## How GPyEDS works and the justification for using it

GPyEDS is an unsupervised machine learning approach used to transform Electron Dispersive Spectroscopy (EDS) maps into phase maps of geochemical variability [1].

We have used it in this study to calculate mineral phase abundances, as an alternative to the time-intensive process of point counting.

How GPyEDS works:

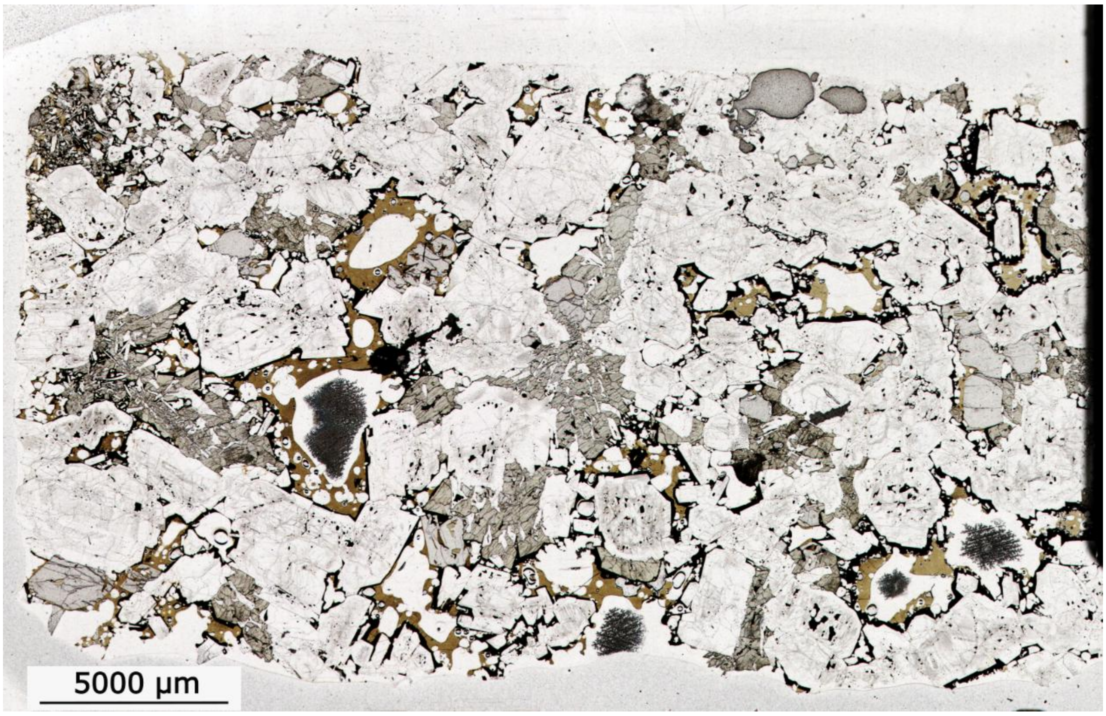
- Make an EDS map of the sample
- Export individual spectral maps – as we studied gabbroic nodules and tholeiitic basalt samples and were interested in plagioclase, olivine and clinopyroxene, we exported Na, Mg, Ca, K, Fe, O, and Al maps
- Load spectral maps into GPyEDS – it uses the spectral maps to determine the chemical composition of each pixel
- Use k means clustering to divide the geochemical latent space into different phases based on chemical composition (we estimate the number of phases from sample petrography)
- In samples with groundmass smaller than the pixel size, we then manually refine the clusters to produce a matrix phase alongside the mineral phases – GPyEDS struggles to group fine groundmass crystals into the correct compositional cluster because the pixels represent multiple crystals of different compositions

How the phase maps were used to calculate mineral phase abundances in tholeiitic basalts:

