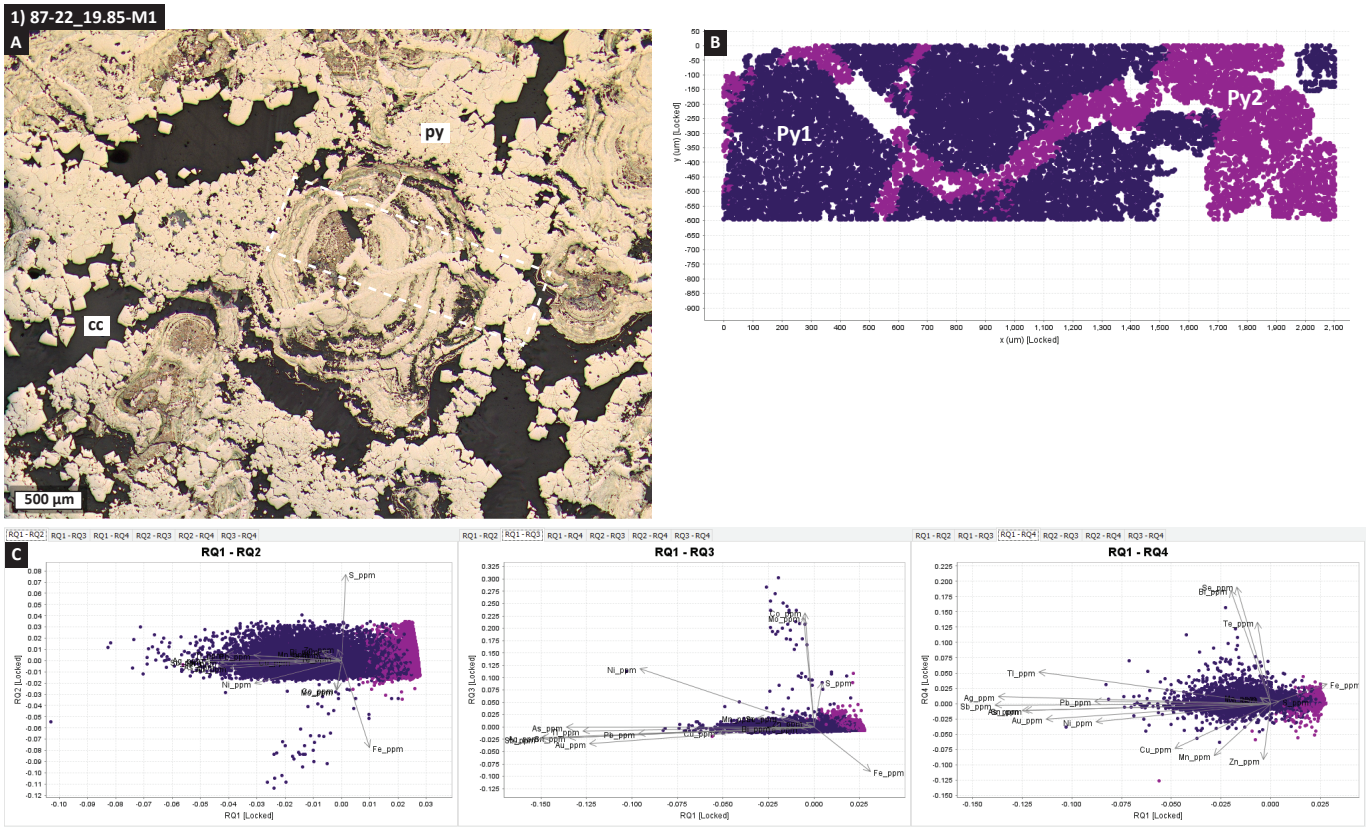

Fig. 1. Sample 87-22_19.85, map 1. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrite groups, distinguished through PCA and K-means clustering. C) PCA biplots showing the distinct compositional characteristics of the various groups.

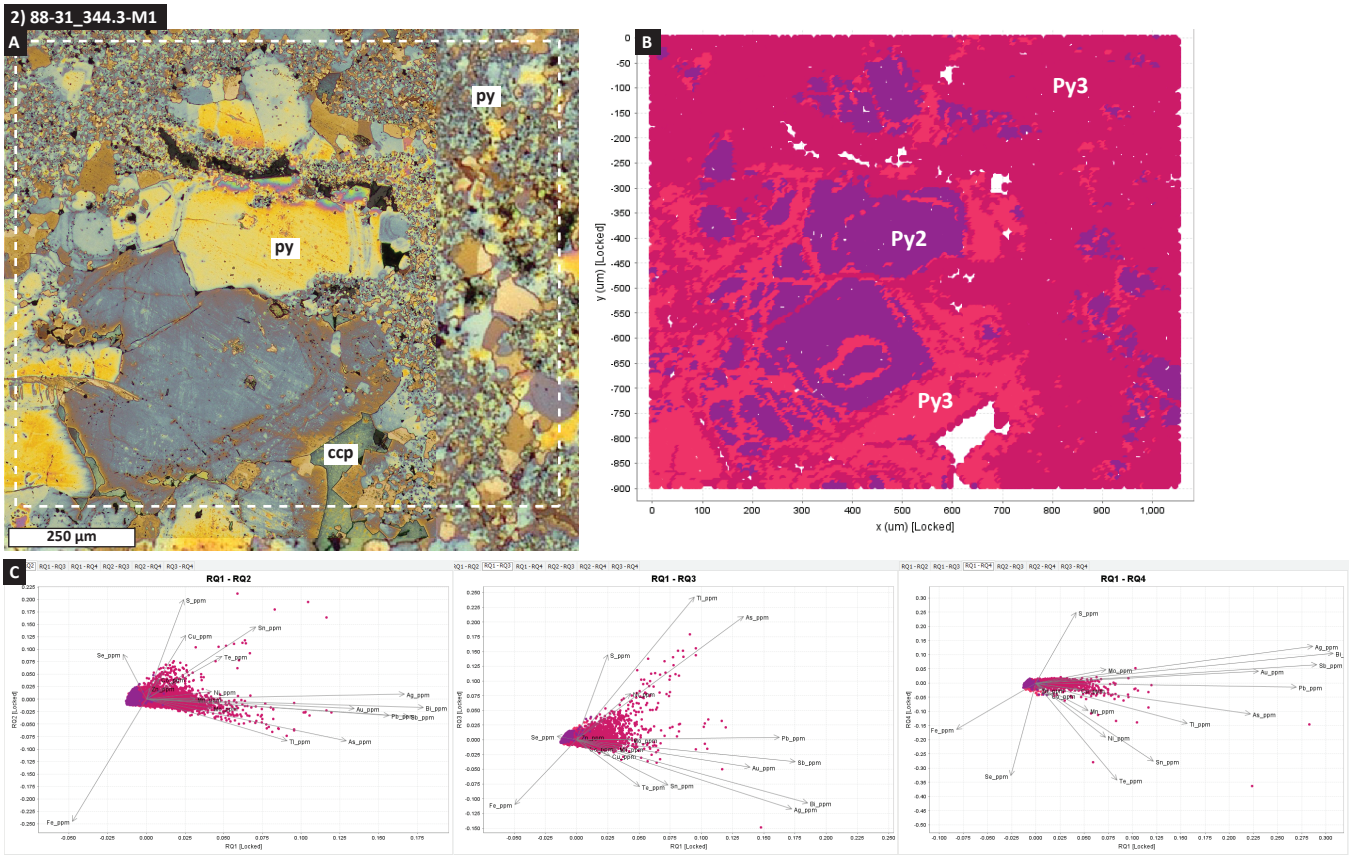

Fig. 2. Sample 88-31_344.3, map 1. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrite groups, distinguished through PCA and K-means clustering. C) PCA biplots showing the distinct compositional characteristics of the various groups.

