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Supplement of

Microscale C-O-S isotope signatures record microbial sulfate reduction in ancient deep subsurface pyrite–calcite–barite assemblages

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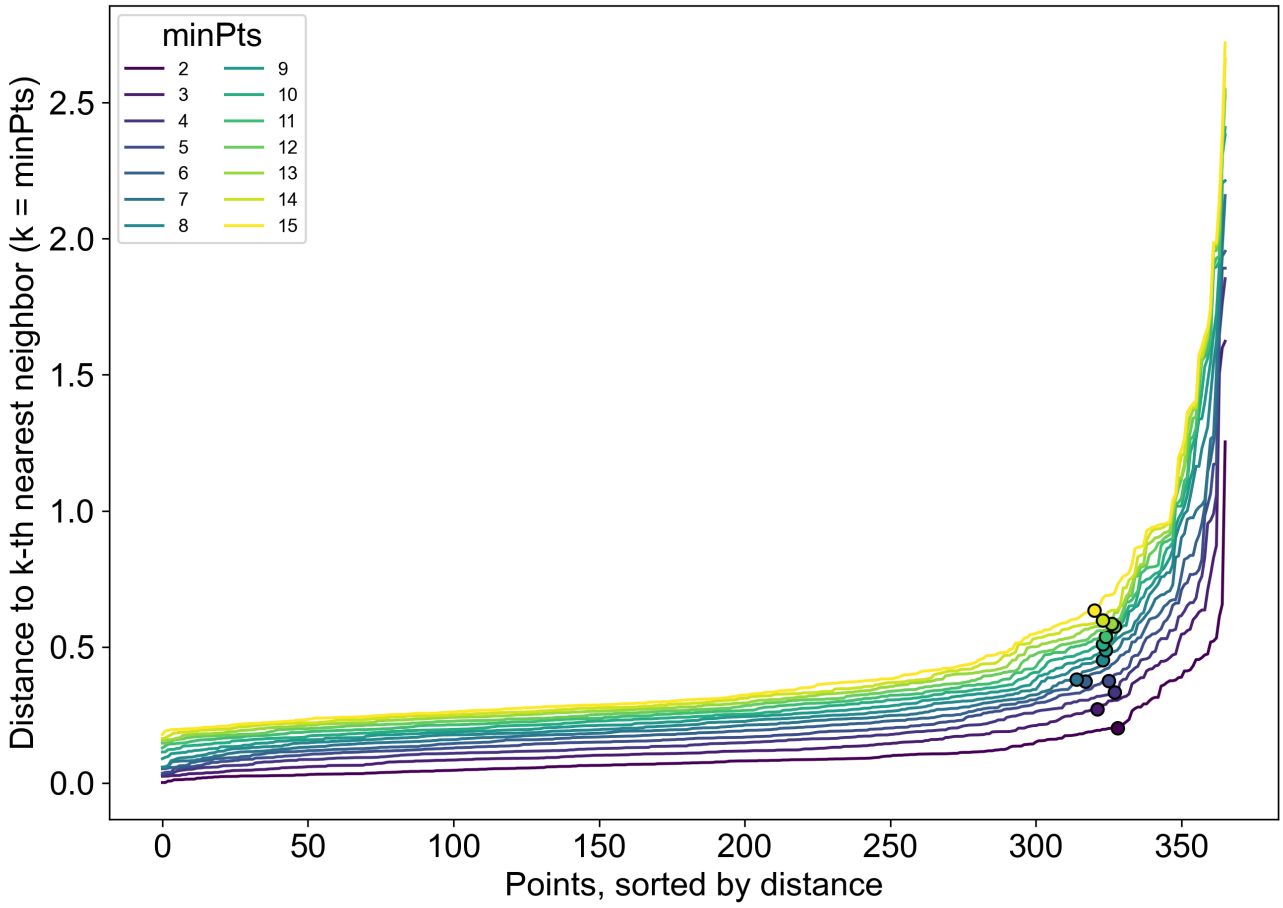


Figure S1: K-distance plot for estimating the neighborhood radius parameter (ε) as a function of the minimum number of points for forming a dense cluster (minPts) for outlier analysis via DBSCAN. The colored dots mark the points of maximum curvature of each respective curve.

