Presenting multivariate statistical protocols in R using Roman wine amphorae productions in Catalonia, Spain

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Highlights

- Geochemical and petrographic data often present different patterns in ceramics.
- We define four protocols for applying multivariate statistics in ceramics.
- We offer two R packages for applying these protocols.
- We demonstrate their performance using a dataset of Roman wine amphorae.
- The fourth protocol is the most effective in evidencing the provenance of materials.

Abstract

Several analytic techniques can provide data for characterizing archaeological ceramics. These data sources are not alternative but rather complementary to each other. They report on different aspects of ceramics concerning the origin of raw materials and the technological processes involved. However, when studies integrate more than one data source, they often do it through textual description and argument, not through a combined statistical analysis.

We aim to help to overcome this situation by presenting four protocols for exploring data on archaeological ceramics. These protocols cover four different paths when interrogating ceramic samples. Protocol 1 aims to assist the definition of chemical reference groups using geochemical compositions, for instance, given by X-ray fluorescence analysis (WD-XRF). Protocol 2 focuses on fabric groups using petrographic examinations, such as in thin-section optical microscopy. Protocol 3 offers a hybrid assessment of provenance, using the integral sum of the two data sources. Last, Protocol 4 consists of the same approach as Protocol 3 but using geochemical data and a selection of petrographic variables that are considered indicative of the origin of raw materials and independent of human factors. We demonstrate their performance by applying them to a well-studied Roman wine amphorae dataset from Catalonia, NE Spain, and contextualising the results. Through a comparison of the results produced by these protocols, we restate the conclusion of Baxter et al. (2008) that a 'mixed mode' approach is preferable to analysing data from different sources separately. Moreover, we argue that treating geochemical data as compositional and petrographic semi-quantitative observations as ordinal variables, when calculating dissimilarity, offers a more complete image of ceramic materials.

The protocols are the synthetic product of several multivariate statistical methods developed for similar purposes in other disciplines, such as geology and ecology. To allow future users to replicate our analysis and apply the protocols, we published online two R packages containing all necessary procedures, from data cleaning to plotting. We also offer in the appendices a tutorial and the example scripts.

Keywords

Ceramics; archaeometric characterization; geochemical composition; petrography; multivariate statistics; R; Roman amphorae

Abbreviations

alr, clr, ilr: additive, centered, isometric log-ratio
CA: correspondence analysis
CHEM : geochemical data
FGs: fabric groups
IND: tag for site-wise outliers (e.g., FEU-IND2 is the second outlier in the Fenals)
NI: neighbour interchange approach to measure dissimilarity in ordinal variables
NMDS: non-metric multidimensional scaling
PCA : principal components analysis
PCoA : principal coordinates analysis
PETRO: mineralogical and petrographic data
PGs: provenance groups
RGs: chemical reference groups
RPCA: robust principal component analysis
RRD: relative rank difference approach to measure dissimilarity in ordinal variables
WD-XRF: X-ray fluorescence analysis
Amphorae formal types:

- D1: Dressel 1
- D2/4: Dressel 2/4
- D7/11: Dressel 7/11
- L2: Lamboglia 2
- Ob.74: Oberaden 74
- P1: Pascual 1
- T1, T3: Tarraconense 1 and 3

1. Introduction

Pottery provenance and technology are well-studied fields in archaeology since they largely contribute to the economic, social and cultural reconstruction of past societies. The examination of the composition and the morphological and technical characteristics of pottery vessels allows making many inferences about them, their creators and users. Typically, we are capable of assessing their provenance and performance characteristics, which informs on the technological skills and traditions involved in their manufacture, trade relationships, the expectations of consumers, etc. (Schiffer and Skibo, 1997, 1987; Sillar and Tite, 2000).

Archaeology is today conceptually and technically well equipped to address this system, given enough evidence (Tite, 2008). Since the 1960s, the incorporation of scientific methods in the study of ancient pottery has been a significant advance in the fields of study. Provenance analysis is used to locate specific pottery designs and technological patterns in particular places and periods, as well as trade relationships between different areas. The investigation through thin-section optical microscopy entails an in-depth study of the geological regions concerned. Provenance can also be accurately established through chemical analysis, although reference databases of the corresponding pottery productions and local raw materials are required. Through a wide range of spectroscopic and microscopic methods, archaeologists can investigate the technological processes involved in pottery manufacture (the procurement and processing of raw materials, forming, finishing, firing, and surface treatments). When approaching pottery artefacts from a long-term perspective, we can address the evolution of pottery making and style, possibly discerning specific cultural and technological patterns. However, contributions are often limited to a partial characterization according to the technical and theoretical backgrounds of the researchers involved. Usually, the plethora of possible analyses will not reach their potential regarding results, if not sufficiently integrated with data obtained with other methods, including qualitative and semi-quantitative data.

Despite the diversity of approaches in studying pottery artefacts, archaeologists should be able to reverse-engineer most technological aspects related to pottery production and use. The end goal of such analyses is to reconstruct the system entangling potters' decisions and constraints—i.e., *chaîne opératoire* defined by Cresswell (1990)—which have both universal and contextual components (Sillar and Tite, 2000).

To our knowledge, the clearest example of the integration of data on archaeological ceramics is the work of Baxter et al. (2008). Their paper successfully illustrates the benefits of combining petrographic and geochemical data to improve classifications based on macroscopic features. Our contribution builds on their conclusions, as we also aim to demonstrate the virtues and limitations of "mixed-mode" analyses. Based on the Baxter et al. (2008) seminal experience, we explored different paths to achieve integration. We focused on statistical methods developed in other disciplines (Filzmoser et al., 2009; Pavoine et al., 2009; Podani, 1999), that exploit computational resources while moving towards reproducible research (Gandrud, 2016; Marwick, 2017). Regarding the processing of geochemical data, we side with those authors that have advocated for log-ratios (Aitchison, 1982; Buxeda i Garrigós, 1999; Martín-

Fernández et al., 2015; Pawlowsky-Glahn and Buccianti, 2011) rather than some form of standardization (e.g., log-scaled). Though not favouring log-ratios, Baxter (2008) summarized this debate with refreshing clarity, identifying arguments that are still valid today.

We synthesize our explorations by presenting a multivariate methodology implemented in R (R Core Team, 2015), which is an entirely free and open-source statistical software widely used in academia. We published an R package online, *cerUB* (Angourakis and Martínez Ferreras, 2017), containing the code required for applying this methodology on comparable datasets. We encourage further extensions and improvements by the community, as we were allowed to do so, particularly regarding the contribution of Pavoine et al. (2009).

The greatest challenge for integration is that, while the geochemical composition is strictly quantitative, both mineralogical and petrographic compositions often go through qualitative assessments before any attempt of quantification, at least within archaeological studies. However, we acknowledge that there are quantitative approaches to petrographic (i.e., point-counting) and mineralogical (i.e., digital image) analyses that are increasingly being used on archaeological ceramics (Quinn 2013). Although beyond the scope of our current proposal, these analyses will be considered for additional protocols in the future.

Once we designed a pottery database reflecting these and other aspects (section 2.2), we explored separate datasets involving different working hypotheses (e.g., provenance diversity, technological change). After much exploration, we define four statistical protocols of multivariate analysis to measure and represent dissimilarity between individual ceramics (section 2.3). The first three address respectively the geochemical composition (protocol 1), the petrographic characterization with data inferred from the mineralogical and petrographic compositions (protocol 2), and both data sources simultaneously (protocol 3). Protocol 4 differs from protocol 3 by selecting variables considered indicative of provenance.

We apply each protocol on a collection of Roman wine amphorae to demonstrate their performance in measuring and visualizing dissimilarity between archaeological ceramics. The collection includes samples found in fifteen workshops in Catalonia, NE Spain, and three shipwrecks sunk along the coast towards Narbonne, SE France (section 2.1). Both workshop productions and amphorae from the ships' cargoes were fully characterized in previous studies (Martínez Ferreras, 2014; Martínez Ferreras et al., 2015, 2013).

Through this approach we expect (a) to provide the analyst with a straightforward image of the pottery variability, thus aiding archaeological classification; and (b) to facilitate the identification of the most relevant factors among variables, to guide future finer analyses. Ultimately, we intend this methodology to be a useful tool for assessing the context of pottery-making, as well as the transport of materials for trade or tribute and the technological change among past societies.

2. Material and methods

2.1. Archaeological materials

The sample consists of a total of 236 Roman wine amphorae (Figure 1, Table 1): 175 found in 15 workshops located in different production areas of the Catalan littoral and pre-littoral depressions, which initiated pottery activity at different times; and 61 recovered in three shipwrecks along the coast towards Narbonne, France.

