**Appendix: Clustering approach to identify seasonality based on δ18Oc and δ13C data in *T. sanchezi***

To test whether grouping of data based on the location within specimen **HU-027** captured the seasonal variability in temperature, the carbonate δ18Oc and δ13C values associated with the clumped isotope analyses on **HU-027** were used to assign statistical clusters. We clustered data within the specimen using K-means and Partitioning Around Medioids (PAM) clustering routines. The K-means routine groups datapoints in the δ18Oc-δ13C space into clusters minimizing the squared Euclidian distance between the points within a cluster using the iterative Hartigan-Wong algorithm coded in the “kmeans” fuction of the “stats” package in R (Hartigan and Wong, 1979; R Core Team, 2023; “stats package - RDocumentation,” n.d.). Clustering was repeated on the same dataset using the Partitioning Around Medioids (PAM) algorithm (Kaufman and Rousseeuw, 1990) using the “pam” function of the “cluster” package (Maechler et al., 2023). We used the Elbow method (Thorndike, 1953) and Silhouette method (Rousseeuw, 1987) to determine that the optimal number of clusters in this dataset was three or four. The Elbow method refers to choosing the point (“elbow”) in the plot of the amount of variance explained by each cluster where adding another cluster has diminishing returns. The Silhouette method picks the number of clusters whereby the Euclidian distance within the clusters in minimized relative to the Euclidian distance between clusters (“silhouette score”;(Rousseeuw, 1987)).

The “Elbow plot” (**Figure 1A**) highlights that increasing the number of clusters beyond 3 or 4 does not significantly reduce the within-cluster variability. At the same time, the Silhouette score (**Figure 1B**) shows a maximum value at three clusters. We therefore decided that three or four is an optimal number of clusters for this stable isotope dataset, which matches with the four location-based groups in the **HU-027** data. The δ18Oc, δ13C and Δ47-based temperature values for different numbers of clusters (three or four) and different clustering algorithms (K-means clustering and the “Partitioning Around Medoids”, or PAM, algorithm) are plotted in **Figure 2**, while clustering based on the locations of samples in the shell results in the pattern shown in **Figure 3**. We found that adding a fourth cluster results in two out of four clusters (spring and autumn clusters) having very similar mean Δ47 values, and that the difference between K-means and PAM clustering is negligible. The δ18Oc, δ13C and Δ47 statistics of all four statistical clustering options as well as the location-based approach are provided in **Table 1**. Overall, clustering by location achieves similar or higher differences in δ18Oc, δ13C and Δ47 between groups.

