VisualEasier - Enhanced visualisation tool in mineral chemistry data analysis through accurate elemental map generation

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Short title: VisualEasier: Elemental Map Visualization Tool

Abstract

VisualEasier is a user-friendly application designed to improve the visualization and interpretation of spatially resolved geochemical data. Developed in the R environment using the Shiny package, it provides a dynamic interface that allows users, regardless of programming experience, to generate high-resolution elemental maps, apply image filters, and perform clustering analysis. The application supports datasets from multiple analytical techniques, such as SEM-EDS, Electron Microprobe, Micro-XRF, and LA-ICP-MS, as long as the input is structured as comma-separated values with pixel-level positional reference. Users can produce individual elemental maps with pixel-by-pixel normalization, generate ternary RGB compositions to explore elemental associations, and apply median or gradient filters to enhance visual features such as grain boundaries or reduce noise. A clustering module based on the k-means algorithm segments the sample into user-defined compositional groups, returning a set of outputs that includes spatial maps, statistical tables, and boxplots for each cluster. All graphical results can be exported in high-quality vectorized PDF format. The flexibility of the system allows users to input normalization references, adapt color palettes, and modify visualization scales. Application on real samples demonstrated the effectiveness of the application in revealing compositional patterns that are not easily identifiable using conventional static plots. The clustering results provided insights into mineralogical domains and potential zoning within the sample, while the filter tools improved the clarity of textural and chemical boundaries. The combination of interactive features, compatibility with multiple data sources, and customizable outputs makes VisualEasier a versatile tool for geologists, mineralogists, and materials scientists seeking to enhance the interpretability of analytical data. The application is particularly valuable in exploratory and research environments where rapid feedback and visual diagnostics play a critical role in decision-making and hypothesis generation.

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46 **Keywords**: Elemental map, MicroXRF, EDS, Mineral Chemistry.

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1. Introduction

The visual representation of elemental distribution is fundamental for a comprehensive understanding in geochemical studies, as accurate spatialization of elemental data allows for a wide range of interpretations and associations. However, outputs from analytical procedures often suffer from low resolution and limit further manipulation such as filtering and personalization to specific research needs. This becomes particularly critical in petrological, mineral exploration and geometallurgical studies, where detailed spatial patterns can indicate zoning, alteration halos, or textural features related to mineralization processes (Bérubé et al., 2018; Caté et al., 2017; Ferreira da Silva et al., 2022a, 2022b; Gazley et al., 2015).

To address these limitations, an attempt was made to enhance the user's capability to understand and manipulate the data, and to provide a more suitable approach for visualization. Visualeasier was developed in the R coding environment, utilizing the Shiny library package (Chang et al., 2025). It offers an intuitive graphical interface, designed especially for users with little or no familiarity with R syntax or programming logic, enabling accessible and efficient data visualization, as well as advanced manipulation through filtering and clustering capabilities.

Through the application, users can generate single-element maps with pixel-per-pixel normalization and apply filters to both single-element and ternary outputs. The ternary map is presented as an RGB composition allowing the selection of three distinct elements. This becomes particularly critical in mineralogical and geometallurgical studies, where detailed spatial patterns can indicate zoning, alteration halos, or textural features related to mineralization processes.

Additionally, a clustering algorithm is used to segment the input sample based on elemental composition, generating a user-defined number of clusters. This output includes boxplots and summary tables describing the elemental characteristics of each cluster, as well as

individual maps highlighting each cluster separately to facilitate interpretation of their spatial distribution. Such clustering outputs are especially valuable in exploratory data analysis, enabling the identification of chemically distinct domains that may correspond to mineral phases, alteration zones, or depositional patterns.

VisualEasier is compatible with any type of spatially resolved mineral chemistry dataset, including SEM-EDS, Electron Microprobe, Micro-XRF, and LA-ICP-MS, once the data is exported in comma-separated values (CSV) format and contains pixel-based positional references. Additional features, such as the conversion of count-per-second (cps) values to concentrations, can be performed when an external reference is provided, preferably the total concentration of the element in the analyzed sample. This flexibility broadens the applicability of the tool across various analytical platforms and sample types.