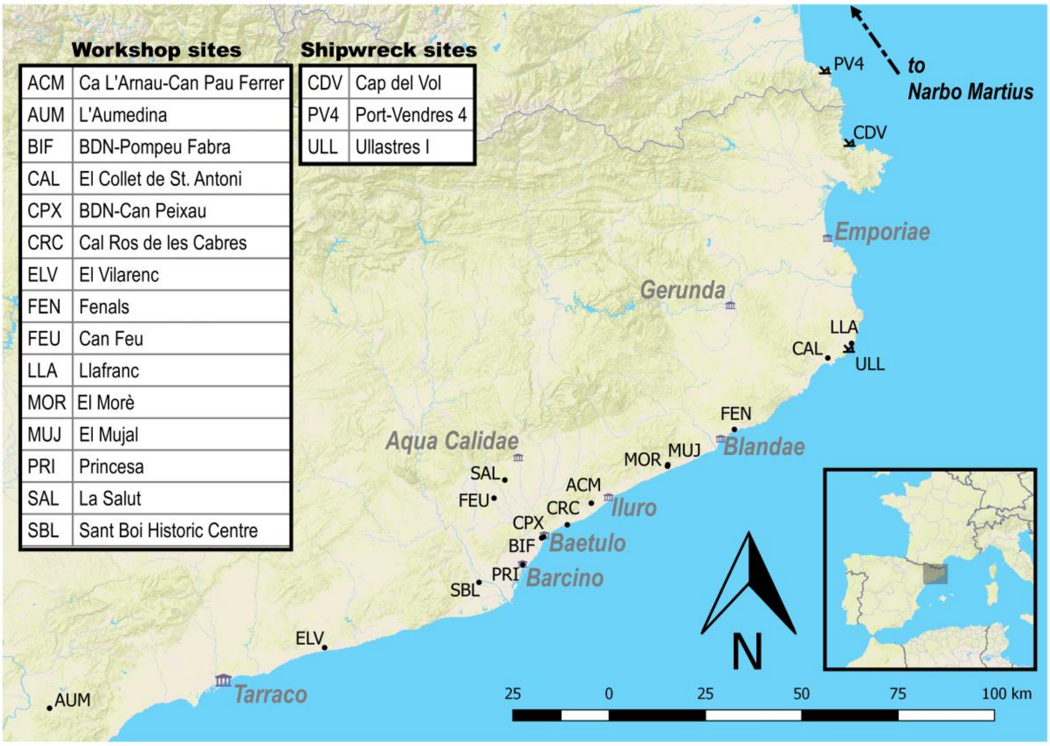

Figure 1. The location of the main Roman settlements in the Catalan coast (NE Spain), the fifteen amphora workshops and the three shipwrecks included in the analysis.

From c. 100 BC to 25 AD, the manufacture of amphorae in the region focused on wine production and export, feeding the maritime trade routes and reaching several port cities, such as *Narbo Martius* (Narbonne) in *Galia Narbonensis* (Martínez Ferreras, 2015).

The collection includes several typological forms of transport amphorae corresponding to specific periods and production areas. The first amphora design consists of a copy of the Dressel 1 (D1) prototype which was by far the most common Italian amphora for wine trade in the western Mediterranean. It existed in the Laietan region (nowadays El Maresme) especially in a few workshops located around the Roman city of *Iluro* (Mataró) such as in ACM. Another isolated production of the D1 type has been identified at La Salut (SAL), located in the western pre-littoral area near the Ripoll River Basin. The area of *Iluro* was also the focus of the introduction in *c*. 50 BC of new variants of an amphora prototype called Tarraconense 1 (T1), in sites such as ACM and MUJ. The workshops at ELV and SAL also produced other variants, which progressively replaced the D1 type.

Site	Location	Category	Chronology	Amphorae types
AUM Aumedina	Tivissa (Ribera d'Ebre)	Wine centre and pottery workshop	30 BC – 1^{st} c. AD	P1, D7/11, Ob.74
ELV El Vilarenc	Calafell (Baix Penedès)	*Villa*, wine centre and pottery workshop	40 BC – 50 AD	D1, T1, T3, P 1, Flat base
SBL Barri Antic	S. Boi Llobregat (Baix Llobregat)	*Villa*, pottery workshop	50 BC –10 AD	P1, D2/4
FEU Can Feu	S. Quirze Vallès (Western Vallès)	*Villa*, wine centre and pottery workshop	20 BC – 50 AD	P1, D2/4
SAL La Salut	Sabadell (Western Vallès)	*Villa*, wine centre and pottery workshop	50 BC –10 AD	D1, T1
PRIN Princesa	Barcelona (Barcelonès)	Suburban pottery workshop	20 BC – 1^{st} c. AD	P1
CPX Can Peixau	Badalona (Barcelonès)	Suburban pottery workshop	40 BC –20 AD	P1
BIF Pompeu Fabra	Badalona (Barcelonès)	Suburban pottery workshop	40 BC – 50 AD	P1, D2/4
CRC Cal Ros Cabres	El Masnou (Maresme)	*Villa*, wine centre and pottery workshop	30 BC – 1^{st} c. AD	P1
ACM CAN Pau Ferrer	Cabrera de Mar (Maresme)	Amphorae accumulation	100 – 75 BC	D1
ACM Ca l'Arnau	Cabrera de Mar (Maresme)	Industrial complex, pottery workshop	100 BC –30 AD	D1, T1, P1
MOR El Moré	S. Pol de Mar (Maresme)	Industrial complex, wine centre and pottery workshop	30 BC –20 AD	P1, D2/4
MUJ El Mujal	Calella (Maresme)	*Villa*, wine centre and pottery workshop	30 BC – 70 AD	T1, P1
FEN Fenals	Lloret de Mar (La Selva)	*Fundus*, pottery workshop	30 BC –80 AD	P1, D2/4
CAL Collet S. Antoni	Calonge (Baix Empordà)	*Fundus*, pottery workshop	30 BC –70 AD	P1
LLA Llafranc	Palafrugell (Baix Empordà)	Industrial complex, wine centre and pottery workshop	30 BC – 1^{st} c. AD	P1, D7/11
PV4 Port-Vendres 4	Port-Vendres (Pyrénées-Orientales)	Shipwreck	40 – 30 BC	P1 and Italian D1 and L2
ULL Els Ullastres	Palafrugell (Baix Empordà)	Shipwreck	25 – 1 BC	P1
CPV Cap del Vol	Port de la Selva (Alt Empordà)	Shipwreck	10 BC – 5 AD	P1

Table 1. The pottery workshops and shipwrecks investigated.

Shortly after, around 40-30 BC, a new amphora design, the Pascual 1 (P1) type was adopted in the Laietan region, in the outskirts of the Roman city of *Baetulo* (nowadays Badalona) (CPX, BIF) and at the lower Llobregat River Valley (SBL). Production of P1 amphorae spread further throughout the territory, which mirrored the peak of wine industry and trade during Augustus' reign. From that time, it was produced in the pottery workshops that emerged in newly organized territories and cities, such as

Barcino (Barcelona) (PRI), *Aqua Calidae* (Caldes de Montbui), the western pre-littoral (FEU), or in the north-eastern (LLA, CAL, FEN, MUJ, MOR) and southern (AUM, ELV) areas.

From 30-20 BC most of the production areas in *Hispania Tarraconensis* started to imitate another Italian prototype for the wine trade, the Dressel 2/4 (D2/4). The manufacture of other minor types such as the Oberaden 74 (Ob74) and Dressel 7/11 (D7/11) designs began at this time, the production of which was limited to the northern and southern areas (Martínez Ferreras, 2014; Miró, 1988).

D1, T1, and P1 types were mainly directed for supplying local and Gaul markets, although the latter also reached military camps in Germania and the southern coasts of Britannia. Even if some D2/4 were traded to Gaul, this type appears to have been mainly diffused at a local and regional level or sent to Italy and other areas of the Roman Empire.

The three shipwrecks selected show the trade *in transito* between a port of departure in NE Spain and a port of destination in southern France, probably at Narbonne (Figure 1). The Port Vendres 4 is one of the several shipwrecks recovered at Port Vendres, south France. Dated to 40-30 BC, it contained an assemblage of Roman wine amphorae from Italy (D1 and L2) and NE Spain (P1), suggesting a trade shipment from a port in the central Catalan coast, probably *Iluro* or *Baetulo*, (Martínez Ferreras et al. 2015). Contrary, Els Ullastres (Palafrugell) and Cap del Vol (Port de la Selva), located in the northern Catalan coast, comprise homogeneous cargoes including only P1 amphorae. Most of the containers have been associated with the pottery workshops located on the outskirts of *Baetulo* and particularly, with BIF (Table 2). Therefore, these two case studies are evidence of the prevalence of the wine amphorae produced at *Baetulo* (Badalona) in the maritime trade to Gaul during the Augustan Age.

2.2. Data formatting

We design a database to enclose and relate common aspects of the study of archaeological pottery from an archaeometric perspective, namely the geochemical, mineralogical, and petrographic compositions, the latter two being registered as qualitative data. However, other important attributes relevant to archaeological interpretations, such as the shape, surface treatment, and mechanical properties could be introduced, if data is available.

The chemical analysis by WD-XRF, the mineralogical analysis by XRD, and the petrographic analysis through thin section optical microscopy allowed the identification of specific chemical reference groups (RGs) along the period of activity of the workshops (Table 2; Martínez Ferreras, 2014).

SITES	RG	AMPHORAE TYPES/SAMPLES*	CaO %	MgO %
AUM (n=10)	AUM-1	P1: AUM-4, 8, 11, 12; D7/11: AUM-14; Ob.74: AUM-17, 20	4.9	5.5
	AUM-2	P1: AUM-5, 10	12.3	4.3
	AUM-IND	P1: AUM-9	5.6	4.3
ELV (n=18)	ELV-1	D1: ELV-2; T3: ELV-7, 9, 15, 52	15.4	3.2
	ELV-2	T3: ELV-45; T1: ELV-51; Flat base: ELV-47, 49	15.7	3.5
	ELV-3	D1: ELV-1; P1: ELV-16, 19, 20, 23, 24, 26, 36	10.7	3.4
	ELV-IND	T3: ELV-28	23.5	2.9