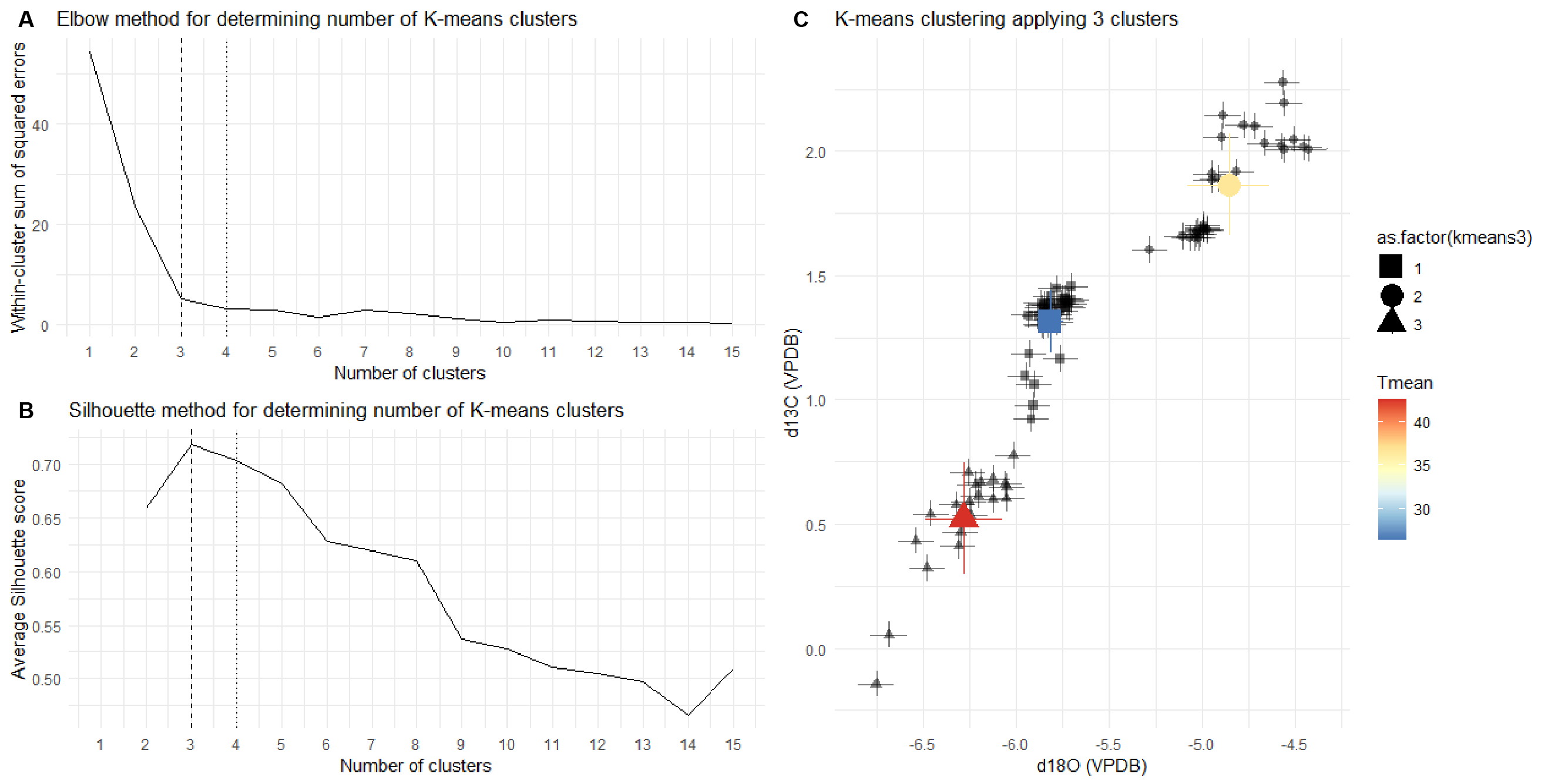


Figure 1: Overview of clustering decision plots using the Elbow (**A**) and