Appendix Seven (digital only): Flixton Island 2 Grouping Analyses Process

1.1 Introduction

The Grouping Analysis tool in the Spatial Statistics toolbox on ArcMap 10.5 was utilised to create visualisations of samples by grouping them into sets of samples most similar in nature to each other and most different in nature from those in the other group(s). It is a form of cluster analysis. This was applied to the layers that contained the attribute data variables that were the elemental readings from ICP-AES and pXRF at Flixton 2. This appendix documents the iterative process used to develop the robust statistical models using Grouping Analysis on ArcMap for the Flixton Island 2 geochemical results. The aim of implementing Grouping Analysis was to consider the relationships between the results and identify groupings of samples with similar elemental compositions, if there were any.

The tool was set up in a manner geared to letting the geochemical data speak for itself. Firstly, groups were set up to have no spatial constraints, thus allowing non-adjacent samples to be grouped. As such, groups would form based on the input elemental variable/s only (data proximity) and not based on their spatial proximity to each other. Secondly, the "Find Seed Locations" option was selected for growing the groups. Seeds, in this case, are the samples from which grouping is templated, so this method means the first seed is randomly selected but then other seeds are selected to maximise the data space between the original seed and themselves. As it is difficult to know what combinations of variables are of relevance in this case, pre-specifying samples with particular elemental compositions to be the seeds of a group is not an option (this is used when you want to find features similar to a particular sample, then you would deliberately grow the group from it).

It is recommended best practice to build up a grouping analysis from a single variable (ESRI n.d.). This gives a sense of which variables are the more significant discriminators in group isolation, as well as results being easier to interpret when there are fewer fields. Furthermore, it is good practice to compare and evaluate repeat runs, on the same variables with the same number of groups, because the random element in identifying the first seed when using Find Seed Locations means there is a potential for different outputs. However, a balance needs to be struck as this can often be a time consuming process that produces an overwhelming amount of data. This was evaluated throughout the process for both datasets.

The default number of groups formed on ArcGIS is 2. It has been recommended by some researchers (Pierre 2014), that another option is to apply Sturge's Rule, C = 1 + 3.3 log (*n*), where C is the number of groups and *n* is the number of features. The ArcGIS tool is also able to statistically evaluate the optimal number of groups (between 2 and 15), based on a measure of the highest pseudo F-Statistics. The 'Evaluate the Optimal Number of Groups' option was checked for at least one run of each variable and number of groups combination, for consideration. The output calculation of the R^2 statistic also further allows for an evaluation of how good the variable is at differentiating the groups, which becomes particularly relevant when considering combinations of elements.

There is an active window while the tool is running that provides some notes on the success of the run and any issues that arose, which were saved as text that is provided as a record at the end of this document. There are two further key outputs produced: The shapefile containing the grouping data and therefore visualising the spatial patterning; and an output report which provides a detailed breakdown of the statistics including the pseudo F-Statistics and R^2 statistics, but also describes the trends in the data that cause the samples to be grouped one way or another. The output report illustrates how each individual variable contributes to the groupings. It provides that as a breakdown for each individual variable in each group and also as a combined parallel box plot (see Figure xxx below) that shows where the average value of the variable falls for each group.

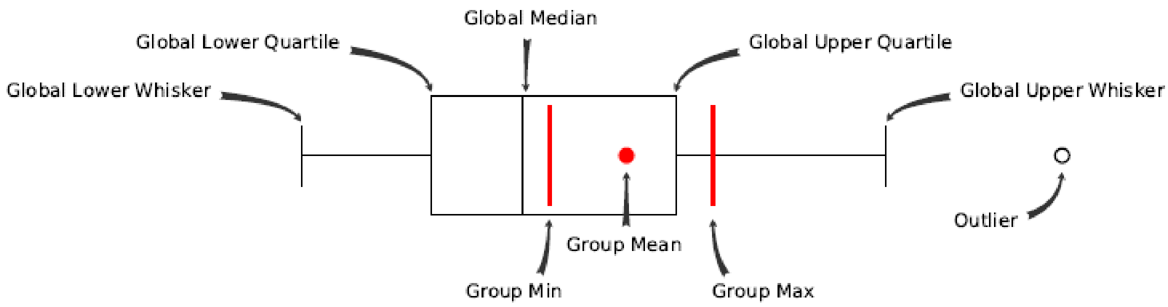


Figure 1. Breakdown of the parallel box plots provided in the output report

1.2 Analysis of Trench 4 ICP-AES Results (from 2012 excavations)

1.2.1 Planning the analysis

Applying Sturge's Rule to the Flixton ICP-AES dataset, C = 1 + (3.3 log (50)) = 6.6066 and therefore 6 or 7 groups are suggested. It was decided that Grouping Analysis would therefore be run on the major and minor elements building up from two groups, to three, to five, then seven to allow a gradual consideration and assessment. The fewer the number of groups, the easier to interpret the results, and this allows teasing out of which elements impact which groupings visually. Then the optimal number of groups as assessed by the tool would be considered and utilised in a run (if it were not two, three, five, or seven groups). Further runs could be made with different numbers of groupings as considered appropriate.

It was demonstrated in chapter six that iron was the major elemental contributor to the samples as measured by ICP-AES, with aluminium, calcium, and magnesium as minor contributors. Barium, potassium, manganese, sodium, phosphorus, sulfur, titanium were trace contributors as well as even smaller measured amounts of silver, arsenic, boron, beryllium, cobalt, chromium, copper, mercury, lanthanum, molybdenum, nickel, lead, antimony, scandium, strontium, vanadium, zinc. As such, it was decided that GA would initially be run on iron, aluminium, calcium, and magnesium, as the major and minor contributors to the samples as read by ICP-AES. Each was run individually initially and then in combination. It was decided to further expand this analysis with the additional integration of manganese and phosphorus. These had been incorporated into the model at Star Carr and this would allow a more nuanced comparison between the results from the two sites to be considered.

It should be noted, that the magnesium measurements appear to have been rounded to the nearest 50 ppm by the commercial laboratory. Therefore, there were only 8 unique values across the 50 readings taken. However, with magnesium contributions being measured at a minimum of 1100 ppm, the results were still deemed to be viable, so this element was still incorporated.

As such, the following is a record of the results from the individual runs that contributed to the development of the model for the major and minor elements in the samples. This includes the grouping analysis runs on the elements individually initially (iron, aluminium, calcium, and magnesium), and then in combination, forming two, three, five, and seven groups and then followed by a run using the statistically suggested optimal number of groups generated by the tool based on the pseudo F-statistic.

1.2.2 Major and Minor Element Grouping Patterns

1.2.2.1 Iron

1.2.2.1.1 Iron: Two groups

Splitting the samples into two groups based solely on iron as a variable did not resolve two spatially contiguous groups naturally (the groups were not spatially constrained so that any patterning reflects the composition of the samples, and is not 'forced' by being grouped by proximity). The red group (referring to the two-group depiction in section 1.2.2.2) mean for iron falls above the global upper quartile, while the blue group mean falls below it. In other words, the red samples tend to be higher in iron than the blue samples. Splitting the samples into two groups based solely on iron as a variable, the red group mean falls above the global upper quartile, while the blue group mean falls below it. In other words, the red samples tend to be higher in iron than the blue samples.

1.2.2.1.2 Iron: Three groups

Here, it can be seen the new red group (N.B. the repeat analyses are unrelated and therefore colours are generated by chance, not based on the previous run of the tool) shows well above the global upper quartile mean readings and is therefore relatively high in iron. These samples from D2 and then A2, Z1, Y0, and Y2 would continue to be grouped together through the five and seven group runs, splitting but remaining in groups next to each other on the box plot in the 15-group run. This appears to be a key, consistent area for relatively elevated iron levels, fitting with the results of the hot spot analysis.

1.2.2.1.3 Iron: Five groups

In this run, the green and yellow group samples were those enhanced and particularly enhanced in iron respectively in D2 and then A2, Z1, Y0, and Y2. These generally tended to cluster in the vicinity of the hot spot although there were a few elsewhere.

The other "group" of note was the purple group. This was one sample from grid square W3 that was unusually low in iron. This would consistently be isolated as a separate group for the seven and 15 run repeats. This low value was not highlighted by the Hot Spot and Cluster-Outlier analyses either, though it would be anomalous for other elements. As such, five groups allowed for identification of this near-anomaly (it was not technically statistically an outlier) that may otherwise have been missed.

1.2.2.1.4 Iron: Seven group and 15 (optimal) group runs

The plots were not informative with this many groups. The samples in D2 and then A2, Z1, Y0 and Y2 remain to be the highest iron level groups relatively and the W3 near-anomaly was identified.

1.2.2.1.5 Overview of iron

While 15 was the optimal number of groups, for just one element this produced a complicated picture that largely confirmed the Hot Spot Analysis and Cluster-Outlier analyses in terms of the relatively readings from D2 and then A2, Z1, Y0,and Y2, but was difficult to read. The three group run identified the main consistent area that was a small number of mostly contiguous samples that were reading similarly elevated in iron, but missed the near-anomaly. The five-group run flagged up a sample consistently low in iron as well (Figure 2).

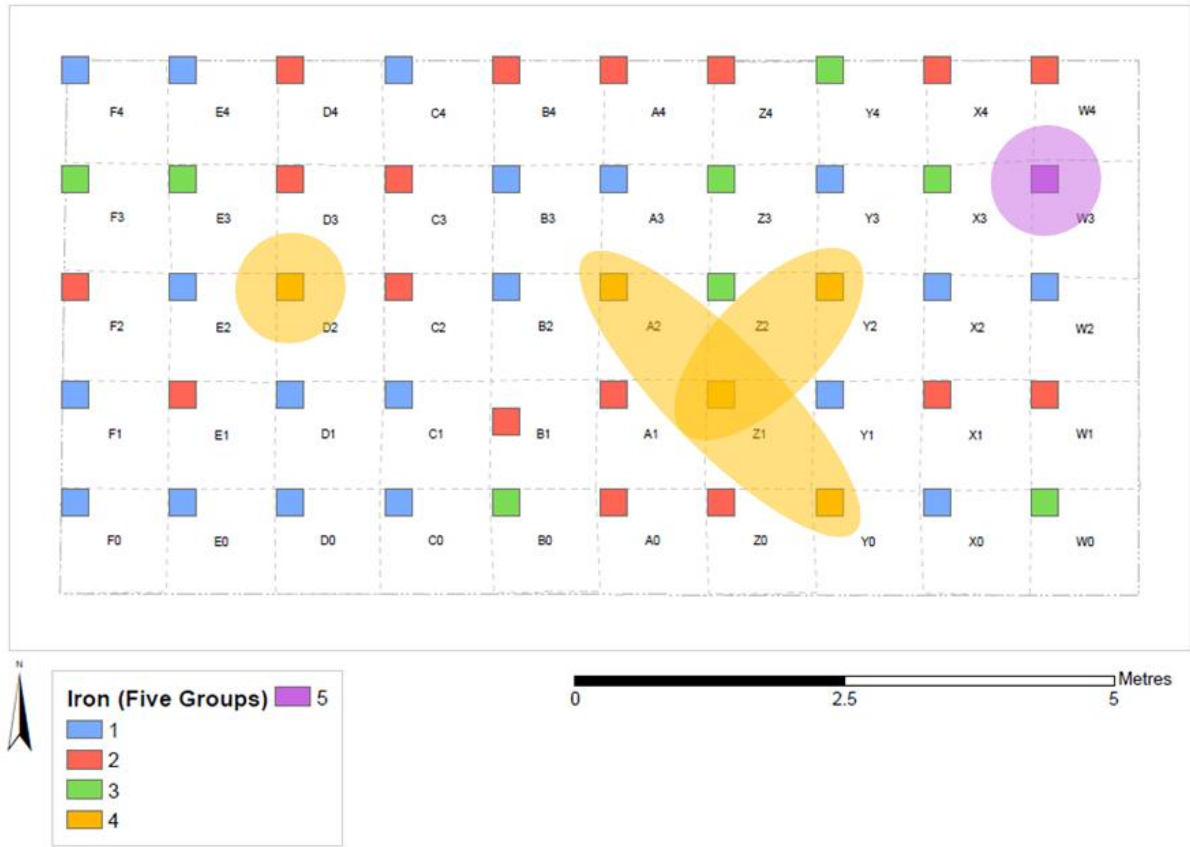
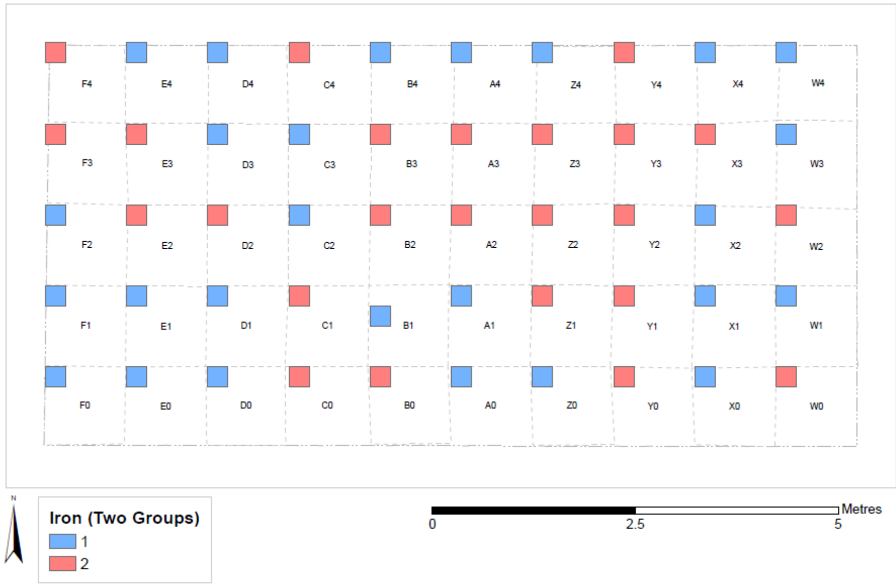
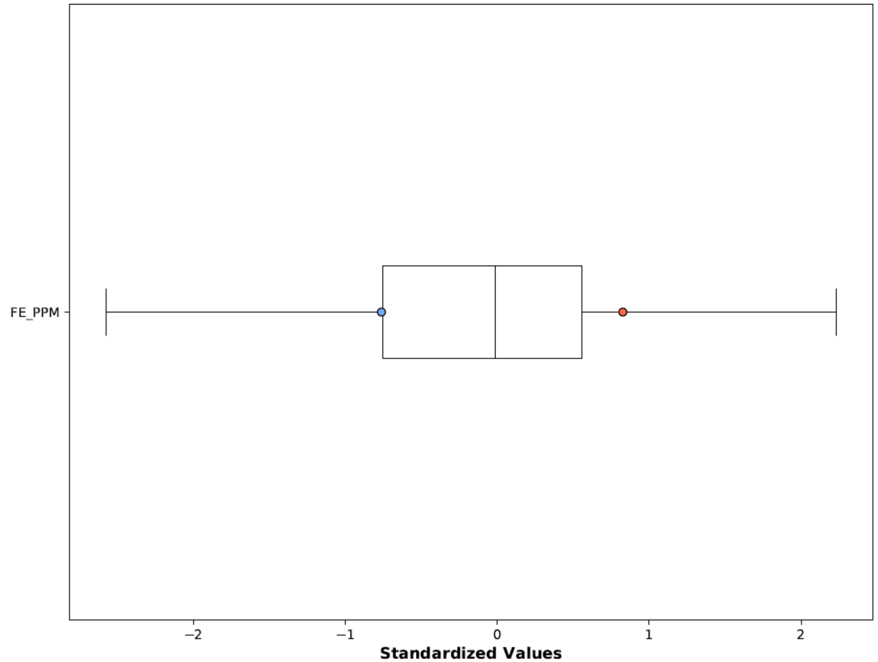


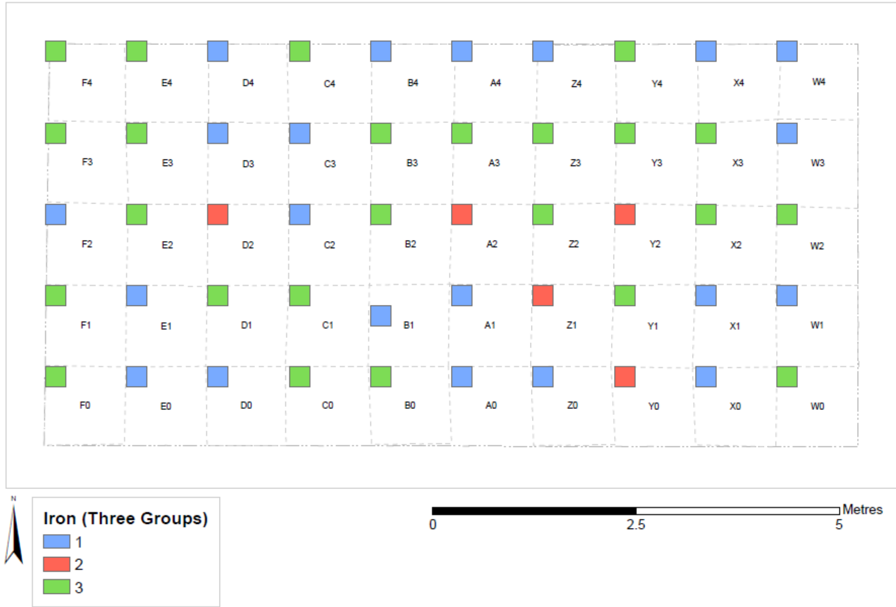
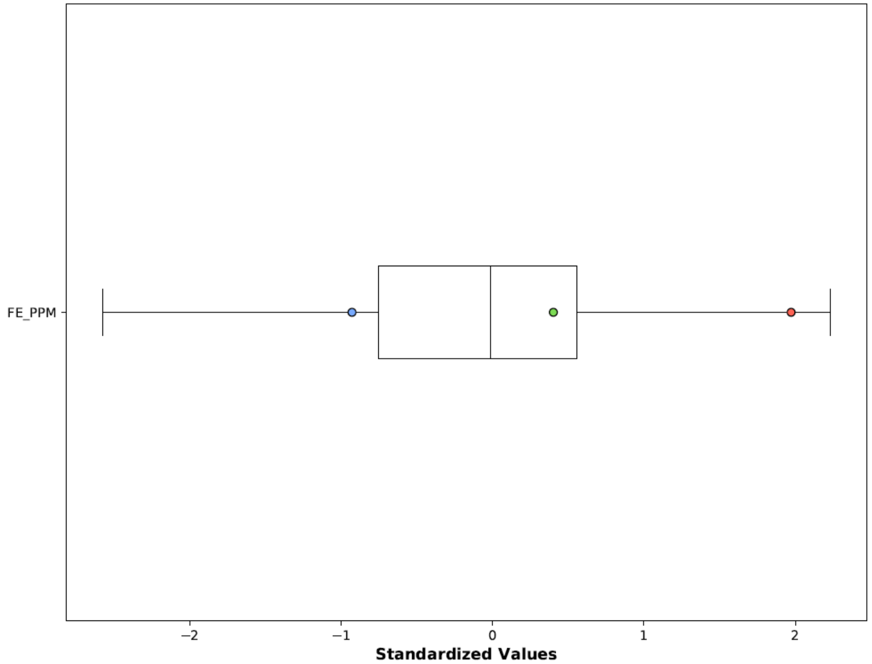
Figure 2. Key patterns in iron levels

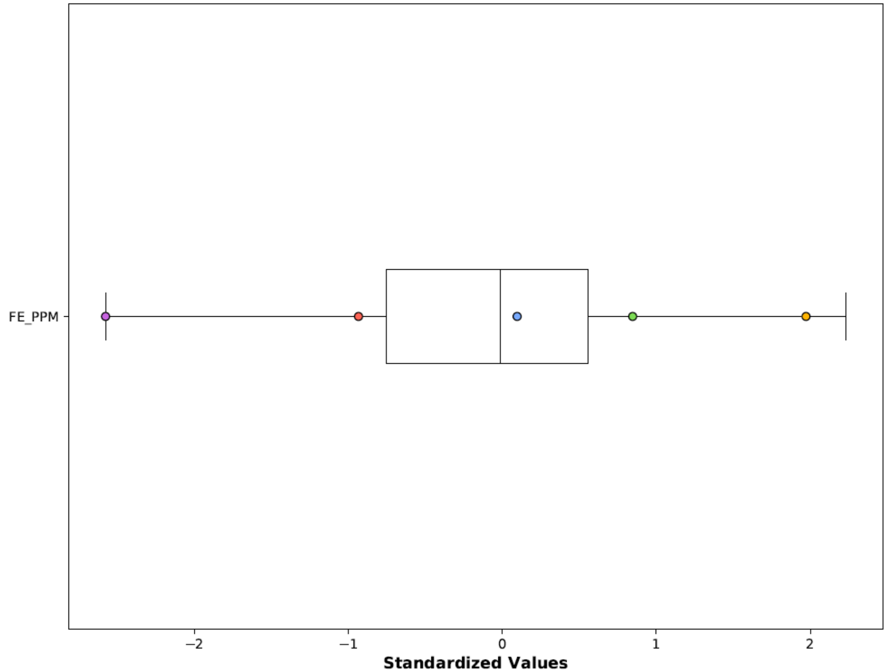
15 being the maximum number of groups that can be recommended reflects that the iron levels were highly variable across the trench, as a higher number of groups was needed to explain the variation adequately (without the added input of other variables being factored in). As essentially what the tool is doing on a single element run is gathering together the samples with the most similar levels of iron into the prespecified number of groups, this is

not surprising. For the minor elements, the plots are provided below but similarly for aluminium, and calcium, the optimal number of groups was again evaluated to be 15. For magnesium, the optimal number of groups dropped to eight because only eight levels of readings were available (as the values were rounded) and as such the eight group model described 100% of the variation.

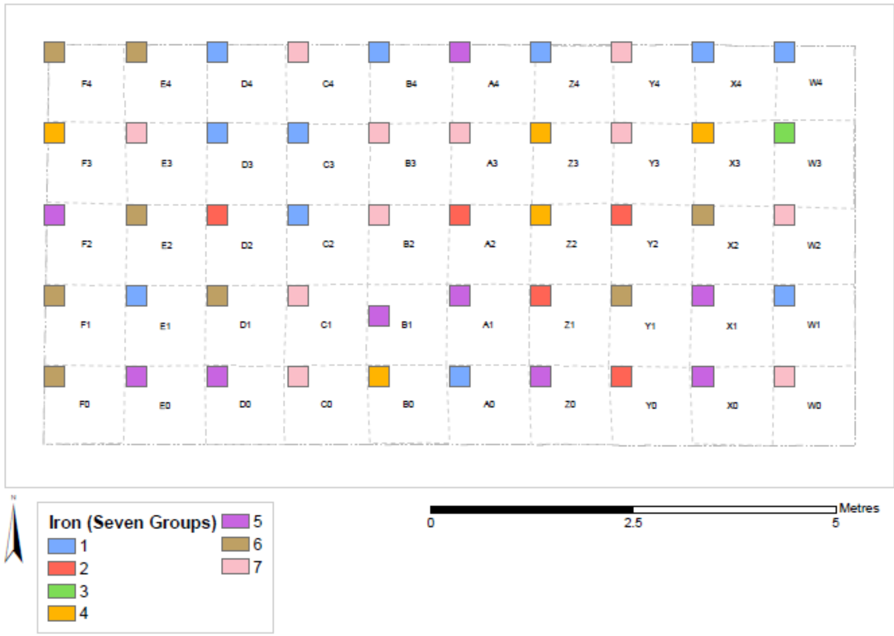
1.2.2.2 Iron: Complete record of repeat runs

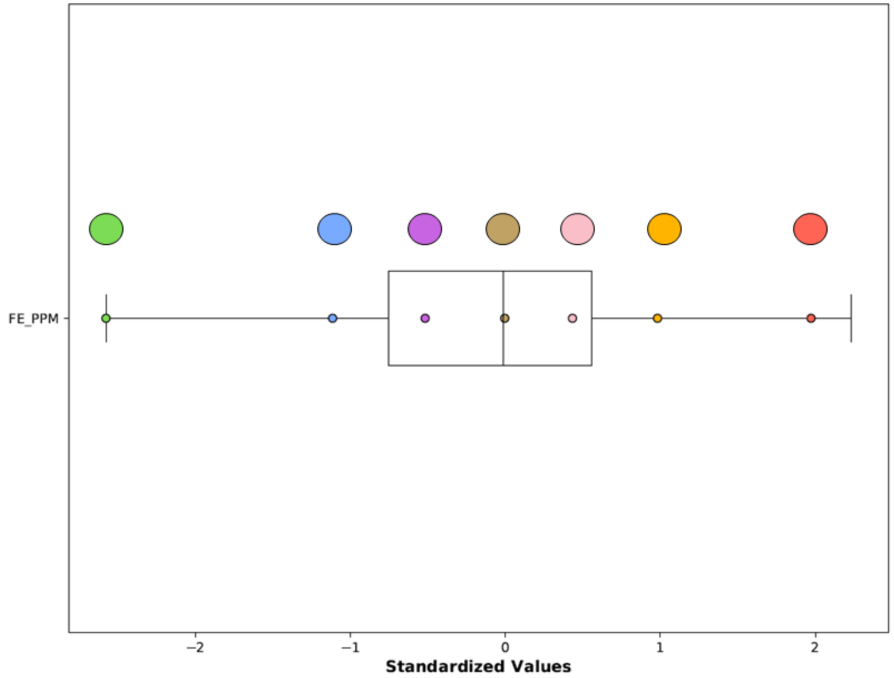
Groups	**Group Composition and Statistics**
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 15. **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.629850 (1.0 meaning it 100% explains differentiation).

Groups	**Group Composition and Statistics**
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 15 (by majority) **How good the variable is at differentiating groups (R^2 statistic):** 0.828151

Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 15 **How good the variable is at differentiating groups (R^2 statistic):** 0.936265

Groups	Group Composition and Statistics





Optimal number of groups (based on highest pseudo F-Statistic): 15 (by majority)

How good the variable is at differentiating groups (R^2 statistic): 0.980631

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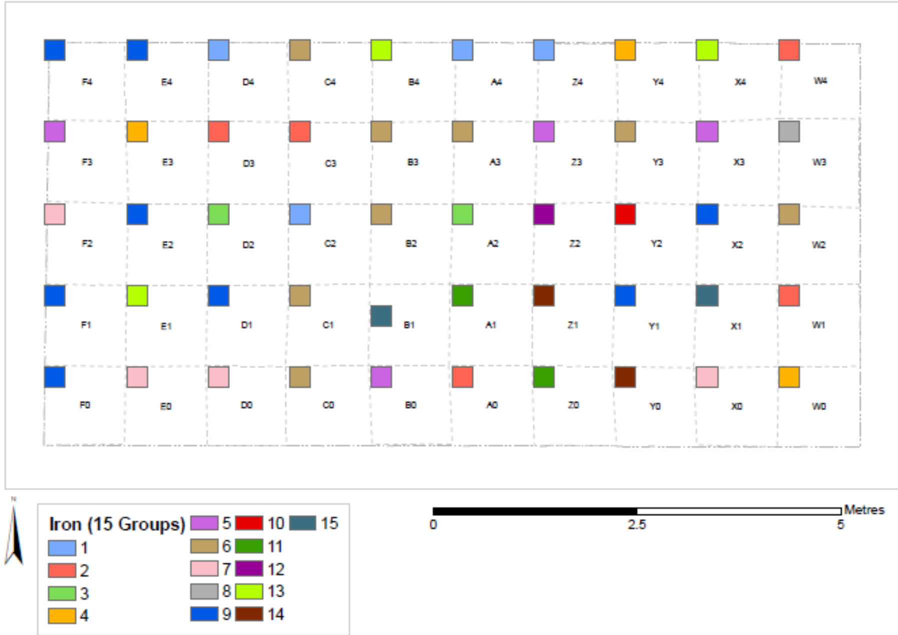

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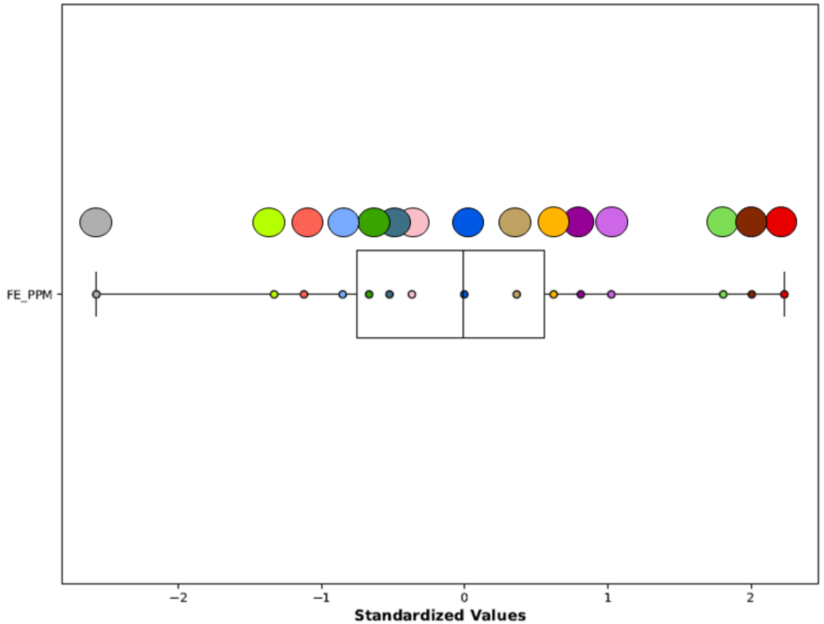

Optimal number of groups (based on highest pseudo F-Statistic): 15

How good the variable is at differentiating groups (R^2 statistic): 0.996959

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1.2.2.3 Aluminium

1.2.2.3.1 Aluminium: Two groups

The two group division was broadly similar to the iron 2 group run, with many of those in the red (higher aluminium) group in the same general areas as those that had been elevated in iron but it was not an exact match.

There was one statistically low outlier flagged immediately but with only two groups being formed, it was included in the lower group in the plot.

1.2.2.3.2 Aluminium: Three groups

A generally contiguous group of high aluminium level samples was identified in green: This included the samples from D2 and A2/Z1/Y2 (as had been consistently high in iron as well) but Y0 was only average in aluminium and this green group was not as tightly confined, including other samples as well.

1.2.2.3.3 Aluminium: Five groups

The five groups allowed the identification of the anomalously low-in-aluminium sample and that was again grid square W3 that had been near-anomalously low in iron.

In addition to this, the high level readings were split into two groups, this time green and yellow. The green group was only two samples in Y1/Y2 so in a similar area to the elevated iron readings but not fully matching. The other samples that had been high in iron were in the next highest aluminium grouping (in yellow), but they again joined with a broader spread of samples high in aluminium.

1.2.2.3.4 Aluminium: Seven group and 15 (optimal) group runs

Again, the seven and 15 group run outputs were complicated. However, the seven group run provided a little more clarity on the high level groupings with Y2 now being isolated as the highest 'group' on its own, then Y1/Z1 and D2. These were split into three separate 'groups', all being the samples highest in aluminium.

1.2.2.3.5 Overview of Aluminium

A small number of samples are elevated, in a similar and close-by pattern to the high iron samples (but not matching, see Figure 3). There tend to be lower values in the western end of the trench, with the exception again of D2. W3 was anomalously low in aluminium, similar to its low value of iron.

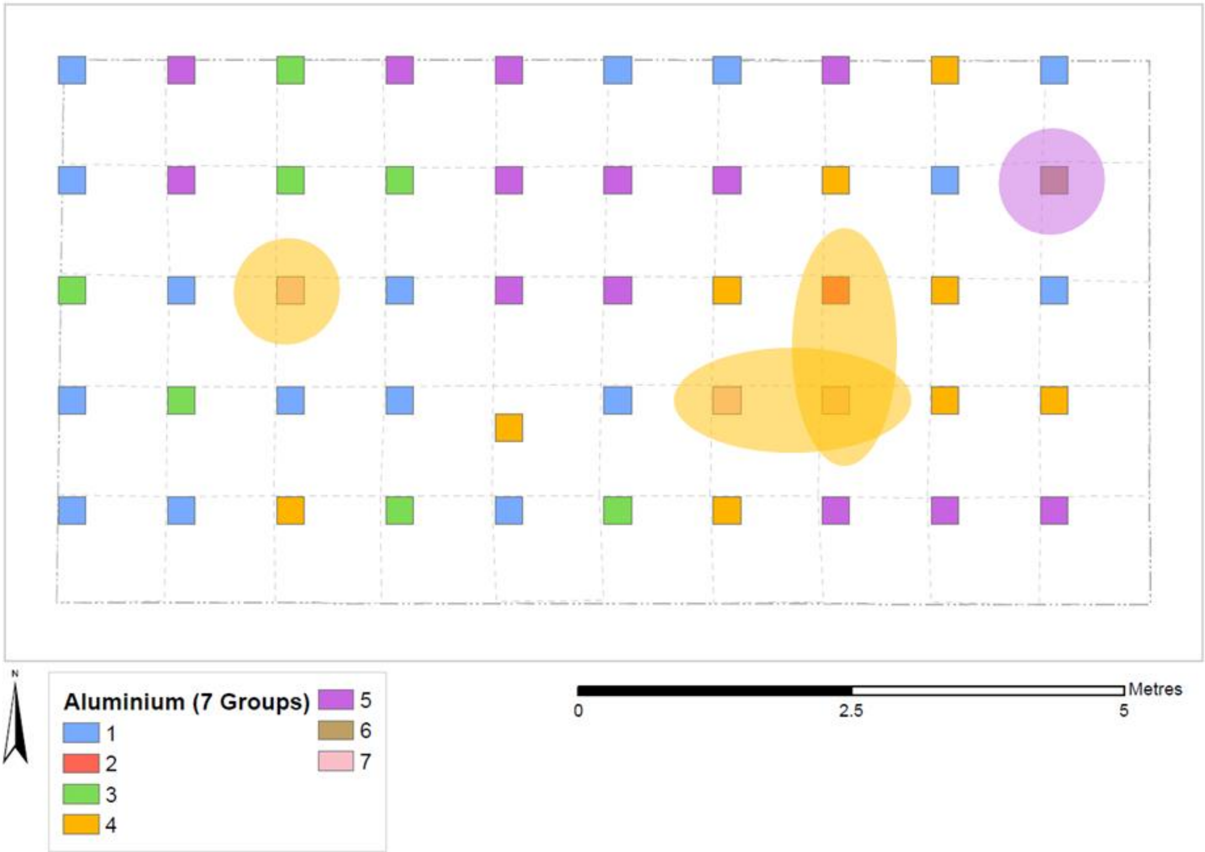

Figure 3. Key patterns in Aluminium levels

1.2.2.4 Aluminium: Complete record of runs

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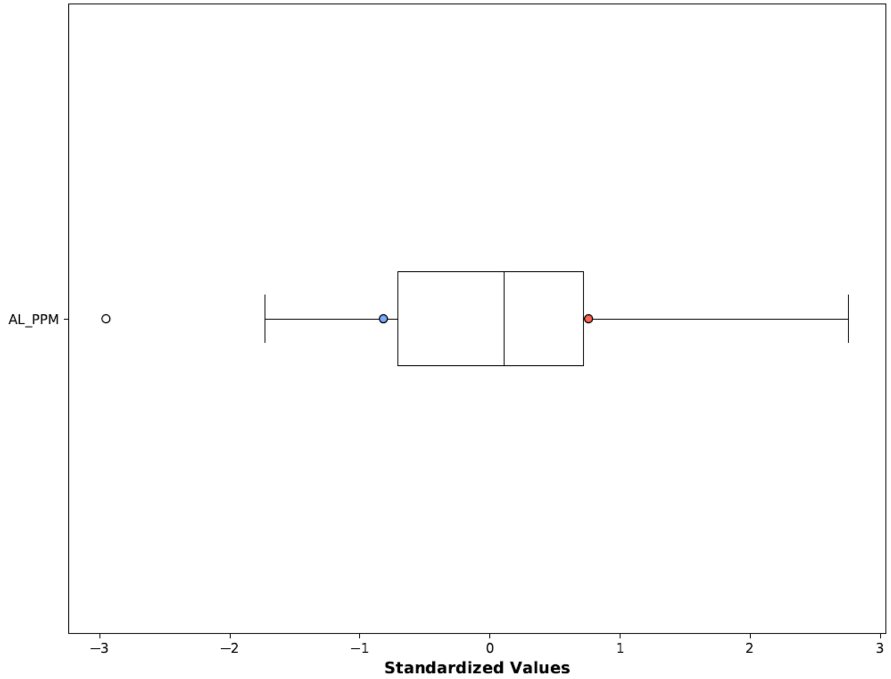
</td><td>