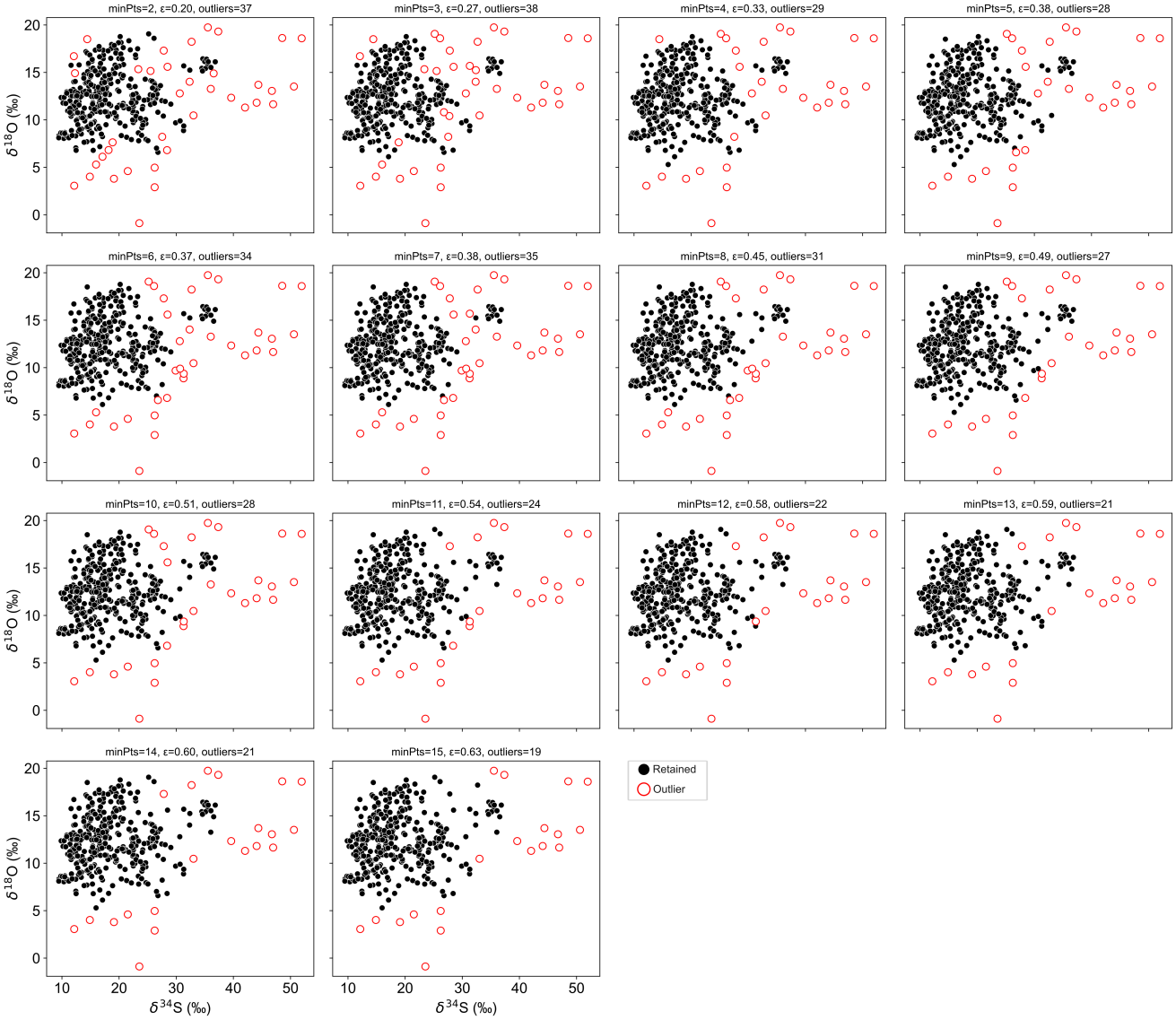


Figure S2: Outlier detection via DBSCAN for minPts values of 2 to 15 and associated ε.