All outputs are available for download in vectorized PDF format. This ensures high-quality graphic representation suitable for inclusion in technical reports, publications, and presentations, expanding the applicability of the tool beyond exploratory analysis. Also, an chemical estimate for each cluster are given, and the mineral composition can be interpreted based on online tools for mineral chemistry processing (e.g. Ferreira da Silva et al., 2021).

2. Implementation

2.1 The R Environment

As part of its development, the application was built using the R programming language. To ensure a robust and comprehensive structure, several additional libraries were incorporated to address specific functional requirements. The core of the application relies on the Shiny package, which handles most of the syntax and enables the creation of an interactive web-based interface. Complementary packages such as shinythemes, tidyverse, readr, reshape2, raster, data.table, patchwork, Cairo, imager, pals, rsconnect, rasterVis, and ggpubr were also integrated (Barret et al., 2025; Chang et al., 2025; Hijmans, 2025; Wickham, 2016, 2014).

These libraries are essential for matrix and dataframe transformations, raster data manipulation, and graphical output generation functions that would not be efficiently achievable using base R alone. Their combined functionality ensured the application could handle multiple data formats, normalize pixel values, apply image filters, and generate publication-ready maps and plots.

2.1.1 The Shiny Application

The development of an application, as previously described, requires the integration of multiple packages and functions. Among them, the Shiny package stands out as the most essential in this scenario due to its unique framework for building interactive web applications in R (Chang et al., 2025). Shiny enables the creation of a dynamic user interface, incorporating widgets, input fields, and action buttons that seamlessly connect the underlying code with the visual presentation delivered to the user (e.g. Figueira et al., 2024; Konrath et al., 2018; Möller et al., 2020). The rendering of various outputs is also handled efficiently through Shiny, integrating the user's uploaded data with processing steps that result in enhanced visualizations of the dataset, such as elemental maps, compositional tables and clustering analyses. Manipulation of datasets and user inputs through Shiny syntax enables a more streamlined workflow, reducing code redundancy and improving structural parallelism. The use of reactive expressions facilitates the development of modular functions and dynamic variable transformations, this allows user inputs to be processed through multiple layers of computation before returning a final output. This programming approach is consistently applied throughout the implementation.

The application's structure is organized into three main processing tab panels (Figure 1): Elemental Map, Filtered Map, and Cluster Map, as well as a Help tab that provides essential guidance for navigation. In each processing tab, the users are presented with several input widgets through which they can specify key parameters required for map generation, found in

most analytical reports. These include selecting which elements to visualize, inputting their weighted percentages, defining the spatial resolution of the analysis (in millimeters), and uploading tabular datasets containing the elemental data.

2.1.2 Elemental Map Function

Initially, in the *Elemental Map* tab, the application generates individual geochemical maps for each selected element. The input data required consists of tabular format files corresponding to each element, along with additional metadata specifying the dimensions of the sampled area, essential for accurate spatial scaling. Furthermore, users can input weighted percentages for each element to perform normalization, which contributes to refining the final visual outputs. Users can also choose from a variety of color palettes to customize the visual output. The main result produced in this tab is a compilation of elemental maps based on the parameters selected. Each map can be individually saved as an image within the application, or collectively exported as a single, vectorized PDF file containing all generated maps in composition.

2.1.3 "RGB and Filtered Maps" Function

The *RGB and Filtered Maps* tab provides image processing tools for both single-element and ternary (RGB composite) maps. For the RGB composite output, the application requires the selection of three different elements, each assigned to a color channel (red, green, or blue) to best suit the desired visualization. Users can apply a median filter to reduce noise or a gradient filter to enhance grain boundaries; both functionalities are implemented using the Imager package. The median filter smooths the image using a 3×3 neighborhood window, computing the median pixel value within this interval. The gradient filter, on the other hand, highlights edges along the x and y axes, making it particularly effective for grain boundaries delimitation. In this tab, the dataset is first normalized and converted into an image object,

which undergoes filtering and further processing. The result image is then transformed back into a data frame format for display as the final output map.