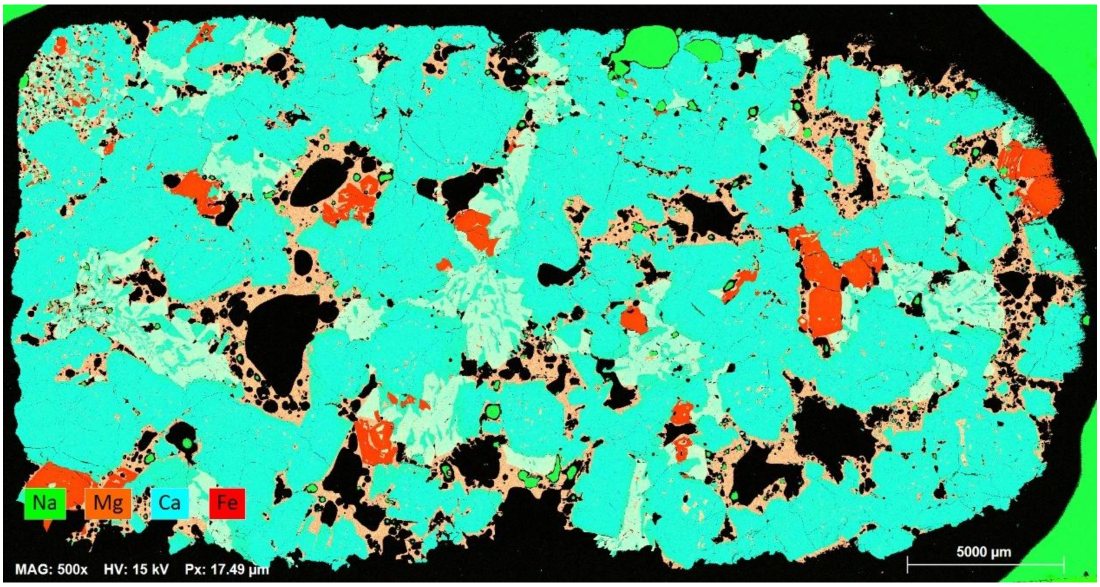
- Create phase maps, typically with four clusters – plagioclase, clinopyroxene, olivine and a matrix phase
- The matrix phase is needed to account for crystals smaller than the pixel size in the EDS maps – in our case the pixel size was 17.49 μm/px
- Export the phase map as a .tiff file for a high-resolution image
- Load the map in ImageJ then threshold the map to isolate each phase
- Apply a size filter to each phase to eliminate noise and any adjacent small crystals that have been merged during k means clustering to produce ‘false’ larger crystals - the size filter used for this study was >25000 $\mu m^2$
- Calculate the area of the total solid fraction, then calculate the area covered by each mineral phase - provides mineral proportion in vol.%

Using this GPyEDS workflow saves significant portions of time compared to the point-counting method, even including the time needed to produce an EDS map for each sample.

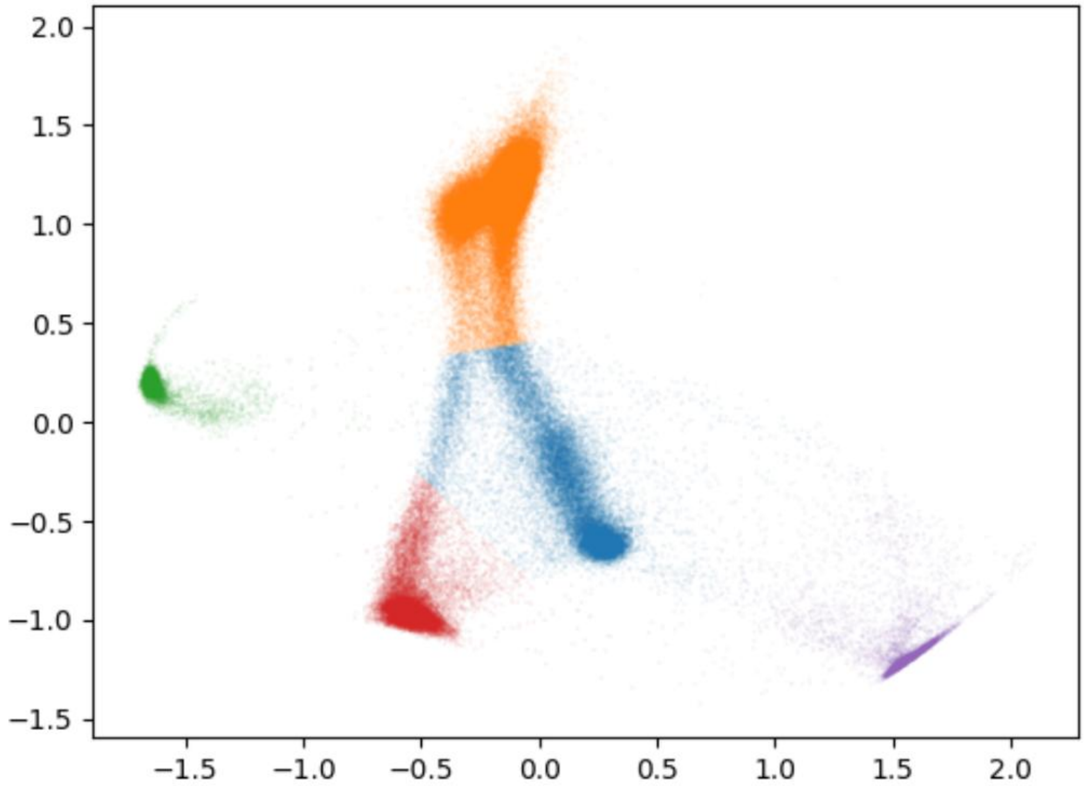
**An example of the GPyEDS workflow for a gabbroic nodule sample compared to a plagioclase-phyric basalt sample**