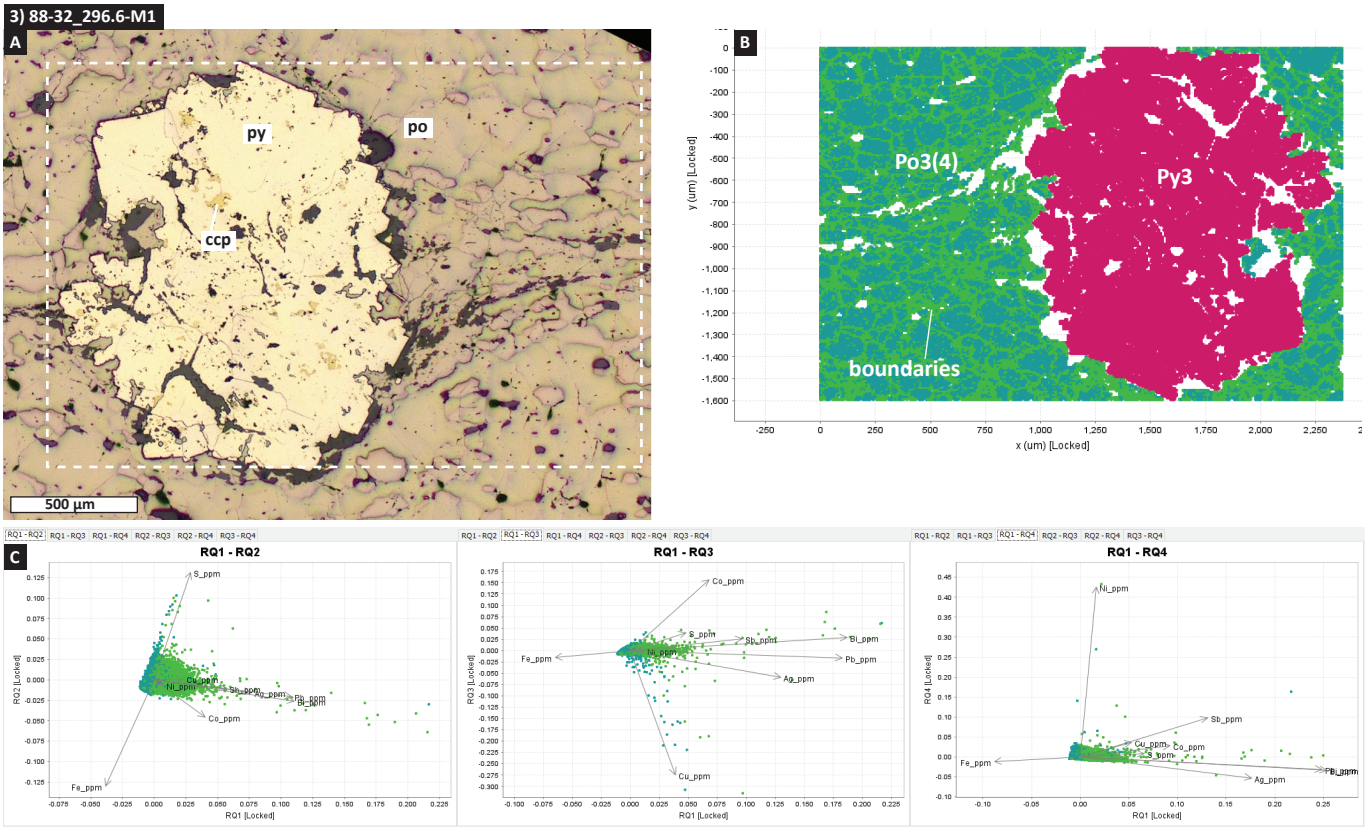

Fig. 3. Sample 88-32_296.6, map 1. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrite and pyrrhotite groups, distinguished through PCA and K-means clustering. C) PCA biplots showing the distinct compositional characteristics of the various pyrrhotite groups (all pyrite here belongs to a single group).

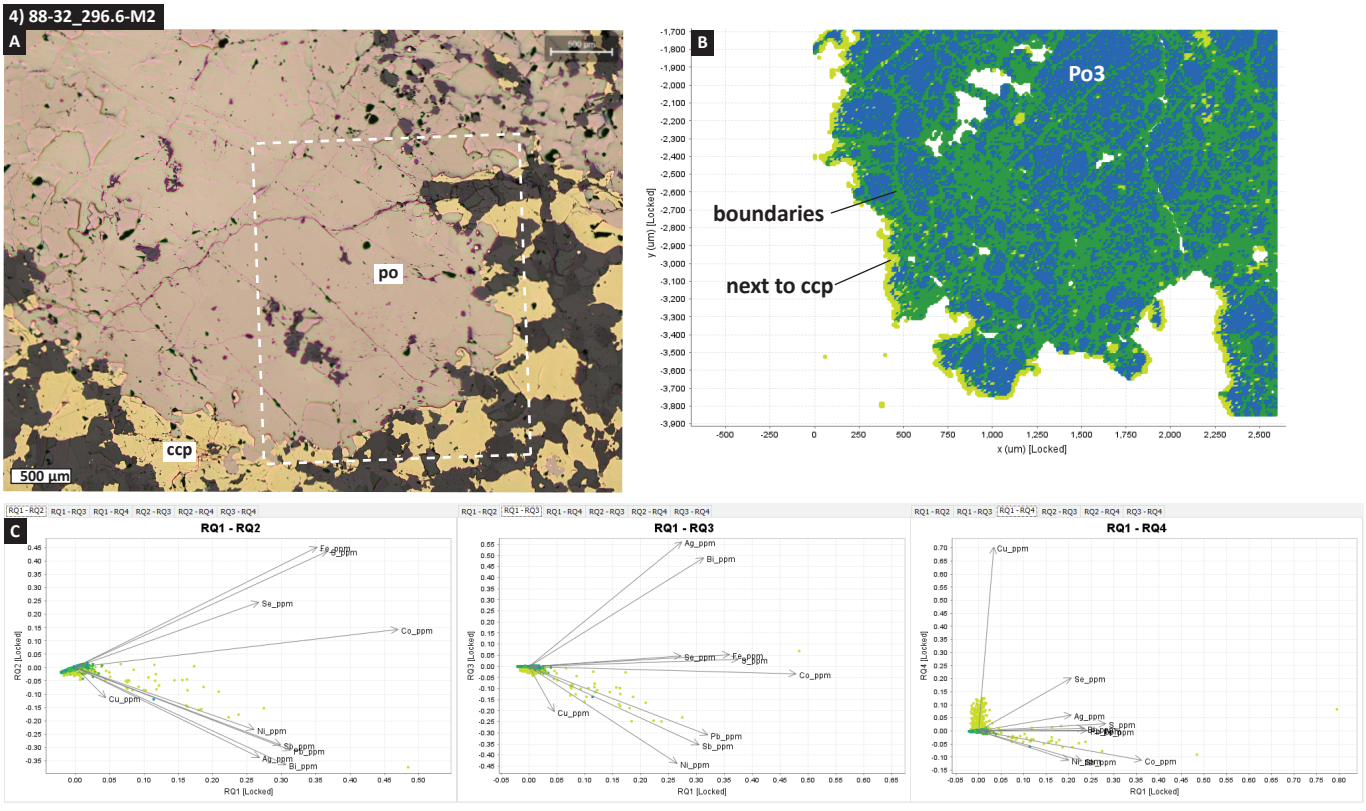

Fig. 4. Sample 88-32_296.6, map 2. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrrhotite groups, distinguished through PCA and K-means clustering. C) PCA biplots showing the distinct compositional characteristics of the various groups.