SBL (n=11)	SBL-1	P1: SBL-1, 6, 11, 24, 28, 32	9.2	1.8
	SBL-2	D2/4: SBL-38 e.s. CALAM, SBL-40 e.s. QVA, SBL-42 e.s. QVA, SBL-43 e.s. SAB, SBL-45 e.s. TH	13.3	1.6
FEU (n=20)	FEU-1A	D2/4: FEU-28, 29	4.9	1.8
	FEU-1B	P1: FEU-15, 17, 18, 19, 26	4.9	1.8
	FEU-2A	P1: FEU-1, 3, 5, 6, 8, 13, 14	14.6	1.8
	FEU-2B	Pointed bases: FEU-38 e.s. CE, FEU-39 e.s. CE, FEU-40 e.s. SEVE, FEU-41 e.s. H	12.5	1.7
	FEU-IND1	P1: FEU-9	1.7	2.3
	FEU-IND2	P1: FEU-16	4.9	1.7
SAL (n=11)	SAL-1	D1: SAL-21; T1: SAL-11, 16; Pointed bases: SAL-25 e.s. MAA, SAL-28 e.s. H	6.4	1.5
	SAL-2	D1: SAL-22; T1: SAL-32	8.2	2.1
	SAL-IND1	Pointed bases: SAL-24 e.s. CA,	12.6	2.8
	SAL-IND2	SAL-26	2.3	1.9
	SAL-IND3	SAL-27	10.6	1.8
	SAL-IND4	SAL-29	7	3.7
PRINC (n=10)	PRINC-1	P1: CSC-54, 55, 58, 59, 65, 66, 67, 70, 91	7.8	1.9
	PRINC-IND	P1: CSC-85	4.8	2.6
CPX (n=11)	CP-A	P1: CPX-4, 8, 33, MRCCP1 e.s. M.PORCI	12.6	6
	CP-B	P1: CPX-10, 13, 18, 42, 48, MRCCP2 e.s. C.ANTESTI	10.3	4
	CP-IND	T1: MRCCP5 e.s. Q.MEVI	12	3.5
BIF (n=21)	BIF-1	P1: BIF-12, 13, 15, 20	11	8.1
	BIF-2	P1: BIF-4, 5, 6, 9, 11, 21, 25, 28	12.3	5.6
	BIF-3	P1: BIF-19, 41, 48; D2/4: BIF-36, 37	14	7.2
	BIF-IND1	P1: BIF-26	6.3	3.6
	BIF-IND2	D2/4: BIF-35	2.9	1.7
	BIF-IND3	BIF-50	17.3	8.4
CRC (n=5)	CRC-1	P1: CRC-2, 19	14.5	6.8
	CRC-2	P1: CRC-8, 18, 24	13.6	4.3
ACM (n=18)	ACM-A	D1: ACM-73, 80, 86, 97, 99 Can Pau Ferrer	5.2	1.9
	ACM-B	D1: ACM-40, 45, T1D: ACM-59, T1E: ACM-3, 61, 63, P1?: ACM-31 Ca l'Arnau	5.4	1.5
	ACM-C	P1: ACM-1, 20, 71, 72 Ca l'Arnau	11.2	1.6
	ACM-IND1	D1: ACM-81 Can Pau Ferrer	7.9	2
	ACM-IND2	ACM-102 Can Pau Ferrer	5.6	1.6
MOR (n=11)	MOR-1	P1: MOR-4, 5, 6, 10	7.8	1.8
	MOR-2	P1: MOR-8, 13, 15; D2/4: MOR-17	4.4	1.8
	MOR-3	D2/4: MOR-11, 18, Pointed base: MOR-20 e.s. CHR	1.8	1.6
MUJ (n=7)	MUJ-1	P1: MUJ-24, 29	1.2	1.4
	MUJ-2	T1A: MUJ- 40, 41, 42, T1C: MUJ-33, 53	1.4	1.3
FEN (n=9)	FEN-A	P1: FEN-11, 25, 26, 27, 29, 31	1.8	1
	FEN-B	D2/4: FEN-36, 37, 38	1	1.3
CAL (n=6)	CAL-A	P1: CAL-2, 3, 25, 28, 32	13.8	1.6
	CAL-B	P1: CAL-5	5.2	1.6
LLA (n=8)	LLA-A1	P1: LLA-9, D7/11: LLA-13	10	1.3
	LLA-A2	P1: LLA-16, 18, 24, 33, D7/11: LLA-10	5.5	1.3
	LLA-IND	P1: LLA-17	11.9	1.7
PV4 (n=13)	PV4-ACM	P1: PV4-1, 2, 4, 11, 16 e.s. TH+S	3.2	2.5
	PV4-MOR	P1 pointed base: PV4-38 e.s. CHR	1.5	1.5
	PV4-MUJ	P1 pointed base: PV4-8 e.s. AM	1.5	1.4
	PV4-BIF	P1: PV4-5, 7, 9	11.7	6.5
	PV4-IND1	P1: PV4-6	6.9	8.2
	PV4-IND2	P1: PV4-13	11.5	3
	PV4-IND3	P1: PV4-14	12.1	2.2

CDV (n=19)	CDV-BIF	P1: CDV-1-11, 13-15, 17-20	11.4	6.6
	CDV-IND	P1: CDV-12	12.6	8.1
ULL (n=19)	ULL-BIF	P1: ULL-1-4, 7, 9-11, 13-16, 18-20, 22	9	8.8
	ULL-IND1	P1: ULL-12	3.2	2.4
	ULL-IND2	P1: ULL-17	8.6	2.2
	ULL-IND3	P1: ULL-21	2.5	1.7
*e.s.: epigraphic stamp				

Table 2. The amphorae examined with indication of the pottery workshops, the groups or productions identified at each one and the average found for CaO and MgO at each group.

The geochemical composition was investigated through WD-XRF using a Philips PW 2400 spectrometer with an Rh excitation source. A total of 25 oxides and trace elements was measured, out of which 16—Fe_2O_3, Al_2O_3, TiO_2, MgO, CaO, SiO_2, Th, Nb, Zr, Y, Ce, Ga, V, Zn, Ni, and Cr—were deemed fit for the analysis of all samples.

The mineralogical composition was examined through XRD using both a Siemens D-500 and a Panalytical X'Pert PRO alpha 1 diffractometers. The crystalline phases were evaluated using the PANalytical HighScore X'Pert software and synthesized as an ordinal variable expressing the approximate firing temperature. Both WD-XRF and XRD measurements were performed at the CCiT-UB laboratory of the University of Barcelona.

The petrographic measurements were performed through the observation of thin-sections under the polarising optical microscope Olympus BX41, using a digital camera Olympus DP70 and the Analysis Five software. Petrographic data concerns the composition and characteristics of the matrix (groundmass) and the microstructure (micromass), especially the frequency, size, shape, type, and distribution of non-plastic inclusions (Whitbread, 1995). The frequency of non-plastic inclusions and voids were estimated by using the comparative tables offered by Matthew et al. (1991). Petrographic analysis registered a total of 115 variables, out of which 43 were not considered in the control study, due to their dependence on known post-depositional perturbations (Buxeda i Garrigós, 1999; Maritan et al., 2009; Maritan and Mazzoli, 2004; Schwedt et al., 2006) or the absence of variance within the selected samples.

In previous studies, we defined fabric groups (FGs), which are broader than RGs, based solely on petrographic data. Provenance groups (PGs), collapse RGs and FGs into a wider spatial criterion: e.g., "AUM" means "was made in L'Aumedina's workshop". In all classifications, we tag the site-wise outliers (IND) separately from the general site groups.

A complete list of petrographic variables names and their values can be consulted in Appendix A.

2.3. Statistical protocols

We defined four protocols using multivariate methods developed and used by mathematicians, geologists, and ecologists (Anderson and Walsh, 2013; Filzmoser et al., 2009; Pavoine et al., 2009; Podani, 1999).

Protocol 1 is designed for analysing geochemical compositions (CHEM) while protocol 2 aims to represent mineralogical and petrographic data (PETRO). Protocol 3 allows the combination of both types of data (CHEM & PETRO) and can be properly called a mixed-mode analysis, after Baxter et al. (2008). Protocol 4 is equivalent to protocol 3 but using a specific selection of variables deemed relevant for identifying provenance (CHEM & $PETRO_{PROV}$), mainly those indicating mineralogical composition. In addition to their data source, protocols vary in three key steps: data transformation, calculation of distance/dissimilarity, and ordination method (Table 3).

Protocol	Protocol 1	Protocol 2	Protocol 3	Protocol 4
Data source	CHEM	PETRO	CHEM & PETRO	CHEM & $PETRO_{PROV}$
Transformation	ilr/clr	ranking	clr & ranking	clr & ranking
Distance	Euclidean	RRD/NI	Extended Gower distance (Euclidean & RRD)	Extended Gower distance (Euclidean & RRD)
Ordination	RPCA	PCoA/NMDS	PCoA	PCoA

Table 3. Statistical protocols

Focusing in CHEM, the protocol 1 first step is to transform counts or percentages given by WD-XRF readings into log-ratios (Aitchison, 1982; Buxeda i Garrigós, 1999; Martín-Fernández et al., 2015; Pawlowsky-Glahn and Buccianti, 2011). Once data is transformed using any log-ratio procedure (alr, clr, or ilr), it is possible to perform PCA using Euclidean distances between log-ratios. However, we do warn that using different log-ratio transformations, as well as any other transformation (normalization, logarithmic), must be taken into account carefully while interpreting results. For easiness and readability, we followed the approach of Filzmoser et al. (2009), which uses a combination of ilr transformation and RPCA. Such treatment empowers the visualisation of compositional data, by compensating for distortions produced by outliers and closure. There are three R packages dedicated to compositional data (zCompositions: Palarea-Albaladejo and Martín-Fernández, 2015; robCompositions: Templ et al., 2011; compositions: van den Boogaart et al., 2014).

When addressing PETRO in protocols 2, 3, and 4, we chose to preserve the original format of variables—i.e., ordinal variables. This practice contrasts with other approaches (Baxter et al., 2008; Cau Ontiveros et al., 2004; Ownby et al., 2014). These used binominal dummy variables instead, thus merely differentiating values (e.g., “common” ≠ “few”) instead of accounting for their order (e.g., “common” > “few”). However, a special treatment is required to measure dissimilarity in ordinal variables. We explored two alternative approaches to this challenge, relative rank difference and neighbour interchange (NI and RRD; Appendix B; Podani, 1999). The essential trait of both methods is that ordinal values are converted into rank scores, which depend not only on ordering (i.e., the sequence of categories) but also on ties (i.e., observations falling into the same category).