2.1.4 Cluster Map Function

The *Cluster Map* tab enables more advanced statistical analysis through the *k*-means clustering algorithm. By default, R implements the method proposed by Hartigan and Wong (1979), which seeks to partition a set of data points into *K* clusters by minimizing the within-cluster sum of squares (WCSS). The algorithm begins with an initial set of *K* cluster centers in *N*-dimensional space and iteratively refines the partitioning by evaluating Euclidean distances between each point and the cluster centroids, transferring points between clusters whenever such a move reduces the WCSS. In the context of geochemical mapping, this optimization procedure supports the delineation of zones with similar elemental compositions, this is particularly effective to highlight mineralogical domains that may not be evident through univariate analysis alone.

This output allows users to interpret spatial patterns in compositional variability by generating not only a composite cluster map but also individual maps for each cluster. Additionally, it provides a statistical overview of cluster compositions through boxplots and summary tables, displaying concentration ranges, means, and standard deviations for each cluster group. These tools enhance the interpretability of the clustering results and offer a quantitative foundation for exploring mineralogical segregation and related geochemical processes.

Figure 1. Application tab panels, from left to right, Elemental Map, Filtered Map, Cluster Map.

2.1.2 Data wrangling

Although the application development relies on some unconventional packages for its structure, the classical data wrangling practices, well established within the R programming community, particularly through the Tidyverse package (Wickham, 2014), represent a fundamental role in this project. Core exploratory data analysis techniques such as data transformation, filtering, and plotting are essential to the implementation of a visualization-oriented application.

Primarily for visualization purposes, the input data passes through several transformations to ensure compatibility with the required parameters. These steps include treating the user input as a matrix, merging datasets from multiple elements, and applying operations such as filtering, column selection, and data binding. This process merges the individual tabular inputs into a more robust and refined dataset, which enables pixel-by-pixel normalization and advanced plotting using the ggplot2 package (Wickham, 2016).

Beyond the data preparation for visualization, the application also performs several statistical summaries, including compositional means, standard deviations, and normalization procedures. These are particularly important because the input data often expressed in count per second (cps) needs to be transformed to represent the percentual part of each element in the total composition of the sample. An essential process for generating both individual and integrated geochemical maps.

3 Input data

To ensure the proper functioning and reliability of the application, the input data must adhere to specific structural and content requirements. Each element to be mapped is represented by a single tabular file in CSV format, containing the results obtained from the analytical procedure. These files must include the count-per-second (cps) values corresponding to the respective

element, as this metric serves as the basis for generating the spatial distributions in the application.

For illustrating this work, the input data were generated using a Micro-X-Ray Fluorescence (MicroXRF) analytical system. The equipment produces individual files for each analyzed element, where each file contains a 2D matrix-like representation of the scanned area. Each row corresponds to a pixel in the image, and each column reports the cps value measured at that point. The positional reference of each pixel is implicit in the row/column structure of the file, preserving the spatial integrity of the measurement.

The MicroXRF output also includes a separate summary file providing the bulk chemical composition of the scanned area, which can be used as a normalization reference. This allows the application to convert cps values into relative concentrations (e.g., in percentage or ppm), when such external reference is available and provided by the user. This conversion enhances the comparability among different elements, supports pixel-by-pixel normalization, and facilitates more quantitative interpretations of the geochemical data.

This data structure, composed of one matrix per element, each in CSV format, plus a reference table, is fully compatible with VisualEasier, enabling efficient and automated generation of elemental maps, RGB composites, and clustering analysis, without the need for manual preprocessing or code manipulation.

Additionally, any mineral chemistry analytical system that meets the aforementioned requirements, such as exporting individual elemental files, providing reference values for converting cps to concentrations, and maintaining spatial positioning of measurements, is compatible with the application and can take full advantage of its functionalities. Example use cases include SEM/EDS mapping, Electron Microprobe analyses, and LA-ICP-MS datasets.

