

TRANSLATING ANALYTICAL PYROLYSIS FINGERPRINTS OF SOIL ORGANIC MATTER TO CLIMATIC VARIABLES



Marco A. Jiménez-González ^{1,2*}, Ana M. Álvarez ², Pilar Carral ², José A. González-Pérez ³, José M. De la Rosa ³, Nicasio T. Jiménez-Morillo ⁴, Francisco J. González-Vila ³, Gonzalo Almendros ¹

*majimenez@mncn.csic.es

(1) National Museum of Natural Sciences (CSIC), c/Serrano 115b, Madrid (Spain)

(2) Autonomous University of Madrid (UAM), c/Francisco Tomás y Valiente 7, Madrid (Spain)

(3) MOSS Group, IRNAS-CSIC, Av. Reina Mercedes 10, Sevilla (Spain)

(4) HERCULES Laboratory, University of Evora, Largo Marquês do Vimioso, 8, Évora (Portugal)

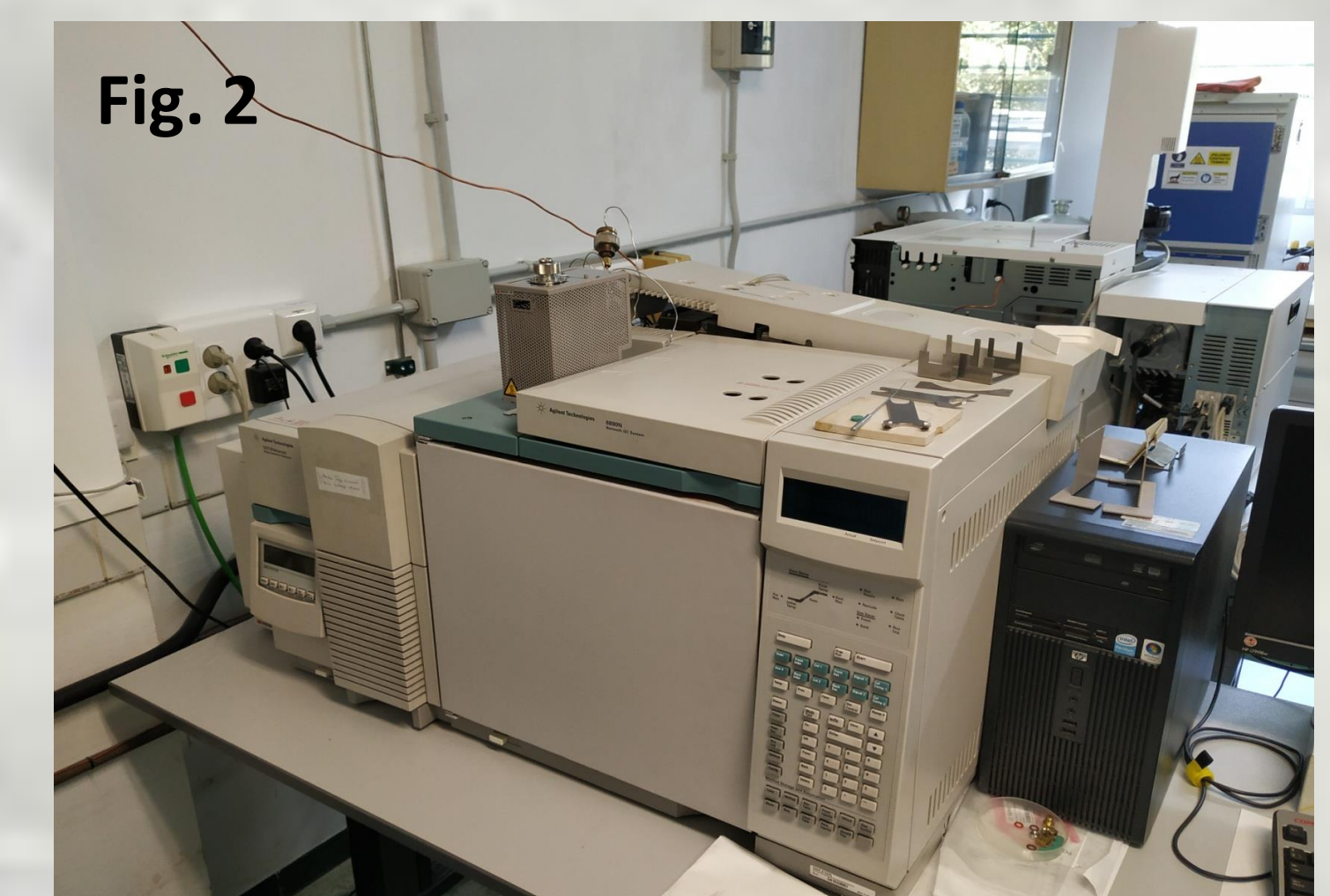
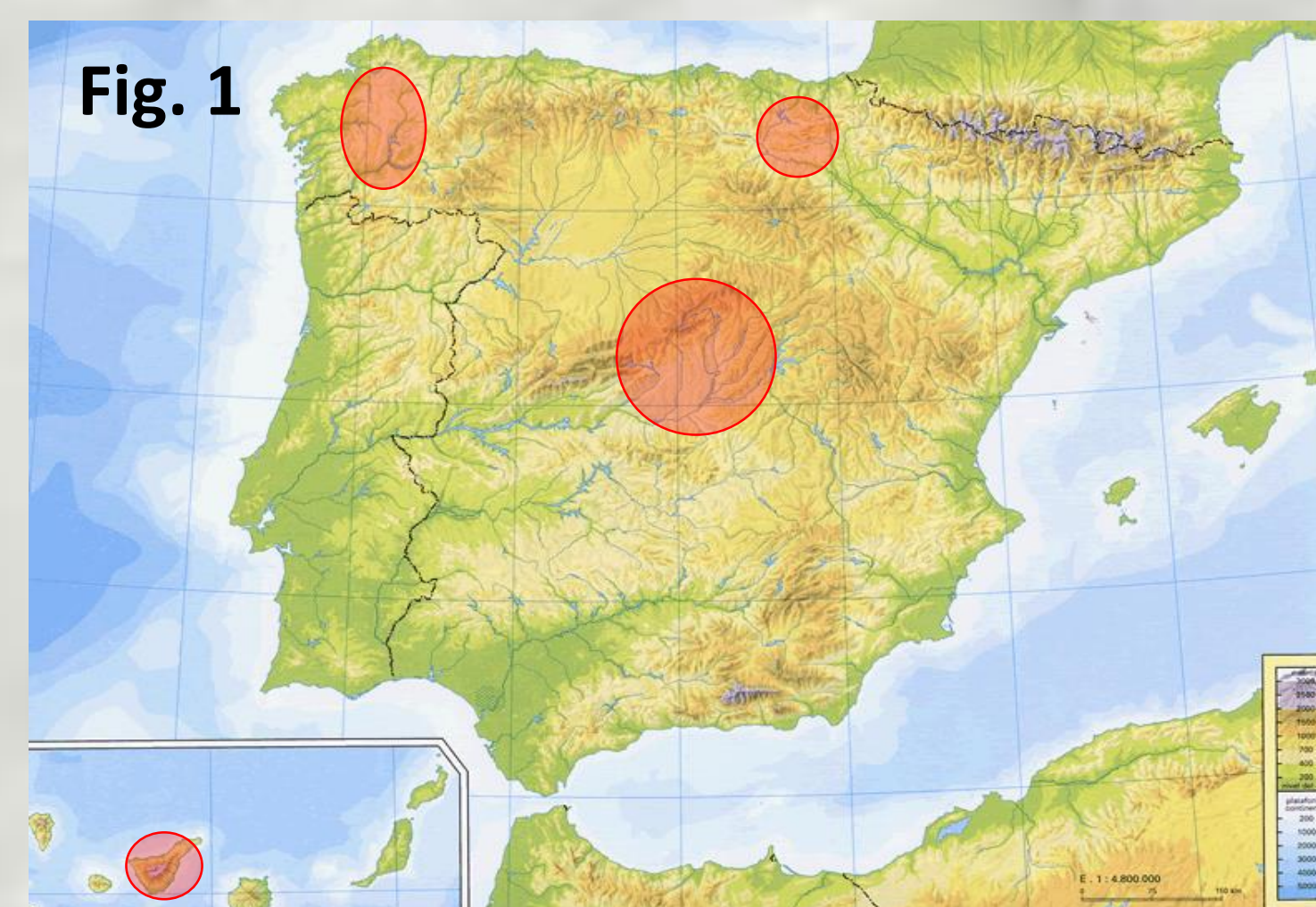