Optimal number of groups (based on highest pseudo F-Statistic): 15
How good the variable is at differentiating groups (R^2 statistic): 0.6205 </td></tr>
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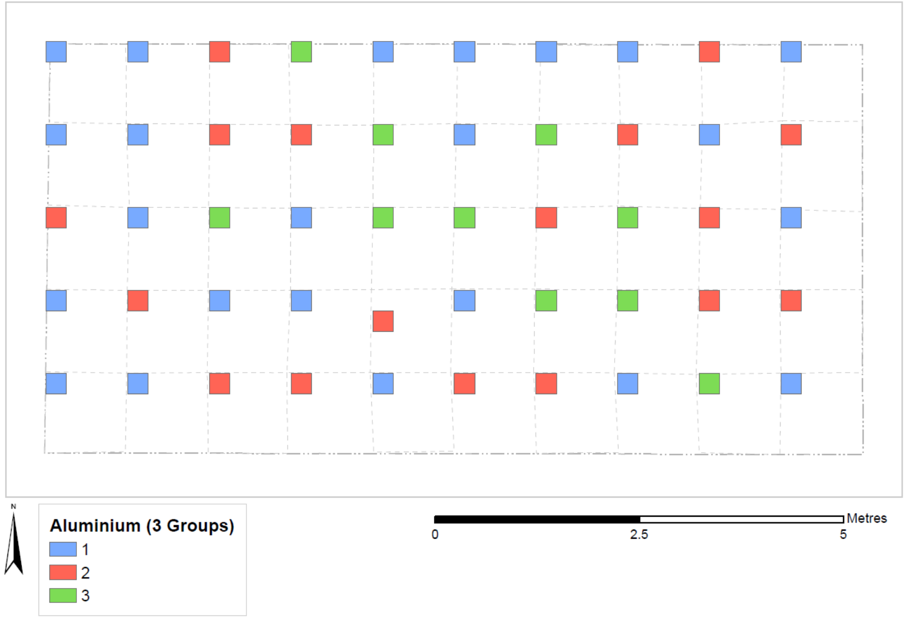
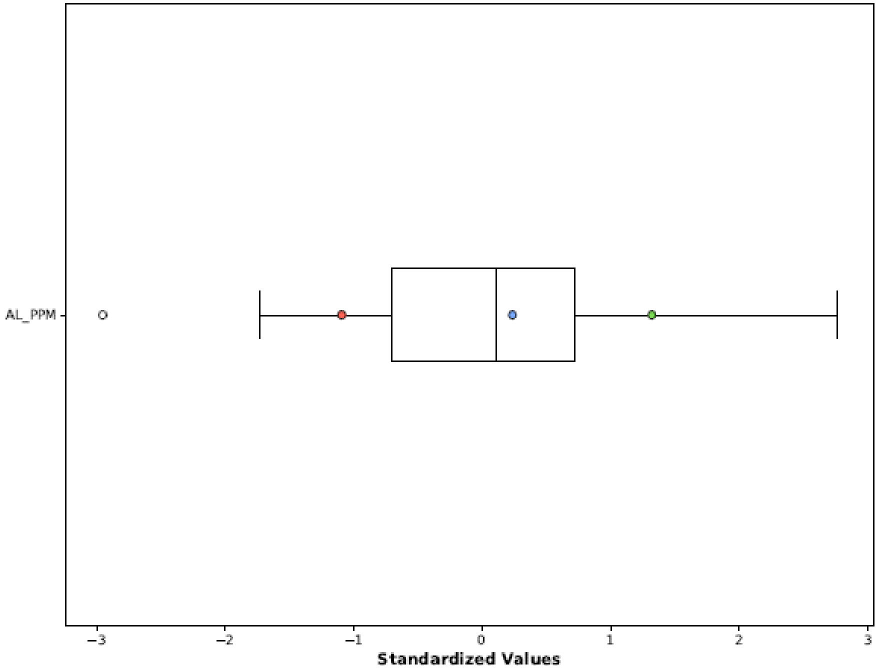
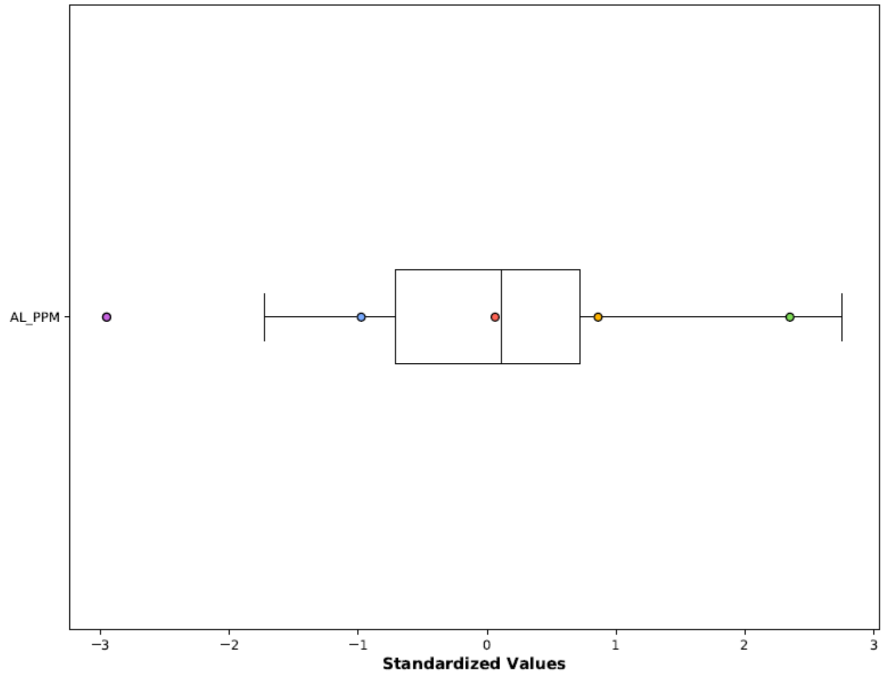
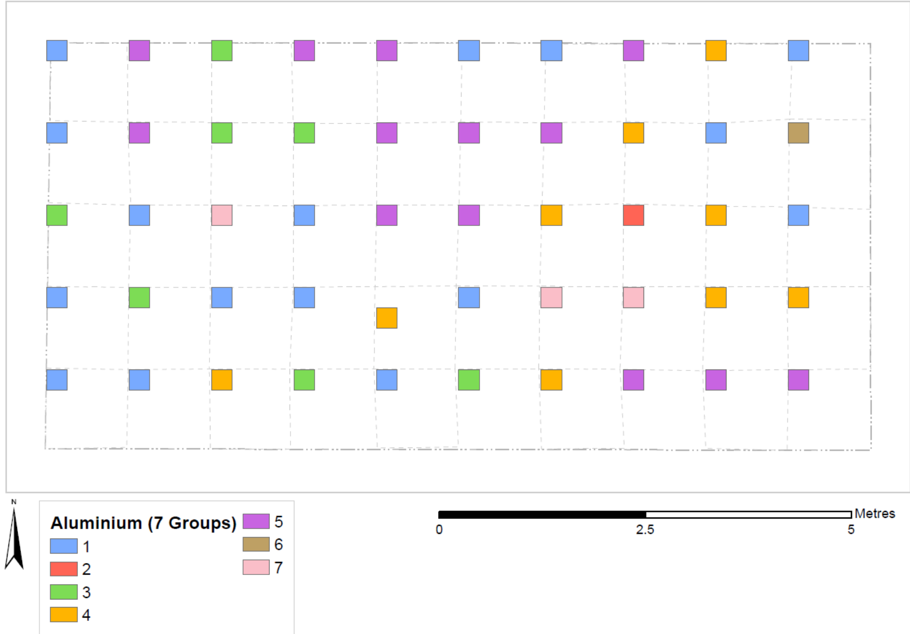
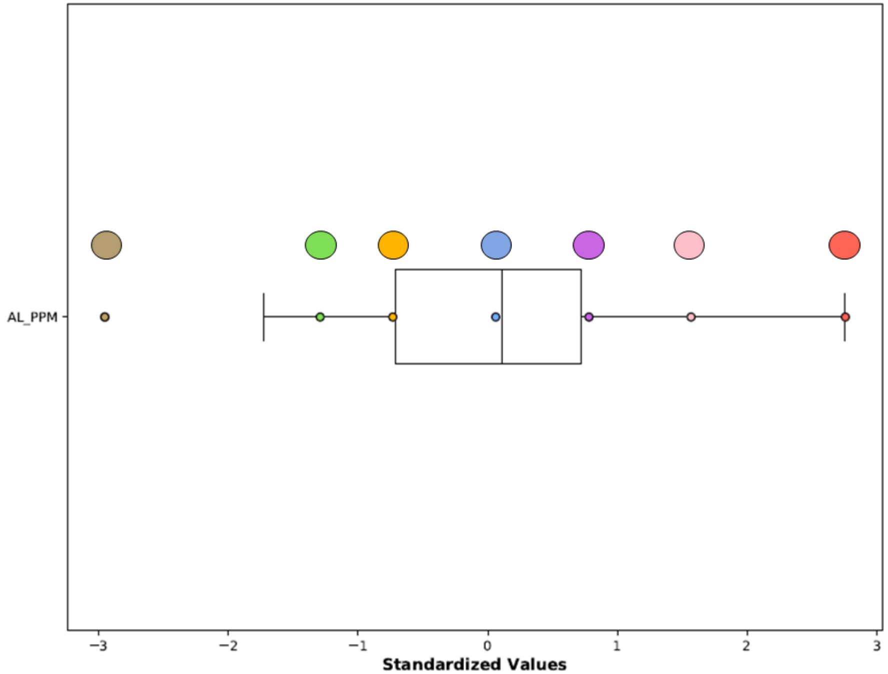
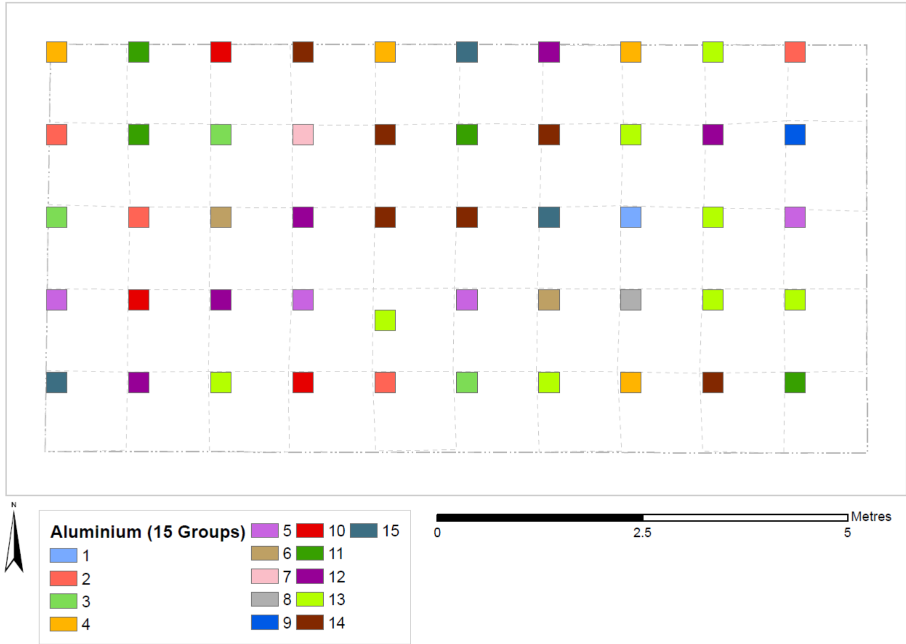
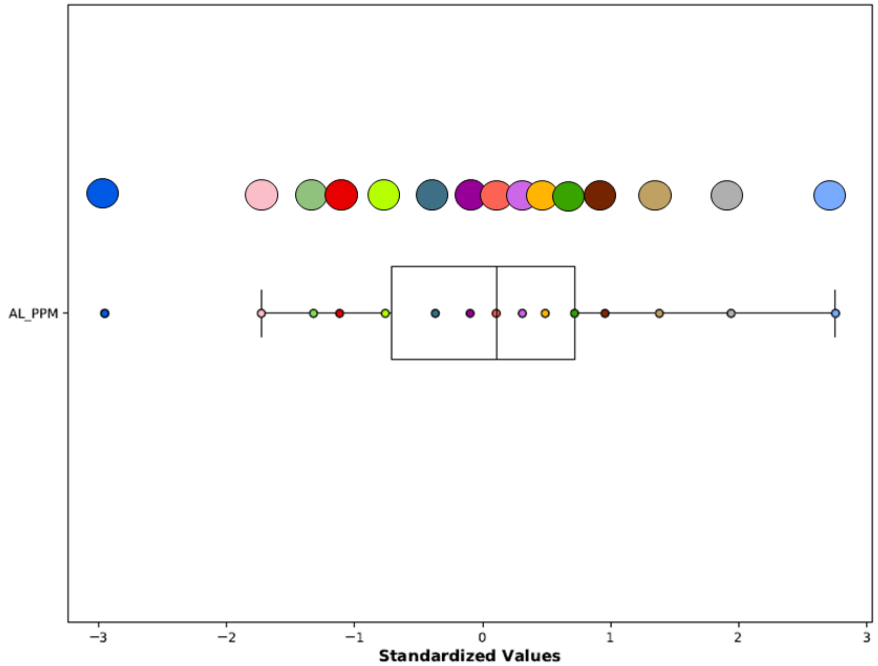
Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 15 **How good the variable is at differentiating groups (R^2 statistic):** 0.7796

Groups	Group Composition and Statistics
	

Optimal number of groups (based on highest pseudo F-Statistic): 15

How good the variable is at differentiating groups (R^2 statistic): 0.9237

Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 15 **How good the variable is at differentiating groups (R^2 statistic):** 0.9633

Groups	**Group Composition and Statistics**
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 15 **How good the variable is at differentiating groups (R^2 statistic):** 0.9972

1.2.2.5 Calcium

1.2.2.5.1 Calcium: Two groups

The two group run for calcium seemed to form a more coherent binary pattern than those for aluminium and iron, with a large area of low calcium (red group) at the centre of the plot at and around grid square B2. Other samples were in the same group from the eastern end of the trench, however. Some of these were those high in iron and aluminium instead. Two anomalies appear in the box plot but was unresolved in the group formations.

1.2.2.5.2 Calcium: Three groups

Three groups resolved the low values around B2 into a smaller group (red), still joined with low values in the eastern end of the trench. Some of these overlapped the areas high in iron and/or aluminium, again.

1.2.2.5.3 Calcium: Five groups

Five groups tightened the B2 low-calcium group up even further (green). The rest of the low-calcium samples were grouped as red. Three high (yellow) samples were grouped together, one of which must be an anomaly. They were not from one area of the trench but grid squares X3, C4, and F0.

1.2.2.5.4 Calcium: Seven group

The seven group run resolved the low anomaly being from square C2 into a group on its own (yellow) while it had previously been included in the low-calcium group around B2 (now more restricted, in brown).

1.2.2.5.5 Calcium: 15 (optimal) groups

The fifteen group was quite complicated and again split the low-calcium group into several low-calcium groups. It did not resolve the high anomaly but kept the three highest samples grouped together.

1.2.2.5.6 Overview of Calcium

The key patterns in calcium was the low-calcium zone around square B2 and the three very high grid squares X3, C4, and F0 (Figure 4).

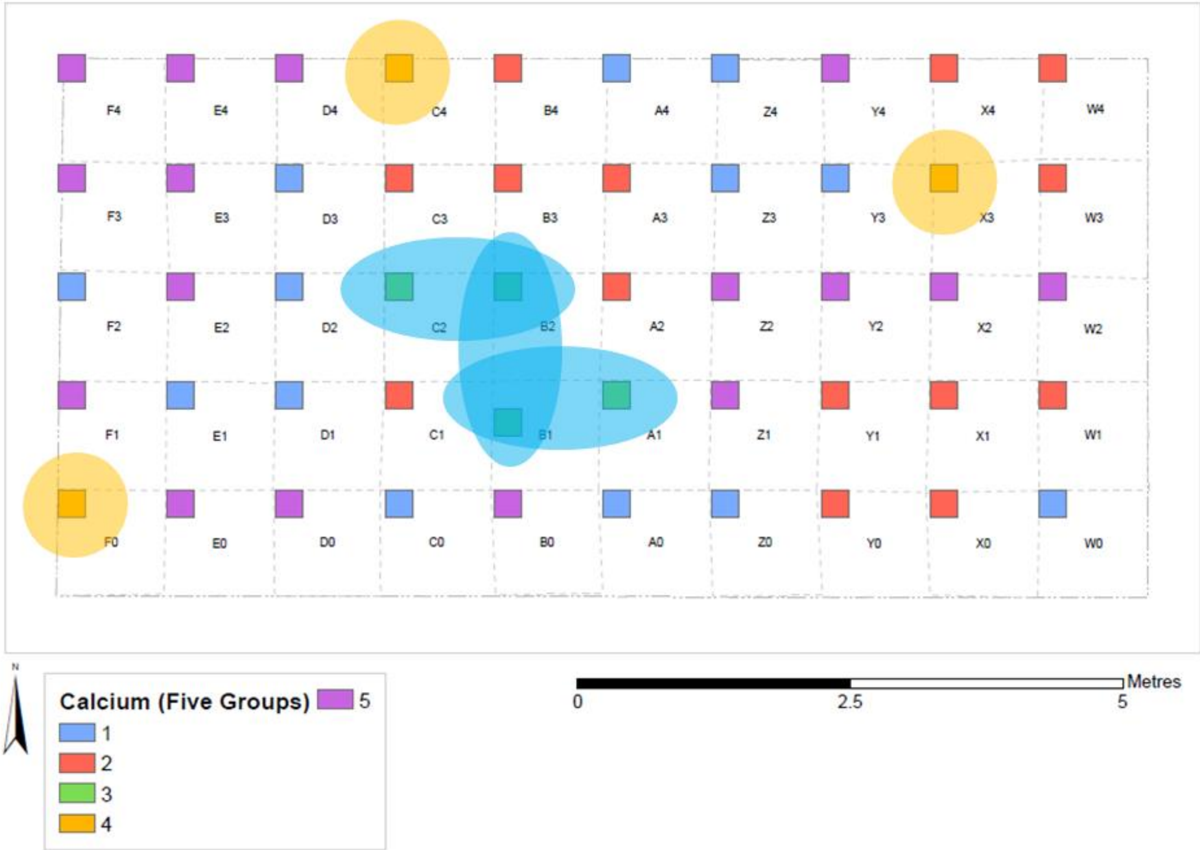


Figure 4. Key patterns in calcium levels

1.2.2.6 Calcium: Complete record of runs

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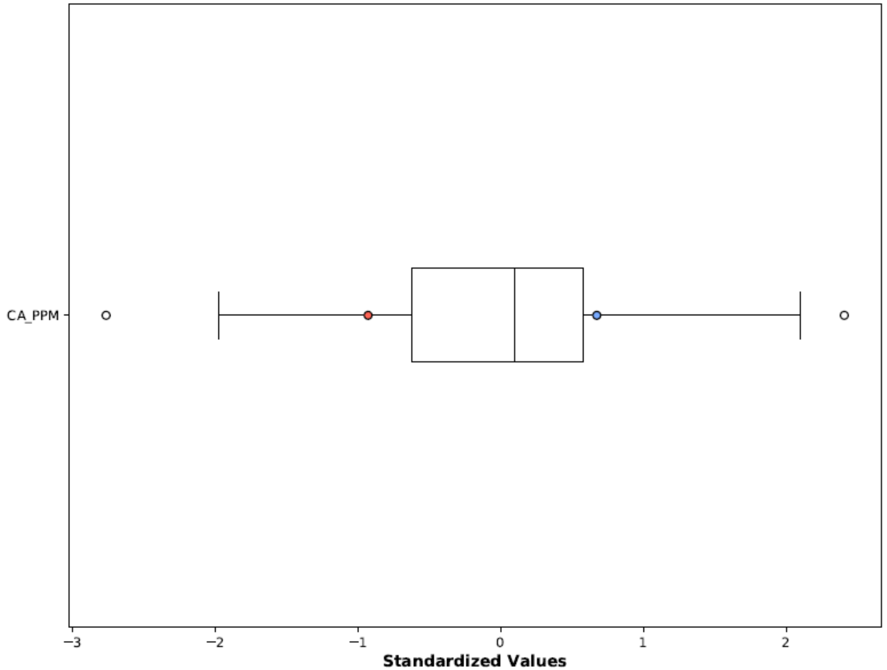
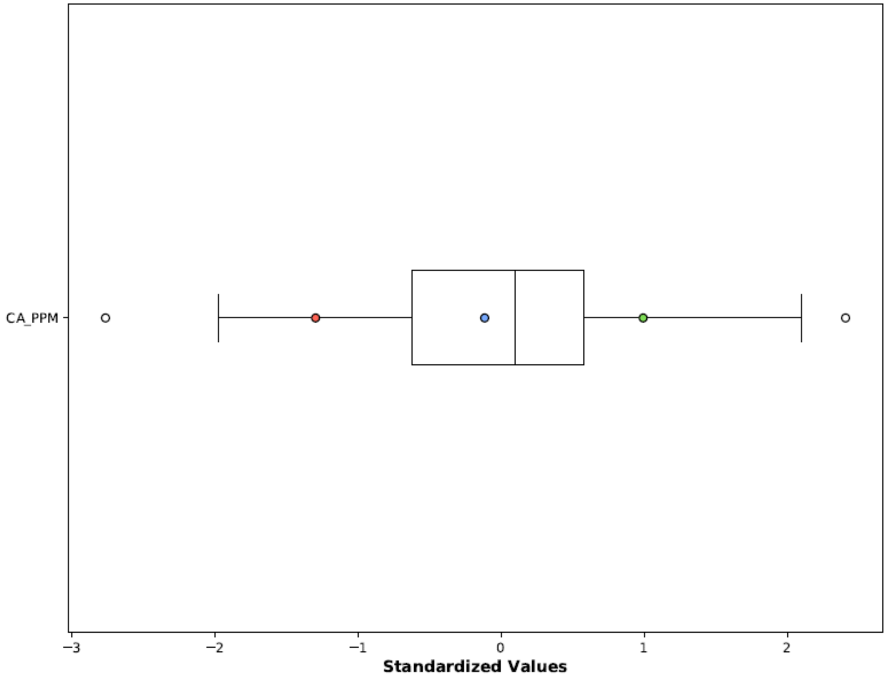
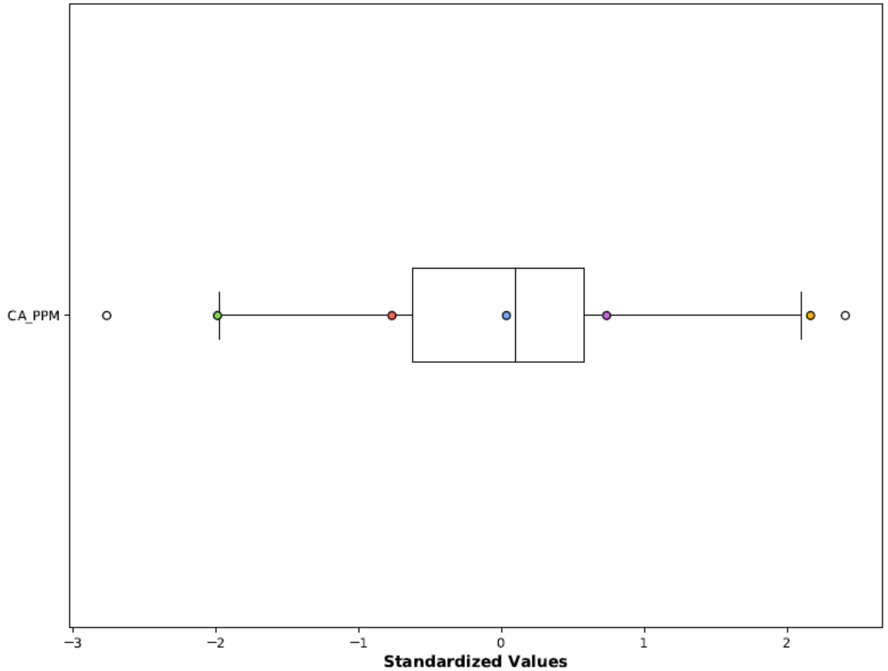
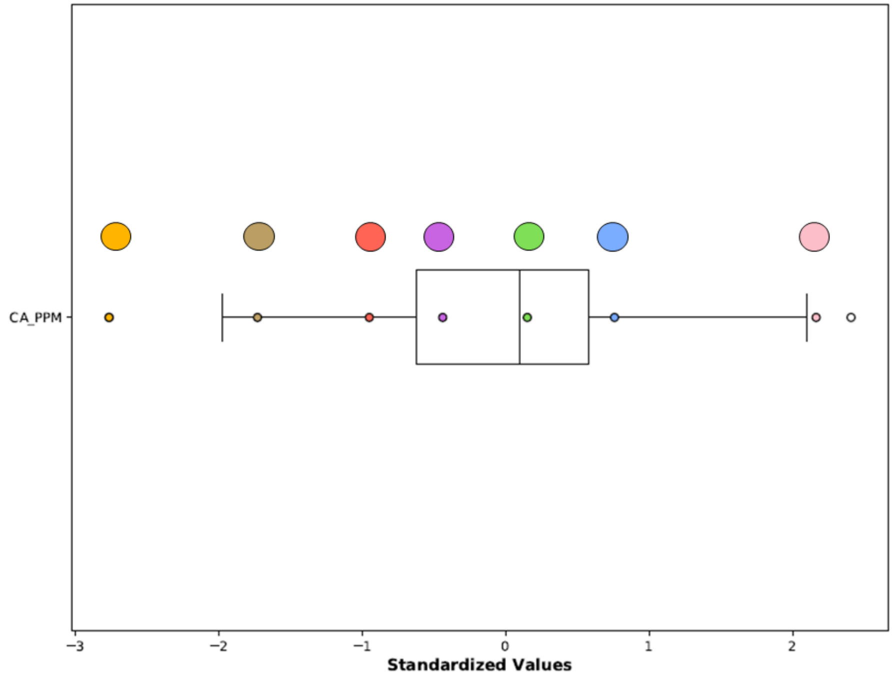
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 13 **How good the variable is at differentiating groups (R^2 statistic):** 0.6257

Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 15 **How good the variable is at differentiating groups (R^2 statistic):** 0.7639

Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 0.9364 **How good the variable is at differentiating groups (R^2 statistic):** 15

Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 15 **How good the variable is at differentiating groups (R^2 statistic):** 0.9707

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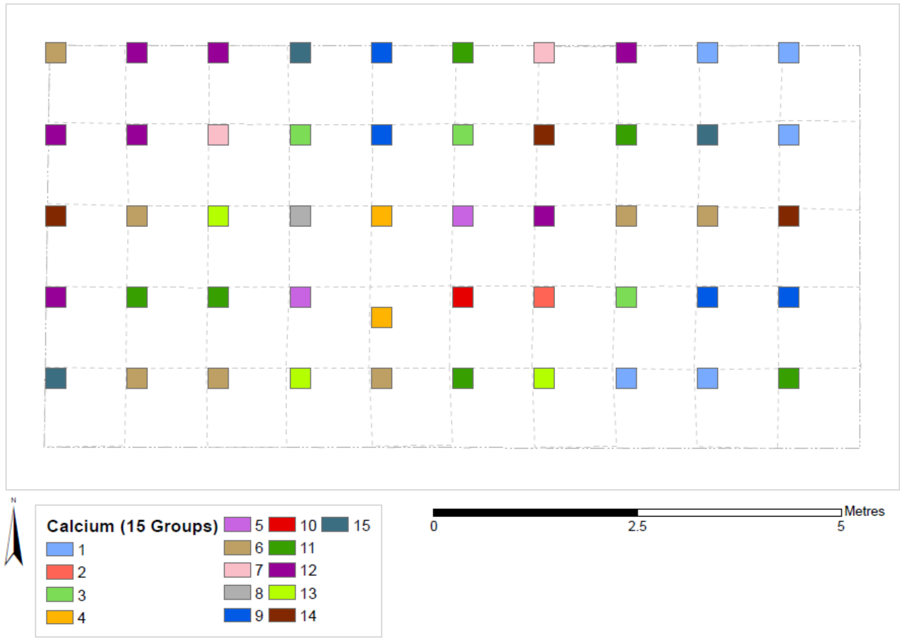

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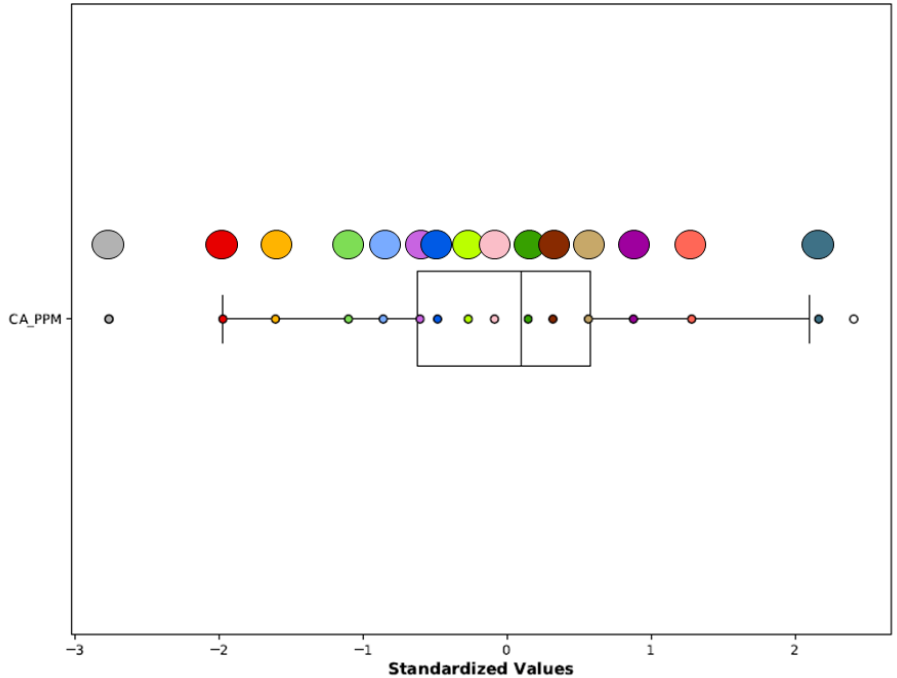

Optimal number of groups (based on highest pseudo F-Statistic): 15

How good the variable is at differentiating groups (R^2 statistic): 0.9943
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1.2.2.7 Magnesium

1.2.2.7.1 Magnesium: Two groups

Generally, the two group analysis on magnesium showed a roughly inverse pattern to the calcium: Where calcium had been low around B2, magnesium was higher. Magnesium was high around Y1, as aluminium had been.

1.2.2.7.2 Magnesium: Three groups

In addition to the high-magnesium samples around B2 and Y1 (but also joined by samples from elsewhere in the trench), the three group run resolved a blue group around W2, in the eastern end of the trench, joined by one sample from the western end (from D3) that was lower in magnesium.

1.2.2.7.3 Magnesium: Five groups

A five group run maintained the low-magnesium group around W2 with D3 (red here). The highest magnesium group samples were around B2 and Y1 still, but the group formation was no tighter so they were linked with other samples from across the trench.

1.2.2.7.4 Magnesium: Seven group

With seven groups, the low-magnesium samples around W2 with D3 was generally maintained, although W3 was again singled out for having lower values than the rest as had happened with iron and aluminium.

1.2.2.7.5 Magnesium: Eight group (optimal)

Eight groups was the optimal, as there were only eight values of magnesium measured. The low-magnesium group (here red) was maintained. One high value was isolated in square X0.

1.2.2.7.6 Overview of Magnesium

There was a broadly contiguous group of low-magnesium samples in the eastern end of the trench, consistently joined by the sample in D3. In addition, grid square W3 was again reading low in this element (Figure 5). This was broadly in keeping with the Hot Spot and Cluster-Outlier analyses.

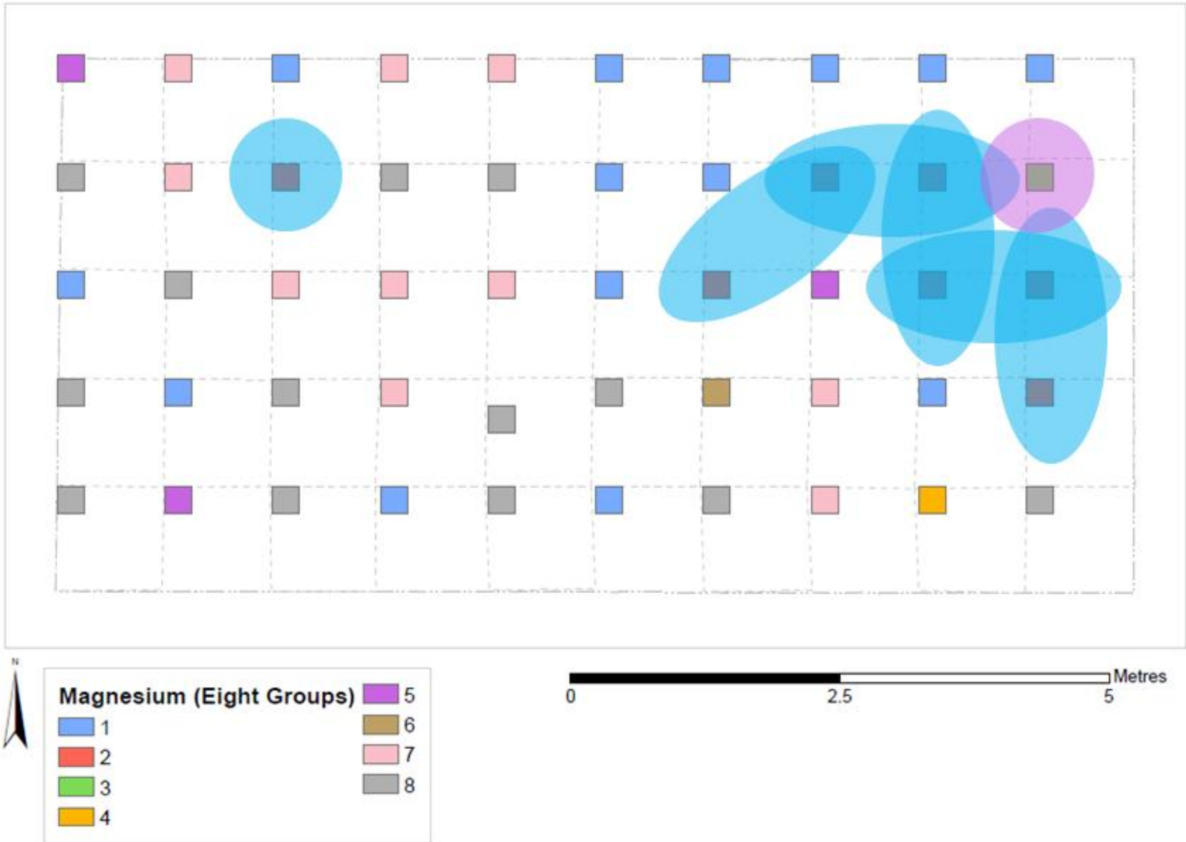

Figure 5. Key patterns in magnesium levels

1.2.2.8 Magnesium: Complete record of runs

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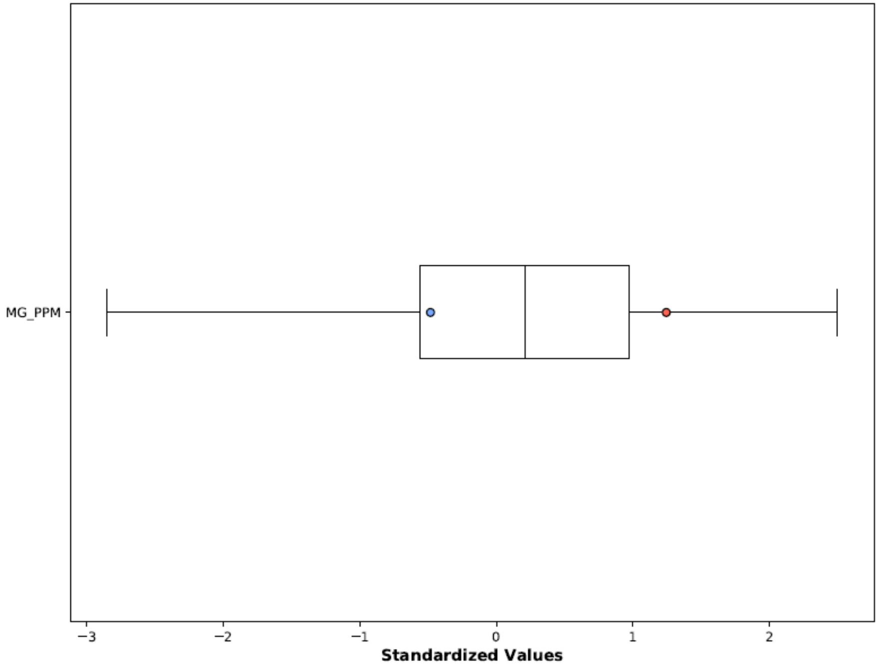
<tr><td></td><td>

Optimal number of groups (based on highest pseudo F-Statistic): 8

How good the variable is at differentiating groups (R^2 statistic): 0.6014</td></tr>
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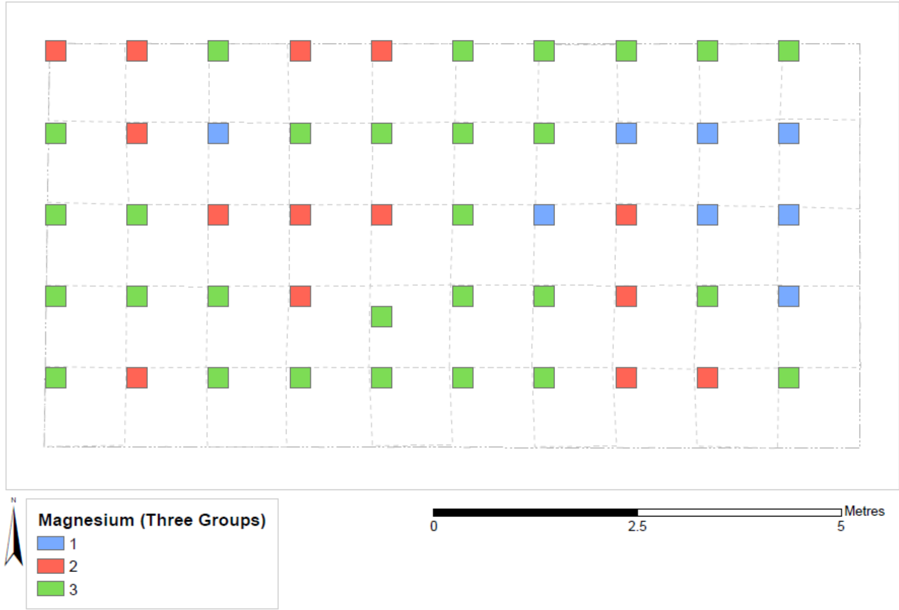
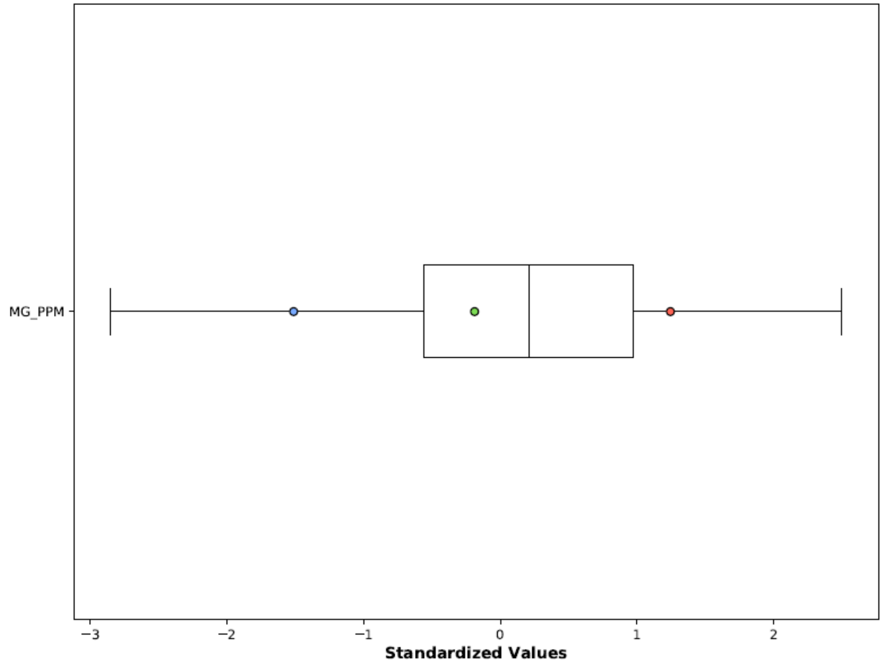
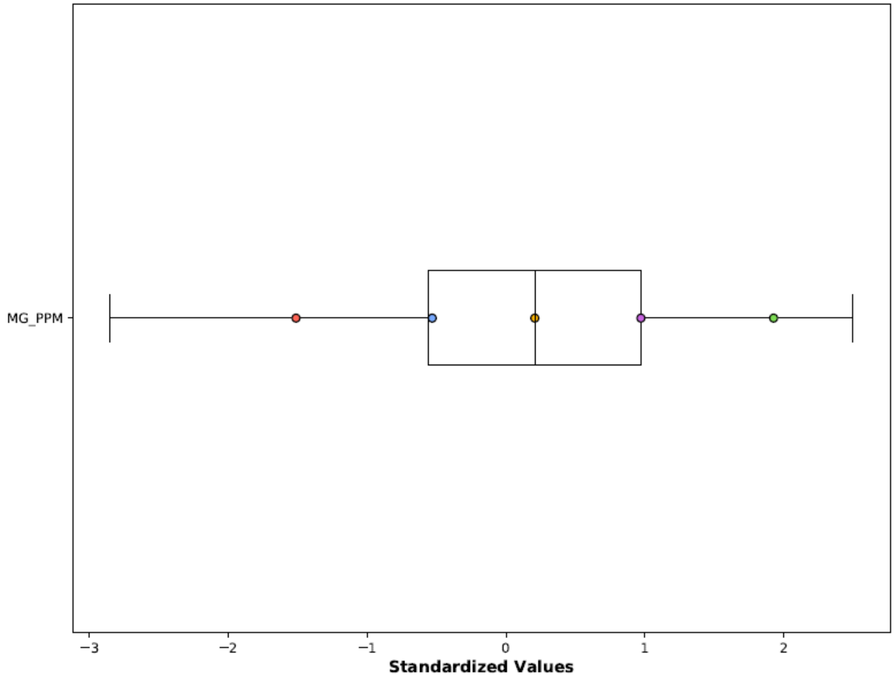
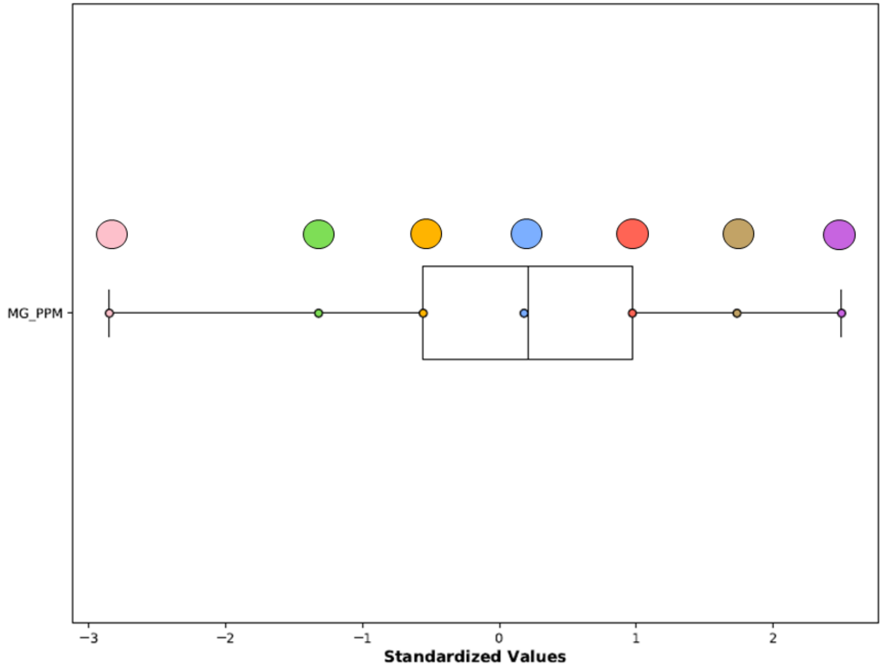
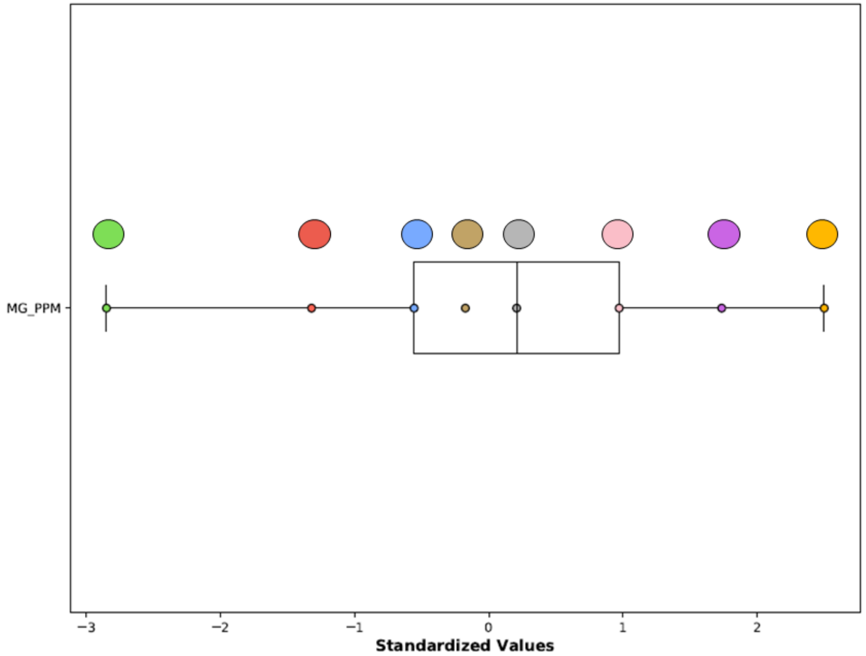
Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 8 **How good the variable is at differentiating groups (R^2 statistic):** 0.8195

Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 8 **How good the variable is at differentiating groups (R^2 statistic):** 0.9476

Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 8 **How good the variable is at differentiating groups (R^2 statistic):** 0.9973

Groups	Group Composition and Statistics
	 **Optimal number of groups (based on highest pseudo F-Statistic):** 8 **How good the variable is at differentiating groups (R^2 statistic):** 1.00

1.2.2.10 Major/Minor Elements Combined Model

1.2.2.10.1 Major/minor elements: Two groups (also optimal)

When analysing the elements in combination, the optimal group suggestion immediately dropped to just two groups. This suggests that overall there is one dominant pattern that prevails, while any other groupings are more subtle.