4. Application results and discussions

To illustrate the functionalities of this application, we used MicroXRF data obtained from samples of sulfide-bearing metamorphosed volcano-sedimentary rocks. These rocks are composed of silicates (e.g., garnet, chlorite, plagioclase, quartz, epidote, tremolite, anthophyllite, among others), various sulfides (e.g., galena, chalcopyrite, sphalerite, pyrite, pyrrhotite), and minor carbonates (identified as zones with high Ca content, once Carbon and Oxygen are not identified). As a result, the analyses contain elemental signals for Fe, Zn, S, Ca, Si, Al, Cu, Ti, Pb, Mg, and several other elements shown in the next sections. These data served as input for testing the different functionalities of the application, with each sample being processed within a dedicated tab panel. Through this structure, it was possible to evaluate the performance, versatility, and accuracy of the application to handle diverse data inputs and visual outputs.

4.1 The Elemental Map tab

Besides enabling the generation of individual elemental distribution maps with enhanced resolution and optimized data scaling, the application also incorporates features aimed at improving accessibility and user experience. One notable implementation is the inclusion of a diverse range of color palettes, including perceptually uniform and colorblind-friendly schemes. These options ensure that the visual interpretation of the data remains effective and inclusive for a broader audience, without compromising the accuracy or clarity of the elemental maps. In the current version, users can choose from five different color pallets (Figure 2): “viridis”, “inferno”, “plasma”, “magma”, or “turbo”.

The normalization allows for a more correlative relationship between different elements, the understanding of elemental spatialization and distribution regarding the visualisation of the whole sample in a compilated product gives the possibility to interpret associations with high accuracy and a more robust general knowledge of the process that thrives through the data.

Figure 2. Elemental Map outputs, viridis, turbo, inferno, magma and plasma palettes.

4.2 The Filtered Map tab

Alongside data normalization, filtering plays a crucial role in the preparation of datasets for a suitable and effective visualization, especially to highlight different aspects of the same sample. In the case of sample 3 (Figure 3), the median filter was applied to the ternary RGB composition to reduce noise and enhance overall readability, while the gradient filter was used on the calcium map to emphasize grain boundaries and structural features. Both filtering strategies contribute to a more accurate and insightful interpretation of spatial patterns. Additionally, the ternary RGB map interface allows users to assign specific elements to each of the red, green, and blue channels, offering flexibility in customization of visual outputs and elemental relationships interpretation from multiple perspectives. On the other hand, the individual elemental map is important for the characterization of a single element and to highlight its distribution with more focus on the single representation in regards to the association between other elements.

Figure 3. Sample 3 Filtered Map outputs, unfiltered, median and gradient filters applied.

4.3 The Cluster Map tab

Finally, the clusterization process is fundamental for a more robust and deeper analysis of the sample to be interpreted (Figure 4). The segmentation of different groups (clusters) within the sample based on the elemental composition resembles the differentiation between various mineral systems. However, it is highly recommended to navigate through the other tabs of the application as an initial approach to better familiarization of the study object, once it is up to

the user to select how many clusters the algorithm will use (*k*). A fewer number of clusters could represent less descriptive groups while a higher number directs the algorithm to differentiate similar compositional areas, or also grouping noise as an individual cluster, this can be seen as a limitation for the application but the flexible processing allows users to attempt clusterization through different cluster numbers until the output is suitable for the intended analysis.

Alongside the main output (A), boxplot plots with compositional information of each cluster (B) associated with the summary panel (tables 1 and 2) are essential for interpretation and works as a quantitative approach to data understanding. While the individual cluster map (D) shows a singular spatial distribution of each cluster. The general compositional aspect of each cluster could bring further interpretations not only about the elemental spatialization of the cluster itself but also about mineralogical inferences.

Although those interpretations are susceptible to the resolution and quality of the input data, the application is sensitive and responsive to the dataset processed, meaning that high-resolution data can amplify the spectrum of possible interpretations, with more cohesive and direct spatialization of the elemental distribution, and consequently, the clusterization.

Table 1. Cluster Map tab compositional mean per cluster table output.

Table 2. Cluster Map tab compositional standard variation per cluster table output.

Figure 4. Sample 4, Cluster Map outputs. A) Cluster Map, B) Cluster Boxplot, C) Individual Cluster Map.

