Interpretation of XRF spectral imaging data using dimensionality reduction combined with clustering algorithms

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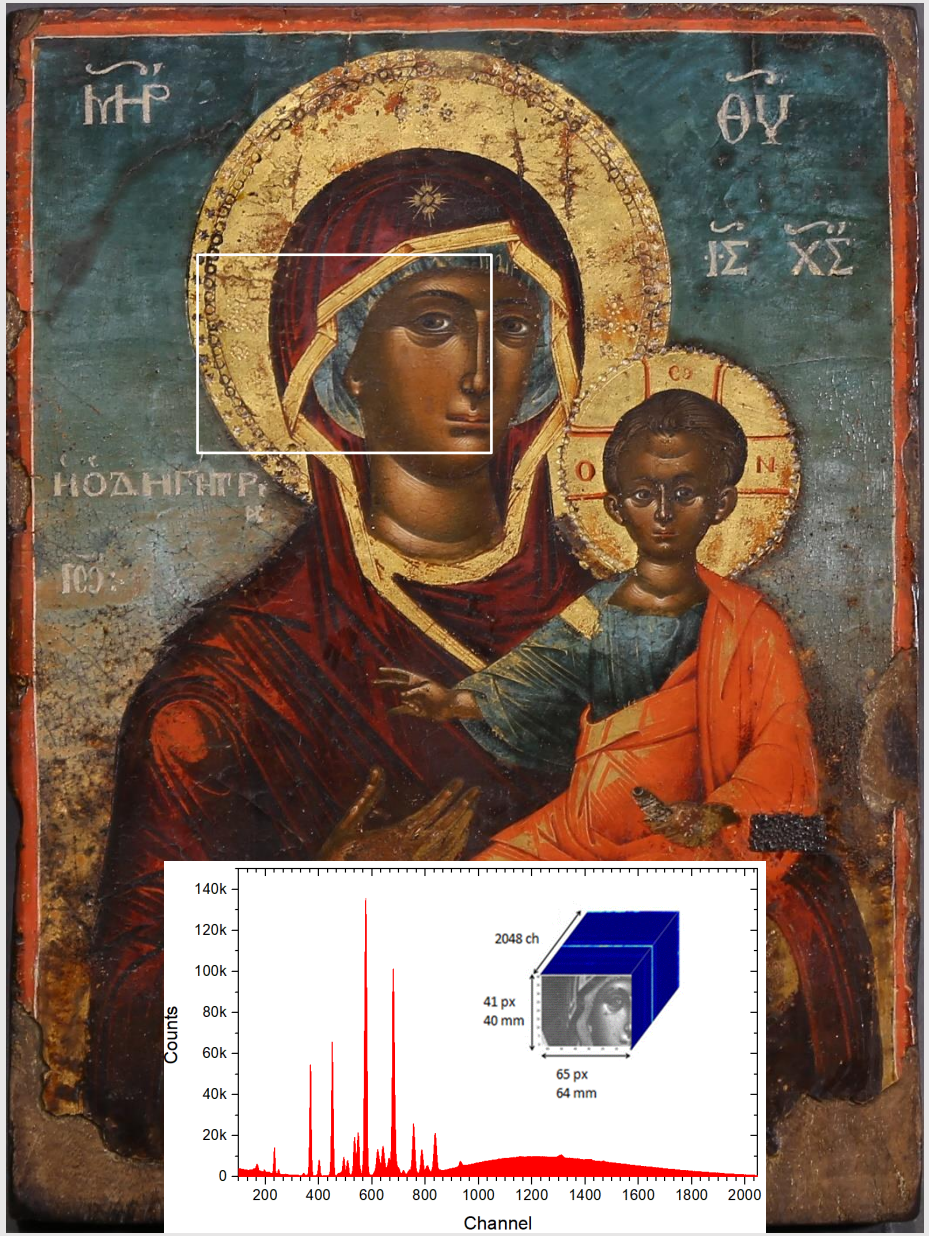
Studied panel painting

- 18th century Greek religious panel painting
- Virgin Mary **“Odigitria”** (Hodēgētria = She who shows the Way)
- originates from **Epirus** region (NW Greece)
- attributed to the famous painters from Kapesovo village **“Kapesovites “ , 28 x 21 cm**
- M1-Mistral (Bruker) micro-X-ray fluorescence spectrometer
- Area of 64 × 40 mm^2 (65 X 41 = 2665 pixels)

