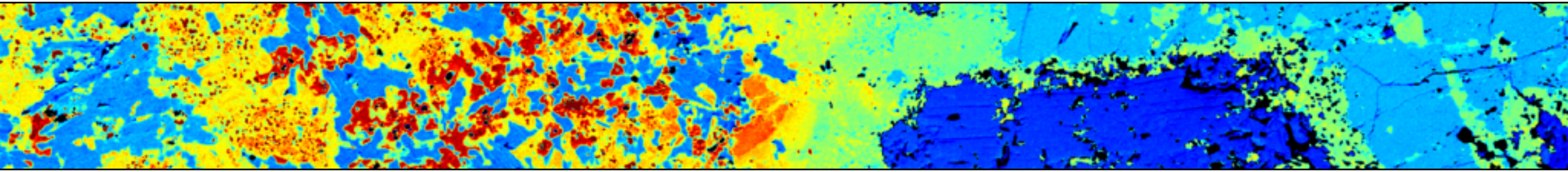

Lecture 3

X-ray map corrections and multi-channel classification

Dr. Pierre Lanari

University of Bern - pierre.lanari@geo.unibe.ch

- Motivation and application examples
- X-ray maps: loading and automated indexation
- Displaying X-ray maps, adjusting color contrast and mineral identification
- Automated classification (normalized and classic methods) for manipulating single-phase data
- Manual adjustment of maskfile using the Binary module
- Manual classification
- Corrections (BRC; IDC; TRC)

Motivation and application examples

Motivations:

1. Quickly retrieve modal abundances from semi-quantitative maps
2. Prepare the X-ray maps (classify and correct) for the analytical standardization

Motivation and application examples

Available online at www.sciencedirect.com

ScienceDirect

Geochimica et Cosmochimica Acta 120 (2013) 496–513

Geochimica et Cosmochimica Acta

www.elsevier.com/locate/gca

REE and Hf distribution among mineral phases in the CV–CK clan: A way to explain present-day Hf isotopic variations in chondrites

Céline Martin [a,*], Vinciane Debaille [b], Pierre Lanari [c], Steven Goderis [a,e], Isabelle Vandendael [d], Frank Vanhaecke [e], Olivier Vidal [f], Philippe Claeys [a]

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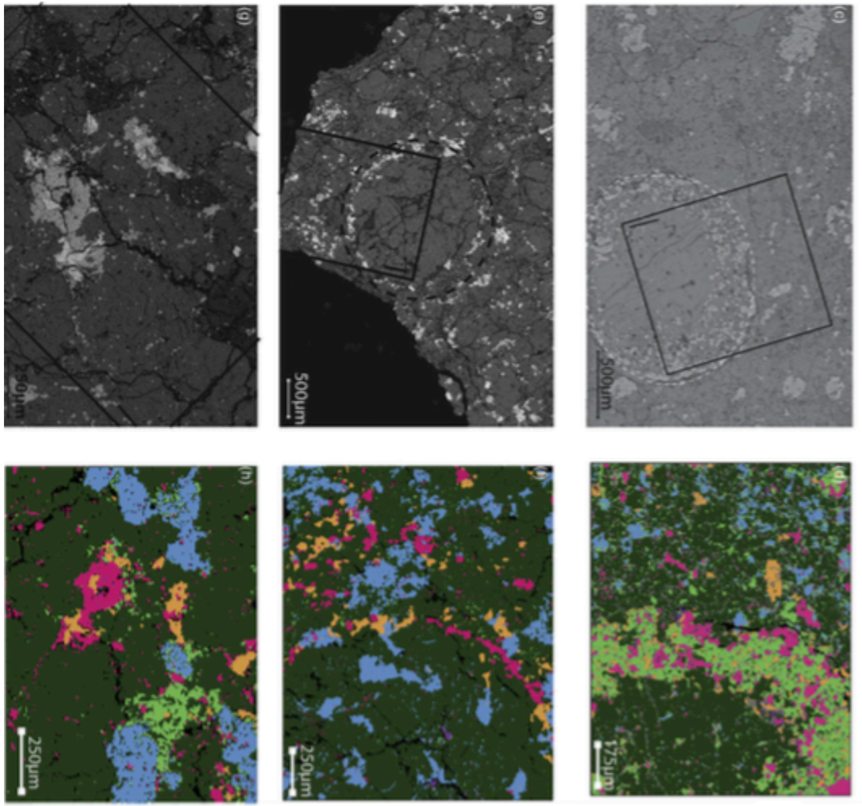
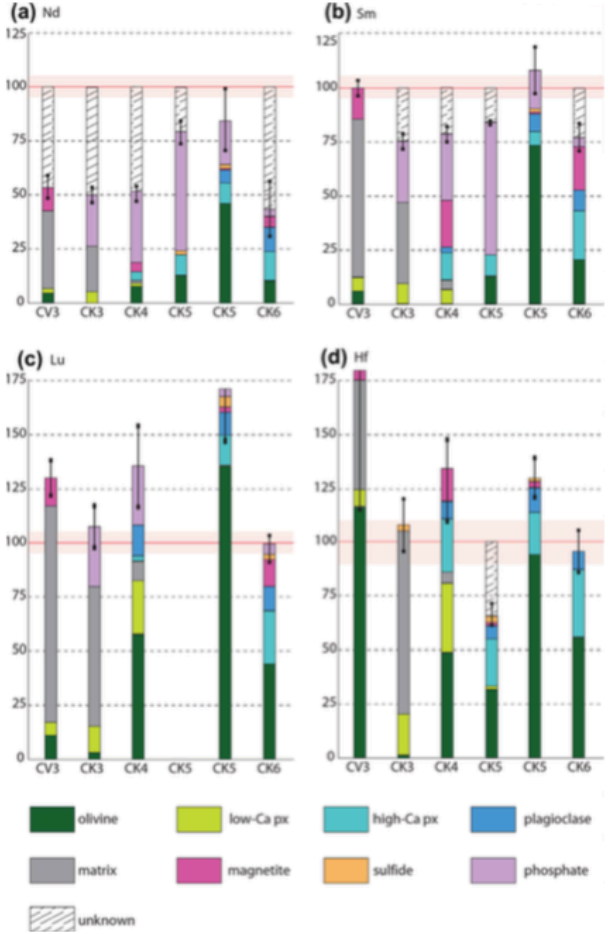
Received 20 September 2012; accepted in revised form 4 July 2013; available online 15 July 2013

Mineral modes from X-ray maps



LA-ICP-MS spot analyses



Martin et al. (2013), GCA

Lithos 282–283 (2017) 262–280

Contents lists available at ScienceDirect

Lithos

journal homepage: www.elsevier.com/locate/lithos

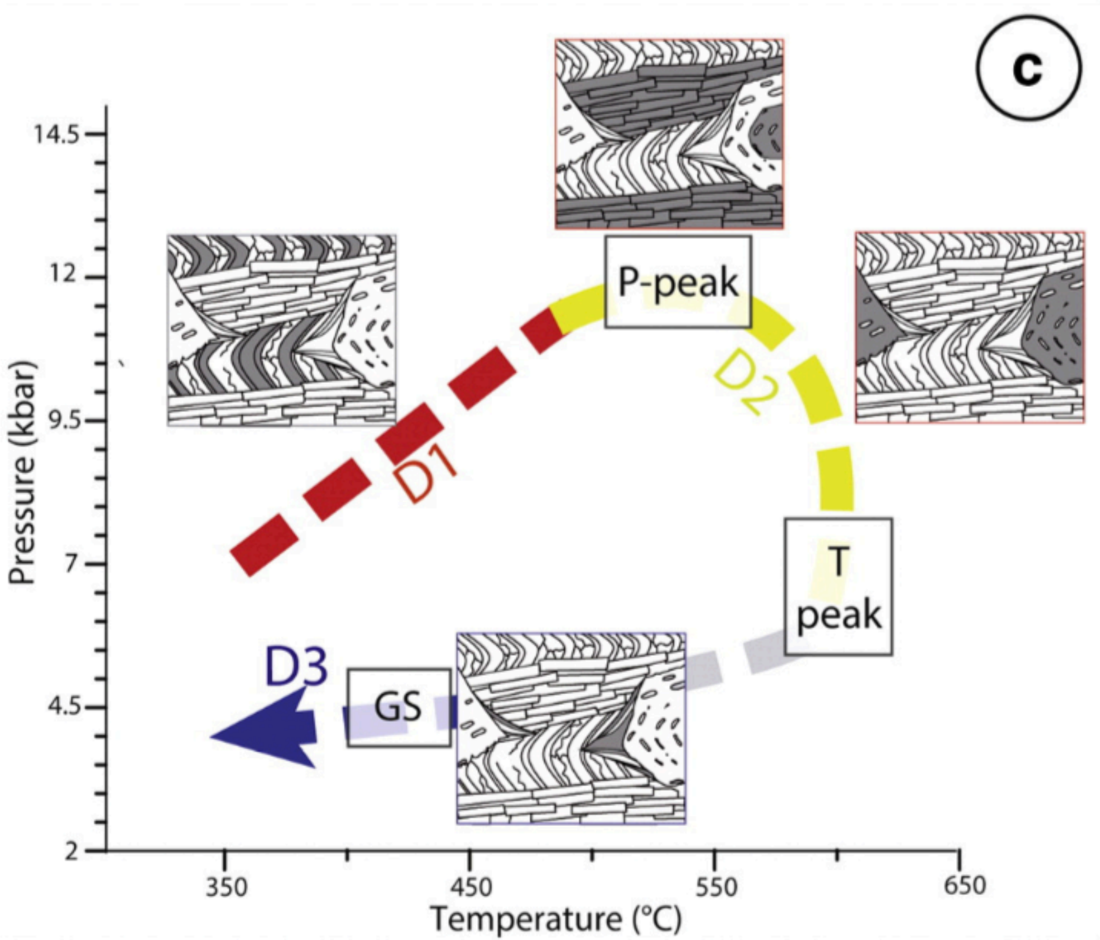
ELSEVIER

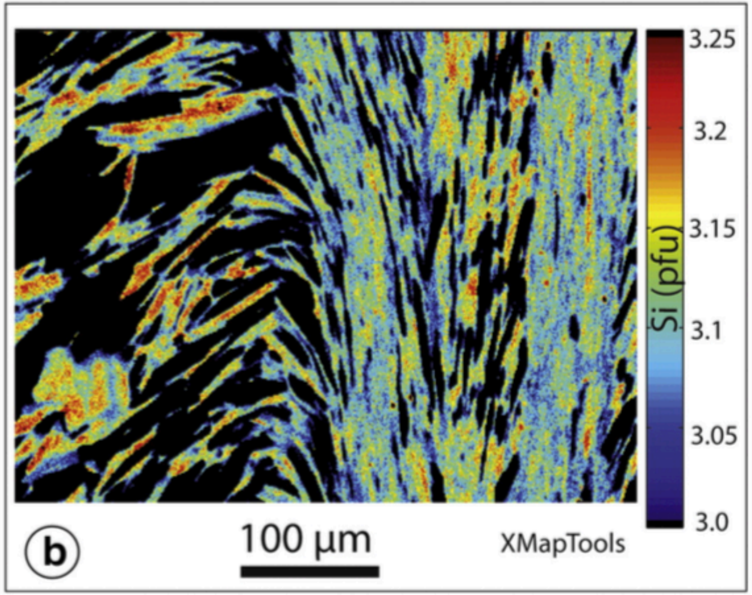
Microstructural vs compositional preservation and pseudomorphic replacement of muscovite in deformed metapelites from the Longmen Shan (Sichuan, China)

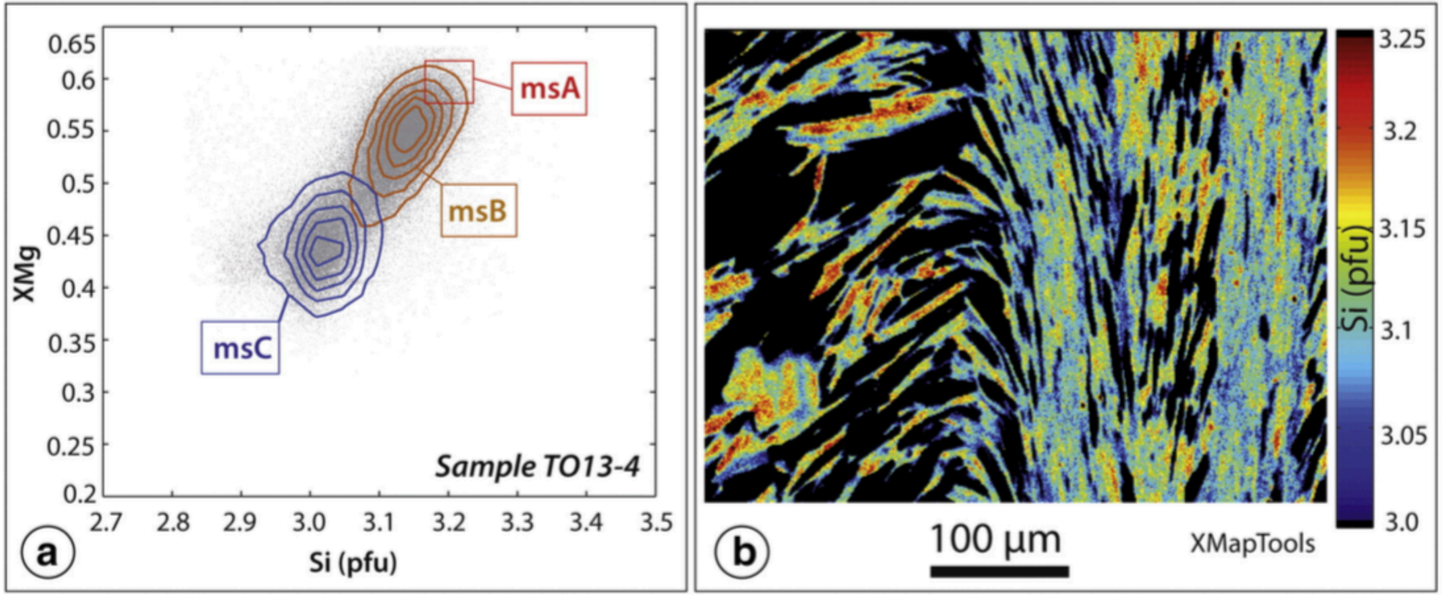
CrossMark

Laura Airaghi [a,*], Pierre Lanari [b], Julia de Sigoyer [a], Stéphane Guillot [a]

[a] Univ. Grenoble Alpes, CNRS, ISTerre, F-38000 Grenoble, France
[b] Institute of Geological Sciences, University of Bern, Baltzerstrasse 1+3, CH-3012 Bern, Switzerland


c
14.5
12
9.5
7
4.5
2
Pressure (kbar)
350
450
550
650
Temperature (°C)
P-peak
D1
D2
T
peak
D3
GS

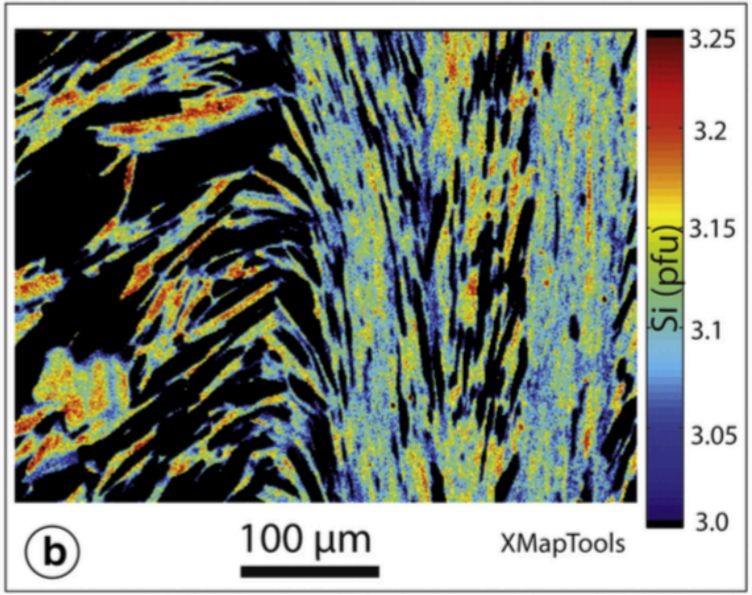

3.25
3.2
3.15
3.1
3.05
3.0
Si (pfu)
b
100 µm
XMapTools



0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
XMg
msA
msB
msC
Sample TO13-4
2.7
2.8
2.9
3.0
3.1
3.2
3.3
3.4
3.5
Si (pfu)
a
3.25
3.2
3.15
3.1
3.05
3.0
Si (pfu)
100 µm
XMapTools
b

Table 3
Degree of muscovite preservation (fraction of pixel surface with a given chemical composition, see text for details).

Microstructural position	ms_A	ms_B	ms_C
Sample: to13-4			
S1 cleavage	0.48	0.52	0
S2 cleavage	0.15	0.80	0.05
P-shadows	0	0	1
Sample: to13-7			
S1 cleavage	0.23	0.77	0
S2 cleavage	0.15	0.85	0
P-shadows	0	0	1
Sample: lm09-223			
S1 cleavage	0	0	1
S2 cleavage	0	0	1
P-shadows	0	0.15	0.85

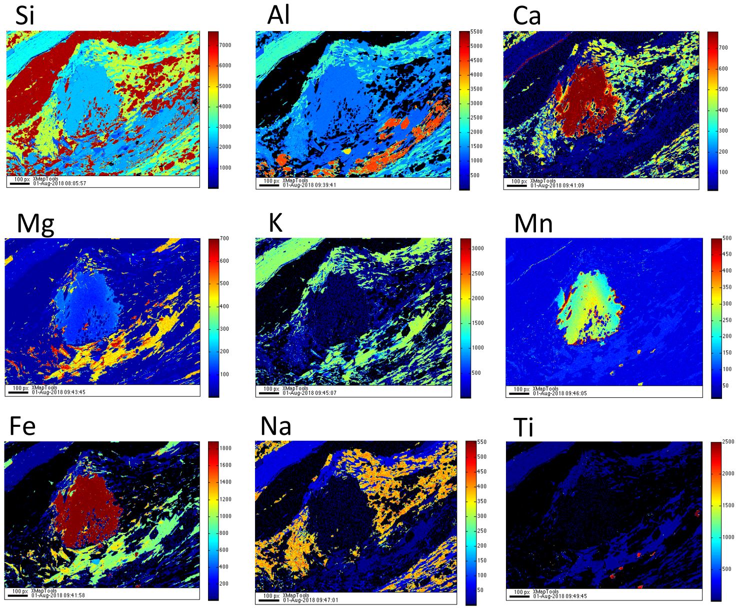


Motivation and application examples

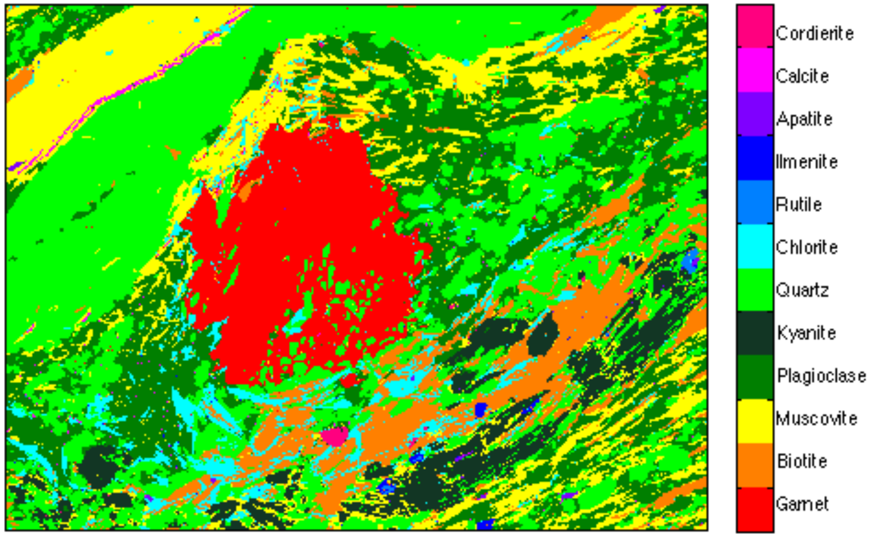
Motivations:

1. Quickly retrieve modal abundances from semi-quantitative maps
2. Prepare the X-ray maps (classify and correct) for the analytical standardization

X-ray maps (multi-channel)



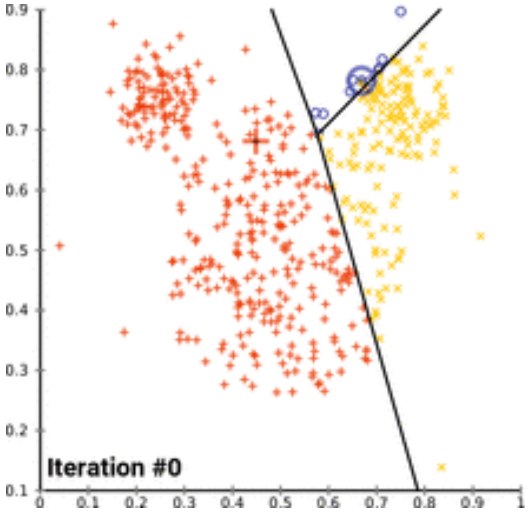
Classified image



Automated classification in XMAPTOOLS: K-means clustering

XMapTools

k-means clustering aims to partition n observations into k clusters in which each observation belongs to the cluster with the nearest mean, serving as a prototype of the cluster



k initial phases compositions

- Number of clusters
- Initial centers of the clusters

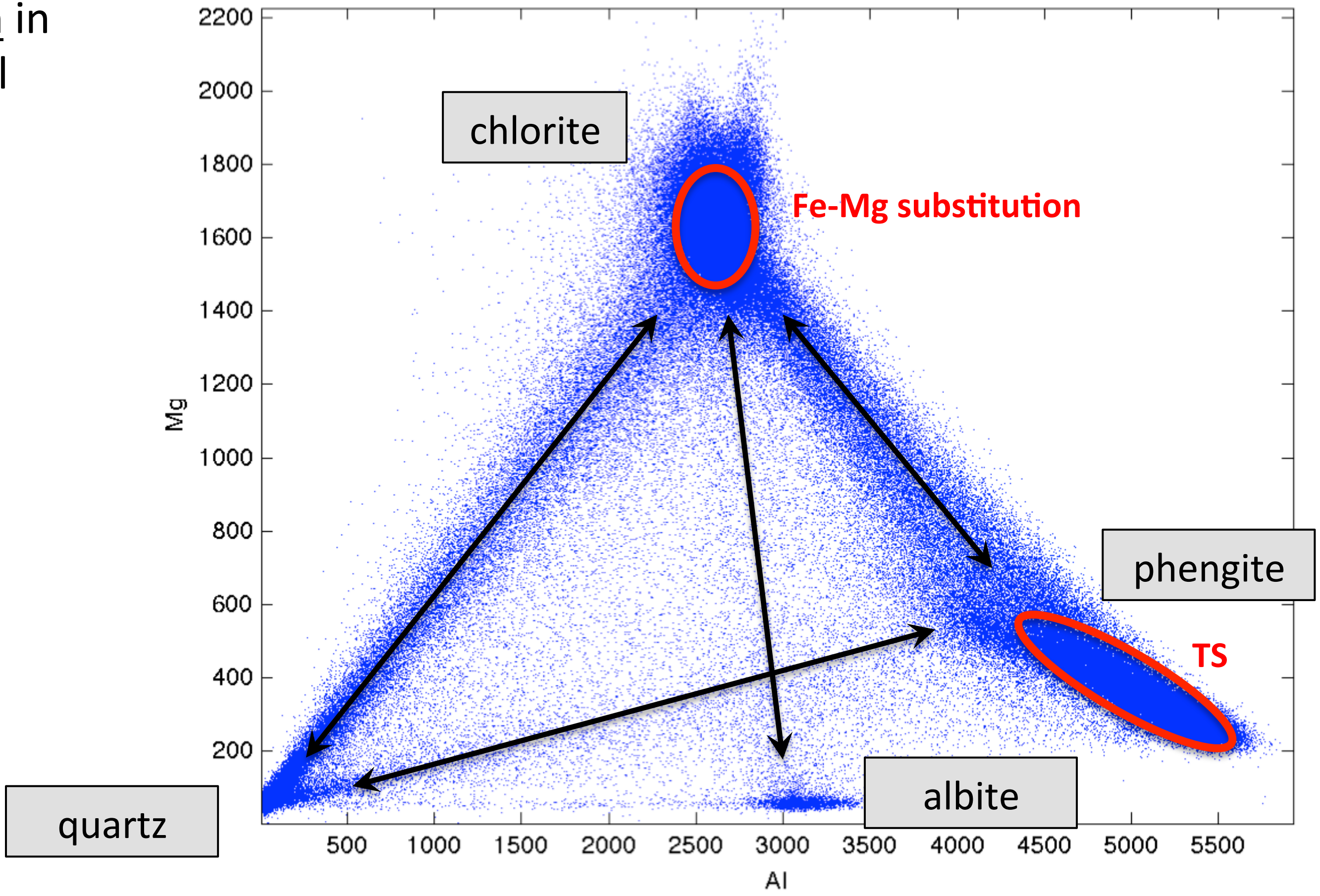
Iterative loop

Allocate all the pixel compositions to the k clusters *(nearest mean)*

Until convergence

Recalculate the centroids positions

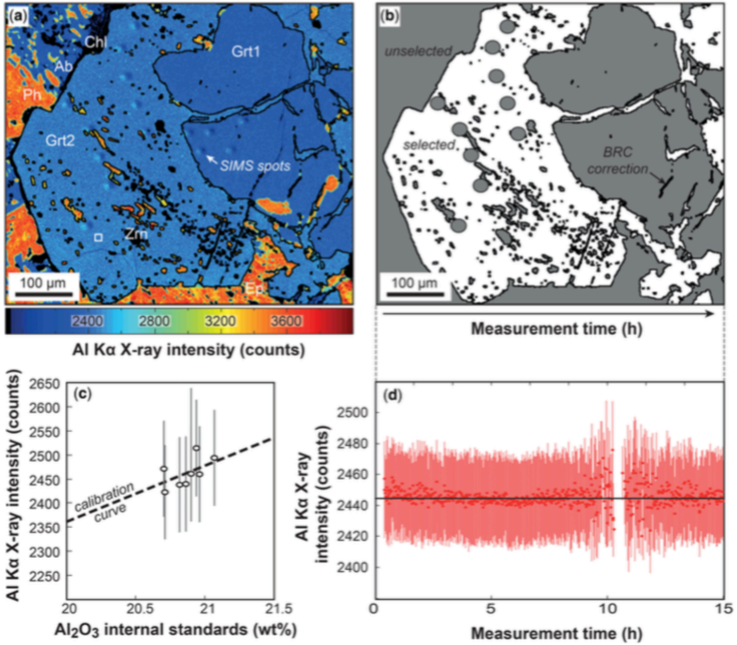
<u>Manual classification</u> in XMAPTOOLS: chemical modules