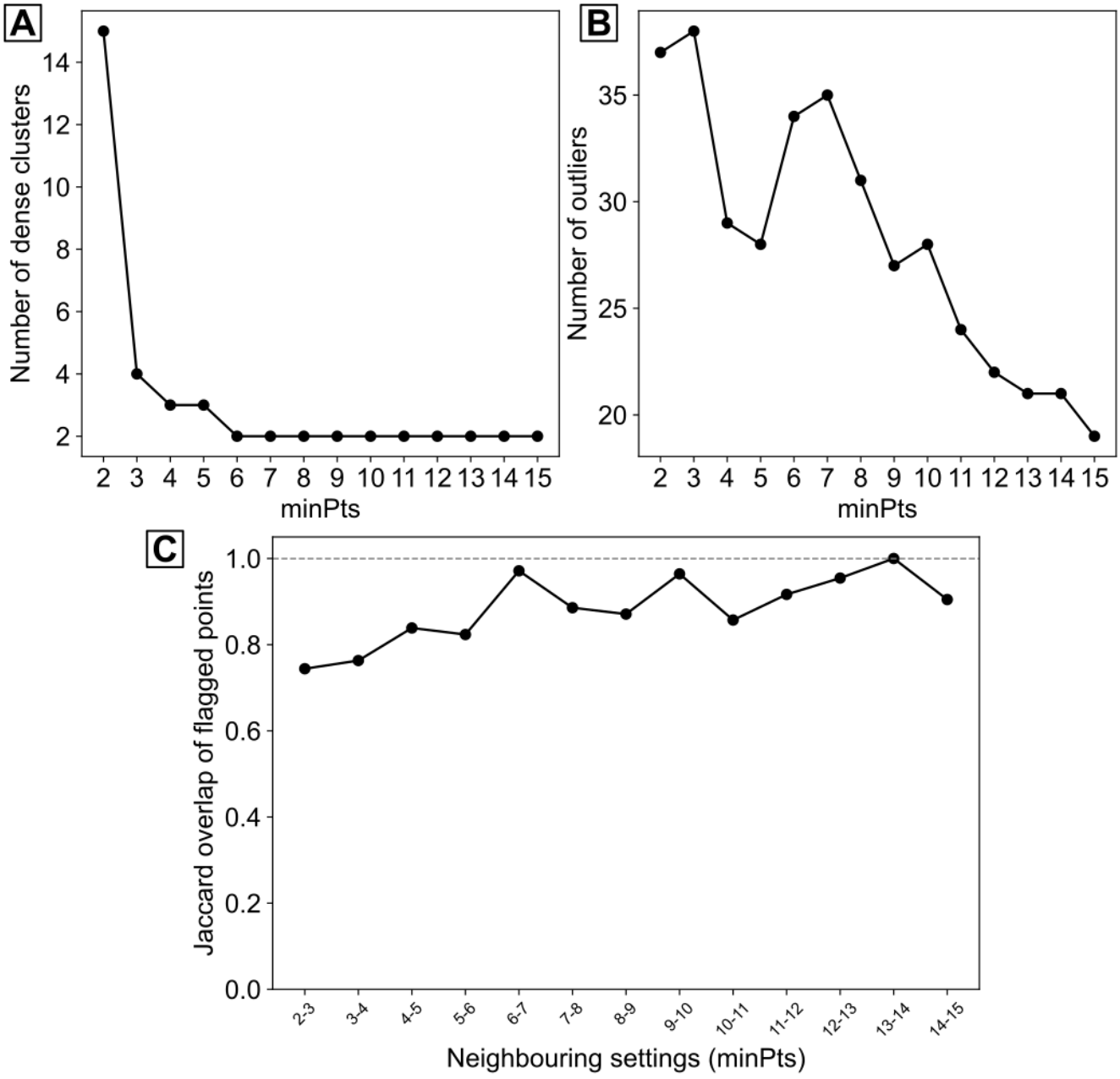


Figure S3: Summary of the sensitivity test for DBSCAN parameters. Low minPts values (2 to 3) and their associated ε lead to a high number of dense clusters and outliers (A-B). The number of outliers (n =21) is stable between minPts of 13 to 14 (B), with a Jaccard overlap of 1.00 (C), suggesting the DBSCAN outlier detection yields identical results in that minPts range. Thus, minPts = 13 was used.

