Compositional data analysis as a potential tool to study the (paleo)ecology of calcareous nannoplankton from the Central Portuguese submarine canyons (W off Portugal)

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Submarine canyons are deep and steep incisions on the continental margins. The physical forcing mechanisms linked with these marine systems, such as the enhancement of upwelling and bottom sediment resuspension, are expected to provide a nutrient source that will increase phytoplankton density (Hickey, 1995, Kampf,2006).

Coccolithophores are the predominant phytoplanktonic group within the calcareous nannoplankton and their sensitivity to a variety of surface water environmental parameters makes them important markers of oceanographic processes and proxies of sea surface water masses and temperatures, productivity and past climate changes (*e.g.* Ziveri et al., 2004; Silva et al., 2008).

In the present work we propose to test compositional analysis (Buccianti & Esposito, 2004; Pawlowsky-Glahn & Egozcue, 2006) as a tool to: a) achieve a clearer distinction between opportunistic coastal-neritic species (r-strategists) and typical oceanic species (k-strategists) in the central Portuguese margin, and b) to identify a coccolith assemblage that might reflect favorable environmental conditions found in the vicinity of the canyon that promotes the productivity of calcareous nannoplankton. Our main difficulty will be in distinguishing the ecological signal from the effects of other environmental factors mentioned before (i.e. advection, dissolution, bottom resuspension). One way to infer the species' ecological inter-relationships is by determining species relative percentages. The main concern is how the closure problem and the inconsistency of percentage determinations will affect our results. Compositional analysis was designed to provide more reliable and thus representative results, since the inference made on the coccolith assemblage features from which the data are drawn is correctly performed from a theoretical point of view (Buccianti & Esposito, 2004). Here, we present the first insights from applying compositional data analysis to coccolith assemblages from 85 surface sediment samples collected from the central Portuguese margin.

1 Introduction

Cocolithophores are the major component of calcareous nannoplankton with an outstanding fossil record provided by open ocean sedimentation (Ziveri et al., 2004). Although this group is generally studied in the oceanic domain where the highest abundances and paleobiodiversity occur, several studies have already proven their ability to profit from the high nutrient conditions driven by coastal upwelling (e.g. Silva et al., 2008). Our research school has been more focused in the occurrence of calcareous nannoplankton in shallower environments (neritic and coastal domain; Cachão & Moita, 2000; Guerreiro et al., 2005; Alday et al., 2006; Narciso et al., 2006) whereby one of our main goals is to investigate the (paleo)ecology of oceanic (K-selected) *vs.* neritic (r-selected) *taxa* along offshore-coastline transects.

As submarine canyons are known for creating regions of enhanced biological productivity (e.g. by enhancement of upwelling near the canyons; Hickey, 1995; Kampf, 2006) our goal is to investigate the role of the Central Portuguese canyons in the (paleo)ecology of calcareous nannoplankton. The Nazaré canyon (NC) and the Lisbon-Setúbal canyon (L-SC) are the two largest canyons cutting across the W Portuguese margin, both exhibiting a transition from erosive proximal to more depositional distal sections (Arzola et al., 2008) and acting as preferential dispersal pathways of particulate matter and attached pollutants from the coast directly to the deep sea

(Richter et al., 2009). Despite these similarities, there are differences between the present day functioning of the two canyons; while active particle resuspension and transport occurs from the upper to the lower NC, the L-SC is mainly trapping vertical particle flux (De Stigter et al., 2007; De Stigter et al., in prep., unpublished data).

Our main difficulty will be in distinguishing the ecological signal from the taphonomical one in such dynamic environments. The correspondence between the living coccolithophore communities and the assemblages preserved in the seabed surface sediments is quite complex and should be carefully considered since the coccolith sedimentary record results from the influence of several environmental factors: (1) phytoplankton productivity in the water column; (2) preferential settling and sorting, merely physically controlled and/or enhanced by biogenic forcing (*e.g.* zooplankton faecal pellets); (3) diagenetic dissolution in the water column and/or within the sediment; and (4) dilution with other sedimentary material. Furthermore, different time-scales are involved along the pathway from the upper photic layer to the bottom; while the coccolithophores observed in the superficial water column represent one instant of the annual productivity, the coccoliths preserved in the sediment-water interface represent the cumulative average of several months or years of productivity, depending on the sedimentation rate.

Determining the species relative percentage values from the absolute abundances (nanno/g) has been the standard analytical approach to circumvent the taphonomic effects and infer the species' ecological inter-relationships independently of the increasing terrestrial dilution effect and/or bottom dynamics near shore. However, the closure problem and the inconsistency of percentage determinations were never tested in terms of how they affect our results and may lead to spurious correlations and biased statistical analysis.