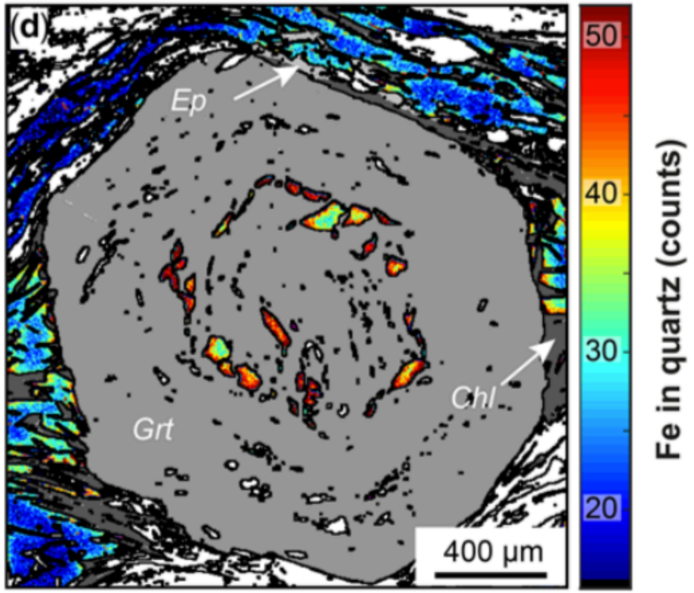
<u>Motivations</u>:

1. Quickly retrieve modal abundances from semi-quantitative maps
2. Prepare the X-ray maps (classify and correct) for the analytical standardization

Drift



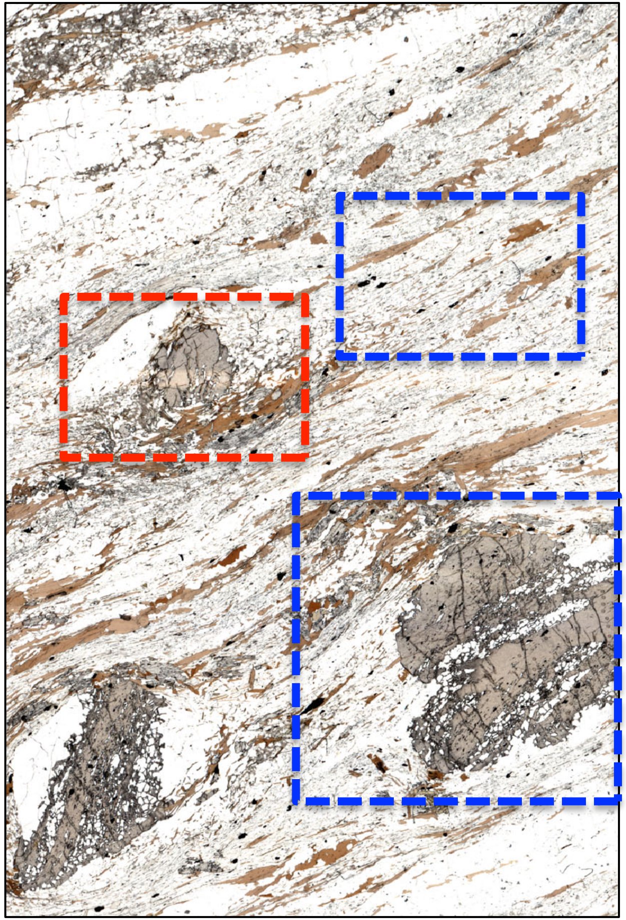
Secondary fluorescence effects



Lanari et al. (2018), GSL

Key steps

- Import the maps into XMapTools
- Identify the mineral phases
- Automated classification
- Manual classification using the Binary module
- Corrections



Sample MA9330

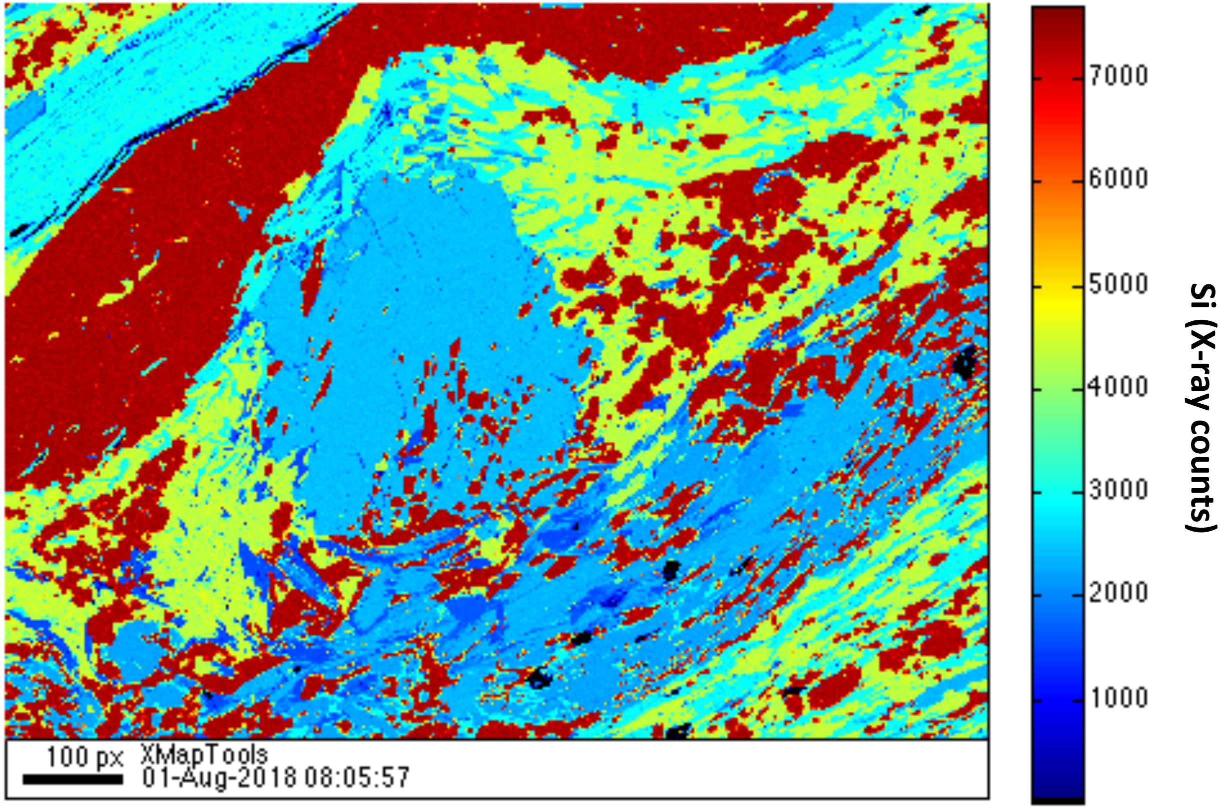
Metapelite from the Central Alps (Switzerland)

Todd & Engi, (1997) JMG; Boston et al. (2017), Lithos

Prograde	garnet, muscovite, quartz, ± plagioclase, ± biotite
Peak	biotite, muscovite, quartz, kyanite, cordierite, plagioclase
Retrograde	biotite, chlorite

Map 1 – Mineral matrix –	1000 x 750 pixels, 6 μm step size 100 ms dwell time – **42 h**
Map 2 – Peak + Retrogression –	1000 x 750 pixels, 6 μm step size 100 ms dwell time – **42 h**
Map3 – Garnet porphyroblast –	1000 x 1000 pixels, 10 μm step size 60 ms dwell time– **33 h**

MOTIVATION AND APPLICATION EXAMPLES

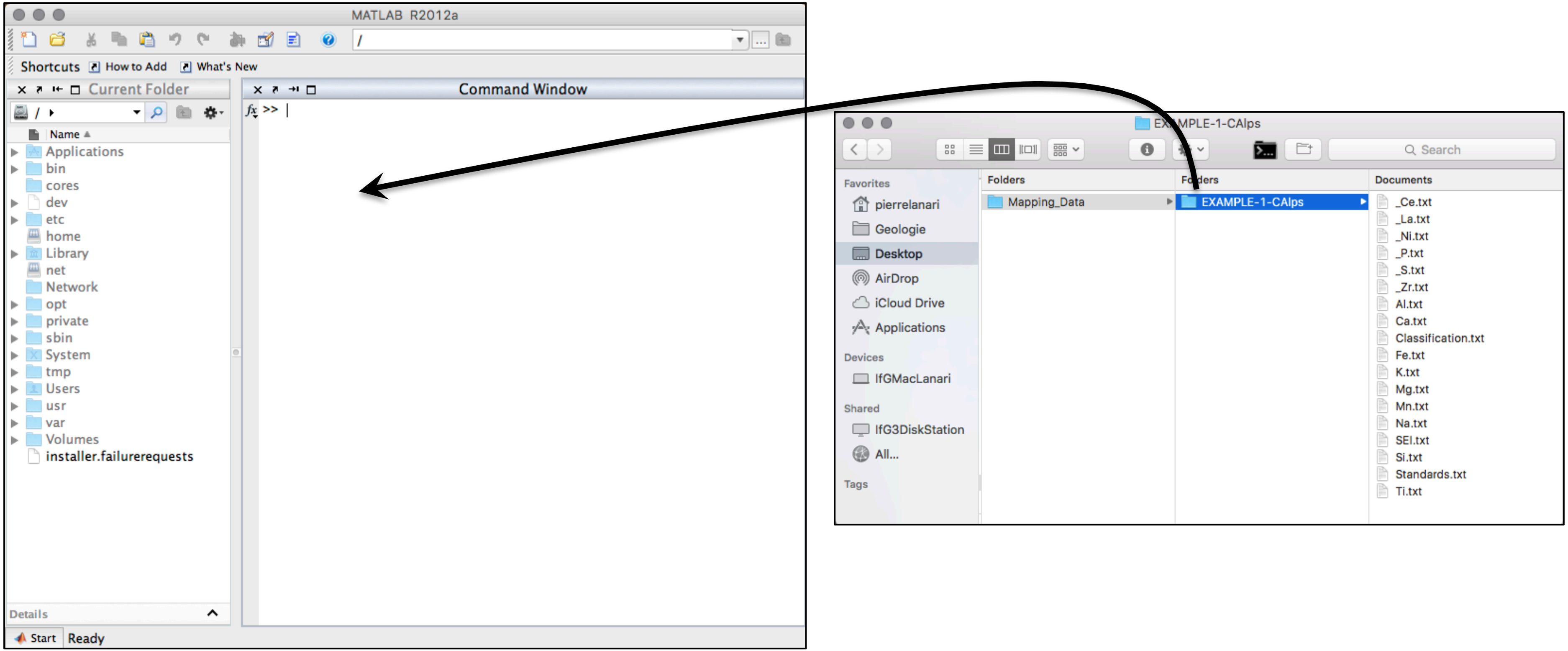


Key steps

- Import the maps into XMapTools
- Identify the mineral phases
- Automated classification
- Manual classification using the Binary module
- Corrections

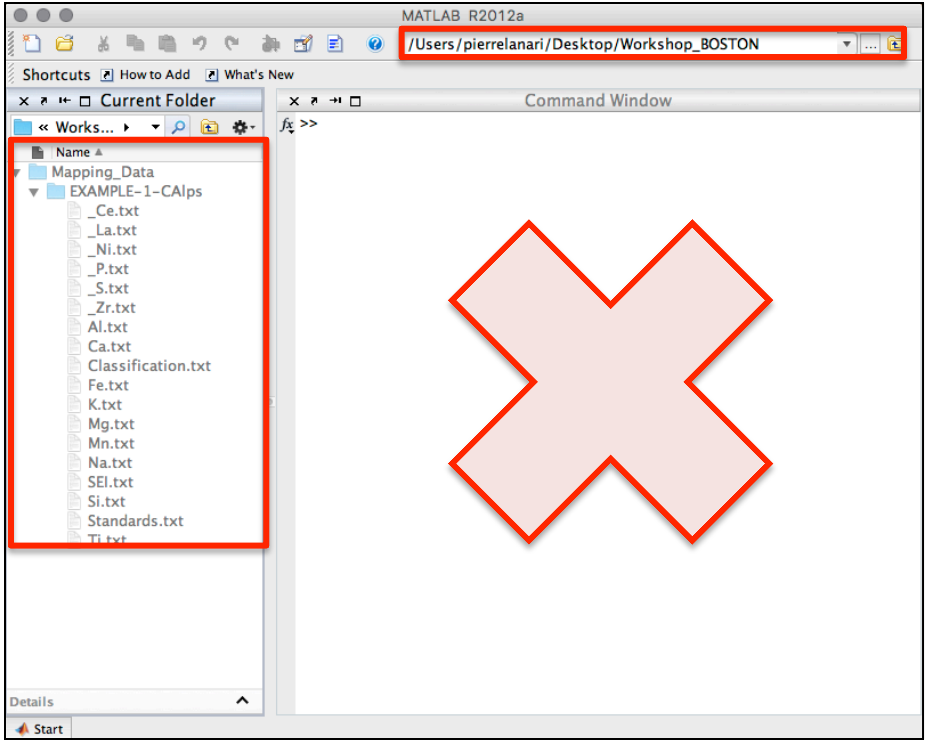
How to launch XMapTools?

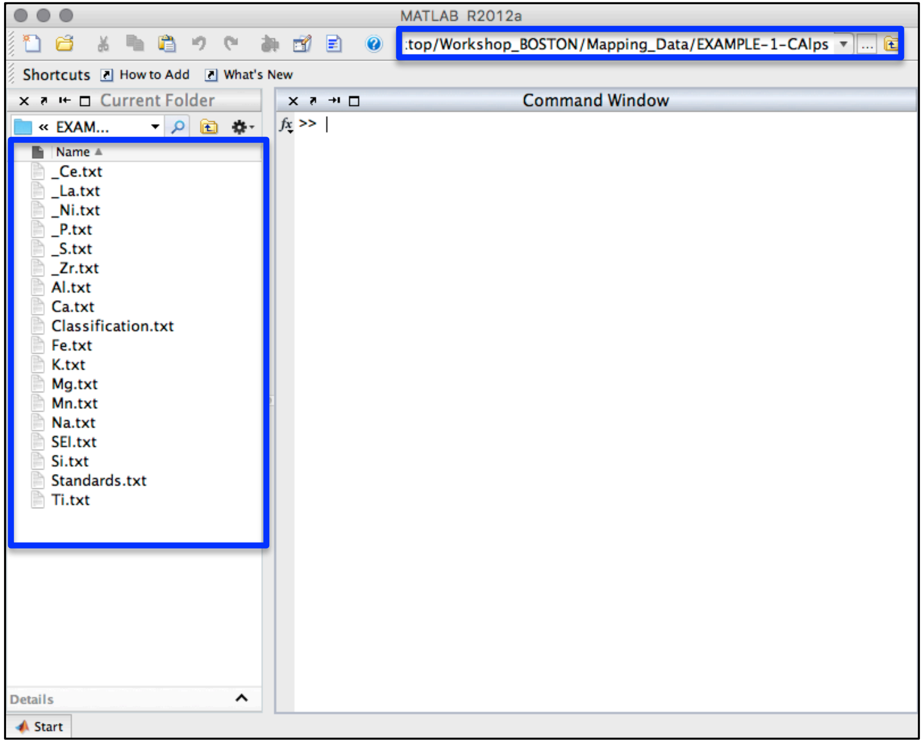
① In MATLAB©, go to the directory *Documents/MATLAB/Mapping_Data/Part1_EPMA/Example-1-CAlps/*



HOW TO LAUNCH XMAPTOOLS?

① In MATLAB©, go to the directory *Documents/MATLAB/Mapping_Data/Part1_EPMA/Example-1-CAlps/*



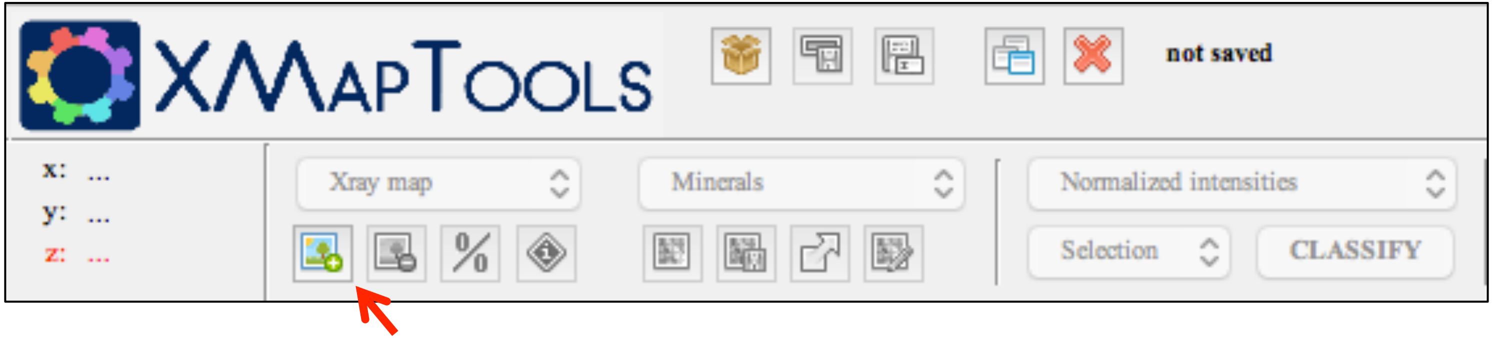


X-RAY MAPS: LOADING AND AUTOMATED INDEXATION

① Launch XMAPTOOLS using the command: *>> XMapTools*

② Import the following X-ray maps using the function *Import map(s)*: _Ce.txt, _La.txt, _Ni.txt, _P.txt, _S.txt, _Zr.txt Al.txt Ca.txt, Fe.txt, K.txt, Mg.txt, Mn.txt, Na.txt, SEI.txt, Si.txt, Ti.txt, TOPO.txt (select automated indexation)

③ Activate the dead time correction (Check 0.cnd for dwell time; dead time: 300 ns) and press *Apply Corrections*



X-RAY MAPS: LOADING AND AUTOMATED INDEXATION

- The list of elements and corresponding oxide is defined in /XMapTools/Program/Dev/Xmap_Default.txt

Xmap_Default.txt

```
!- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
!                                                                !
!                    XMAPTOOLS Default File                      !
!             Last update (8.01.2018),   Pierre Lanari           !
!                                                                !
!- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
!
! Element / element / Oxide / OXIDE
! EDIT WITH CAUTION (No empty line without the comment symbol (!)
!
!
Na  na  Na2O    NA2O
Mg  mg  MgO     MGO
Al  al  Al2O3   AL2O3
Si  si  SiO2    SIO2
P   p   P2O5    P2O5
S   s   SO2     SO2
F   f   FO2     FO2
Cl  cl  Cl2O    CL2O
K   k   K2O     K2O
Ca  ca  CaO     CAO
Ti  ti  TiO2    TIO2
V   v   V2O5    V2O5
Cr  cr  Cr2O3   CR2O3
Mn  mn  MnO     MNO
Fe  fe  FeO     FEO
Co  co  CoO     COO
Ni  ni  NiO     NIO
Cu  cu  CuO     CUO
Zn  zn  ZnO     ZNO
Zr  zr  ZrO2    ZRO2
Ag  ag  AgO     AGO
Cd  cd  CdO     CDO
Sn  sn  SnO2    SNO2
Ce  ce  Ce2O3   CE2O3
As  as  As2O5   AS2O5
Sb  sb  Sb2O3   SB2O3
Cs  cs  Cs2O    CS2O
La  la  La2O3   LA2O3
Nd  nd  Nd2O3   NdO2
Pb  pb  PbO     PBO
Sr  sr  SrO     SRO
Th  sr  ThO2    THO2
U   u   UO2     UO2
Yt  yt  Y2O3    Y2O3
!Yt is Y (must be different that 'Y' coordinate)
Sm  sm  Sm2O3   SM2O3
Gd  gd  Gd2O3   GD2O3
Dy  dy  Dy2O3   DY2O3
```