5. Final remarks

The application offers a wide range of possibilities for the visual interpretation of geochemical data, providing a robust tool for identifying meaningful connections between elemental distribution and mineralogical processes. The application is divided into multiple tabs, each with a specific purpose, which enables a complete and structured analysis of the sample. Although the combined use of all tabs provides a more thorough visualization, the system remains flexible. Each tab functions independently, allowing the user to upload data directly and focus on the aspect of interest. This structure ensures that users can work with the most relevant tools for their analysis, without relying on a fixed workflow.

Moreover, the application not only enhances visualization but also facilitates its transferability, as users can export the results in vectorized PDF format. This feature supports both detailed image analysis and straightforward export in other image formats directly through the interface.

Despite the fact that its performance depends on the quality of the input datasets, users who provide well-processed and reliable data can fully benefit from its analytical potential. In addition, the concise and modular structure of the application allows for straightforward future implementations, especially as community feedback contributes to further improvements. This includes not only computational enhancements, but also adaptation to a broader variety of analytical datasets and sample types.

Availability

The source code for VisualEasier is freely available for download and use under an open license via GitHub at: [https://github.com/lucasamesquita/Visualeasier]. Users are encouraged to explore, adapt, and contribute to the ongoing development of the tool. Additionally, an online version of the application will soon be available on the Geological Survey of Brazil's official application platform: https://apps.sgb.gov.br, allowing users to run the tool directly from a web browser without requiring local installation.

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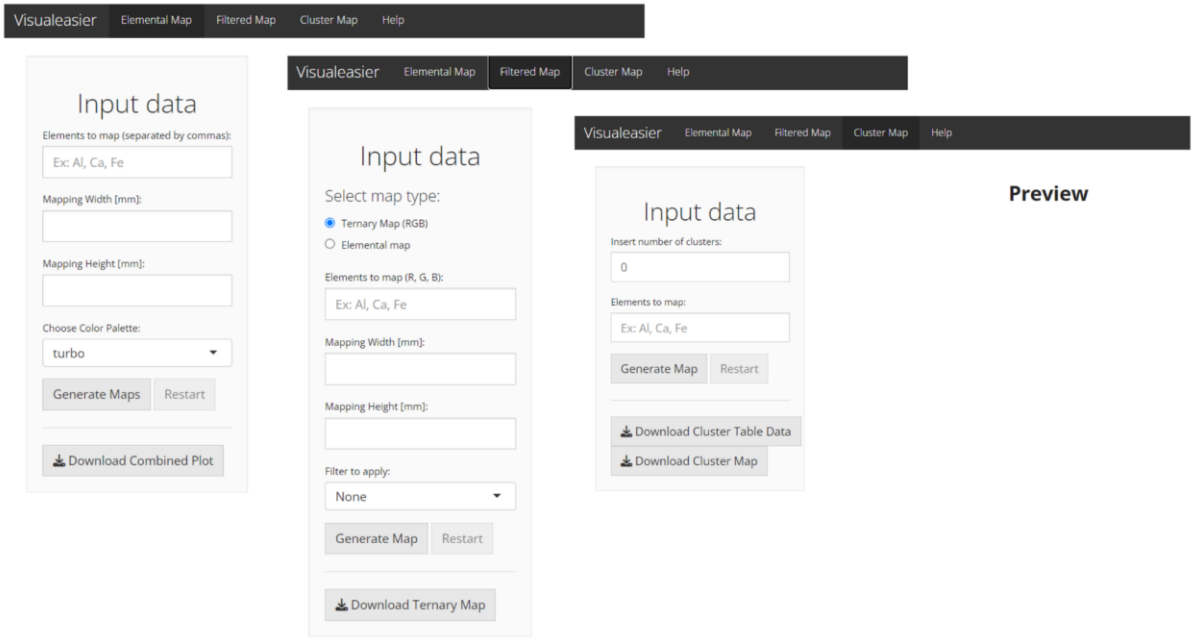