Silhouette (**B**) method.

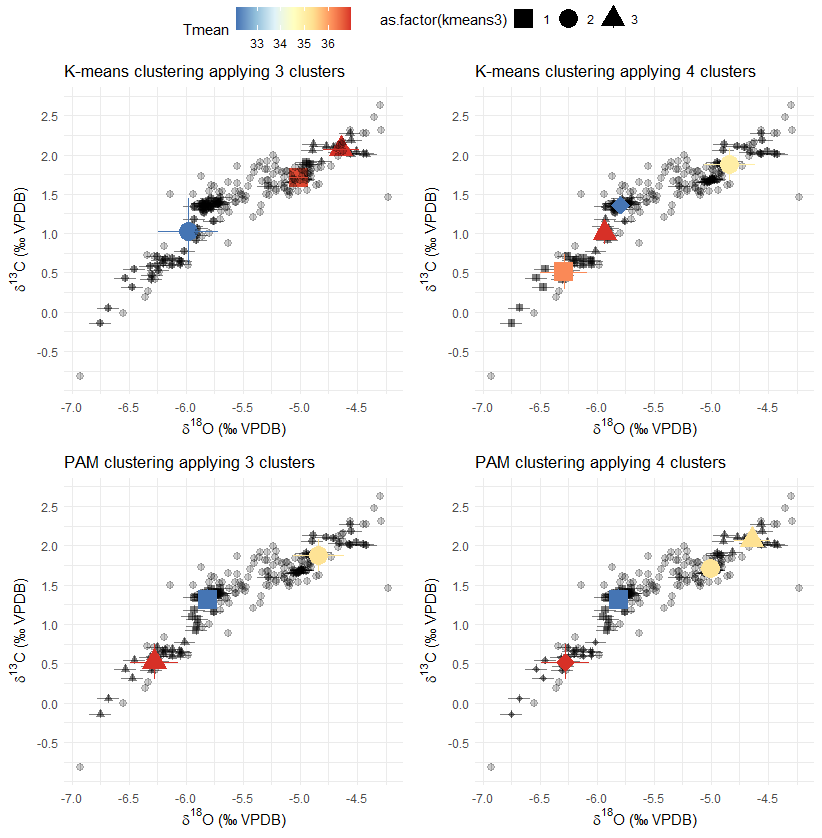
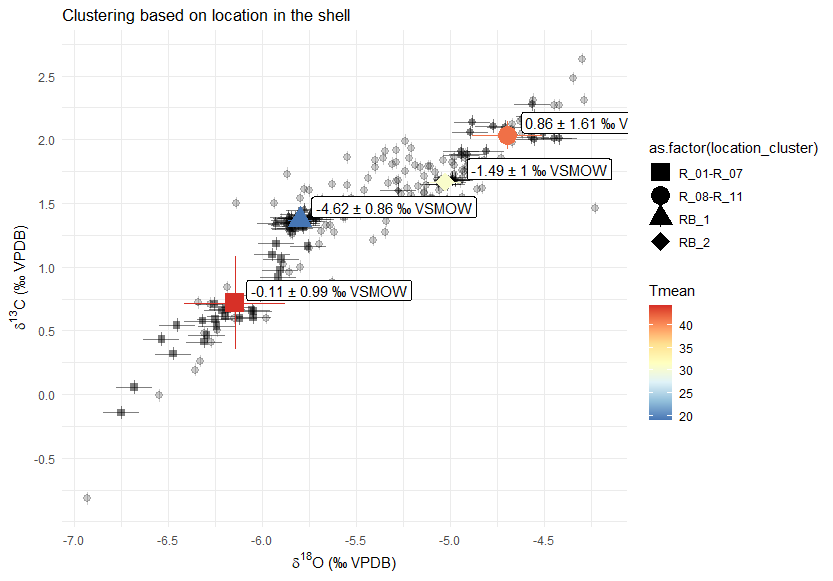