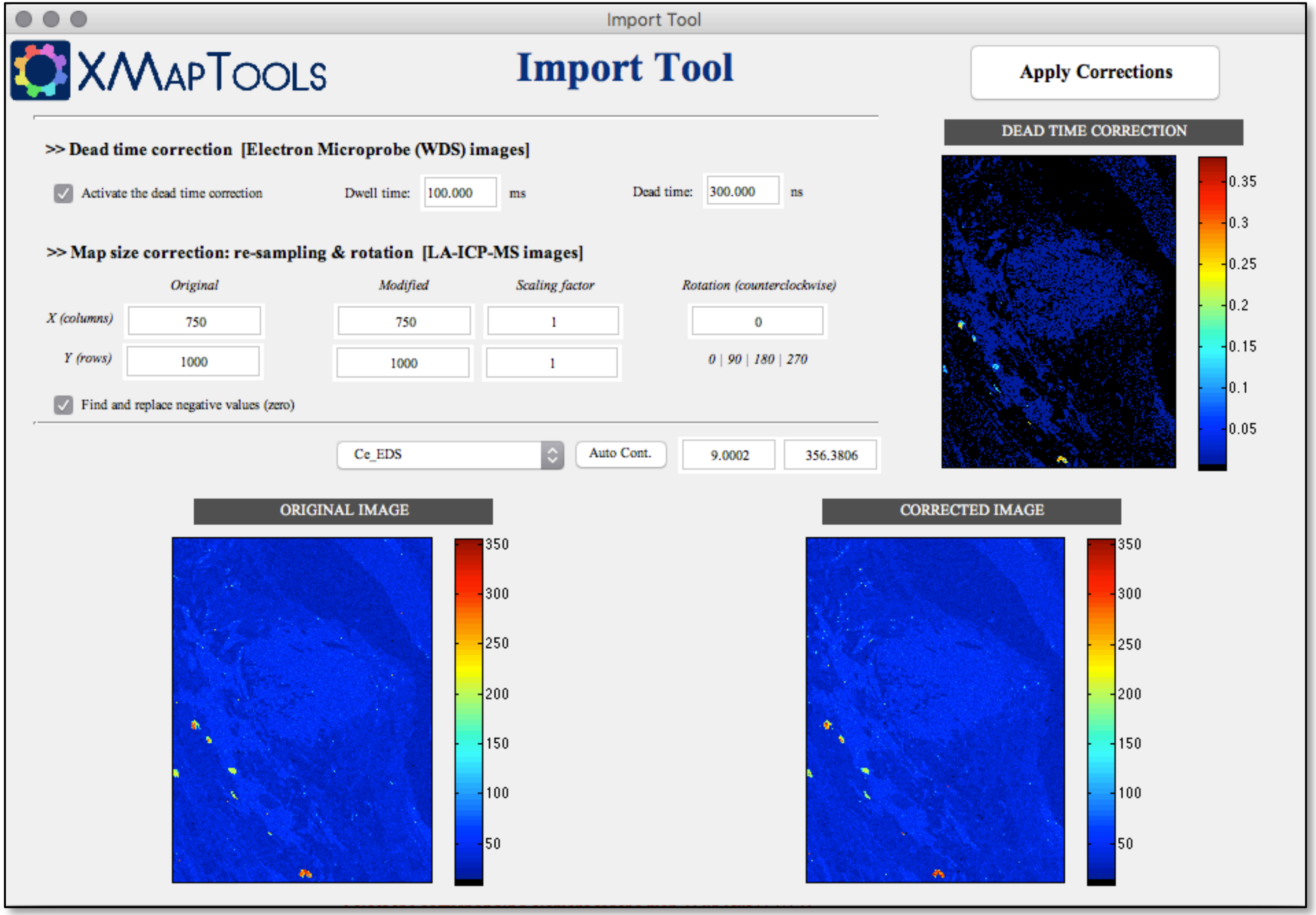
Xmap_Default.txt

```
Pr  pr  Pr2O3   PR2O3
Au  Au  Au2O3   AU2O3
!
!
! The following isotopes are available for LA-ICP-MS data
!
7Li     7li     Li  LI
9Be     9be     Be  BE
11B     11B     B   B
12C     12C     C   C
13C     13C     C   C
23Na    23na    Na  NA
24Mg    24mg    Mg  MG
25Mg    25mg    Mg  MG
27Al    27al    Al  AL
28Si    28si    Si  SI
29Si    29si    Si  SI
31P     31p     P   P
34S     34S     S   S
35Cl    35cl    Cl  CL
39K     39k     K   K
43Ca    43ca    Ca  CA
44Ca    44ca    Ca  CA
45Sc    45sc    Sc  SC
47Ti    47ti    Ti  TI
49Ti    49ti    Ti  TI
51V     51v     V   V
52Cr    52cr    Cr  CR
53Cr    53cr    Cr  CR
55Mn    55mn    Mn  MN
56Fe    56fe    Fe  FE
57Fe    57fe    Fe  FE
59Co    59co    Co  CO
60Ni    60ni    Ni  NI
65Cu    65cu    Cu  CU
66Zn    66zn    Zn  ZN
69Ga    69ga    Ga  GA
71Ga    71ga    Ga  GA
72Ge    72ge    Ge  GE
73Ta    73ta    Ta  TA
74Ge    74ge    Ge  GE
75As    75as    As  AS
77Se    77se    Se  SE
81Br    81br    Br  BR
82Se    82se    Se  SE
85Rb    85rb    Rb  RB
88Sr    88sr    Sr  SR
89Y     89y     Yt  YT
90Zr    90zr    Zr  ZR
```

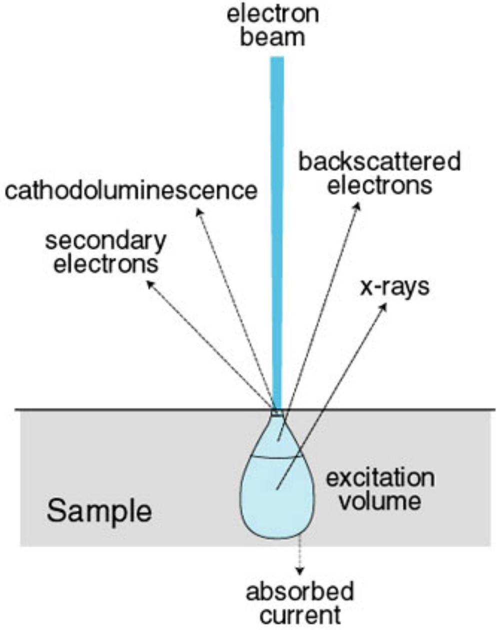
Xmap_Default.txt

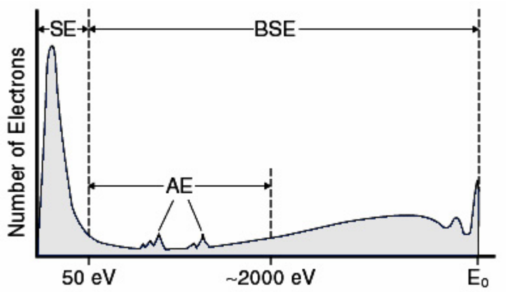
```
192Os   192os   Os  OS
193Ir   193ir   Ir  IR
195Pt   195pt   Pt  PT
197Au   197au   Au  AU
202Hg   202hg   Hg  HG
205Tl   205tl   Tl  TL
204Pb   204pb   Pb  PB
206Pb   206pb   Pb  PB
207Pb   207pb   Pb  PB
208Pb   208pb   Pb  PB
209Bi   209bi   Bi  BI
232Th   232th   Th  TH
238U    238u    U   U
!
! The following oxides are available to load standardized X-ray
maps.
! The function TTQuanti (Transfert to Quanti) can be used to
transfert
!      the data from the X-ray to the Quanti parts.
!
! We used _s because this name will be unused (correspondance with
std name of elements).
!
SiO2    sio2    SiO2_s   SIO2_s
TiO2    tio2    TiO2_s   TIO2_s
Al2O3   al2o3   Al2O3_s  AL2O3_s
FeO     feo     FeO_s    FEO_s
MnO     mno     MnO_s    MNO_s
MgO     mgo     MgO_s    MGO_s
CaO     cao     CaO_s    CAO_s
Na2O    na2o    Na2O_s   NA2O_s
K2O     k2o     K2O_s    K2O_s
!
! The following elements are for metaloids.
!     - Fe_m is X-ray data for Fe metal [Name of X-ray images].
!     - Fe_ms is Fe metal standardized (Wt% of Fe) [Name of
elements for the point analyses].
!
Fe_m    fe_m    Fe_ms   FE_MS
Cu_m    cu_m    Cu_ms   CU_MS
!
! The following labels are for the BSE, SEI and TOPO images
! They should not be standardized but they can be trasnfered to
Quanti and Result
!       using TTQuanti button.
!
BSE     bse     BSE_s   BSE_s
SEI     sei     SEI_s   SEI_s
TOPO    topo    TOPO_s  TOPO_s
```

X-RAY MAPS: LOADING AND AUTOMATED INDEXATION



BSE, SEI AND TOPO MAPS





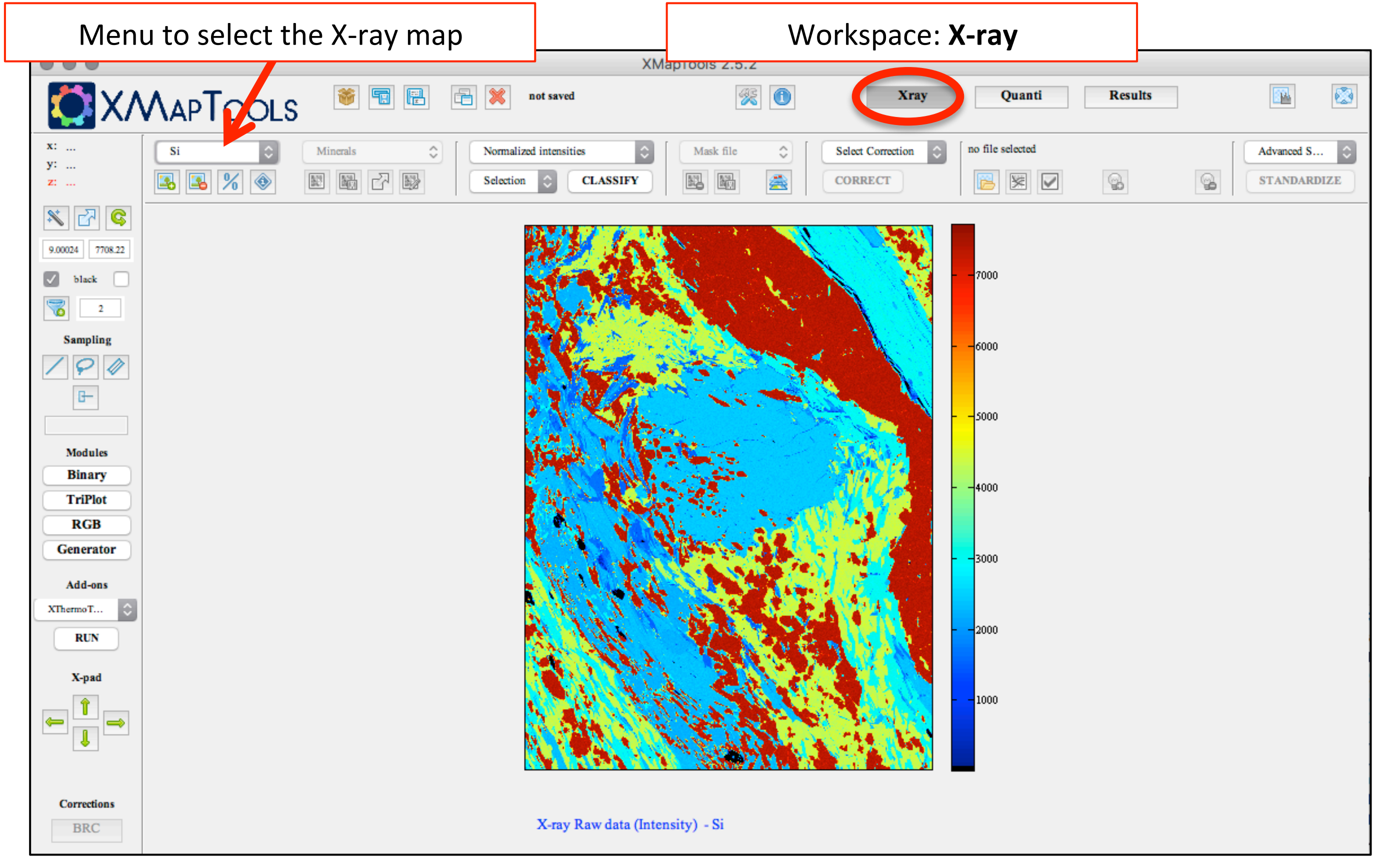
Backscattered electrons (BSE) high energy primary electrons scattered from the entry surface. Most BSE have energies slightly lower than that of the primary electron beam E0 (mostly elastic + inelastic scattering). The fraction of beam electrons backscattered from a sample, depends strongly on the sample's average atomic number, Z, reflecting the increasing charge of the atomic nuclei.

Secondary electrons (SE) are sample electrons mobilized through inelastic scattering (i.e., involving transfer of energy from the beam electrons to the atoms of the specimen) by beam electrons overcome the surface energy barrier and escape from the sample. They have lower energies (<50 eV; majority <10 eV) compared to back-scattered electrons. The escape depth of secondary electrons is only about 1/100 of that for backscattered electrons for incident beam energies in the range 10-30 keV. SE are useful in studying the surface characteristics of the sample.

Everhart-Thornley (E-T) detector for topographic contrast: This detector analyze the BSE (negatively biased E-T detector) or both BSE + SE (positively biased E-T detector). The E-T detector is mounted on one side of the sample chamber receiving a highly directional view of the specimen. As a result, when imaging a fractured surface, the faces directly in the line-of-sight of the detector appear brighter than the other faces

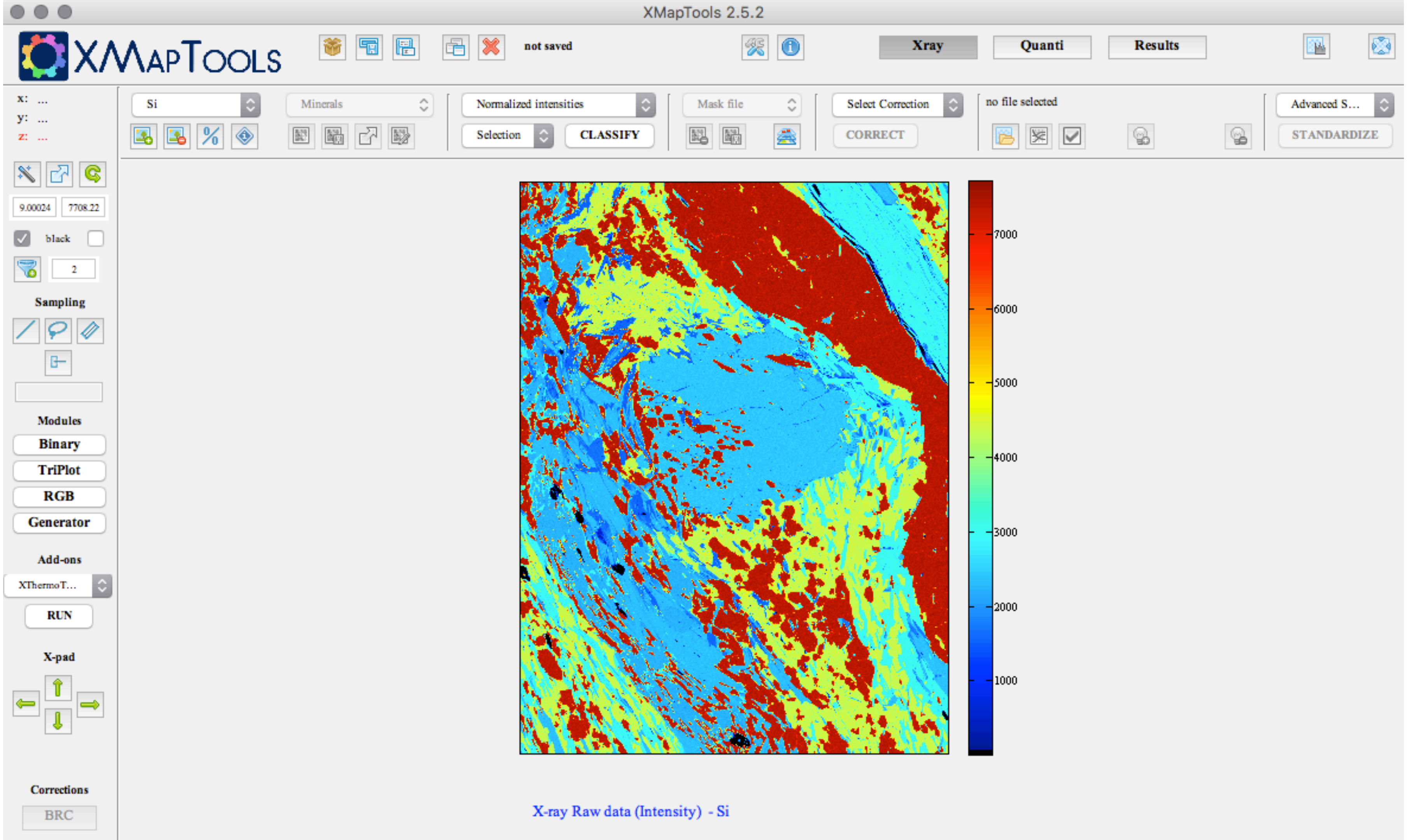
X-RAY MAPS: LOADING AND AUTOMATED INDEXATION

- Display the X-ray map Si:



Key steps

- Import the maps into XMapTools
- Identify the mineral phases
- Automated classification
- Manual classification using the Binary module
- Corrections

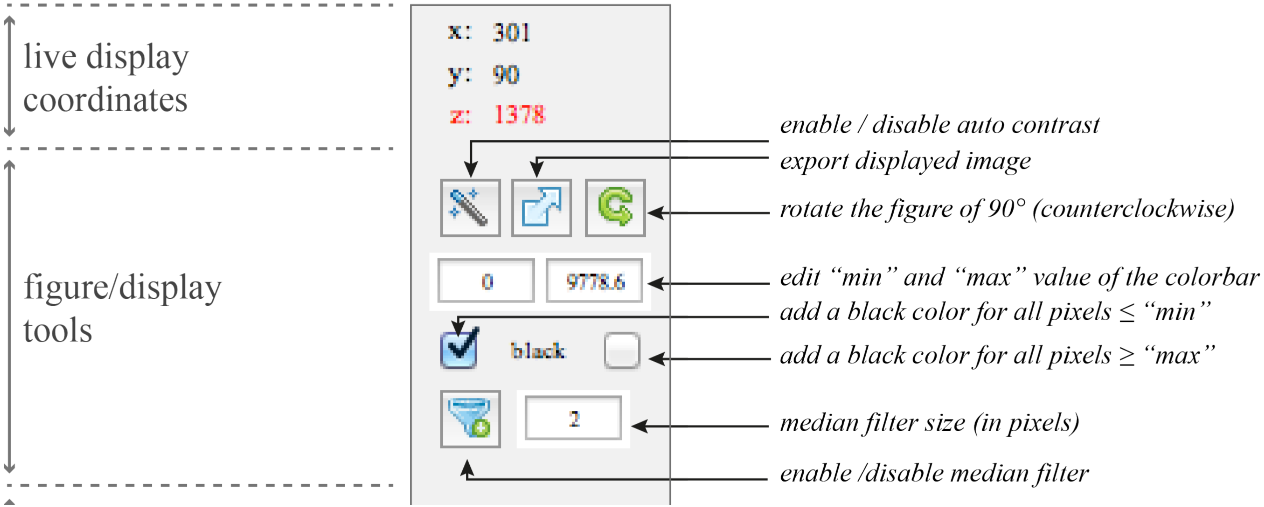

XMapTools 2.5.2
XMAPTOOLS
not saved
Xray
Quanti
Results
x: ...
y: ...
z: ...
Si
Minerals
Normalized intensities
Selection
CLASSIFY
Mask file
Select Correction
CORRECT
no file selected
Advanced S...
STANDARDIZE
9.00024
7708.22
black
2
Sampling
Modules
Binary
TriPlot
RGB
Generator
Add-ons
XThermoT...
RUN
X-pad
Corrections
BRC
7000
6000
5000
4000
3000
2000
1000
X-ray Raw data (Intensity) - Si

IDENTIFICATION OF MINERAL PHASES

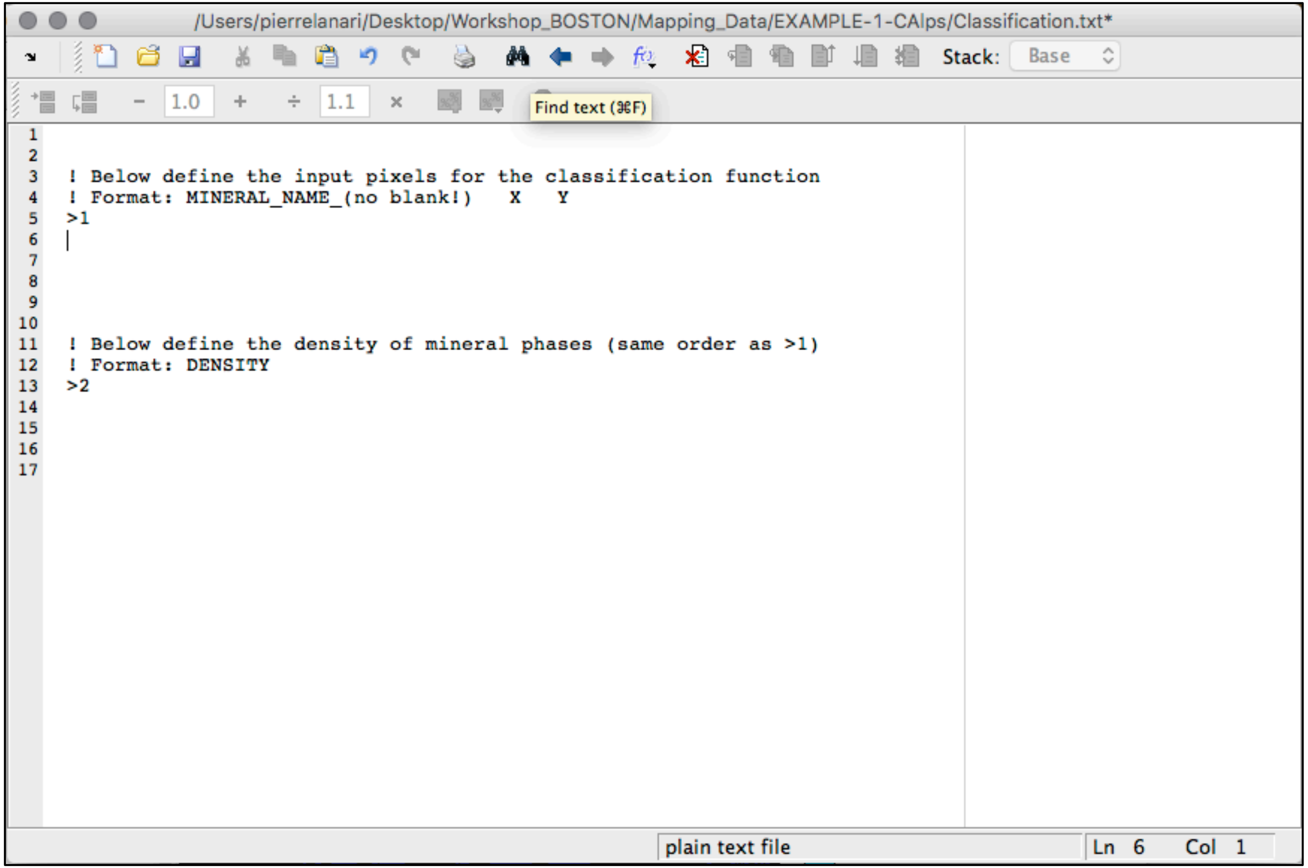
① Use the rotate function to rotate the image by 90°

② Quickly go through all the maps using the auto-contrast function to automatically adjust the limits of the colorbar. Every time you recognize a new phase, report the coordinates of a reference pixel in the file *Classification.txt*