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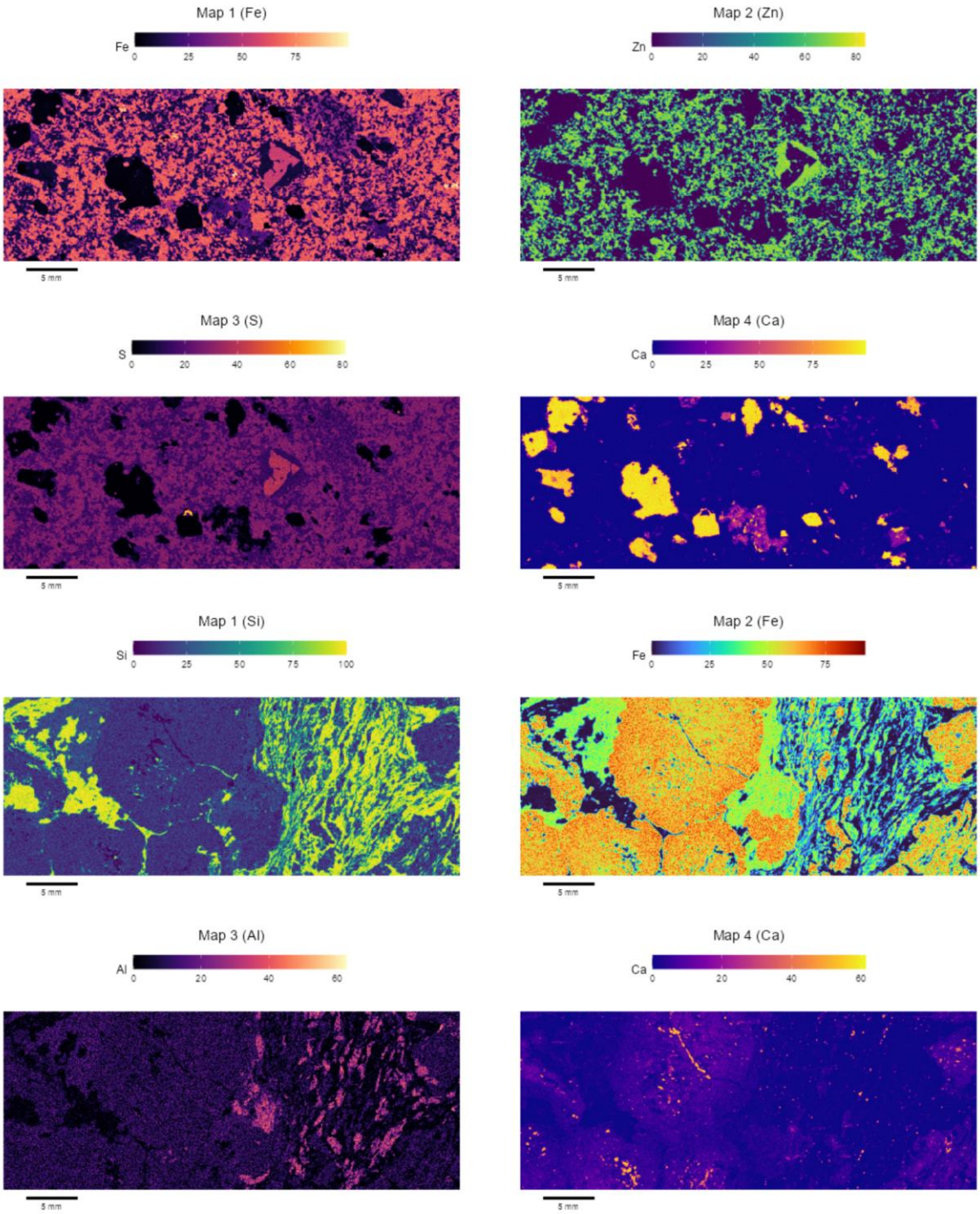
379 FIG 1


Map 1 (Fe)
Fe
0
25
50
75
Map 2 (Zn)
Zn
0
20
40
60
80
5 mm
Map 3 (S)
S
0
20
40
60
80
Map 4 (Ca)
Ca
0
25
50
75
Map 1 (Si)
Si
0
25
50
75
100
Map 2 (Fe)
Fe
0
25
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20
40
60