The samples fall into two groups based on the four elements combined. The pattern was generally similar in all four repeats. In the binary split of the data, all four elements were lower in the blue group (repeats 1, 2, 3, red group in repeat 4), with a greater difference between the iron and aluminium averages. This does not appear restricted to one area of the trench but forms in diagonal bands northwest to southeast alternately across the full width of the trench (four of each colour). The R^2 statistics confirm that iron and aluminium account for the majority of the differentiation between the defined groups. There were generally two parallel groups of those with lower levels overall and those with higher levels overall in all later (higher number grouping) runs, but as other groups were split out, the averages the parallel strands represented got closer to the global averages for the elements, and samples retained in these groups were generally mixed throughout the trench between the groupings separated out as more distinct. It is suggested therefore, this is a general background signal.

This also suggests that any localised patterning would not be dominantly associated with particular enhancement or depletion of either iron or aluminium but would depend on the levels of less highly present elements generally.

1.2.2.10.2 Major/minor elements: Three groups

Separating out a third group, produces a more interesting pattern that may be due to a localised process (natural or anthropogenic) occurring. There is a pattern of generally mixed and distributed blue and green samples which reflect a pattern similar to the binary split (with the blue group being higher on average for all four elements than the green group samples). Just west of centre of the trench (around B2) and in the southeast of the trench (Y1/X0) there are two pockets of the third, red, group samples which have slightly above (global) average magnesium and aluminium, slightly below average results of iron, but most significantly, well below average readings for calcium. This reflects those low and the one anomalously low reading identified in the calcium-only groupings, and shows the significance of this depletion relative to all other low spots in the combined elements. Calcium has a much higher R^2 statistic, demonstrating how it is more relevant in differentiating these groups than in the binary division.

1.2.2.10.3 Major/minor elements: Five groups

Using the colours from the first repeat run for ease of discussion, the blue and green groups continue to seem to reflect the general background variation, being dispersed through the trench, with the blue group being generally higher in all four elements than the green group that runs parallel. However, the purple and red groups seem to be of more interest for identifying potential areas of anthropogenic alteration to the soils. The purple group mostly overlies the area just to the west of centre (around B2) and in the southwest of the trench at Y1. These samples reflect those much lower in calcium again, with slightly above average magnesium and aluminium, and near to/just below average iron levels. The red group here is always in grid squares adjacent to the purple group but it is only slightly below the average in calcium. This group, in contrast, shows significantly higher than average readings in aluminium and iron, however. The yellow group is four samples, all from around the edges of the trench and in different regions of the trench. They are all marked by being high in magnesium and low in iron. At this stage, the fact they are four isolated samples does not suggest a tightly localised process is causing this signature to appear. It might suggest that groups are being made for the sake of the higher number of groupings, rather than being meaningful in any way. The repeat runs did not produce the isolation of the four samples due to higher magnesium content alone. The R^2 statistics confirm that magnesium is contributing more to the definition of these groups than before and all four are being incorporated into the model better.

1.2.2.10.4 Major/minor elements: Seven groups

Again utilising the colours in the first run to start discussion, the pink and green groups seem to represent the underlying overall variation patterning, with the pink group being moderately higher than average in all elements, particularly iron and aluminium, and the green being the opposite. Samples of these colours are dispersed throughout the trench.

The red group is defined by being very low in calcium and slightly low in iron, while being moderately high in magnesium and slightly high in aluminium. This is again in the area around B2 and Y1/X0, as well as the sample from B4. This was repeated in the other runs being the yellow, green, and brown groups sequentially.

At this stage, the sample in W3 gets isolated (brown) as does the sample in Y2 (purple). The sample in Y2 is particularly high in magnesium, iron, and aluminium, along with slightly elevated levels of calcium. The sample in W3 is the opposite, being very low in magnesium, iron, and aluminium, and moderately low in calcium. These could be amplified exaggerations of the general split in the samples (as demonstrated by the pink and green group profiles in this run), or they could be samples with genuine enhancement or depletion but this would need consideration with the other evidence to support this being from a specific activity or other process.

The blue group is interesting because it is moderately high in calcium, slightly high in iron, but then slightly low in aluminium and moderately low in magnesium. This is a small cluster of samples in the northeast quadrant of the trench around X4, sandwiched between the W3 and Y2 oddities. It also follows the general pattern of W3, just significantly higher in all absolute values but with calcium being the dominant element of the four, followed by much lower values of the other three. This could be an area of interest in terms of the ratio of calcium to magnesium, rather than it being about specific enhancement or depletion of either. The variations in aluminium and iron in these samples could relate more to these being more variable in the soils naturally.

The R^2 statistics suggest that iron, aluminium, and magnesium are the variables most responsible for defining the groups in this model, though calcium still has an R^2 statistic of greater than 0.5. To put it another way: iron, aluminium, and magnesium variability is better described by this model than the calcium variability. The model is still oversimplified for calcium. This is likely due to the fact that at seven groups, the two anomalies (one low, one high) in the calcium dataset are still incorporated into broader groups.

1.2.2.10.5 Overview of major/minor elements combined

Aluminium and iron seem to be naturally highly variable in the samples and dominate general variations across the trench. Two areas of potential activity/process do seem to flag up through the incorporation of calcium and magnesium, however, in the vicinities of the red group and blue group in the seven group run (Figure 6).

Returning to the individual element plots temporarily, neither iron nor aluminium had immediate patterning in their two group runs (which fits with the interpretation that they are generally more highly variable across the trench). In contrast, the groupings formed based on just calcium and aluminium looked less mixed on their individual two group plots, and the areas flagged there fitting broadly with the red and blue grouped samples in the seven group run on the combined major/minor element set. Consideration of the relative elemental composition of these latter groups confirmed they were notable for their calcium or magnesium patterning (the difference between Ca and Mg being balanced differently to other samples, if not notably enhanced or depleted in one or the other).

That is not to say iron and aluminium are not affected in these areas; the patterns seen in just those elements do relate to the areas of interest identified in the combined elements runs. It is just more difficult to distinguish variations in iron and aluminium that might be due to specific processes as separate from the natural variations of these elements in the soil. There has not been a process that has enhanced/depleted iron or aluminium in the soil to such a level and in such a way that it has preserved and become a dominant signal.

As such, two areas of interest were identified from the combined element modelling in the vicinities of the red group and the blue group, but as these were not significant enough to overcome the natural variations in iron and aluminium in the two group run; they will need to be combined with the artefactual and geophysical evidence to support their being considered an area of alteration. Even if so, it would need to be considered whether this process was anthropogenic, and furthermore whether it was Mesolithic or a more recent effect. It does provide two patterns to explore further however.

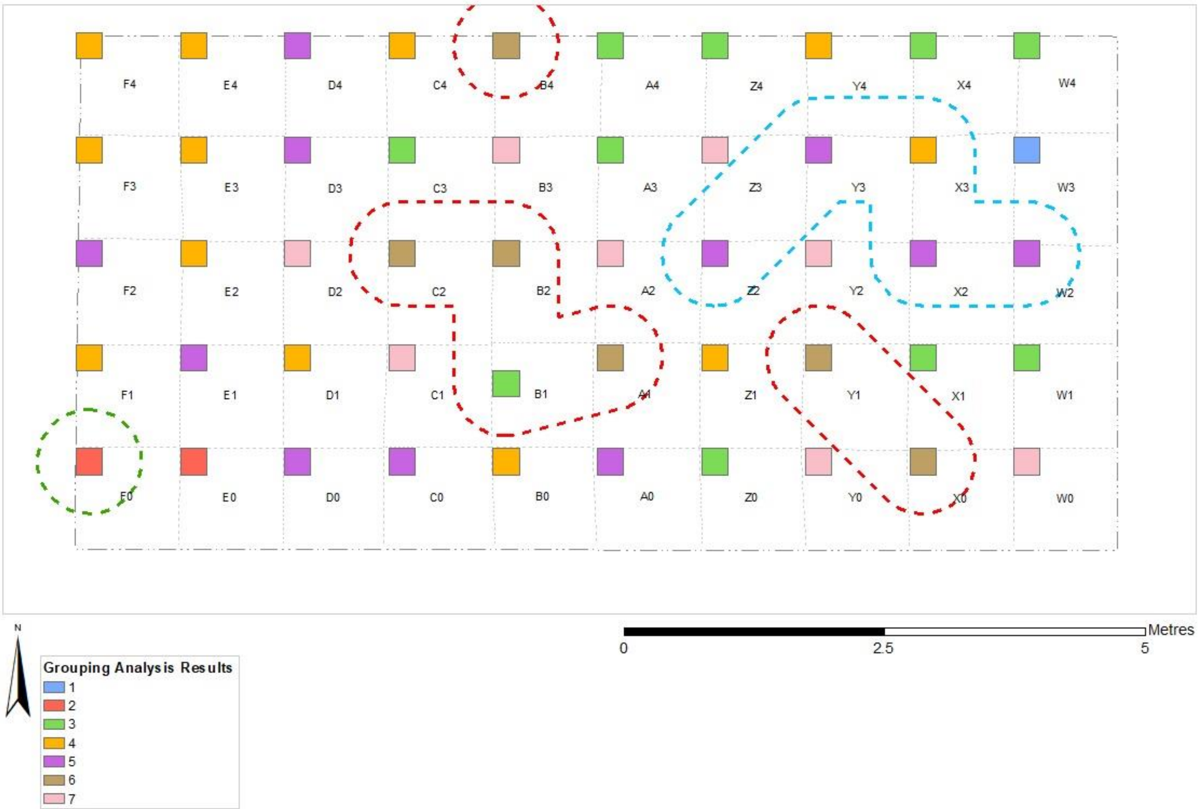


Figure 6. Combined major/minor elemental patterning across trench 4

1.2.2.11 Major and minor elements combined: Complete record of repeat runs

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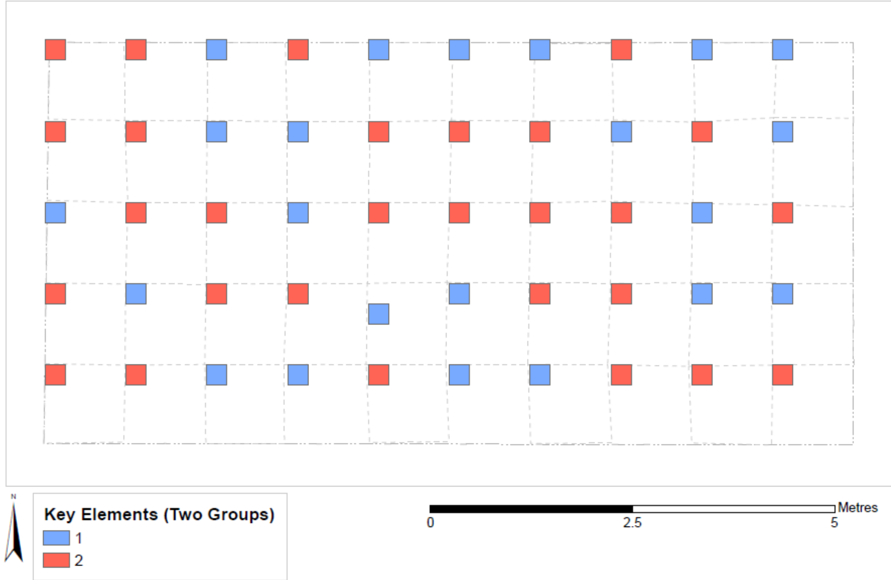
2 (also optimal number)



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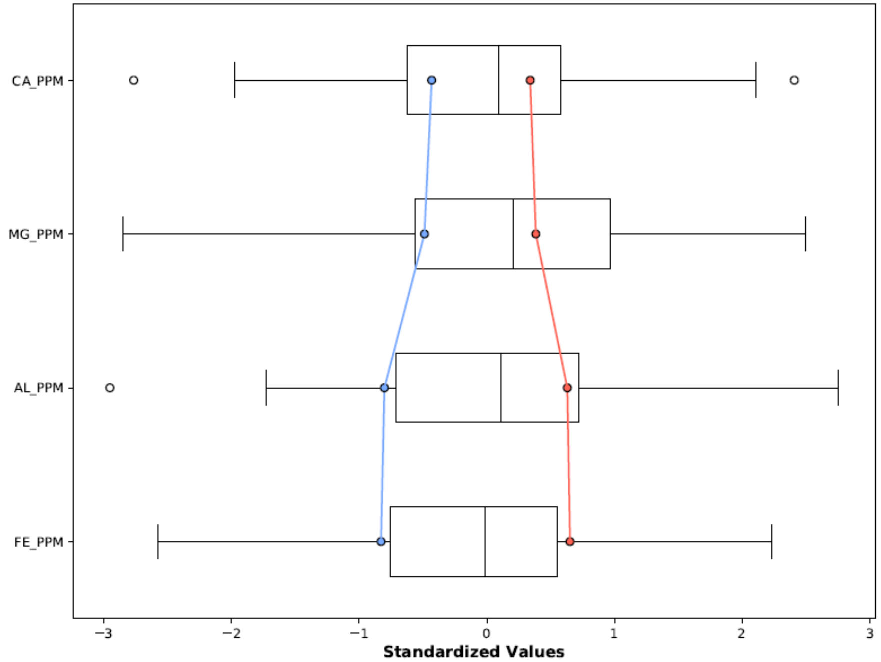

Optimal number of groups (based on highest pseudo F-Statistic): 2

How good the variable is at differentiating groups (R^2 statistic):

Fe: 0.5394; Al: 0.5056; Mg: 0.1874; Ca: 0.1467

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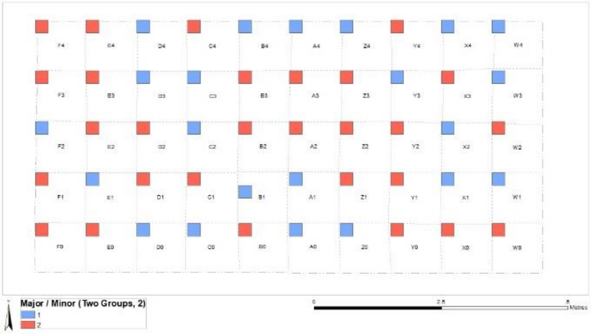
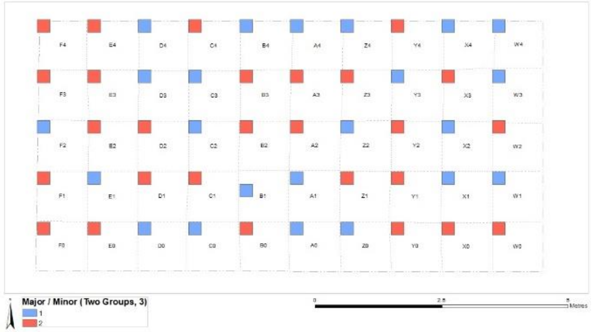
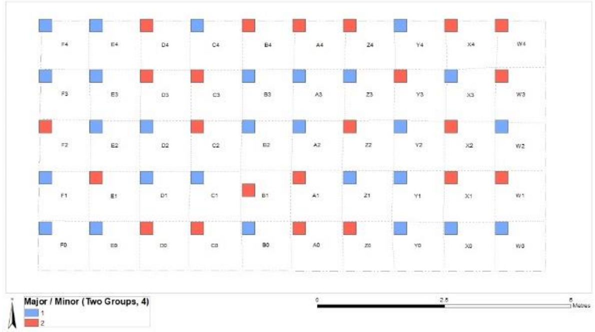
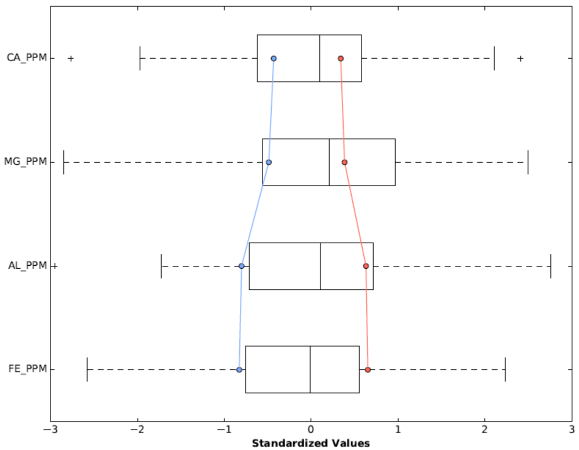
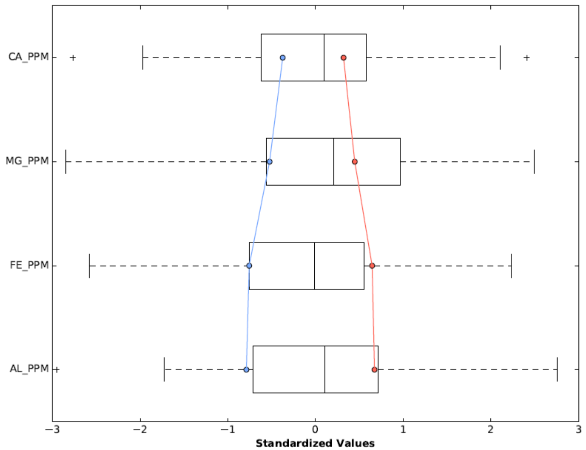
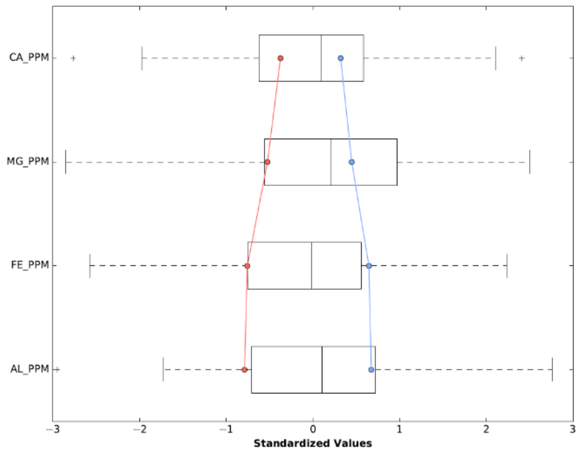
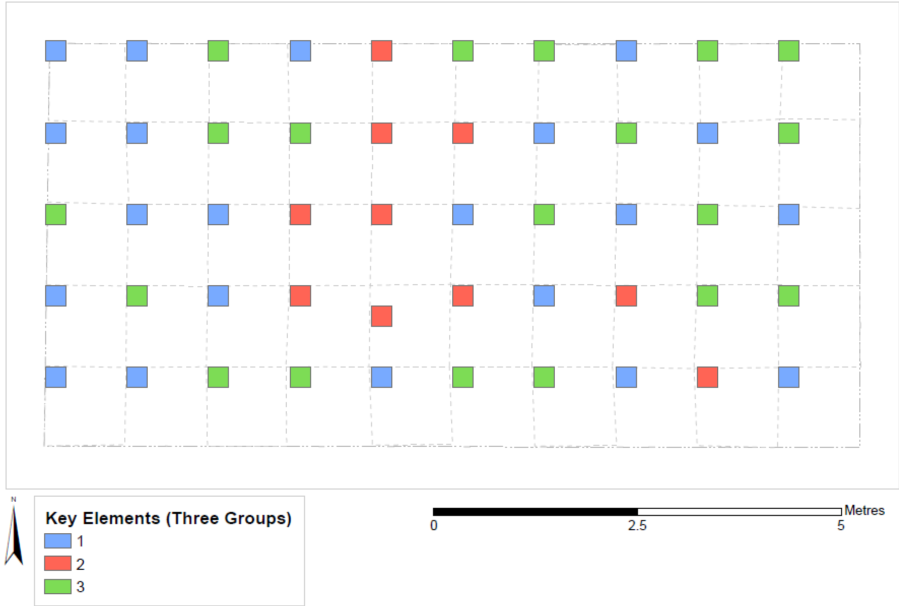
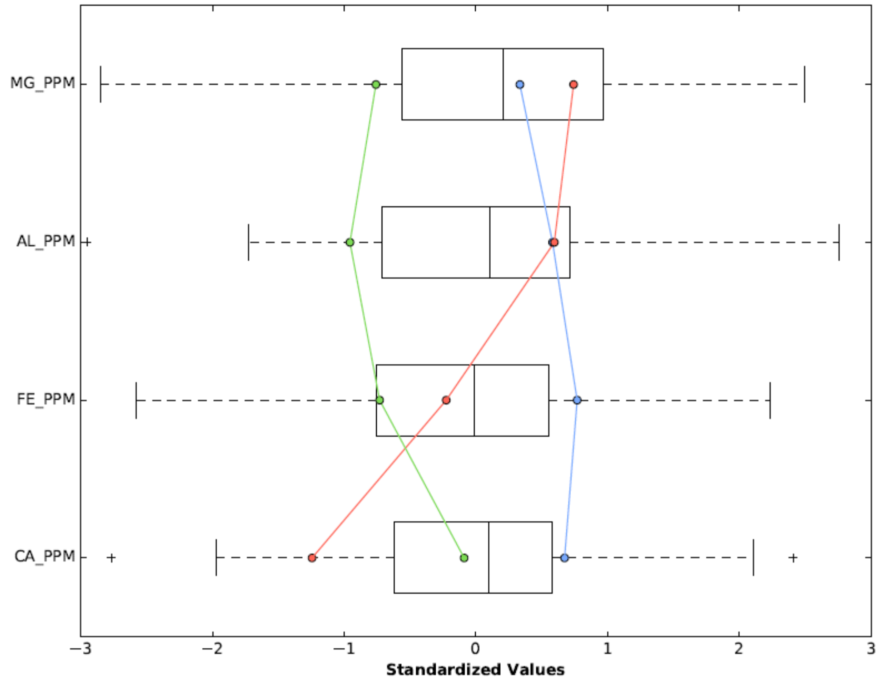
		
		

Groups	Group Composition and Statistics
3  	 **Optimal number of groups (based on highest pseudo F-Statistic):** 2 **How good the variable is at differentiating groups (R^2 statistic):** Fe: 0.4613; Al: 0.5605; Mg: 0.3756; Ca: 0.5028

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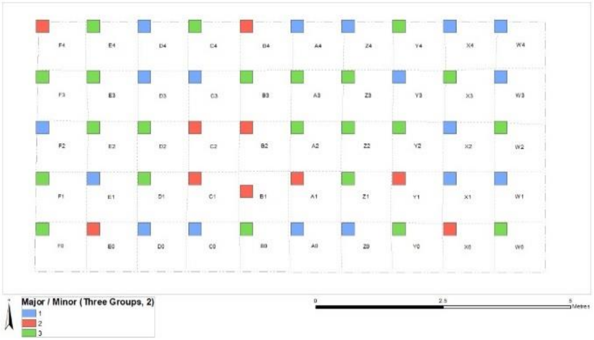	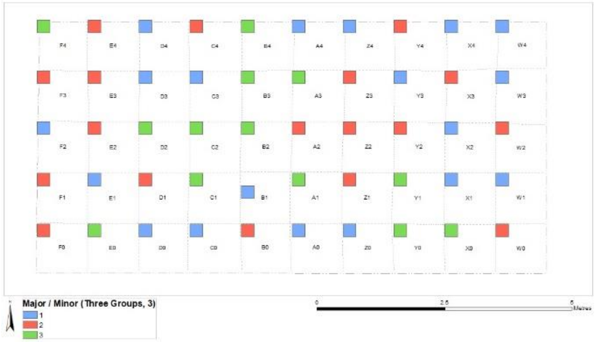	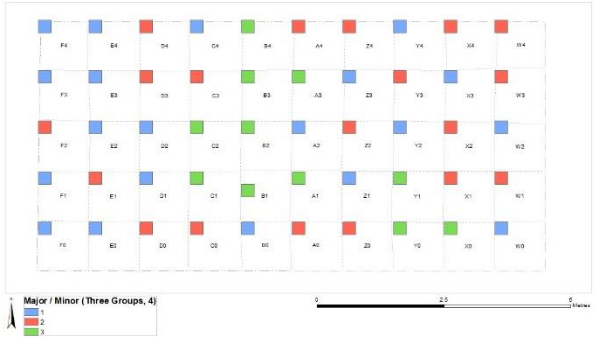
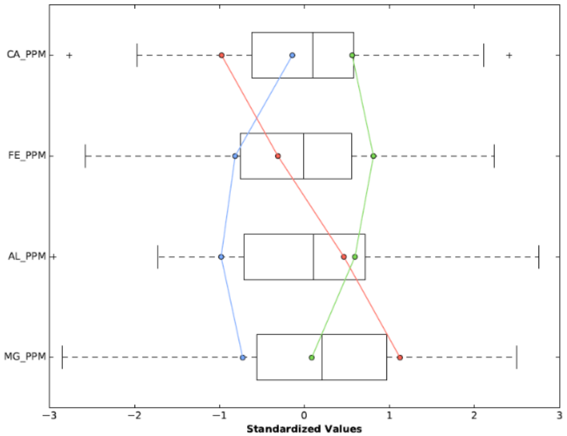	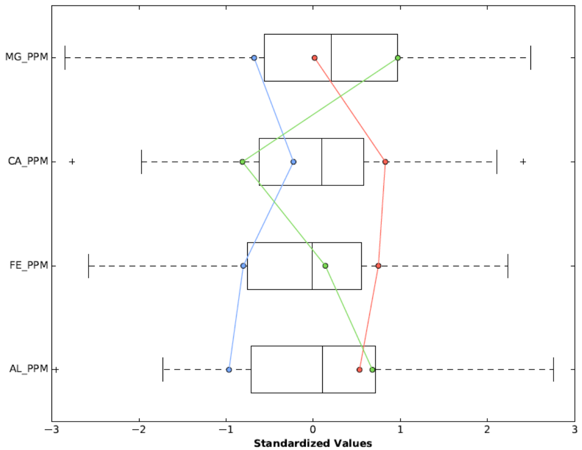	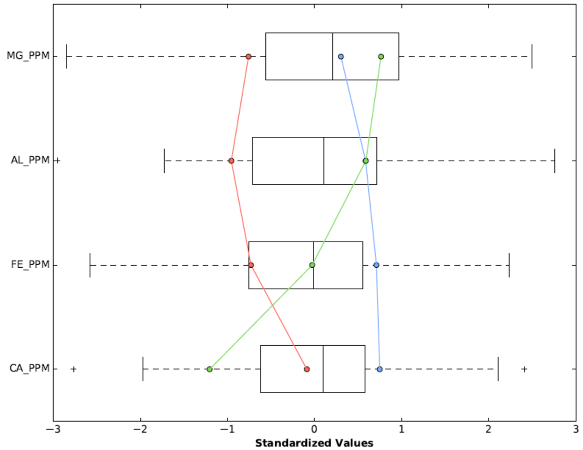

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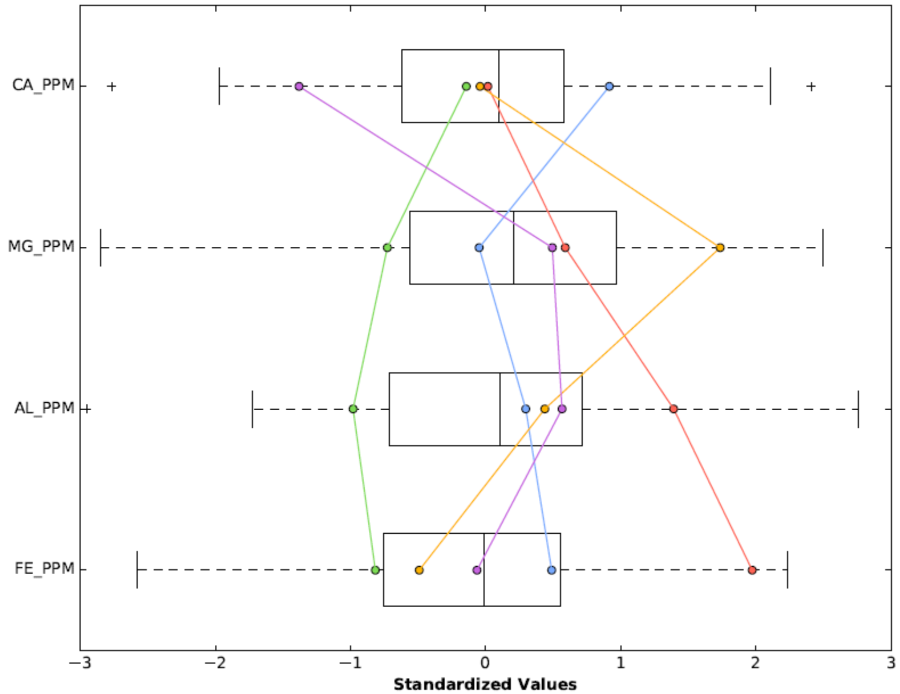
</td><td>