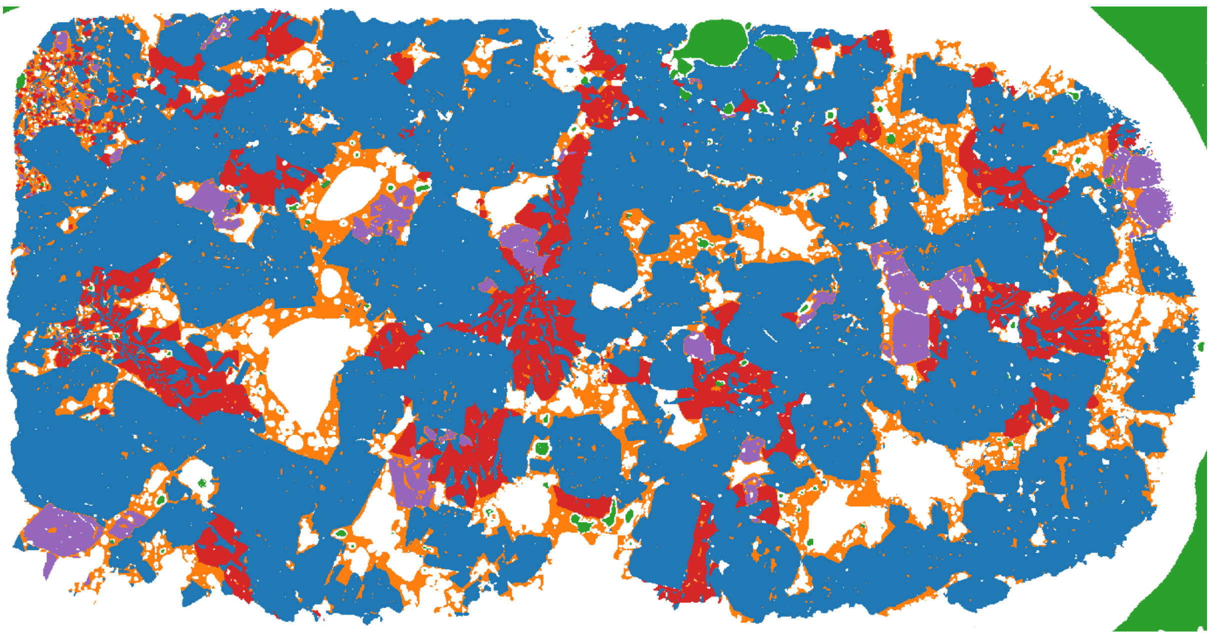

1. PPL image of sample BRA-10-01, a gabbroic nodule



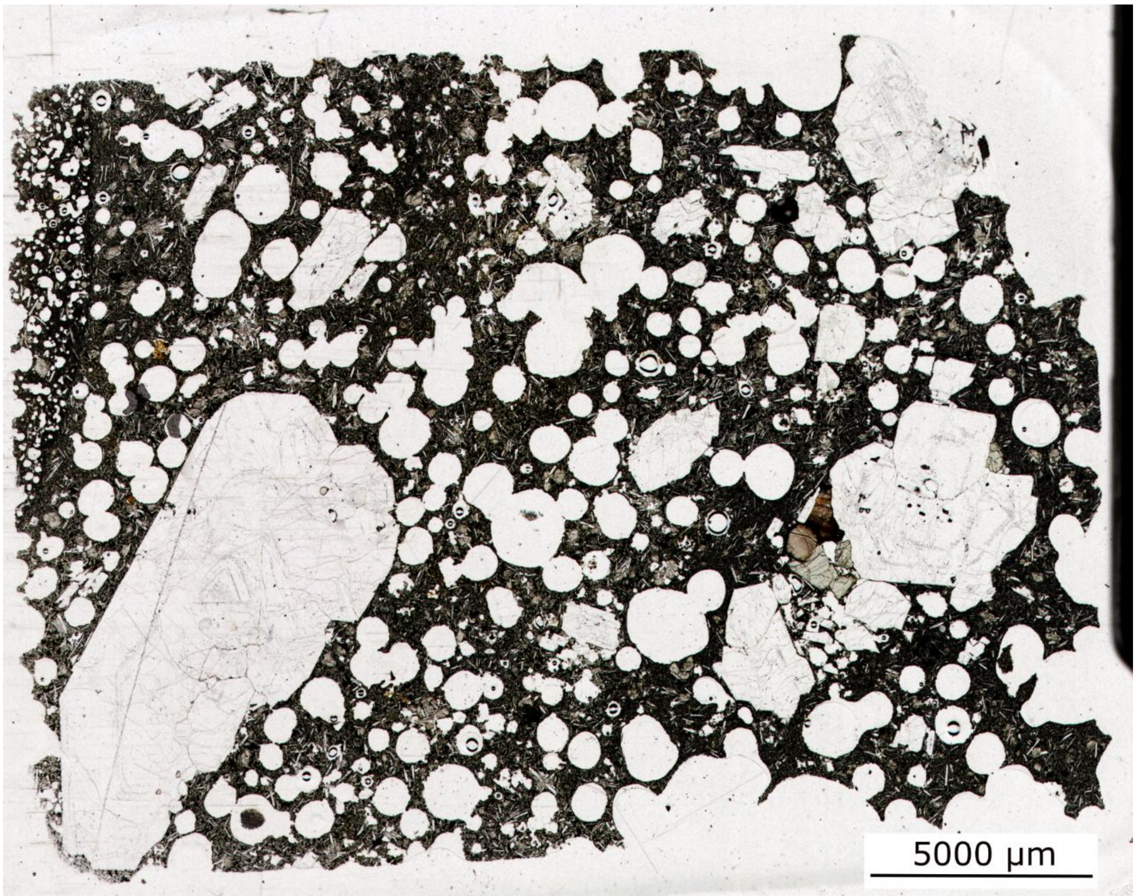

2. A composite EDS map of BRA-10-01: plagioclase is turquoise, olivine is red, clinopyroxene is mint green, glass is pink