INTRODUCTION

The progressive degradation of soils due to climatic factors in conjunction with unsuitable environmental management and agricultural practices is a global issue of current interest. In particular, the progressive degradation of soil structure, which is associated to soil organic matter (SOM) depletion with an important cementing capacity, is responsible for an increased risk of soil erosion and the substantial loss of physical and chemical fertility of soils, mainly in semiarid environments. Presumably, all these aspects are reflected in the molecular SOM composition. Previous studies have evidenced that a correlation exists between the carbon content and the relative abundance of specific SOM constituents, e.g., alkane homologous series or lignin-derived methoxyphenols. This study aims to identify molecular descriptors of the SOM, which can vary significantly as a function of aridity levels.

MATERIAL AND METHODS

A total of 30 soil samples were collected from different areas of Spain (Fig. 1). The sampling was carried out in the topsoil (0–10 cm) where the SOM content is higher. The SOM was analyzed by pyrolysis - gas chromatography mass spectrometry (Py-GC/MS) of whole soil samples (Fig. 2).



RESULTS AND DISCUSSION

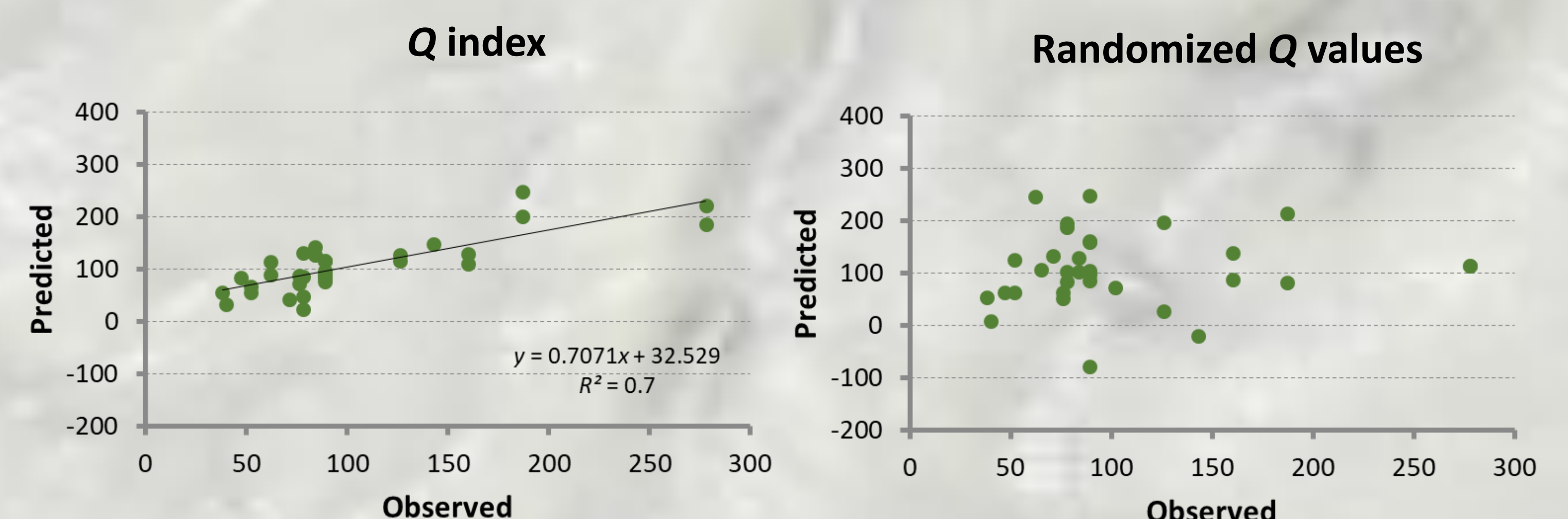
In order to assess desertification levels we used the Emberger's index (Q). This index was calculated from the annual rainfall and temperatures average for each soil sampling point. A total of 193 pyrolytic compounds were identified, and used as predictor variables in partial least squares (PLS) regression models forecasting the Emberger's index.