③ Delete the maps that are not needed



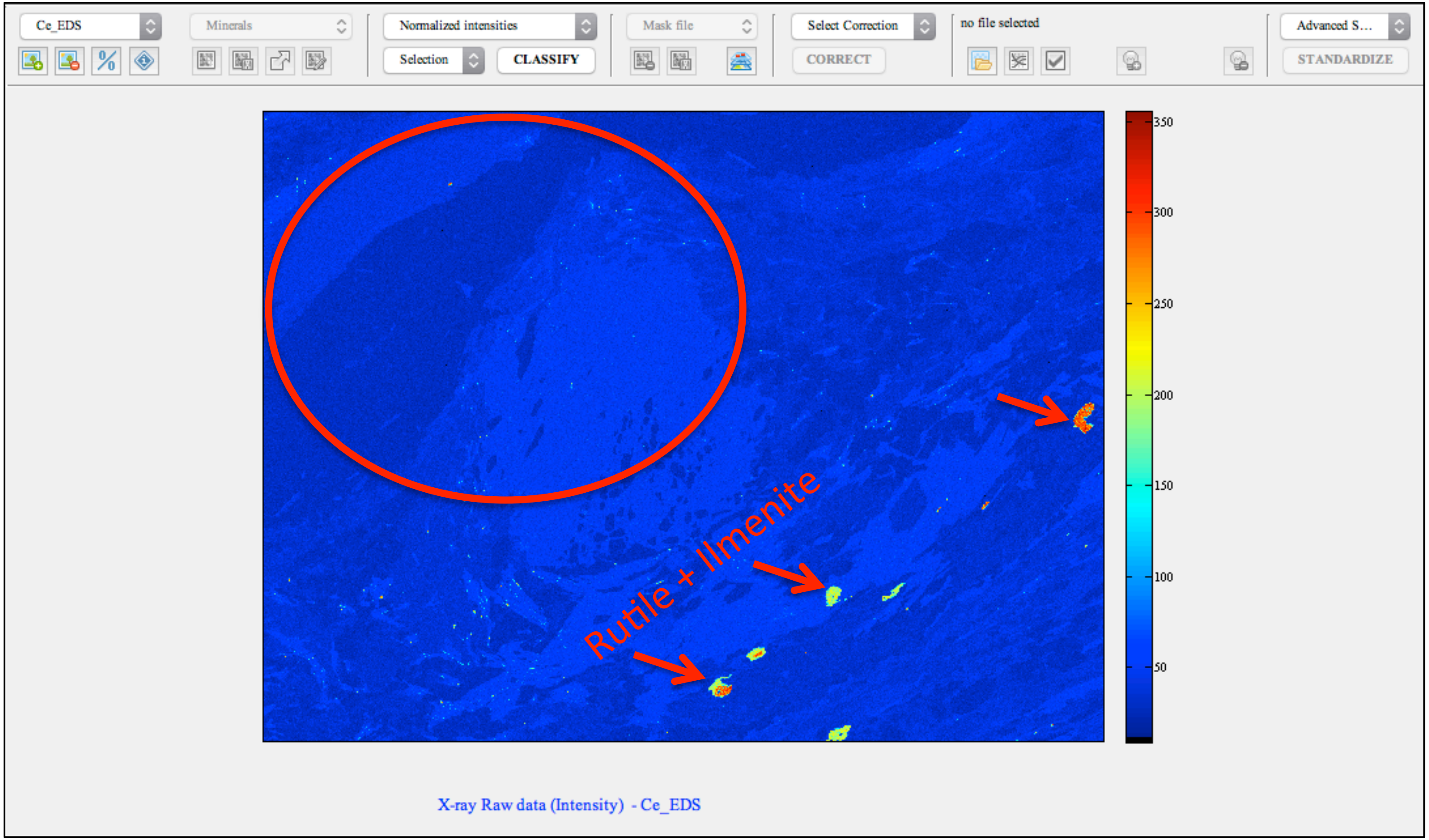
IDENTIFICATION OF MINERAL PHASES

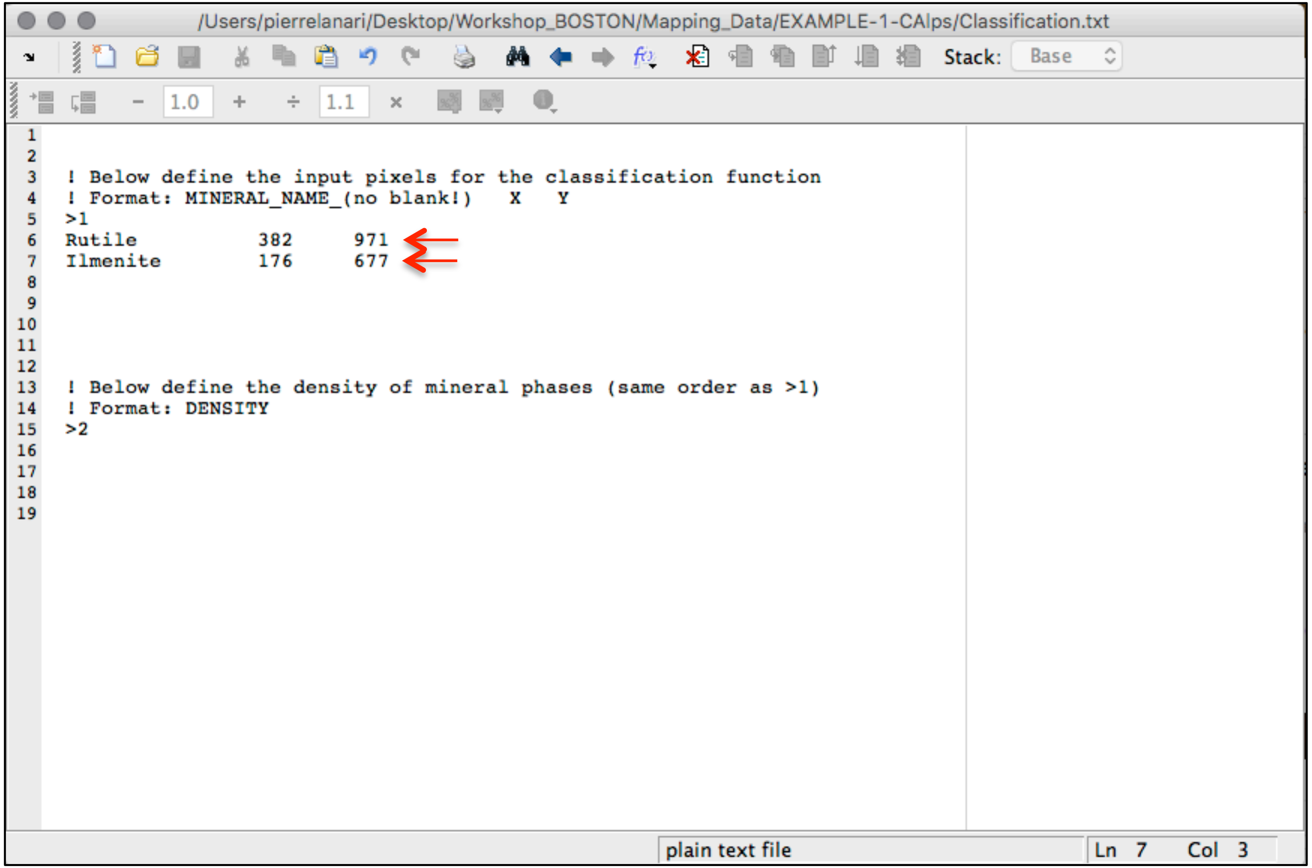



```


! Below define the input pixels for the classification function
! Format: MINERAL_NAME_(no blank!)    X    Y
>1





! Below define the density of mineral phases (same order as >1)
! Format: DENSITY
>2
```

IDENTIFICATION OF MINERAL PHASES

Ce
La



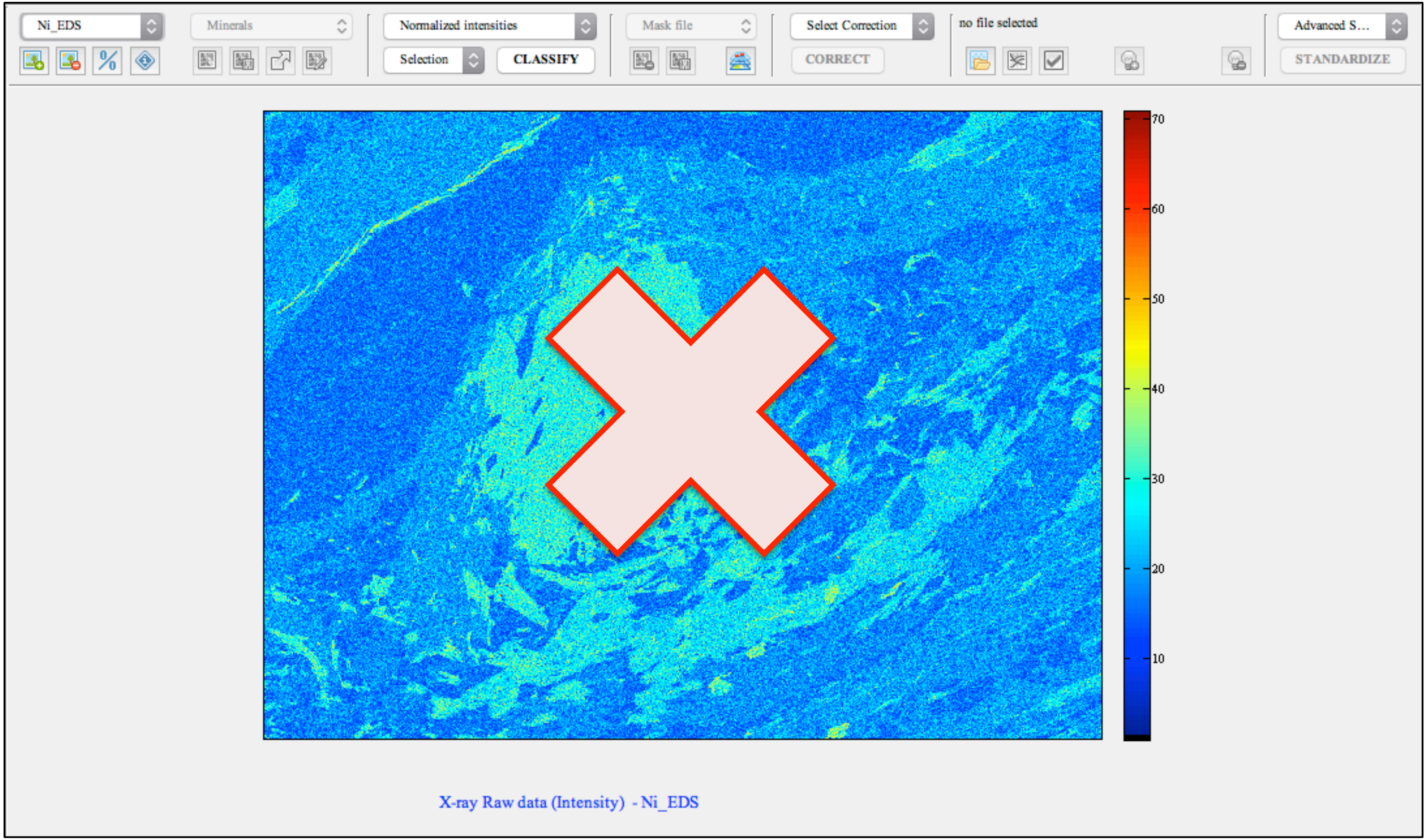

/Users/pierrelanari/Desktop/Workshop_BOSTON/Mapping_Data/EXAMPLE-1-CAlps/Classification.txt
Stack: Base
! Below define the input pixels for the classification function
! Format: MINERAL_NAME_(no blank!) X Y
>1
Rutile 382 971
Ilmenite 176 677
! Below define the density of mineral phases (same order as >1)
! Format: DENSITY
>2
plain text file
Ln 7 Col 3