Figure 2: Result of clustering in δ18Oc-δ13C space using K-means and PAM techniques. Small black symbols represent individual stable isotope measurements in the **HU-027** dataset while large symbols with horizontal and vertical error bars indicate the means and standard deviations of variability within the clusters. The lightly shaded round symbols show incrementally sampled δ18Oc and δ13C data. Colours indicate the clumped isotope-based temperature average for each cluster on the scale indicated on the right-hand side. Statistics of the clusters are provided in **Table 1.**



**Figure 3**: Result of clustering in δ18Oc-δ13C space based on the location in the shell. Small black symbols represent individual stable isotope measurements in the **HU-027** dataset while large symbols with horizontal and vertical error bars indicate the means and standard deviations of variability within the clusters. The lightly shaded round symbols show incrementally sampled δ18Oc and δ13C data. Colours indicate the clumped isotope-based temperature average for each cluster on the scale indicated on the right-hand side. Labels show the mean δ18O values of the precipitation fluid (δ18Ow) based on combined clumped and oxygen isotope analyses. Statistics of the clusters are provided in **Table 1.**

**Table 1**: Statistics of clusters using K-means (**A**; three clusters and **B**; four clusters) and PAM (**C**; three clusters and **D**; four clusters) methods of clumped isotope measurements in specimen **HU-027**. Clumped isotope, δ18Ow and temperature uncertainties on mean cluster values are reported as 95% confidence levels. Uncertainties on δ18O and δ13C are reported as one standard deviation.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Cluster** | **N** | **δ18Oc­**  **(‰VPDB)** | **δ13C**  **(‰VPDB)** | **Δ47**  **(‰I-CDES)** | **T**  **(°C)** | **δ18Ow**  **(‰VSMOW)** |
| **K-means (3 clusters)** | | | | | | |
| 1 | 20 | -6.28 ± 0.21 | 0.52 ± 0.22 | 0.546 ± 0.011 | 42.6 ± 4.2 | -0.53 ± 0.98 |
| 2 | 30 | -4.85 ± 0.22 | 1.86 ± 0.20 | 0.564 ± 0.012 | 36.6 ± 4.6 | -0.21 ± 1.08 |
| 3 | 36 | -5.81 ± 0.07 | 1.32 ± 0.13 | 0.594 ± 0.014 | 26.3 ± 4.8 | -3.16 ± 1.03 |
| **K-means (4 clusters)** | | | | | | |
| 1 | 28 | -4.84 ± 0.22 | 1.88 ± 0.20 | 0.563 ± 0.013 | 36.9 ± 4.8 | -0.13 ± 1.12 |
| 2 | 35 | -5.81 ± 0.07 | 1.33 ± 0.11 | 0.598 ± 0.013 | 24.7 ± 4.3 | -3.49 ± 0.95 |
| 3 | 17 | -6.18 ± 0.14 | 0.63 ± 0.12 | 0.543 ± 0.014 | 44.3 ± 5.7 | -0.12 ± 1.15 |
| 4 | 4 | -6.61 ± 0.13 | 0.17 ± 0.26 | 0.540 ± 0.042 | 45.4 ± 17.1 | -0.36 ± 3.16 |
| **PAM (3 clusters)** | | | | | | |
| 1 | 36 | -5.81 ± 0.07 | 1.32 ± 0.13 | 0.594 ± 0.014 | 26.3 ± 4.8 | -3.16 ± 1.03 |
| 2 | 28 | -4.84 ± 0.22 | 1.88 ± 0.20 | 0.563 ± 0.013 | 36.9 ± 4.8 | -0.13 ± 1.12 |
| 3 | 20 | -6.28 ± 0.21 | 0.52 ± 0.22 | 0.546 ± 0.011 | 42.6 ± 4.2 | -0.53 ± 0.97 |
| **PAM (4 clusters)** | | | | | | |
| 1 | 36 | -5.81 ± 0.07 | 1.32 ± 0.13 | 0.594 ± 0.014 | 26.3 ± 4.8 | -3.16 ± 1.03 |
| 2 | 15 | -5.01 ± 0.08 | 1.71 ± 0.10 | 0.564 ± 0.020 | 36.8 ± 7.5 | -0.32 ± 1.50 |
| 3 | 13 | -4.64 ± 0.16 | 2.07 ± 0.09 | 0.562 ± 0.018 | 37.0 ± 6.6 | 0.08 ± 1.39 |
| 4 | 20 | -6.28 ± 0.21 | 0.52 ± 0.22 | 0.546 ± 0.011 | 42.6 ± 4.2 | -0.53 ± 0.97 |
| **Based on sample location** | | | | | | |
| RB\_1 | 27 | -5.80 ± 0.06 | 1.37 ± 0.04 | 0.614 ± 0.012 | 19.2 ± 3.8 | -4.62 ± 0.86 |
| RB\_2 | 14 | -5.03 ± 0.08 | 1.67 ± 0.02 | 0.577 ± 0.013 | 31.0 ± 4.5 | -1.46 ± 0.95 |
| R\_1 – R\_7 | 29 | -6.15 ± 0.27 | 0.72 ± 0.36 | 0.543 ± 0.010 | 44.2 ± 4.0 | -0.11 ± 0.99 |
| R\_8 – R\_11 | 16 | -4.70 ± 0.18 | 2.04 ± 0.11 | 0.552 ± 0.020 | 41.5 ± 7.8 | 0.86 ± 1.61 |

The clusters created from the clumped isotope dataset of specimen **HU-027** highlight the relationship between δ18Oc values in *T. sanchezi* and the temperature and δ18Ow values reconstructed from clumped isotope thermometry (**Figure 4**). Interestingly, while the lowest δ18Oc values in *T. sanchezi* are associated with the highest temperatures, as one would expect assuming a constant δ18Ow value throughout the year, the highest δ18Oc values do not represent the coldest season. This suggests that the Saiwan environment in the Late Campanian experienced significant seasonal variability in δ18Ow values, with excursions towards very low δ18Ow values (-4.63 ± 0.86 ‰VSMOW) in the coldest season, far removed from the commonly assumed δ18Ow value of -1 ‰VSMOW past greenhouse periods (Shackleton, 1986).

A screenshot of a graph

Description automatically generated

**Figure 4**: Relationship between **A)** temperature and δ18Oc values and **B**) δ18Ow and δ18Oc values in T. sanchezi shell based on four clusters of clumped isotope analyses through specimen **HU-027** grouped by location of the samples in the shell cross section. Uncertainties on mean cluster values are reported as 95% confidence levels. The curved dashed lines with grey shading highlight the result of a loess filtering through the data to find the most likely shape of the δ18Oc-temperature and δ18Oc-δ18Ow relationship and its 95% confidence level. The horizontal dashed line in **B** indicates the common assumption of a constant δ18Ow value of -1‰VSMOW throughout the year in the ice-free Late Cretaceous.

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