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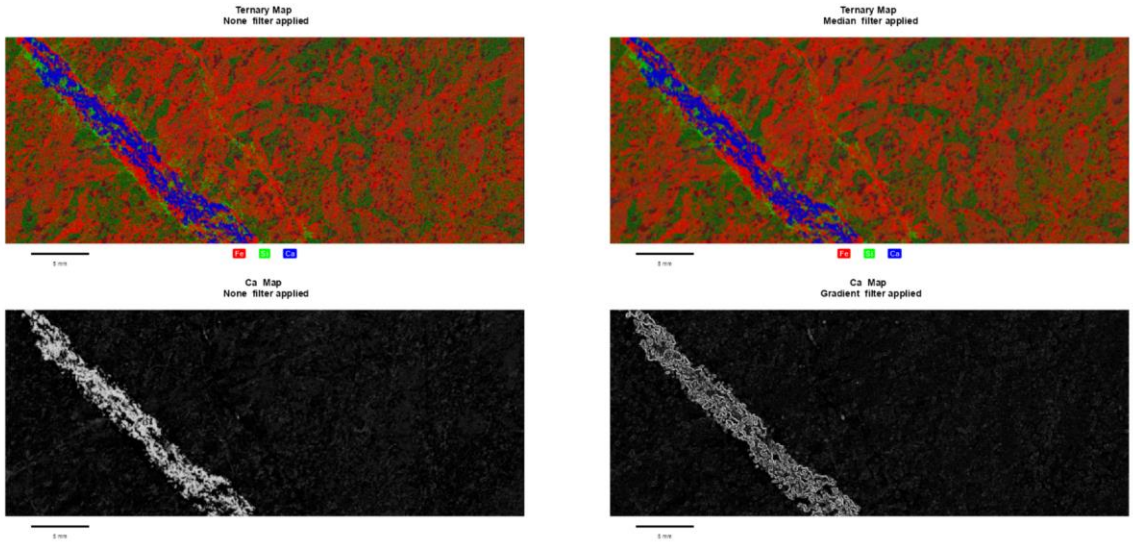
381 FIG 2



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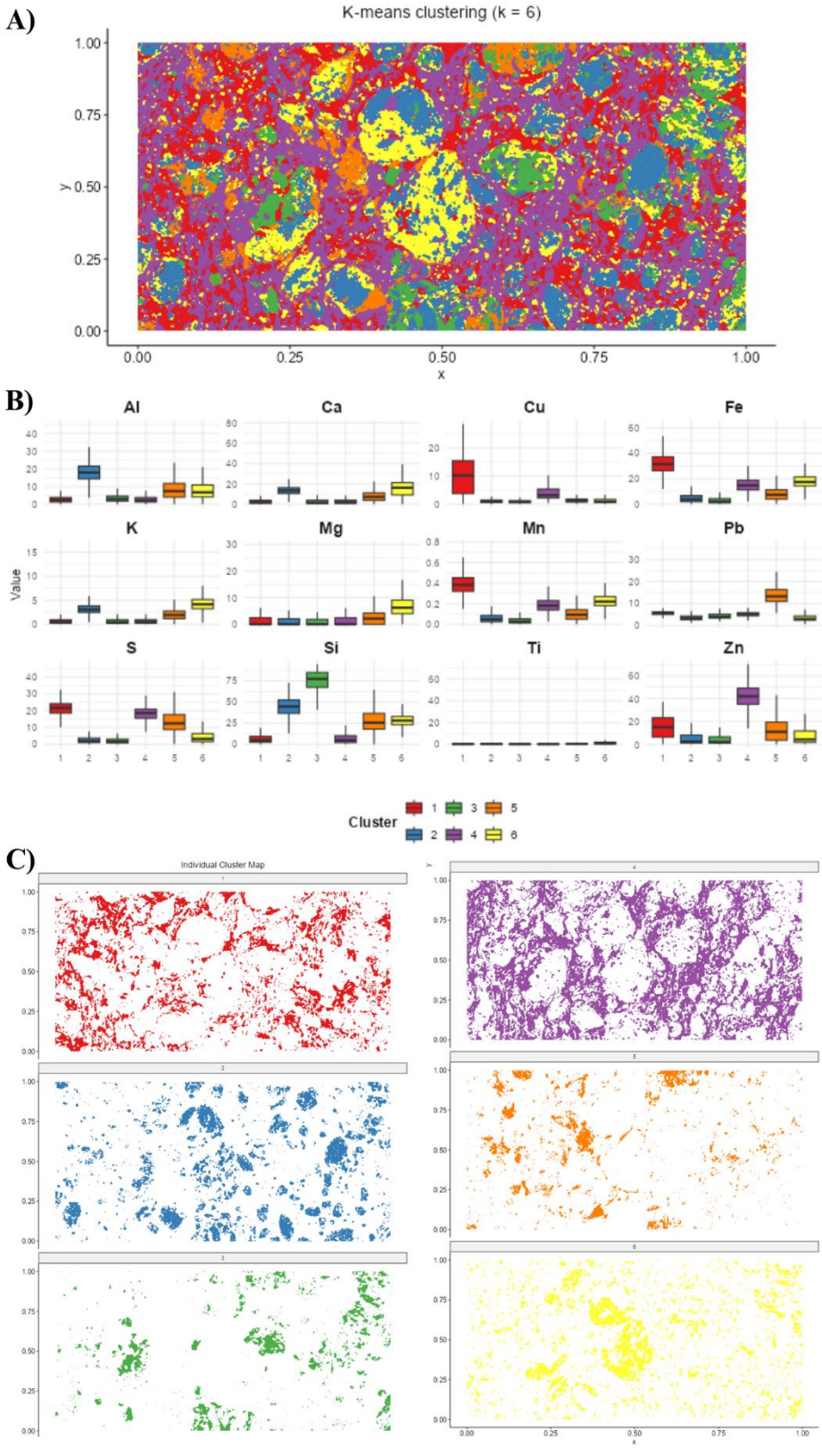
383 FIG 3