In the present study we want to test the Compositional Data Analysis (CODA) (Buccianti & Esposito, 2004; Pawlowsky-Glahn & Egozcue, 2006) in our data, by comparing results from the absolute and relative abundances (nanno/g and percentages, relatively) with the *Clr* values and compositional balances computed from CODA. The differences and similarities between the three approaches will be analysed and discussed.

2 Material and Methodology

The calcareous nannoplankton assemblages were determined from 85 surface sediment samples (top 0.5 or 1cm of 85 of box- and multicores) collected along six transects crossing the central Portuguese continental margin in approximately E-W direction (Figure 1): (1) two transects covering the NC and L-SC; (2) two transects covering a complete coast – open ocean section off Cape Mondego and Cape Sines, and (3) one transect covering the open continental slope of Estremadura Spur. Slides were prepared following the random settling procedure (Flores & Sierro, 1997) and observed under optical polarizing microscope (Olympus BX-40), at 1250× magnification. A minimum of 300 individual nannoliths was counted and identified in each slide to characterize calcareous nannoplankton assemblages and determine their absolute abundances, expressed as nannoliths per gram (nanno/g), calculated according to the following equation:

$$(1) \quad N = n \times \frac{V}{Vp} \times \frac{Pa}{Oa} \times \frac{1}{W}$$

Where, N = nanno/g, n = number of counted nannoliths, V = volume within the glass bottle (10.000μl), Vp = volume pipetted and injected into the Petri dish, Pa = Petri dish area, Oa = observed area (obtained by the number of vision fields, VF, at the microscope, multiplied by the unit area correspondent to the microscope field of vision; 1 FV Olympus BX-40 = 0.,02 mm2), and W = weight of the sediment sample.
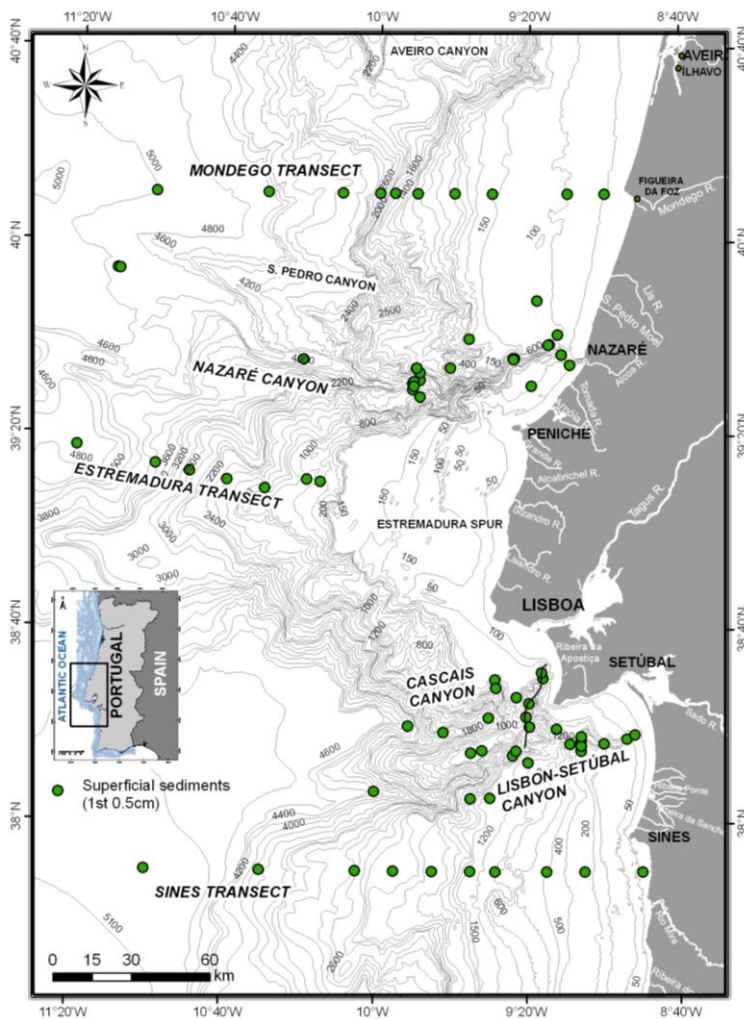
Figure 1. Geographical location map.

To minimize effects of diagenetic dissolution, only the larger and more resistant species (>3 micron) were considered for this study. We will target six species of coccolithophores, based on previously acquired knowledge on their ecological preferences: *Coccolithus pelagicus* (Cp), *Helicosphaera carteri* (Hc) and *Gephyrocapsa oceanic* (Go) are considered to be well adapted to more neritic/coastal environments, while *Gephyrocapsa muellerae* (Gm), *Calcidiscus leptoporus* (Cl), *Umbilicosphaera sibogae, Umbellosphaera irregularis* and *Rhabdosphaera* spp. are considered to be typically oceanic (Cachão, 1993; Cachão & Moita 2000; Guerreiro et al., 2005; Silva et al., 2008).