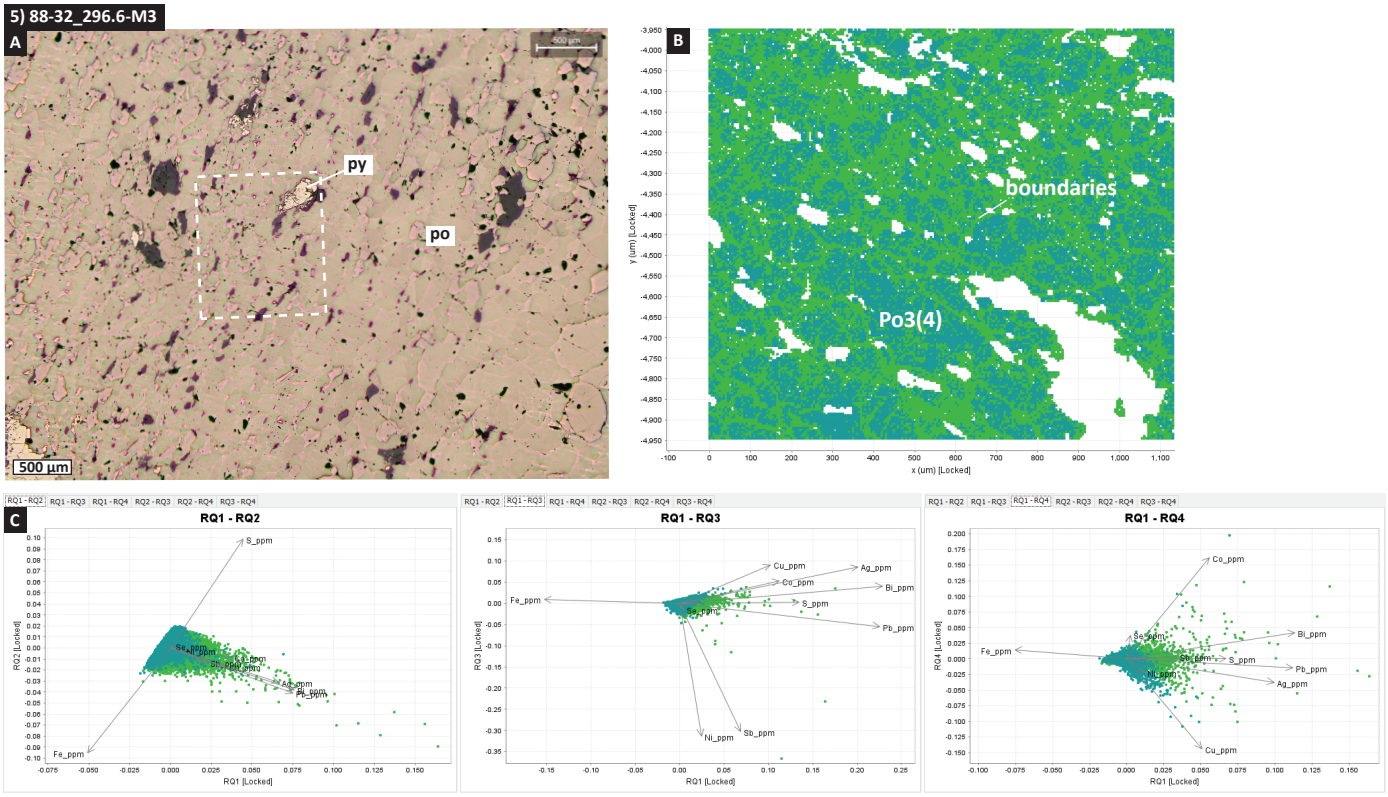

Fig. 5. Sample 88-32_296.6, map 3. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrrhotite groups, distinguished through PCA and K-means clustering. C) PCA biplots showing the distinct compositional characteristics of the various groups.

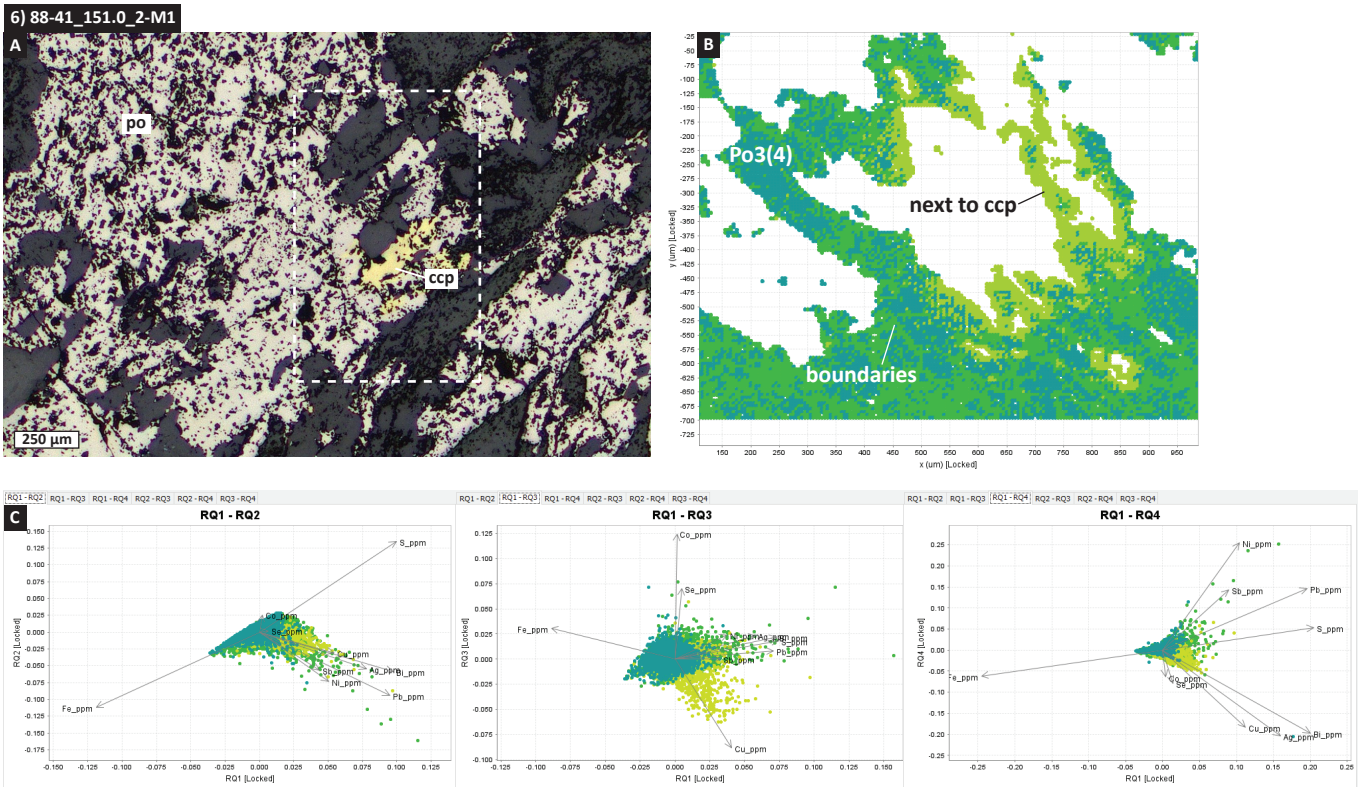

Fig. 6. Sample 88-41_151.0_2, map 1. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrrhotite groups, distinguished through PCA and K-means clustering. C) PCA biplots showing the distinct compositional characteristics of the various groups.

