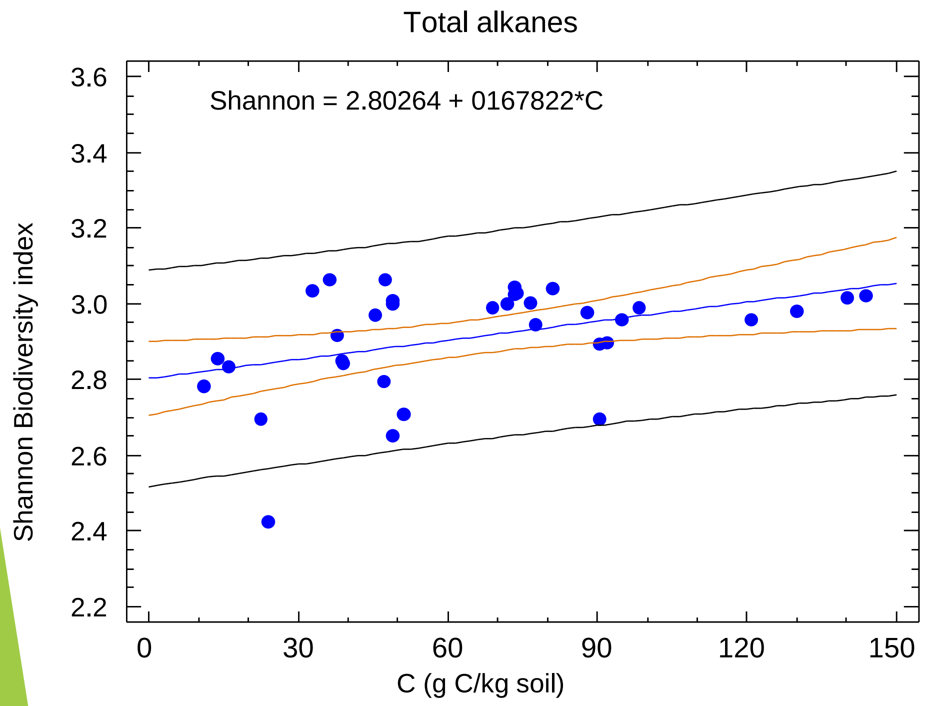


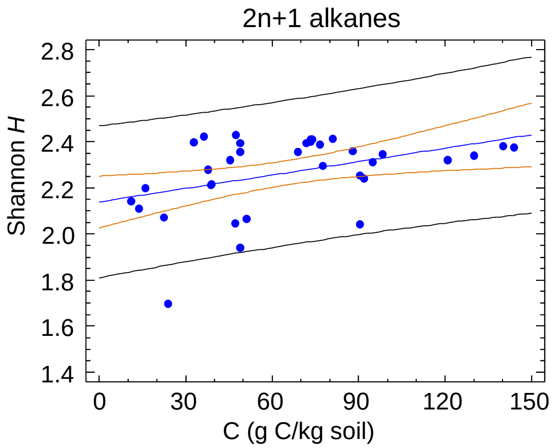


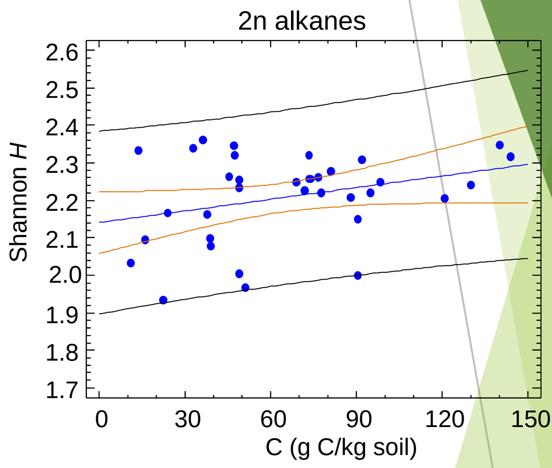
Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

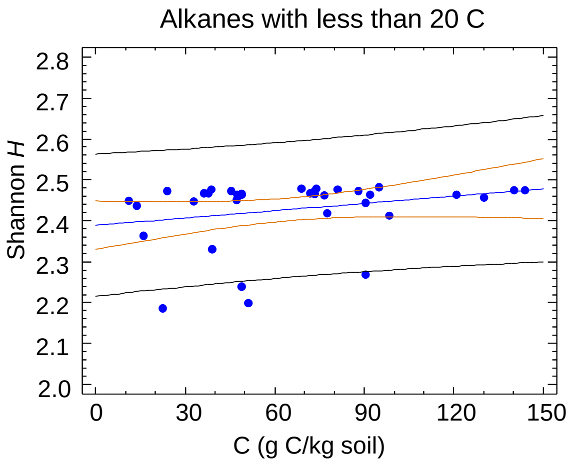
Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

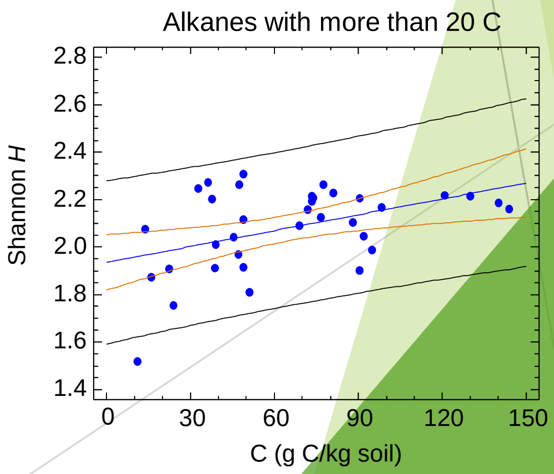
After calculating a series of molecular proxies derived from the analysis of pyrolytic alkanes, including the Shannon Wiener biodiversity index, correlations with the soil organic carbon content were examined