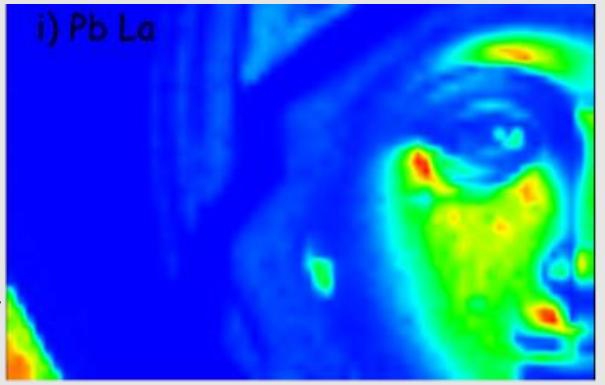


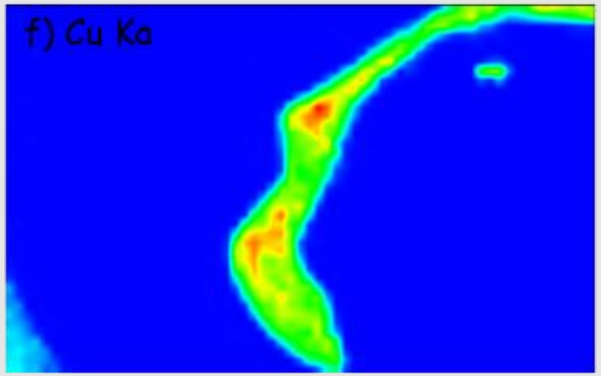
Spectroscopic Analysis

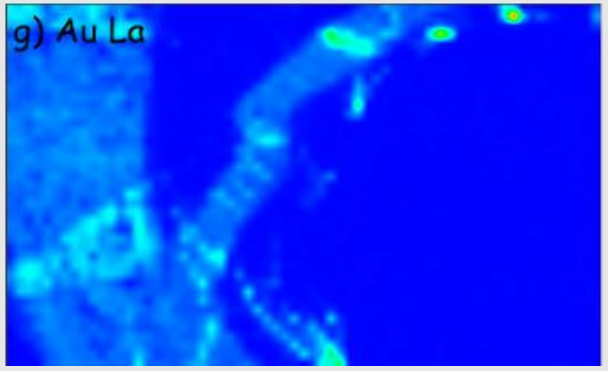
- data were analyzed using the PyMCA

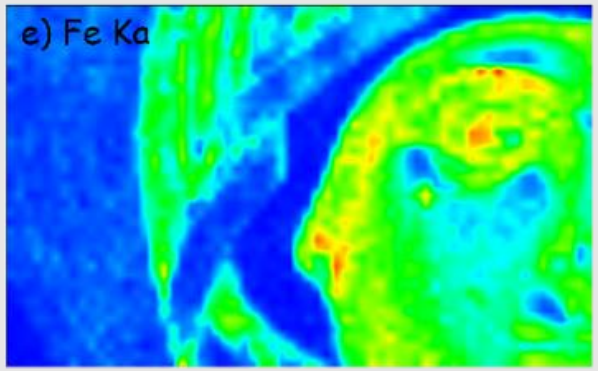
- elemental distribution maps of

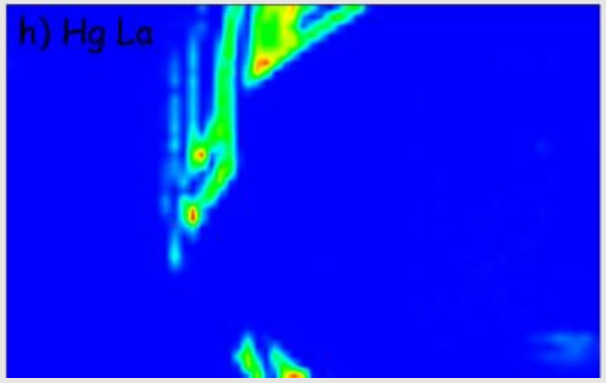
Pb, Cu, Au, Fe, Hg and Ca

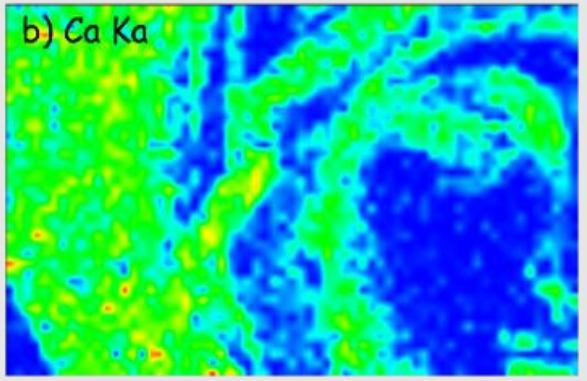










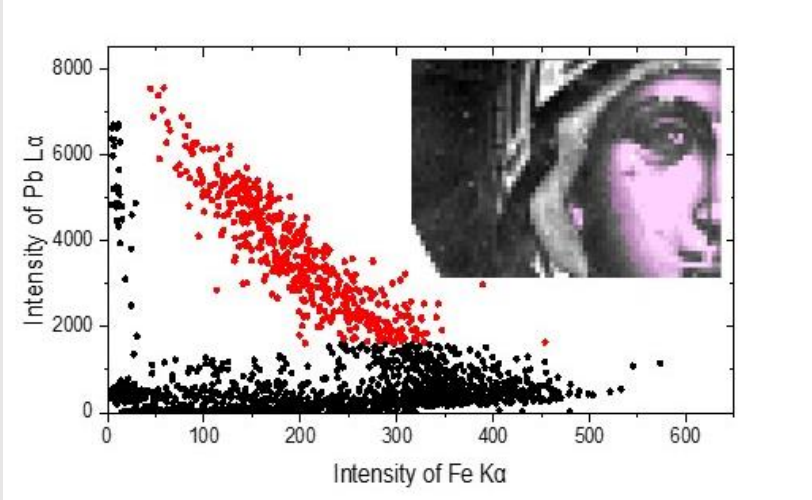


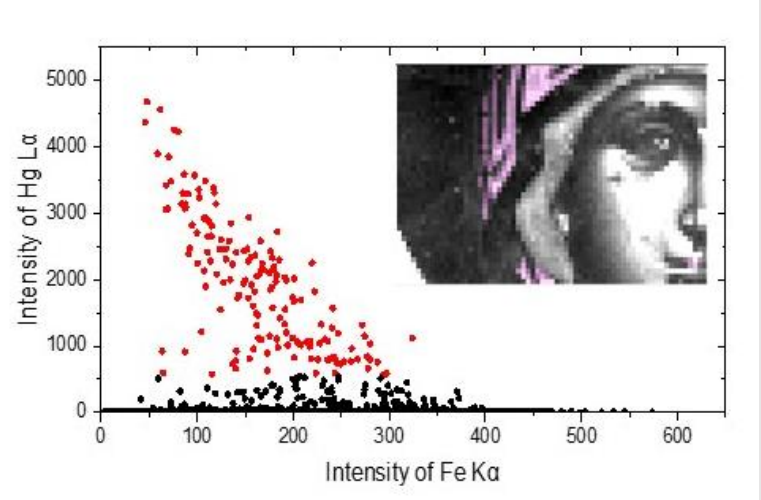
Spectroscopic Analysis

- Transitions intensity scatter plots, spatial correlations

  Left) Pb relative to Fe

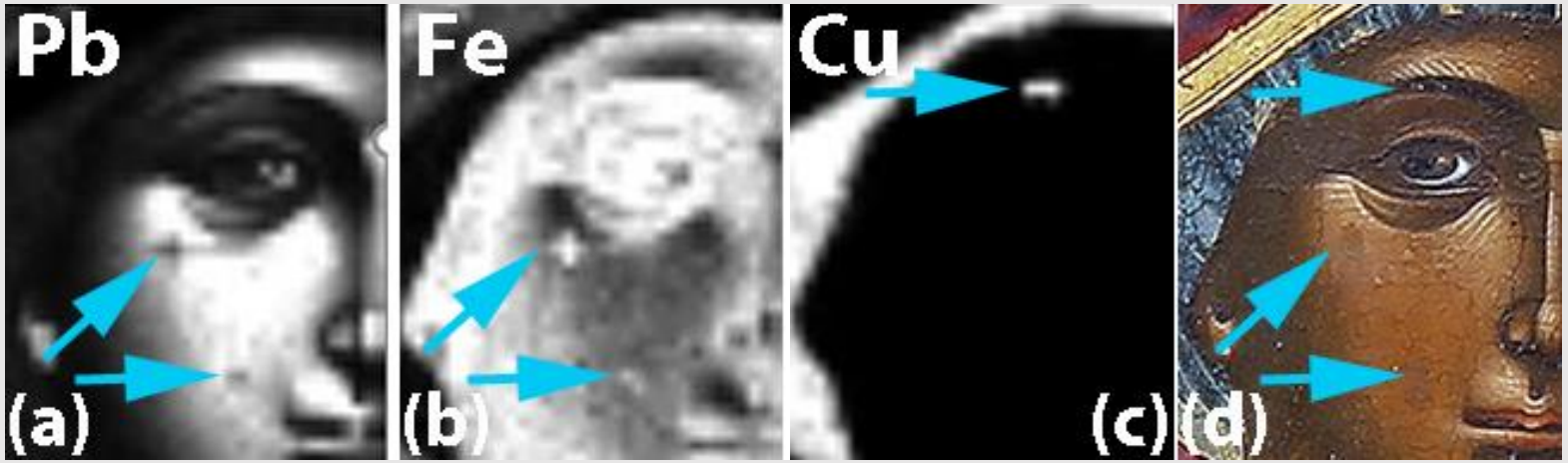
  Right) Hg relative to the Fe





- Preservation of the artifact

Two intensity irregularities on the area of Virgin Mary's cheek **(a, b)**
Copper shows a spot of high intensity on the Virgin Mary's eyebrow **(c)**



Clustering

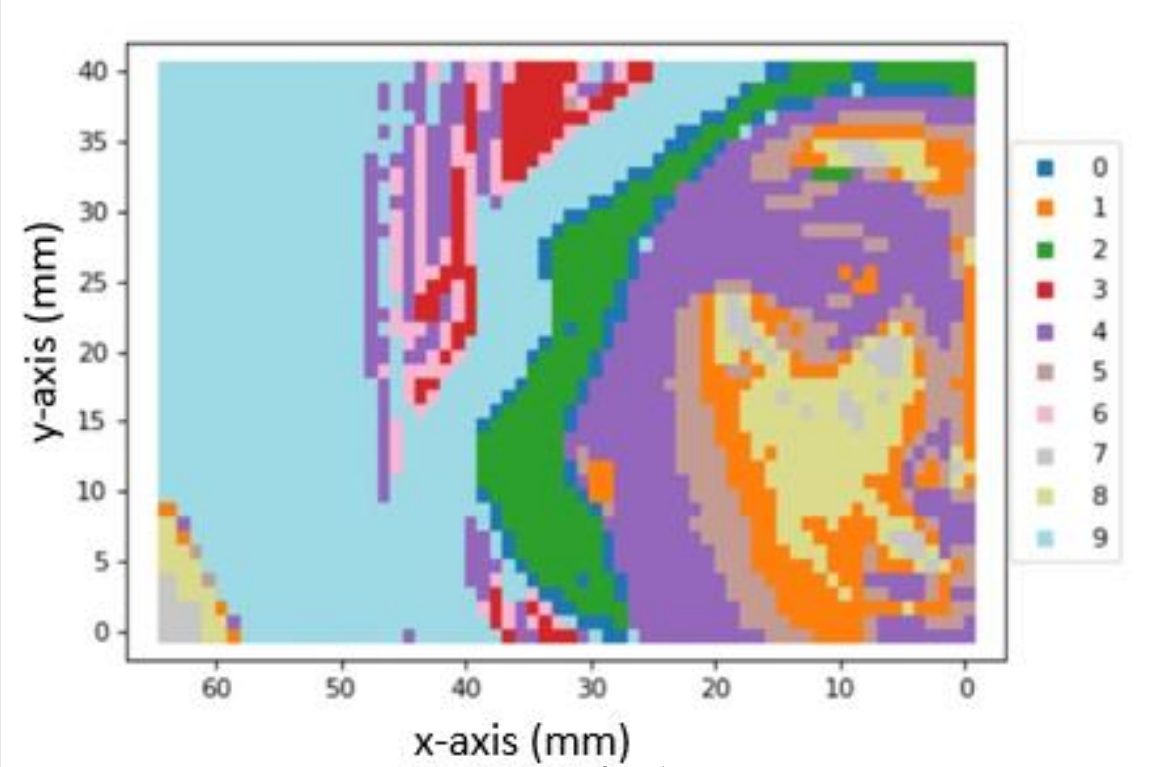
Object:

- Organize the spectral information
- Groups of spectra that shape similarities defining a distance measure (Euclidean, Manhattan ,Minkowski or Hamming)
- Each cluster can be summarized by a representative spectrum, the cluster centroid
- K-means algorithm for clustering

- **Step1:** Choose the number of K
- **Step2:** Randomly select any K data points as cluster centers
- **Step3:** Calculate the distance between each data point and each cluster center
- **Step4:** Assign each data point to some cluster
- **Step5:** Re-compute the center of newly formed clusters
- **Step6:** Keep repeating Step3 to 5 until a stopping criteria is met

k-means

- The most popular clustering method due to its simplicity and low computational complexity O(n)
- $X=\{x_1,x_2,\ldots,x_{2665}\}$ is the spectra dataset, where each x_i is a spectrum vector in $\mathbb{R}^{2048}$ vector space
- In our case the number of clusters is not known
- Use of the Silhouette criterion (K=10, score≈0.52)

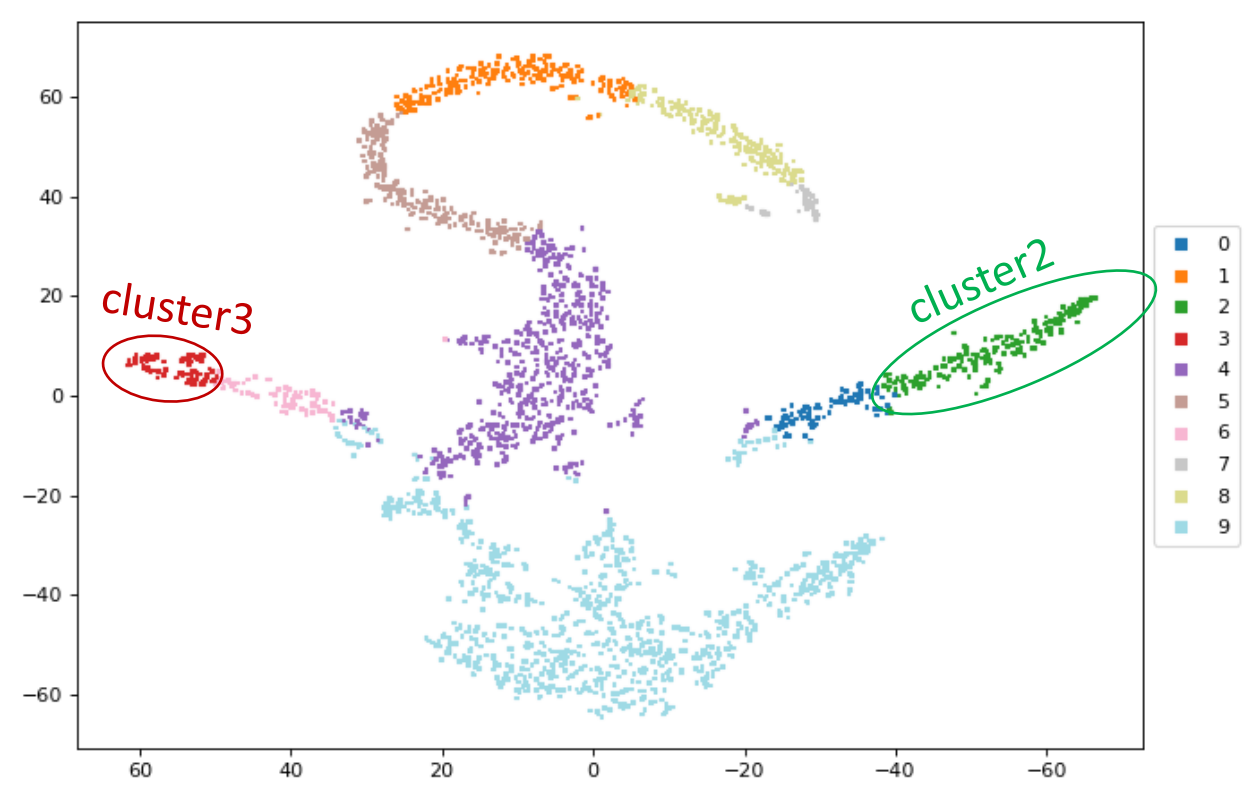


Mapping of clusters

Visualization

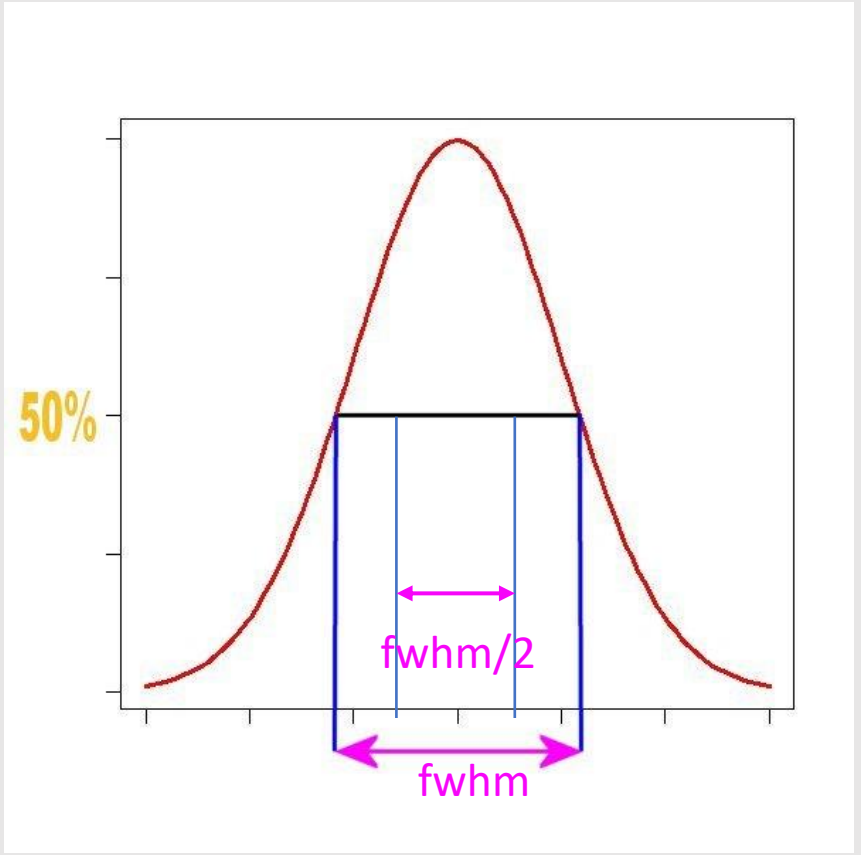
- Dimensionality reduction methods to project each high dimensional spectrum vector to a two-dimensional vector
- Next the two-dimensional projections permits spectra visualization
- $\mathbb{R}^{2048} > \mathbb{R}^{25}$ PCA (Principal Component Analysis)
- $\mathbb{R}^{25} > \mathbb{R}^{2}$ t-SNE (t-Stochastic Neighbor Analysis)