IDENTIFICATION OF MINERAL PHASES

Ni

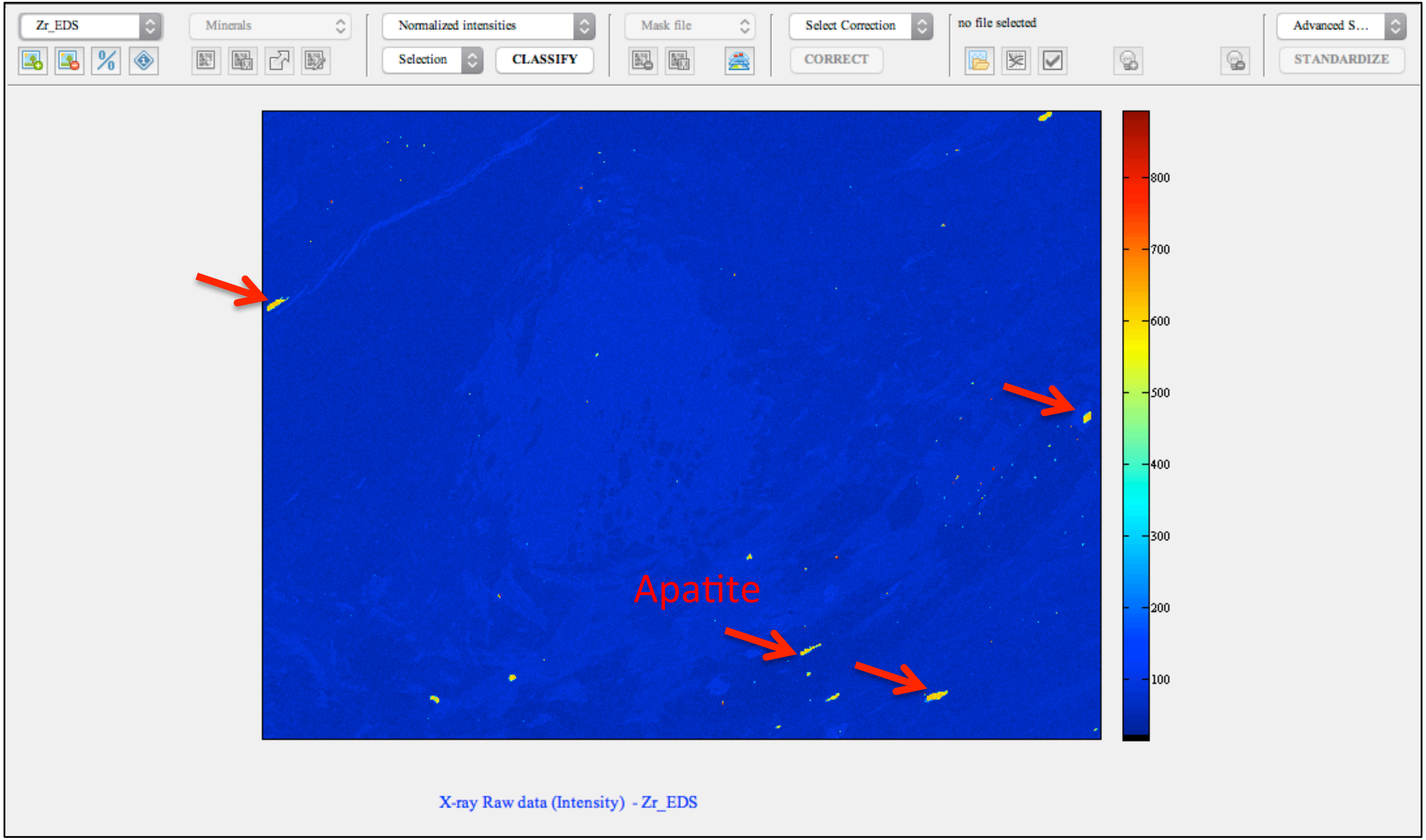
P

S

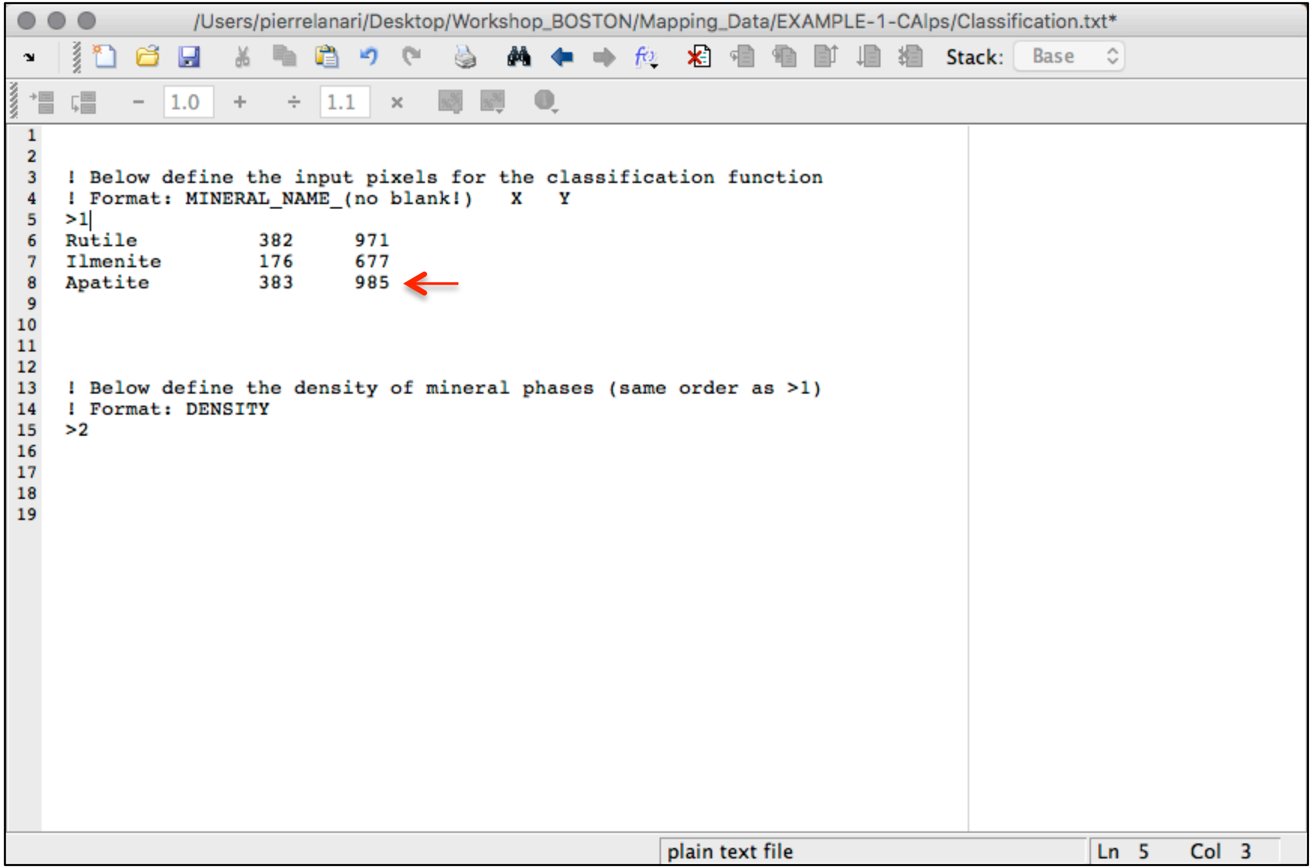


IDENTIFICATION OF MINERAL PHASES

Zr

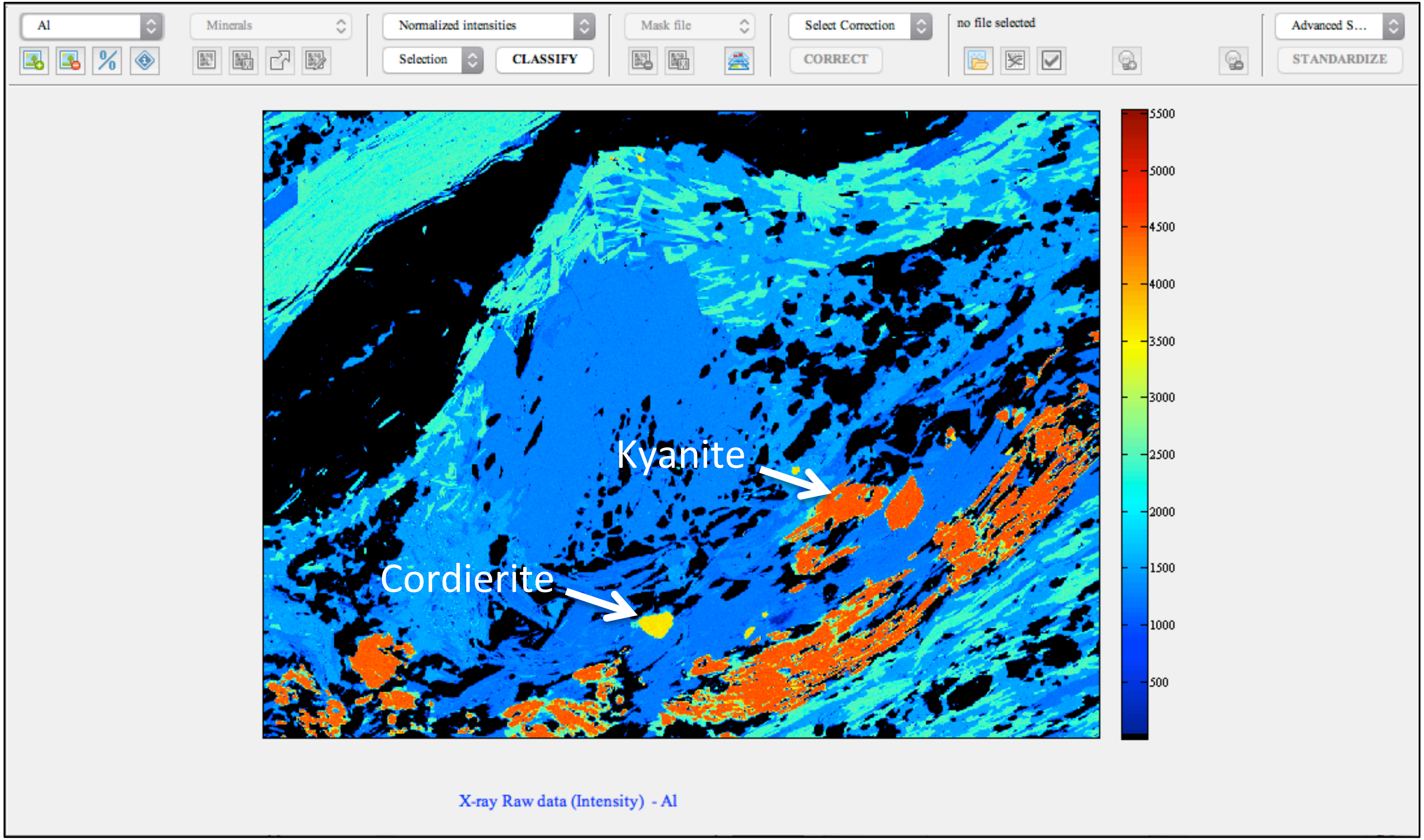


IDENTIFICATION OF MINERAL PHASES

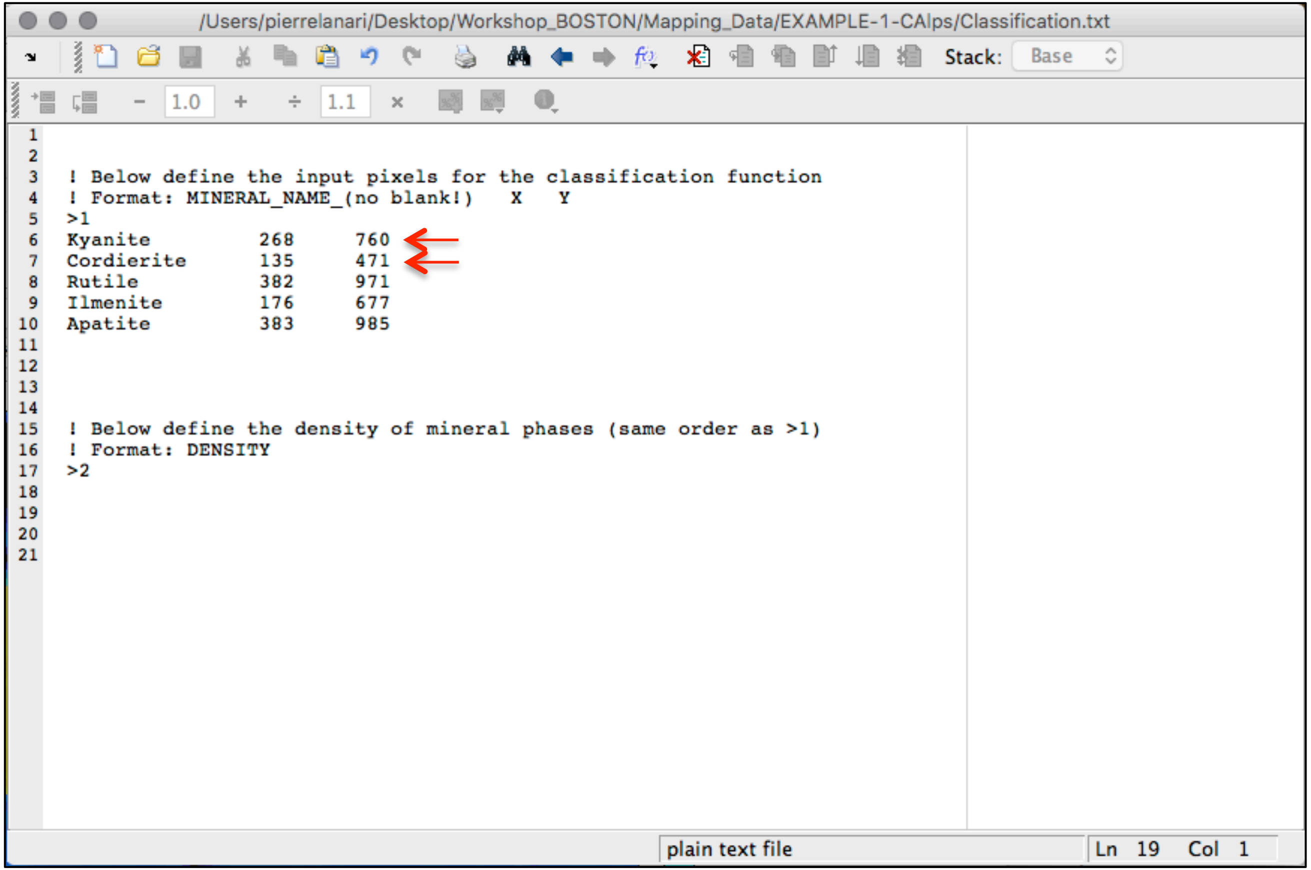


IDENTIFICATION OF MINERAL PHASES

Al

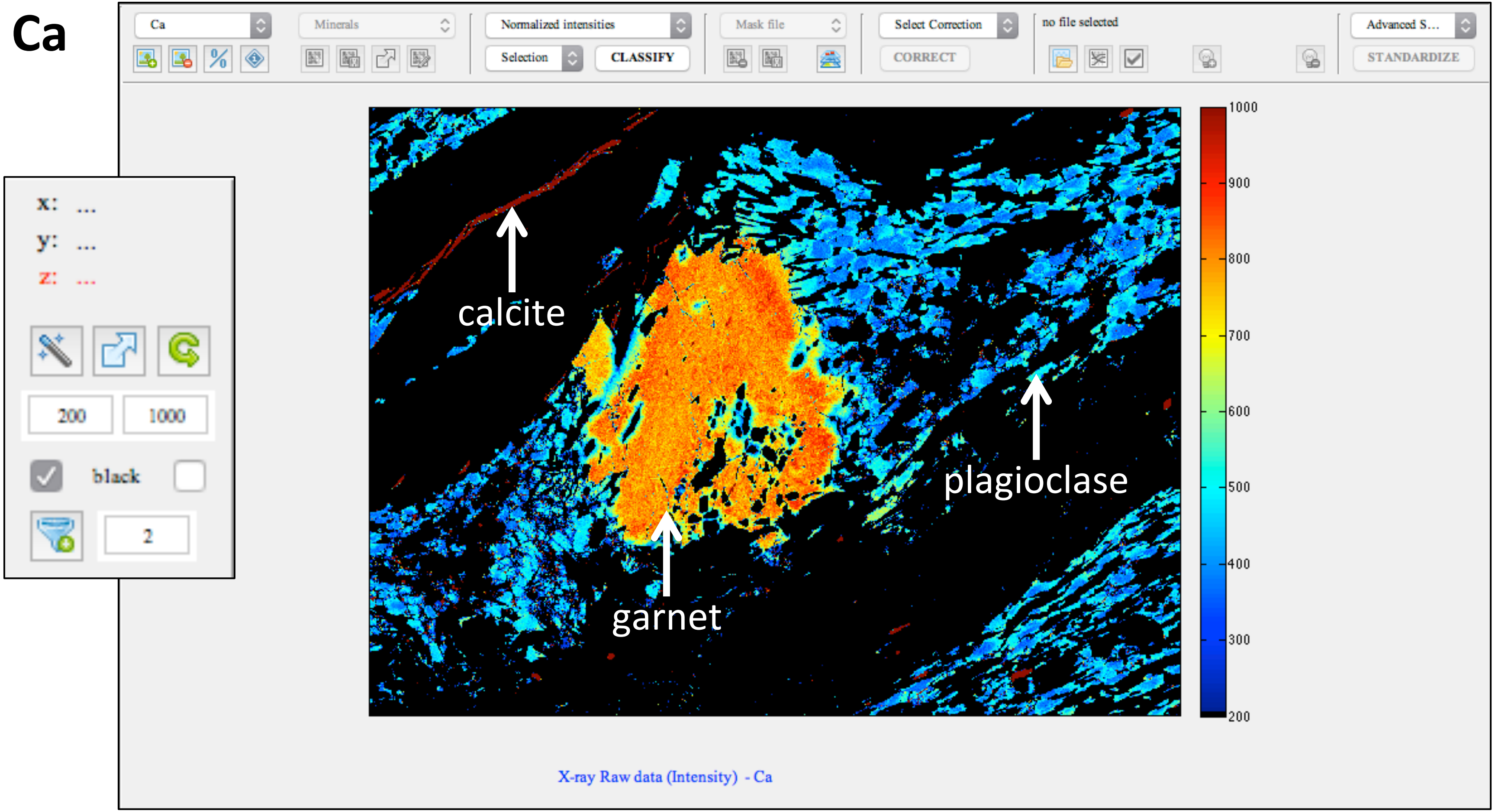


Identification of mineral phases

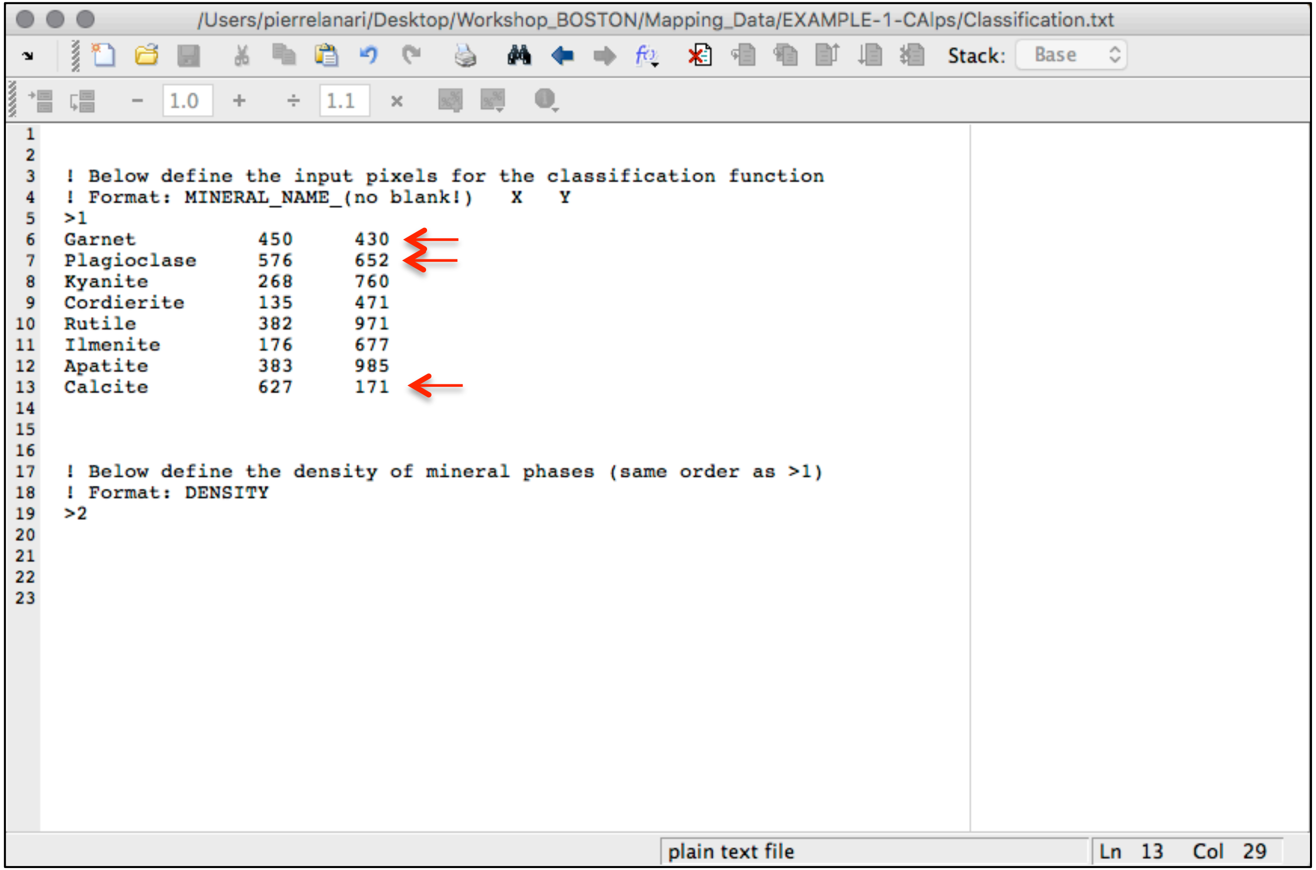



```
! Below define the input pixels for the classification function
! Format: MINERAL_NAME_(no blank!)    X     Y
>1
Kyanite          268      760
Cordierite       135      471
Rutile           382      971
Ilmenite         176      677
Apatite          383      985




! Below define the density of mineral phases (same order as >1)
! Format: DENSITY
>2
```

IDENTIFICATION OF MINERAL PHASES



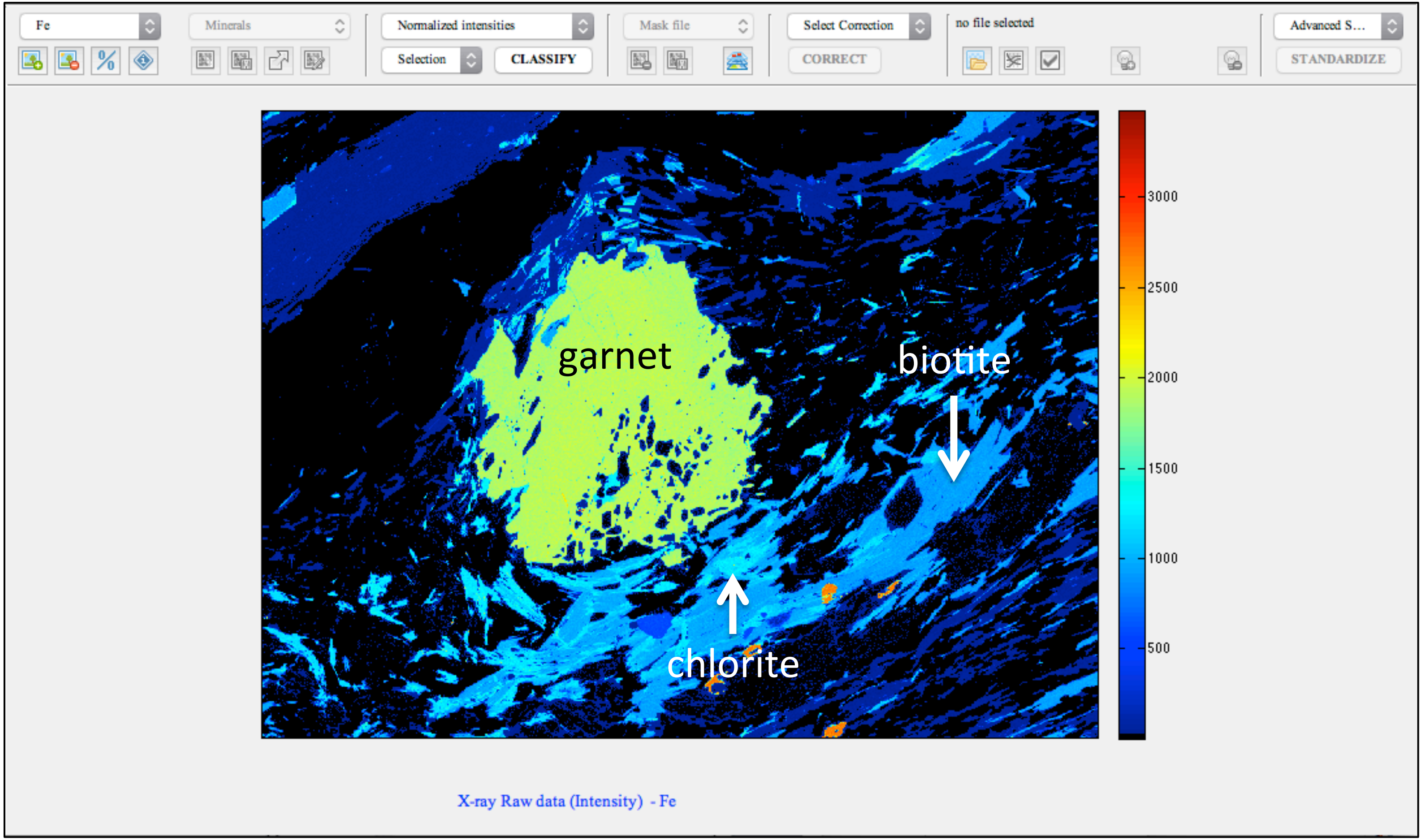
IDENTIFICATION OF MINERAL PHASES




```


! Below define the input pixels for the classification function
! Format: MINERAL_NAME_(no blank!)    X    Y
>1
Garnet          450     430
Plagioclase     576     652
Kyanite         268     760
Cordierite      135     471
Rutile          382     971
Ilmenite        176     677
Apatite         383     985
Calcite         627     171



! Below define the density of mineral phases (same order as >1)
! Format: DENSITY
>2
```

IDENTIFICATION OF MINERAL PHASES

Fe



IDENTIFICATION OF MINERAL PHASES

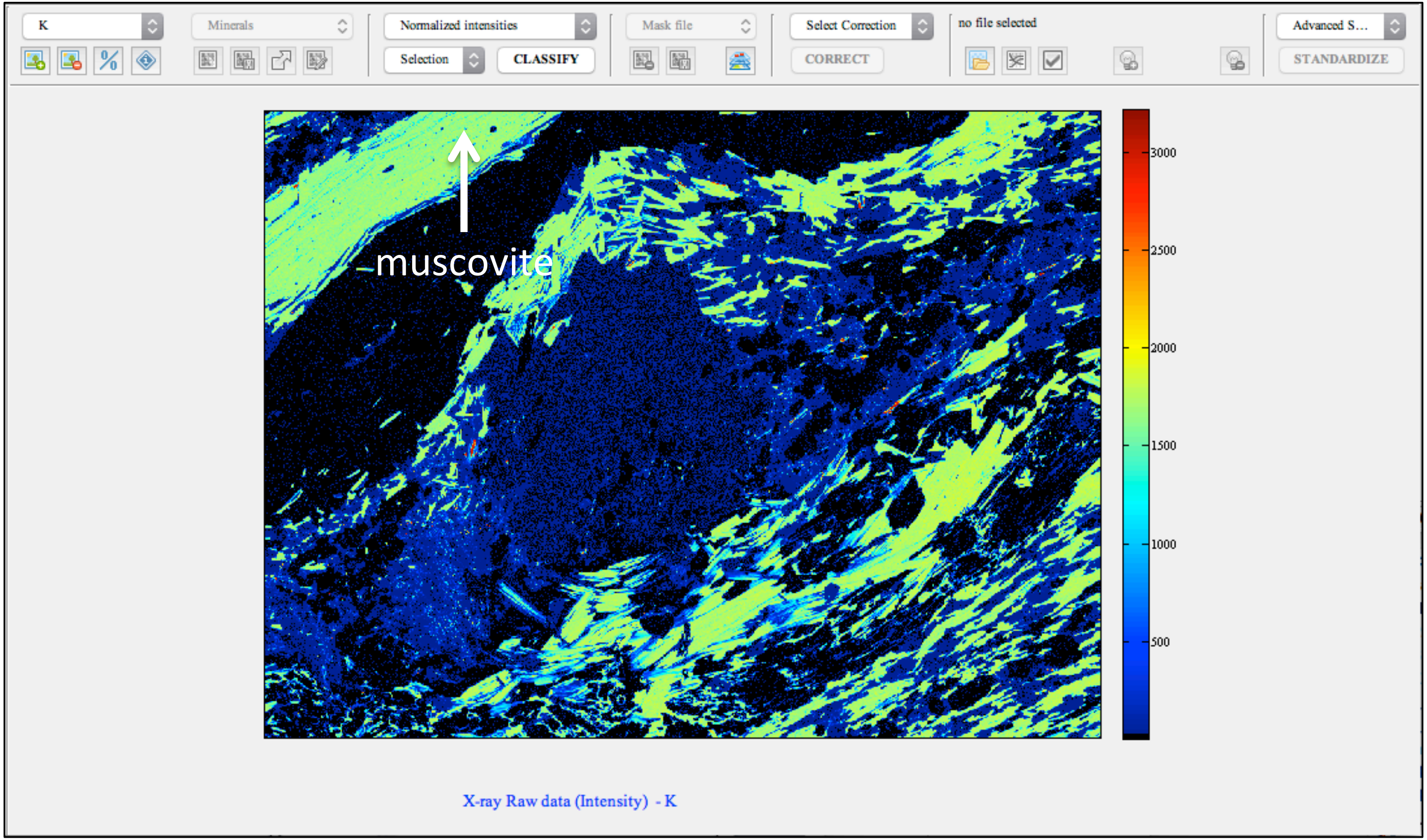
/Users/pierrelanari/Desktop/Workshop_BOSTON/Mapping_Data/EXAMPLE-1-CAlps/Classification.txt

```


! Below define the input pixels for the classification function
! Format: MINERAL_NAME_(no blank!)    X    Y
>1
Garnet          450     430
Biotite         323     855
Plagioclase     576     652
Kyanite         268     760
Chlorite        205     556
Cordierite      135     471
Rutile          382     971
Ilmenite        176     677
Apatite         383     985
Calcite         627     171



! Below define the density of mineral phases (same order as >1)
! Format: DENSITY
>2
```

plain text file   Ln 23   Col 1

IDENTIFICATION OF MINERAL PHASES

K



IDENTIFICATION OF MINERAL PHASES

/Users/pierrelanari/Desktop/Workshop_BOSTON/Mapping_Data/EXAMPLE-1-CAlps/Classification.txt

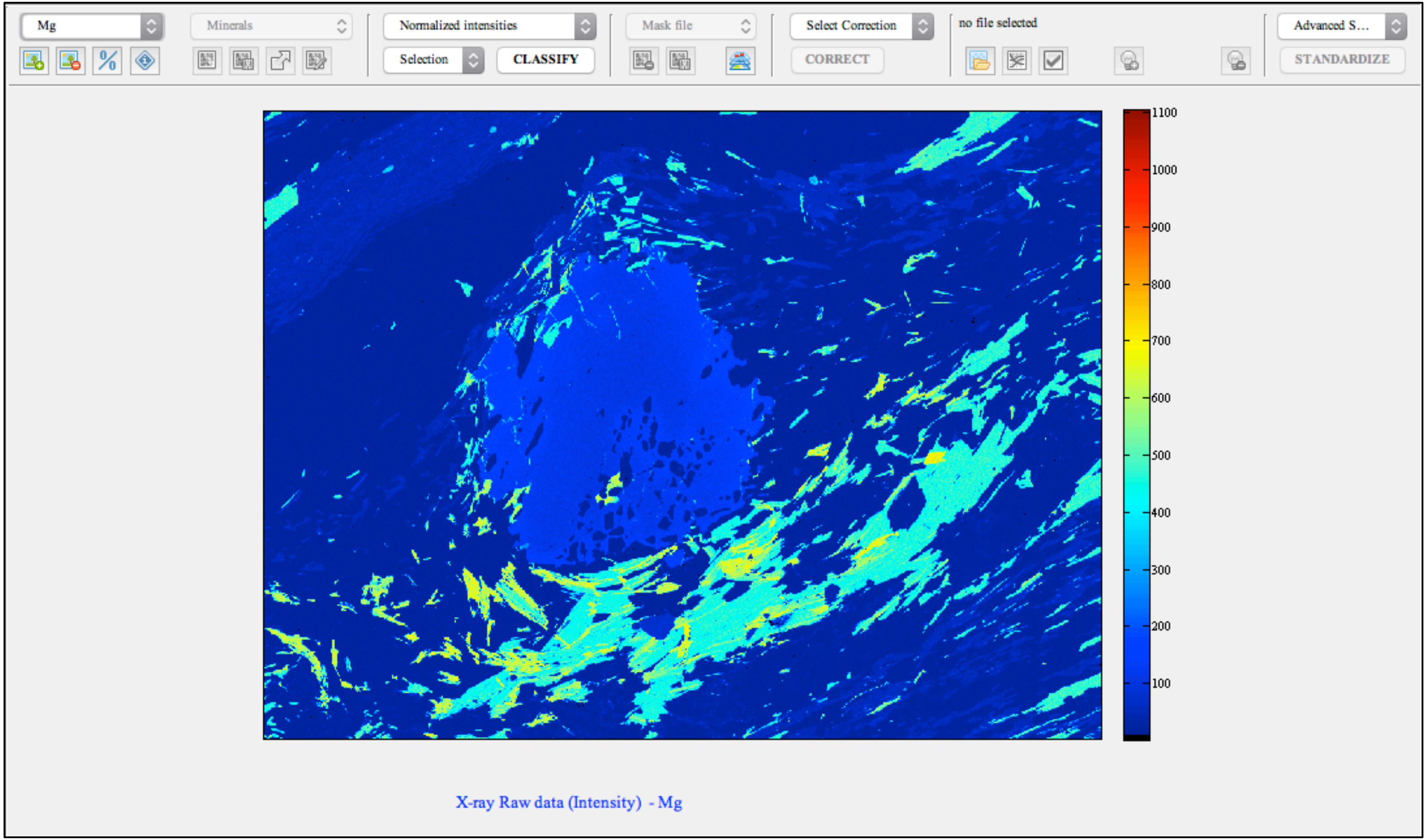
Stack: Base

```


! Below define the input pixels for the classification function
! Format: MINERAL_NAME_(no blank!)    X    Y
>1
Garnet            450     430
Biotite           323     855
Muscovite         615     85
Plagioclase       576     652
Kyanite           268     760
Chlorite          205     556
Cordierite        135     471
Rutile            382     971
Ilmenite          176     677
Apatite           383     985
Calcite           627     171



! Below define the density of mineral phases (same order as >1)
! Format: DENSITY
>2
```