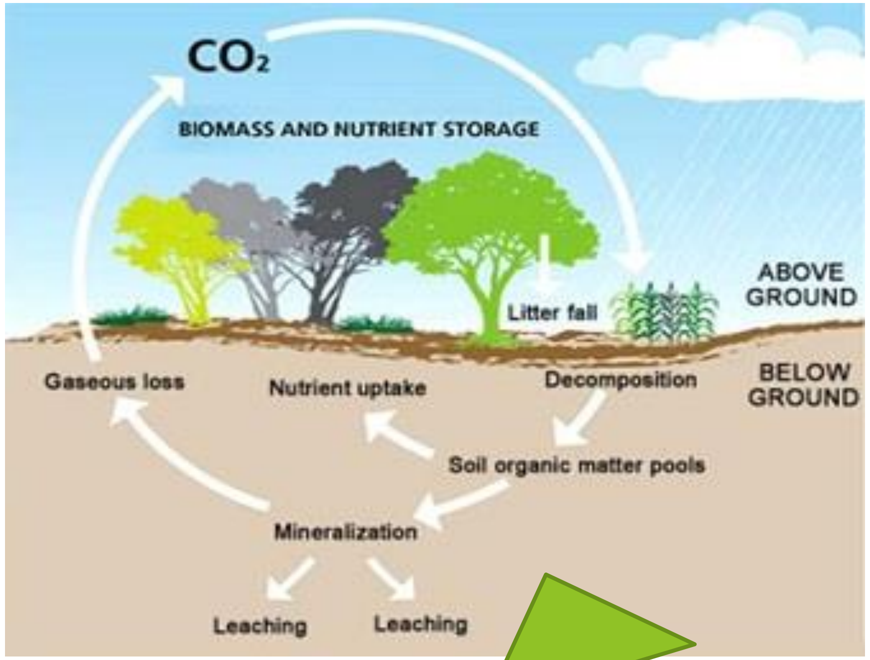


Significant (*P*< 0.05) correlations were found between soil organic C content and several groups of *n*-alkanes !!!

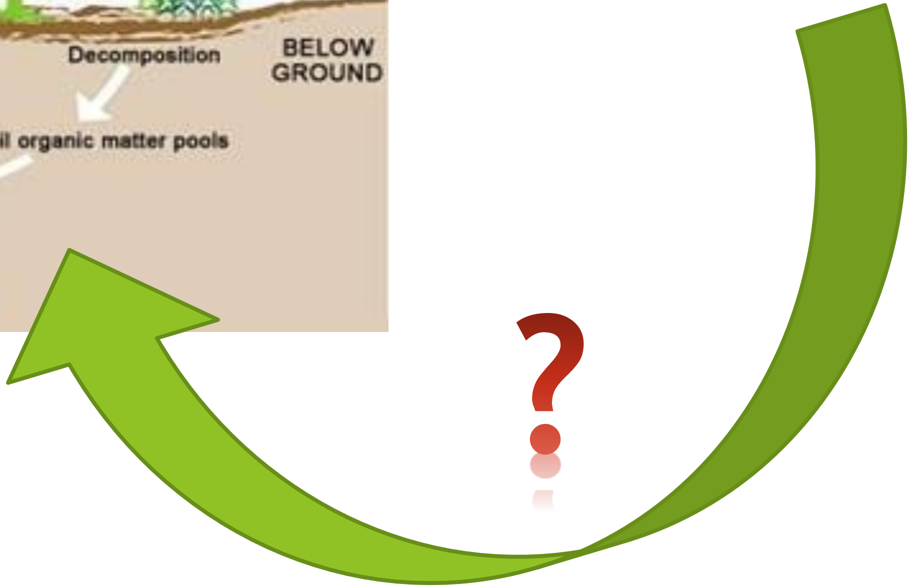
Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Introduction



The factors involved soil C sequestration, which is reflected in the highly variable content of organic matter in the soils, are are not yet completely understood.



Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Molecular biodiversity in pyrolytic compounds

It is hypothesized that the molecular composition of soil organic matter can play a role on its biodegradability and consequently in the variable amount of C stored in the soils. For this reason, lipid composition could be very important source of proxies for soil C sequestration. The biodiversity of this molecular composition may reflect the complexity of the soil biota and its bearing as regards biodegradation and humification processes, which in turn is associated to the organic carbon content.