Dissimilarities given by NI generally do not satisfy the axiom of triangle inequality (i.e., they are not metric). Therefore, NI can be used in protocol 2, dealing only with ordinal variables, but it is incompatible with the integration of Euclidean distances, as in protocols 3 and 4. In turn, RRD dissimilarities can be analysed with metric techniques and so we used this approach to measure dissimilarity in PETRO variables in protocols 2 through 4.

Protocols 2 through 4 calculate the overall dissimilarity between observations using a version of Gower's distance (Gower, 1971; Appendix B), extended and implemented in R language by Pavoine et al. (2009). Similarly to Baxter et al. (2008) 'mixed mode' approach, they named this methodology as the "mixed-variables coefficient of distance" which was presented with their original R code.

The extended Gower distance enables protocols 3 and 4 to combine CHEM and PETRO in the same distance coefficient. CHEM numeric variables contribute with Euclidean distances between pairs of clr, and PETRO ordinal variables with RRD between pairs of rank scores. By modifying Pavoine et al. (2009) original script, it was possible to equal the weights of the two sets of variables (CHEM, PETRO), so that the distance represents the exact middle ground between the patterns displayed in protocols 1 and 2. We then project the resulting distance matrix in 2D and 3D through PCoA.

The 2D and 3D projections generated by each protocol are complemented with PERMANOVA and PERMDISP2 tests (Anderson and Walsh, 2013), which together evaluate the significance of the separation between given groups. These tests are good supplements to ordination methods (PCA, PCoA) because both use the entire multidimensional variability present in distance matrices, part of which is invisible in graphic projections (biplots).

PERMANOVA assesses the probability of the null hypothesis of no difference among group centroids (i.e., small p values indicate significant separation). However, PERMANOVA is unreliable when there is heterogeneity of dispersions, which confounds effects of group location and dispersion. PERMDISP2 tests the null hypothesis of heterogeneity of dispersions, ignoring the position of group centroids. If homogeneity of dispersion can be assured (PERMDISP2: p-value < 0.05), PERMANOVA may be considered a reliable test for significant separation among groups. Both tests are possible using the *vegan* package in R (Dixon, 2003; Jari Oksanen et al., 2016): the *adonis* function and the *permtest* function (applied to *betadisper* function results).

The statistical protocols presented here include methods already available in one or more existing packages in R. However, we aim to facilitate their use for archaeologists. In this sense, accompanying this study, we present two R packages that are fully documented and freely available.

The *cerUB* package contains all necessary functions to follow the protocols and apply them to other comparable datasets (Angourakis and Martínez Ferreras, 2017). It includes the dataset presented here (amphorae), as a working example but also for ease of reproducibility.

The *biplot2d3d* package (Angourakis, 2017) combines the functionalities of several R packages to generate 2D and 3D projections of ordination methods (biplots; Gabriel, 1971), allowing for centralized control of many graphic parameters. We used four features particular to this package:

1. We opted to detach the location of the 'second' plot of a biplot (i.e., the arrows), move it to the bottom-right corner, and re-scale it to avoid overlapping points;

2. To reduce the number of variables represented in protocols using petrographic data (>80 variables), we filtered those that did not project well in the first two dimensions (less than 50% of the maximum covariance among all variables).

3. We added a representation of eigenvalues (bottom-left corner), which are interpretable as the proportion of variance captured in every dimension (i.e., the first two or three bars being the dimensions of the plot). Additionally, we indicate this proportion as the percentage of variance explained by the visible dimensions.

4. We mark groups with inertia ellipses, which correspond to 95% confidence ellipses whenever we assume that group members were drawn from normal distributions for all input variables. We advise that this may not be reasonable for groups that are either too small or contain subgroups, in which case ellipses should be interpreted simply as graphic summaries of the group's cloud of points. We also add the "star" representation of groups, i.e. every point connected by a line to the centroid.

We offer a full walkthrough for installing and using the *cerUB and biplot2d3d* packages (Appendix C) and the corresponding R scripts (Appendix D); both are also available in a GitHub page (https://andros-spica.github.io/cerUB_tutorial/). Besides having published them in Zenodo.org, we maintain their open source code in GitHub repositories (github.com/Andros-Spica/cerUB, github.com/Andros-Spica/biplot2d3d). All analyses and plots presented here were made using R 3.4.1.

3. Results

3.1. Determining production centres

Aiming to test their usefulness for defining productions from pottery centres, we applied protocols 1 through 4 only to samples found in workshops. The classifications displayed in biplots and tested with PERMANOVA and PERMDISP2 vary depending on the range of the input data (i.e., RGs in protocol 1 and 3, FGs in protocol 2, and PGs in protocols 4).

In Protocol 1 (Figure 2; Appendix E.1), the amphorae are distributed forming clusters consistent with the previously defined RGs. Most IND sherds are isolated or close to other sites' RGs. The main factors causing this distribution are the CaO and MgO values. As already detected, the P1 produced around *Baetulo* has the highest MgO content (Buxeda i Garrigós et al., 2002; Martínez Ferreras, 2014).

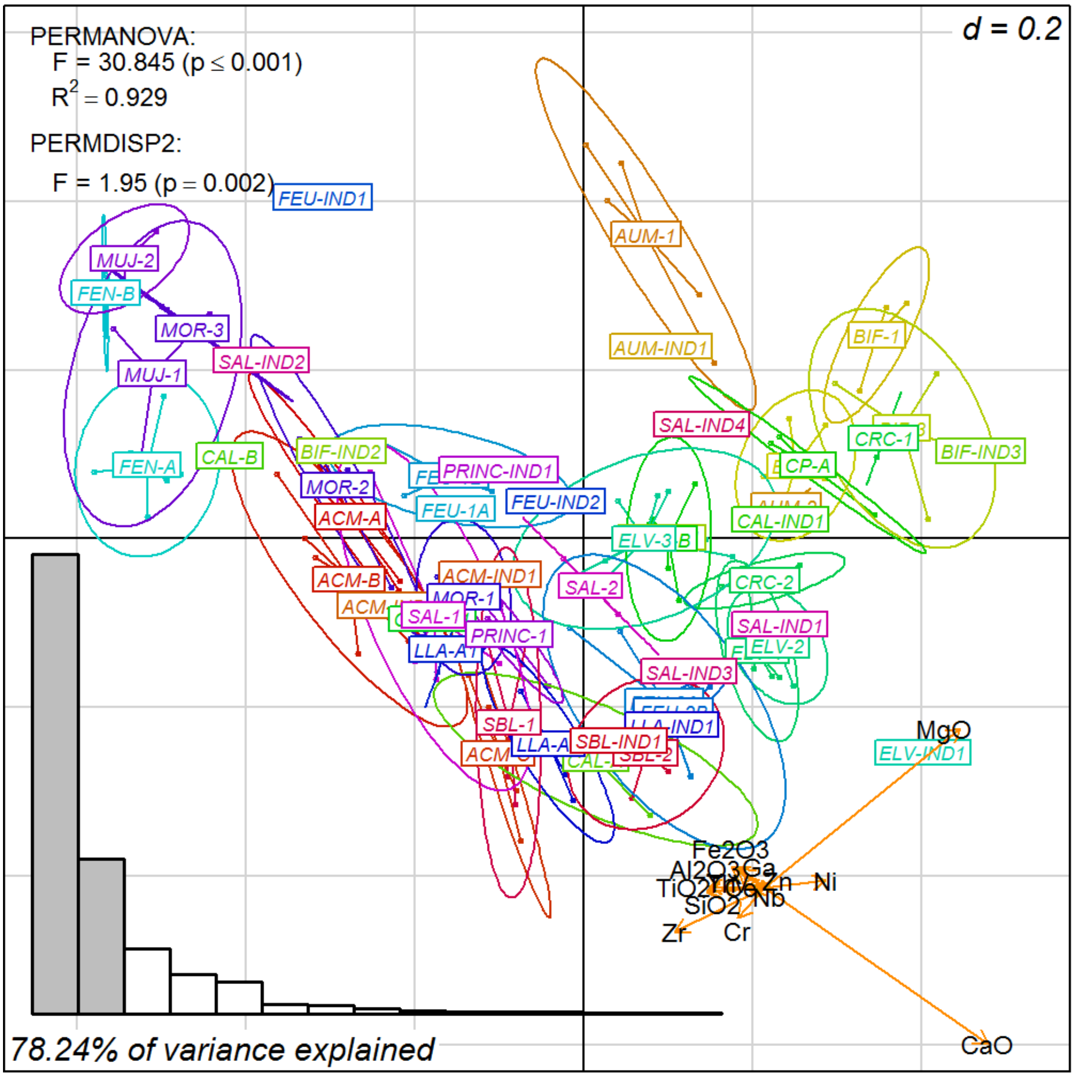

Figure 2. Protocol 1 results concerning the samples of all amphorae workshops included in the study. The plot shows the best 2D projection, the horizontal and vertical axes respectively containing the first and second principal components. The RGs are labelled and distinguished by colour.

Some workshops procured and processed raw materials differently. In CAL, the first D1 and T1 were produced using Fe-rich clays, while the latter P1 correspond to calcareous pastes. In MOR and FEU, the earlier P1 (MOR-1, FEU-2A, and FEU-2B) exhibit higher CaO content than the latter P1 and D2/4 (MOR-2, MOR-3, FEU-1A, and FEU-1B) which were made with Fe-rich clays. The variability within a workshop has usually been interpreted as diversity of local raw materials used over time (Vila Socias et al., 2009). Such variability causes the RGs of some workshops to be relatively dispersed. Still, large clusters emerge with workshops geographically close, thus using similar raw materials; i.e., those located around *Blandae* (MUJ and FEN) or *Baetulo* (CPX, BIF and CRC; Buxeda i Garrigós et al., 2002; Martínez Ferreras, 2014; Vila Socias, 2011). In other cases, RGs of different production sites and areas overlap because they exhibit many similarities in their chemical composition, especially in CaO and MgO; i.e., ACM-C, SBL-1 and LLA-A2.