Optimal number of groups (based on highest pseudo F-Statistic): 2
How good the variable is at differentiating groups (R^2 statistic):
Fe: 0.7203; Al: 0.6326; Mg: 0.5056; Ca: 0.5636</td></tr>
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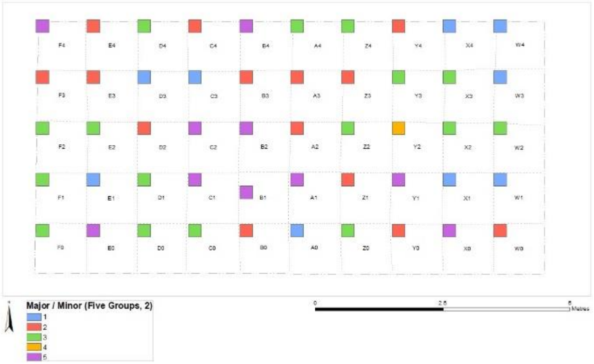
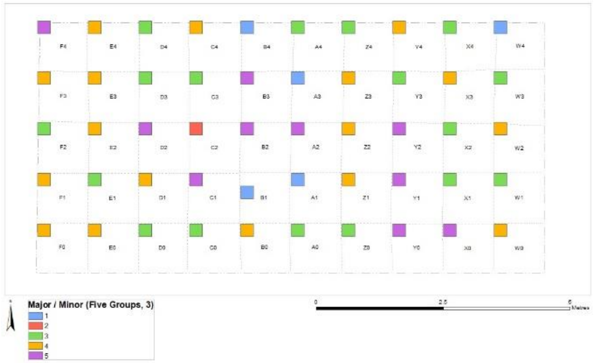
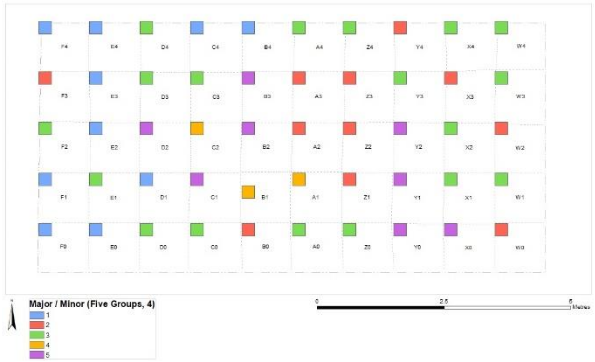
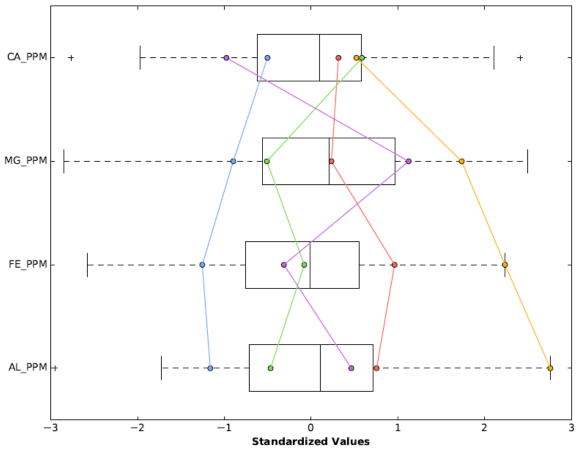
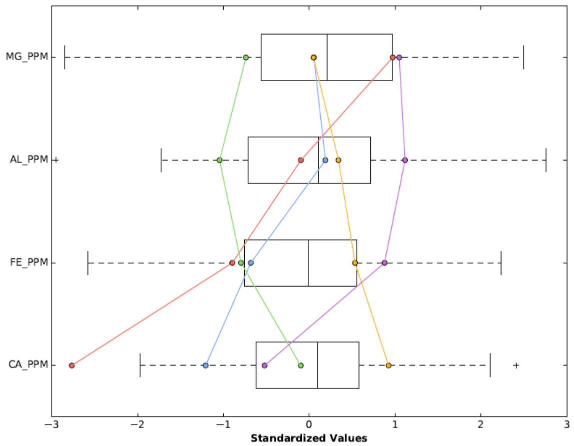
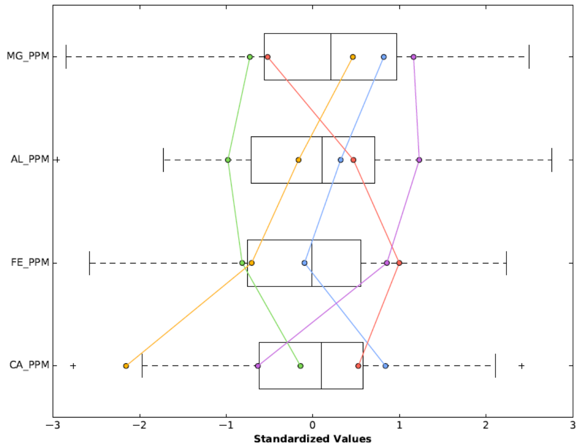
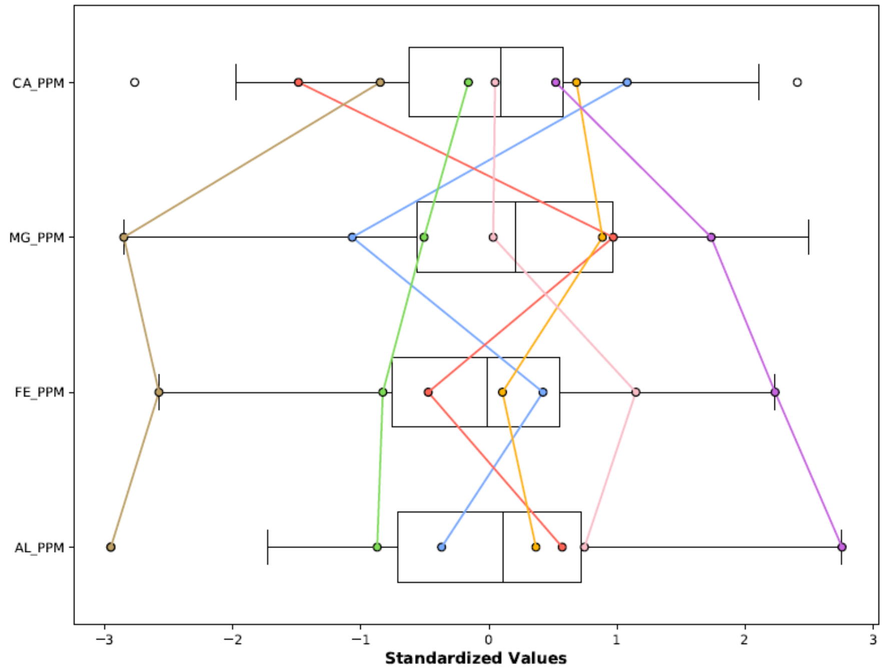
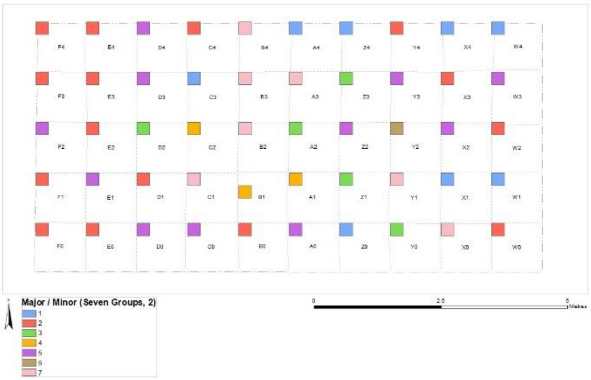
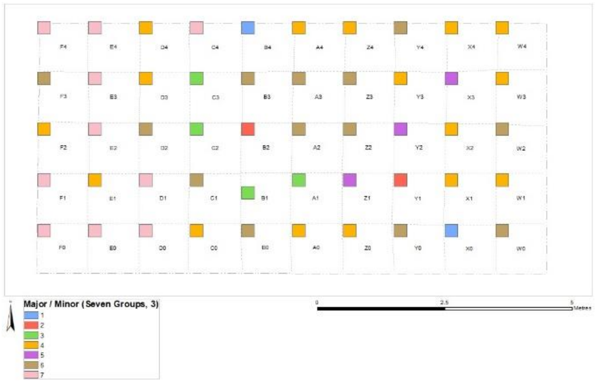
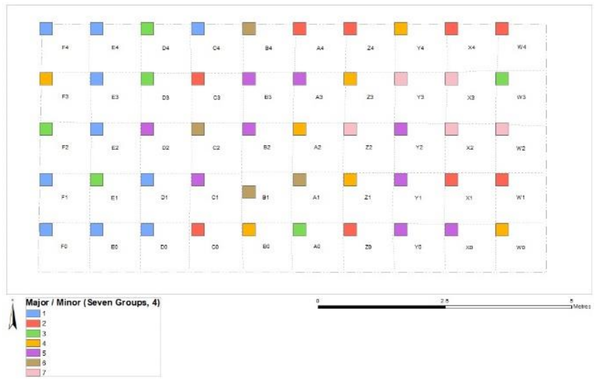
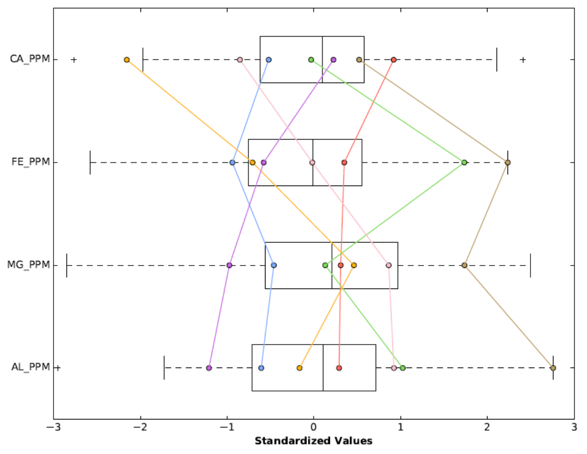
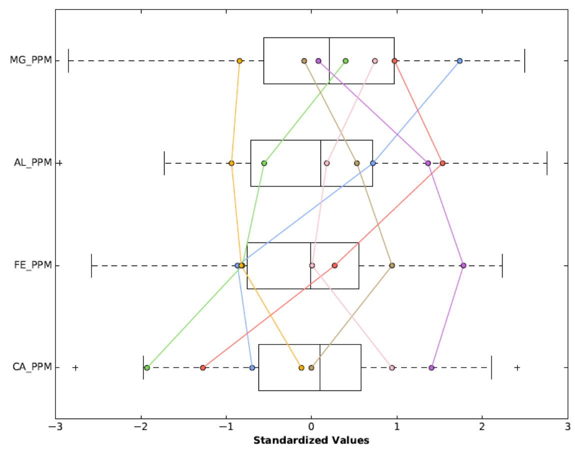
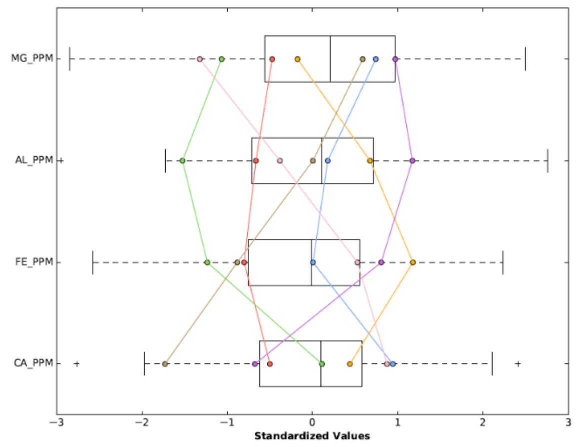
		
		

Groups	Group Composition and Statistics
7  	 **Optimal number of groups (based on highest pseudo F-Statistic):** 2 **How good the variable is at differentiating groups (R^2 statistic):** Fe: 0.7829; Al: 0.7633; Mg: 0.7099; Ca: 0.5615

Repeat 2	Repeat 3	Repeat 4
		
		

1.2.2.12 Manganese

1.2.2.12.1 Manganese: Two groups

The two groups showed the samples did have some degree of contiguity between those samples higher than manganese and those lower. It was not a mixed plot as the iron and aluminium plots had been but more like the calcium two-group plot.

1.2.2.12.2 Manganese: Five groups

This highlighted (in the form of the purple group) two restricted groups of low manganese, one of which was the area of B2 which had been flagged as an area of interest by the previous analyses. This area had also been low in calcium and magnesium.

1.2.2.12.3 Manganese: Seven groups

This further reinforced the groupings established by the five group run, showing the two low manganese groups (pink and red) in the same grid squares as before (Figure 7). Readings high in manganese (green and purple) were adjacent to each other but spread throughout the trench.

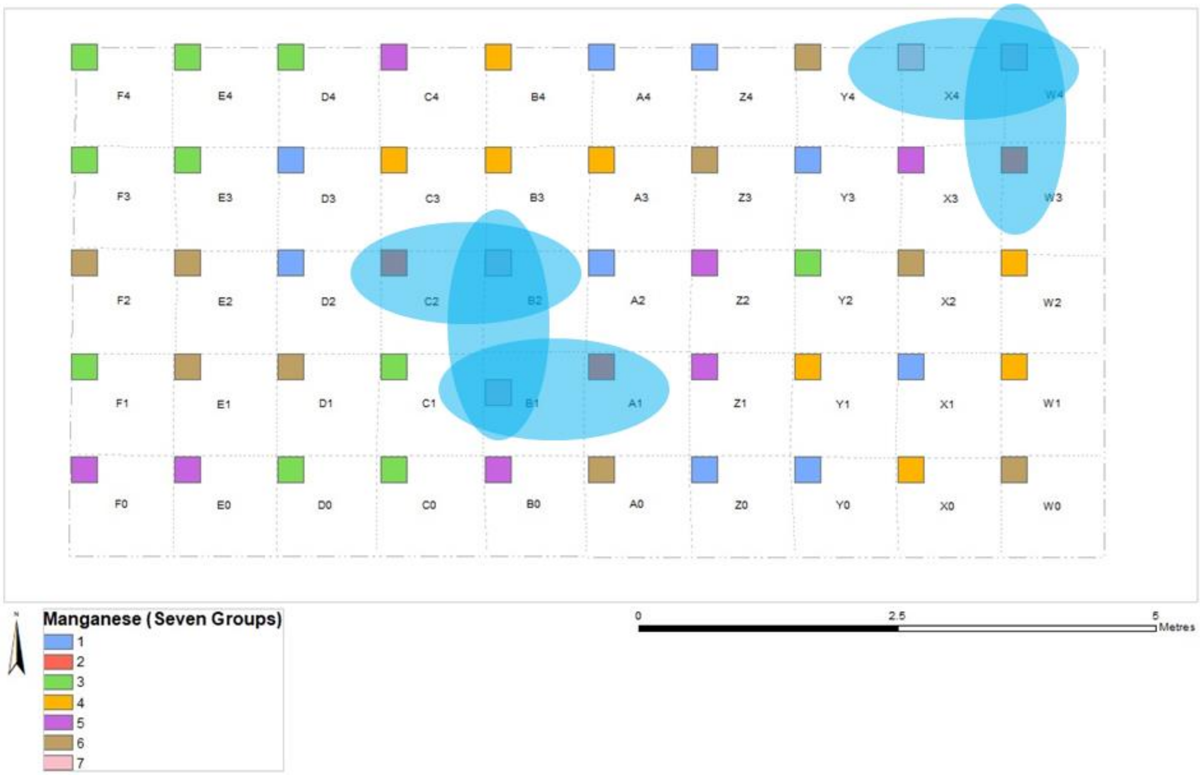


Figure 7. Key groupings based on manganese levels

1.2.2.13 Manganese: Complete record of repeat runs

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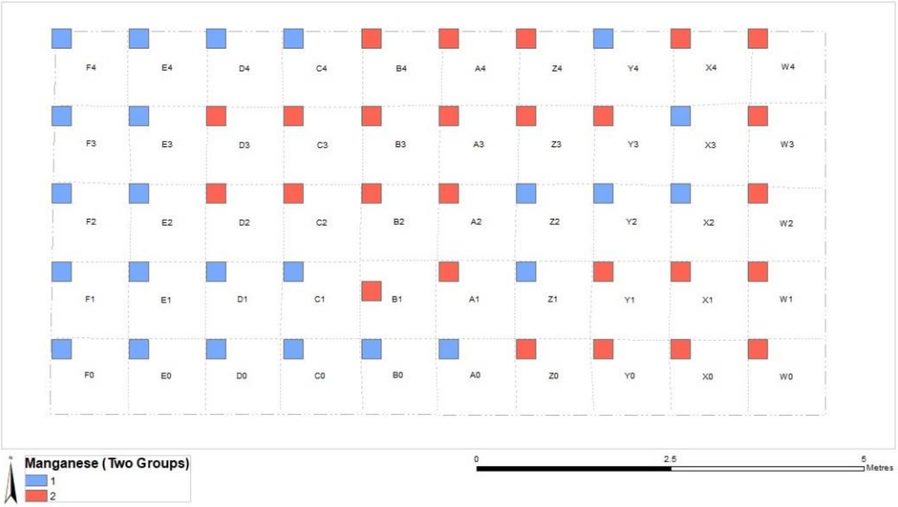	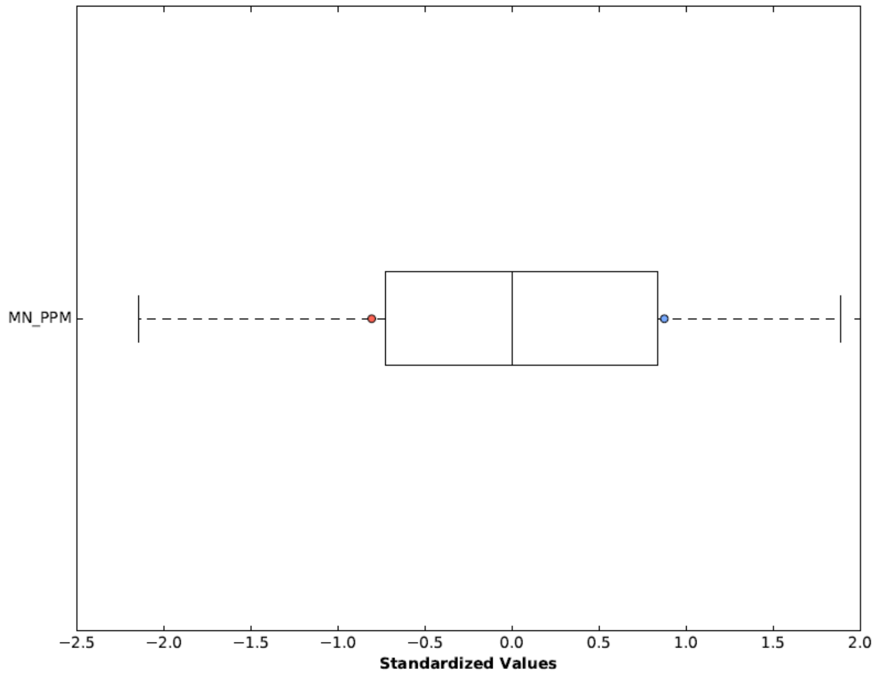 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.7056

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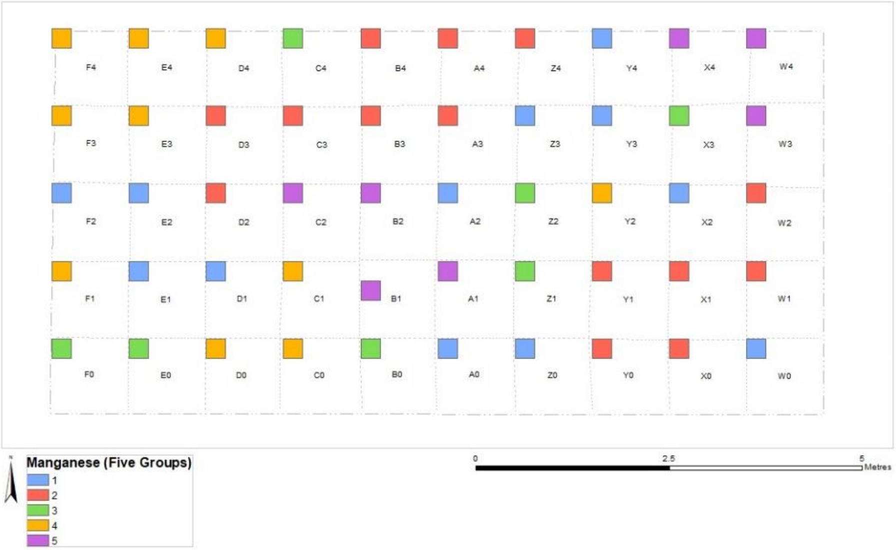

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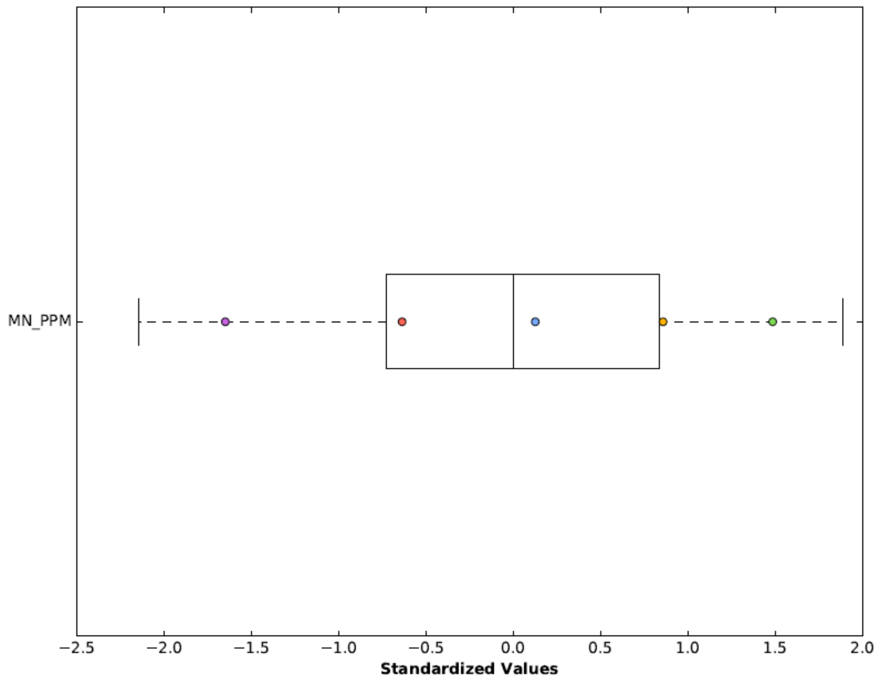

The R^2 statistic that suggests how good the variable is at differentiating these groups: 0.9546
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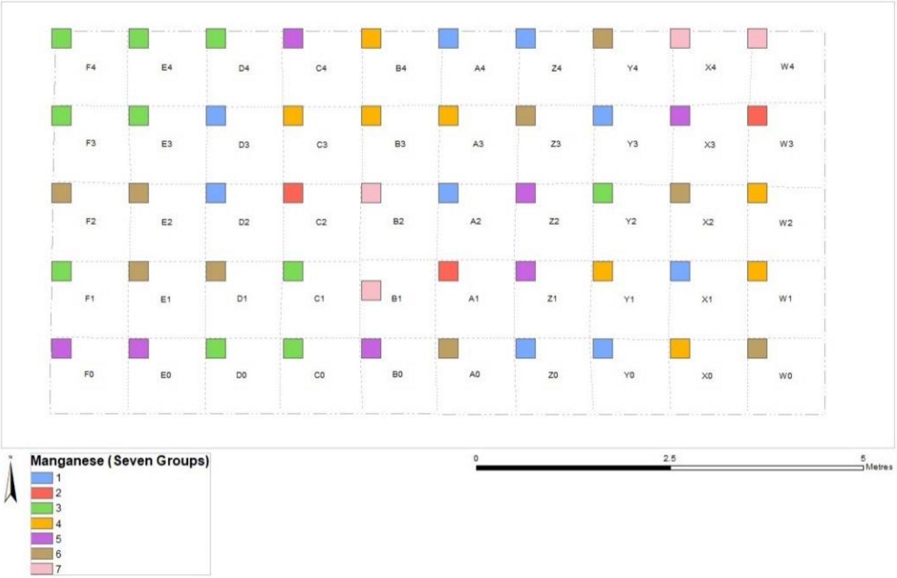
<tr><td>
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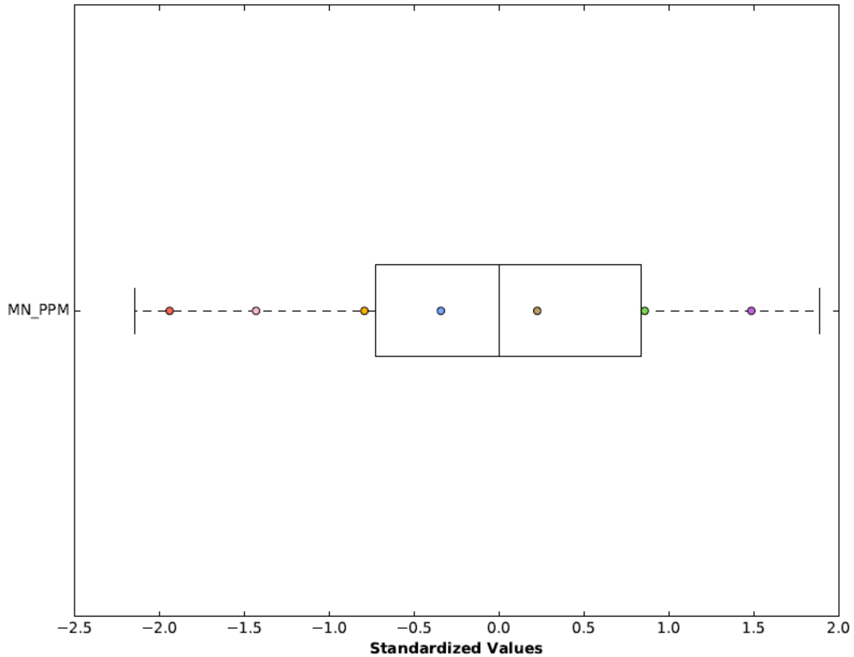
<td>

The R^2 statistic that suggests how good the variable is at differentiating these groups: 0.9769</td></tr>
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1.2.2.14 Phosphorus

1.2.2.14.1 Phosphorus: Two groups

The phosphorus two group run showed a clear distinction of a high phosphorus group in the southwest corner of trench 4.

1.2.2.14.2 Phosphorus: Five groups

The five group run showed the southwest area to be anomalously high in phosphorus, surrounded by values of the next highest phosphorus value group. Then there is an area of depleted samples in the region around B2, as had been for calcium, magnesium, and manganese as well as in the northeast corner as had been the case for manganese.

1.2.2.14.3 Phosphorus: Seven groups

The seven group run (Figure 8) further reaffirmed the five group run: Three isolated groups (blue, red, brown) formed the three highest phosphorus value samples and they were all in the southwest corner. In addition, the low phosphorus value group (green) was in the B2 area and northeast corner. The general regions of the trenches were generally slightly below average in the northeast quadrant of the trench, and gradually getting higher until in the region of the high values in the southwestern corner of the trench, i.e. the eastern end of the trench was generally lower in phosphorus than the western end.

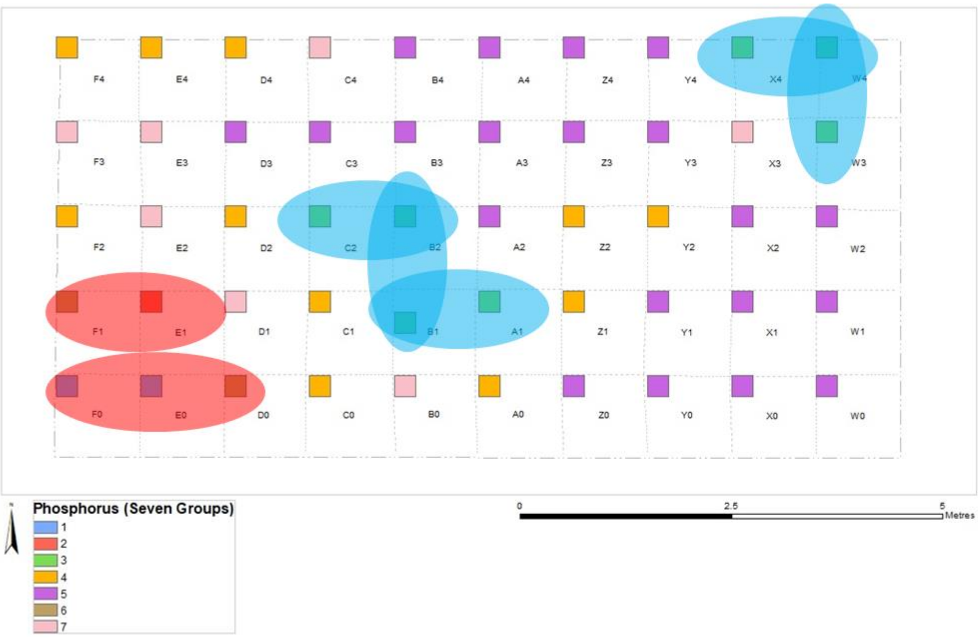

Figure 8. Key groupings based on phosphorus levels

1.2.2.15 Phosphorus: Complete record of repeat runs

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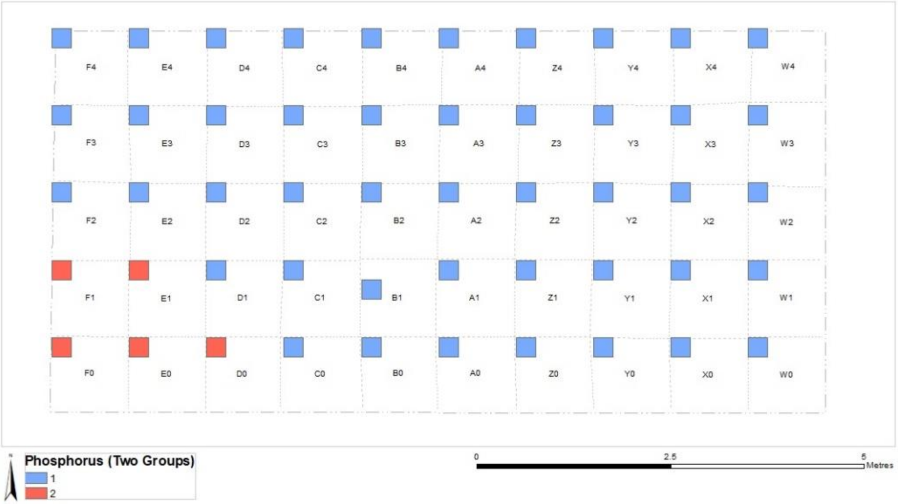	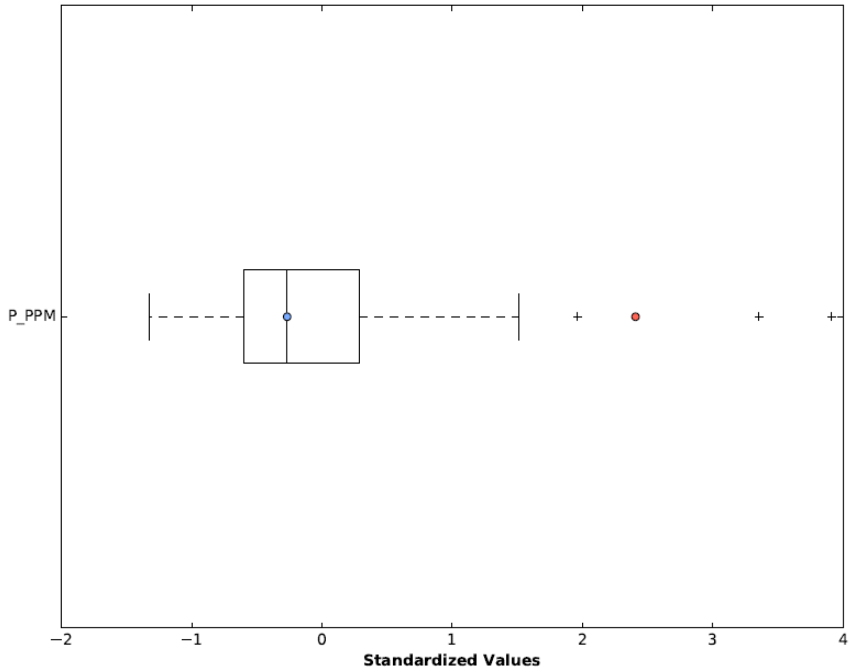 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.6435

<table>
<tr><th>Groups</th><th>Group Composition and Statistics</th></tr>
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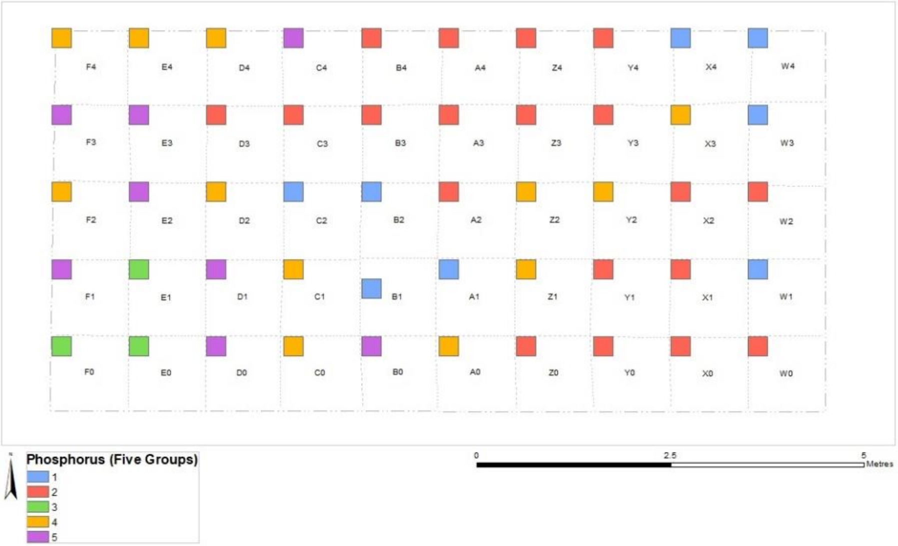

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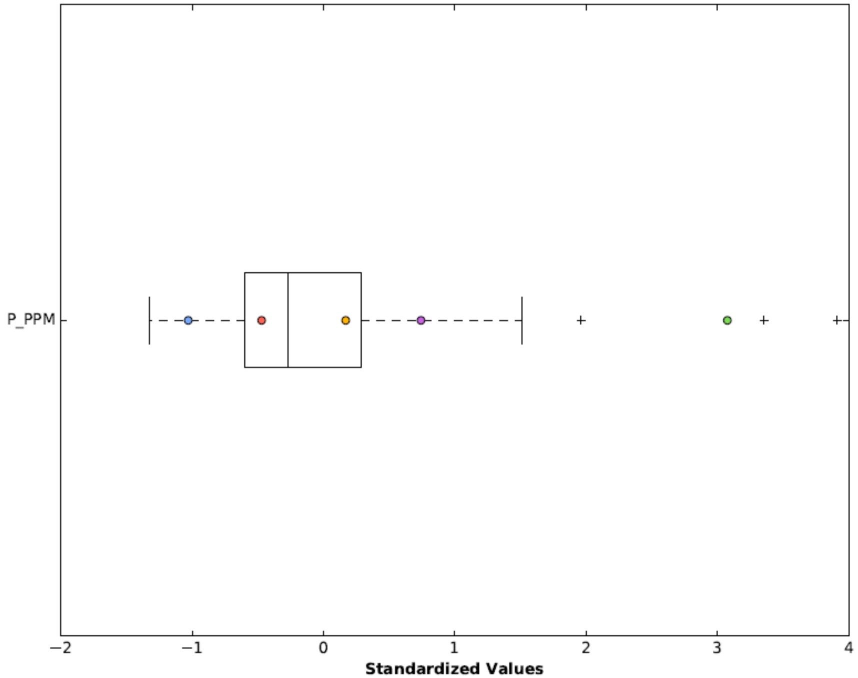

The R^2 statistic that suggests how good the variable is at differentiating these groups: 0.9164

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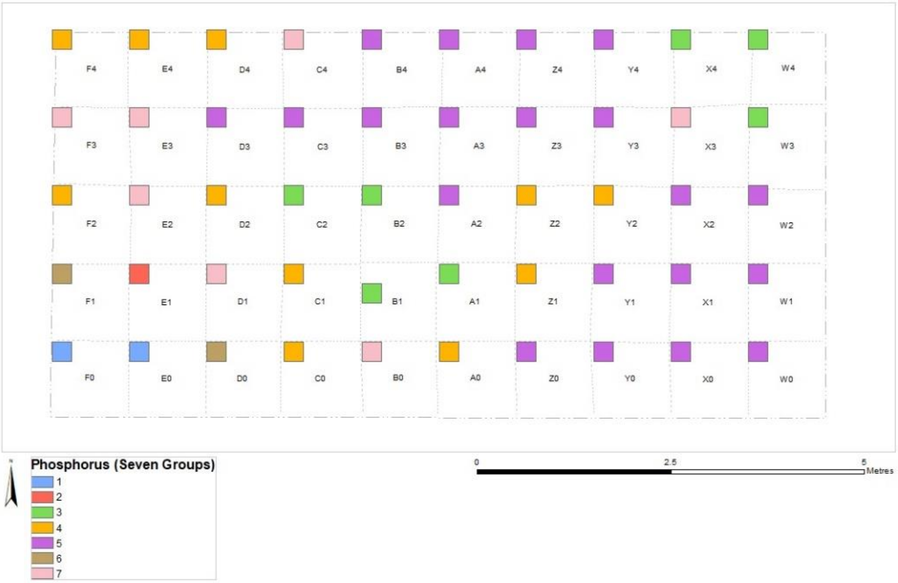
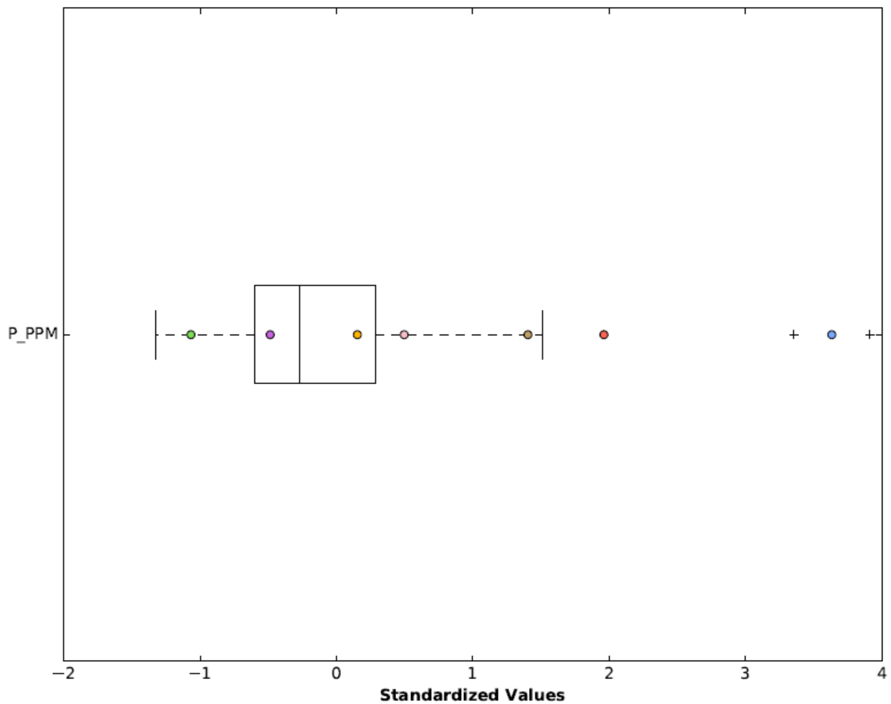
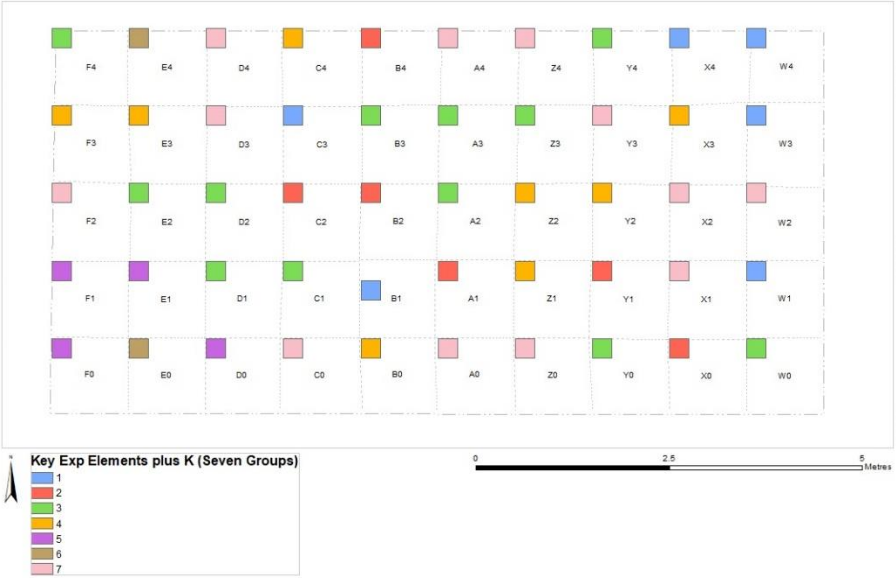
Groups	Group Composition and Statistics
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.9770

1.2.2.16 Major/Minor Elements Expanded Combined Model

The notes for this model are included as part of the main body of text (chapter seven).

A run was conducted with potassium added as a variable as well, as had been done at Star Carr, but this just resulted with a grouping being dedicated to the two samples that had different readings of potassium to all the other samples which were all the same (lower) value as had been identified in the exploratory analysis of just this element. It was not run as an individual variable through grouping analysis for this reason but it may have corresponded with other patterning in some way when combined with other variables so it was incorporated in the combination model. It had no effect on the general identification of the areas of interest (which still flagged up around grid square B2 and the southwest and northeastern corners of the trench).