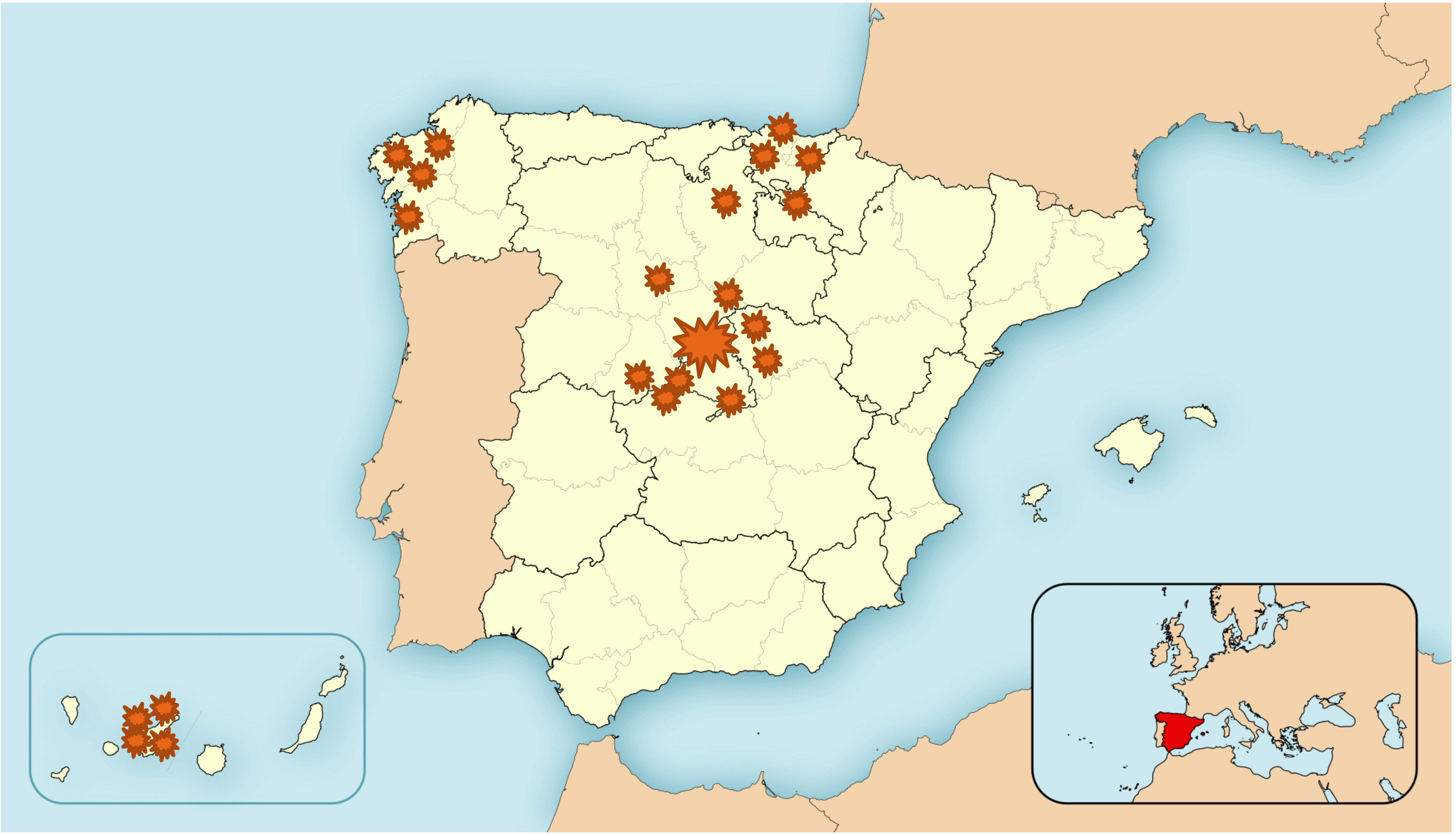
In this case we calculate different indices to assess the possible relationships between the molecular composition of the pyrolytic assemblages of soil alkanes and the total carbon in the soil (viz, C preference index (odd-to-even C ratio), chain length, linear-to-branched, different biodiversity indices, etc).

In particular biodiversity would be considered as an index for formation in soil of complex and chaotic organic matter forms, recalcitrant to enzymatic processes. Such a complexity would be associated to the high performance of the soil C sequestration.

Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Sampling area



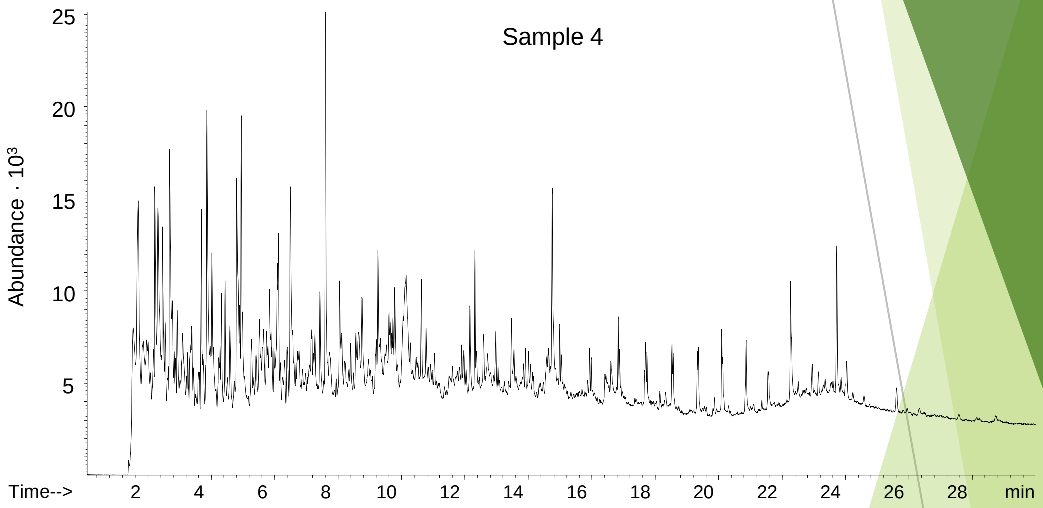
A total of 35 topsoil samples were collected in representative sites with different soil organic carbon content and physical properties.

Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Pyrolysis-gas chromatography-mass spectrometry (Py-GC/MS)

500 ºC



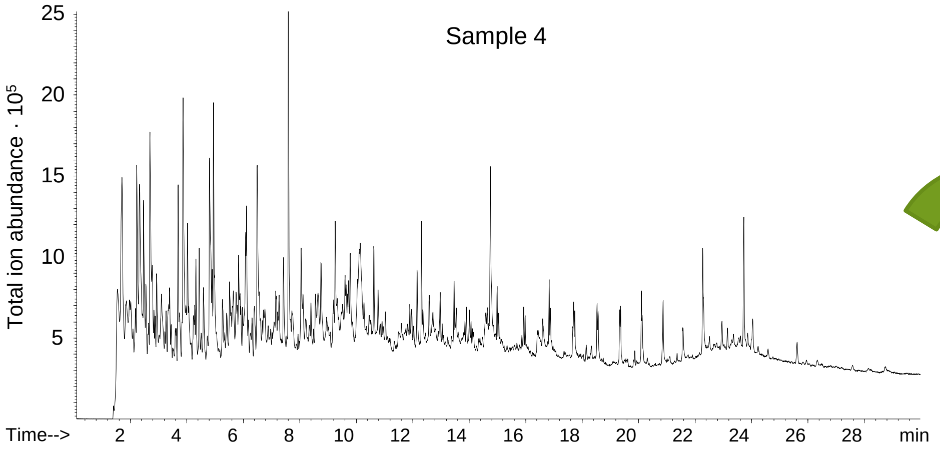
Soil samples were subjected to analytical pyrolysis (Py-GC/MS), a technique not requiring previous isolation or chemical treatment; in this analysis bulk soil samples were used.