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385 FIG 4

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Cluster	Percentage of Rock Composition	Si (wt %)	Zn (wt %)	Fe (wt %)	S (wt %)	Ca (wt %)	Al (wt %)	Pb (wt %)	Cu (wt %)	Mg (wt %)	K (wt %)	Ti (wt %)	Mn (wt %)
1	18,8	7,093	15,203	32,315	21,073	2,856	2,618	5,679	10,263	1,414	0,692	0,399	0,394
2	14,8	44,523	6,016	4,874	2,733	13,139	18,04	3,82	1,321	1,301	3,249	0,742	0,061
3	6,9	75,303	5,185	3,173	2,346	2,635	3,449	4,569	1,132	1,058	0,648	0,462	0,04
4	38,6	7,472	41,882	15,236	18,01	2,859	2,577	5,324	4,132	1,292	0,685	0,343	0,187
5	6,7	28,652	12,423	8,046	13,706	7,841	8,285	13,973	1,586	2,592	2,02	0,776	0,1
6	14,2	28,659	7,641	18,061	4,329	15,217	7,791	3,663	1,493	6,737	4,273	1,911	0,227

TABLE 1

Cluster	Si (wt%)	Zn (wt%)	Fe (wt%)	S (wt%)	Ca (wt%)	Al (wt%)	Pb (wt%)	Cu (wt%)	Mg (wt%)	K (wt%)	Ti (wt%)	Mn (wt%)
1	7,142	9,58	8,071	4,436	2,882	2,448	1,113	6,812	1,92	0,649	0,694	0,099
2	10,805	7,285	3,8	2,351	4,981	5,249	1,764	1,335	1,642	1,124	1,206	0,047
3	11,609	6,495	3,056	2,096	2,824	2,645	1,887	1,186	1,445	0,631	0,972	0,038
4	7,595	9,684	5,26	4,169	2,921	2,497	1,483	2,633	1,836	0,642	0,688	0,064
5	14,497	9,362	4,989	6,723	5	5,324	4,102	1,362	2,835	1,14	1,155	0,062
6	8,538	7,545	5,822	3,329	8,026	4,79	1,904	1,598	3,856	1,468	3,606	0,071

TABLE 2