1.2.2.16.1 Major and minor elements expanded including potassium

<table>
<tr><th>Groups</th><th>Group Composition and Statistics</th></tr>
<tr><td>


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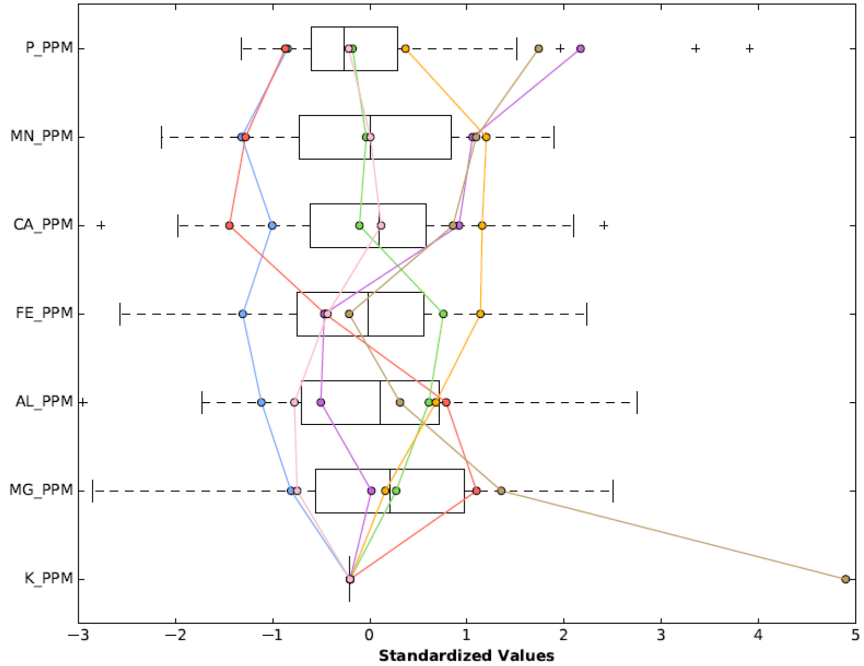
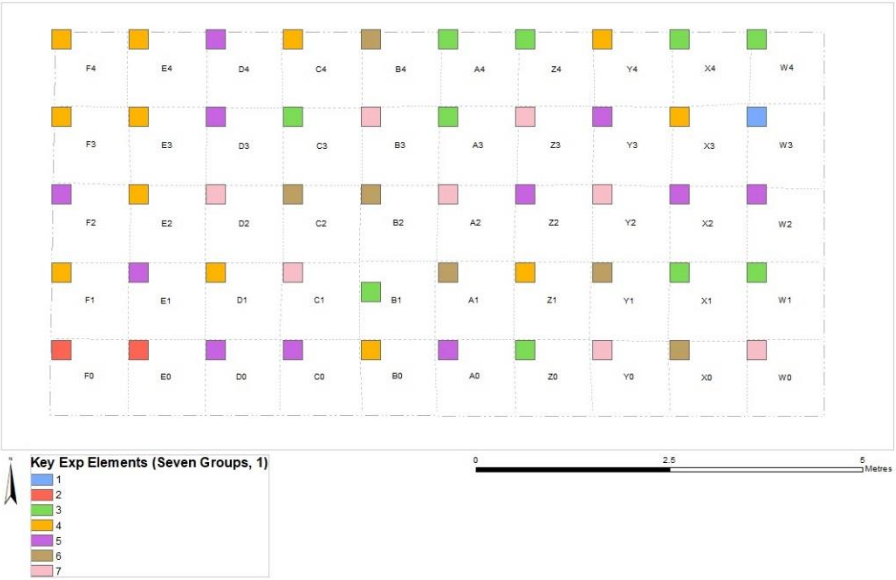


Optimal number of groups (based on highest pseudo F-Statistic): 5

The R^2 statistic that suggests how good the variable is at differentiating these groups: K: 1.0; Mn: 0.7736; P: 0.7153; Ca: 0.6889; Fe: 0.6411; Al: 0.5555; Mg: 0.4533
</td></tr>
</table>

1.2.2.16.2 Major and minor elements expanded excluding potassium

<table>
<tr><th>Groups</th><th>Group Composition and Statistics</th></tr>
<tr><td>



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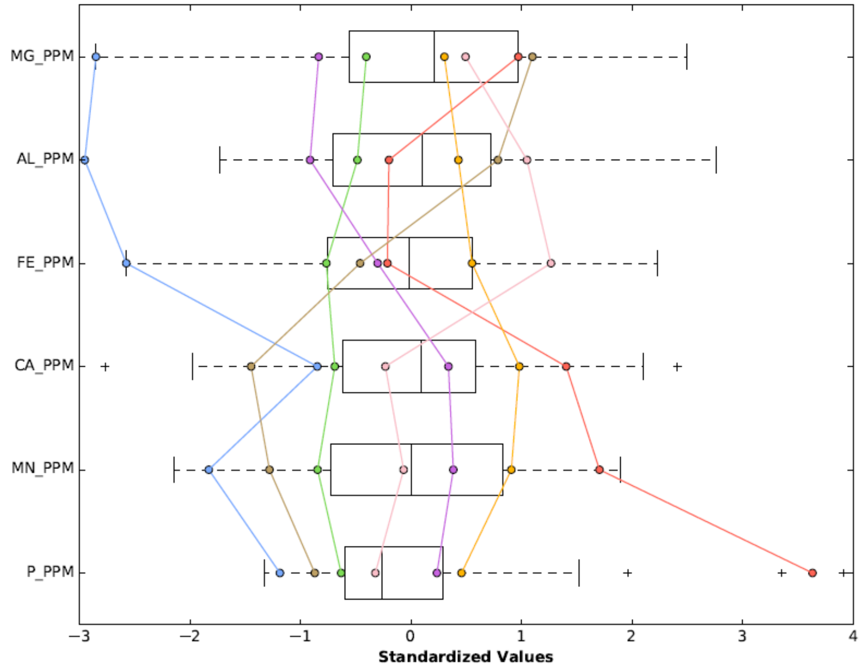
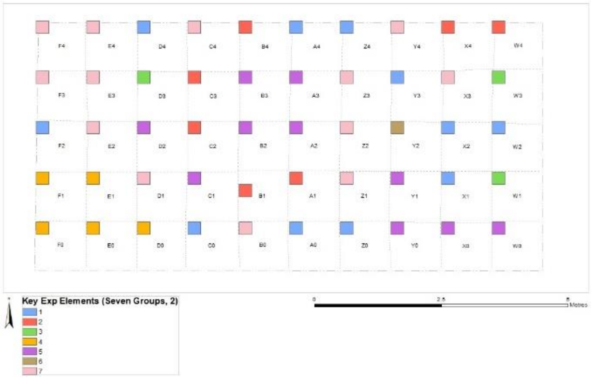
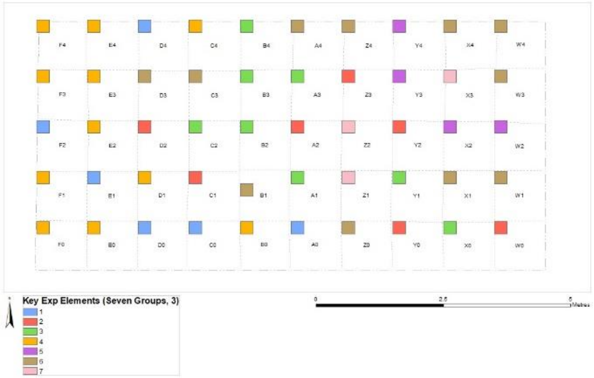
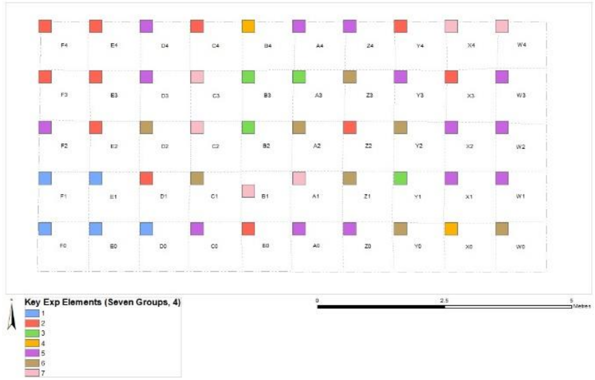
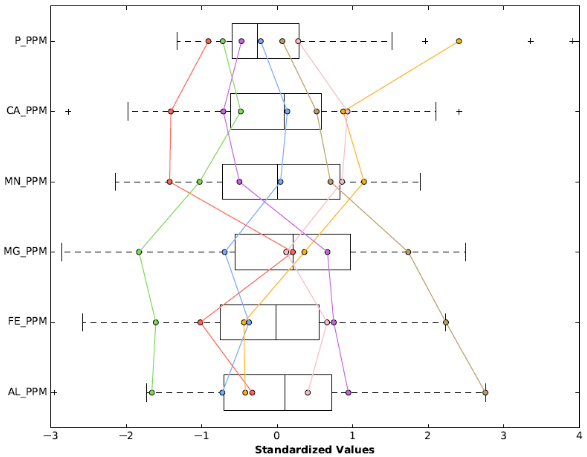
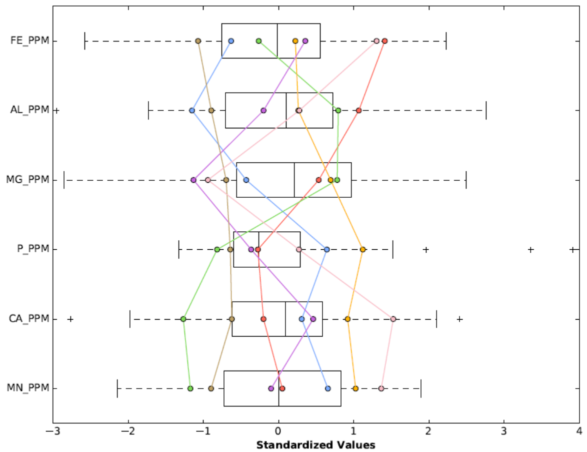
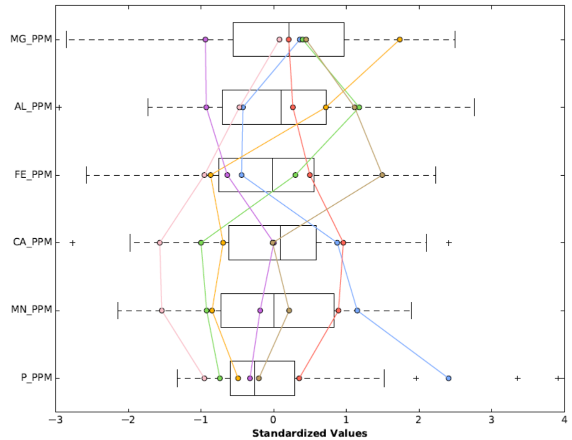


Optimal number of groups (based on highest pseudo F-Statistic): 3

The R^2 statistic that suggests how good the variable is at differentiating these groups: P: 0.8056; Mn: 0.7535; Ca: 0.7039; Al: 0.7007; Fe: 0.6272; Mg: 0.5921

</td></tr>
</table>

Repeat 2	**Repeat 3**	**Repeat 4**
		
		

1.3 Analysis of Trenches 11, 12(N), and 15 Field pXRF Results (from 2014 excavations)

1.3.1 Planning the analysis

It was demonstrated in chapter six that silicon, aluminium and iron were the major elemental contributors to the samples as measured by pXRF in the field, with calcium, potassium, and titanium as minor contributors. Measured trace elements included sulfur, zirconium, phosphorus, vanadium, manganese, chromium, strontium, zinc, rubidium, tantalum, cadmium, yttrium, silver, nickel, thorium, lead, niobium, copper, mercury, molybdenum, bismuth, arsenic, and uranium. Chlorine had one reading that would have classified it as a minor contributor, but it was suspected this was an anomaly from contamination or otherwise and therefore here it is treated as a trace element. As with the ICP-AES results from trench 4, GA would initially be run on the major/minor contributors individually initially and then combined.

In developing the model for the ICP-AES data, two group runs were of assistance in demonstrating whether there was any obvious immediate enhancements or depletions that overcame the natural variances in the elements across the trench. Three groups usually isolated areas of potential activity even when there was no clear pattern that overcame natural variation in the elements in the two group run, but it did not allow for identification of anomalies. Five and seven groups were usually most helpful in identifying key patterns with the additional flexibility allowing anomalies to be drawn out. Fifteen groups were often very complicated and while identifying a lot of nuances in the data, were not particularly helpful as they overcomplicated key trends that might potentially be of interest, for example you might get three groups formed because they were all very enhanced in one element, just to different degrees but specifying the high number of groups forced an unnatural split. In addition to this, evaluating the optimal number of groups was not fruitful for individual elements because the tool had too little to base the groups on. This was only worth consideration for the multi-elemental analysis and at that stage the number of groups was usually within the ranges already covered by the repeat runs. As the incorporation of selected other elements based on the work at Star Carr had successfully complemented the results from the ICP-AES at Flixton 2, it was decided to expand to include those elements reading as trace elements in the pXRF as well. The combination model would immediately incorporate these rather than it being segregated.

As such, with the Flixton Field pXRF results a slightly different approach was adopted. By Sturge's Rule, $C = 1 + (3.3 \log (345)) = 9.3748$ and therefore 9 groups are suggested using this rule. It was decided that grouping analyses would therefore be run on the major/minor elements individually for just two and five groups, to provide a general impression. Optimal groups would not be run. Then for the combined model, four repeat runs of two, five, and nine groupings would be run.

1.3.2 Major and Minor Element Grouping Patterns

1.3.2.1 Silicon

1.3.2.1.1 Silicon: Two groups

Generally, trenches 11 and 12(N) were higher in silicon than trench 15. The southern end of both trenches, particularly trench 11 had lower values, however. The opposite was seen in trench 15, with only areas around grid squares I-4 and I-5 being in the higher group.

1.3.2.1.2 Silicon: Five groups

Increasing the groupings to five gave a complicated picture (Figure 9). A pocket of readings grouped into the particularly low silicon group was in the base of trench 11. There were two pockets of high readings in the centre and north of that trench. In trench 12(N), a similar pattern is seen with the southern end being in the lower silicon groups, but there being a pocket of higher readings in the centre of the trench. In trench 15, generally readings are slightly or moderately depleted in silicon, but there is a pocket in the south of the trench around H-5 that had samples assigned to the highest silicon groupings. The possible feature grid squares were assigned to mixed grids.

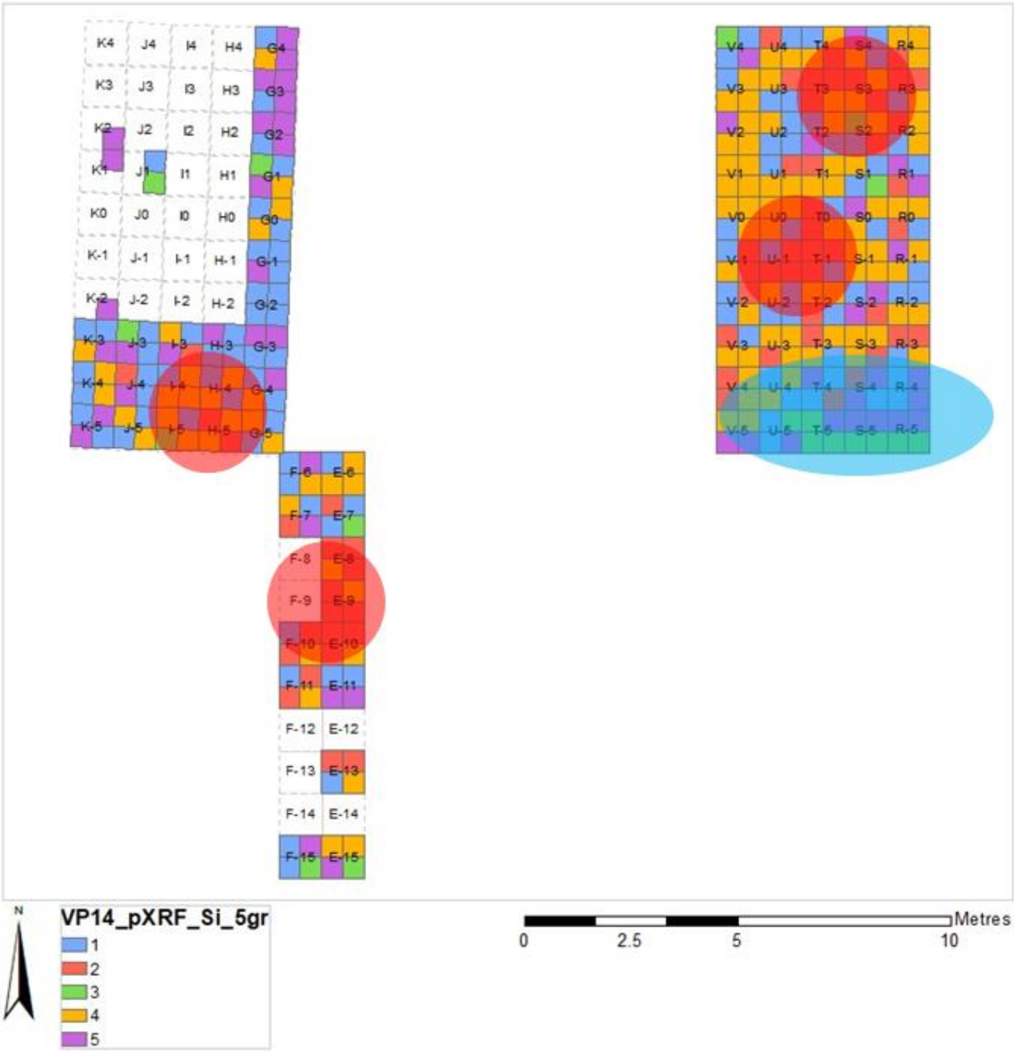
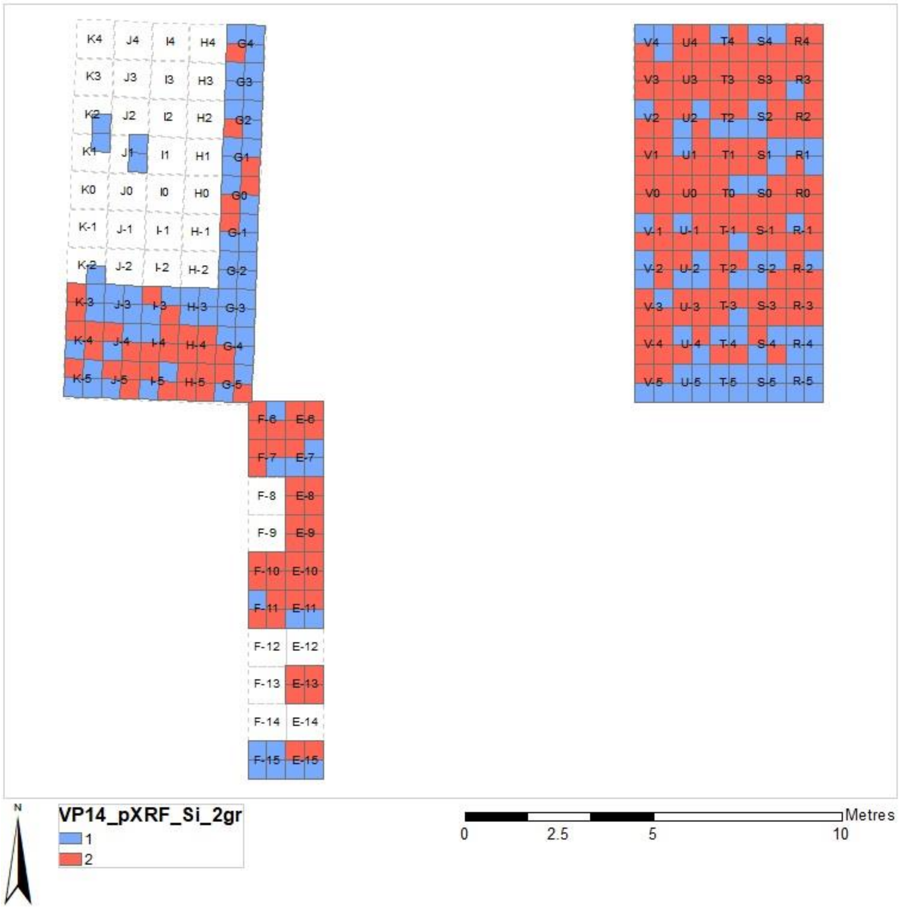
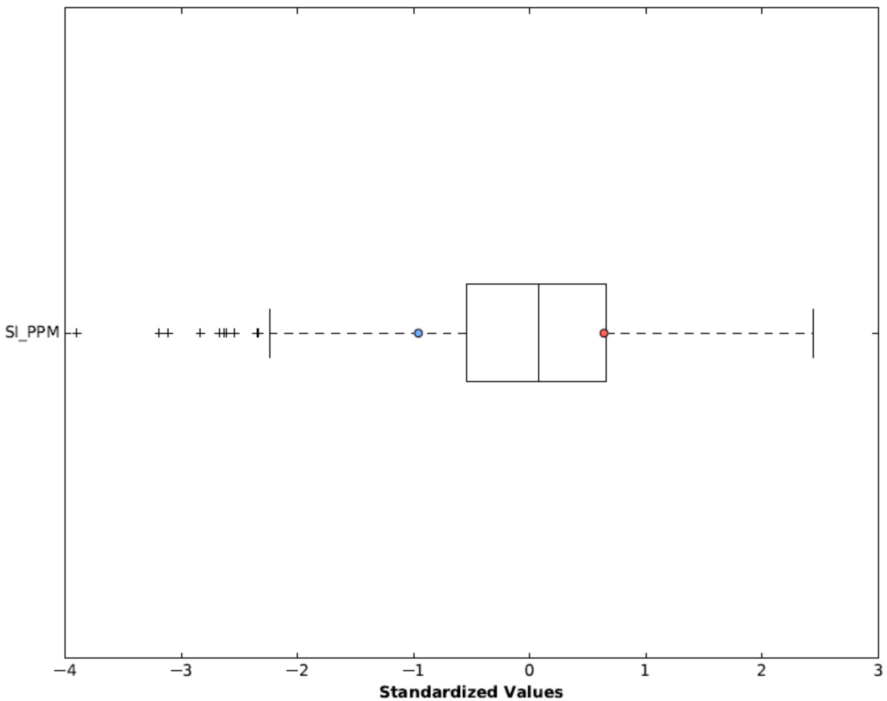
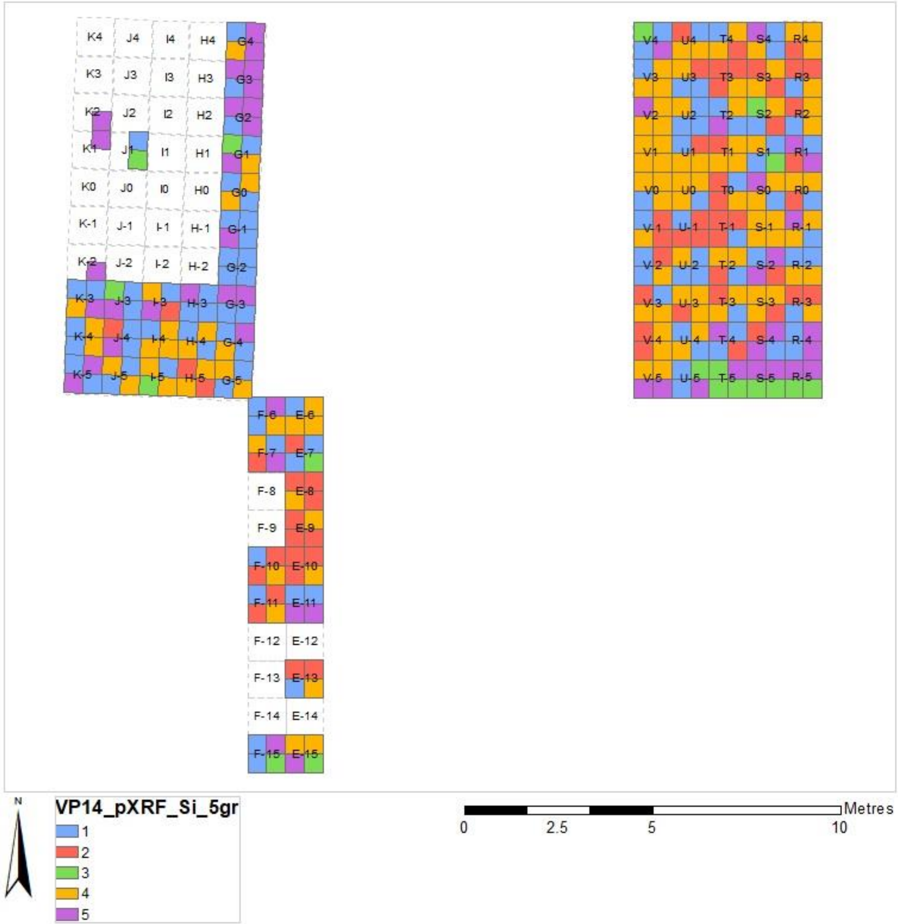
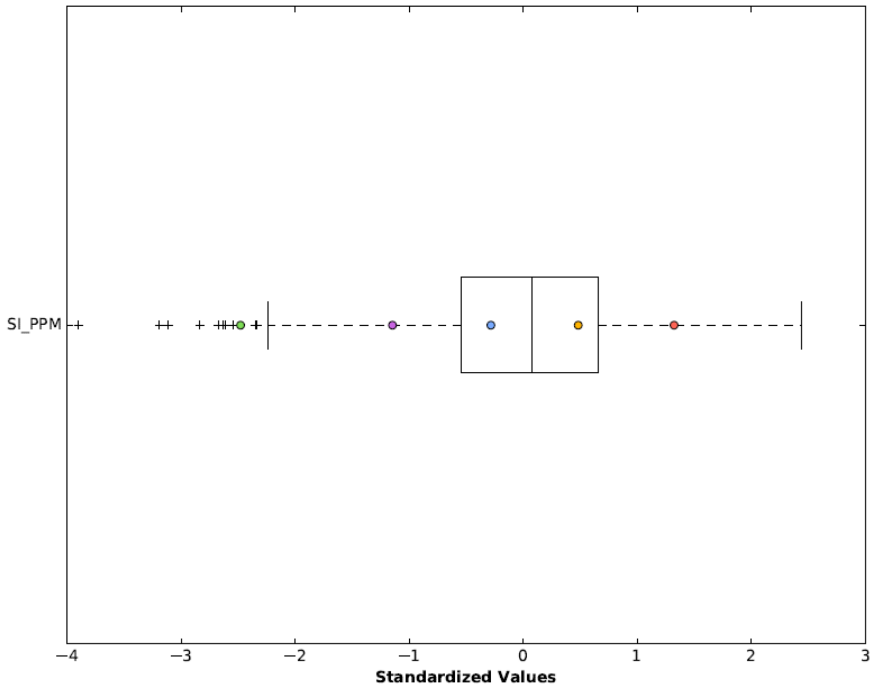


Figure 9. Summary of the key patterns in the silicon readings

1.3.2.2 Silicon: Complete Record

Groups	**Group Composition and Statistics**
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.6129

Groups	Group Composition and Statistics
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.9264

1.3.2.3 Aluminium

1.3.2.3.1 Aluminium: Two groups

Trench 11 is generally lower in aluminium in the south and higher in the north. Most of trench 12(N) is lower in aluminium. Trench 15 is generally higher in aluminium with no patterning to the samples grouped in the lower (red) group.

1.3.2.3.2 Aluminium: Five groups

The lowest aluminium grouped samples (red) tend to be clustered at the southern end of trench 11 and perhaps a little to the north of that (Figure 10). There are a lot of samples in the highest aluminium grouping (yellow) possibly at the southern end of trench 15 around I-5 and H-5 again, but there is one red sample there also. There are other yellow samples throughout trench 15 but none in trench 11. The signal from trench 12(N) is mixed, as is that from the separate feature grid squares in the northwest of trench 15.

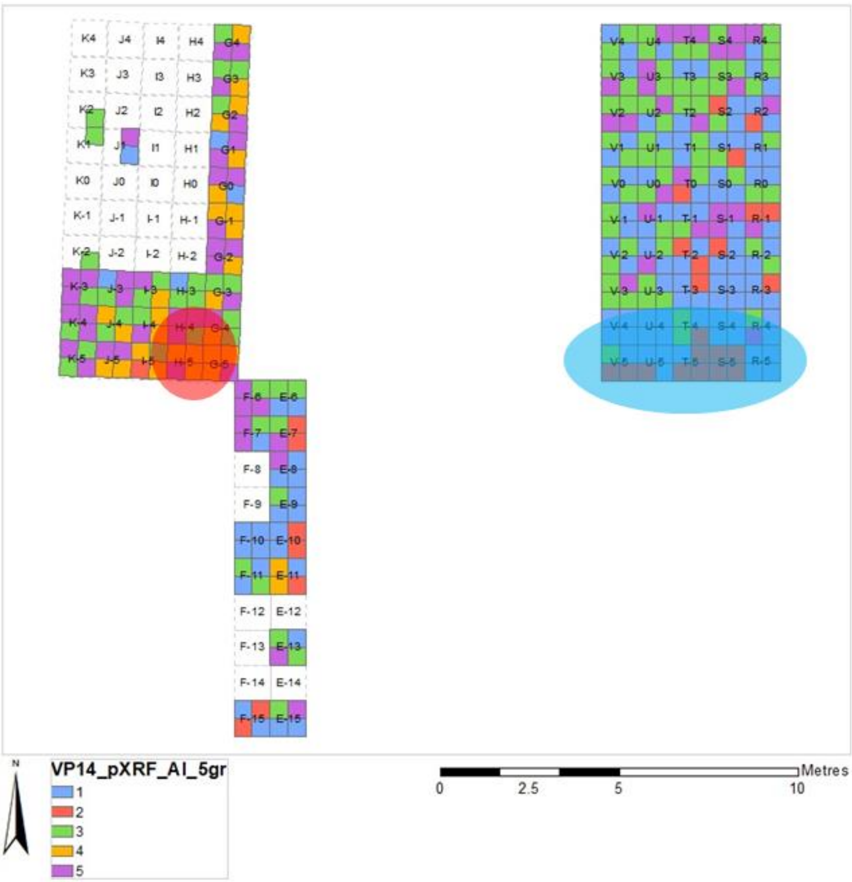
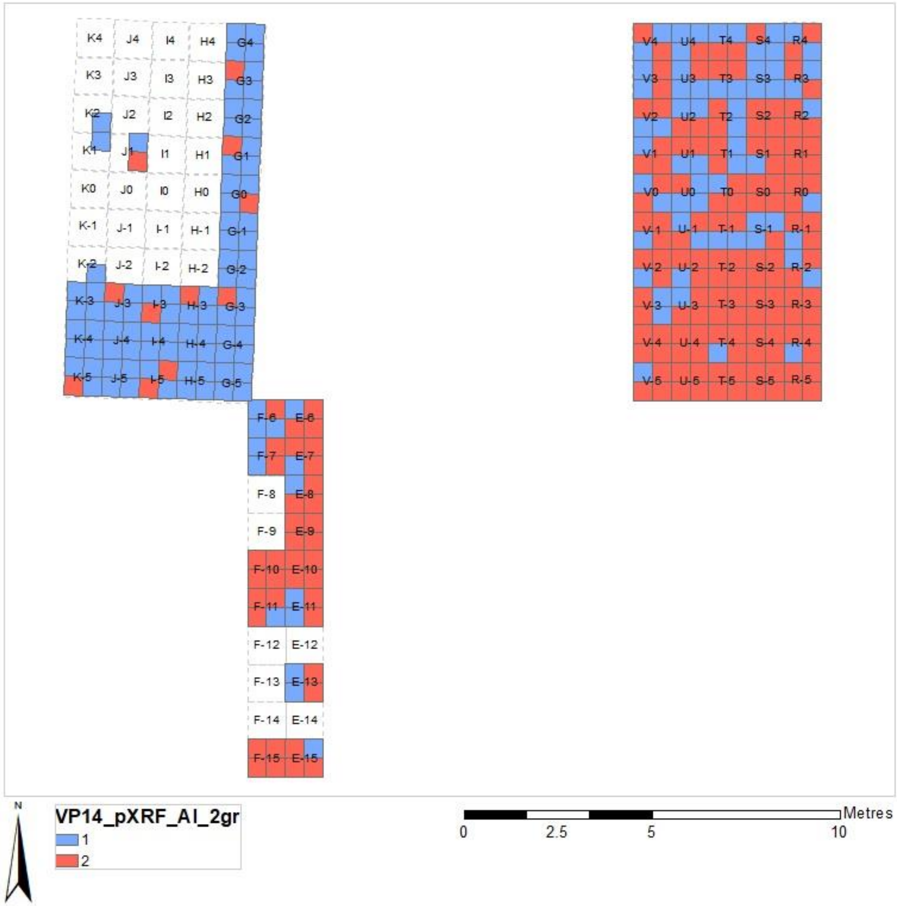
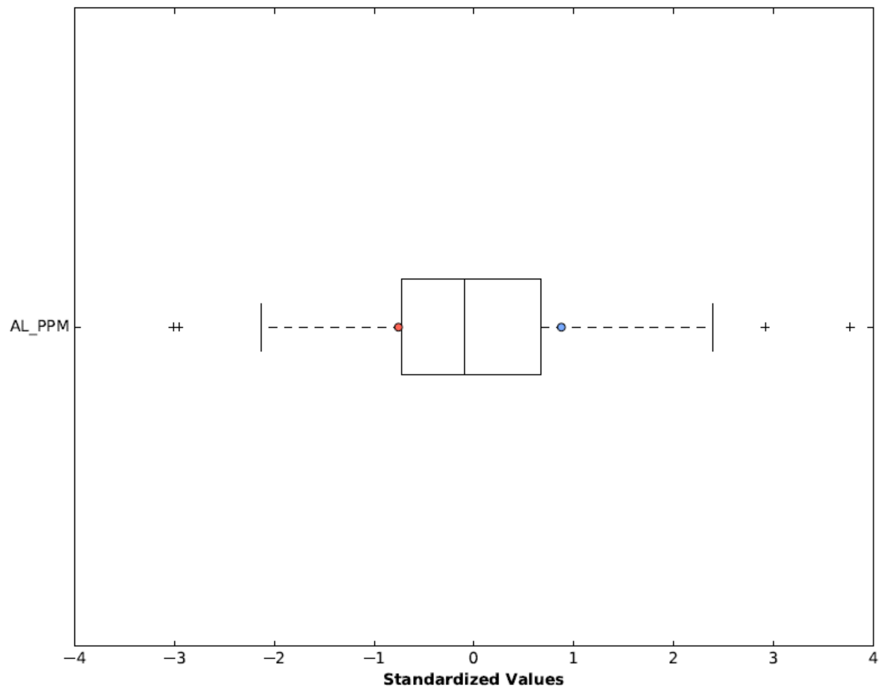
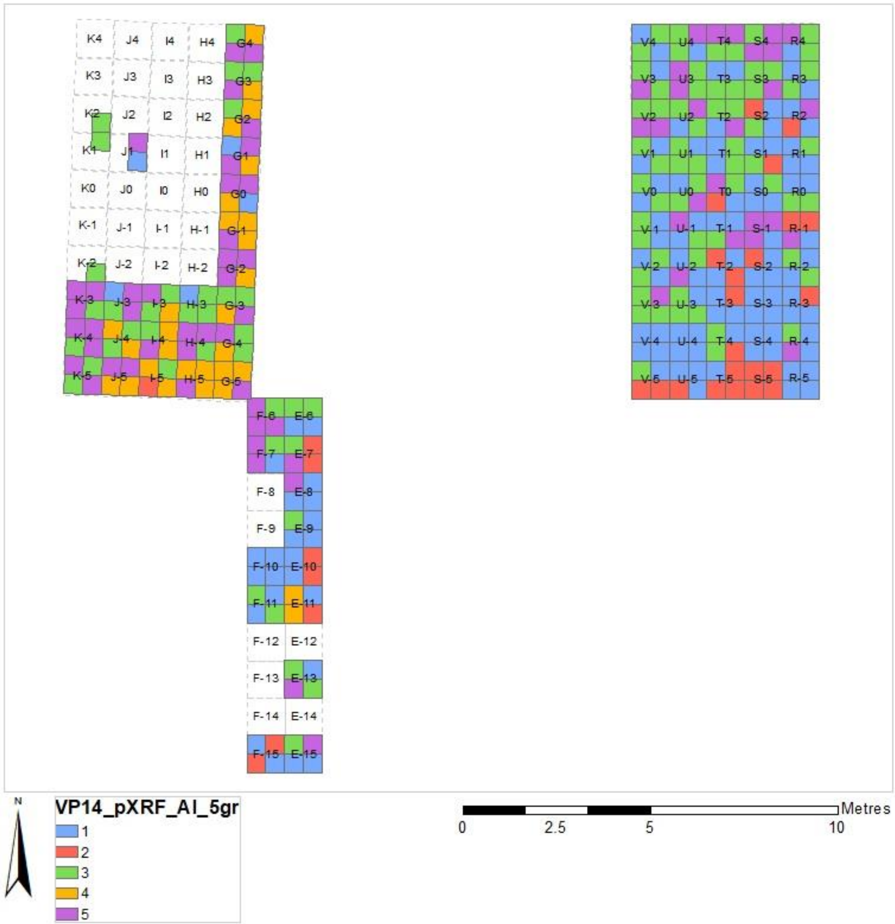
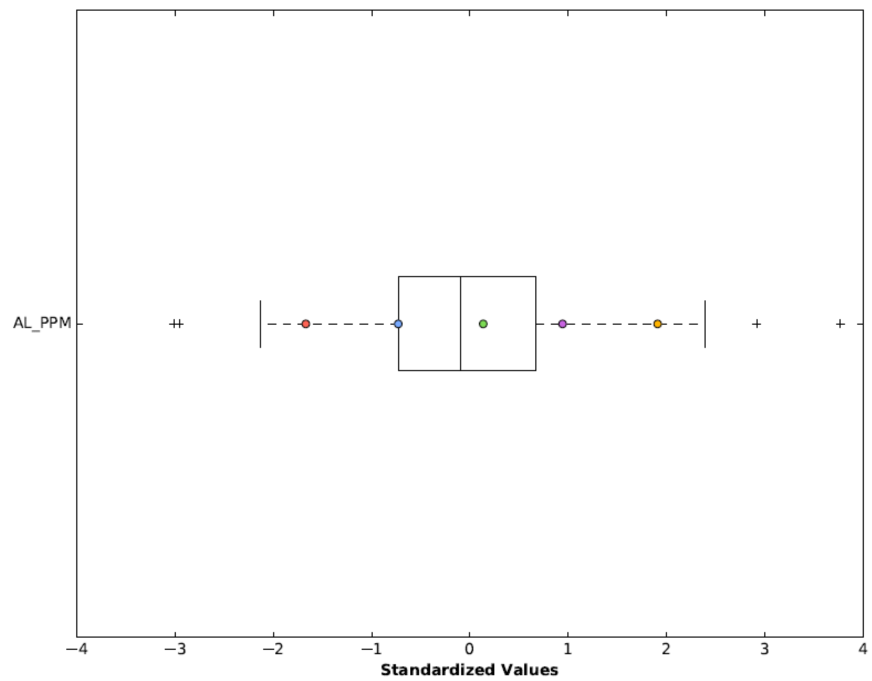


Figure 10. Summary of the key patterns in aluminium

1.3.2.4 Aluminium: Complete Record

Groups	**Group Composition and Statistics**
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.6627

Groups	Group Composition and Statistics
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.9137

1.3.2.5 Iron

1.3.2.5.1 Iron: Two groups

The southeast corner of trench 11 is generally part of the lower iron (red) group, while the northern half is more mixed. Most of trench 12(N) is in the low iron group. There is also an area of lower iron in the end of trench 15, though this trench is generally also mixed.

1.3.2.5.2 Iron: Five groups

Most of the lowest iron group samples (yellow) are in the southern end of trench 11, particularly towards the southeast corner Figure 11. In contrast, there is a pocket of highest iron group samples around U-2 in the middle of an area with many yellow samples. The other two trenches are generally mixed but with higher iron levels, perhaps in the vicinity of J-5 and I-5 in trench 15 and in the middle of trench 12(N). The feature grid squares in the north of trench 15 were average or moderately enhanced in iron.