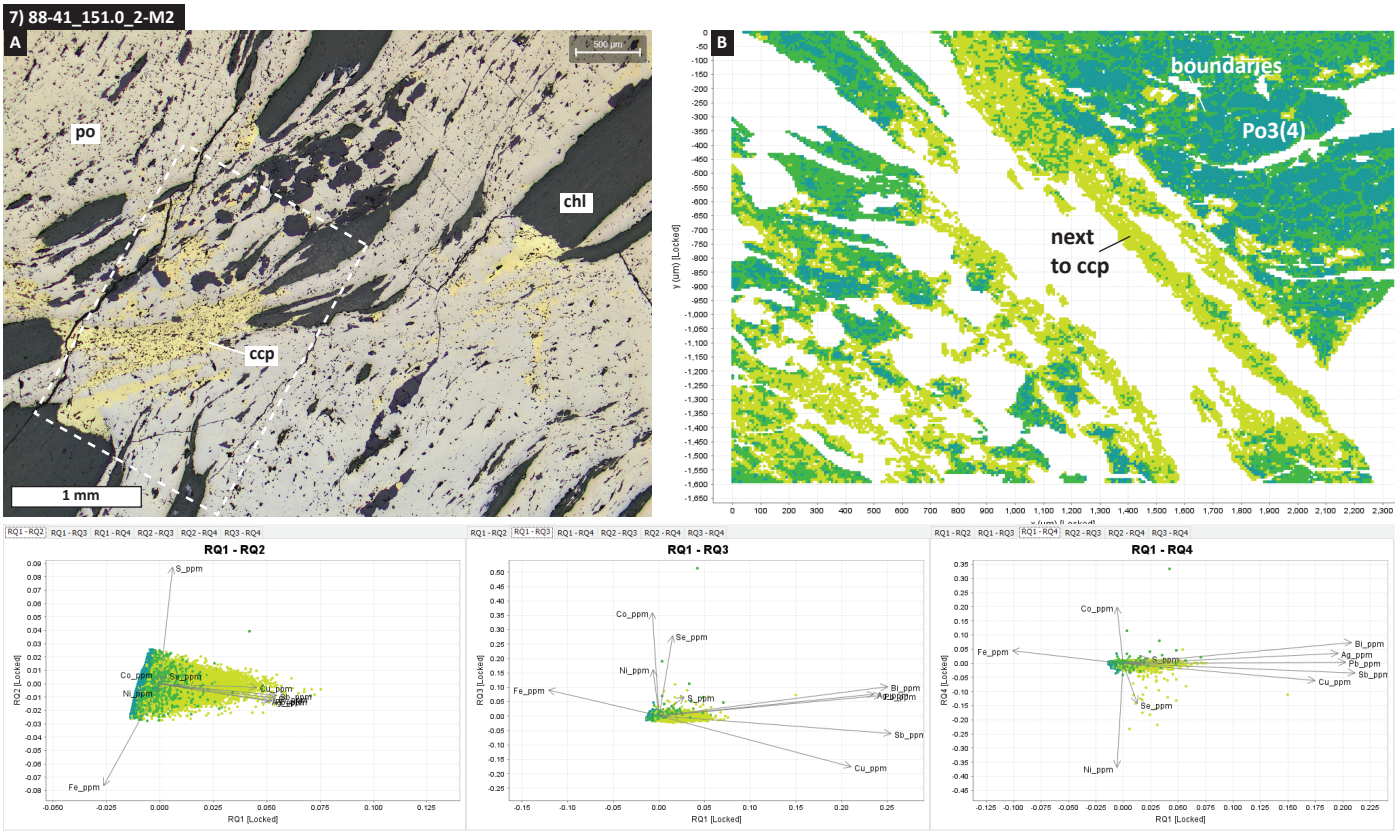

Fig. 7. Sample 88-41_151.0_2, map 2. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrrhotite groups, distinguished through PCA and K-means clustering. C) PCA biplots showing the distinct compositional characteristics of the various groups.

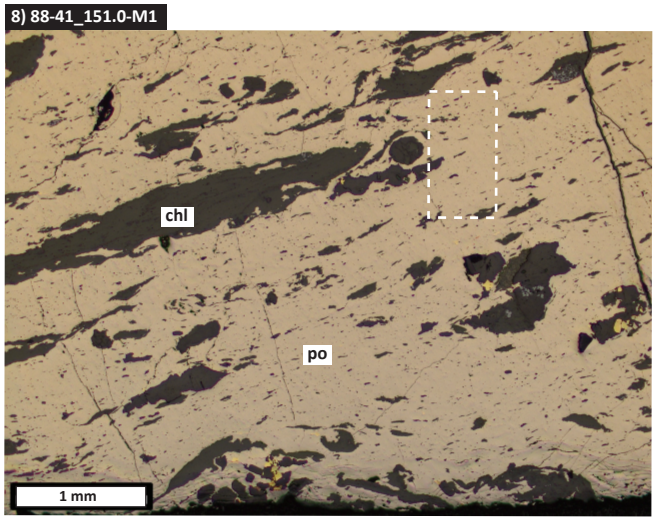

Fig. 8. Sample 88-41_151.0, map 1. Photomicrograph showing location of LA-ICP-MS map. No PCA or K-means clustering was applied to this map.

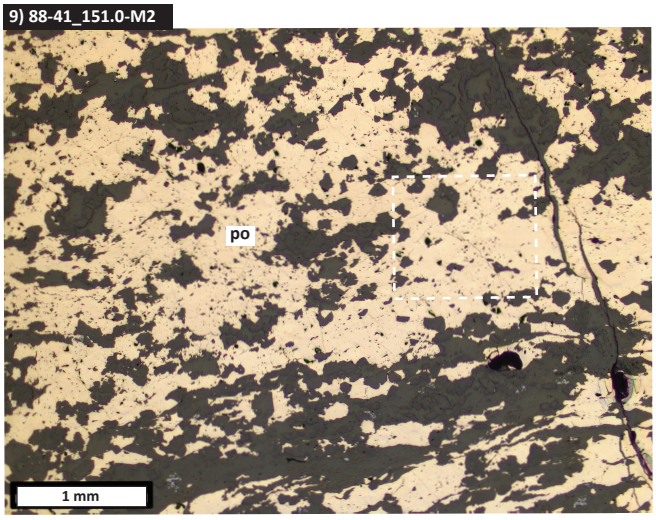

Fig. 9. Sample 88-41_151.0, map 2. Photomicrograph showing location of LA-ICP-MS map. No PCA or K-means clustering was applied to this map.