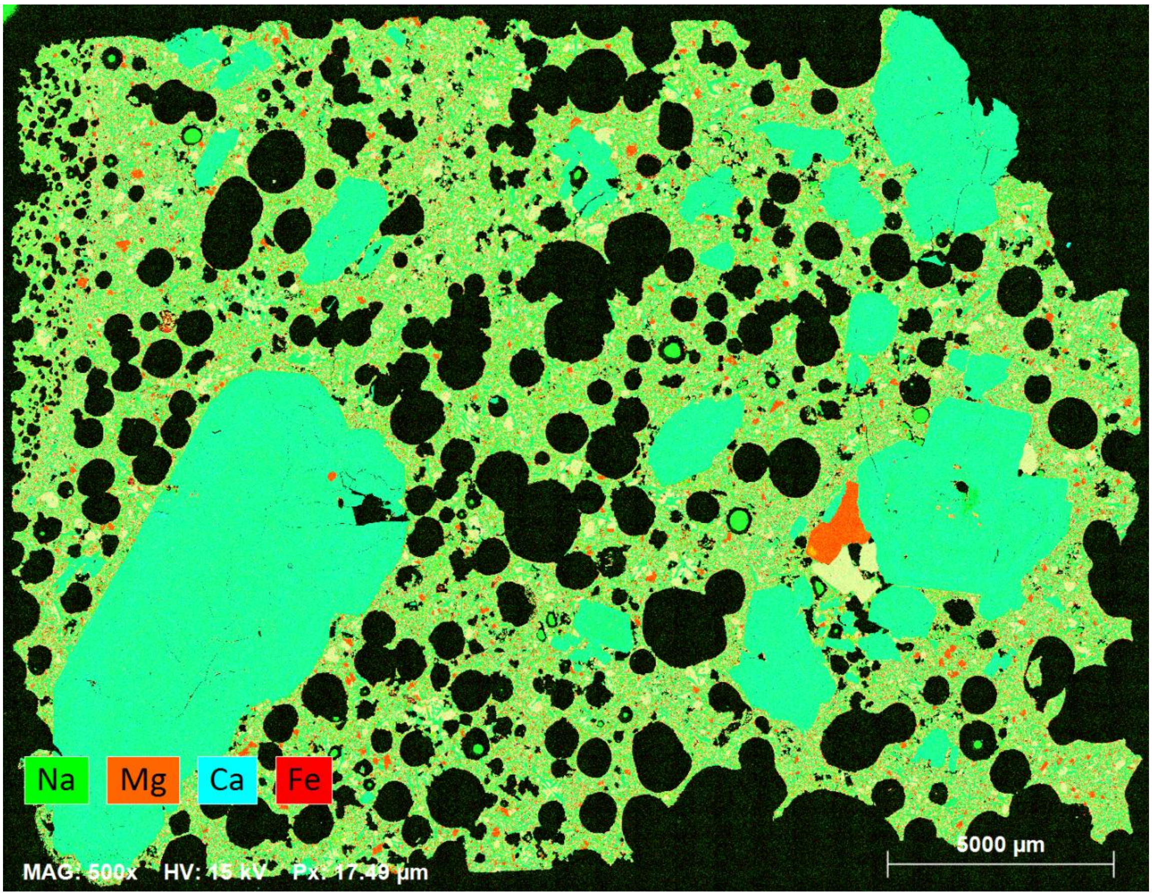

3. The geochemical latent space of sample BRA-10-01 in GPyEDS - plagioclase is blue, olivine is purple, clinopyroxene is red, matrix glass is orange, green is resin