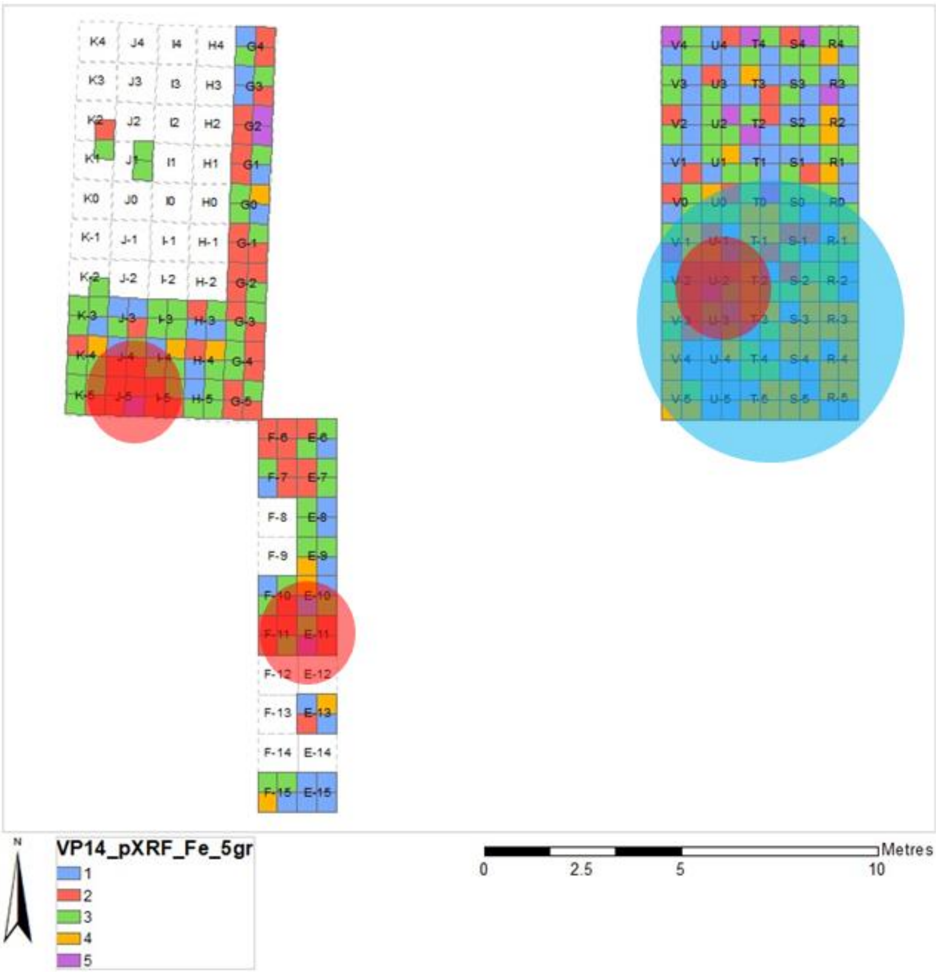


Figure 11. Key patterns in iron groupings

1.3.2.6 Iron: Complete Record

<table>
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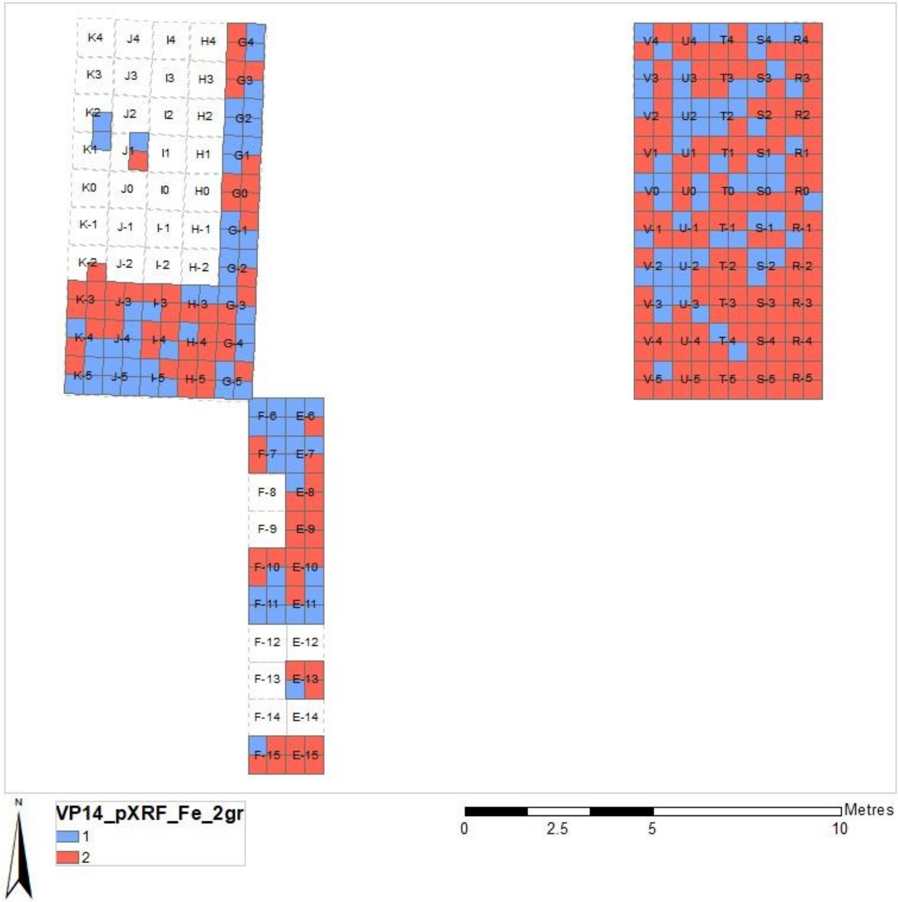

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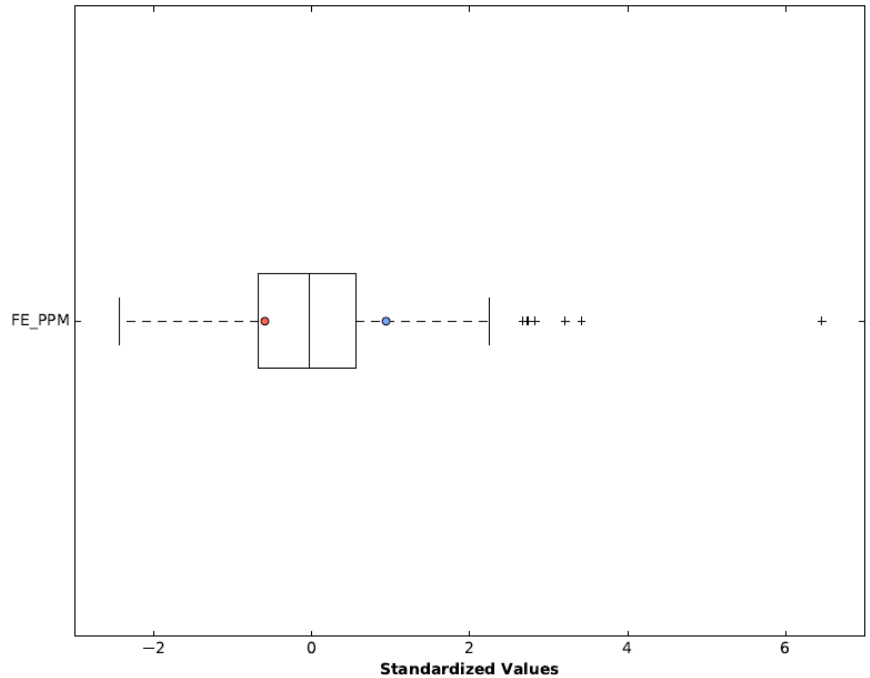

The R^2 statistic that suggests how good the variable is at differentiating these groups: 0.5599
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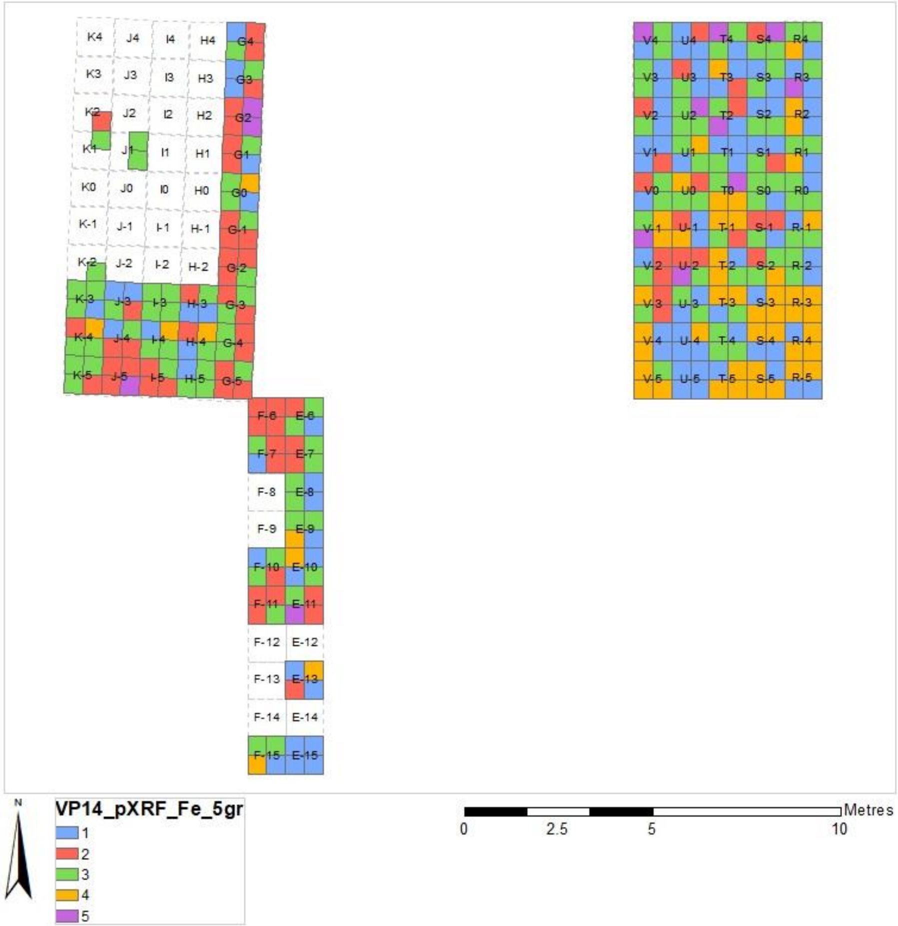

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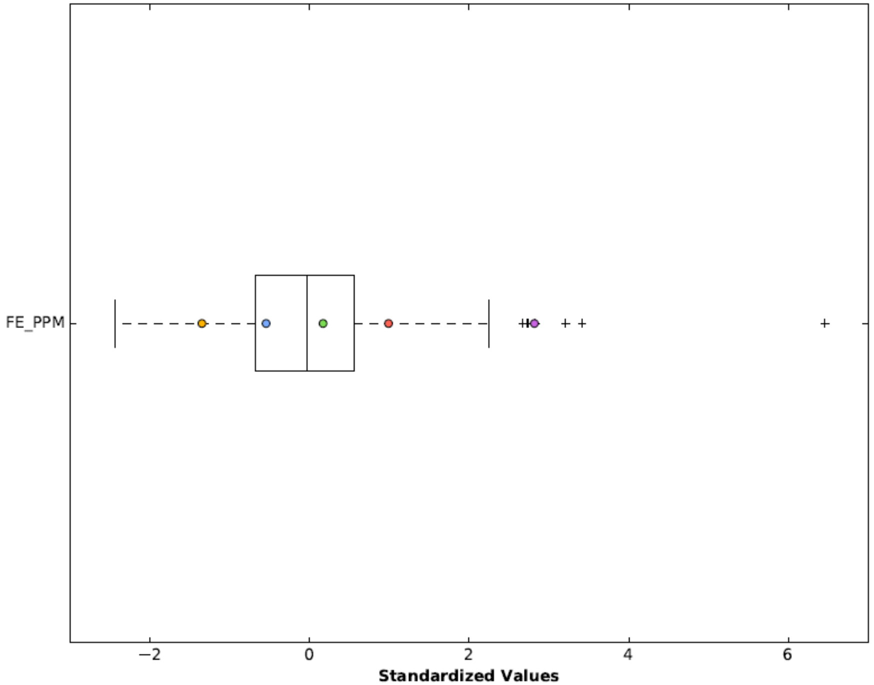

The R^2 statistic that suggests how good the variable is at differentiating these groups: 0.8811
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</table>

1.3.2.7 Calcium

1.3.2.7.1 Calcium: Two groups

All trenches were quite mixed. The southeastern corner of trench 11 was generally in the higher calcium group (blue), as was the southwestern corner of trench 15 in the approximate vicinity of K-3/K-4/J-4. Trench 12(N) was generally mixed although there were two possible pockets of higher calcium readings around grid squares E-8 and in the southern end of the trench in grid squares F-15 and E-15.

1.3.2.7.2 Calcium: Five groups

In trench 11, the southeast corner samples were assigned to the second highest calcium group (green), although none fell into the high calcium outlier group (yellow). In addition, diagonally across the centre of the trench there was a general spread of the lowest calcium group (red) samples. Trench 12(N) was generally mixed of average or slightly enhanced/depleted values, with occasional high group values from the yellow outlier group. Trench 15 seemed to have an area of high calcium grouped values (yellow, green, mixed with average and slightly depleted) in the vicinity of J-4. The rest of that trench was a mix but with many of the lowest calcium group values (red). The features in trench 15 were from a mix of groups.

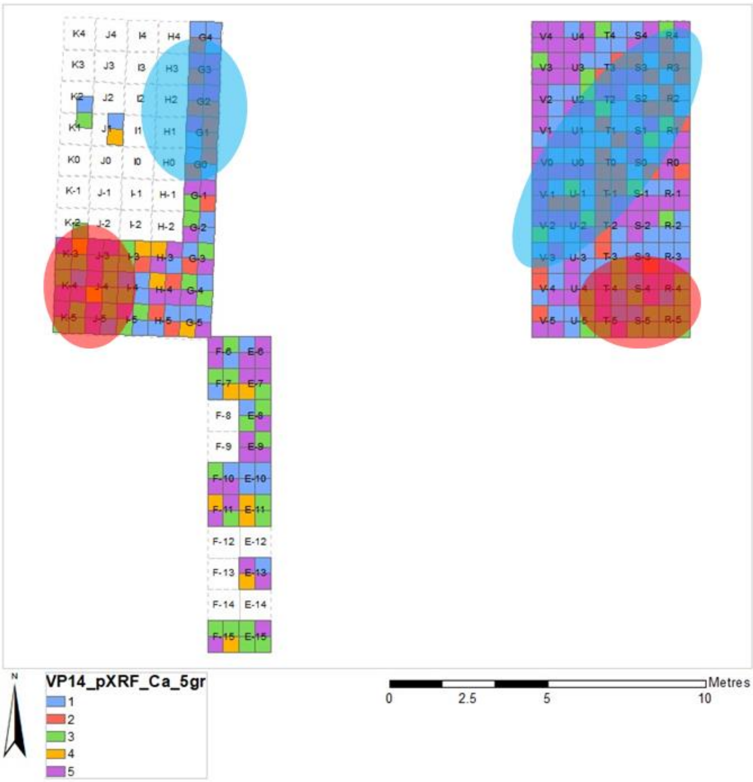
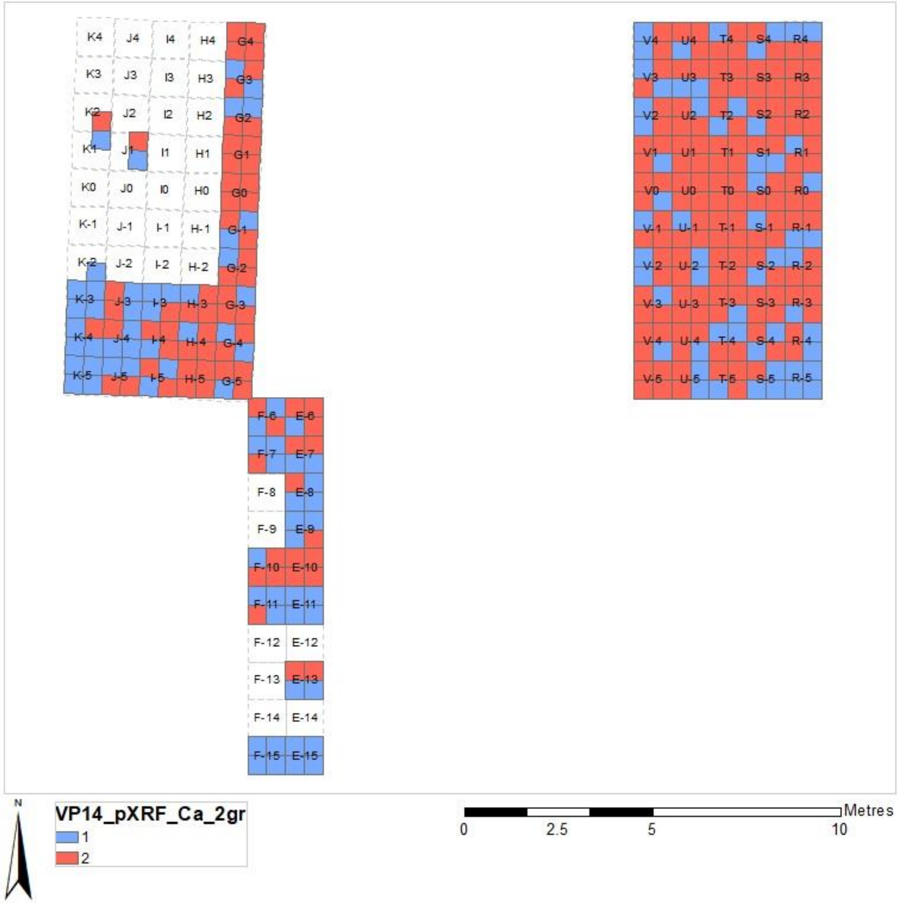
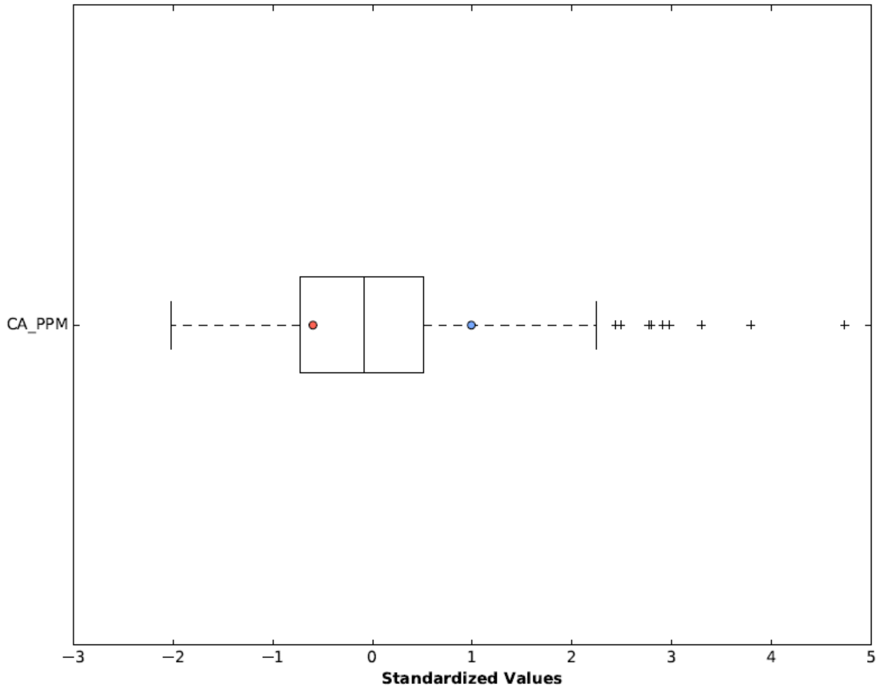


Figure 12. The key patterns in the groupings based on calcium

1.3.2.8 Calcium: Complete Record

Groups	Group Composition and Statistics
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.5929

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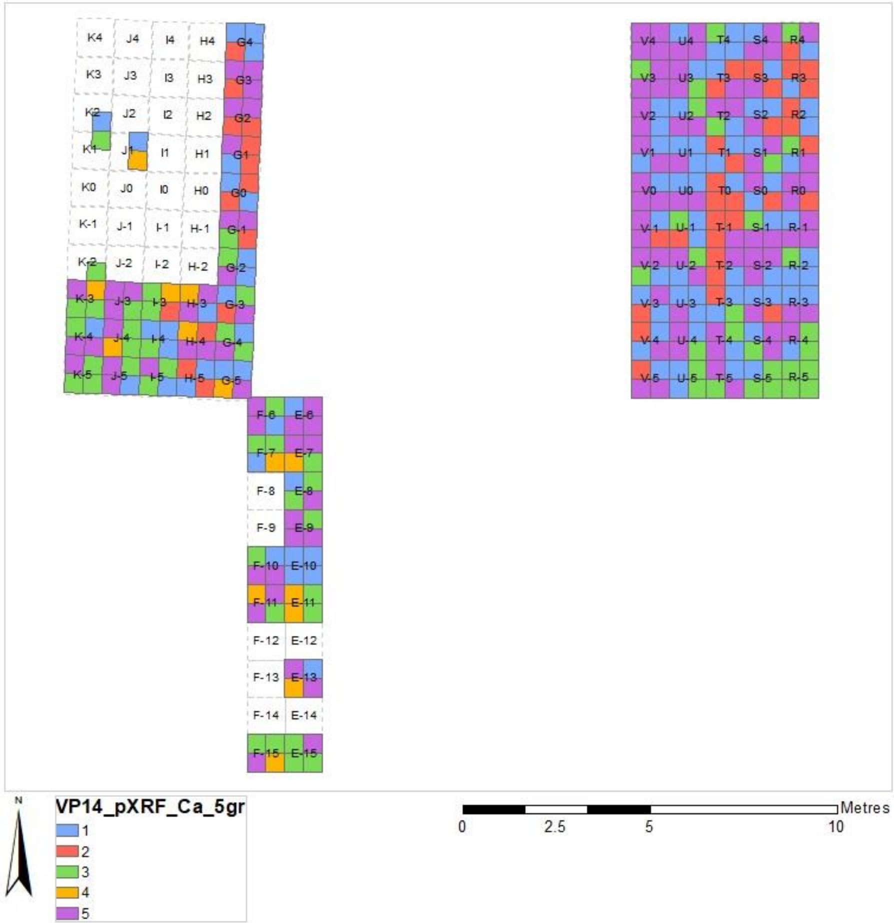

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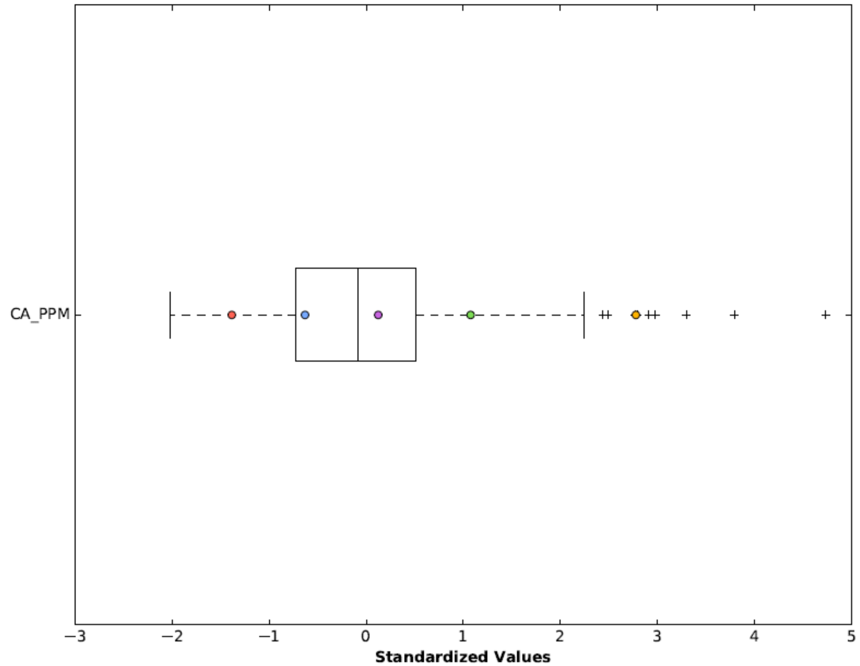


The R^2 statistic that suggests how good the variable is at differentiating these groups: 0.9096
</td></tr>
</table>

1.3.2.9 Potassium

1.3.2.9.1 Potassium: Two groups

All trenches were mixed although trench 15 had mostly higher potassium group samples (red), while trenches 11 and 12(N) were mostly lower potassium.

1.3.2.9.2 Potassium: Five groups

The high potassium anomaly group (yellow) was only three samples that were scattered in trenches 11 and 15 (Figure 13). There were two areas of slightly greater density of the lowest potassium group samples (purple) in the southeast of trench 11, and the middle of trench 12(N) around grid square E-9, but these were not very distinct and still quite mixed. The features were mixed again as well.

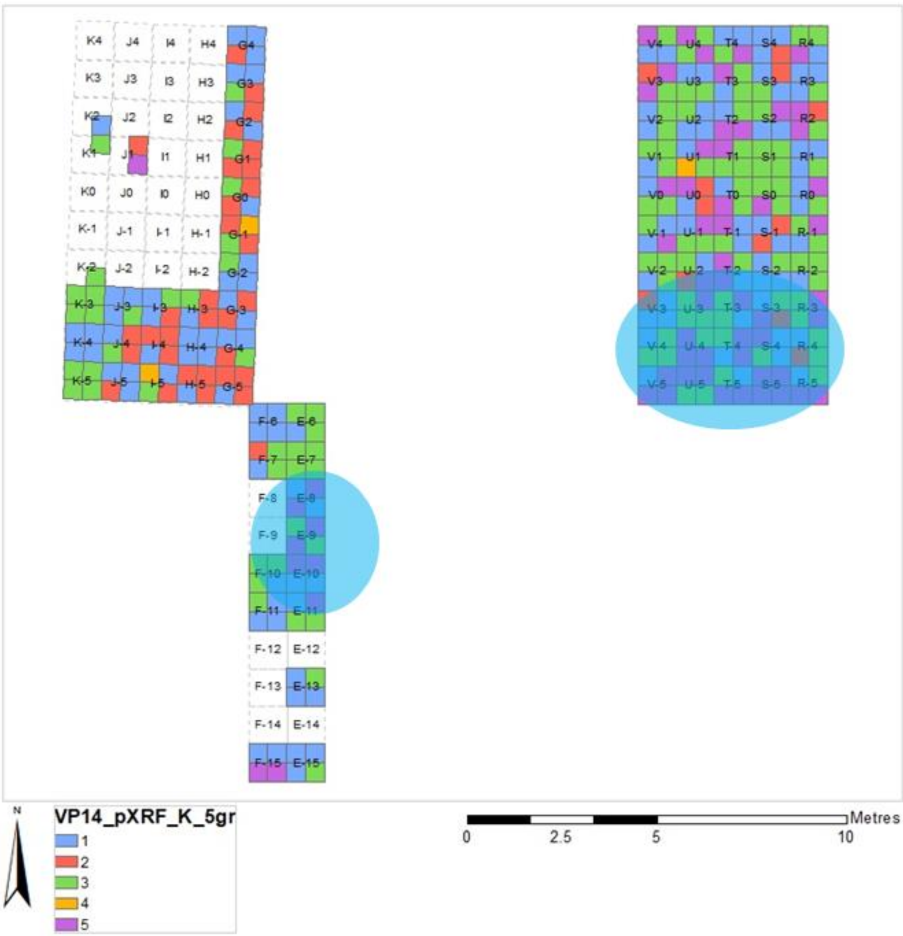
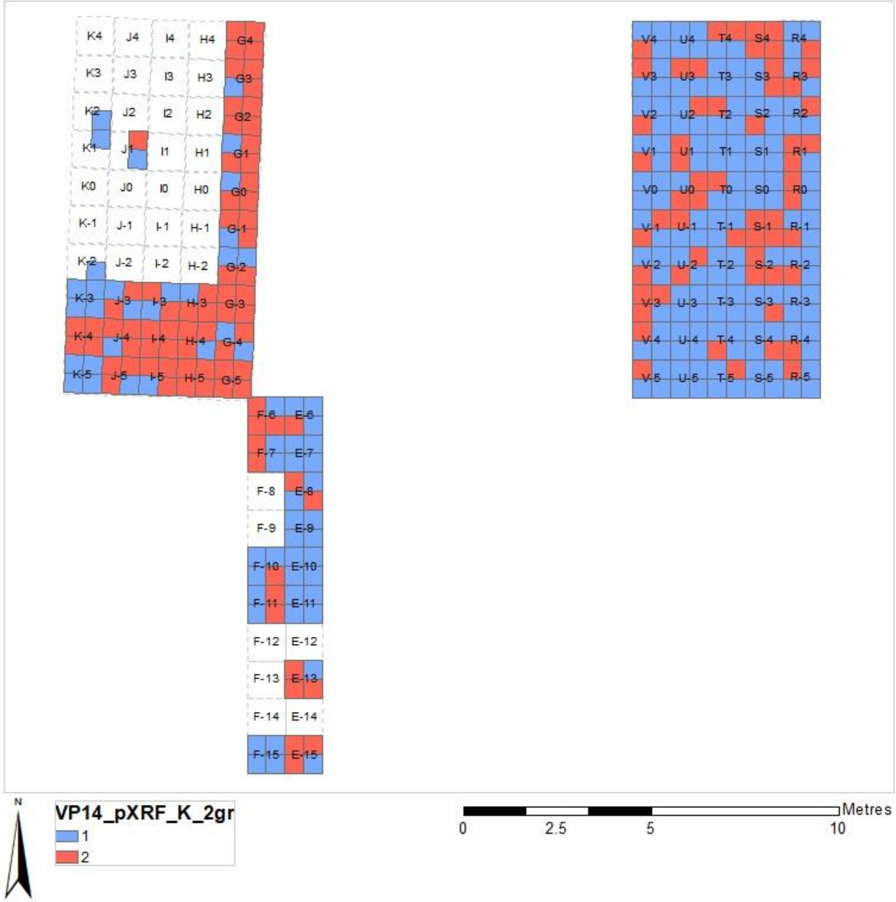
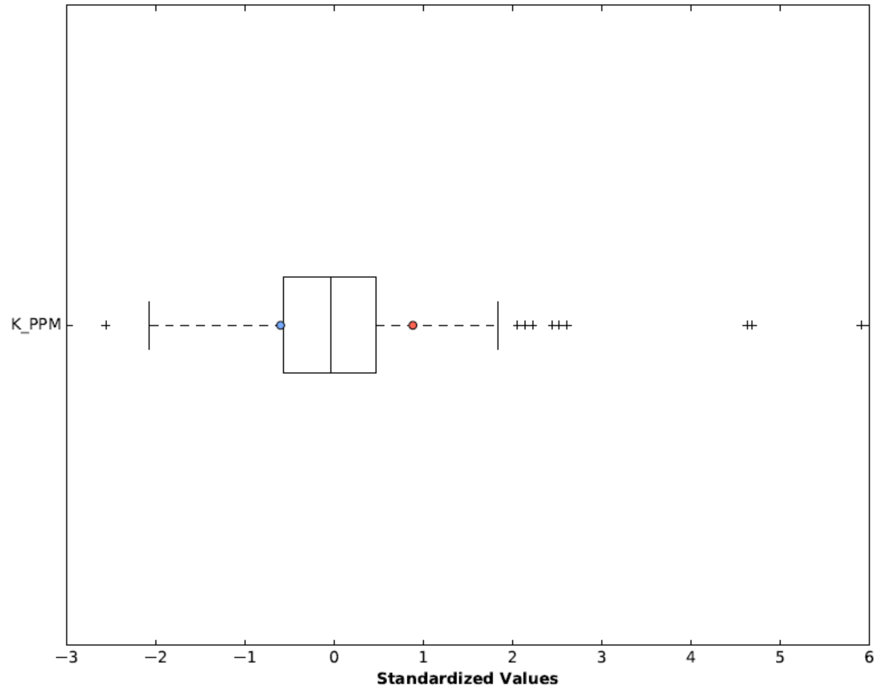
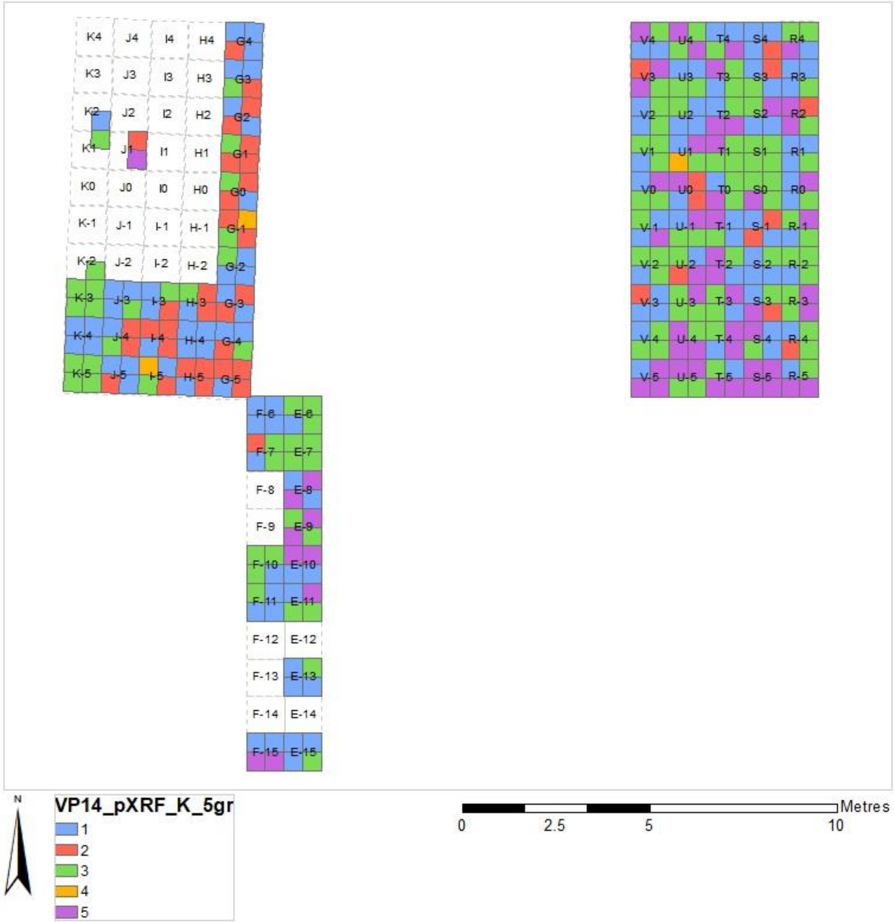
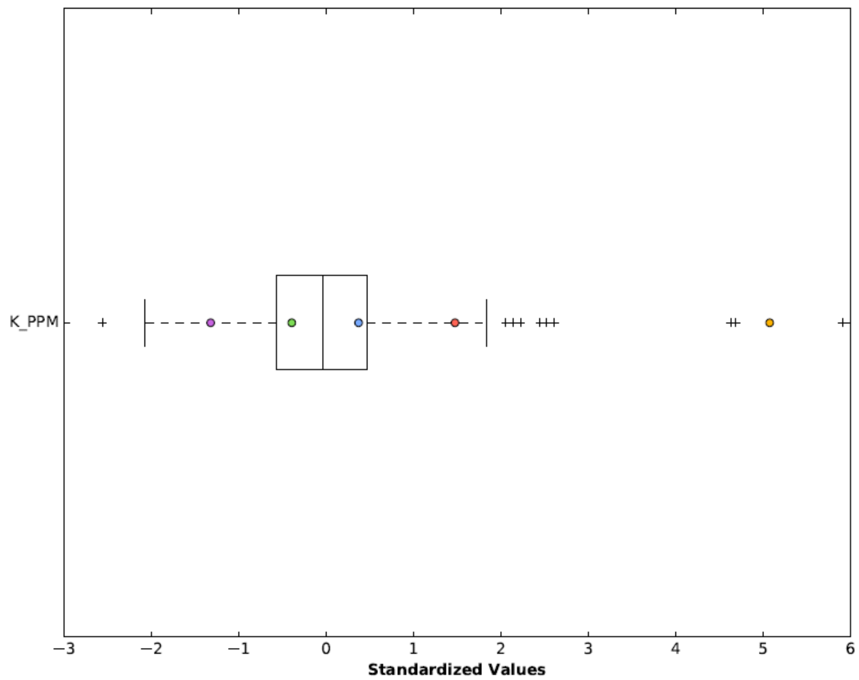


Figure 13. The patterns of groups based on potassium

1.3.2.10 Potassium: Complete Record

Groups	Group Composition and Statistics
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.5311

Groups	Group Composition and Statistics
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.9112

1.3.2.11 Titanium

1.3.2.11.1 Titanium: Two groups

All trenches were mixed, although the southeast corner of trench 11 was made of the lower titanium group samples (blue). The southern end of trench 15 and trench 12(N) samples were generally grouped into the higher titanium group (red).

1.3.2.11.2 Titanium: Five groups

The lowest titanium group samples (yellow) were only found in trenches 11 and 12(N) (Figure 14). They were densest in the southern end of trench 11. Immediately above that area in trench 11, there was an area of highest and second highest titanium group samples (red and green respectively). Trench 12(N) was overall very mixed. Trench 15 had an area of highest and second highest titanium group samples too in the vicinity of squares I-4/H-4/H-5. The samples from the features in the north of trench 15 were either slightly depleted or slightly enhanced in titanium.