The low calcareous amphorae from the workshops located around *Iluro* and *Blandae* form another cluster. It comprises amphorae of the T1 (MUJ-2), P1 (MUJ-1 and FEN-

A), and D2/4 (FEN-B) types, also joined by one of the pointed bases from La Salut (SAL-IND2). This cluster exhibits the lowest CaO (1-2%) of the dataset, together with low MgO and high Fe_2O_3, Al_2O_3, SiO_2, Zr, and Y. Nevertheless, amphorae from FEN present lower TiO_2 and V, and higher Cr values. Most of the D2/4 from MOR (MOR-3) resemble these productions, although they exhibit lower Cr and higher Zn. The P1 from MOR (MOR-2) are low to border calcareous (4% CaO), while the earlier production of this type (MOR-1) appears to be calcareous (7-8% CaO).

In ACM, the production of different types of amphorae also entailed changes in raw materials procurement or processing. For instance, the D1 and T1 (ACM-A and ACM-B) exhibit 4-7% CaO and high Fe_2O_3, Al_2O_3, TiO_2, Y, and Ce. Their composition is similar to MOR-2, though with higher Cr. The P1 and D2/4 from FEU (FEU-1A and FEU-1B) resemble ACM's but containing higher Zn and Ni. We could attribute the P1 PRINC-IND found at Barcelona to FEU productions. The D1 and T1 from SAL (SAL-1) are border calcareous (6.4% CaO) with high TiO_2 and Zr. Instead, SAL-2 is more calcareous and exhibits lower Zr and Cr.

The P1 from PRINC (PRINC-1) and LLA (LLA-A1) are also border calcareous to calcareous with low Fe_2O_3 and Al_2O_3. LLA-A1 presents lower MnO, TiO_2, and MgO, and higher Cr. It differs from LLA-A2 because the latter exhibits higher CaO (10%). The calcareous P1 LLA-A2 is similar to CAL-A, ACM-C, and SBL-1. Ce is higher in ACM-C, while Ni and Cr are more abundant in SBL-1. The D2/4 from SBL (SBL-2) exhibits lower Zr and Cr, and present similarities with the P1 from FEU (FEU-2A and FEU-2B), except for their higher SiO_2. One of the pointed bases from SAL (SAL-IND-3) also resembles these two FEU RGs.

The P1 discussed above differ from those produced at the Besòs River Valley, through their MgO content. Amphorae from CP (CP-A and CP-B) and BIF (BIF-1, BIF-2, and BIF-3) consist of calcareous pastes (10-14% CaO) with low Al_2O_3, SiO_2, and Ga, and high MgO (4-8%). As previously suggested, amphorae from *Baetulo* resemble those found at CRC (CRC-1/2), located north of the Roman city (Buxeda i Garrigós et al., 2002).

Regarding the southern workshops near *Tarraco* (Tarragona), some RGs present a relatively unique chemical composition, i.e., the D1, T3, and flat-bottom amphorae from ELV-1 and ELV-2 and the P1 from AUM-1. The first two present calcareous pastes (15-16% CaO) with high Ni and low Al_2O_3, SiO_2, Ce, and Ga, while the third exhibits 5% CaO, the highest K_2O (5%), high MgO (5.5%) and Ni, and low SiO_2, Ba, Zr, and Ce. Nevertheless, the P1 from ELV-3 contain higher Ce and Zn and are closer to the P1 from CP-B. Moreover, the two amphorae included in group AUM-2 exhibit higher CaO (12%), Sr, and Cu and approach the products from *Baetulo*.

We mentioned the interesting cases of those IND sherds found in one workshop but allegedly produced in another. However, most INDs (AUM-IND1, FEU-IND2, BIF-IND1, BIF-IND3, ACM-IND1, and ACM-IND2) are linked with the RGs of their respective sites. They probably correspond to productions that were not well characterised, or were made in nearby workshops not yet investigated or discovered. Only two samples, FEU-IND1 and ELV-IND1, don't match with any RG and so their provenance remains indeterminate.

In protocol 2, the separation of FGs is more consistent with their textural characteristics and with the geographical location of the pottery workshops (Figure 3; Appendix E.2). For instance, the amphorae from the southern workshops (AUM and ELV) are tightly clustered because they consist of fine to medium-fine fabrics with moderately abundant aplastic inclusions (≤ 0.5 mm grain-sized; lower L2; Figure 4). The predominant inclusions are quartz (L43), K-feldspar, and plagioclase derived from granitoids. Foraminifers, micritic calcite (L27), and sparite in some samples, all presenting various states of decomposition, are frequent. Phyllosilicates (L36), metamorphic and sedimentary rock fragments (L24, L33) are common to few. The raw materials used were the local Pleistocene alluvial deposits and piedmont terrains constituted by marls, calcarenites, and biomicrites from the Miocene.

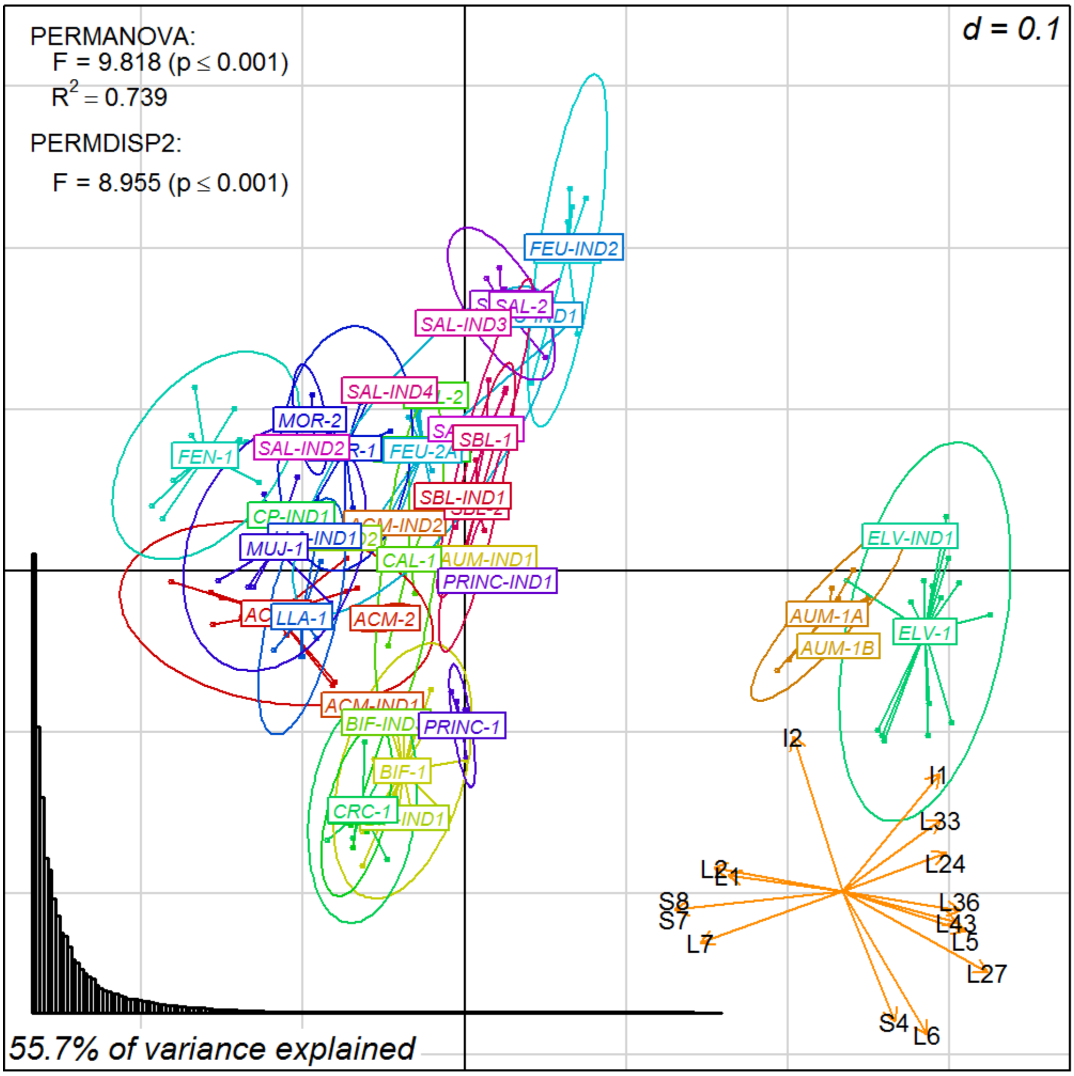

Figure 3. Protocol 2 results concerning workshops samples. The plot shows the best 2D projection, the horizontal and vertical axes respectively containing the first and second principal coordinates. The FGs are labelled and distinguished by colour. Consult Appendix A for variable codes.

The coarser, low calcareous D1, T1, and P1 from the workshops located around *Iluro* and *Blandae* —ACM-1 MOR-1 and MOR-2, MUJ-1, and FEN-1— appear on the opposite side. These workshops exploited raw materials from the Quaternary fluvial-torrential deposits extending in the narrow plain between the coastal mountains and the

Mediterranean Sea. The clayey matrix is rich in iron oxides, and inclusions are moderately abundant, ranging in size from fine-grained to very coarse-grained sand (≤ 0.25-2 mm grain-sized; higher L2). They include predominant granitic rock fragments (L7) derived from the Carboniferous-Permian coastal mountain system and crystals detached from these rocks, mainly quartz, K-feldspar, plagioclase, and biotite together with few to common amphibole and epidote (Figure 4). Partly or totally decomposed microfossils and calcite (micrite) are common to rare in fabrics ACM-1, MOR-1 and LLA-1. MOR-1 and MOR-2 exhibit few metamorphic rock fragments. Moreover, clinopyroxene crystals are present (few) in LLA-1derived from the Quaternary alkaline-volcanic complex located to the west. Although overlapping in 2D, ACM-1 and LLA-1 are well differentiated in 3D.