Analytical pyrolysis has been extensively used in the structural research on the molecular composition of the soil organic matter.

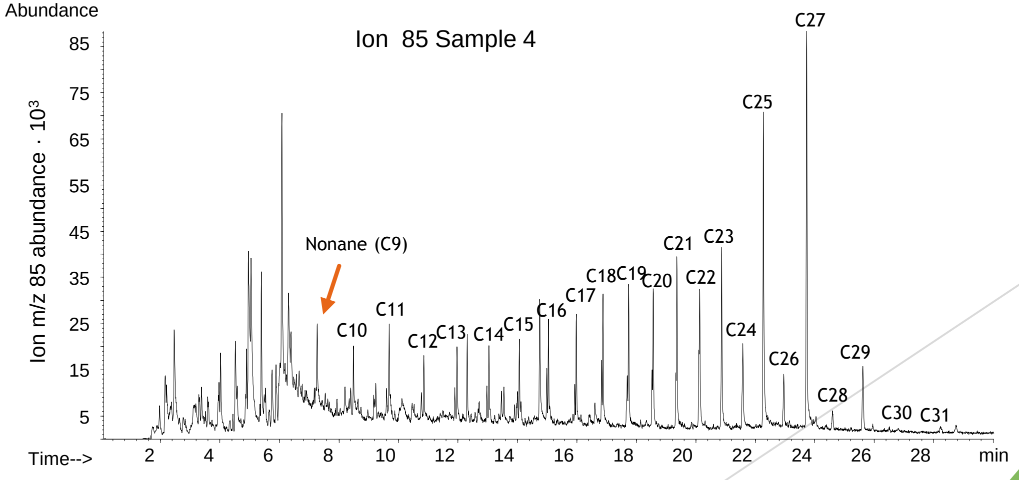
Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Pyrolysis-gas chromatography-mass spectrometry (Py-GC/MS)



In this case we used the ion trace at m/z 85 to identify the *n*-alkanes in pyrolysates from whole soil organic matter.

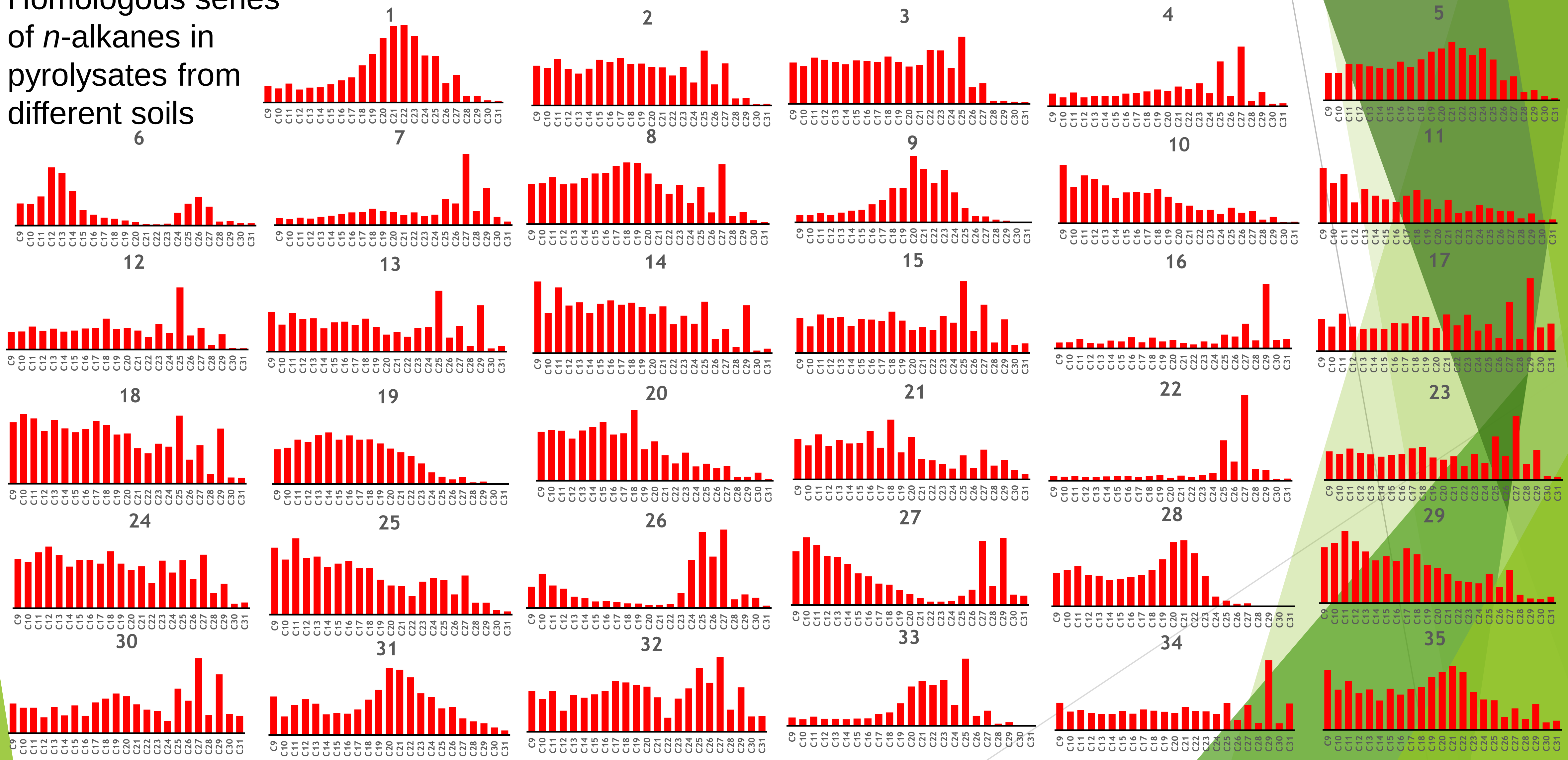


Finally, with the peak area integration values, we can compare the total abundances of *n*-alkanes of each sample.

Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Homologous series of *n*-alkanes in pyrolysates from different soils



Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Shannon Wiener index (*H*)

As a heterogeneity measure, the Shannon index takes into account the degree of evenness in species abundance. Typical values are between 1.5 and 3.5.

In this work we calculated Shannon Wiener indices for five different groups of alkanes.

- Total alkane range: from C9 (nonane) to C31 (hentriacontane)
- Odd C-numbered alkanes
- Even C-numbered alkanes
- Alkanes with more than 20C
- Alkanes with less than 20C

Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

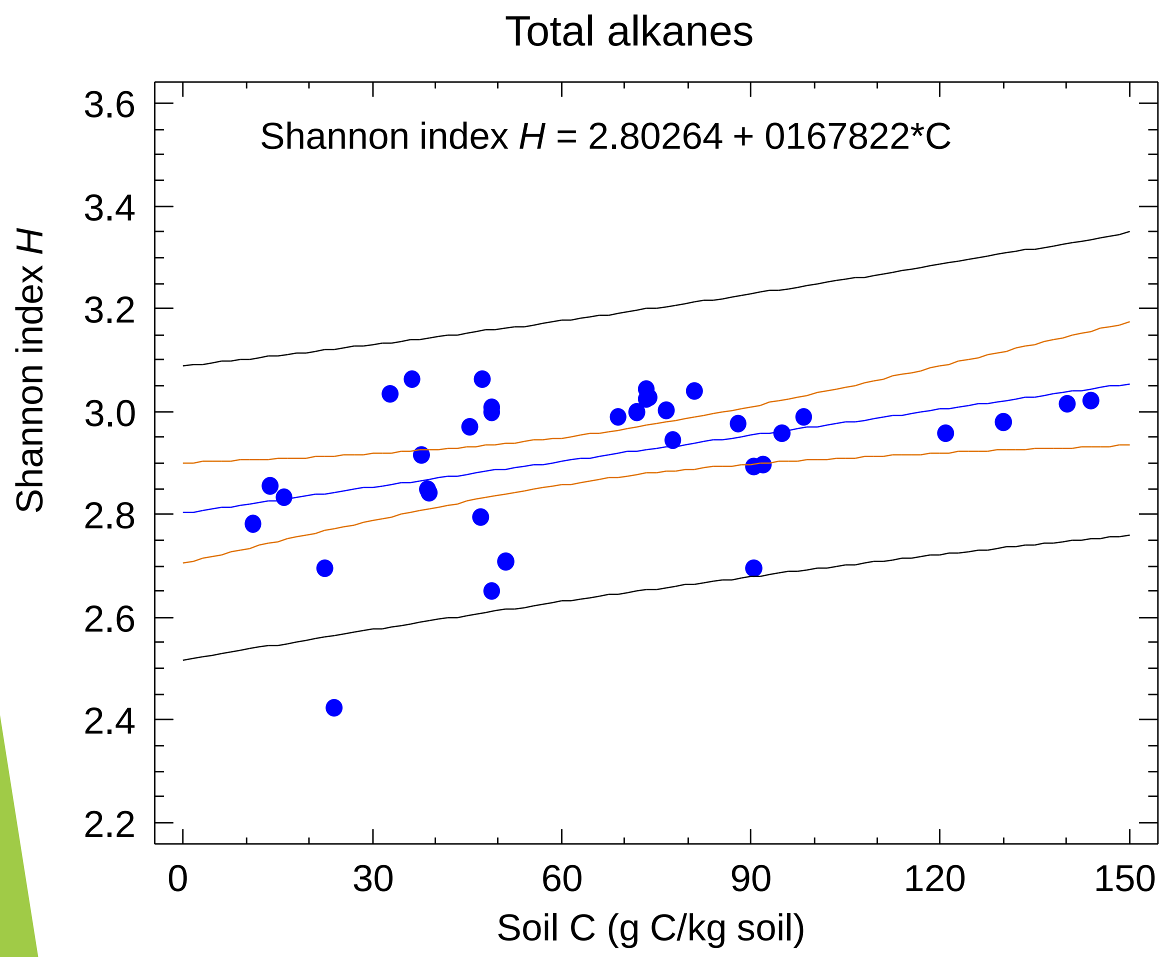
	Shannon Wiener index (H)				
Sample	**Total alkanes**	**Odd C-numbered alkanes**	**Even C-numbered alkanes**	**Less than 20C**	**More than 20C**
1	2.8421	2.2156	2.0777	2.3303	2.0103
2	2.9906	2.355	2.2481	2.4786	2.0909
3	2.9587	2.3117	2.2205	2.4823	1.9887
4	2.8958	2.2394	2.3092	2.4643	2.0472
5	2.9997	2.3551	2.2558	2.4663	2.1167
6	2.6959	2.0716	1.9345	2.1853	1.9084
7	2.8567	2.1103	2.3338	2.4362	2.0732
8	2.9776	2.3594	2.2085	2.4729	2.1034
9	2.7095	2.0651	1.9676	2.199	1.8098
10	2.8936	2.2547	2.1496	2.4446	2.2062
11	2.9439	2.2963	2.2209	2.418	2.2646
12	2.9702	2.3208	2.2622	2.4729	2.0431
13	3.001	2.3866	2.2608	2.4618	2.1261
14	2.9988	2.3955	2.2255	2.4685	2.1572
15	3.0446	2.4103	2.3202	2.473	2.2138
16	2.7945	2.0455	2.3463	2.4519	1.968
17	3.0616	2.4237	2.3617	2.4673	2.2729
18	3.0266	2.4091	2.2563	2.4787	2.2093
19	2.8499	2.2122	2.0985	2.4773	1.9106
20	2.9145	2.2789	2.1614	2.467	2.2014
21	3.0095	2.3942	2.2349	2.4634	2.3082
22	2.4221	1.6977	2.1659	2.4722	1.7551
23	3.0216	2.3742	2.3167	2.4754	2.1606
24	3.0395	2.4136	2.2776	2.476	2.2268
25	2.9814	2.3386	2.2406	2.4567	2.2155
26	2.6521	1.9405	2.0035	2.2385	1.916
27	2.8335	2.1998	2.0955	2.3637	1.8716
28	2.7811	2.1408	2.0323	2.4493	1.5167
29	2.9567	2.3205	2.2053	2.4646	2.2189
30	3.0359	2.3962	2.3398	2.4473	2.2464
31	2.9904	2.3447	2.2482	2.4121	2.1677
32	3.0618	2.4285	2.3199	2.4641	2.2641
33	2.6938	2.0419	1.9996	2.2682	1.9003
34	3.0153	2.3825	2.3479	2.4741	2.1859
35	3.0236	2.4019	2.2579	2.4652	2.1942

With the total abundances calculated for the different *n*-alkanes released by pyrolysis from each soil sample, and using the software "Species Diversity & Richness II version 2.5" we obtained the values of *H*. These values are different for each group of *n*-alkanes.

Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Simple regression (Shannon vs C) for total alkanes



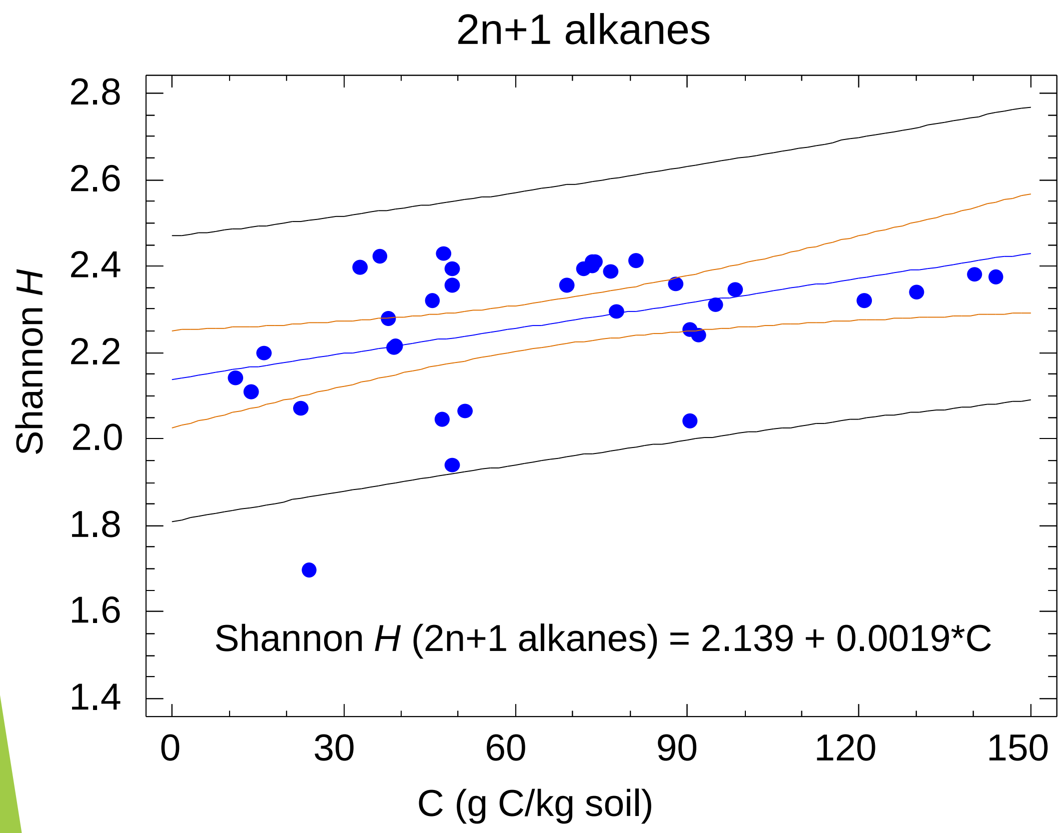
In the linear correlation models between alkane biodiversity and total soil organic C, the *P*-value is 0.014, *i.e.,* there is a statistically significant relationship between *H* and C at the 99% confidence level.

The higher the alkane biodiversity, the greater the amount of organic C stored in the soil

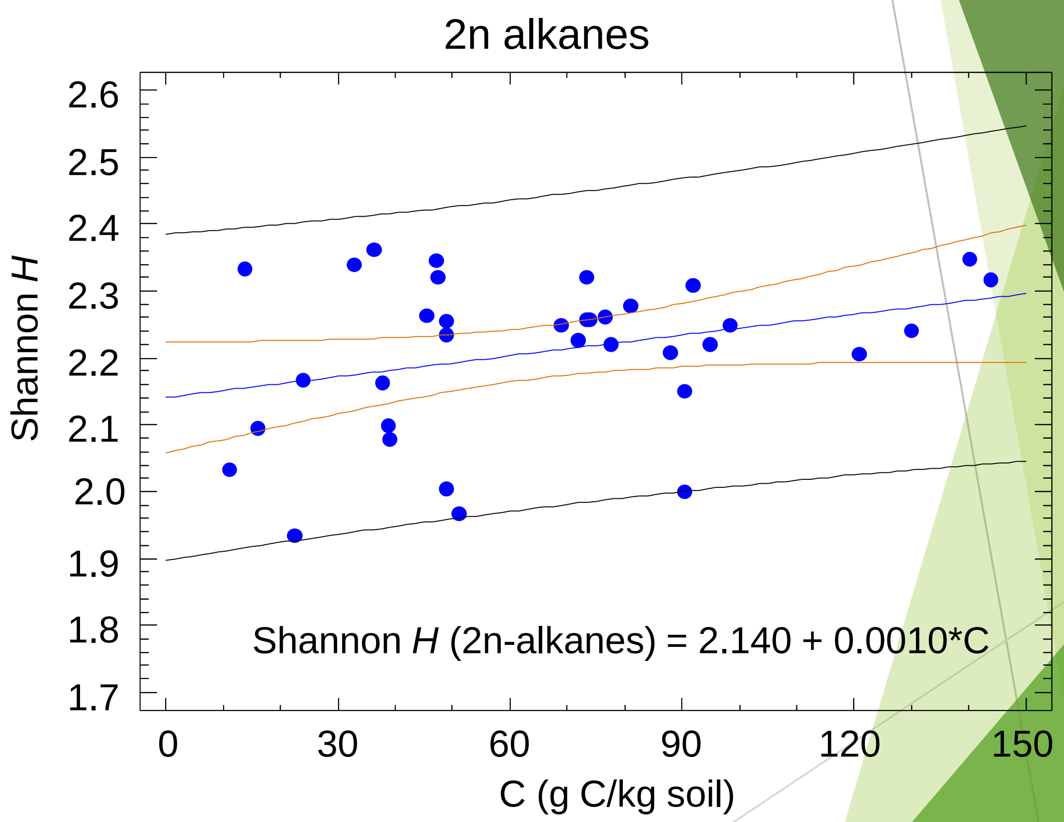
Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Simple regression (Shannon vs C) for 2n+1 and 2n C-numbered alkanes