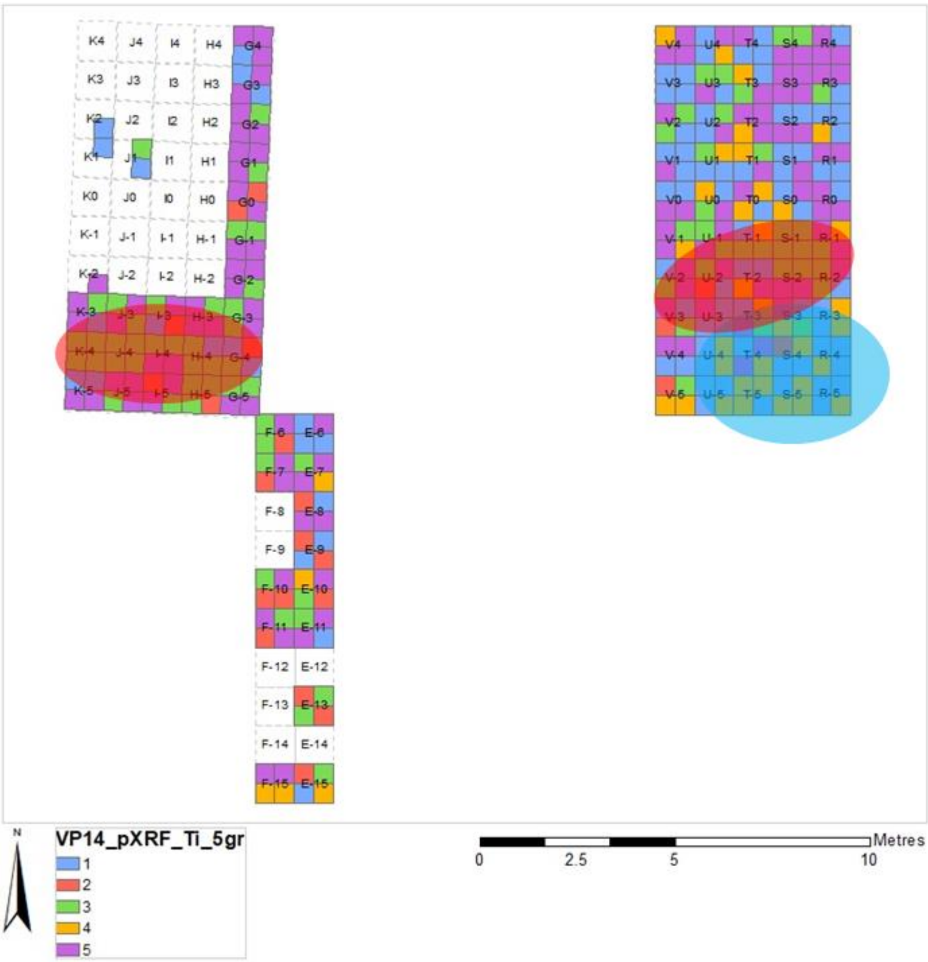
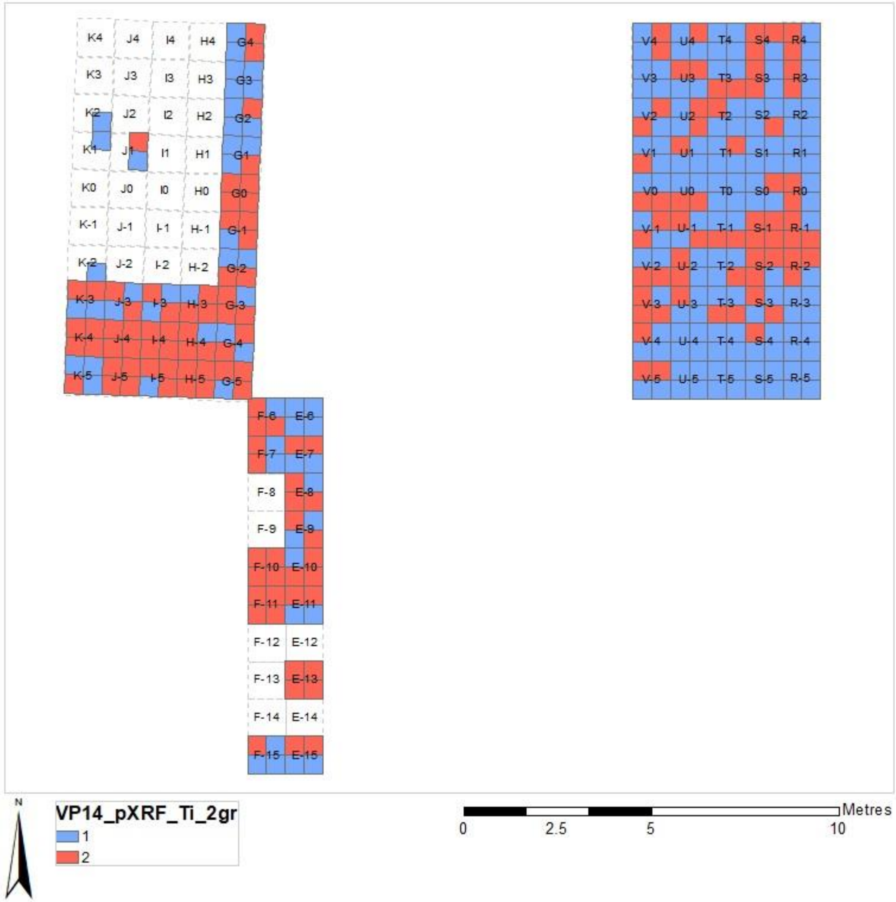
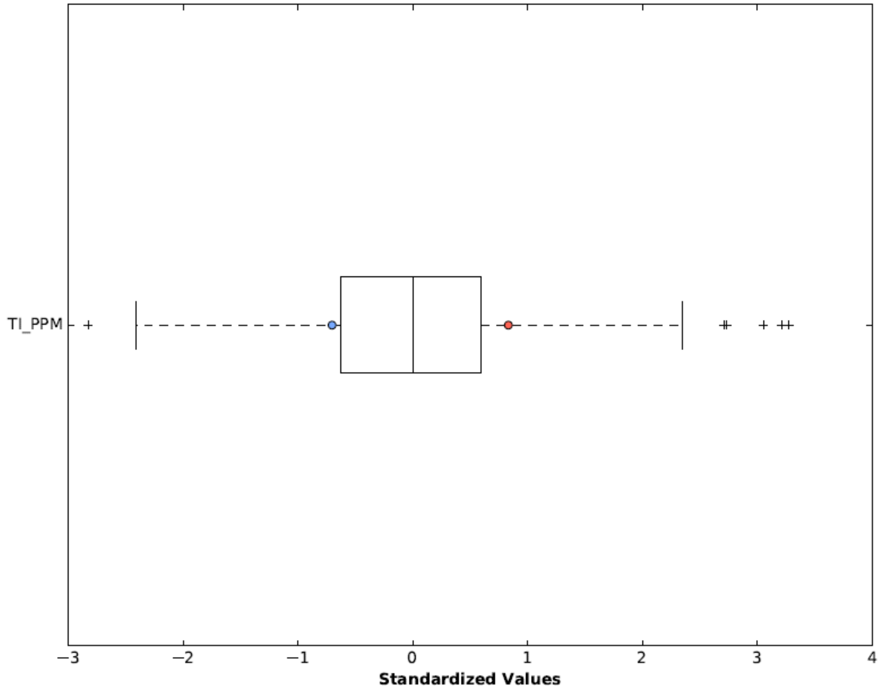
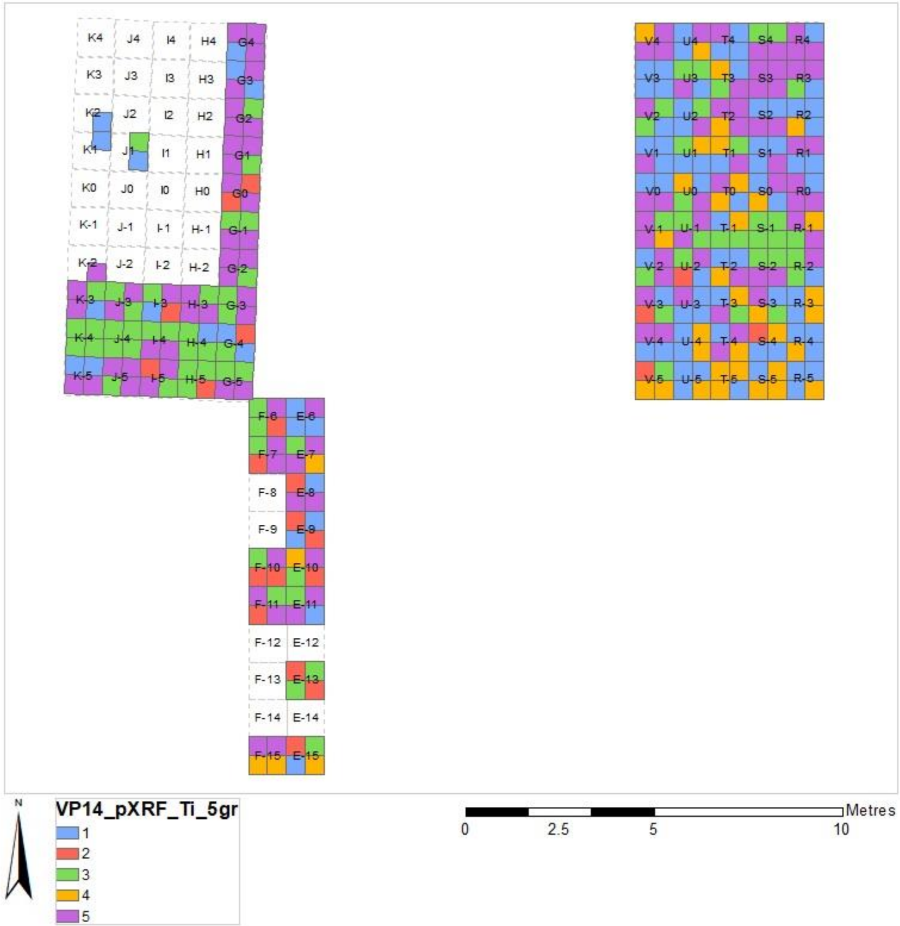
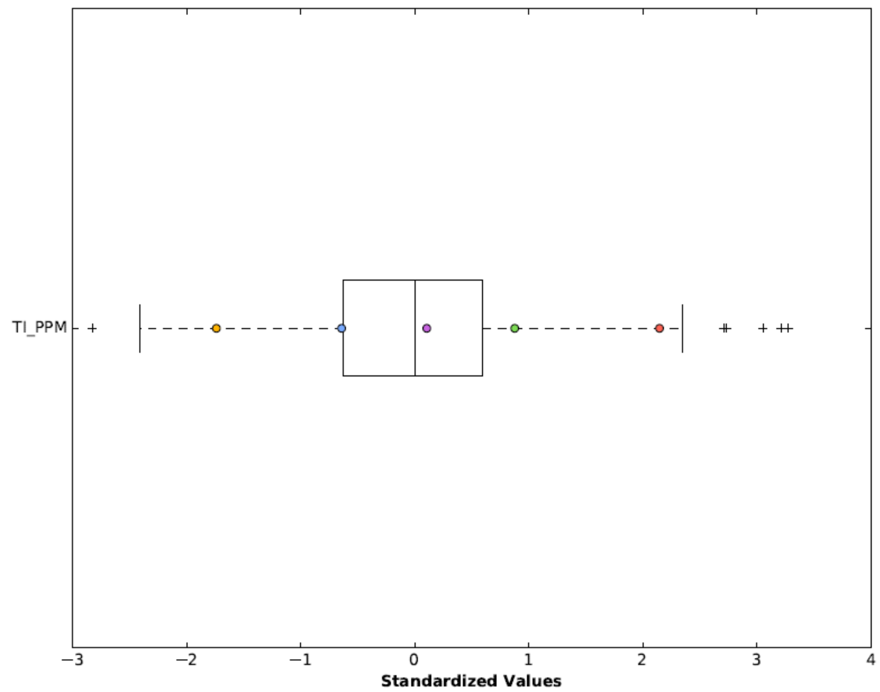


Figure 14. Key patterns in the groupings based on titanium

1.3.2.12 Titanium: Complete Record

Groups	**Group Composition and Statistics**
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.5851

Groups	**Group Composition and Statistics**
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.9203

1.3.2.13 Manganese

1.3.2.13.1 Manganese: Two groups

All trenches were mixed between the two groups. Trench 11 samples were generally in the lower group overall, although there was an area in the centre of the trench that were from the higher group. The southern samples from trench 15 were generally put into the higher group, as were those from the northern end of trench 12(N).

1.3.2.13.2 Manganese: Five groups

The trenches and the features were all generally mixed. There were possible pockets of higher manganese group samples, one in the northern end of trench 11, one in the northern end of trench 12(N), and two in the southern end of trench 15 but these were not very clear.

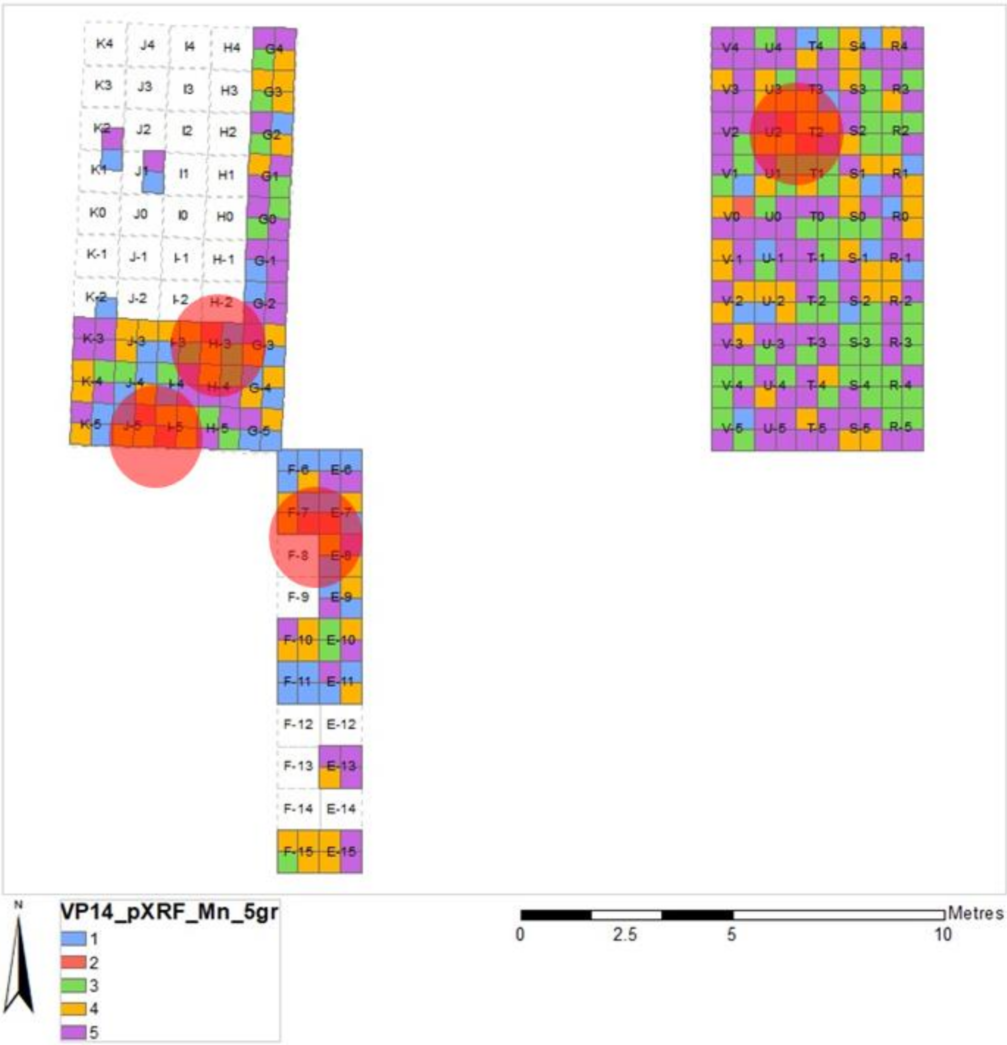
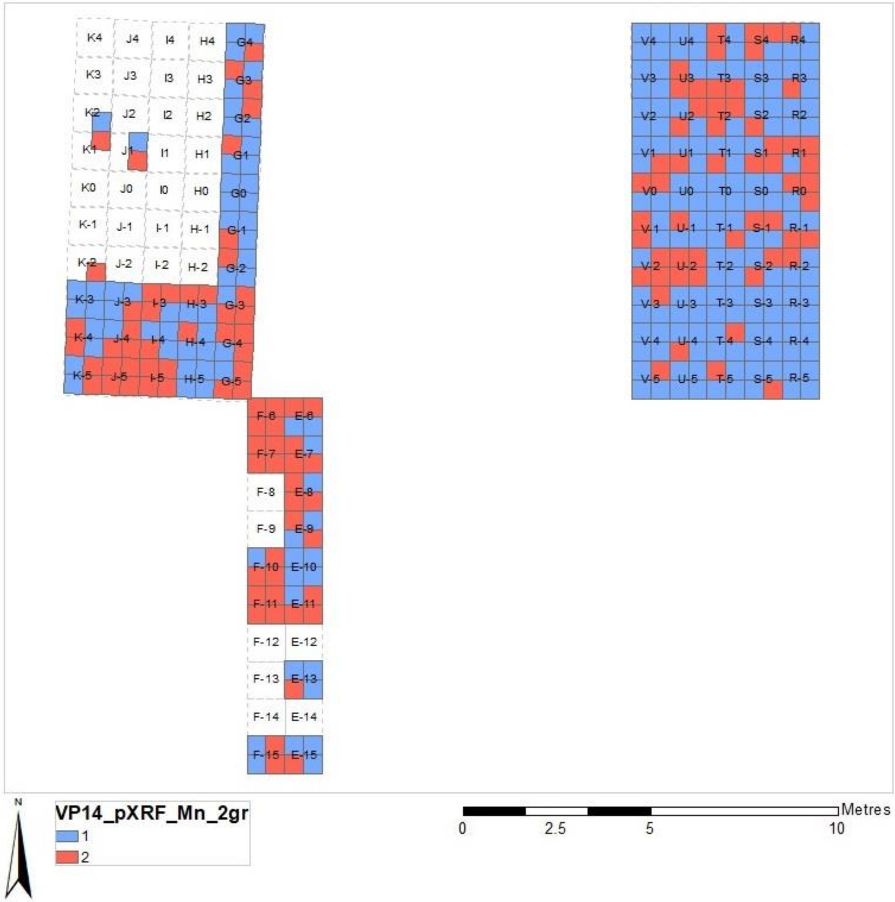
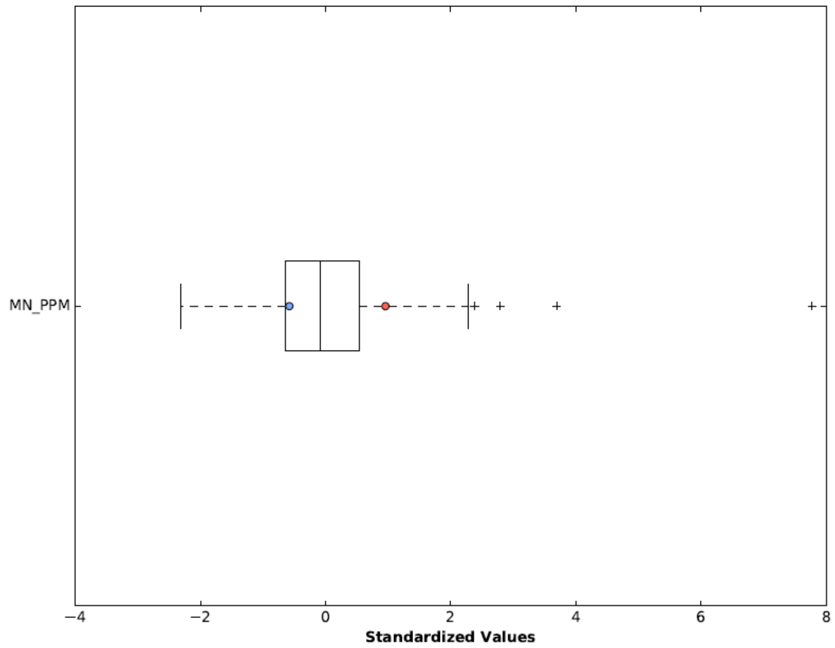
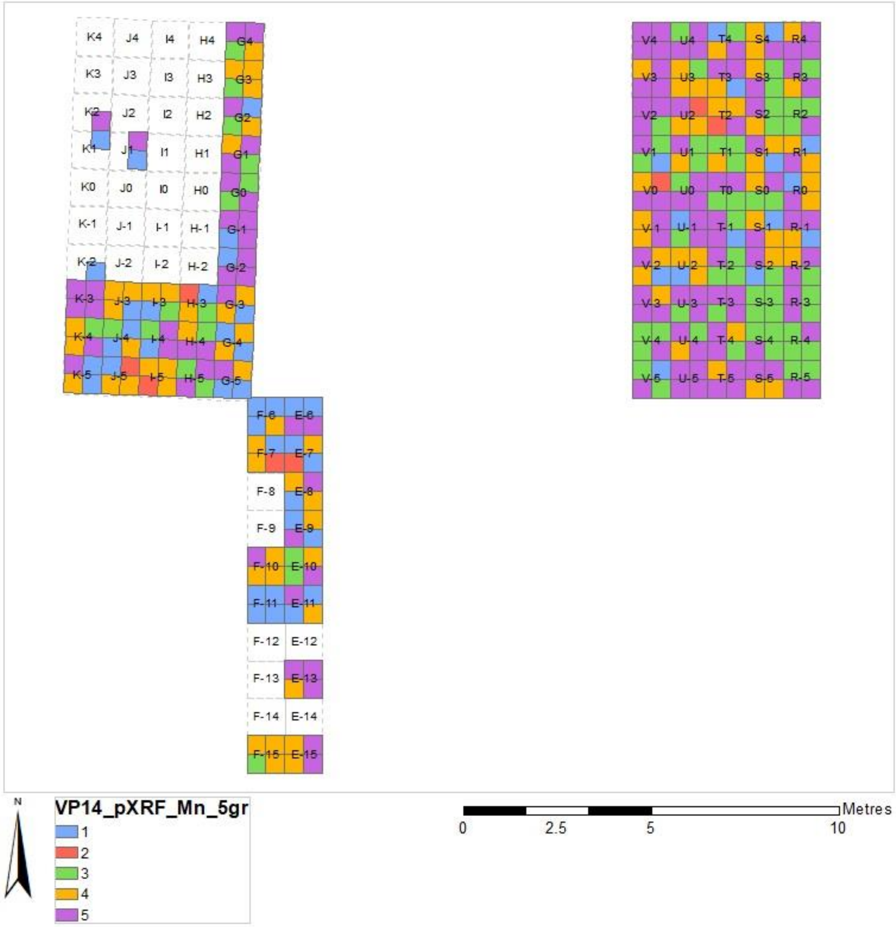
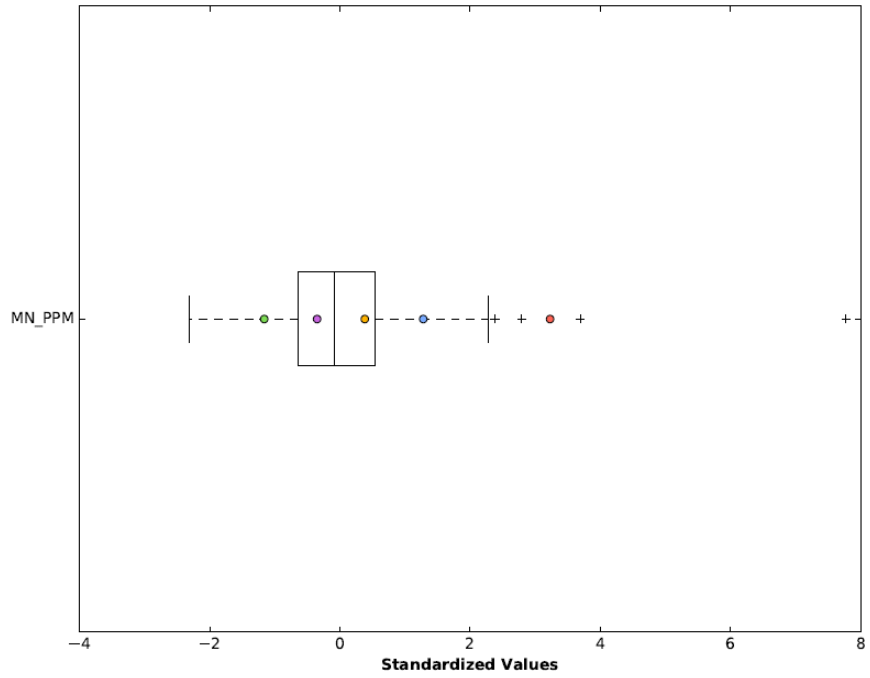


Figure 15. Groupings based on manganese readings

1.3.2.14 Manganese: Complete Record

Groups	**Group Composition and Statistics**
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.5537

Groups	Group Composition and Statistics
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.8487

1.3.2.16 Phosphorus

1.3.2.16.1 Phosphorus: Two groups

Trench 11 was generally lower in phosphorus, with the southeastern corner of it being in the higher group in contrast. The trench 12(N) and 15 samples were generally in the higher group category but were overall mixed.

1.3.2.16.2 Phosphorus: Five groups

The southeast corner of trench 11 and a small pocket of samples in the middle of the trench around grid square R1 were in the lower of the two moderately enhanced groups (blue), in contrast to the rest of the trench which was the lowest, but only slightly depleted, phosphorus group that most of the rest of the trench was assigned to (green) (Figure 16). The other trenches were generally mixed although with more of the higher phosphorus group samples (purple) in the southern end of trench 15 and the northern end of trench 12(N). The highest phosphorus group samples were all seemingly anomalies and found in every trench. The features were from the two moderately enhanced groups.

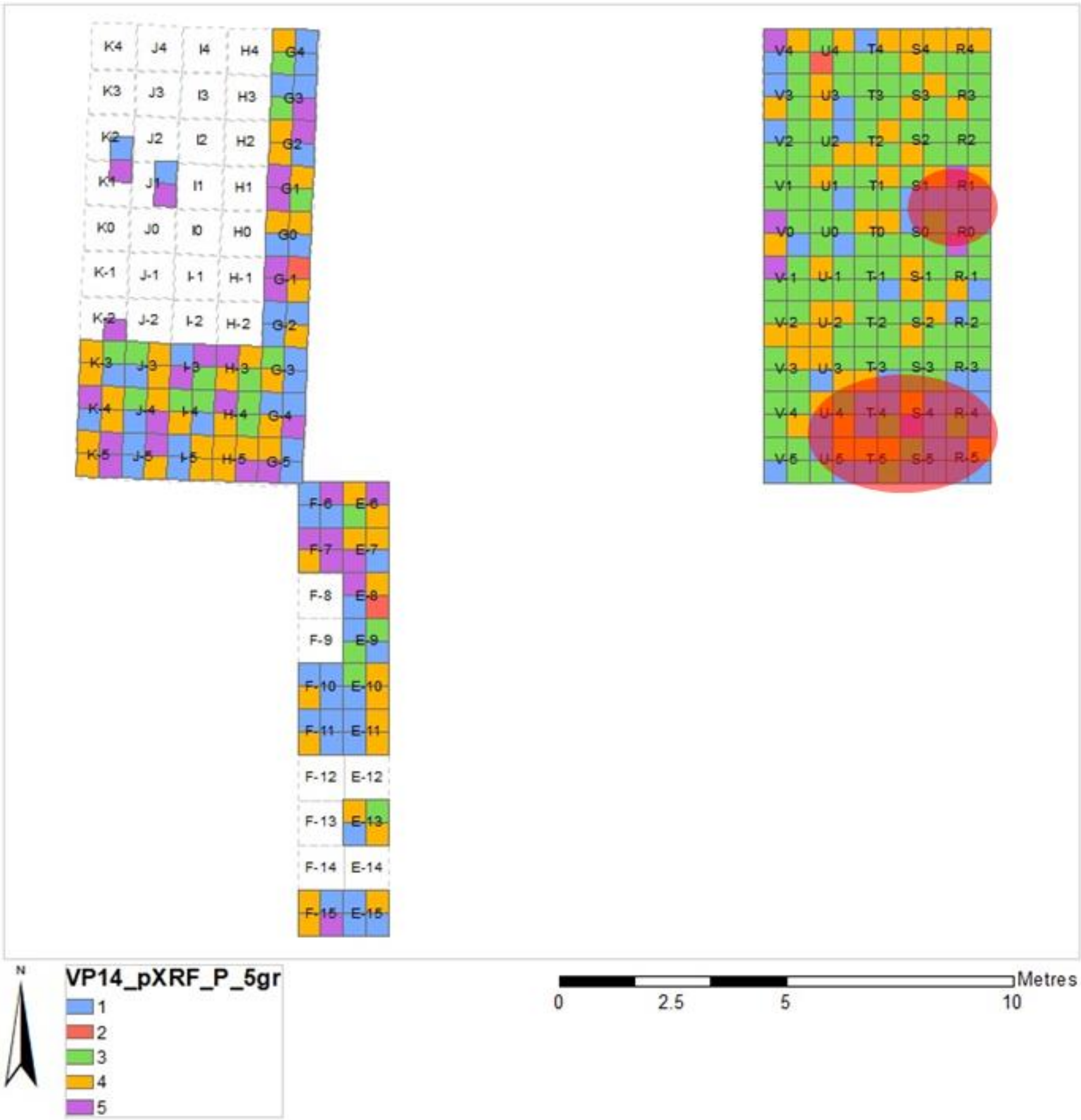
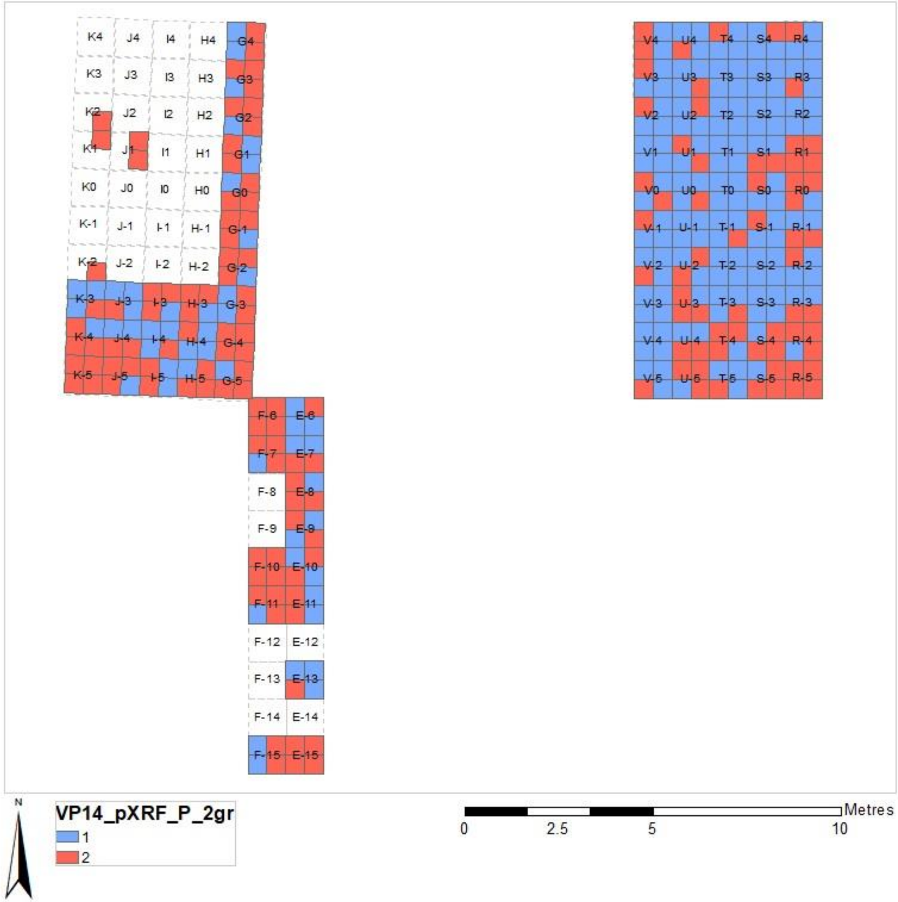
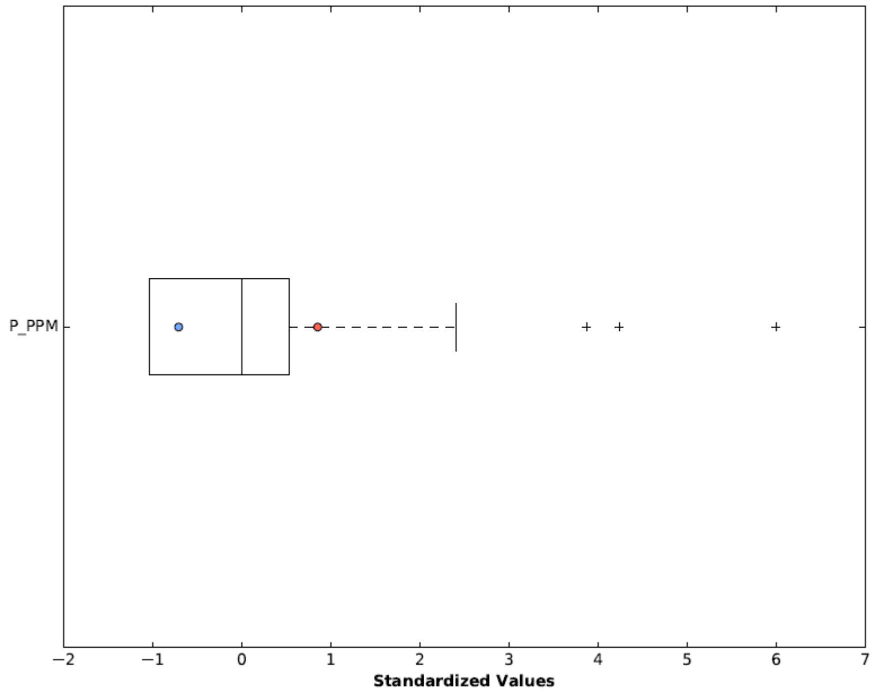


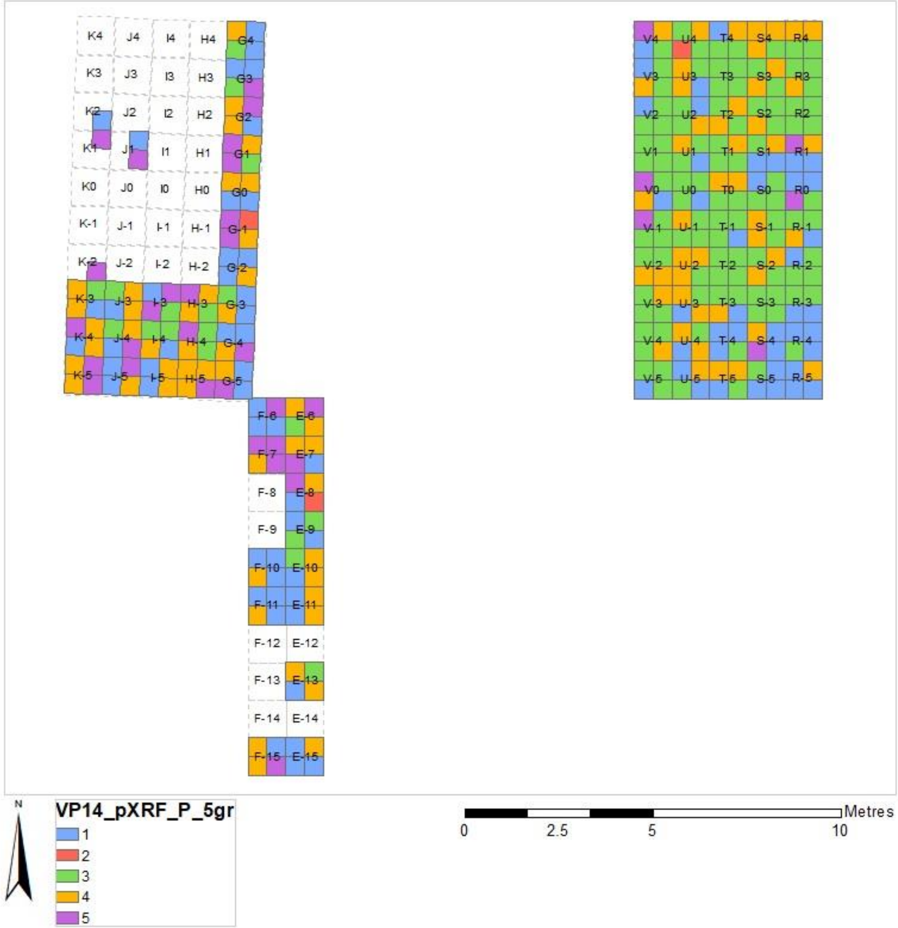
Figure 16. Groupings based on the phosphorus values

1.3.2.17 Phosphorus: Complete Record

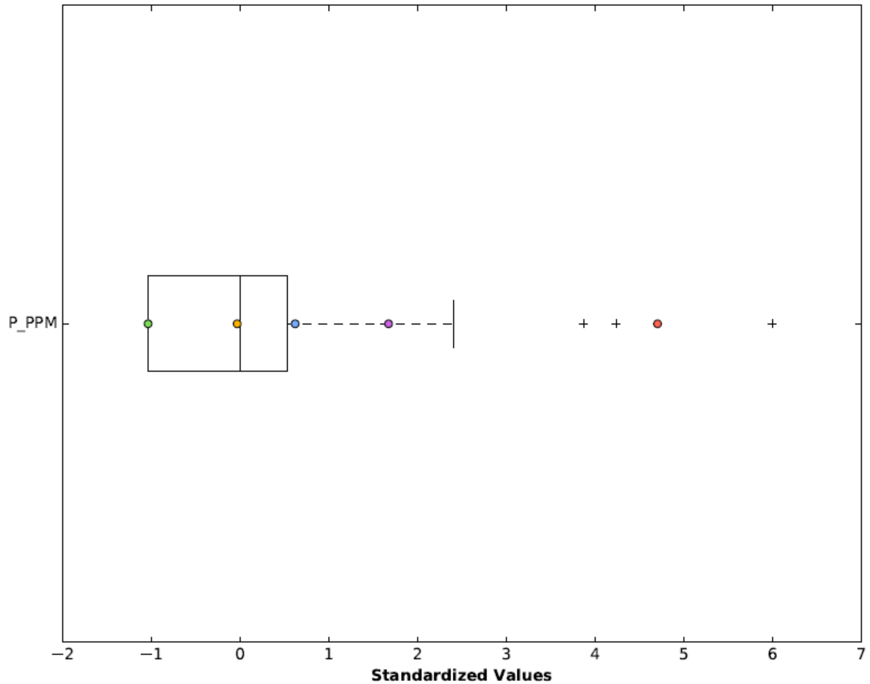
Groups	Group Composition and Statistics
	 **The R^2 statistic that suggests how good the variable is at differentiating these groups:** 0.6046

Groups	Group Composition and Statistics

Groups



Group Composition and Statistics



The R^2 statistic that suggests how good the variable is at differentiating these groups: 0.9562

1.3.2.18 Major/Minor Elements with Mn and P Combined Grouping Analysis

1.3.2.18.1 Two group run and repeats

The two groups are characterised by one group being higher in silicon on average but lower in everything else (blue in the first run), and vice versa for the other group (the red group). It is likely that the reason the averages are proportionally lower in the other elements (because it must be remembered these are averages of parts per million, not an average of the numbers of atoms themselves) is because at least some of that proportion is taken up by the additional silicon. Manganese, phosphorus, iron, and calcium only have high outliers and the former three also have more of a difference between the averages of the two groups, indicating these elements have greater value ranges and are therefore more variable across the trenches. Potassium, titanium, and aluminium have both high and low outliers and are moderately variable in that the group averages are closer to the global average than for Mn, P, and Fe, but the difference is greater than that between the calcium and silicon averages. The difference between the two groups being that one is greater in silicon is diminished by the fact that the difference between the average silicon readings between the two groups is the smallest difference between averages explored here.

The two group run identifies that trench 11 is generally different to trenches 12(N) and 15, in that most of its samples are grouped into the higher silicon group, while the inverse trend is seen in the other trenches. In particular, the southern end of trench 11 seems to have the greatest density of samples grouped into the higher silicon group. The rest of the trench is a little more mixed. The feature squares are in keeping with the rest of trench 15, being grouped into the lower silicon group.

The repeats are all consistent with the trends highlighted for the first run.

One thing to note is that the R^2 values are all lower than 0.4 implying this model is a greatly oversimplified representation, particular for silicon which only has an R^2 statistic of 0.0440. It is interesting therefore that the optimal number of groups as evaluated by the tool was deemed to be two, despite this. The higher group models produce better R^2 values than this.

1.3.2.18.2 Five group run and repeats

The five grouping run highlights the importance of running at a greater number of groups, even though the tool suggest two was the optimal number (shown in Figure 17 for the key grouping run). In allowing separate groups to form, the southeastern corner of trench 11 actually groups in all five-group repeat runs as being the only solid presence of samples grouped into a significantly low silicon grouping, the blue group in the first of the runs, even though this end appeared to be dominated by high silicon grouped samples in the two-group runs. This is counter-intuitive but not illogical: The averages for silicon in the two-group runs were close together, presumably being drawn closer together by the interaction of the low silicon samples in trench 11 on the statistical spread of the apparently high silicon group, and the majority of samples from trench 11 must have on average been more similar to each other due to the other elements overall than to the samples placed in the group with lower silicon in general. As such, this confirms the issues with the two-group outputs that were suggested by the R^2 statistics. The R^2 statistics are still quite low, however, ranging between 0.5819 for aluminium down to 0.4233 for manganese.

As such, the southern end of trench 11 and particularly the southeastern corner of that trench is grouped as being generally the lowest silicon samples, joined by moderately or slightly depleted aluminium, potassium, and titanium compared to the global average, near average (slightly depleted or enhanced) iron, manganese and phosphorus, and moderately elevated calcium (blue group). There is a second, smaller pocket of similarly grouped samples midway up the trench around grid square R1. This is generally confirmed in the other runs (in one run, the phosphorus levels of the group formed are on average moderately enhanced instead). Immediately to the north of this is an area, there is an area more in keeping with the originally suggested trend: these samples are usually grouped into the highest average silicon group (red in the first run) which can be slightly up to highly enhanced levels but always the highest of the options, which are characterised by being slightly or moderately depleted in the other elements which is much more in keeping with the original profile of the samples from that trench. The northern half of the trench meanwhile is generally assigned to a group characterised by being near global average in all elements (green in the first run). These trends are also confirmed in the repeat runs.