$$Q = \frac{100 \times P}{(M^2 - m^2)}$$

where P = annual precipitation (mm); M = average of the highest temperature of the warmest month, m = average of the lowest temperature of the coldest month

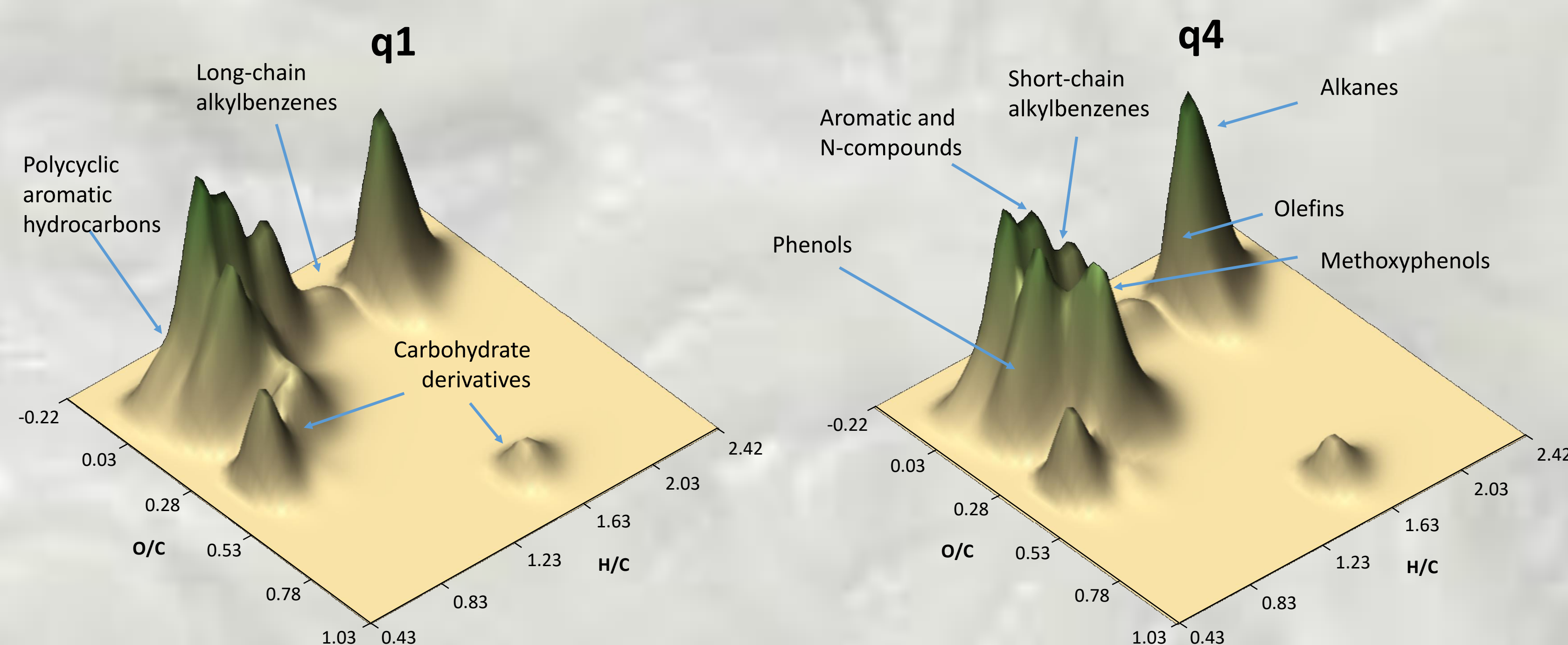
Partial least squares regression (PLS)

The PLS was used to explore the utility of the pyrolytic compounds as predictors of the Emberger's index and to verify if there is a relationship between SOM composition and aridity index. Randomized Emberger's index values were used to check for overfitting in the model.