plain text file   Ln 24   Col 1

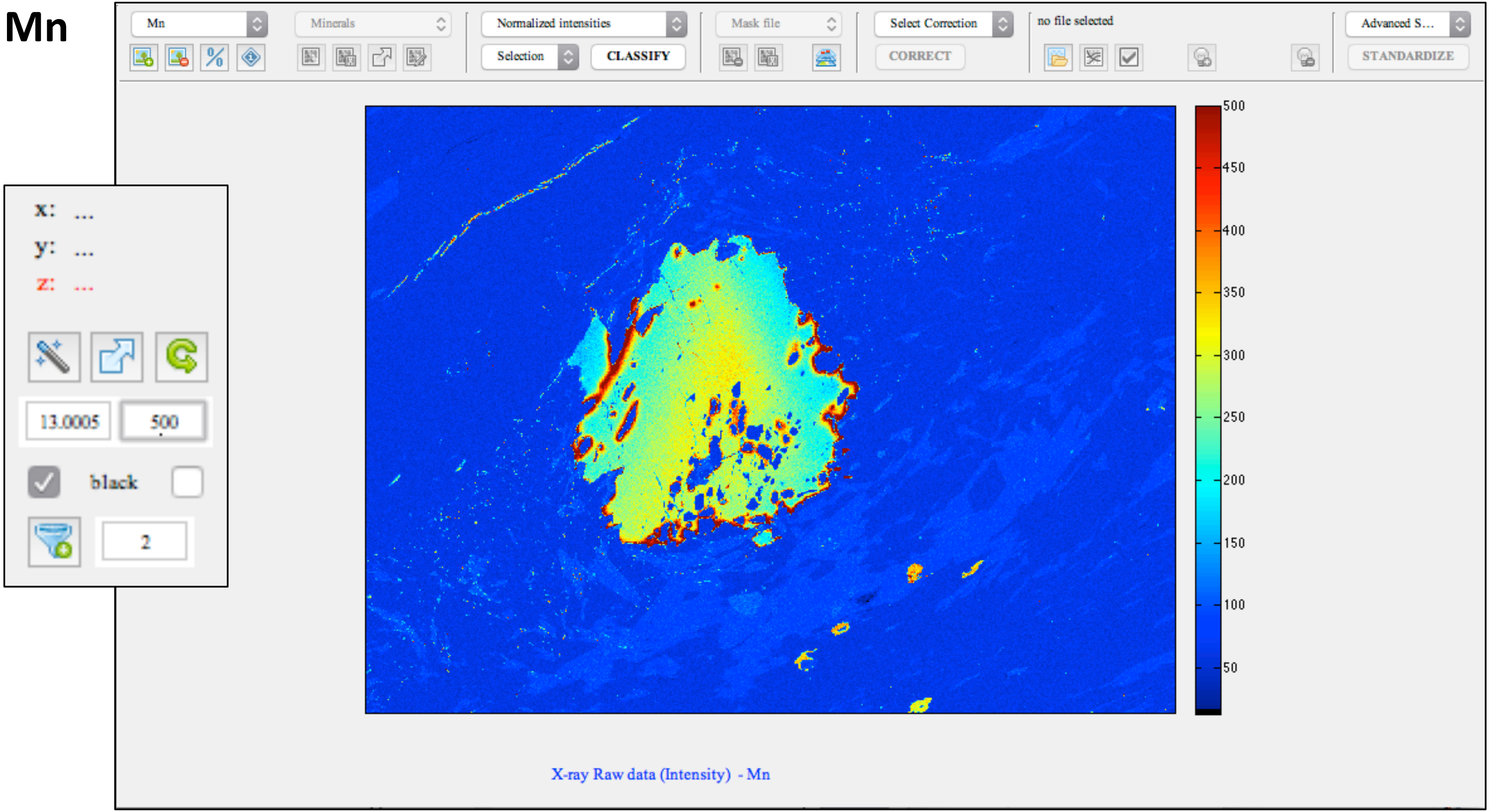
IDENTIFICATION OF MINERAL PHASES

Mg



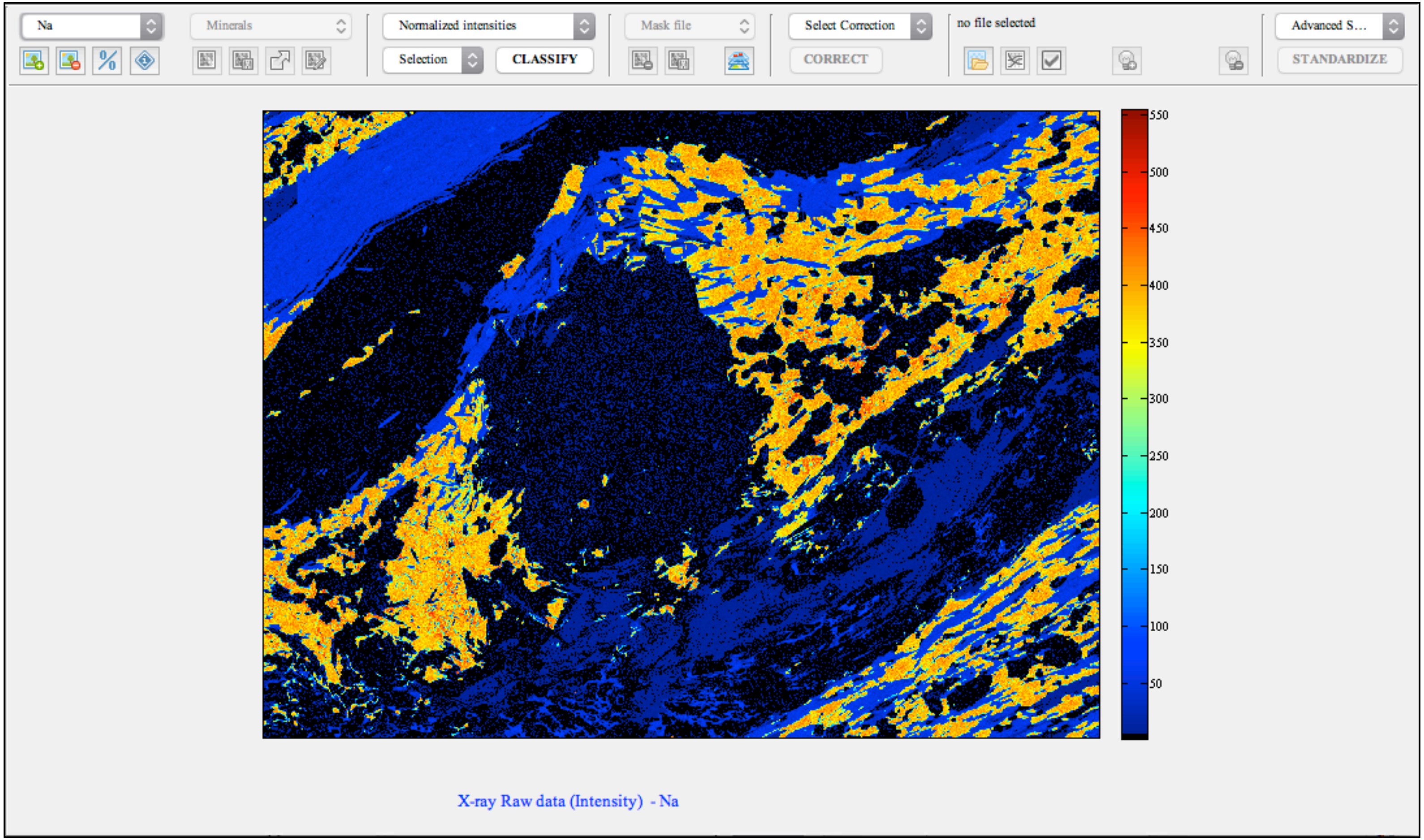
IDENTIFICATION OF MINERAL PHASES

Mn



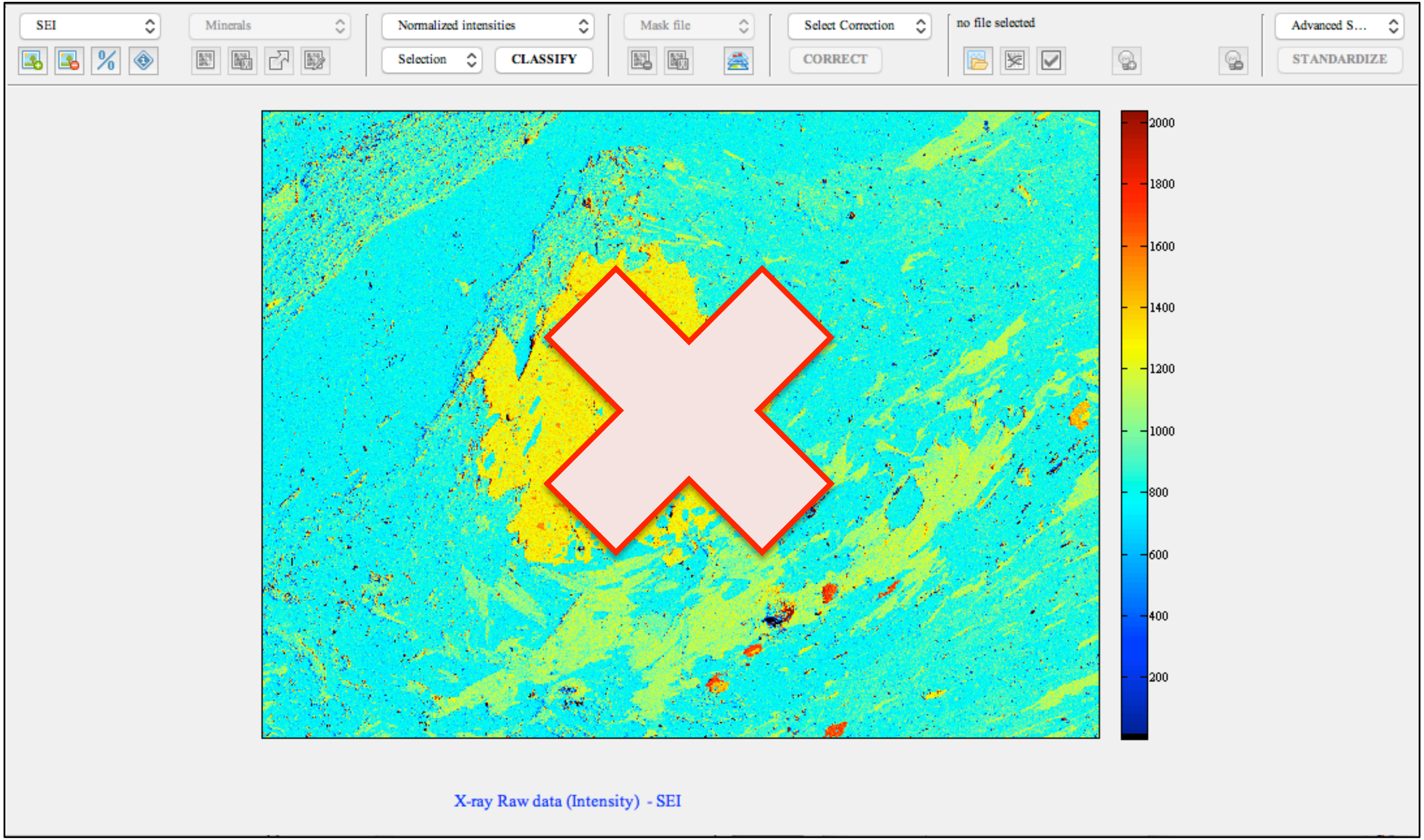
IDENTIFICATION OF MINERAL PHASES

Na



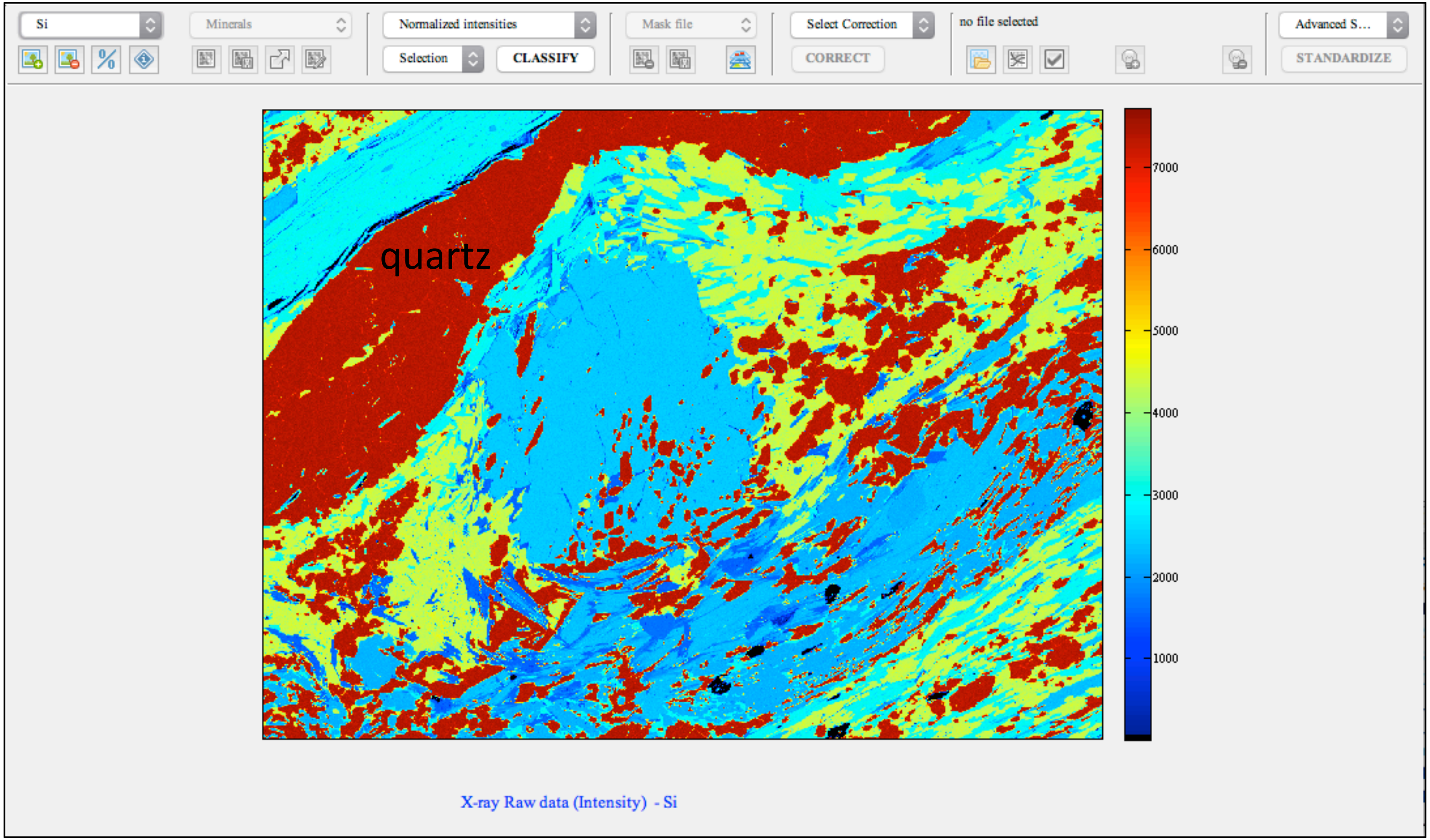
IDENTIFICATION OF MINERAL PHASES

SEI

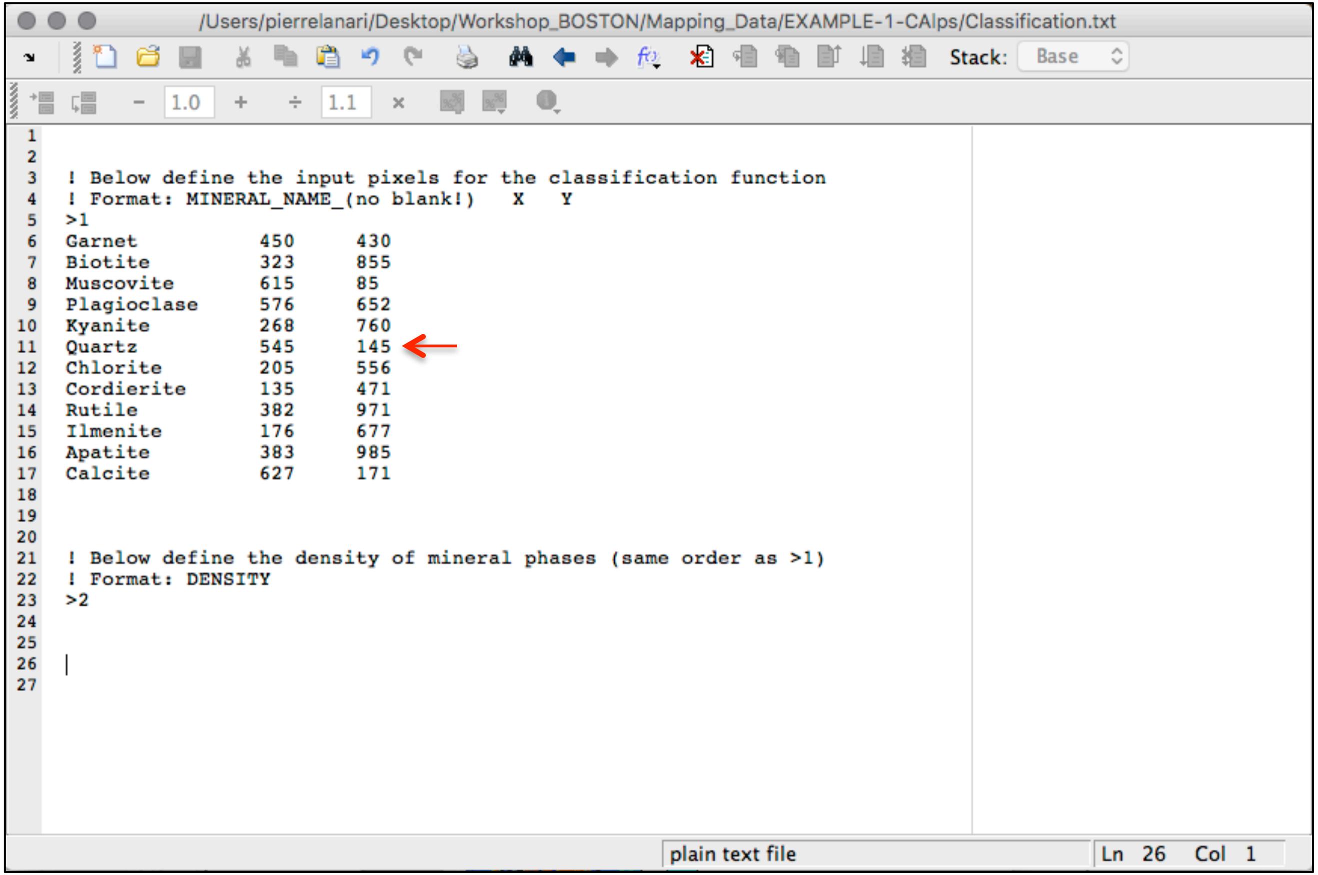


IDENTIFICATION OF MINERAL PHASES

Si



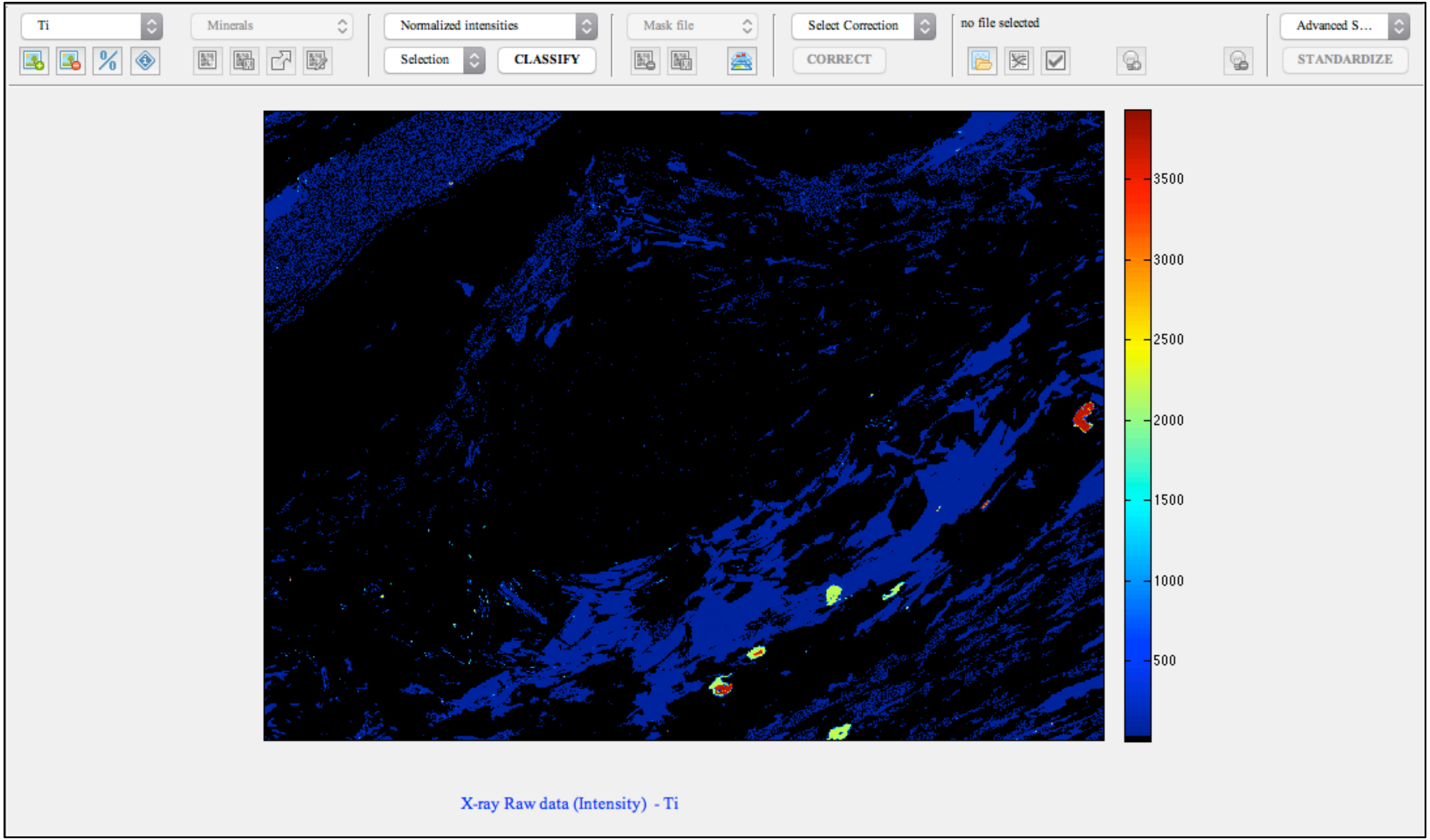
IDENTIFICATION OF MINERAL PHASES




```


! Below define the input pixels for the classification function
! Format: MINERAL_NAME_(no blank!)    X    Y
>1
Garnet          450     430
Biotite         323     855
Muscovite       615     85
Plagioclase     576     652
Kyanite         268     760
Quartz          545     145
Chlorite        205     556
Cordierite      135     471
Rutile          382     971
Ilmenite        176     677
Apatite         383     985
Calcite         627     171



! Below define the density of mineral phases (same order as >1)
! Format: DENSITY
>2
```