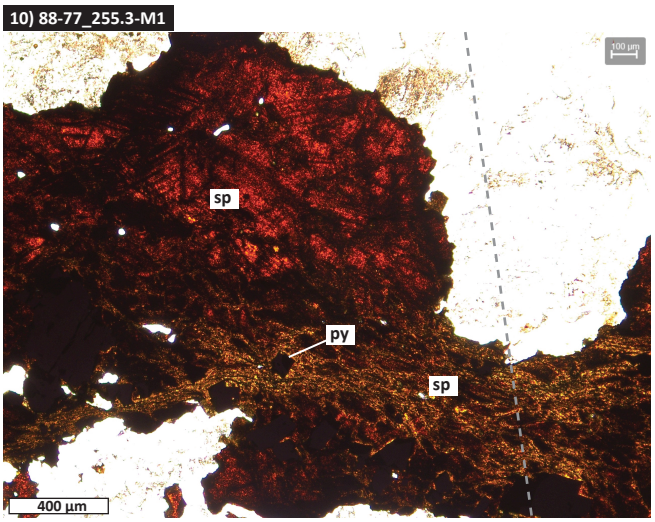

Fig. 10. Sample 88-77_255.3, map 1. Photomicrograph showing location of LA-ICP-MS map. No PCA or K-means clustering was applied to this map.

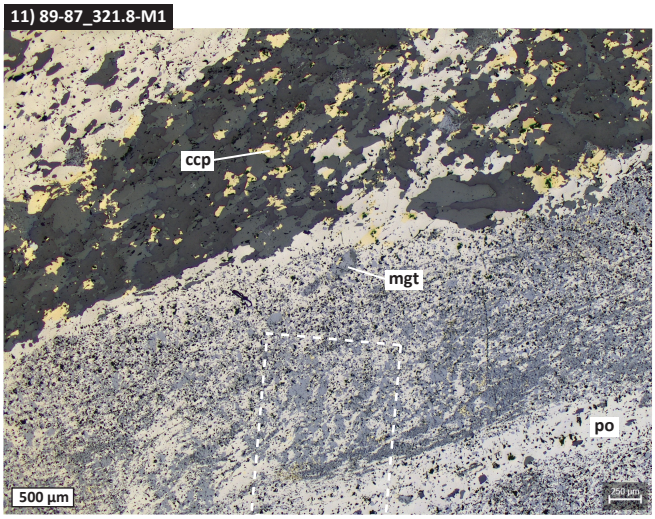

Fig. 11. Sample 89-87_321.8, map 1. Photomicrograph showing location of LA-ICP-MS map. No PCA or K-means clustering was applied to this map.

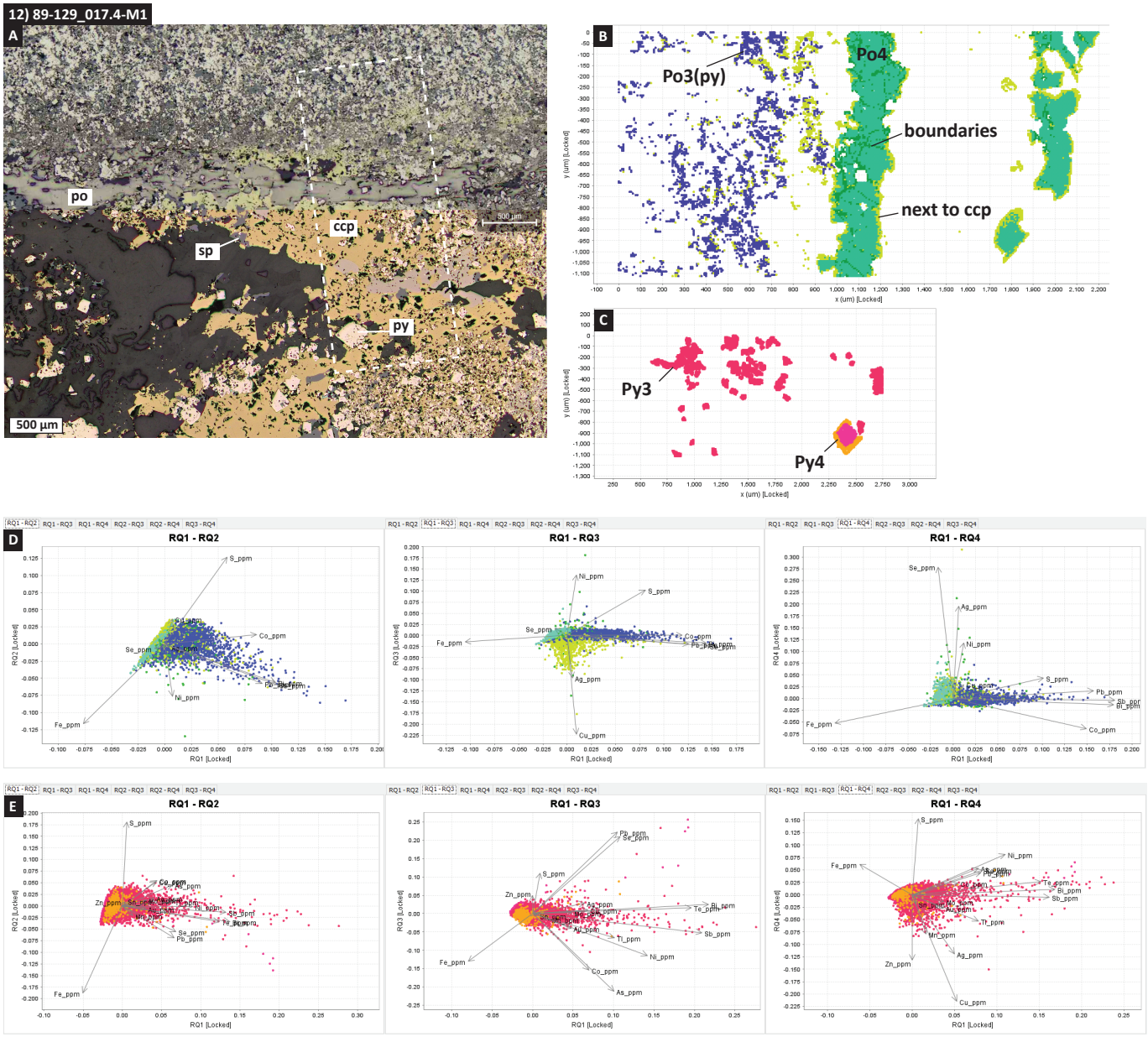

Fig. 12. Sample 89-129_017.4, map 1. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrrhotite groups, distinguished through PCA and K-means clustering. C) Map of the same area, showing colour-coded pyrite groups. D) PCA biplots for pyrrhotite showing the distinct compositional characteristics of the various groups. E) PCA biplots for pyrite showing the distinct compositional characteristics of the various groups.