Taking into account that waters offshore Portugal register a weak coccolithophore ecological signal from oceanic warm currents driven along the Azores current (Cachão *et al.*, 2000) *U. sibogae, U. irregularis, Rhabdosphaera* spp. were grouped into one single taxonomic variable (UUR).

The species relative percentage values and all the subsequent calculations were determined from the absolute values and made by taking rigorously into account the sample space of compositional data (i.e. data matrices whose rows sum to 100%).

Firstly, we performed a comparison between the three possible approaches to investigate the (paleo)ecological behavior of the selected 6 species: absolute abundance values (nanno/g) *vs.* percentage values (Σ 6 spp(%) = Cp(%) + Hc(%) + Go(%) + Cl(%) + Gm(%) + UUR(%) = 100%) *vs.* ***clr*** values, where $Clr_{(i)} = LN(sp_{(i)} \times g(x))$ and g(x) is the sample geometric mean, calculated as

$$g(x) = \sqrt[n]{(sp1\% \times sp2\% \times ... \times spn\%)}$$, where *n* is the number of species, in our case 6. Nanno/g, percentage values and ***clr*** values of each species were plotted against the distance of each station to the coastline (expressed in km) and compared.

Secondly, five compositional balances were determined by applying a sequential binary partition (SBP) to the selected species, based on our previously acquired knowledge on their (paleo)ecological preferences. The SBP was performed by taking the whole group (6 species) and dividing it into two groups (e.g. 3 oceanic spp. *vs.* 3 neritic/coastal spp.). The resulting balance (β1) reflects the (geometric) mean behavior of the first group *vs.* the (geometric) mean behavior of the second group. Each group was subsequently divided again until each group was represented by one single species. The five calculated compositional balances (β) are calculated according to the following equations:

$$(2) \; \beta 1 \; \{Cl, Gm, UUR\} \; vs \; \{Cp, Hc, Go\} = \sqrt{\frac{3 \times 3}{3 + 3}} \times LN \frac{\sqrt[3]{Cl \times Gm \times UUR}}{\sqrt[3]{Cp \times Hp \times Go}}$$

$$(3) \; \beta 2 \; \{Cl, UUR\} \; vs \; \{Gm\} = \sqrt{\frac{2 \times 1}{2 + 1}} \times LN \frac{\sqrt[2]{Cl \times UUR}}{\sqrt[1]{Gm}}$$

$$(4) \; \beta 3 \; \{Cp, Hc\} \; vs \; \{Go\} = \sqrt{\frac{2 \times 1}{2 + 1}} \times LN \frac{\sqrt[2]{Cp \times Hc}}{\sqrt[1]{Go}}$$

$$(5) \; \beta 4 \; \{Cl\} \; vs \; \{UUR\} = \sqrt{\frac{1 \times 1}{1 + 1}} \times LN \frac{\sqrt[1]{Cl}}{\sqrt[1]{UUR}}$$

$$(6) \; \beta 5 \; \{Cp\} \; vs \; \{Hc\} = \sqrt{\frac{1 \times 1}{1 + 1}} \times LN \frac{\sqrt[1]{Cp}}{\sqrt[1]{Hc}}$$

3 Results and Discussion

3.1 Comparison between different analytical approaches

3.1.1 Species absolute abundances (nanno/g)

A general decrease of nanno/g values towards the coastline is visible from the plots of the six species, especially in the case of Cl (Figure 2). Such trend probably reflects the preferential oceanic nature of such phytoplanktonic organisms and in addition the increasing effect of terrestrial dilution and bottom sedimentary dynamics (e.g. resuspension transport, dissolution, diagenesis) as we move towards the coast. Both factors will affect all the six studied species, thus eventually masking the species' ecological inter-relationship. Therefore, using the species absolute abundances appears to enhance the taphonomic effects over the ecological signal.

Still it is apparent that such phenomena act differently in each studied transect; the W – E decreasing gradient is more evident along the ocean-coast transects than along the canyon transects. All species display higher nanno/g values in the upper canyons than in the adjacent margins at the same distance from the coastline. This indicates the role of the canyons either as morphological traps for particles in transit along the shelf, or as typical oceanic environments cutting across the continental shelf and bringing typical oceanic ecological conditions towards the coastal zone. Furthermore the canyons may be promoting/enhancing upwelling conditions near the coast (e.g. Hickey, 1995; Kampf, 2006).