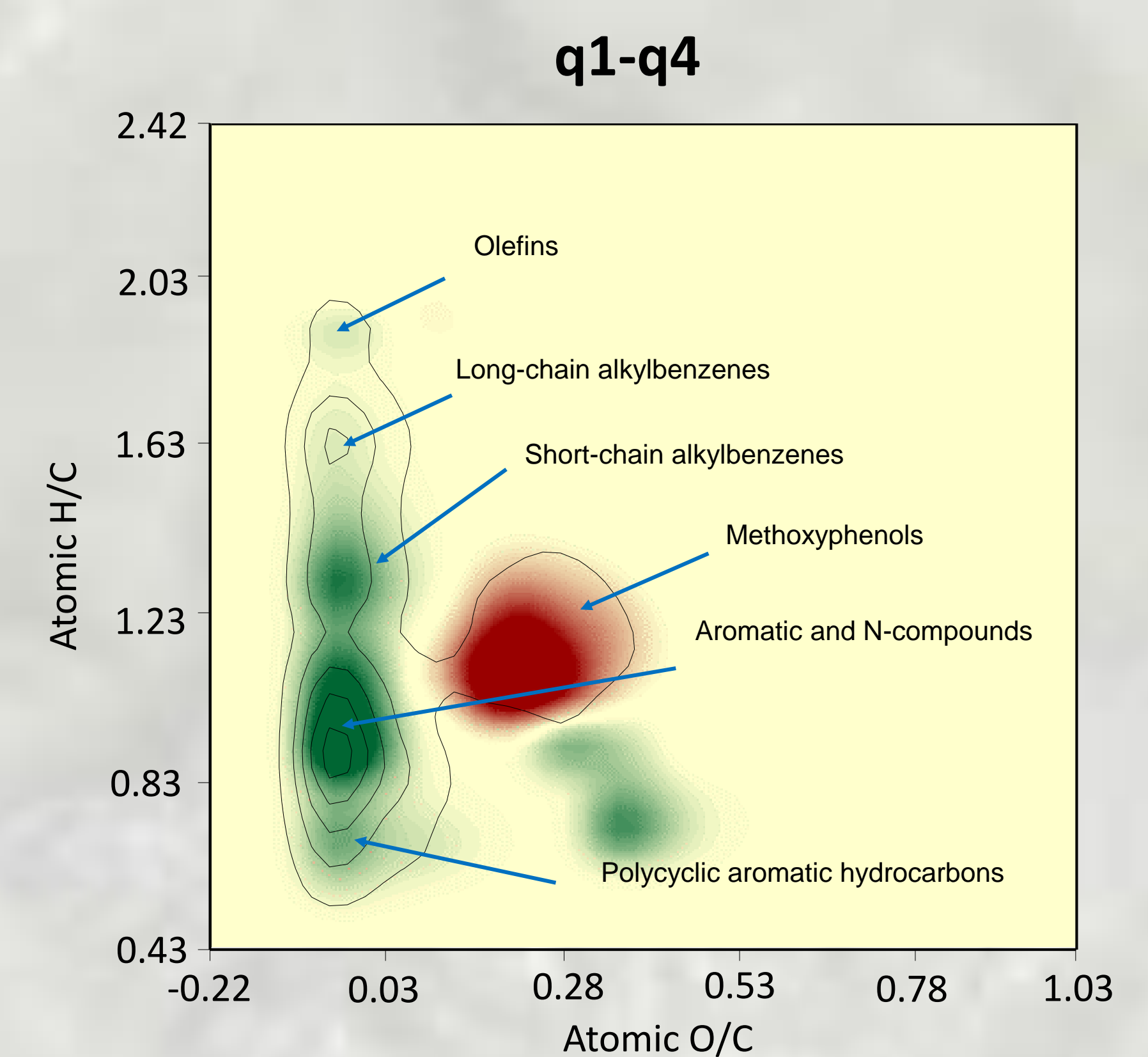
Composition of soil organic matter (SOM) in different soils

Samples were ordered according to the Emberger's indices in the corresponding sampling points, then the average compound composition of the SOM of the 1st quartile (q1) and the 4th quartile (q4) were selected. The subtraction between compounds proportions from soils of these extreme quartiles (q1-q4) was represented in a 2D van Krevelen diagram where products that accumulate in humid climate appear in green colour, and those that are more characteristic of warm climate appear in red.