Data Visualization in two dimensions



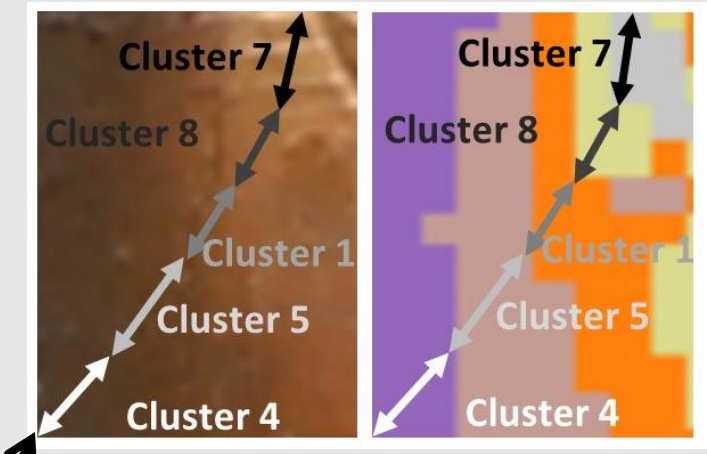
Cluster Interpretation

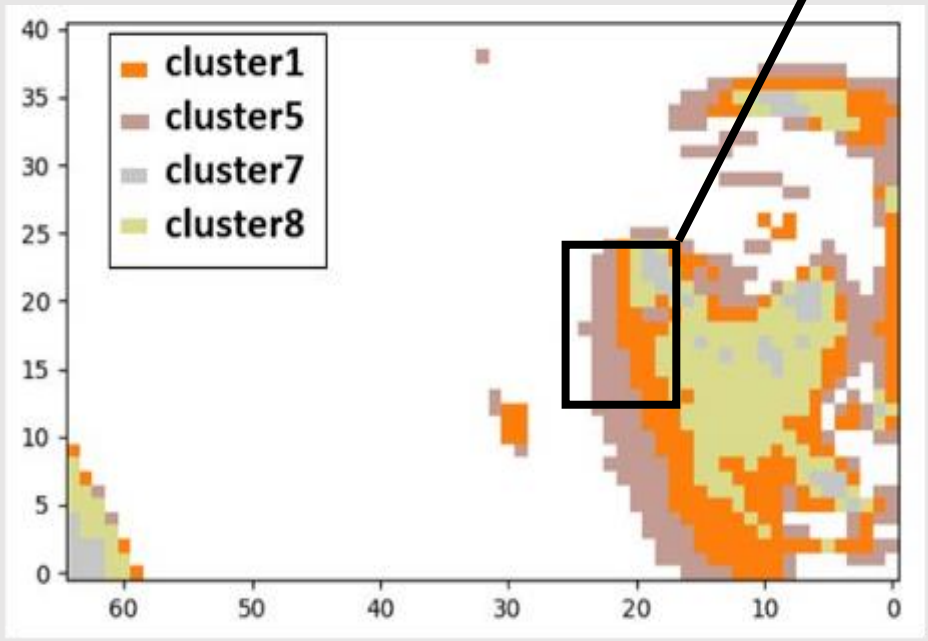
- The representative spectrum (centroid) of each cluster was evaluated
- The transition intensities were estimated by the region of interest method (ROI)
- Energy range was selected equal to ±fwhm⁄2 to avoid overlap of L X-ray transitions of the elements Au, Hg and Pb

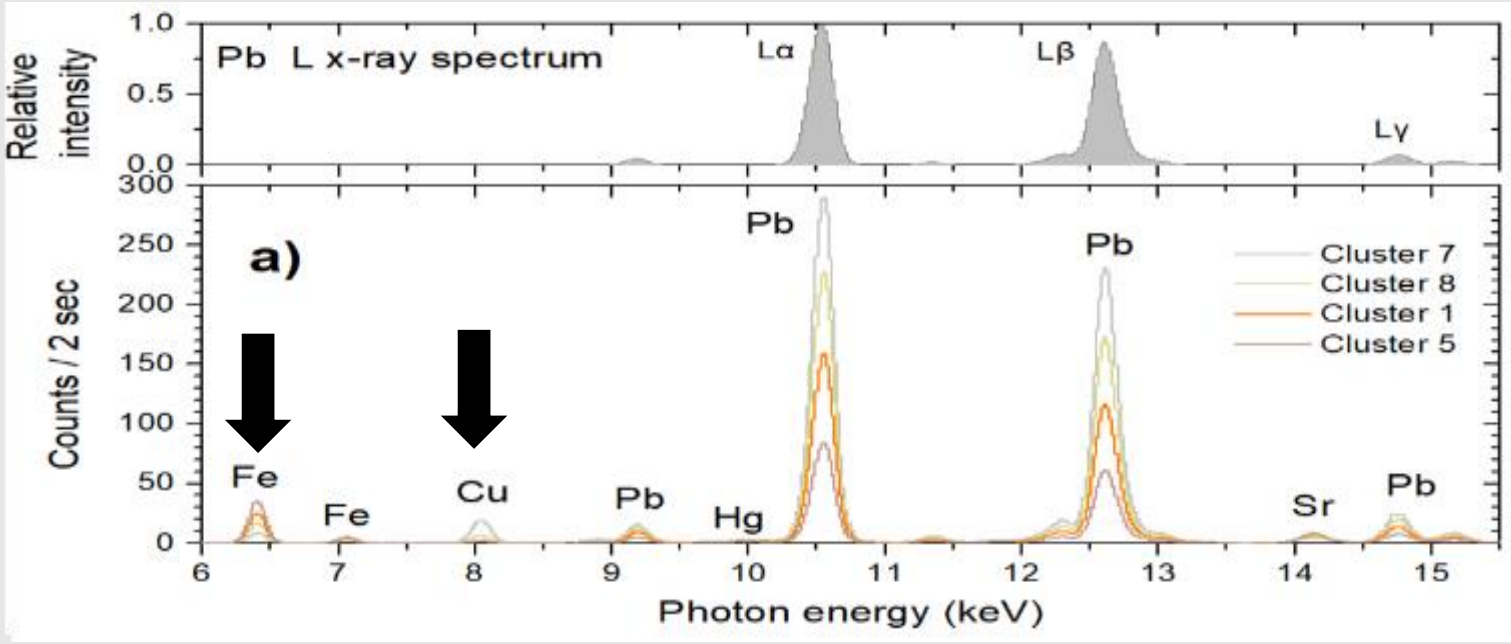


Transition	Transition centroid (eV)	fwhm (eV)	Low Energy (eV)	High Energy (eV)
Fe Kα	6405	142	6334	6476
Cu Kα	8046	155	7968	8124
Au Lα	9713	169	**9629**	**9797**
Hg Lα	9989	171	**9904**	**10074**
Pb Lα	10551	175	**10464**	**10638**