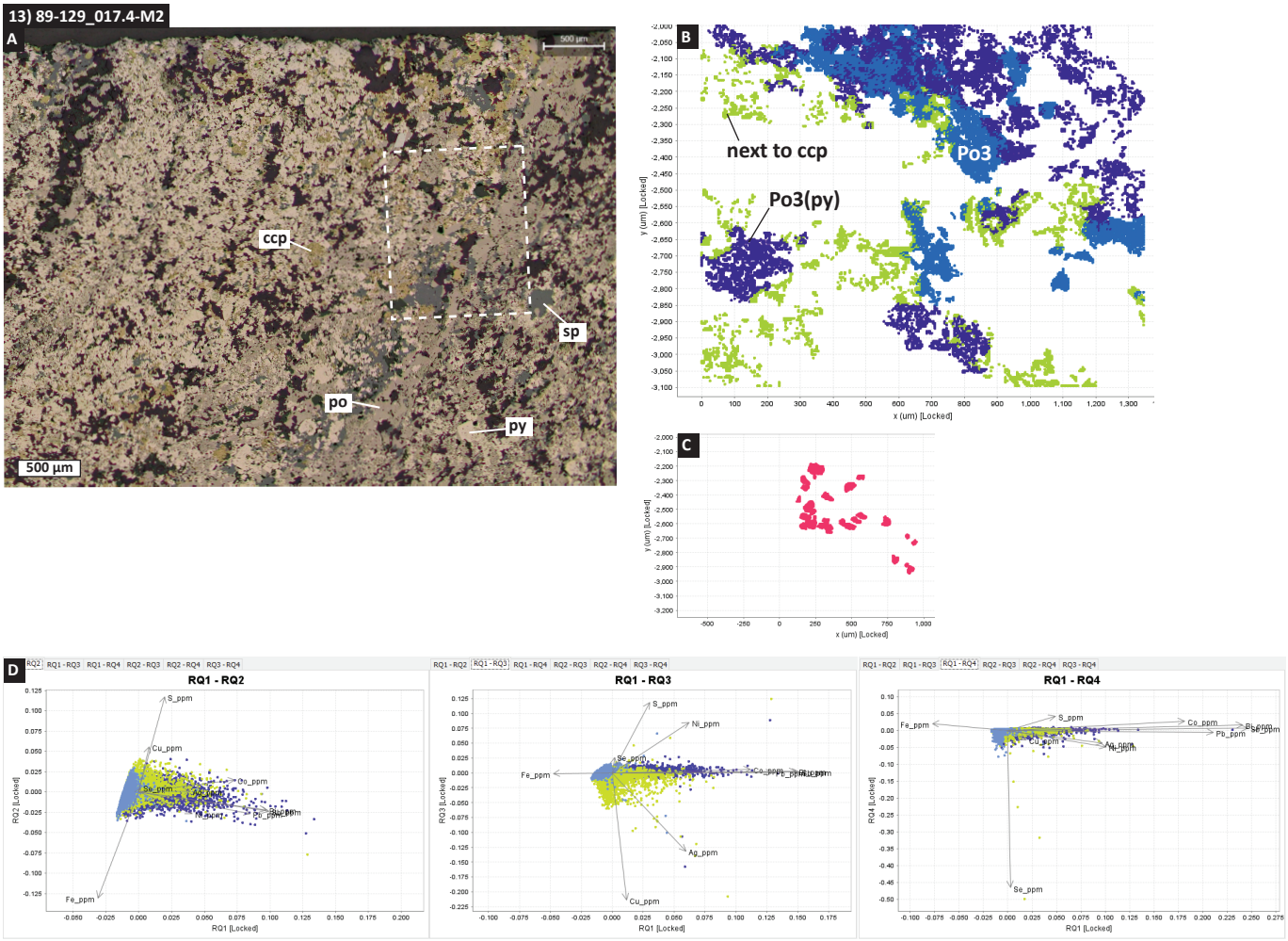

Fig. 13. Sample 89-129_017.4, map 2. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrrhotite groups, distinguished through PCA and K-means clustering. C) Map colour-coded for pyrite groups. D) PCA biplots for pyrrhotite showing the distinct compositional characteristics of the various groups (all pyrite here belongs to a single group).

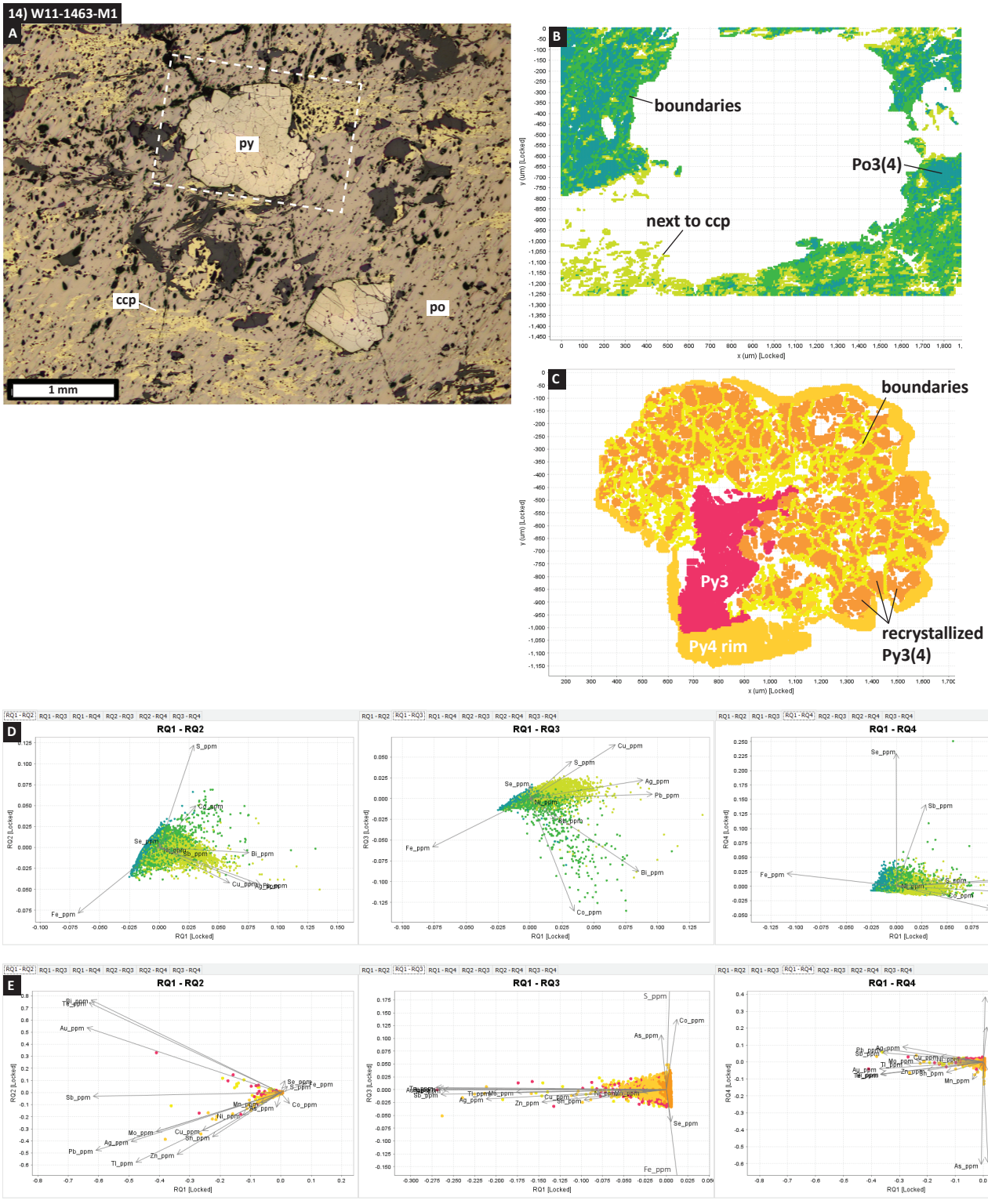

Fig. 14. Sample W11-1463, map 1. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrrhotite groups, distinguished through PCA and K-means clustering. C) Map colour-coded for pyrite groups, distinguished through PCA and K-means clustering. D) PCA biplots for pyrrhotite showing the distinct compositional characteristics of the various groups. E) PCA biplots for pyrite showing the distinct compositional characteristics of the various groups.