P-value= 0.014

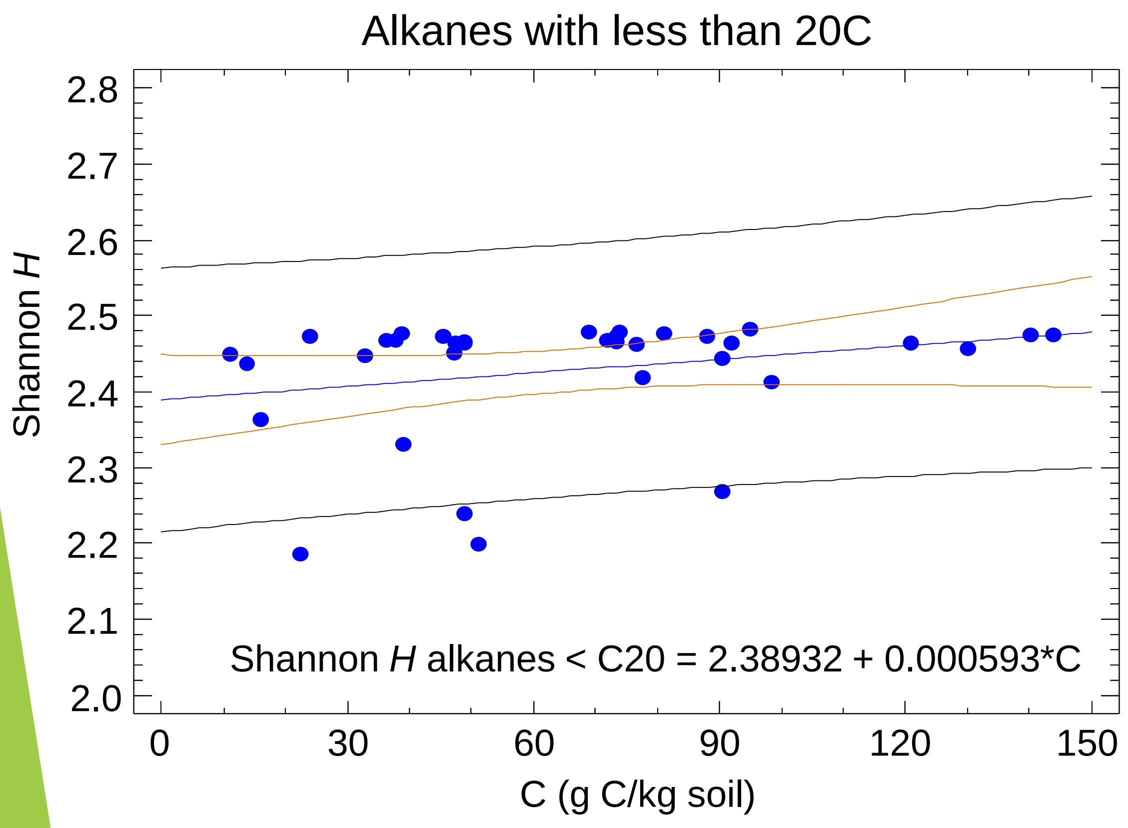


P-value= 0.069

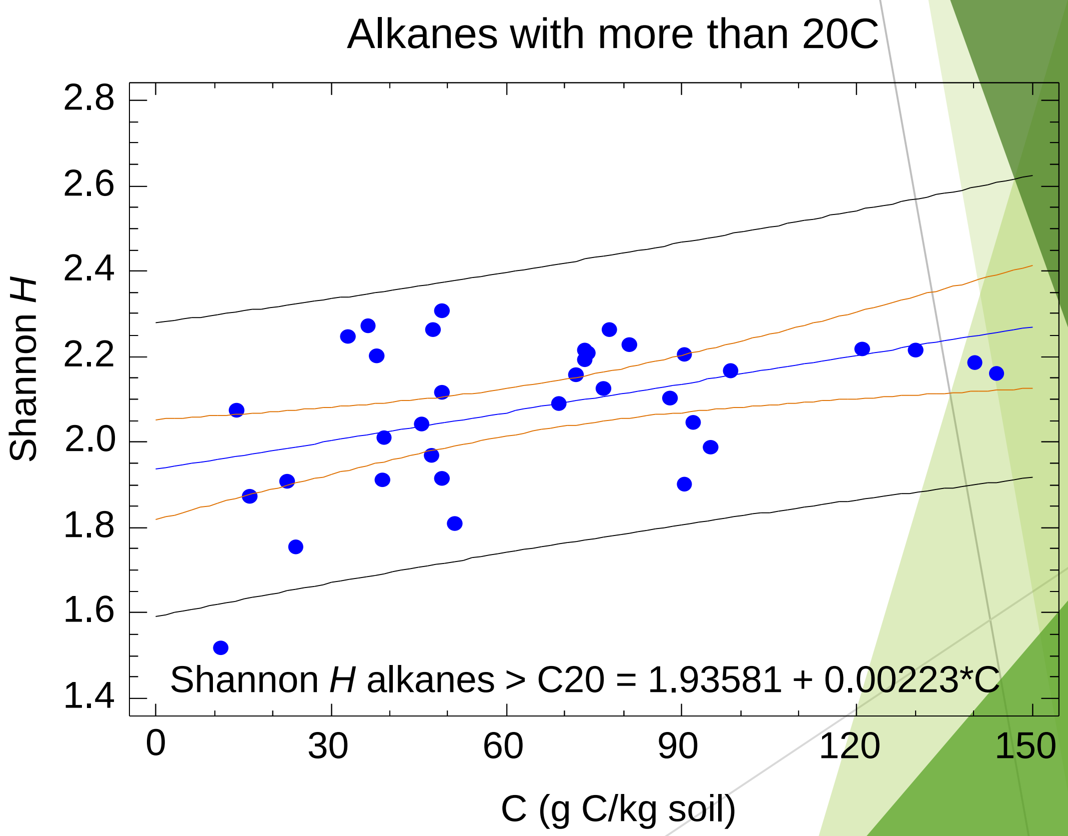
Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Simple regression (Shannon vs C) for alkanes <20C and >20C