Much of the trench 15 samples are placed into a grouping characterised by particularly high potassium and aluminium, but also moderately or slightly high iron and titanium on average (yellow group in the first run). There is one sample in the second repeat run that is placed into a single-sample grouping for being anomalously high in potassium and also phosphorus but in all other runs this was subsumed into the general groups of the trench, and in that run the group the majority of the rest of the samples are placed in is still characterised by enhanced potassium, aluminium, and to a lesser extent titanium and iron so it does not seem to have a great bearing on the profile of that main group. The southwestern corner of trench 15 is generally a little different to the rest of trench 15, being mixed but more akin to the northern end of trench 11 (mainly green grouped in the first run). There are more samples here placed into a group that is moderately elevated in calcium, phosphorus, manganese and iron (purple in the first run) but it is not a solid signal.

Trench 12(N) is generally mixed, although the southern end of it features several samples grouped into the low silicon group similar to the southeastern corner of trench 11. There are samples there grouped into the high silicon group and other groups also though. In the centre of trench 12(N), there is a pocket of generally green (all elements near average) grouped samples. The northern end of trench 12(N) is akin to the southern end of trench 15 but again mixed.

1.3.2.18.3 Nine group run and repeats

The nine group model largely reinforced the five group model patterns, with many of the areas just being split into complicated, heterogeneous patterns of the groups with near average readings. Trench 11 still splits into three regions in its southeast corner (grey in the first run), centre (light blue), and northern half (mixed). Trench 12 is also similar with the southern end featuring samples in the same group as those from the southeastern corner of trench 11, the centre sometimes being included in a group with moderately enhanced titanium and silicon (dark blue), and the northern end being grouped with samples from trench 15.

The patterning in trench 15 is more complicated and less consistent between the runs. There is an area in the southeastern corner, paired with another block of samples in the northern transect (red or purple in the first run). These are variably characterised with slightly or moderately enhanced potassium as well as slight enhancements of other elements in various combinations. These areas are generally encircled in samples of mixed groupings with high aluminium, iron, titanium and/or potassium (brown), or enhanced calcium, phosphorus, manganese, and/or iron, possibly with reduced silicon (pink) (samples like these characterising the northern end of trench 12 as well). Then there are samples grouped into those with near average groupings that make up the southwestern end of the trench. As such while this distinguishes some different patterning, the chemical composition changes related to this are very subtle and how they are grouped is much more dependent on the random seed initiation than the other patterns that are more consistent between runs.

The R^2 statistics were still generally a bit low, ranging between 0.6673 (for aluminium) down to 0.5025 (for manganese).

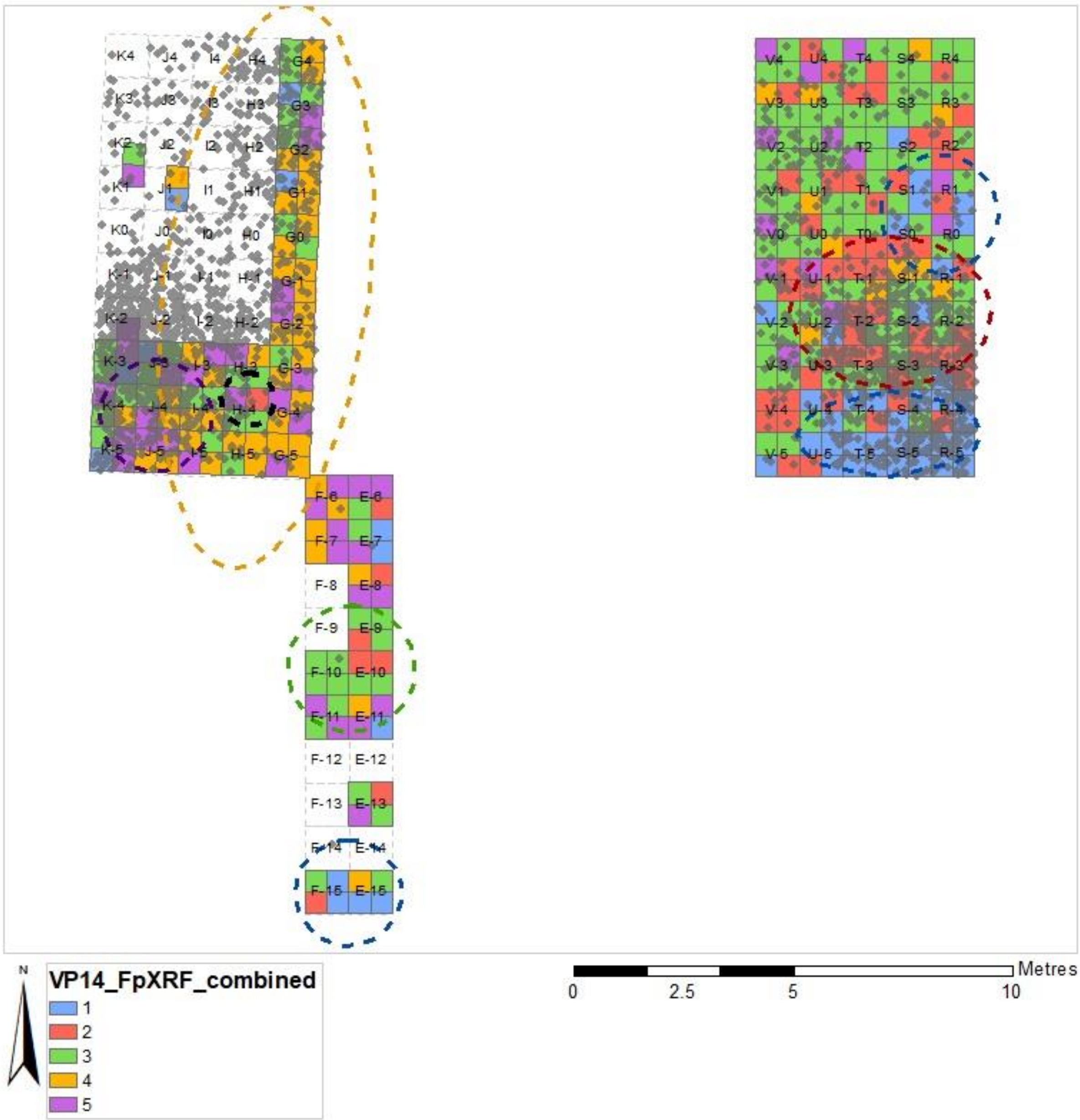


Figure 17. Summary of the key patternings identified in the combined model

1.3.2.19 Major and minor elements expanded: Complete Record

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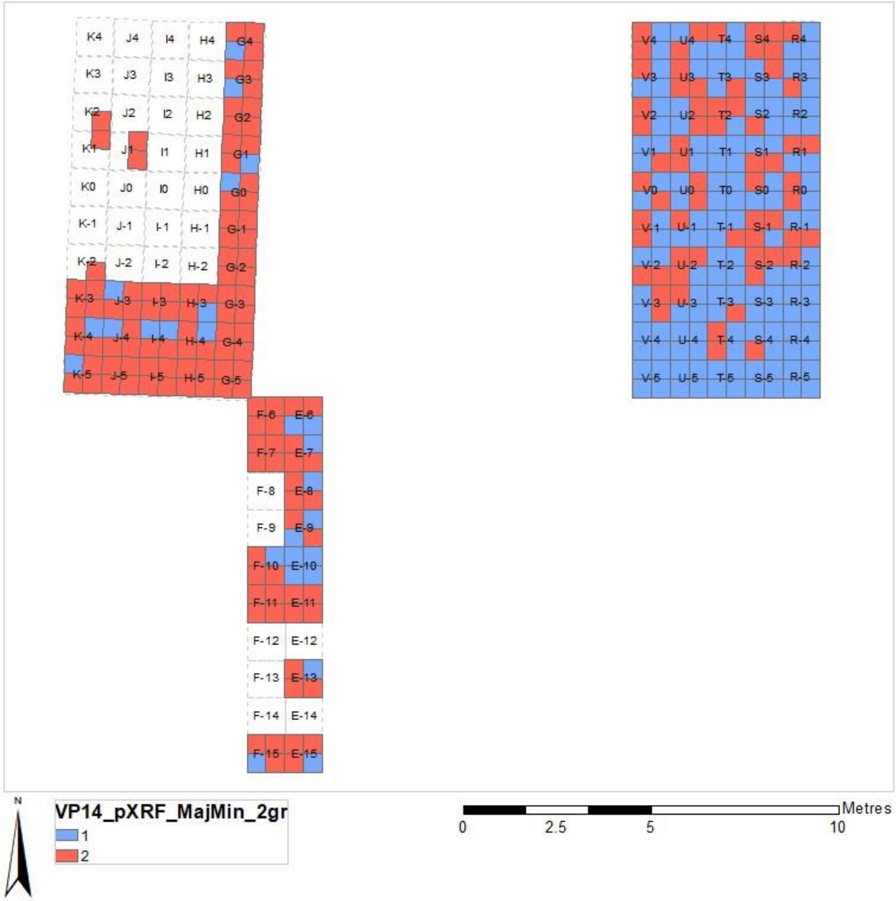

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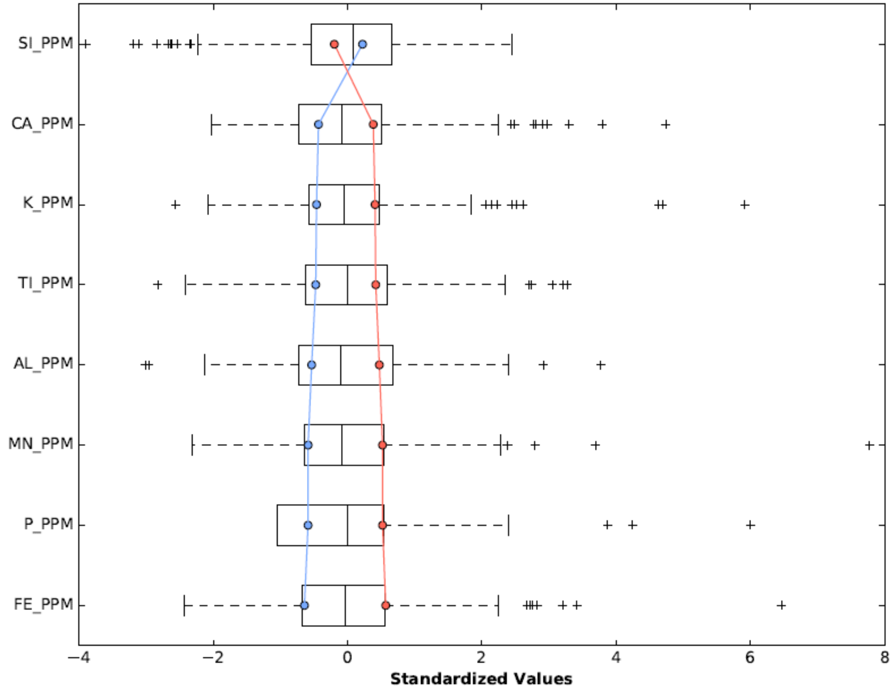

Optimal number of groups evaluated: 2

The R^2 statistic that suggests how good the variable is at differentiating these groups: Fe: 0.3652; P: 0.3065; Mn: 0.3059; Al: 0.2531; Ti: 0.1990; K: 0.1892; Ca: 0.1657; Si: 0.0440
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2 Group Repeats

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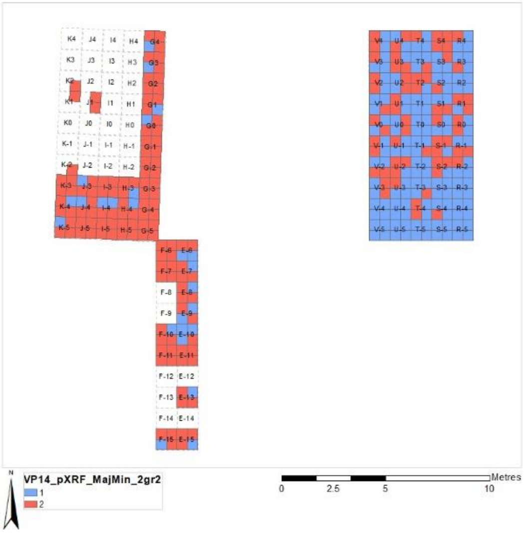	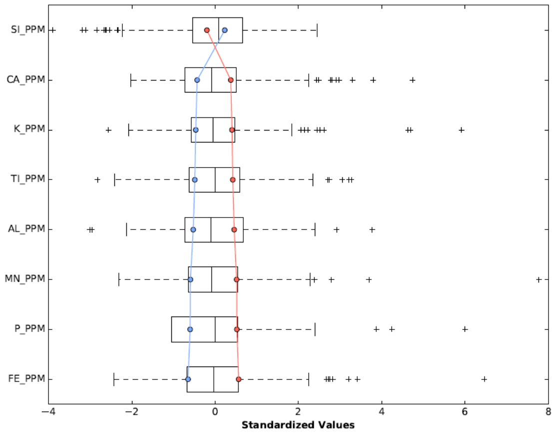
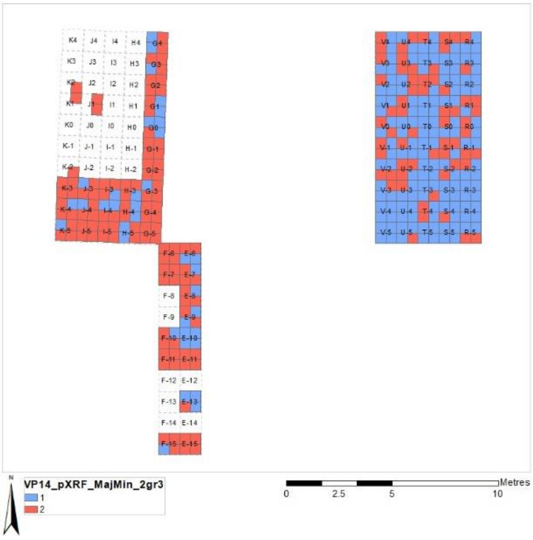	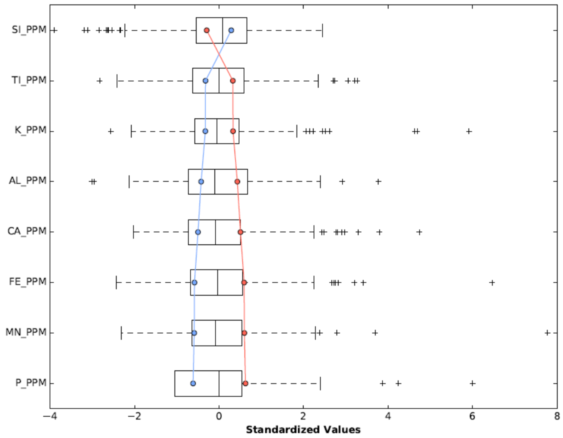

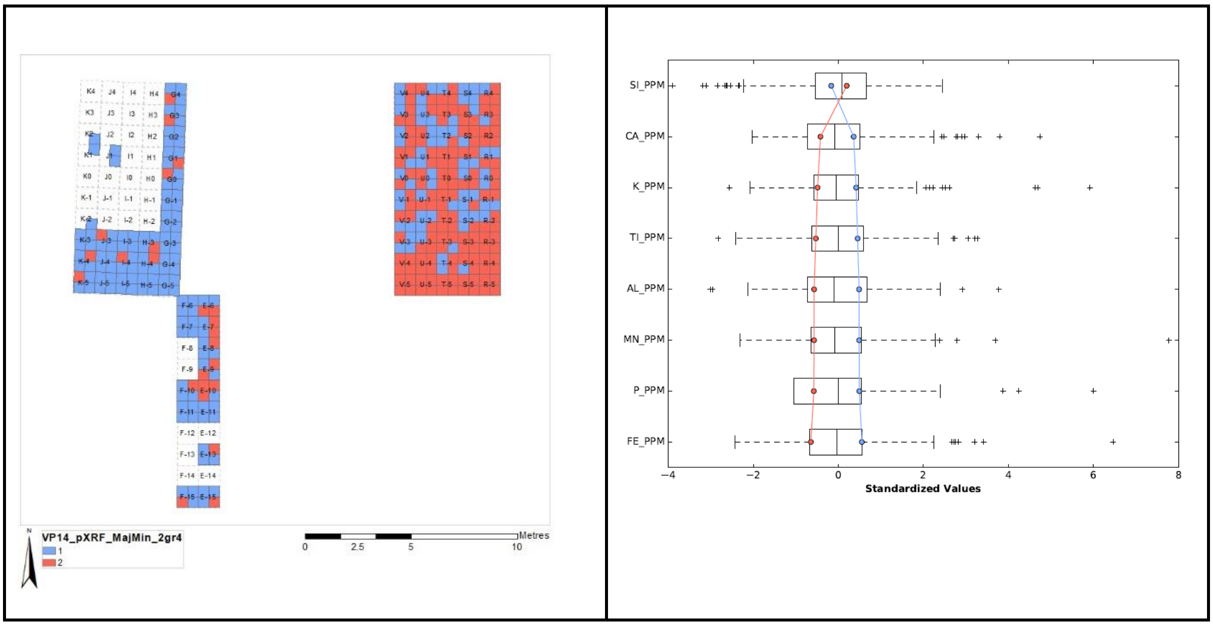
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CA_PPM
K_PPM
TI_PPM
AL_PPM
MN_PPM
P_PPM
FE_PPM
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0
2
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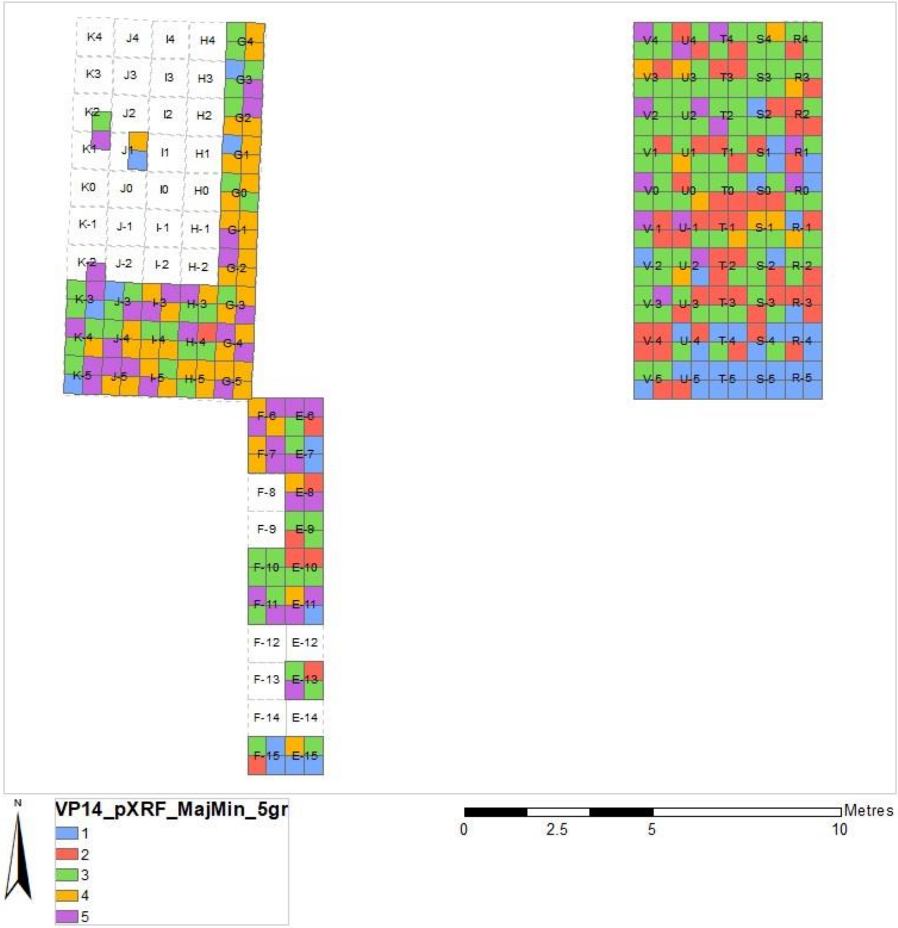
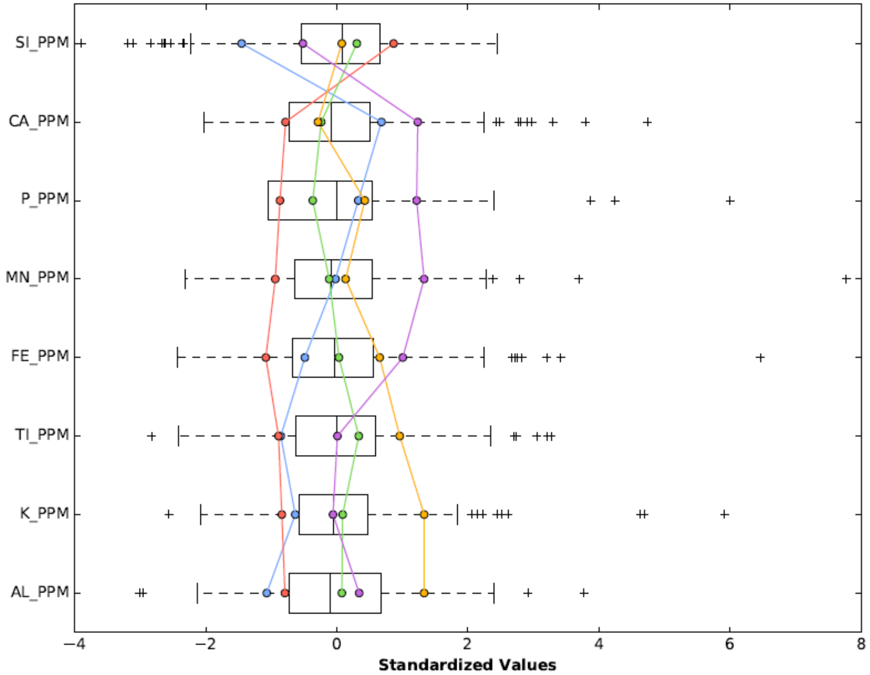
6
8
Standardized Values

Groups



Group Composition and Statistics



Optimal number of groups evaluated: 2

The R^2 statistic that suggests how good the variable is at differentiating these groups: Al: 0.5819; Si: 0.5087; K: 0.4751; Fe: 0.4612; P: 0.4449; Ti: 0.4370; Ca: 0.4313; Mn: 0.4233

5 Group Repeats

<table>
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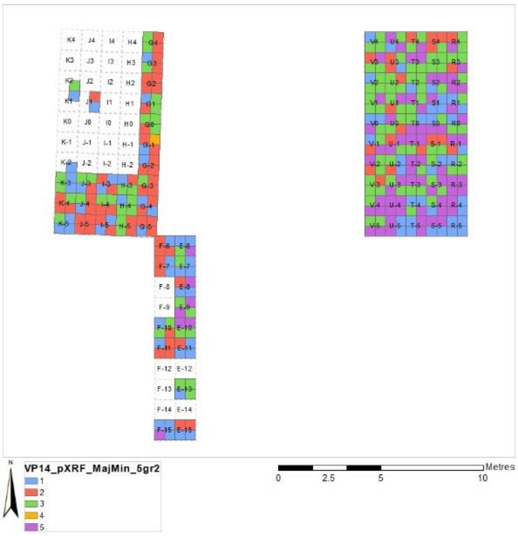

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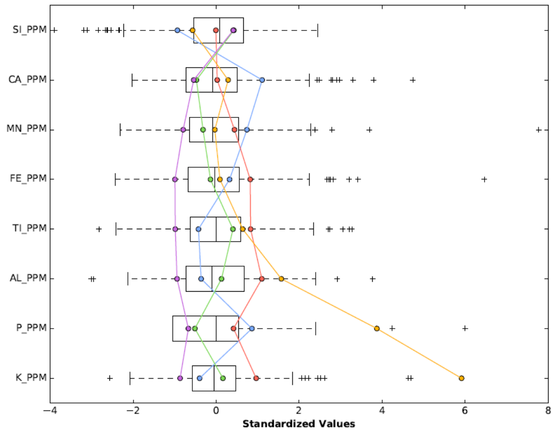

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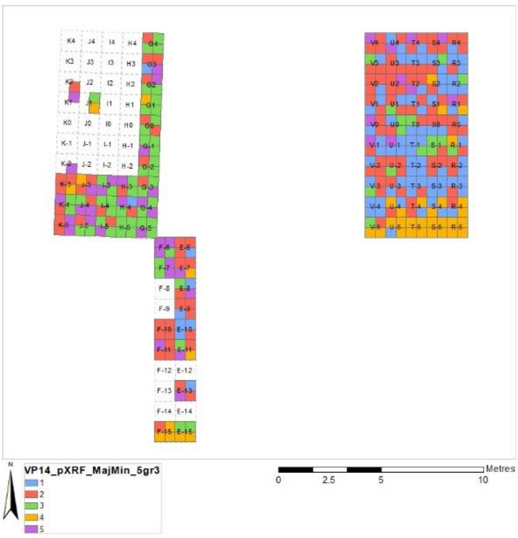

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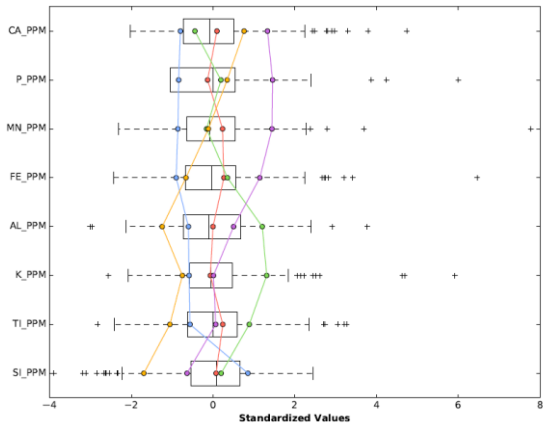

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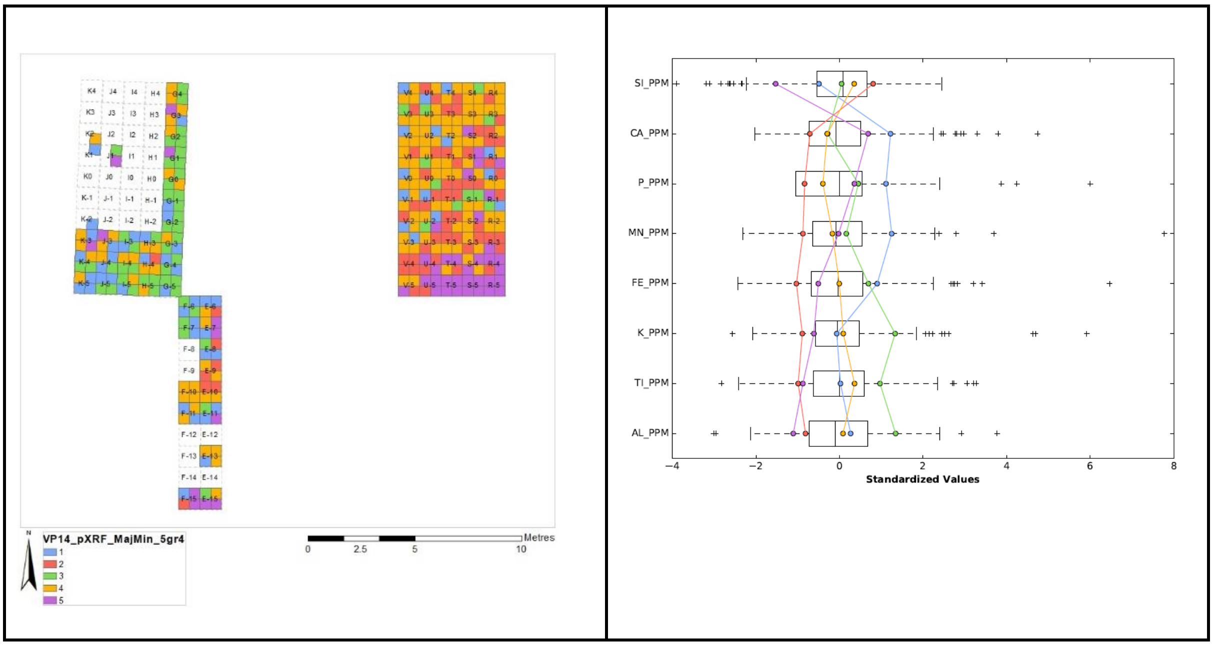
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CA_PPM
P_PPM
MN_PPM
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4
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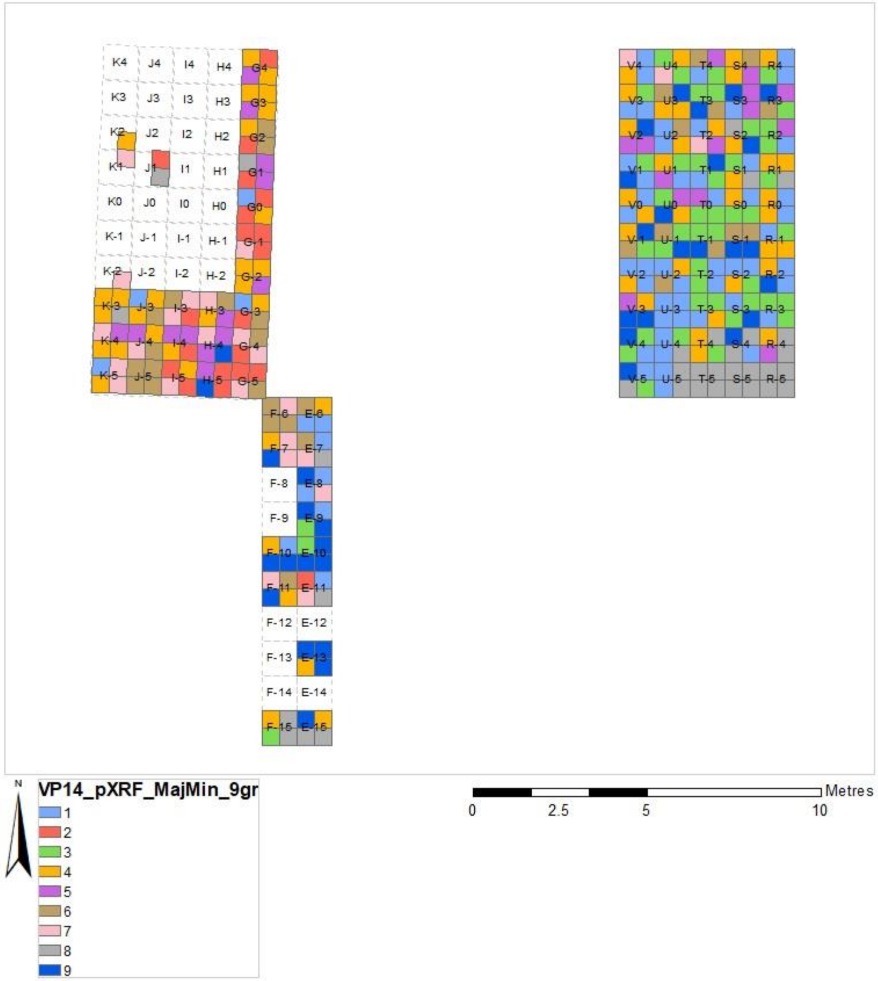
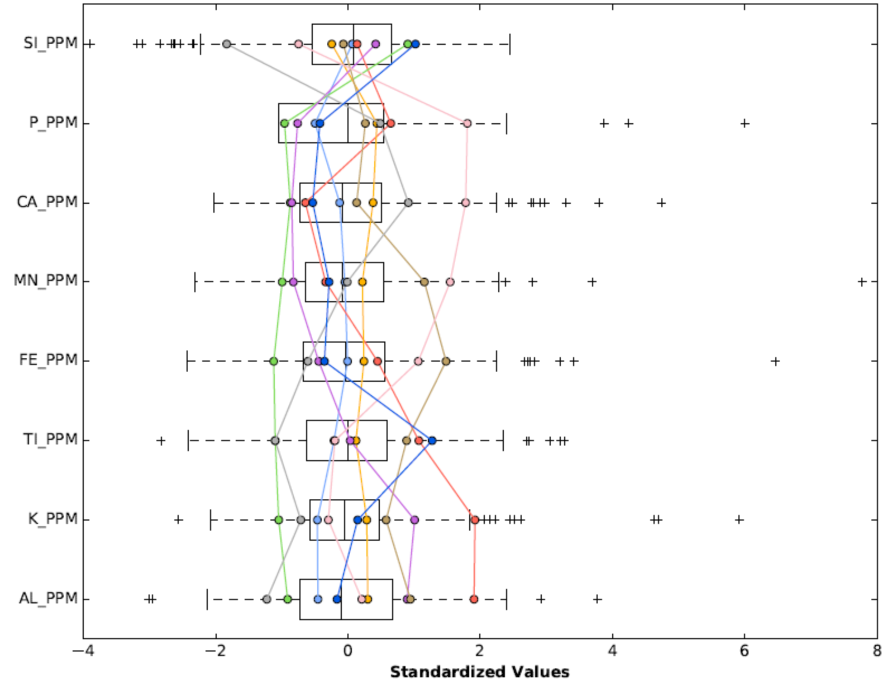
8
Standardized Values

Groups	Group Composition and Statistics

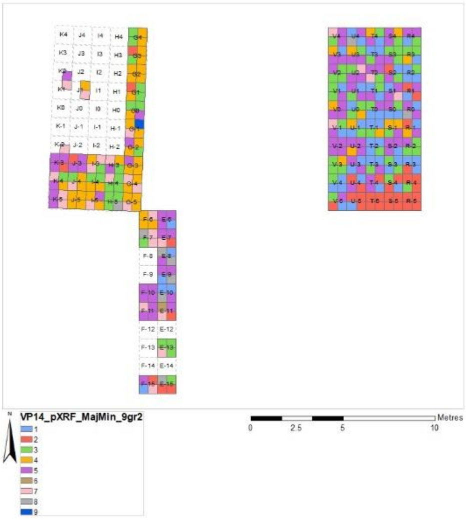
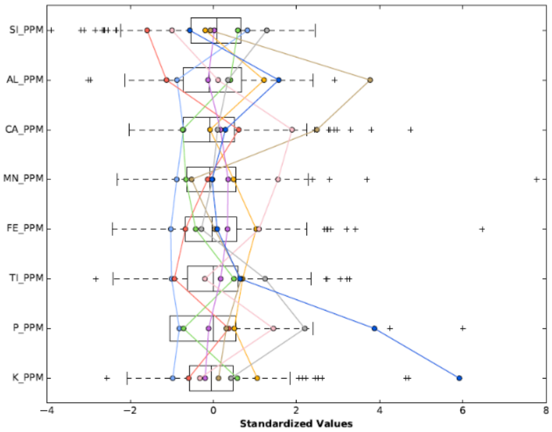
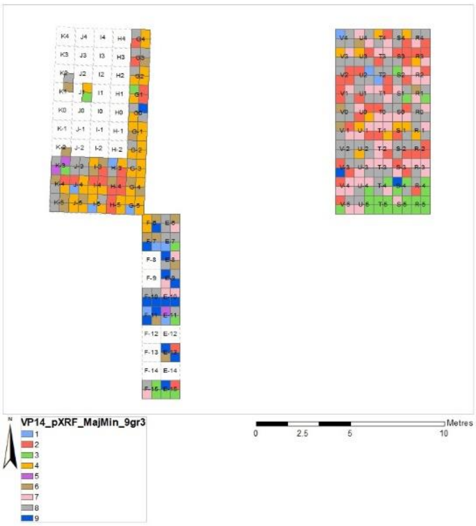
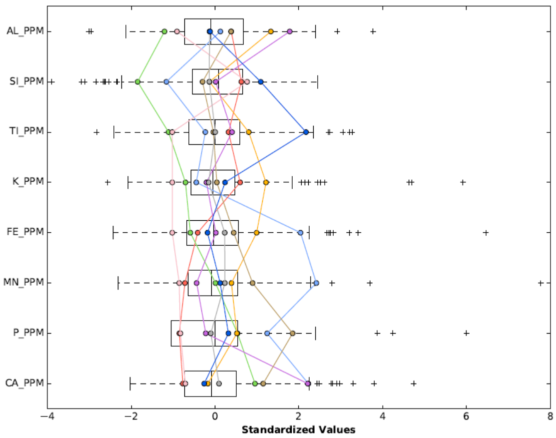


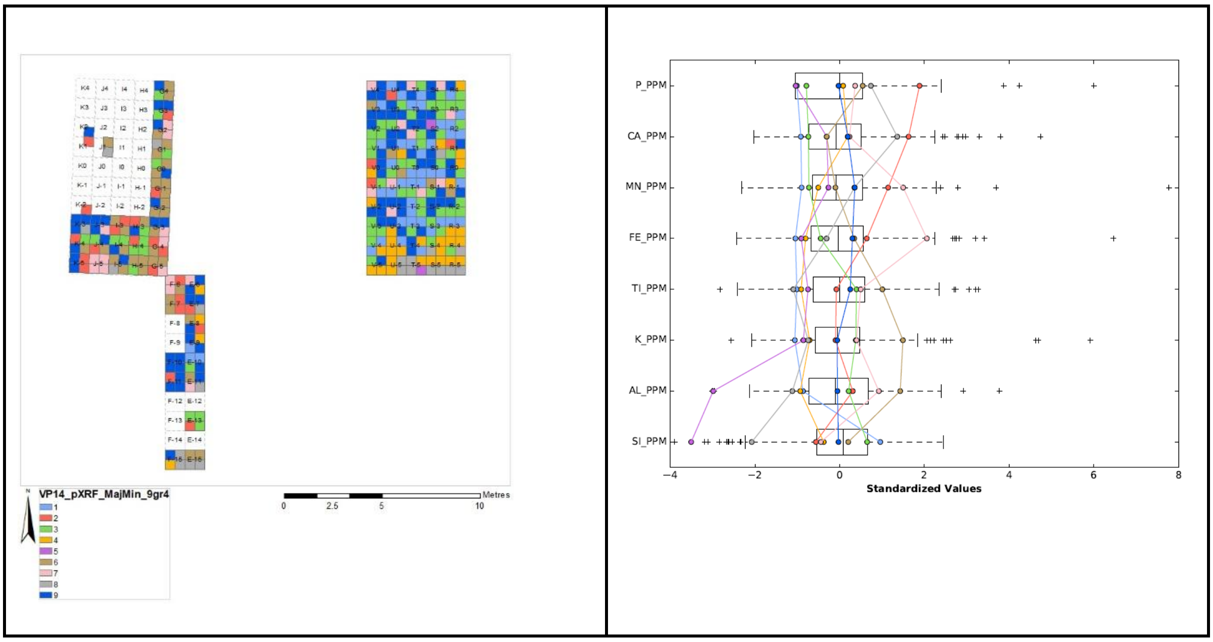


Optimal number of groups evaluated: 2

The R^2 statistic that suggests how good the variable is at differentiating these groups: Al: 0.6673; Si: 0.6097; Ti: 0.6013; K: 0.5793; P: 0.5560; Ca: 0.5528; Fe: 0.5339; Mn: 0.5025

7 Group Repeats

Group	**Box Plot**
	
	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AL_PPM
SI_PPM
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Standardized Values