All the species are generally more abundant in the upper L-SC than in the upper NC. This difference may result from dilution caused by the extremely high terrigenous sediment input in NC (De Stigter et al., 2007), while L-SC is mainly trapping vertical particle flux (De Stigter, in prep., unpublished data) and thus potentially providing better conditions to preserve the (paleo)ecological signal.

3.1.2 Species relative abundances (%)

A quite clear W-E gradient is evident from the distribution of the coccoliths relative abundances (%), namely a clear increase of the neritic/coastal species (Go and Hc) towards the coast, with the higher values located in the upper reaches of the canyons; Cp also reveals this general trend although weaker than the latter. Cl displays the opposite trend, clearly decreasing towards the coast; Gm and UUR display the same general decreasing trend, although less evident than Cl. The neritic/coastal species are particularly well represented in the upper NC while the oceanic species are more abundant in the upper L-SC (Figure 3).

The Mondego and Sines transects frequently show different (opposite?) trends which may be

related to differences in the bottom morphological/hydrodynamic conditions along the two transects (i.e. the Mondego transect has a much rougher bottom morphology than the Sines transect) and/or the presence of a N – S ecological gradient (more temperate and neritic/coastal species north of NC *vs*. more warm subtropical species south of S-LC).

All the species (except Cp) are clearly more abundant in the upper reaches of the canyons than in the adjacent W-E transects, at the same distance to the coastline.

As previously referred in section 3.1.1, this may reflect either (1) the role of the canyons as morphological traps of particles (taphonomic signal) and/or (2) the fact that both canyons are bringing typical oceanic ecological conditions into the coastal zone that will increase productivity of coccolithophores near the coast, (3) the enhancement of coastal upwelling (with subsequent increase of nutrients availability) in the upper canyons.

However, the canyons have different coccolith assemblages: L-SC has higher values of oceanic species while NC has higher values of neritic/coastal species. This indicates that each canyon has its particular ecological imprint closely related with each canyon's dynamics; (1) the higher values of neritic/coastal species in NC agrees with a more active and proximal canyon system which the opportunistic species (r-selected) are better adapted to; on the other hand, (2) the higher values of oceanic species in L-SC agrees with the hypothesis that this canyon represents a calmer environment, mainly trapping particles from vertical flux, and thus more favorable for the species with preference for stratified oceanic waters (K-selected).

3.1.3 Compositional Data Analysis (*clr* values)

The same general W – E trend obtained from species percentage values is also evident from CoDA results, with Hc and Go (and Cp) increasing towards the coastline and Cl and URR (and Gm) increasing in offshore direction (Figure 4). Go, Hc and Cl are the species that most clearly reflect the W – E gradient. Still, these relationships and trends are more pronounced using *Clr* values, since a lower dispersion between the different studied transects is visible.

Hc and Go are more abundant in the upper NC than in the upper L-SC. Cp is quite consistent all along the W – E section, both in the transects and canyons, except on Estremadura Spur where a conspicuous minimum is registered. Of the three oceanic taxa, Cl is the one showing the strongest W – E decreasing gradient.

Cl and UUR are more abundant in the upper L-SC and Sines transect in comparison with the upper NC and Mondego transect.

The general decrease of Gm towards the coast is quite evident in the Sines transect but it shows a very weak variation along the whole W – E section in the other sectors. This suggests that Gm is quite well adapted to both oceanic and coastal/neritic conditions.

All species show a W – E trend in the Estremadura Spur somewhat similar to the trend in the deeper part of the Mondego and Sines transect, except for what concerns Cp and Gm.

3.2 Compositional balances

β1 represents the (geometric) mean behavior of the oceanic species (Cl, UUR and Gm) *vs*. the (geometric) mean behavior of the neritic/coastal species (Hc, Go and Cp) and clearly shows a decreasing trend towards the coastline, particularly off Cape Sines and Cape Mondego, followed by NC. In the L-SC a more flattened trend is observed, confirming that this submarine canyon represents a more oceanic environment near the coast in comparison with the adjacent margin areas, and also with NC. The higher abundance of coastal/neritic species north of NC *vs*. the higher abundance of oceanic species south of NC is also visible here (N – S ecological gradient) (Figure 5).