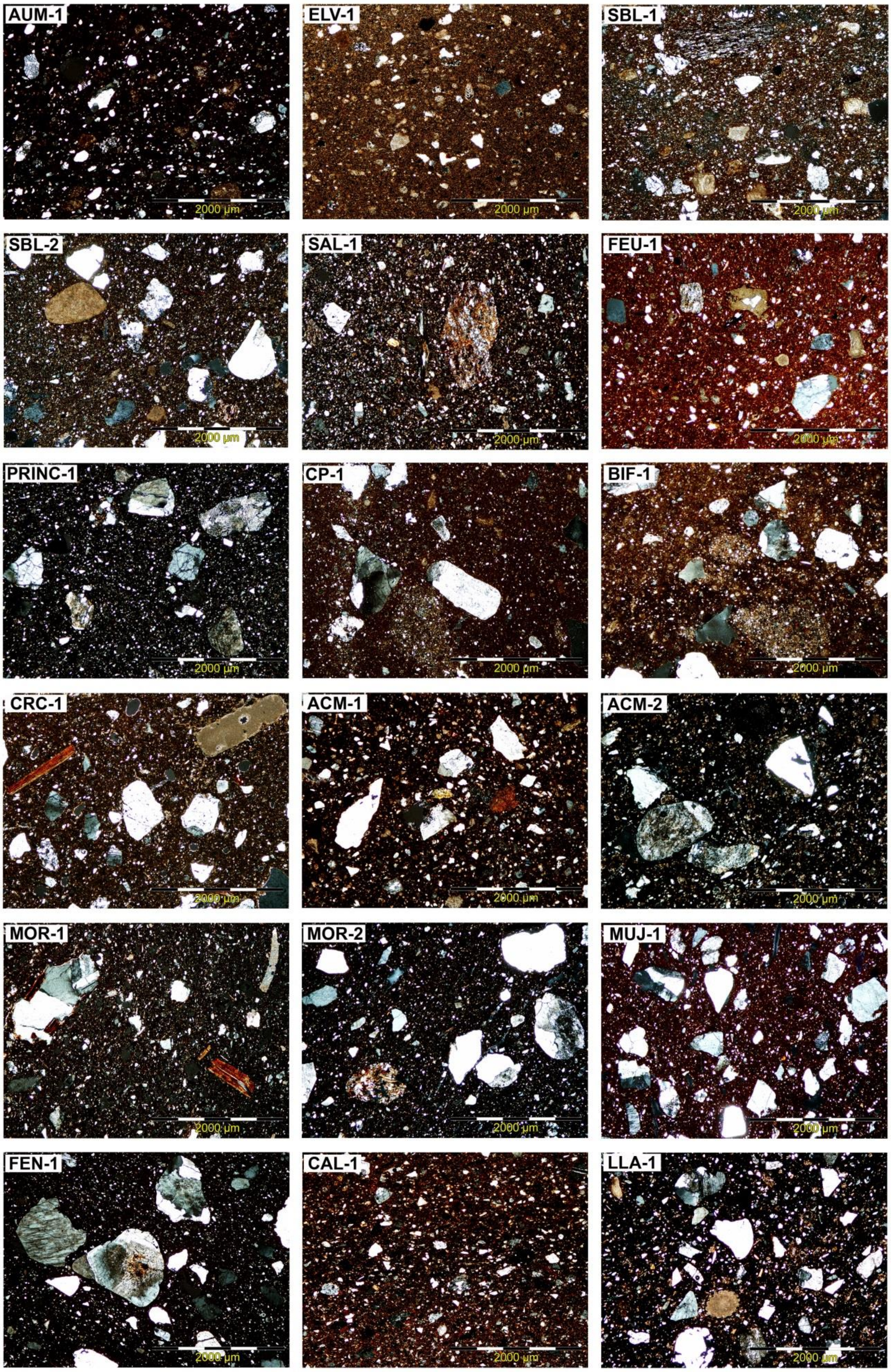

Figure 4. Microphotographs of the FGs 40X, XPL

A few P1 from CAL (CAL-2) are close to those of *Iluro* and *Blandae* because it corresponds to a medium coarse, border calcareous fabric with few microfossils and frequent crystals derived of granitoids. The other P1 from this workshop (CAL-1) are not too different, though they have a Ca-rich matrix with predominant inclusions of grain size fine to medium-fine (Vila Socias and Martínez Ferreras, 2015). Despite its finer inclusions, the petrographic composition of CAL amphorae resembles that of the P1 from ACM (ACM-2).

The fabrics attributed to the sites near the Ripoll River Basin (FEU-1, SAL-1, and SAL-2), as well as some “IND” sherds from these sites, are clustered because they consist in medium-to-coarse, border calcareous to calcareous fabrics. The clayey sediment is rich in iron oxides, with the presence of some nodules of calcite (micrite) and microfossils, especially in SAL-2. Most of the inclusions are metamorphic and sedimentary rock fragments, together with crystals derived from granitoids. They constitute the fluvial-torrential Miocene and Quaternary clayey sediments of the Ripoll River Valley formed by the erosion of the littoral and pre-littoral mountain ranges.

FEU-2 and the productions from the Lower Llobregat basin (SBL-1 and SBL-2) and Barcelona (PRINC-1) unite because they all are calcareous, coarse fabrics. FEU-2 comprises P1 and pointed bases with epigraphic stamps that were produced using Ca-rich clays with abundant medium to very coarse grain-sized aplastic inclusions. In this case, granitic and metamorphic rock fragments predominate, quartz and feldspars are frequent, and limestone and fragments of sedimentary rocks are scarce. The P1 from SBL-1, SBL-2, and PRINC-1 have in turn a Fe-rich clay matrix with carbonates and moderately abundant inclusions, which primarily consist of granitic rock fragments, crystals derived from these rocks, metamorphic rock fragments and, to a lesser extent, sedimentary rock grains. These materials come from the Quaternary alluvial clayey sediments deposited in the Lower Valley of the Llobregat River.

The coarse FGs from CP and BIF, in *Baetulo* (CP-1 and BIF-1), and CRC (CRC-1) are clustered apart because they exhibit a characteristic calcareous matrix with aggregates of calcareous, silty sediment. The aplastic inclusions are relatively abundant and consist of coarse and very coarse granitic rock fragments and crystals derived from these rocks —quartz, plagioclase, K-feldspar, amphibole, and epidote— along with calcareous nodules (micrite). Sandstone and metamorphic rock fragments are few or absent at CP-1.

Protocol 3 represents an amalgam of the technological characteristics of productions and their provenance, by combining all CHEM and PETRO variables (Figure 5, Appendix E.3).

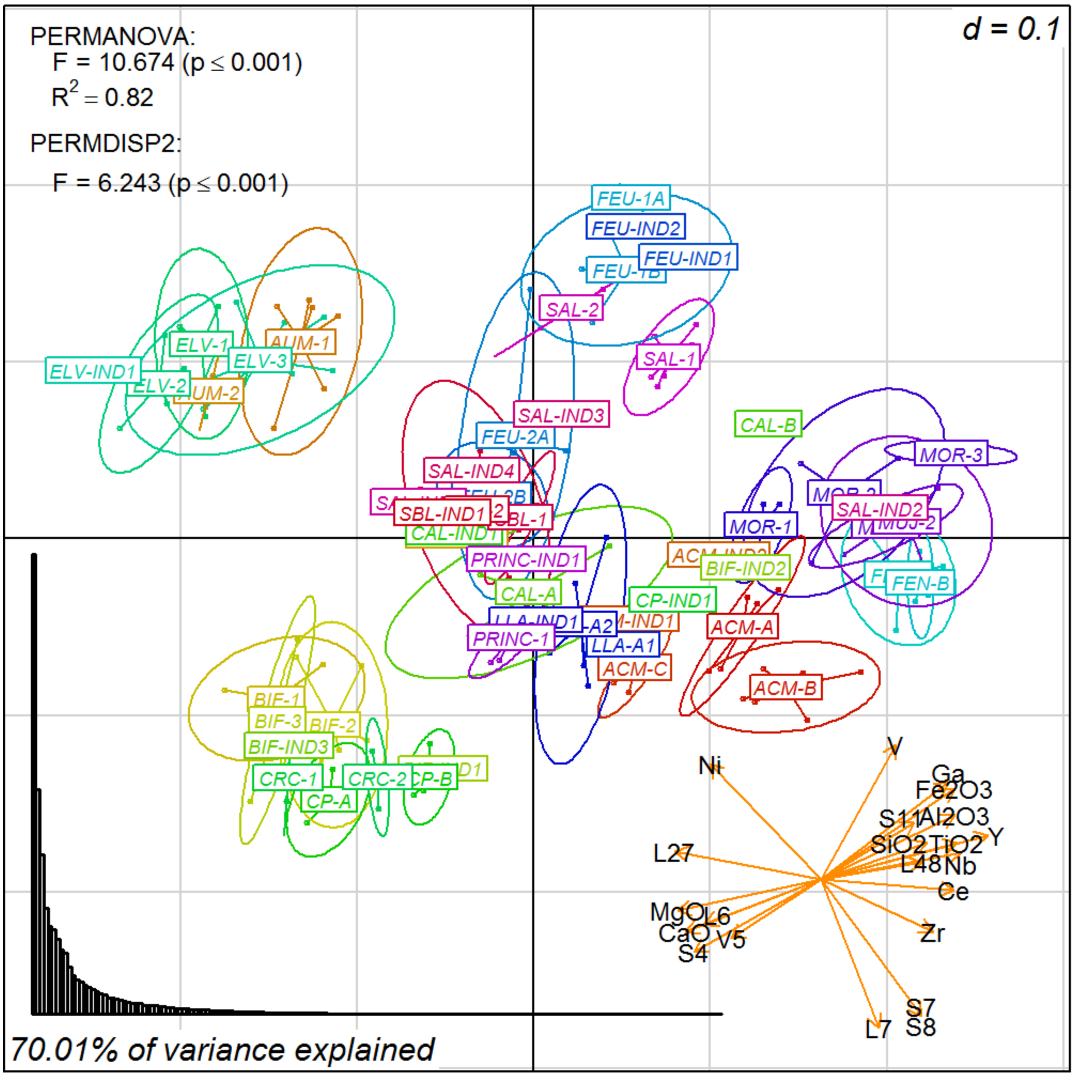

Figure 5. Protocol 3 results concerning the workshops samples. The plot shows the best 2D projection, the horizontal and vertical axes respectively containing the first and second principal coordinates. The RGs and the site outliers are labelled and distinguished by colour. Consult Appendix A for variable codes.