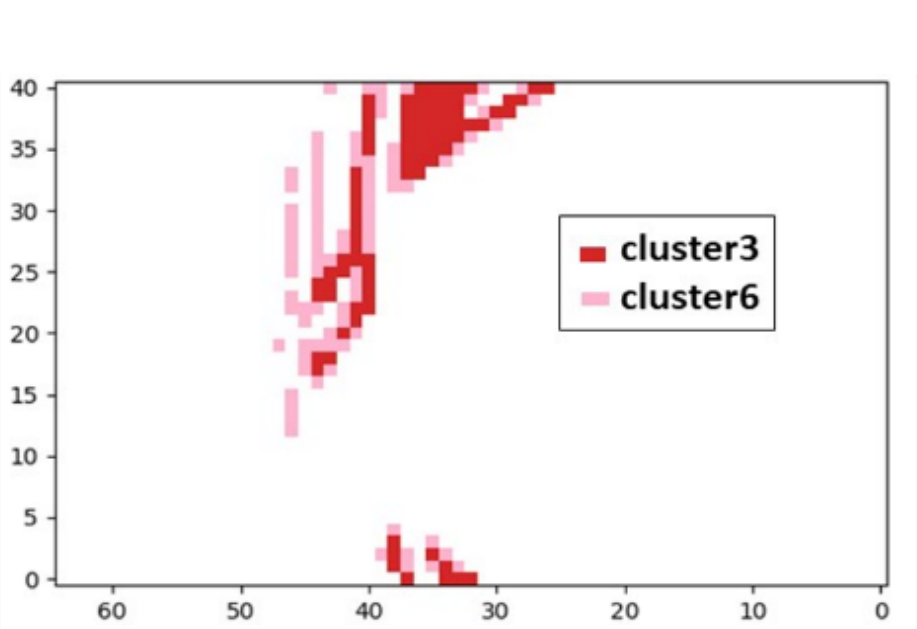
Cluster Interpretation

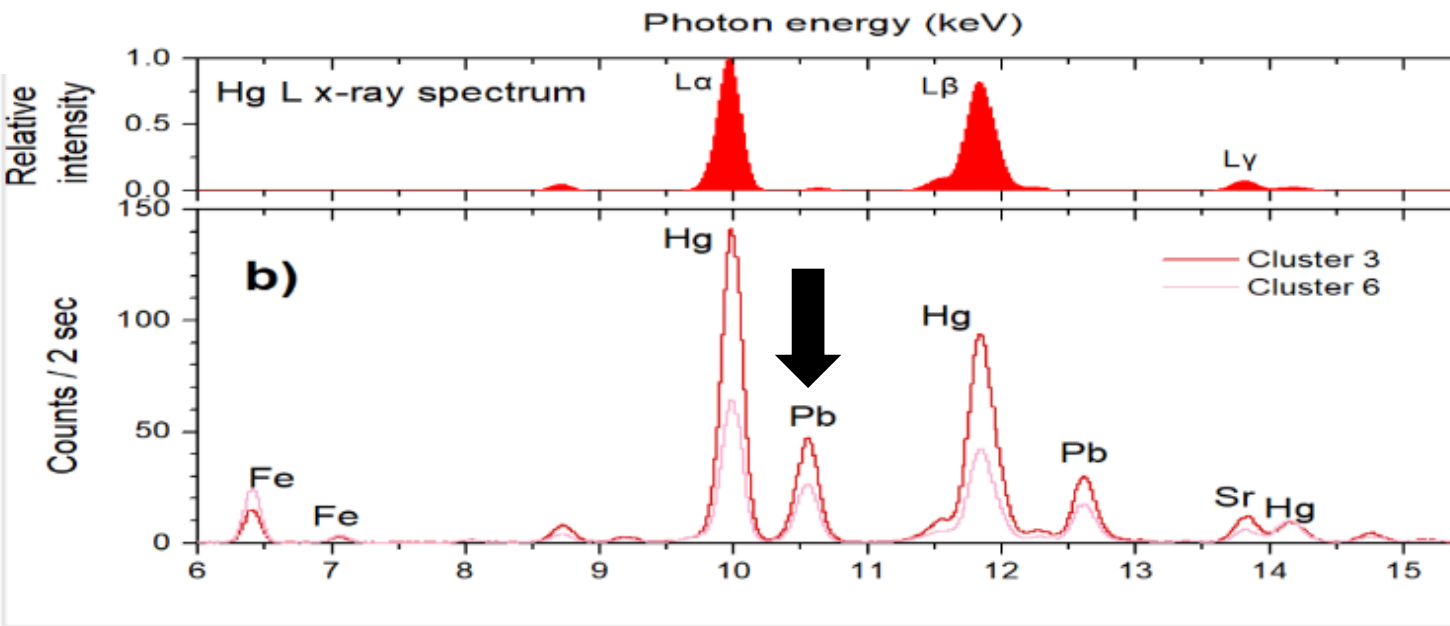


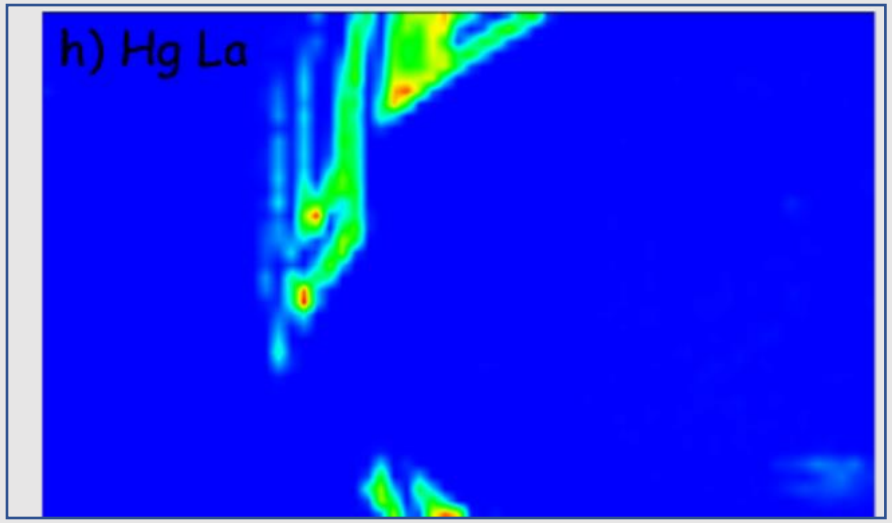


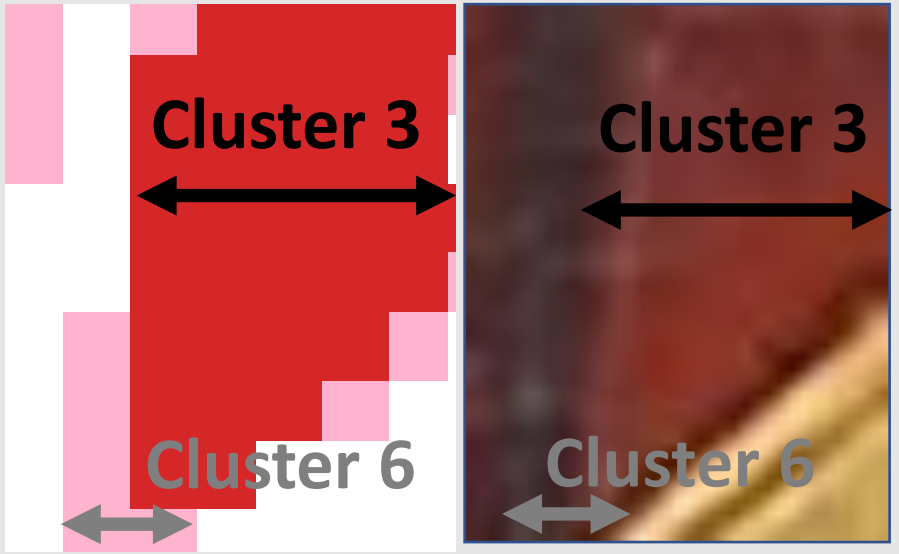


Cluster Interpretation