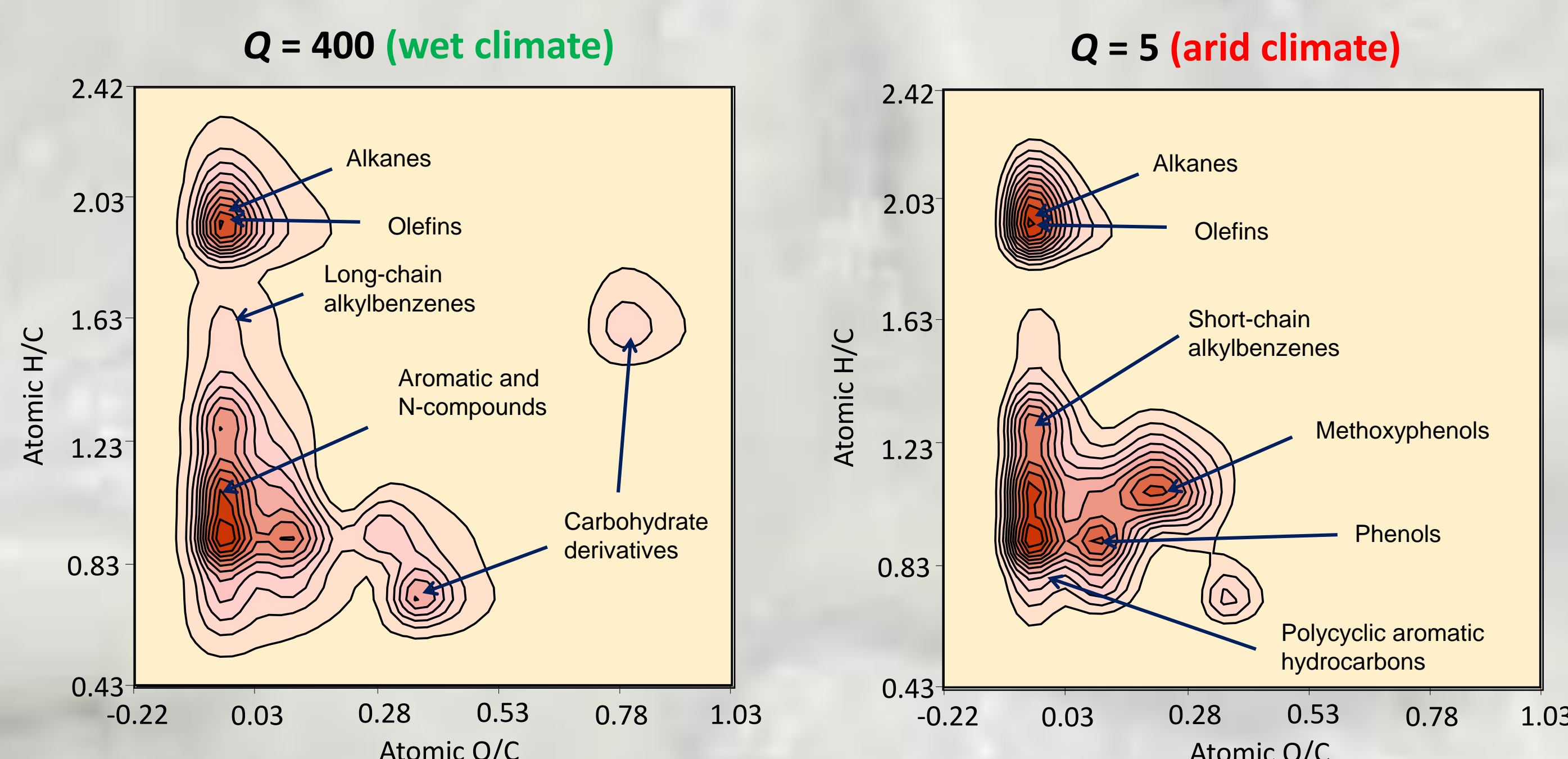


Subtraction between compounds proportions (q1-q4)

Student's t values at $P < 0.1$ are also shown as a superimposed contour diagram.



Simulation models were carried out to predict the composition of the SOM for extreme climatic scenarios of high or low aridity. i.e., extreme humid conditions ($Q = 400$) and extreme arid conditions ($Q = 5$).



CONCLUSIONS

The Py-GC/MS present a large potential not only as fingerprinting technique, but also to identify the origin and transformation of the SOM and to monitor environmental changes reflected in its molecular composition. In this case, it could be demonstrated that a reduced set of the 193 major pyrolysis compounds had an interesting value as bioclimatic proxies.