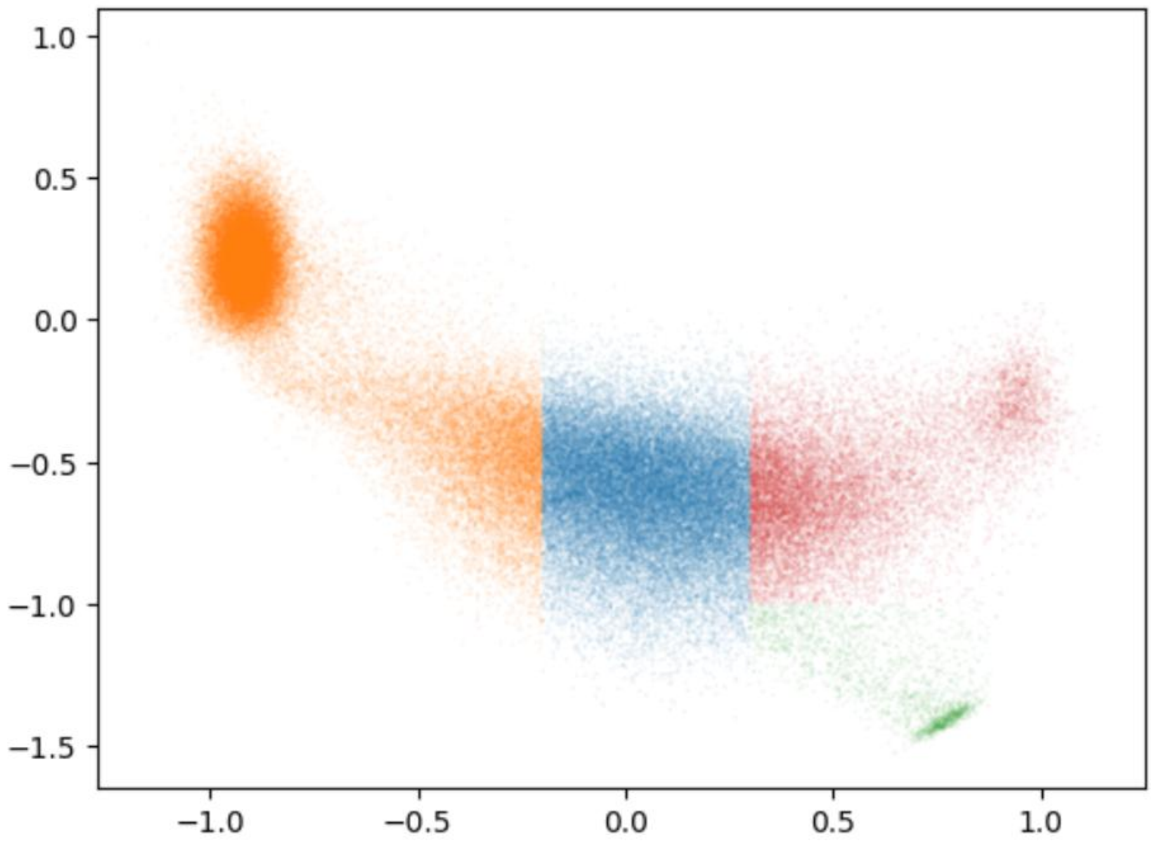
4. A GPyEDS phase map of BRA-10-01: plagioclase is blue, olivine is purple, clinopyroxene is red, matrix glass is orange, green is resin