β2 represents the (geometric) mean behavior of Cl and UUR *vs*. the (geometric) mean behavior of Gm, and suggests a clear decrease of Cl and UUR towards the coast in the Mondego transect and NC, while in the L-SC and Sines transect differences in the ecological behavior of the three oceanic species are less evident. Also here it is visible that Cl and UUR are slightly more abundant in the upper reaches of the L-SC in comparison with NC. Moreover it may also indicate that, among the
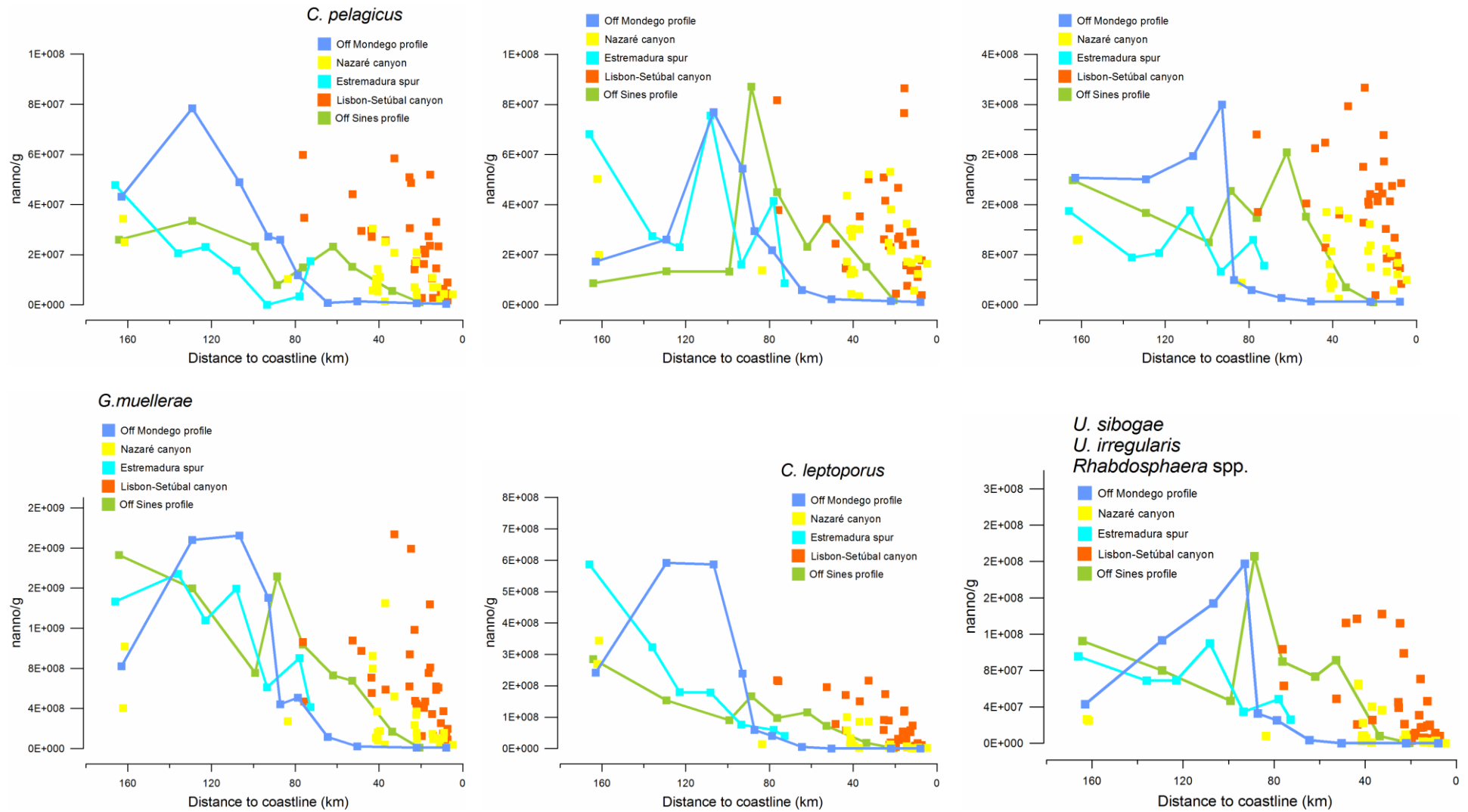
Figure 2: Species absolute abundances (nanno/g) plotted against distance to the coastline (m).
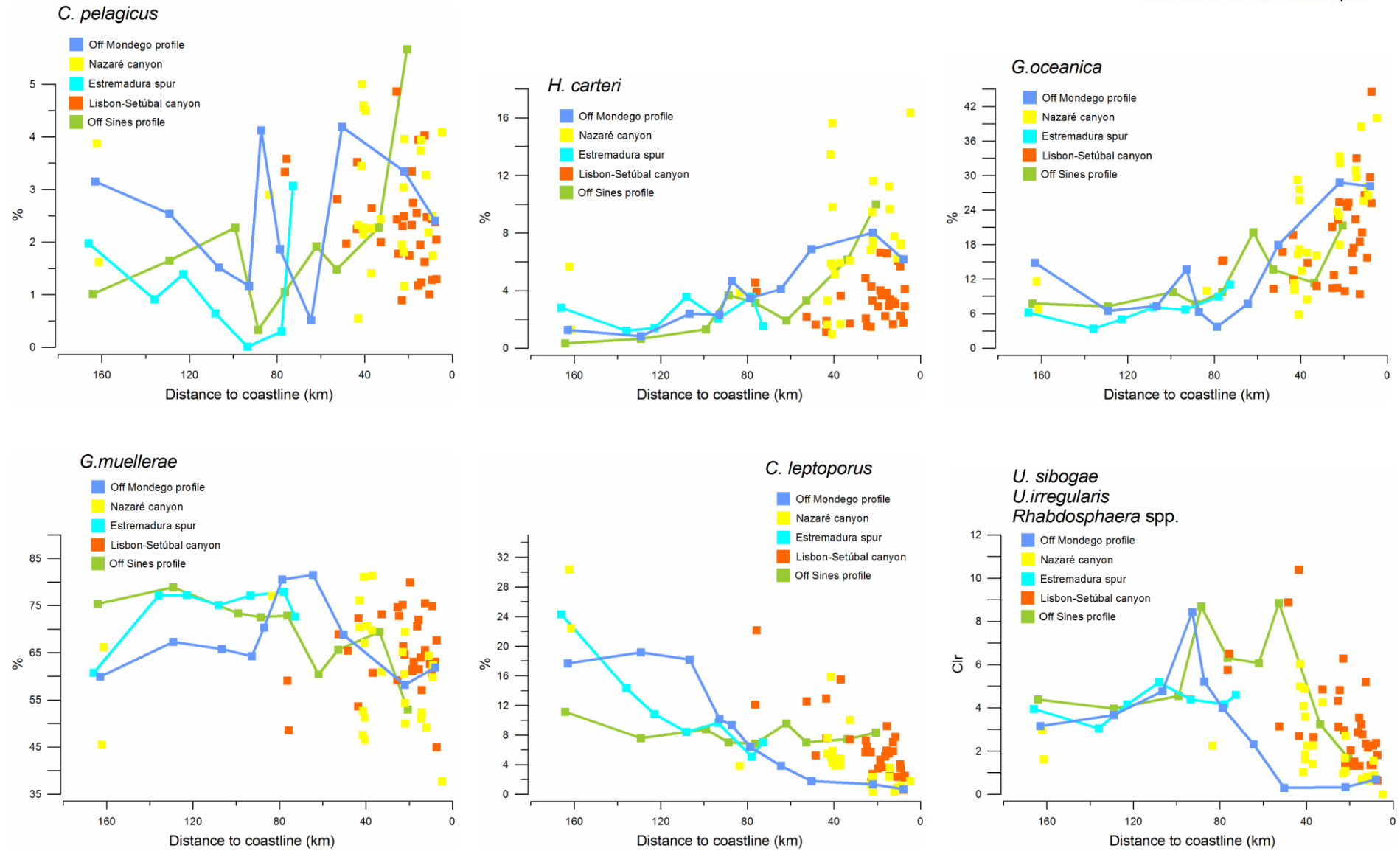
Figure 3: Species relative abundances (%) plotted against distance to the coastline (m).