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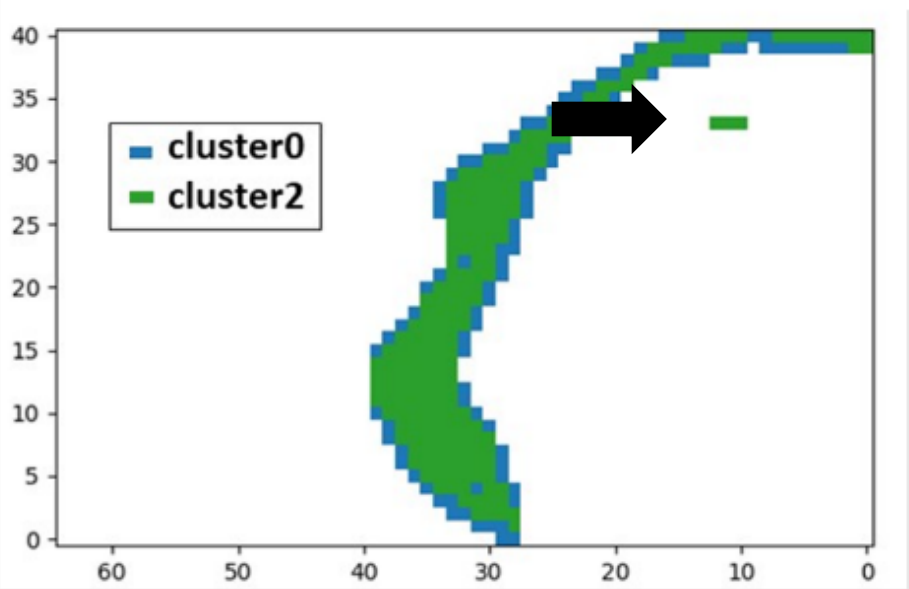
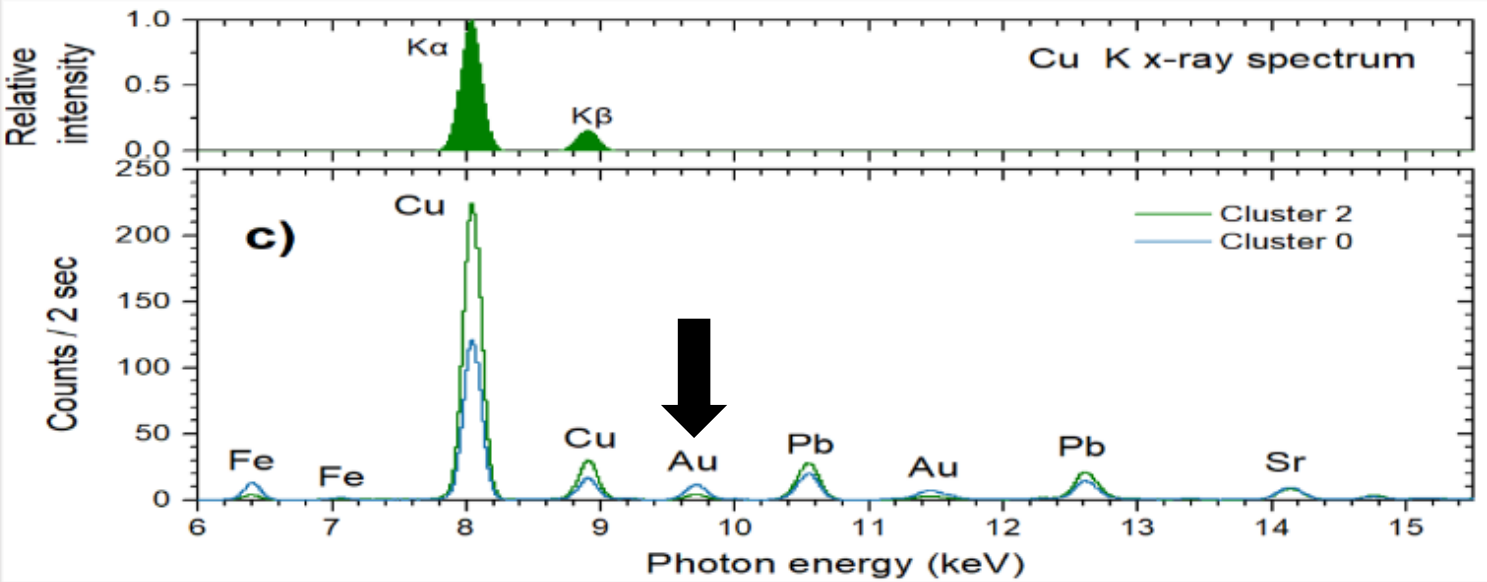
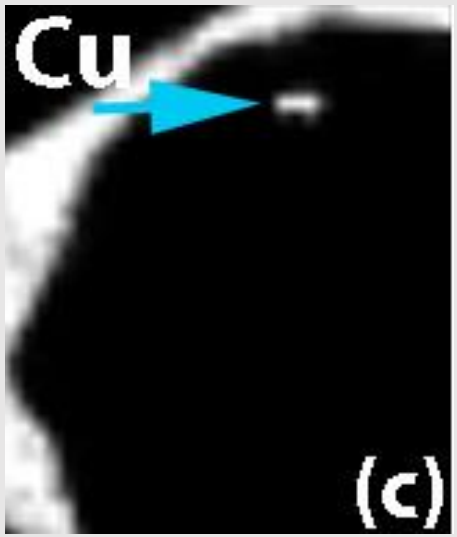
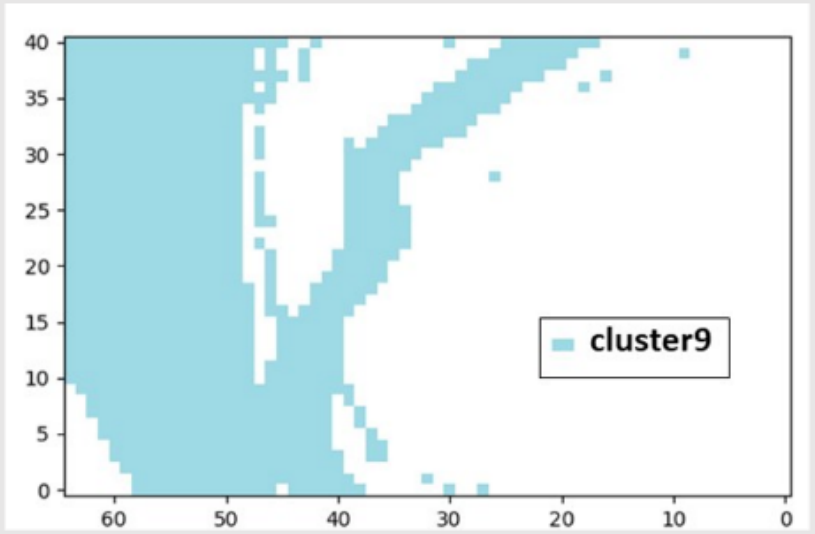