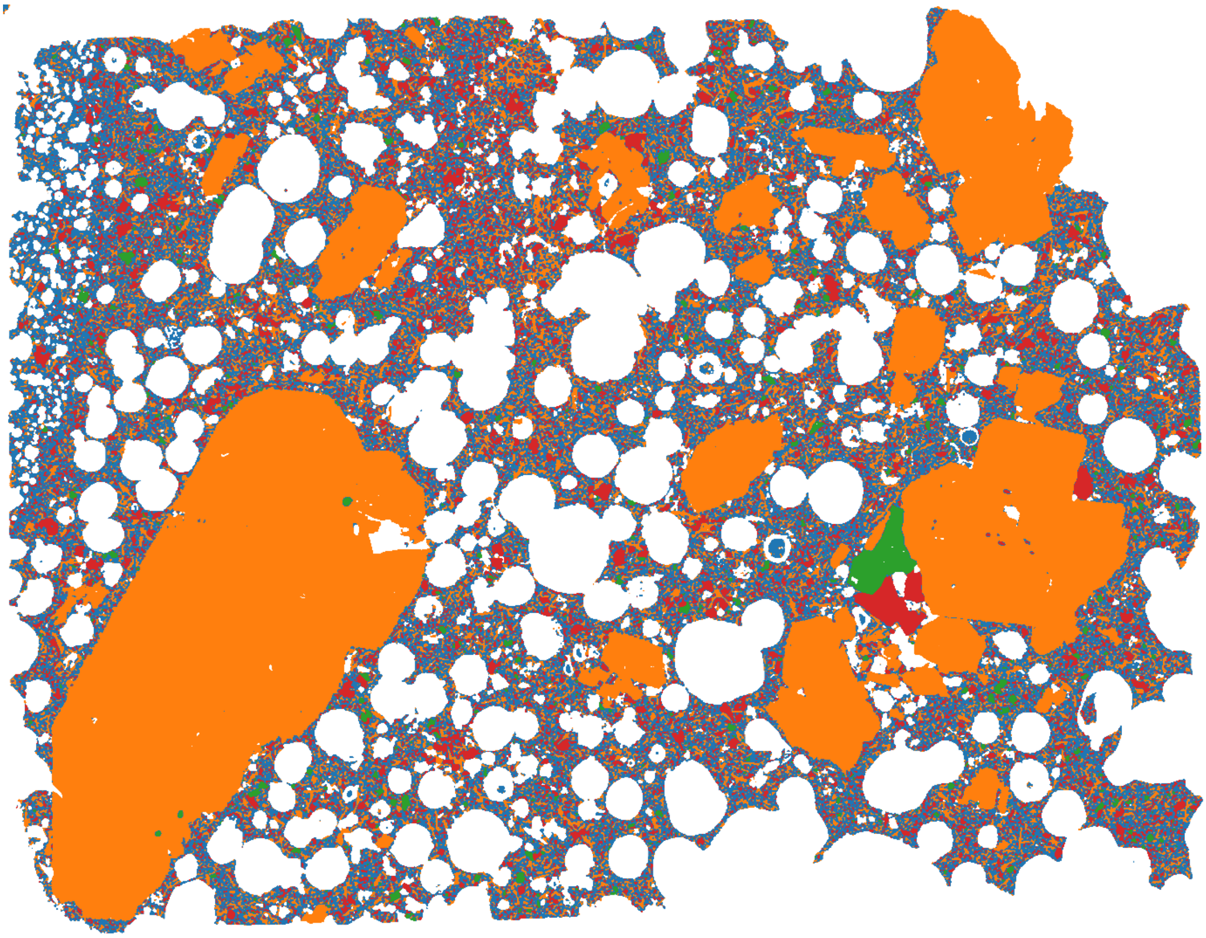

1. A PPL image of sample 1288-7, a plagioclase ultra-phyric basalt




2. A composite EDS map of 1288-7: plagioclase is bright green, olivine is red, clinopyroxene is yellow




3. The geochemical latent space of sample 1288-7 in GPyEDS: plagioclase is orange, olivine is green, clinopyroxene is red, and the matrix phase is blue



4. A GPyEDS phase map of sample 1288-7: plagioclase is orange, olivine is green, clinopyroxene is red, and the matrix phase is blue

## References


[1] Toth et al. (2025). JGR: MLC 2(4).