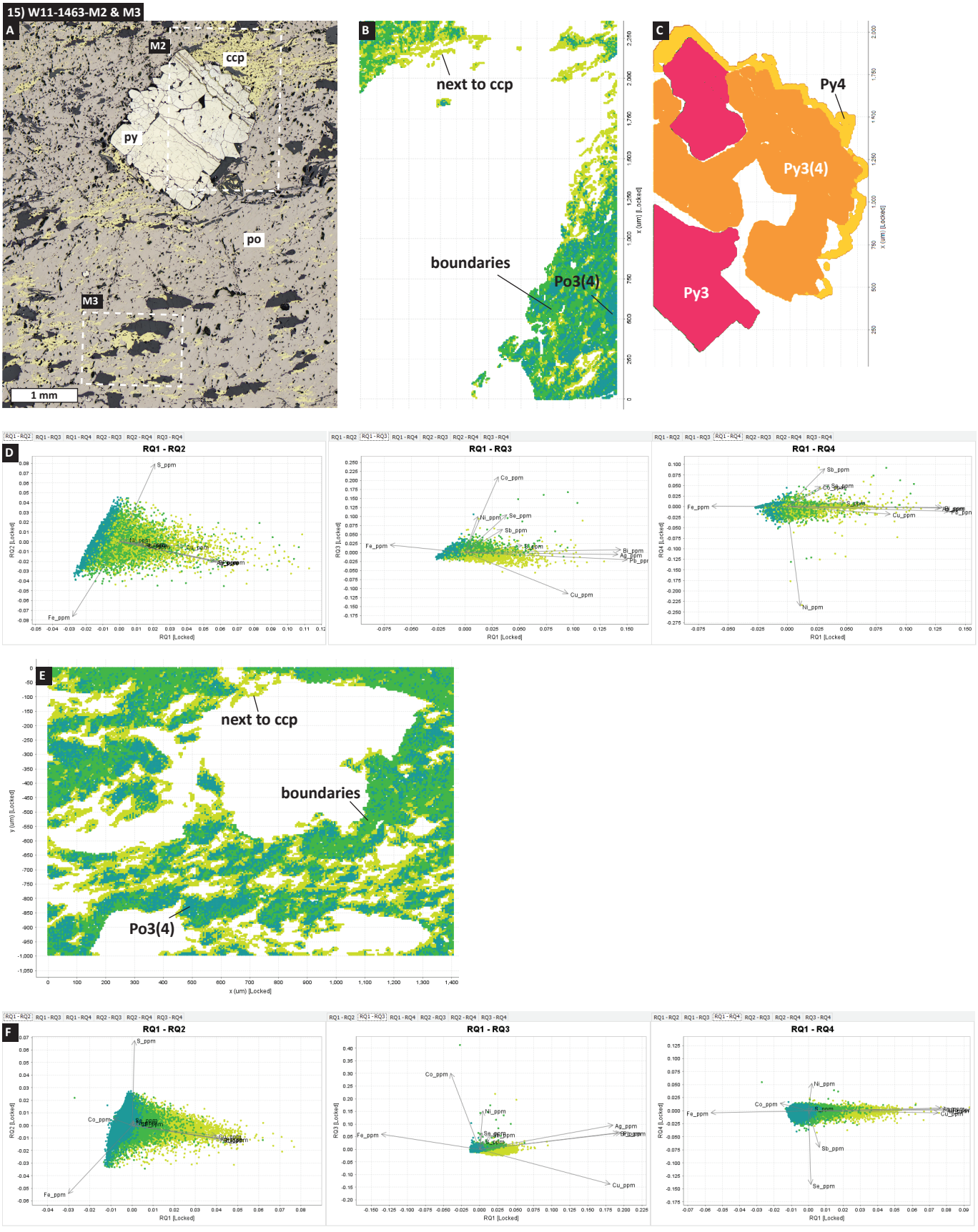

Fig. 15. Sample W11-1463, maps 2 and 3. A) Photomicrograph showing locations of LA-ICP-MS maps. B) Map 2, colour-coded for pyrrhotite groups, distinguished through PCA and K-means clustering. C) Map 2, colour-coded for pyrite groups, distinguished through PCA and K-means clustering. D) Map 2, PCA biplots for pyrrhotite showing the distinct compositional characteristics of the various groups. PCA and K-means clustering were not used on pyrite in Map 2, because they failed to accurately distinguish the different groups. Instead, they were manually selected. E) Map 3, colour-coded for pyrrhotite groups, distinguished through PCA and K-means clustering. F) Map 3, PCA biplots for pyrrhotite showing the distinct compositional characteristics of the various groups.

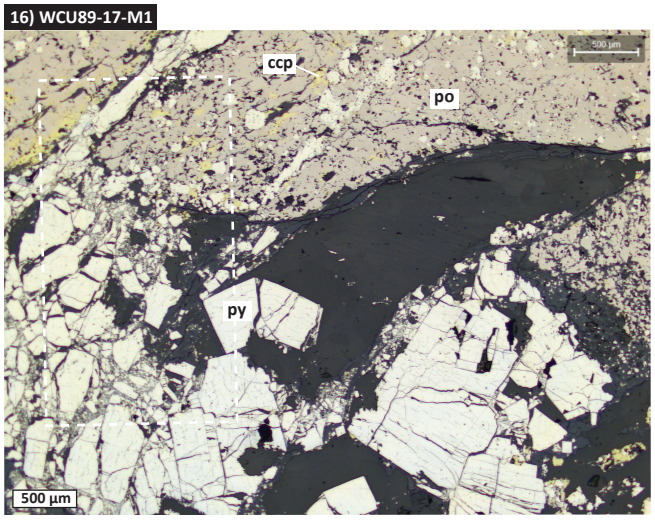

Fig. 16. Sample WCU89-17, map 1. Photomicrograph showing location of LA-ICP-MS map. No PCA or K-means clustering was applied to this map.