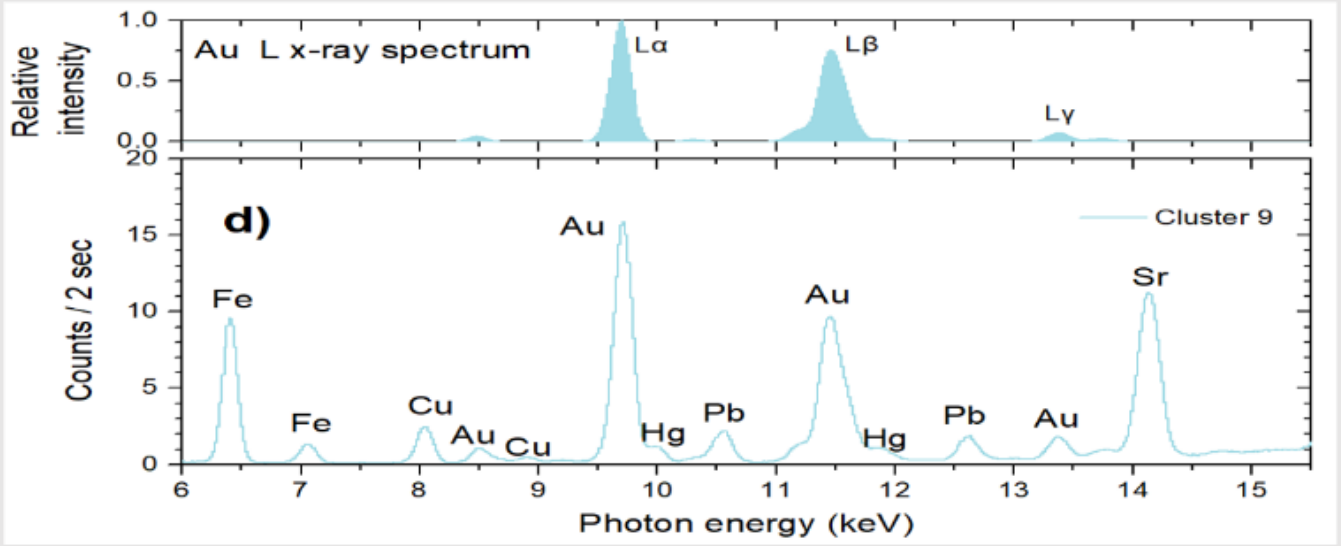


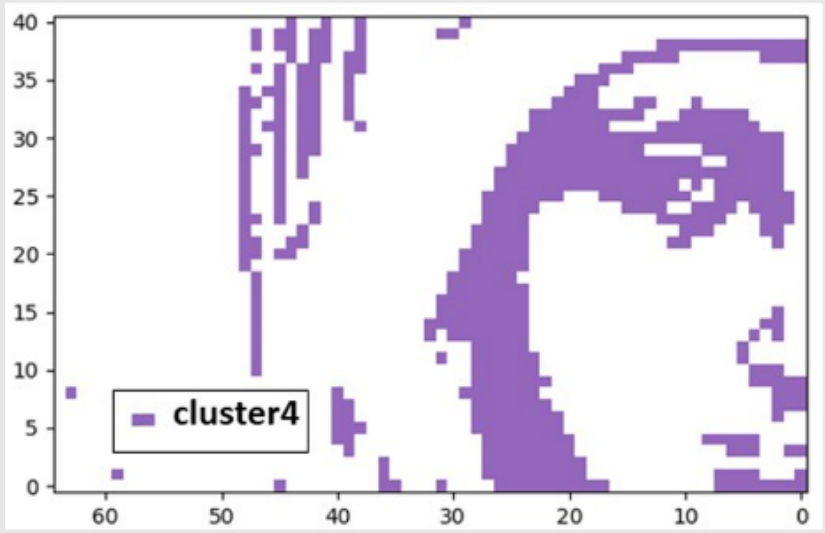


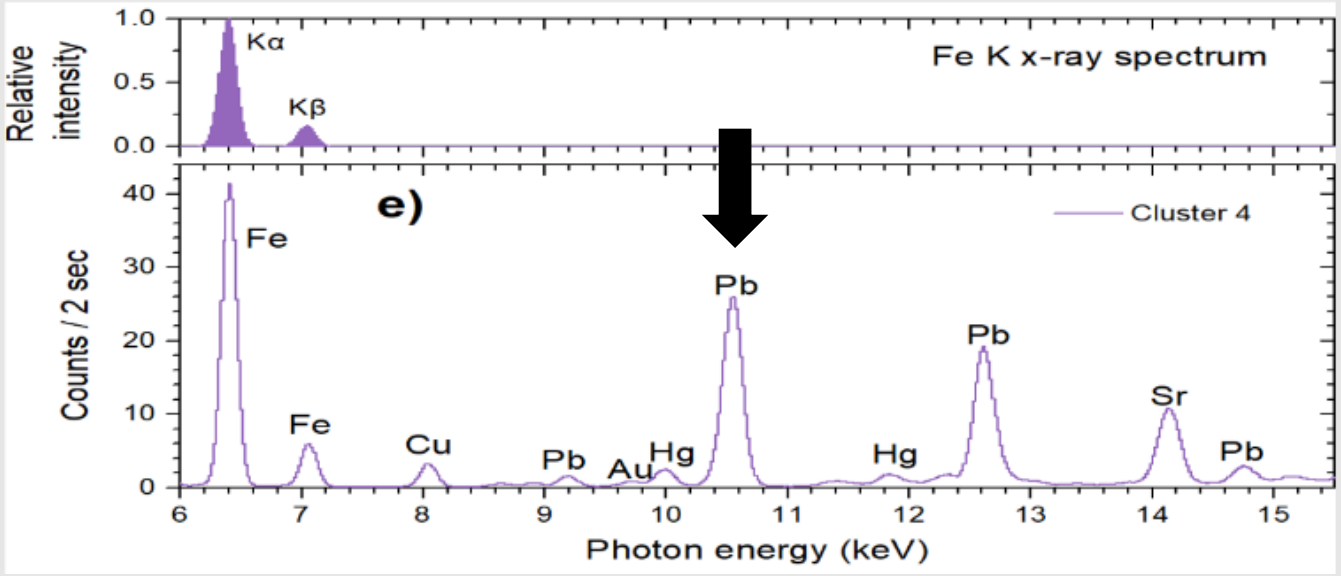
Presence of copper in the region of the Virgin Mary's eyebrow that reveals the later intervention

Cluster Interpretation









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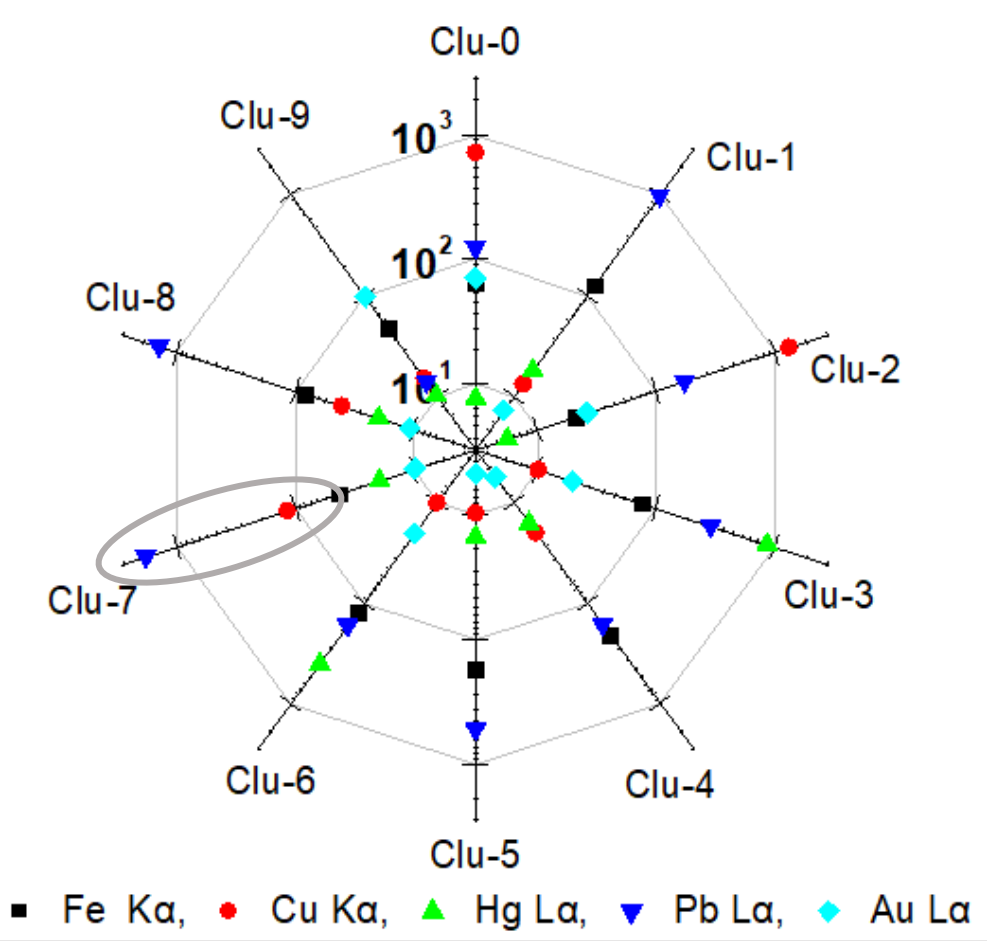