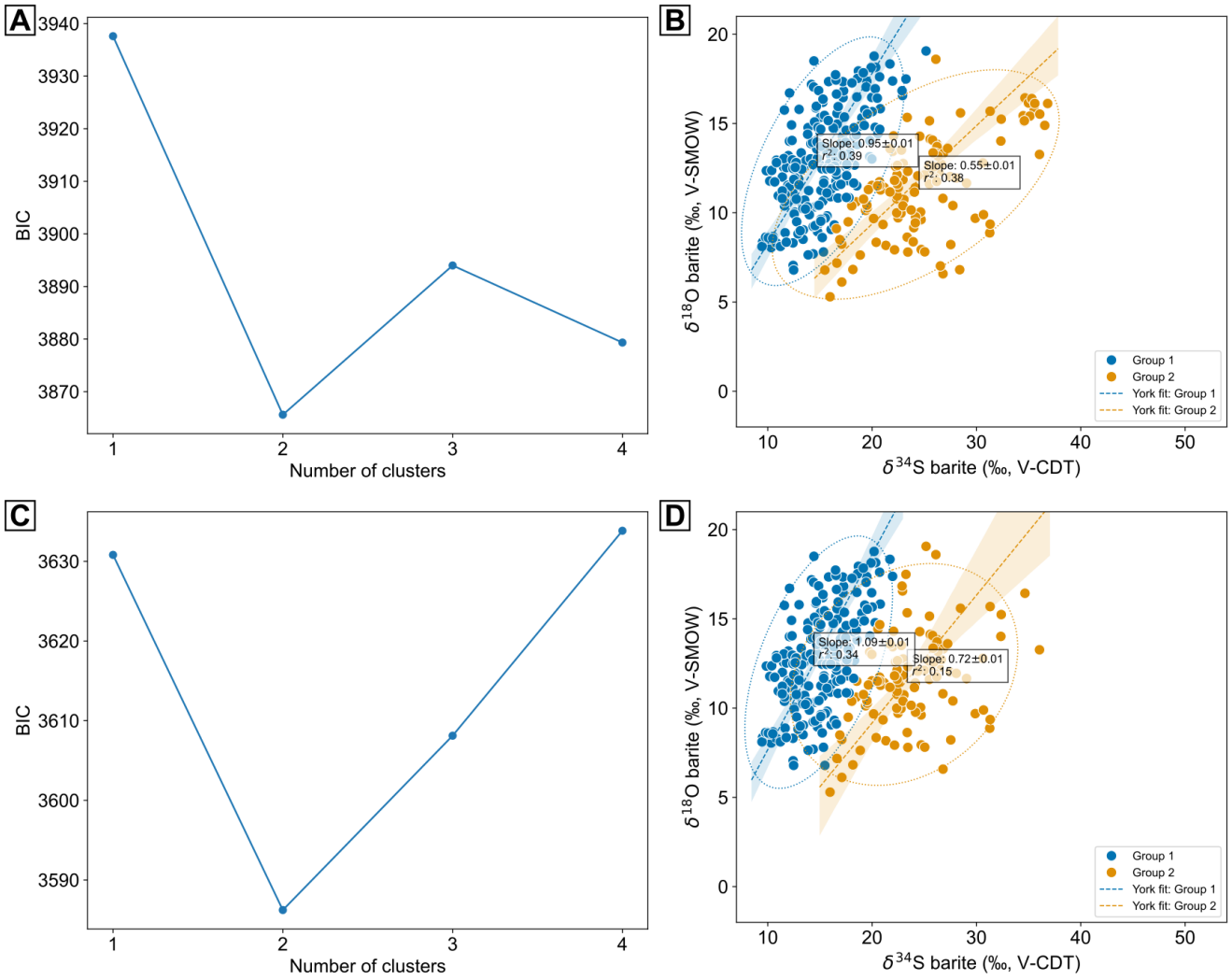


Figure S4: Sensitivity test of the Gaussian Mixture Modeling (GMM) approach against the influence of the two localities using the outlier-cleaned dataset. A: Bayesian Information Criterion (BIC) as a function of the number of clusters used for GMM of data from Laxemar and Forsmark. B: Results of GMM and York regression of the resulting clusters of data from Laxemar and Forsmark. C: BIC as a function of the number of clusters used for GMM of data from Laxemar only. D: Results of GMM and York regression of the resulting clusters of data from Laxemar only. The shaded areas in (B) and (D) are uncertainty envelopes with a 95% confidence interval. The dotted envelopes in (B) and (D) represent the areas containing 95% of the cluster's probability mass. The axis ranges in (B) and (D) match those in Fig. S2 for comparability.