The southern workshops (AUM and ELV) stand out from the others. The most distinctive characteristic is their fine fabrics, predominantly calcareous, with an abundance of carbonates, especially foraminifers, quartz, feldspars, and metamorphic and sedimentary rock fragments.

Workshops near *Iluro* and *Blandae* (ACM, MOR, MUJ, and FEN) differ because of their Fe-rich clays with coarse aplastic inclusions primarily derived from granitoids and abundant biotite, consistent with high Fe_2O_3, Al_2O_3, and SiO_2. The amphorae from the Lower Besòs Basin (CP, BIF and CRC), already well distinguished with protocols 1 and 2, are completely detached from the other workshops. In protocol 3, their position is due to both their petrographic properties (coarse fabrics with a predominance of carbonates and crystals and rock fragments derived from granitoids in a Ca-rich clay matrix) and their high CaO and MgO contents, which are consistent with the presence of dolomite outcrops in the area.

FEU and SAL form another cluster. The D1 and T1 from SAL are close to the border calcareous P1 and D2/4 from FEU (FEU-1A and FEU-1B). Less distinguished, the calcareous P1 and pointed bases with stamped marks from FEU (FEU-2A and FEU-2B) share significant compositional similarities with the D2/4 from SBL (SBL-2). They consist of calcareous, coarse amphorae, with granitoids, metamorphic and sedimentary rock fragments and carbonates resulting in high CaO and low Fe_2O_3, Al_2O_3, MgO, and Cr. The P1 from SBL (SBL-1) differ from SBL-2 because they contain higher Zr, Ni, and Cr. They chemically resemble the P1 of PRINC-1, but the lithological constituents of the aplastic inclusions are equivalent to those observed in the D2/4 from SBL-2.

The northern workshops (CAL and LLA) are difficult to individualize. The calcareous P1 (CAL-A and LLA-A2), which contain foraminifers and bivalves, match those of SBL-1 and PRINC-1. On the other hand, the border calcareous P1 and D7/11 of LLA-A1 are closer to the calcareous P1 of ACM-C.

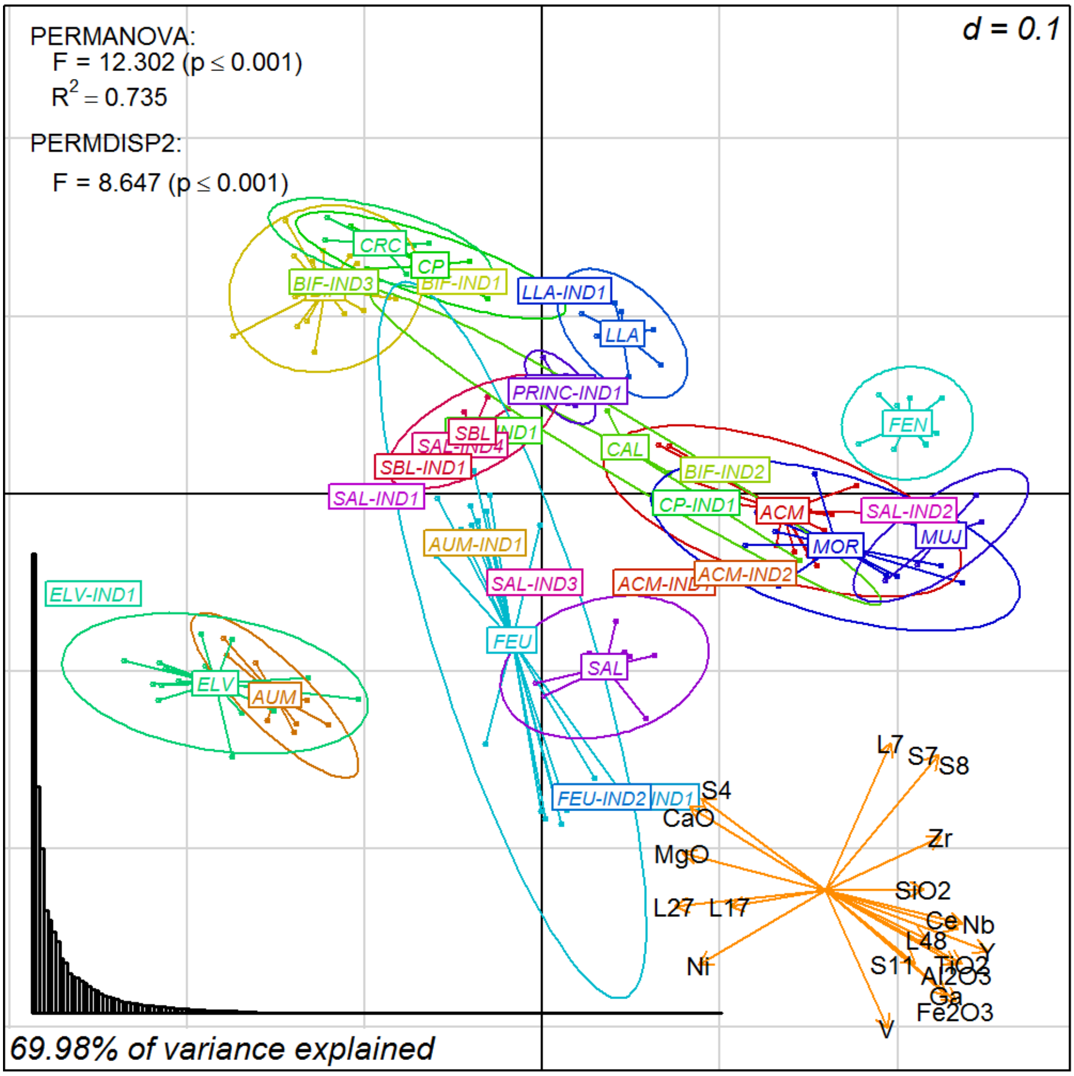

Figure 6. Protocol 4 results concerning the workshops. The plot shows the best 2D projection, the horizontal and vertical axes respectively containing the first and second principal coordinates. The general PGs and the site outliers are labelled and distinguished by colour. Consult Appendix A for variable codes.

To assess the provenance as accurately as possible, protocol 4 considers only variables that characterize raw materials (CHEM & $PETRO_{PROV}$). The resulting biplot (Figure 6; Appendix E.4) were not as discriminative as expected. This is due to the still high multidimensionality of the data—note the many long arrows pointing different directions. Even so, several productions are individualised and most positions are consistent with the PGs.

Particularly well defined are the workshops placed near the Ebro River and *Tarraco* (AUM and ELV), in the lower Besòs River Basin near *Baetulo* (CP, BIF, CRC), and in the Laietan region near *Iluro* and *Blandae* (ACM, MOR, MUJ, FEN). CP, BIF, and CRC exploited Holocene deposits and Miocene marls from the plain that are deltaic, fluvial, torrential and marine. The presence of carbonates in the clayey pastes conferred pale brown to yellowish colours after firing. Instead, the amphorae produced in ACM, MOR, MUJ, and FEN consist in reddish fabrics because the Laietan potters employed the Fe-rich clayey sediments from Quaternary fluvial-torrential deposits that cover the littoral plain. These areas have specific geological constituents, and their amphorae productions are well differentiated while the variability within each zone is very low.

Unfortunately, not even protocol 4 can satisfactorily separate all productions within each region. Nonetheless, this treatment proved to be useful to discern among the amphorae manufactured in the Ripoll River Basin (FEU and SAL), even when they exhibit a high variability in shapes and composition within their workshops. It also allowed individualizing LLA, PRINC, and SBL, which overlap in other protocols. CAL remains the only workshop that overlaps in 2D with geographically unrelated productions.

3.2 Determining provenance: Shipwreck case studies

Protocol 4 proved to be the most effective treatment for individualizing provenance. Therefore, we used it to explore the origin of amphorae from the three shipwrecks considered in this study.