oceanic species, Gm is the one better adapted to more coastal regions (Figure 5).

β3 represents the (geometric) mean behavior of Cp and Hc *vs*. the (geometric) mean behavior of Go, and suggests no significant difference in the ecological behavior between these three neritic/coastal species along the whole W-E section. Still, in the near shore part, the NC and Sines transect have slightly higher abundances of Cp and Hc than the L-SC and Mondego transect. In the offshore part, the NC and Estremadura Spur transect show the higher values of Cp and Hc. A positive and a negative anomaly of Cp+Hc are observed in the middle of the Mondego and Estremadura Spur transects, respectively (Figure 5).

β4 represents the (geometric) mean behavior of Cl *vs*. the (geometric) mean behavior of UUR, and suggests a weak decrease of Cl towards the coast, except in the L-SC and off Sines. A very high value of β4 is recorded in the upper NC. The L-SC shows no clear gradient due to high variability of values (Figure 5).

β5 represents the (geometric) mean behavior of Cp *vs*. the (geometric) mean behavior of Hc, and suggests no significant ecological difference between these two species in onshore-offshore direction, although a slight general decrease of Cp towards the coast is visible. Cp is generally more abundant in the L-SC while Hc is more abundant in the NC. A distinct minimum of Cp is recorded in the Estremadura Spur transect (Figure 5).

4 Preliminary conclusions

A quite clear W – E distribution gradient of calcareous nannoplankton, is visible in all the five studied transects. Such gradient suggests that the sediment samples did preserve the ecological signal despite the influence of several *post-mortem* processes affecting the coccoliths and the major differences in the environmental settings of each transect (e.g. canyons *vs*. off canyons). It is particularly well represented by the increase of neritic/coastal species (Hc and Go) and decrease of oceanic species (Cl and UUR) towards the coast. This is visible in both the relative percentages, *Clr* values and the compositional balances.