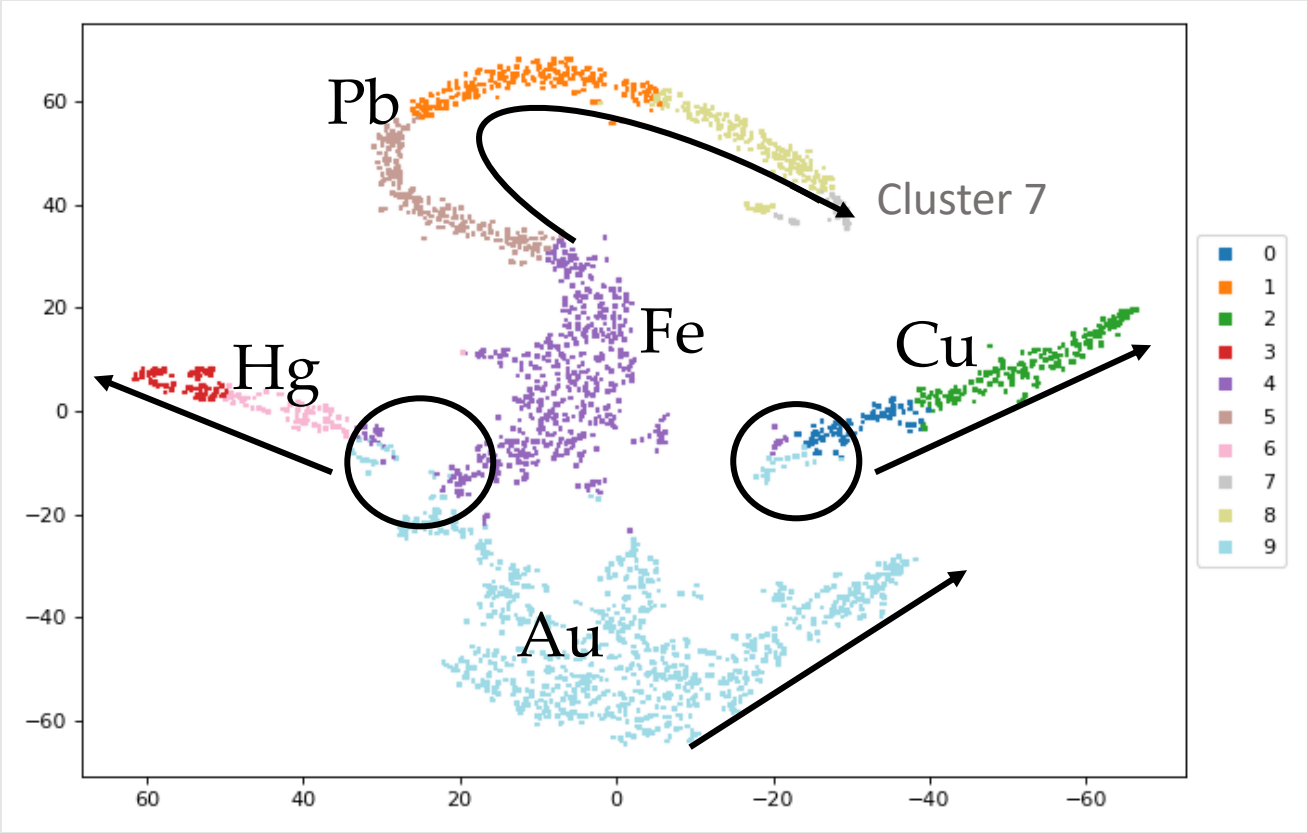

Future work

Journal of *Imaging*

MDPI

Article

Scanning X-ray fluorescence data analysis for the identification of Byzantine icons' materials, techniques, and state of preservation

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Abstract: X-ray fluorescence (XRF) spectrometry has proven to be a core, non-destructive, analytical technique in cultural heritage studies mainly because of its non-invasive character and ability to rapidly reveal the elemental composition of the analyzed artifacts. Moreover, X-rays penetrate deeper into matter than the visible light, allowing thus further analysis that may eventually lead to the extraction of information that pertains to the substrate(s) of an artifact. The recently developed scanning macroscopic X-ray fluorescence method (MA-XRF) allows for the extraction of elemental distribution images. The present work aimed to compare two different analysis methods for interpreting the large number of XRF spectra collected by scanning X-ray fluorescence spectroscopy. The measured spectra were analyzed in two ways: a fully spectroscopic approach, and an exploratory data analysis approach. The potentialities of the applied methods are showcased on a notable 18th-century Greek religious panel painting. The fully spectroscopic approach analyses separately each one of the measured spectra and leads to the construction of single-element spatial distribution images (element maps). The statistical data analysis approach leads to the grouping of all spectra into distinct clusters with common features and afterward dimensionality reduction algorithms help to the reduction of thousands of channels of XRF spectra in an easily perceived dataset of two-dimensional images. The two analytical approaches allow extracting detailed information about the used pigments, paint layers and pigment mixing (i.e., painting technique) and restoration interventions/state of preservation.

Keywords: MA-XRF, elemental maps, clustering, dimensionality reduction, painting statigraphy, pigments, panel painting

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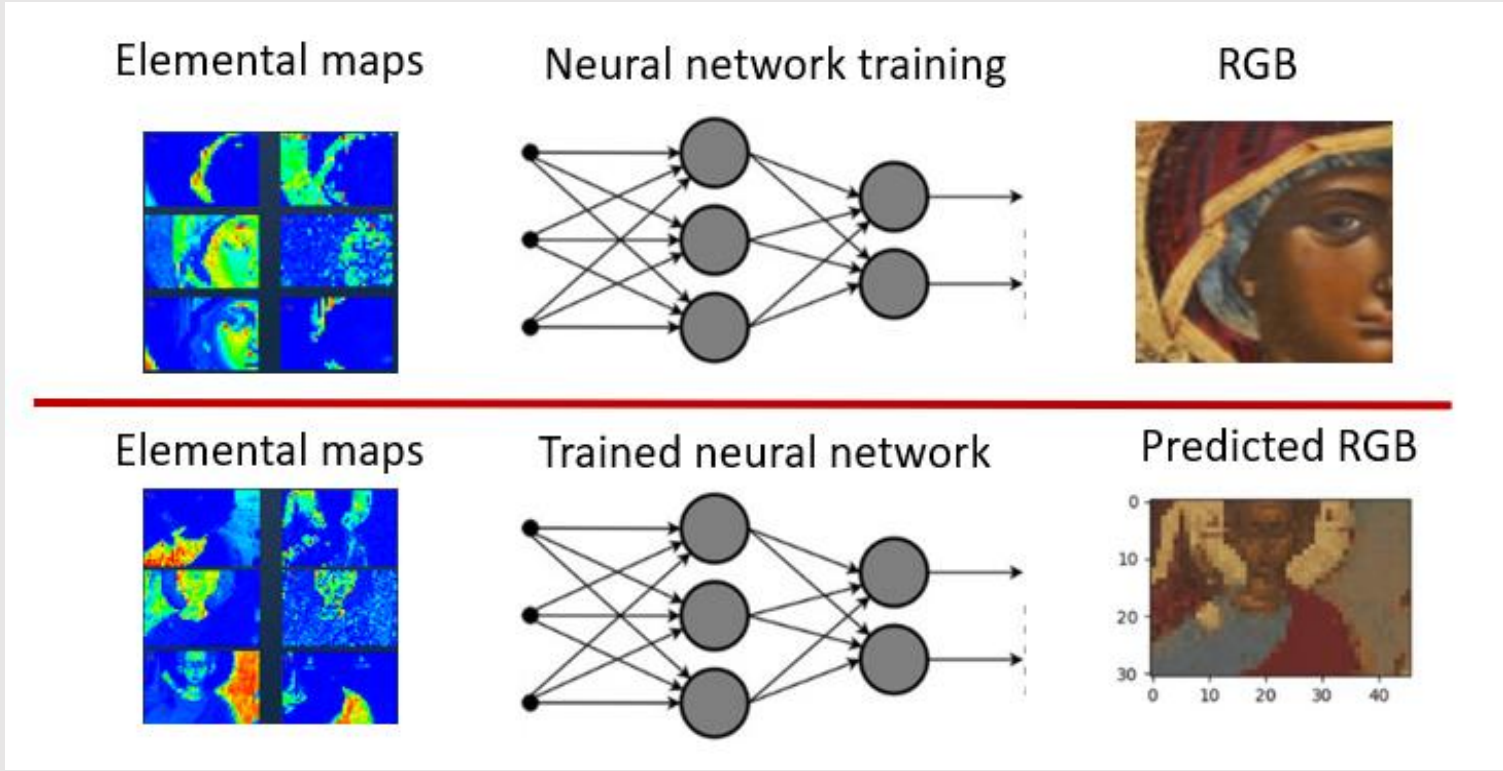
1. Introduction

XRF spectrometry is extremely valuable in the field of cultural heritage materials' investigation mainly because it offers a rapid, accurate and non-invasive elemental characterization [1]. Being able to penetrate deeper into matter than the visible light, X-rays allow for a more sophisticated analysis that can eventually lead to the extraction of information pertaining to the substrate(s) of an artifact. What is more, one can retrieve extremely useful information as regards paintings' materials and techniques through the generation of XRF elemental distribution maps by scanning macroscopic X-ray fluorescence set ups (MA-XRF), an approach that is indeed increasingly applied [2-5]. The data acquisition during a MA-XRF measurement results to large number of spectra (from

MA-XRF and machine learning techniques for digital image restoration



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Thank you for your attention!

Questions…