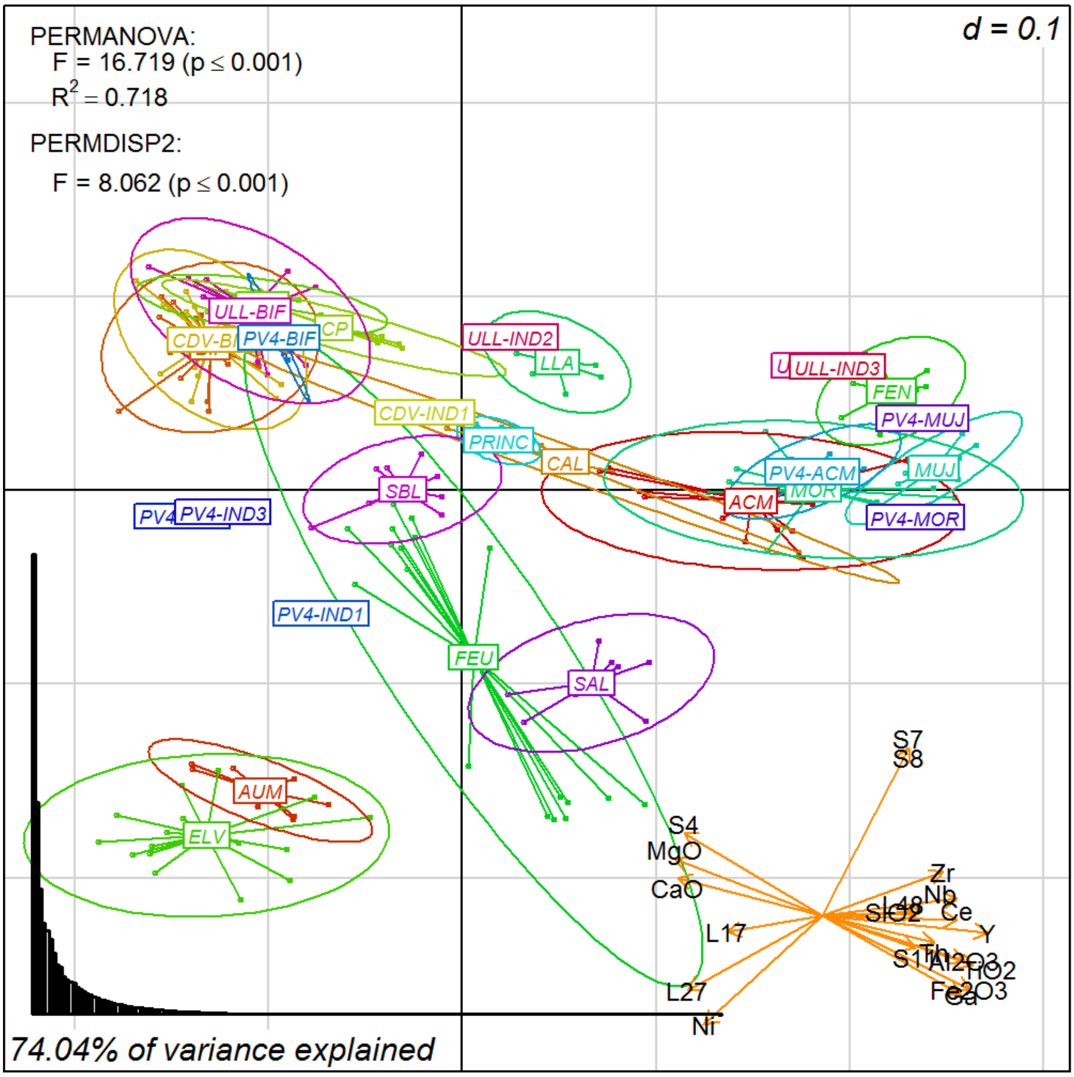

Figure 7. Protocol 4 results concerning both workshops and shipwrecks samples. The plot shows the best 2D projection, the horizontal and vertical axes respectively containing the first and second principal components. The general PGs and the shipwreck outliers are labelled and distinguished by colour. Consult Appendix A for variable codes.

As expected, the biplot (Figure 7; Appendix E.5) shows that most of the P1 from CDV (CDV-BIF) and ULL (ULL-BIF), dated to the Augustan Age, match the amphorae produced at the lower Besòs River Basin (CP, BIF and CRC). Two of the containers with unknown origin from ULL (ULL-IND1/3) resemble the low calcareous productions from MUJ and FEN, while ULL-IND2 is closer to the productions of LLA. CDV-IND1 appears related to the amphorae produced at the lower Llobregat River Valley (SBL) and *Barcino* (PRINC). Despite the varied provenance of these amphorae, the port of departure of these ships was probably the coastal city of *Baetulo* since most of the cargo originated in either one of the two workshops found on the outskirts of the city (BIF, CP).

Dated in earlier times (between 40-30 BC), the provenance of the amphorae found in PV4 is more diverse. Some low and border calcareous amphorae (PV4-ACM, PV4-MOR, and PV4-MUJ) present similar chemical and petrographic composition with the products of different workshops located in the territory of *Iluro* and *Blandae* (i.e., ACM, MOR, and MUJ). Other vessels are associated with the workshops in *Baetulo* (PV4-

BIF), and three (PV4-IND1/2/3) are isolated due to major chemical and petrographic differences compared to the PGs considered.

4. Discussion

The goal of this paper has been to present an explorative methodology for analysing the variability of archaeological ceramics. We intended to offer alternative protocols that drawn information from different data sources and follow different statistical treatments. Building on the conclusions of Baxter et al. (2008), we experimented with a new version of what they named the mixed-mode approach, i.e., the combination of geochemical composition and petrographic data into the same multivariate analysis. Their proposal included using raw chemical data and converting petrographic ordinal data into binominal dummy variables, and the application of PCA or CA for visualization. The approach we advocate here differs in that geochemical data is treated as compositional data, by applying log-ratio transformations, and that the ordinal variables normally used as petrographic data can contribute to more systematic analysis without sacrificing the ordering information. In this sense, our proposal employs techniques developed in other disciplines that, in our assessment, produce more satisfactory and integral images of ceramic materials.

Our confidence in the protocols presented here comes from their performance summarizing the variability of the Roman wine amphorae as shown above. Overall, there is a good match between prior classifications (RGs, FGs, and PGs) and the 2D/3D projections generated by each protocol. Additionally, all PERMANOVA and PERMDISP2 results are significant, under any reasonable criterion (in all cases p-values are much less than 0.01), meaning that the classifications given are satisfactory group hypotheses according to the distances calculated in each protocol.

Except in protocol 1 where there is much overlap, 2D projections consistently separated the two southern workshops (ELV, AUM), the three *Baetulo*-Besòs river workshops (BIF, CP, CRC), four of the Laietan workshops (ACM, MOR, MUJ, FEN), and, in lesser degree, the two inland workshops (SAL, FEU). The least differentiated groups were those containing samples from SBL, PRINC, and CAL, which never lay too far from the projection centre.

By comparing the results of the four protocols, we also aimed to present an independent confirmation of the main conclusion in Baxter et al. (2008), which states that the 'mixed mode' approach to archaeological ceramics is superior to considering data sources separately. Indeed, the results obtained with protocols 3 and 4 confirmed that integrating *chemical* and *petrographic* data can aid characterization and the detection of groups in space and time. Furthermore, we concluded that a more selective multivariate analysis is a better strategy for answering specific questions—i.e., choosing those variables known to indicate the provenance of materials in protocol 4.

To the date, several studies in pottery archaeometry use more than a single analytic method, typically WD-XRF and petrographic observations. In this sense, they are already following a 'mixed mode' approach. However, datasets originating from different sources are rarely put together into the same database or go through the same statistical analysis, if at all. By publishing online the *cerUB* and *biplot2d3d* packages, we offer an opportunity for those researchers that have access to different analytic methods but lack the know-how required for applying and visualizing more sophisticated multivariate statistics (including ordinal variables). Moreover, by establishing these four protocols under the same framework, we allow for straightforward comparisons between their results, which is useful for defining and testing typologies based on different aspects of the data.

Despite what, in our opinion, are clear advantages of applying these protocols, we did detect possible caveats in doing so. First, the applicability of protocols 2 through 4 requires petrographic observations to be annotated in a database. Due to the amount of work this entails, petrographic variables may not be available for all archaeological samples recovered. However, it is indispensable that observations entering the database take the form of ordinal variables rather than other qualitative textual assessment. Additionally, the functions in *cerUB* package assume that petrographic data were named and entered following the same system used by us (Appendix A). However, as we have shown here, it is not necessary to input all petrographic variables in our list since protocols can manage any smaller set of variables.

Also, if the analyst has access to a reliable quantitative petrographic method (e.g., point-counting), other versions of protocols 2, 3, and 4 could be developed to only handle sets of numeric variables rather than using ordinal variables. In the case of using point counting, these alternative protocols would certainly be less complex, requiring solely the scaling to sample total (in case totals vary among samples) and a log-ratio transformation, given that the input data is strictly compositional (as defined in Aitchison, 1982).

Another critical warning concerns the nature of multivariate representations (e.g., biplots), not only in our protocols but when using any ordination method (e.g., PCA, CA, PCoA). We cannot interpret a multivariate projection as bivariate. Multivariate means multidimensional, which implies that the distance between two points in two dimensions cannot account for their distance in a third dimension, the same way that a single blueprint cannot represent a two-story building. Biplots of the first two principal coordinates display the most complete 2D representation that the method can calculate with the data given.

For instance, in protocol 1 (Figure 2), the 2D projection explains almost 80% of the total variability, which in turn is mostly contributed by CaO and MgO. In this case, we may read more safely the position of points in terms of more or less CaO or MgO content. Conversely, when there are many variables, the two most explicative dimensions may correlate with several of them, what is represented in a biplot as a star of long arrows pointing out many directions. In this kind of context, variables ‘compete’ with each other to order the points according to their criterion. This is the case in protocol 2 (Figure 3), where the orientation of inclusions (I2) has a clear readability while interpreting, for instance, the presence-abundance of chert (L33) can be misleading. The Appendix section C.8 explains this more thoroughly.

With this paper we hope to provide general archaeologists with a tool for accessing a straightforward image of the variability of their ceramic materials, thus assisting archaeological classification. However, this is an exploratory tool, and it is not designed to replace finer analyses of geological provenance and material science. Nor do we suggest dismissing other classical multivariate approaches, which are also readily available in R (Baxter, 2016). In this sense, the end products of the protocols (i.e., an R list object) contain a distance matrix that can be further used in other multivariate methods, such as discriminant and cluster analysis. We do not discard the possibility of applying this type of methodology in other archaeological materials and we encourage future development in this direction.

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