In addition to this general pattern, each transect has its own ecological signature, probably closely related with their particular oceanographic and/or ecological dynamics: (a) the upper canyon reaches always higher abundances than the adjacent margin areas; (b) the NC is more favorable to coastal/neritic (r- selected) species while L-SC shows a higher abundance of oceanic species (K-selected).

While NC is a very active submarine canyon cutting across the entire shelf almost to the beach, the L-SC is more distant from the coast, with it's head located at the shelf-break and thus providing more favorable conditions for typical oceanic species.

Along the Mondego transect coastal/neritic (Hc, Go) and temperate (Gm) species are relatively more abundant while along the Sines transect oceanic warm water species (UUR and Cl) are more abundant. On Estremadura Spur a W – E ecological gradient is observed which is very similar to that of the lower part of the Mondego and Sines transect for all species except Cp and Gm.

Although there is consistency in the general W – E trend obtained from both percentage and CODA (*clr* values and compositional balances), a lower scatter of values was obtained from the latter suggesting that Compositional Data Analysis is able to extract the real ecological trends and thus to perform more accurate (paleo)ecological interpretations on the calcareous nannoplankton assemblages from the central Portuguese margin. In the near future results presented here will be properly integrated with data from sediment grain-size and sediment accumulation rates, in order to evaluate the reliability of such (paleo)ecological trends.
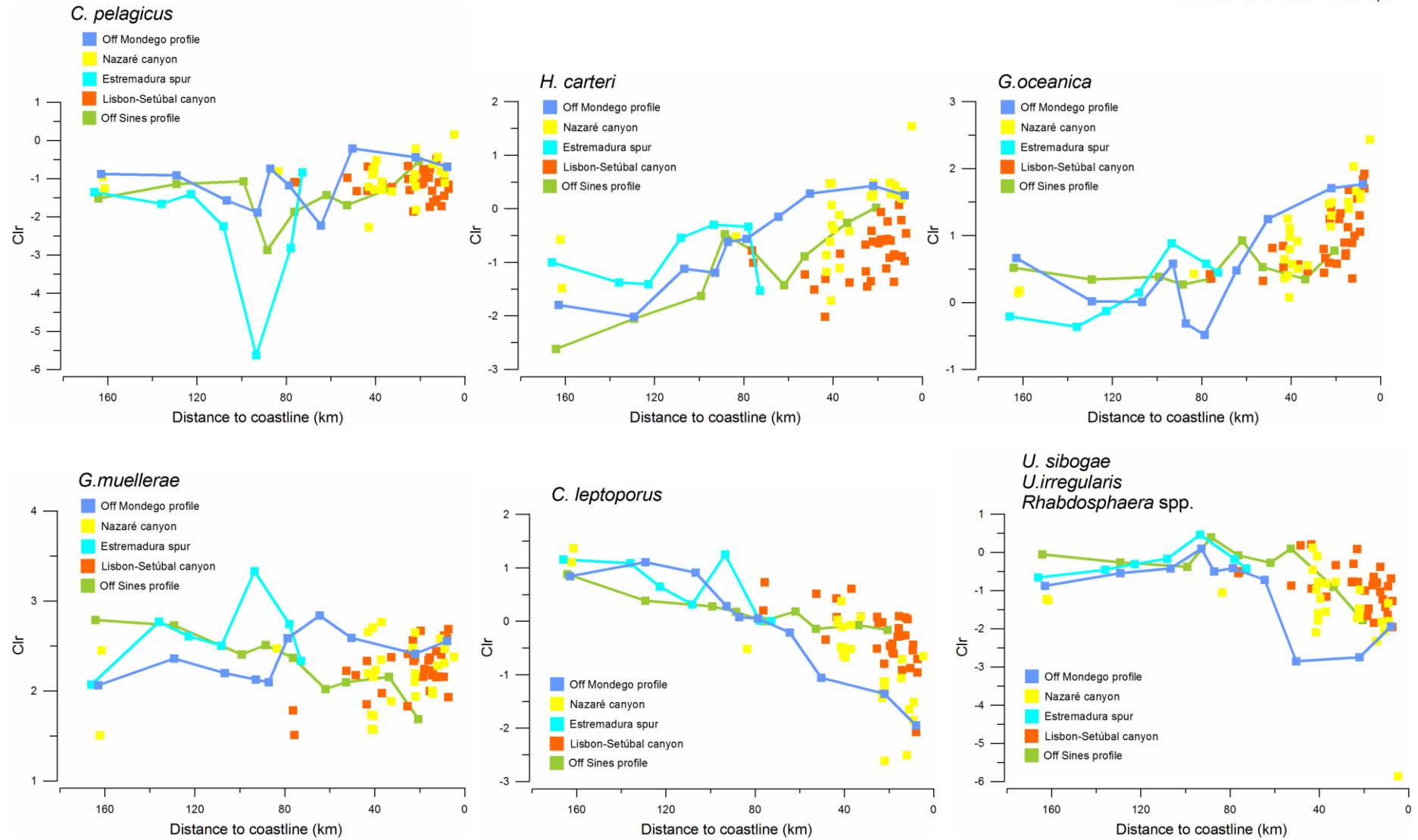
Figure 4: *Clr* values (CODA) plotted against distance to the coastline (m).
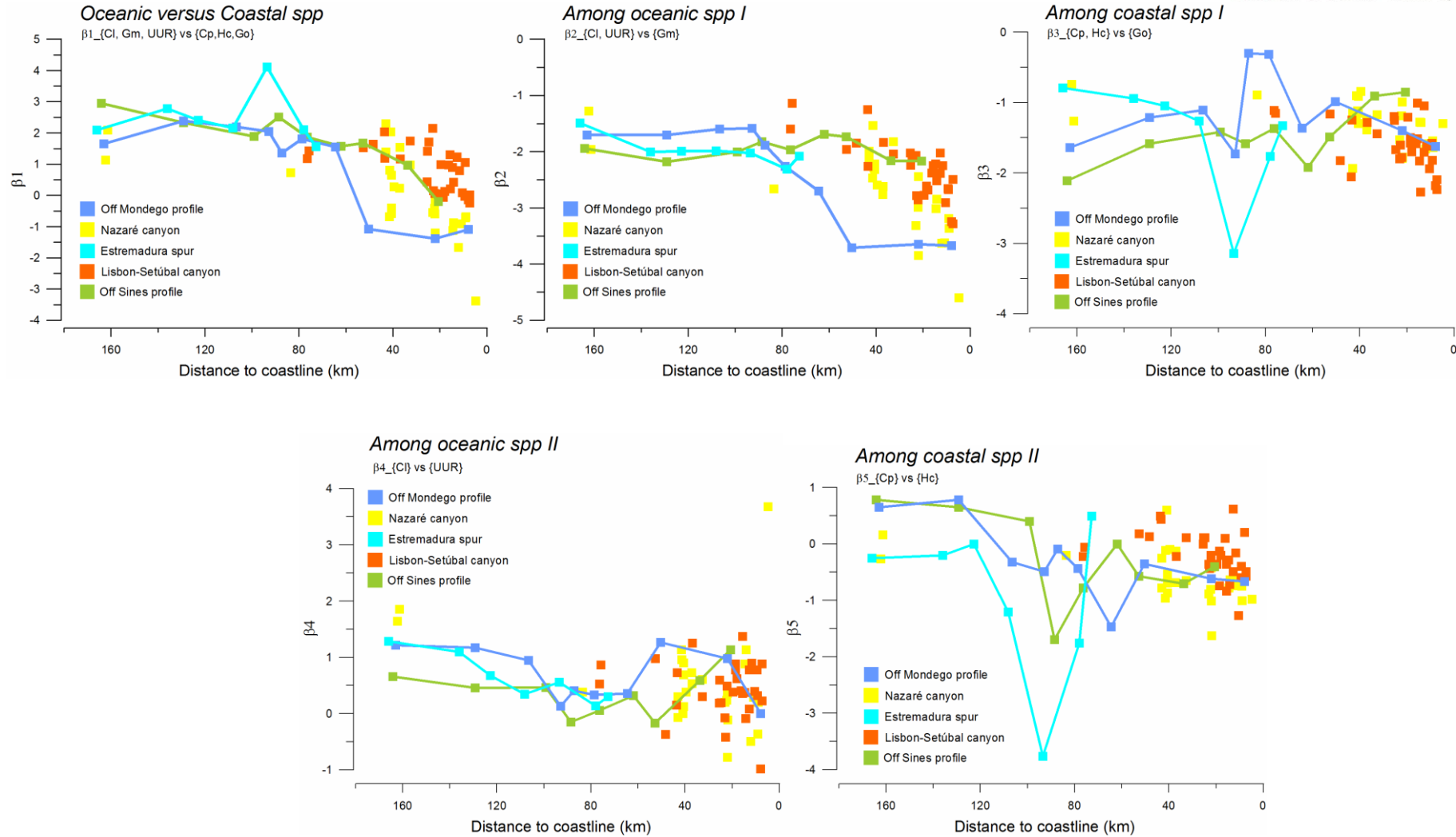
Figure 5: Compositional balances (CODA) determined by a Sequential Binary Partition (SBP) applied to an initial vector represented by six species (oceanic: Cl, UUR, Gm; and neritic/coastal: Cp, Hc, Go)

Acknowledgments

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