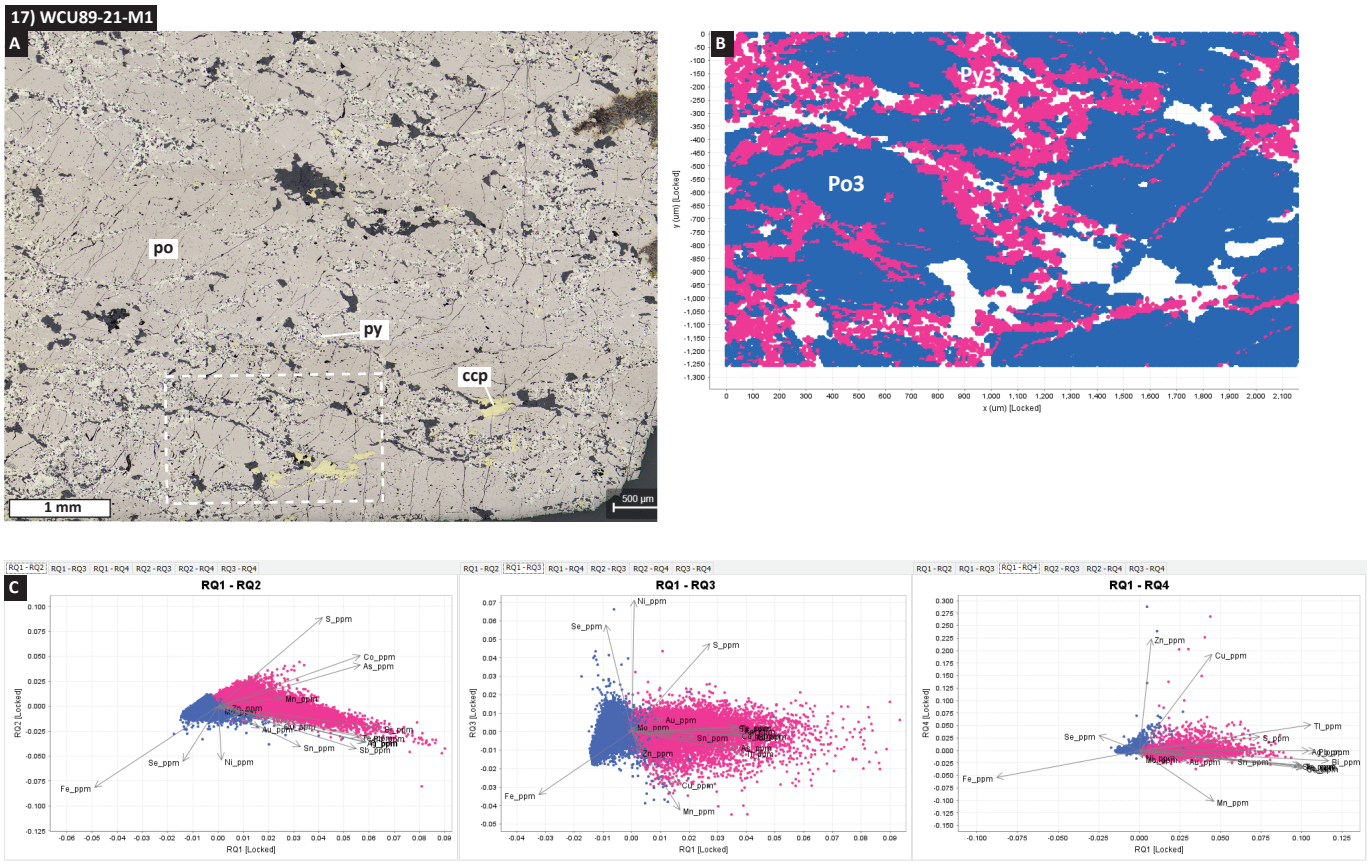

Fig. 17. Sample WCU89-21, map 1. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrite and pyrrhotite, distinguished through filtering. C) PCA biplots showing the distinct compositional characteristics of the pyrite and pyrrhotite (only 1 pyrite group and 1 pyrrhotite group are present in this sample).

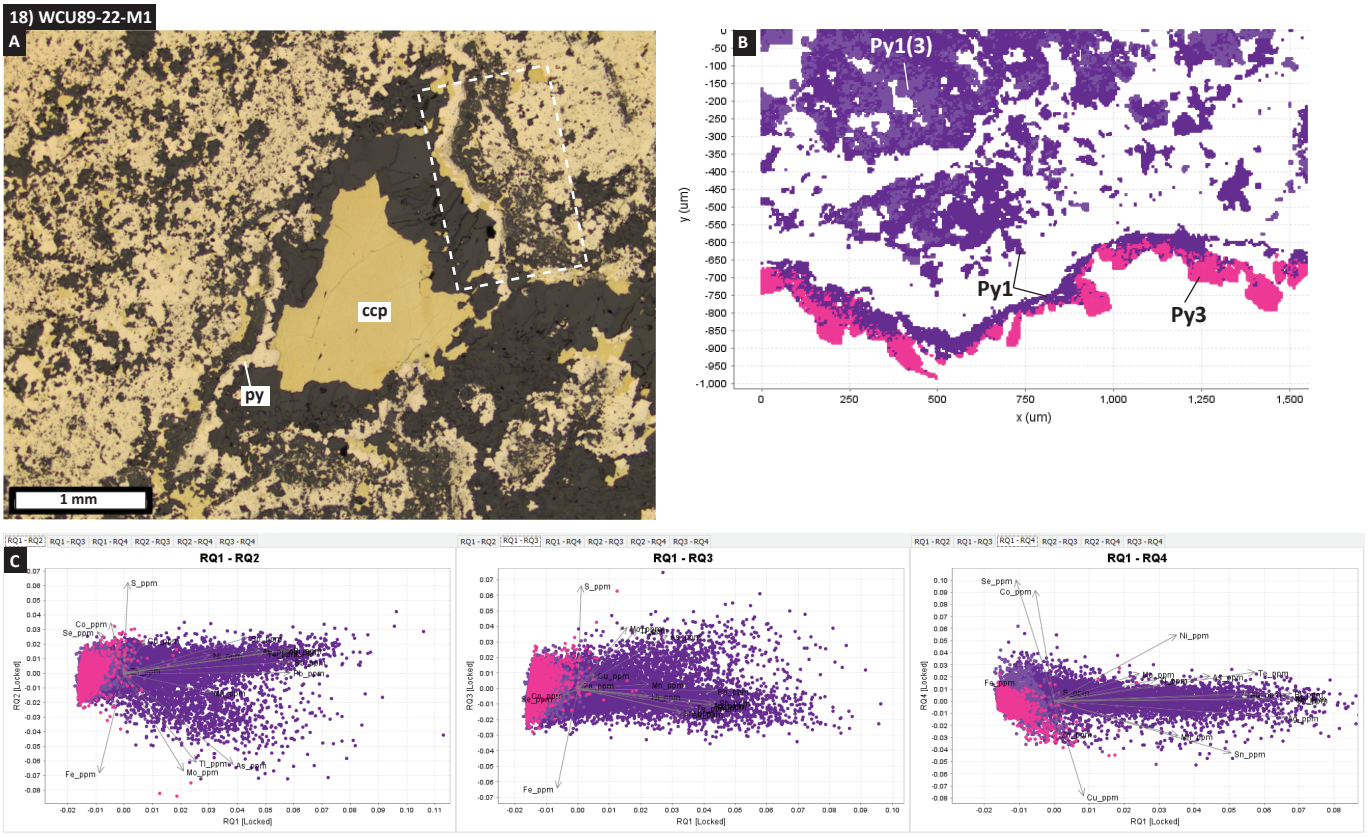

Fig. 18. Sample WCU89-22, map 1. A) Photomicrograph showing location of LA-ICP-MS map. B) Map colour-coded for pyrite groups, distinguished through PCA and -means clustering. C) PCA biplots showing the distinct compositional characteristics of the various groups.

Legend

- Py1
- Py1(3)
- Py2
- Py3
- Py3(4)
- Py4
- Po3(py)
- Po3
- Po3(4) deformed
- Po4 in fold hinges
- Grain- & subgrain boundaries
- Next to Ccp

Mineral Abbreviations

cc: calcite, ccp: chalcopyrite, chl: chlorite, mgt: magnetite, po: pyrrhotite, py: pyrite, sp: sphalerite,

Other Abbreviations

EBSD: electron backscatter diffraction
LA-ICP-MS: laser ablation - inductively coupled plasma - mass spectrometry
PCA: principal component analysis