P-value= 0.141

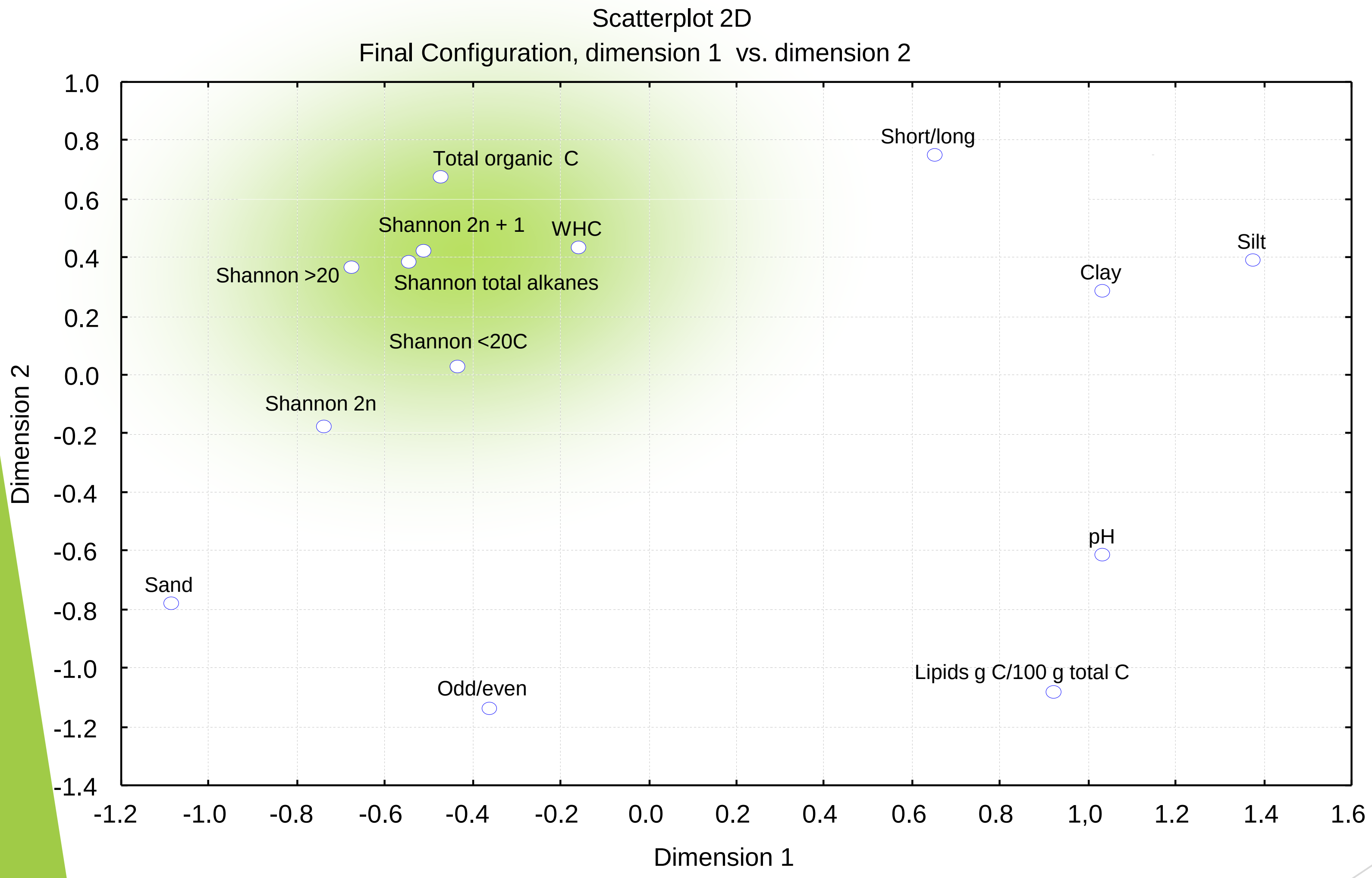


P-value= 0.007

Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Multidimensional scaling (MDS)



Multidimensional scaling illustrates the more or less close relationship between soil C concentration and molecular proxies derived from the analysis of soil lipids. For this statistical treatment the 1- Pearson *r* index was used as distance measure. Of the different factors considered, the Shannon's diversity indices calculated from the molecular assemblages of alkanes were those more significantly paralleling the observed values soil organic C.

Improved chemometric methodologies for the assessment of soil carbon sequestration mechanisms

Jiménez-González et al. MNCN-CSIC. Madrid (Spain)

Conclusion

The results show that a relation exists between the molecular composition of alkanes and the organic C content of the soils.

Although the total content of alkanes show a significant relationship with the soil C content, these correlations are more significant in the case of the odd-C numbered and the long-chain (> C20) *n*-alkanes, which present low *P*-values (0.014 and 0.007 respectively).

With the present exploratory approach we can forecast factors involved in the soil C sequestration process, despite unraveling the exact mechanisms of C stabilization would require additional research. Nevertheless, the chemometric approach used was especially helpful in the assessment of the extent to which these factors can be relevant at this respect.