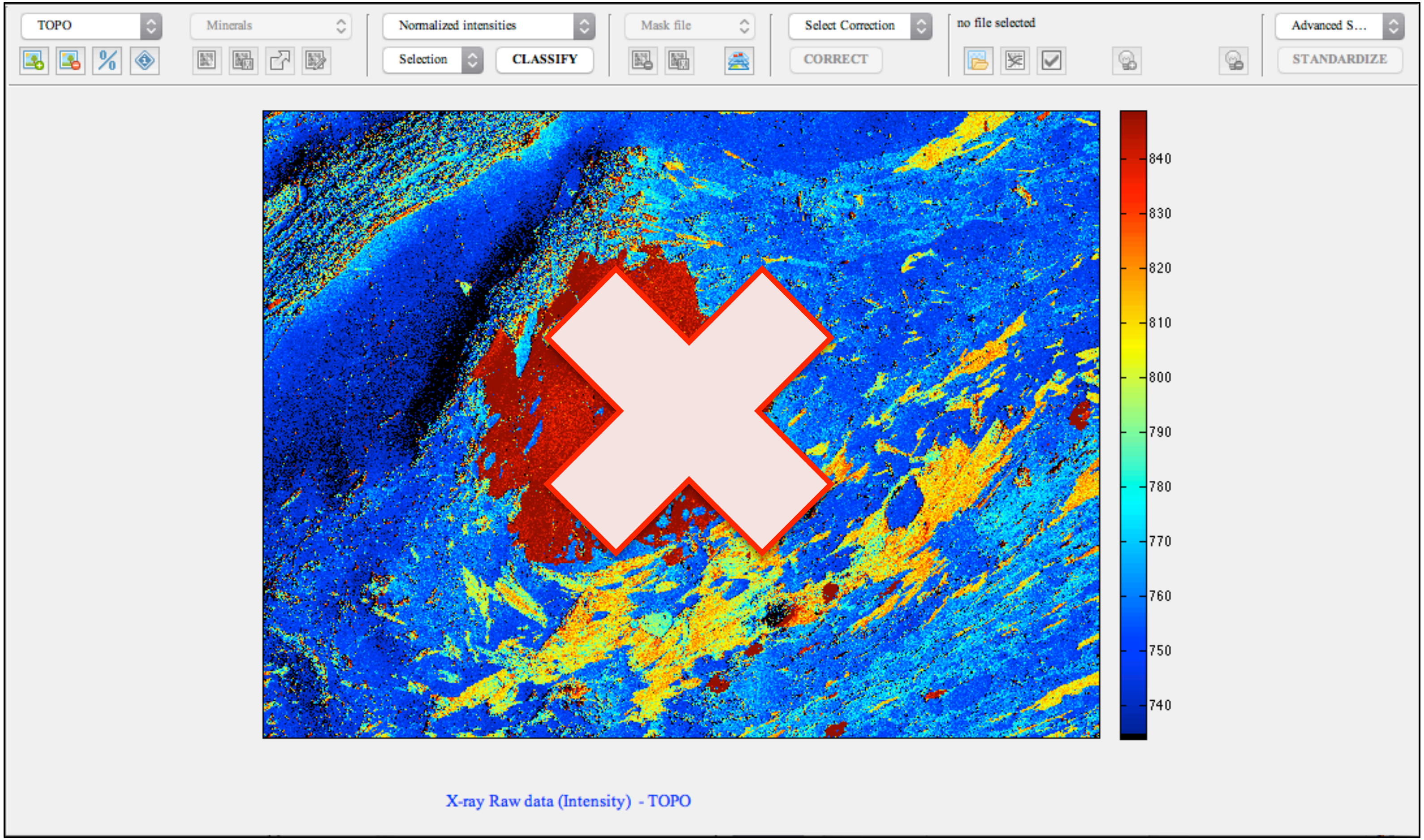
IDENTIFICATION OF MINERAL PHASES

Ti

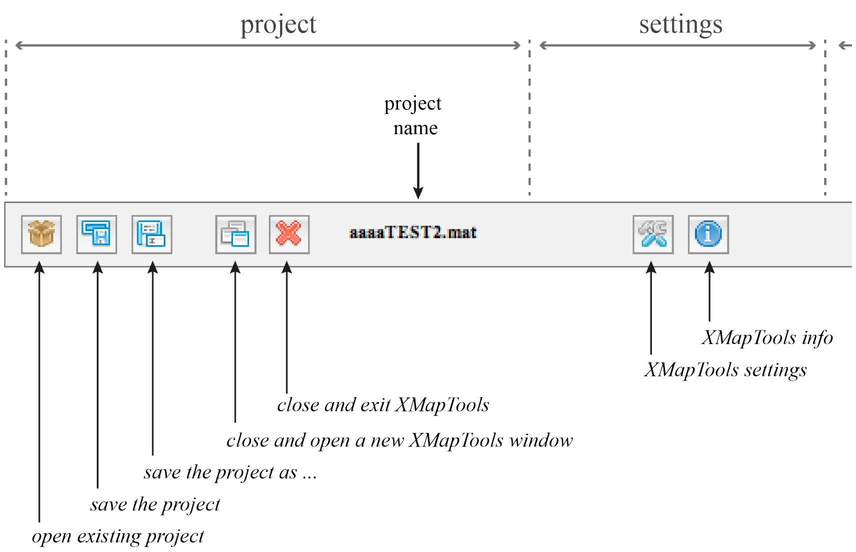


IDENTIFICATION OF MINERAL PHASES

TOPO



IDENTIFICATION OF MINERAL PHASES



① Save the project (aaa.mat)

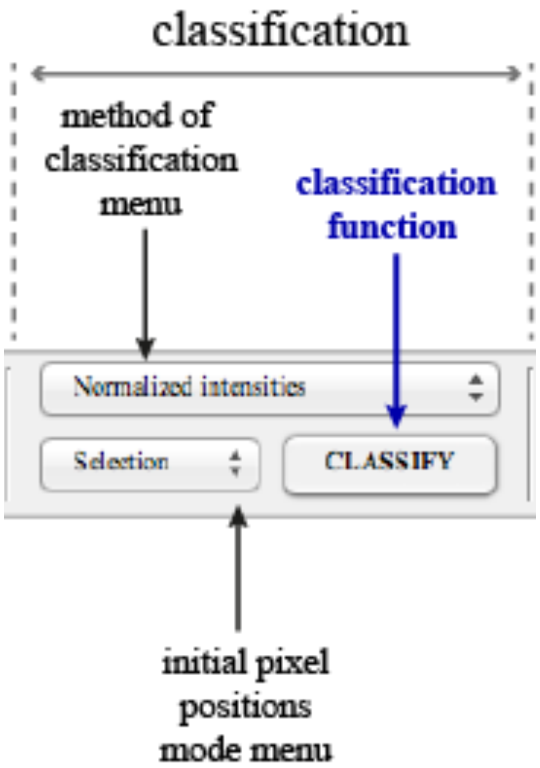
② Close XMAPTOOLS

③ Launch XMAPTOOLS and load your project using the command: >> *XMapTools open aaa*

Key steps

- Import the maps into XMapTools
- Identify the mineral phases
- Automated classification
- Manual classification using the Binary module
- Corrections

Automated classification (normalized and classic methods)



① Select the method "Normalized intensities" and the mode "file" in the classification menus

② Press CLASSIFY

③ Follow the instructions given by the program. In this example, Mn is excluded from the classification; system: Ce, La, Zr, Al, Ca, Fe, K, Mg, Na, Si, Ti

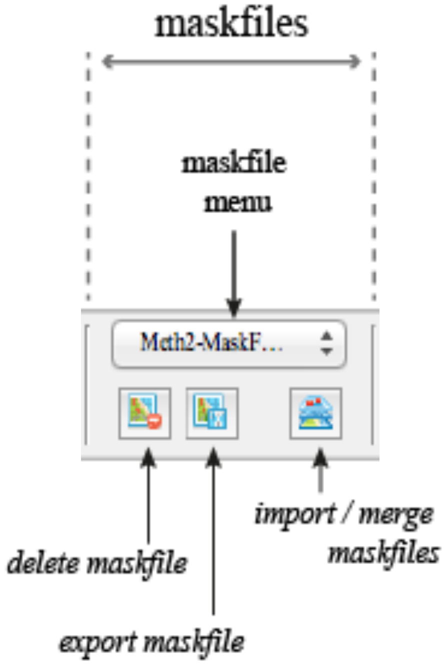
If you want to use the mode "selection", you need to find a map on which all the phases are visible in order to define the reference pixels of each phase.

➢ The classification function generates a maskfile

AUTOMATED CLASSIFICATION (NORMALIZED AND CLASSIC METHODS)

1	1	1	2	2	3	3	1	1	1
1	1	2	2	3	3	4	1	1	1
1	2	2	3	3	4	4	4	1	1
2	2	3	3	4	4	4	4	4	1
2	2	2	3	3	4	4	4	2	2
2	2	2	3	3	1	4	2	2	2
3	3	3	3	1	1	1	1	2	2
3	3	3	1	1	1	1	1	1	3

4	Garnet
3	Chlorite
2	Plagioclase
1	Quartz

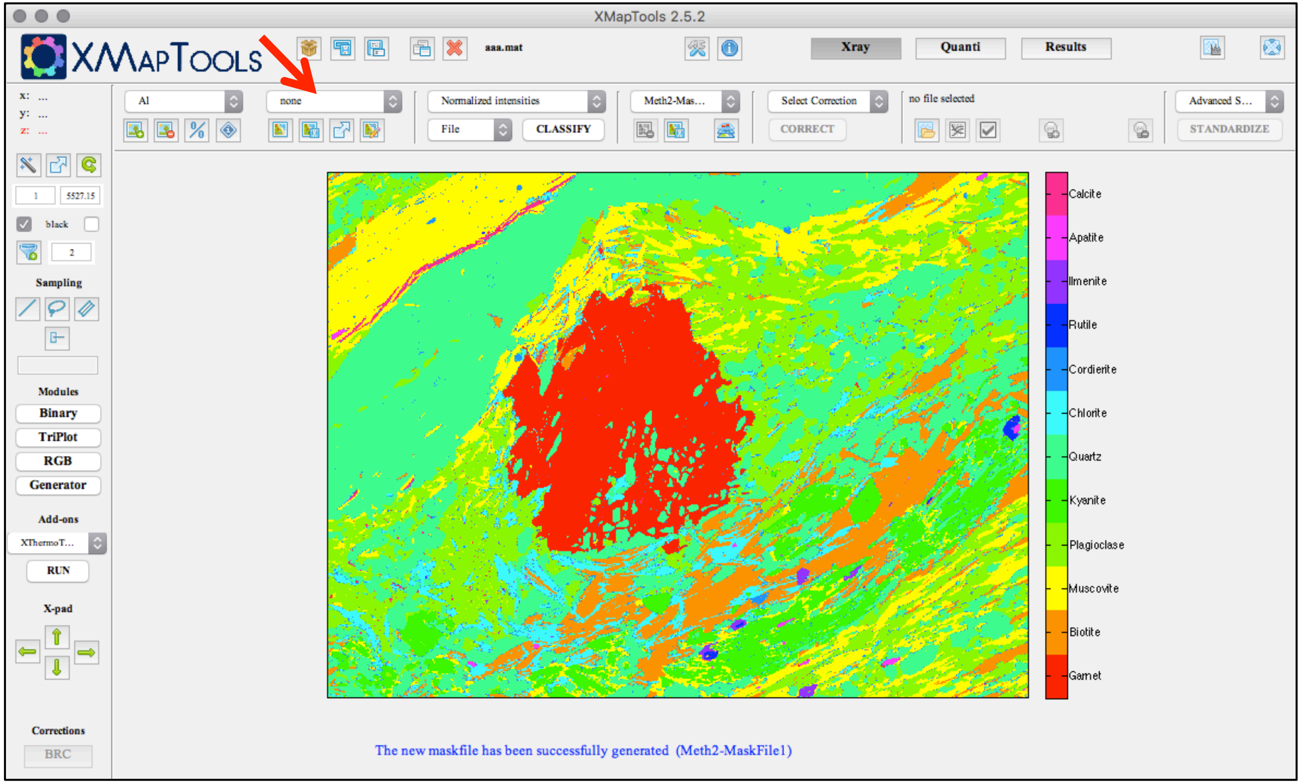


Note:

It is possible to select and manipulate maskfiles using the maskfile menu and the corresponding buttons

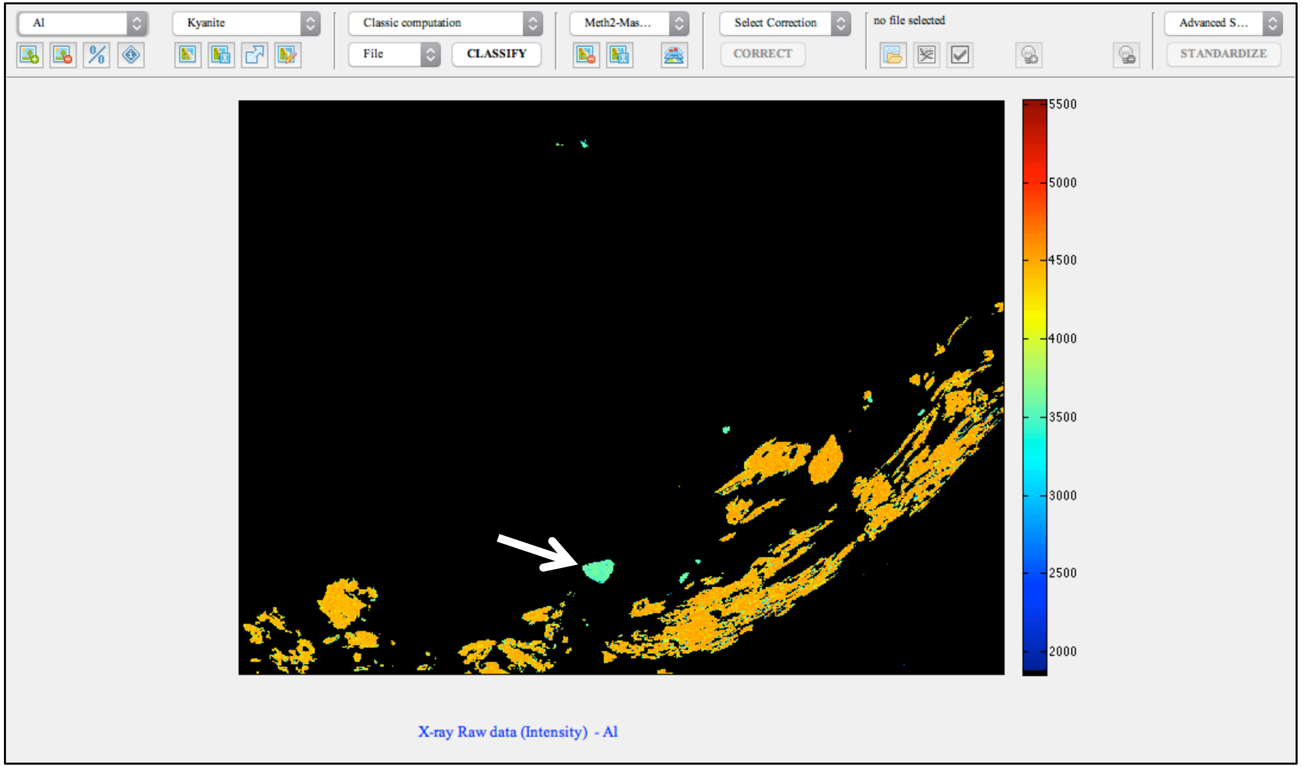
AUTOMATED CLASSIFICATION (NORMALIZED AND CLASSIC METHODS)

④ Check the classification by displaying each phase

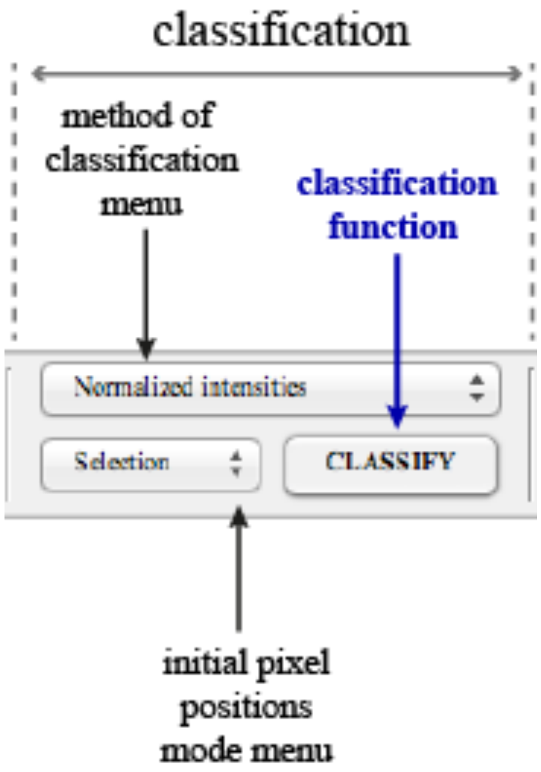


AUTOMATED CLASSIFICATION (NORMALIZED AND CLASSIC METHODS)

④ Check the classification by displaying each phase



AUTOMATED CLASSIFICATION (NORMALIZED AND CLASSIC METHODS)



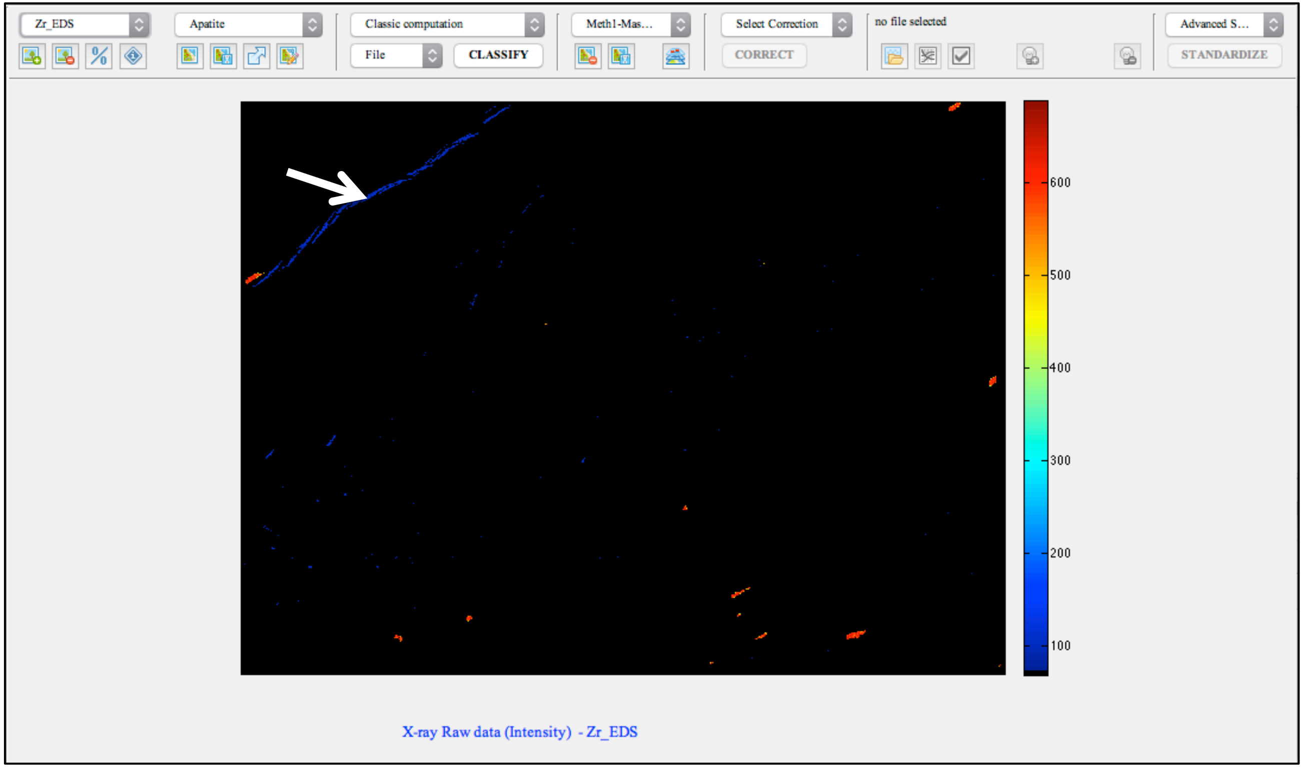
① Select the method "Classical computation" and the mode "file" in the classification menus

② Press CLASSIFY

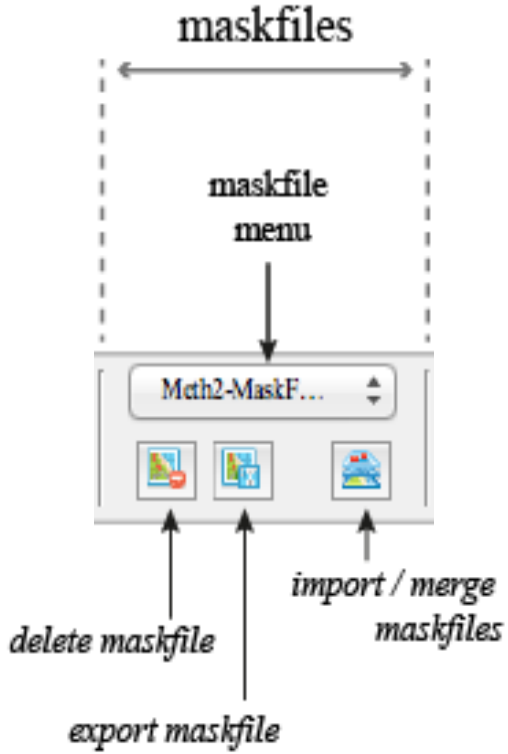
③ Follow the instructions given by the program. In this example, Mn is excluded from the classification; system: Ce, La, Zr, Al, Ca, Fe, K, Mg, Na, Si, Ti

AUTOMATED CLASSIFICATION (NORMALIZED AND CLASSIC METHODS)

④ Check the classification by displaying each phase

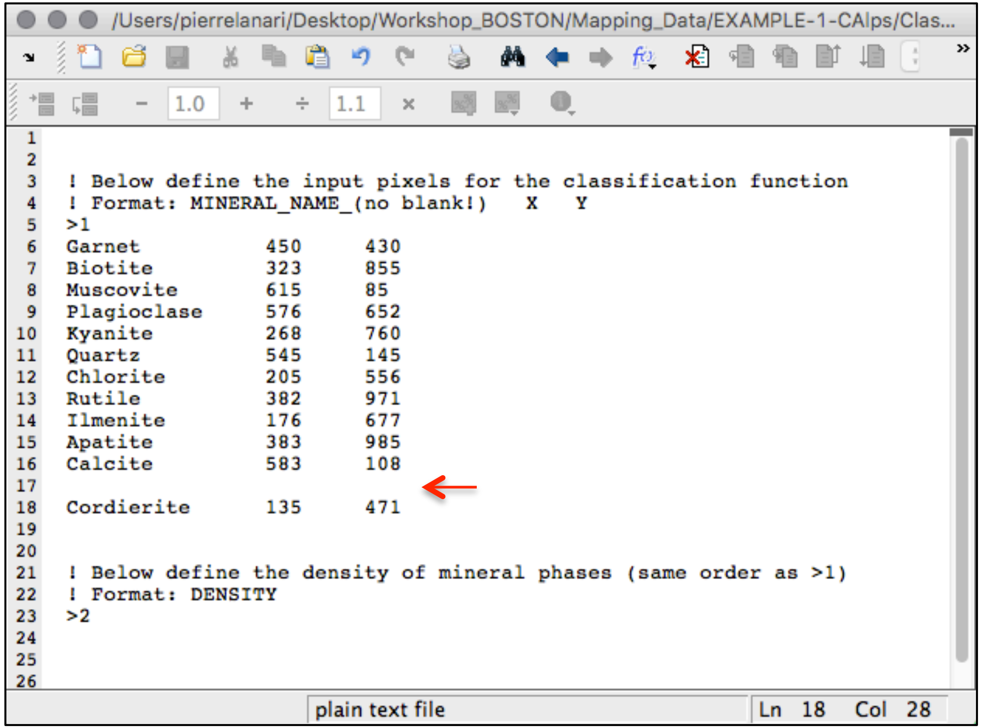


AUTOMATED CLASSIFICATION (NORMALIZED AND CLASSIC METHODS)

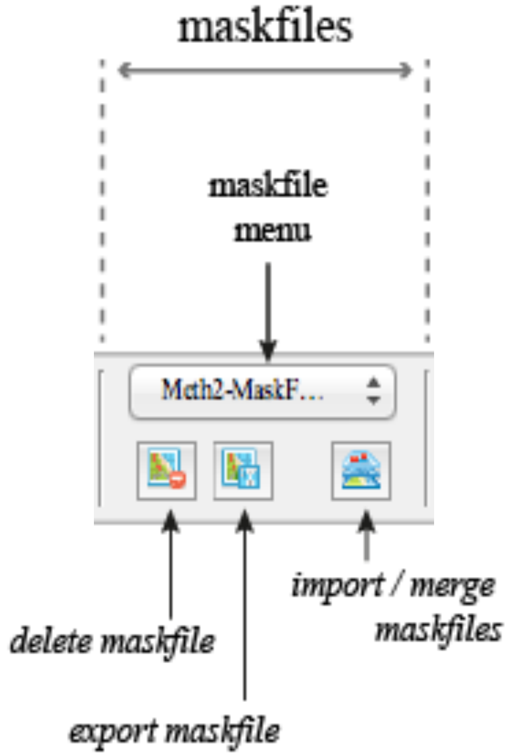


① Delete the second maskfile (*Meth1-MaskfFile2*, classic computation)

② Remove Cordierite from the list in Classification.txt



AUTOMATED CLASSIFICATION (NORMALIZED AND CLASSIC METHODS)



① Delete the second maskfile (*Meth1-MaskfFile2*, classic computation)

② Remove Cordierite from the list in Classification.txt

③ Select the method "Normalized intensities" and the mode "file" in the classification menus

④ Press CLASSIFY

⑤ Follow the instructions given by the program. In this example, Mn is excluded from the classification; system: Ce, La, Zr, Al, Ca, Fe, K, Mg, Na, Si, Ti

⑥ Export the maskfile (all masks) as "AutoClassificationNoCrd.txt"

- All the pixels are classified (no zero)
- The pixels of kyanite and cordierite are in mask number 5, *kyanite*

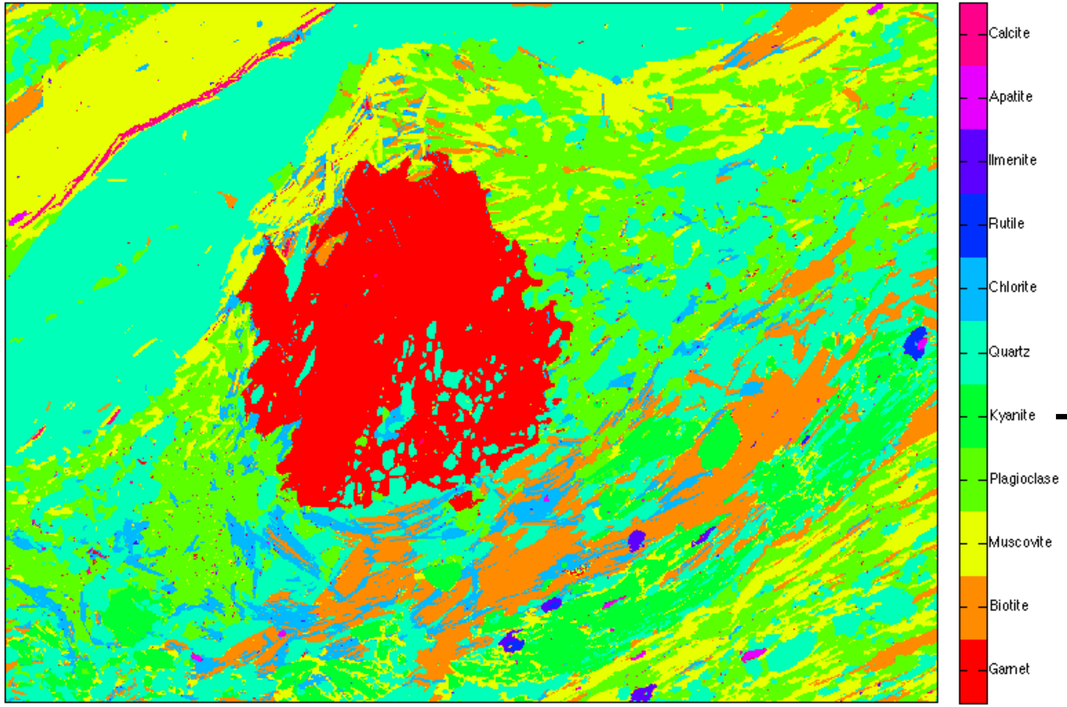
Save the project

Key steps

- Import the maps into XMapTools
- Identify the mineral phases
- Automated classification
- <u>Manual classification using the Binary module</u>
- Corrections

Manual adjustment of maskfile

Automated classification (normalized)



Binary module

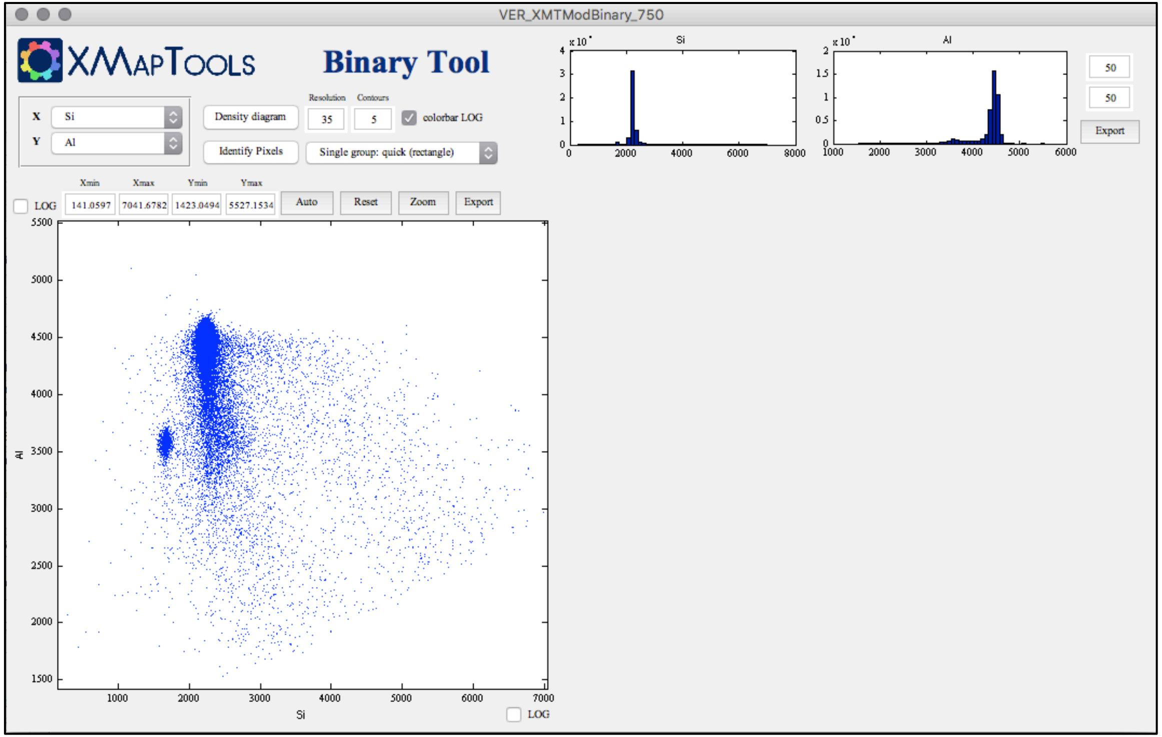
kyanite + cordierite

Create a new mask

MANUAL ADJUSTMENT OF MASKFILE

① Select the phase kyanite

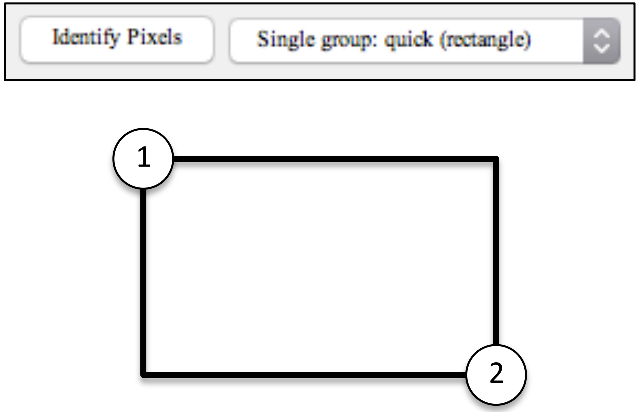
② Open the chemical module “Binary”

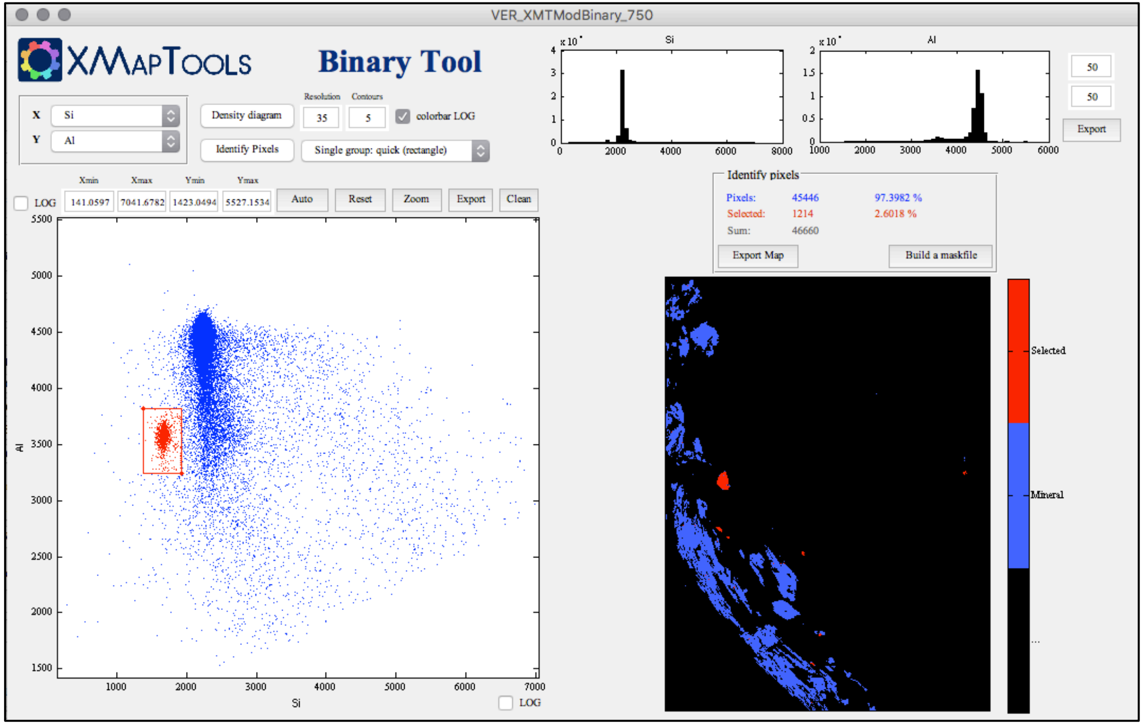


Manual adjustment of maskfile

③ Plot the pixel compositions in a diagram *Si vs Al*

④ Use the identify pixel tool "single group: quick (rectangle)" to select the pixels of cordierite



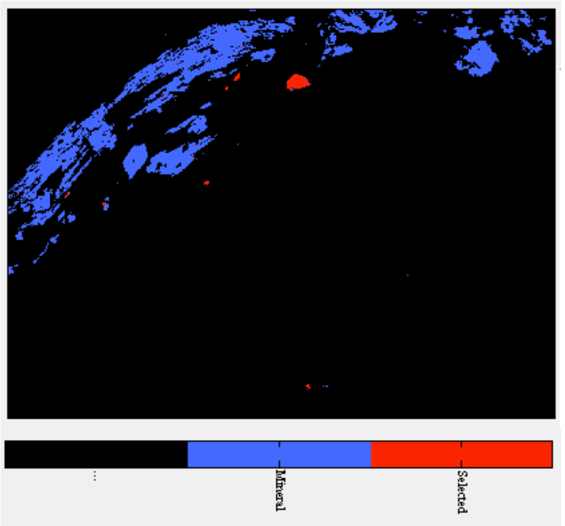


MANUAL ADJUSTMENT OF MASKFILE

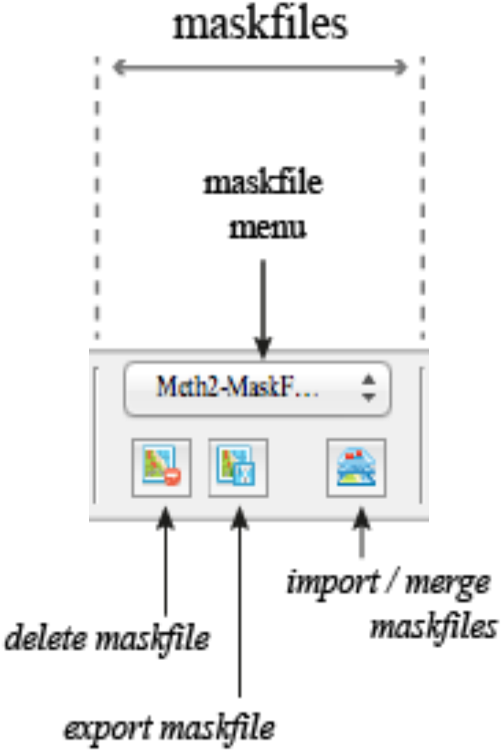
⑤ Press "*build a maskfile*" and generate a new maskfile "*Cordierite.txt*"; Note: it is important to only export the selected pixels. Edit the name of the mask "*Selection_1*" to "*Cordierite*"

⑥ Close the Binary module

⑦ In XMAPTOOLS, import and merge the two maskfiles



kyanite + cordierite

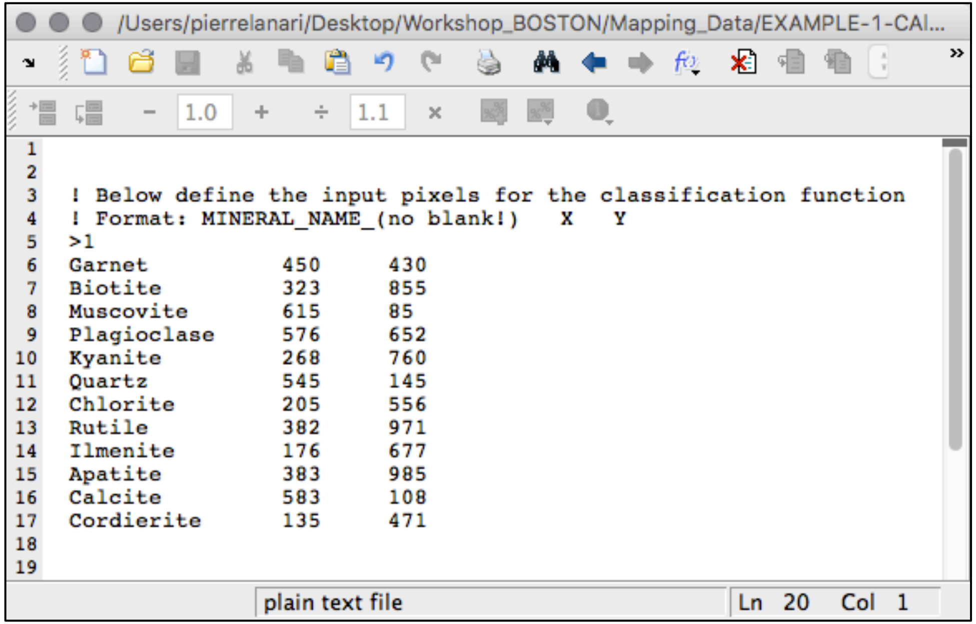


MANUAL ADJUSTMENT OF MASKFILE

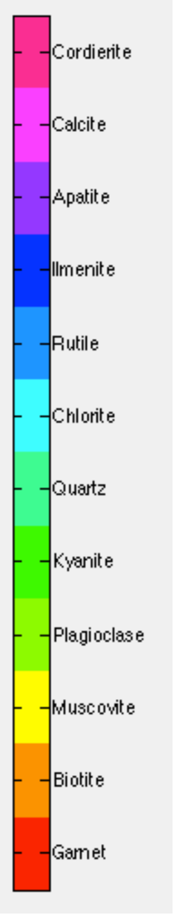
⑧ Check the classification by displaying each phase

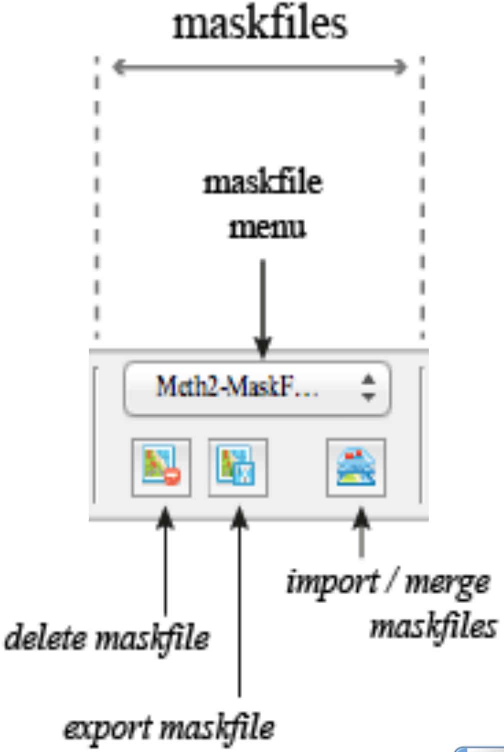
⑨ Delete the other maskfiles

⑩ Update the file *classification.txt*




```
! Below define the input pixels for the classification function
! Format: MINERAL_NAME_(no blank!)    X    Y
>1
Garnet          450     430
Biotite         323     855
Muscovite       615     85
Plagioclase     576     652
Kyanite         268     760
Quartz          545     145
Chlorite        205     556
Rutile          382     971
Ilmenite        176     677
Apatite         383     985
Calcite         583     108
Cordierite      135     471
```



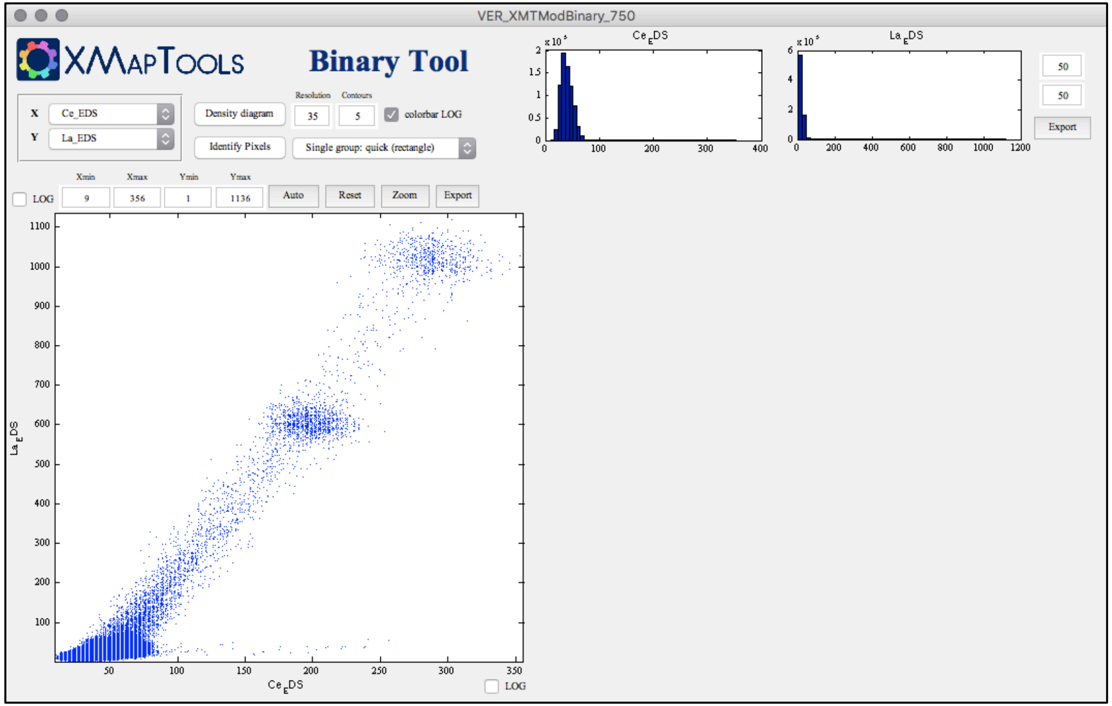


Save the project

Manual classification with the Binary module

① Select "none" in the *phase menu*

② Open the chemical module "Binary"

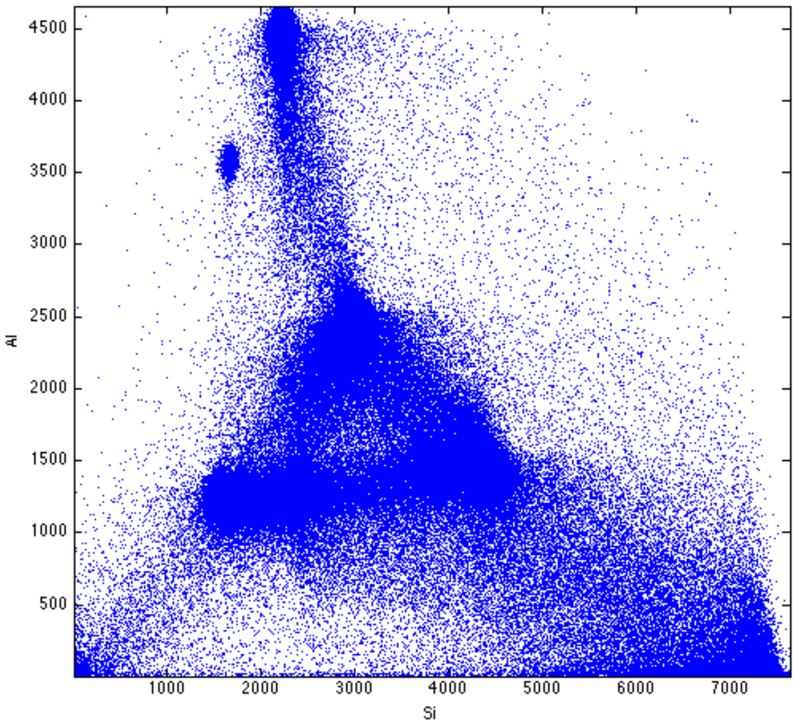


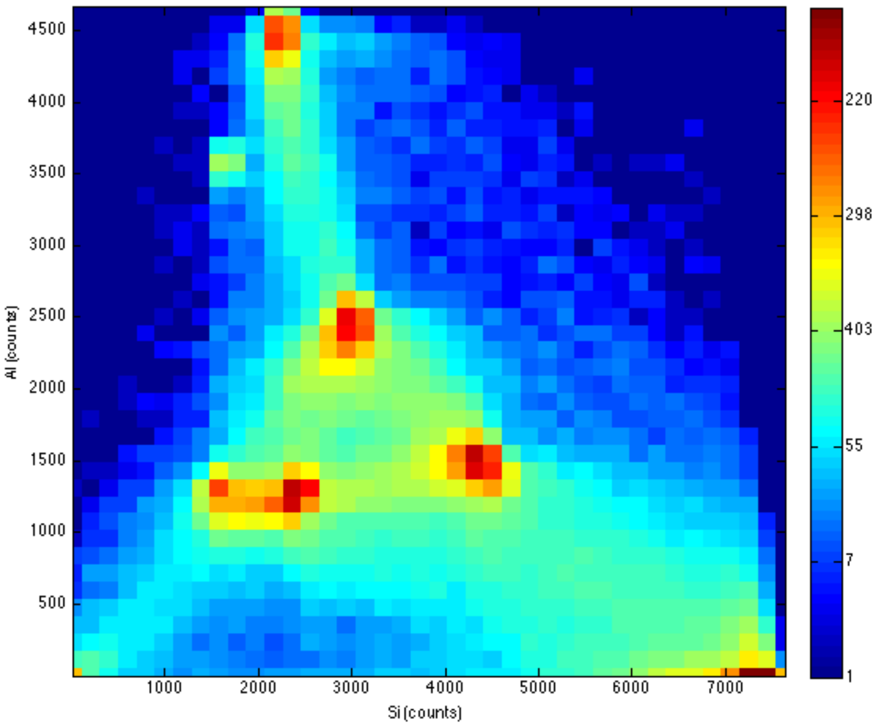
In this case the compositions of all the pixels have been sent to the Binary module

MANUAL CLASSIFICATION WITH THE BINARY MODULE

① Plot again *Si vs Al* and press "auto" to adjust the axis limits

② Compute a density map of this diagram with a resolution of 40 px

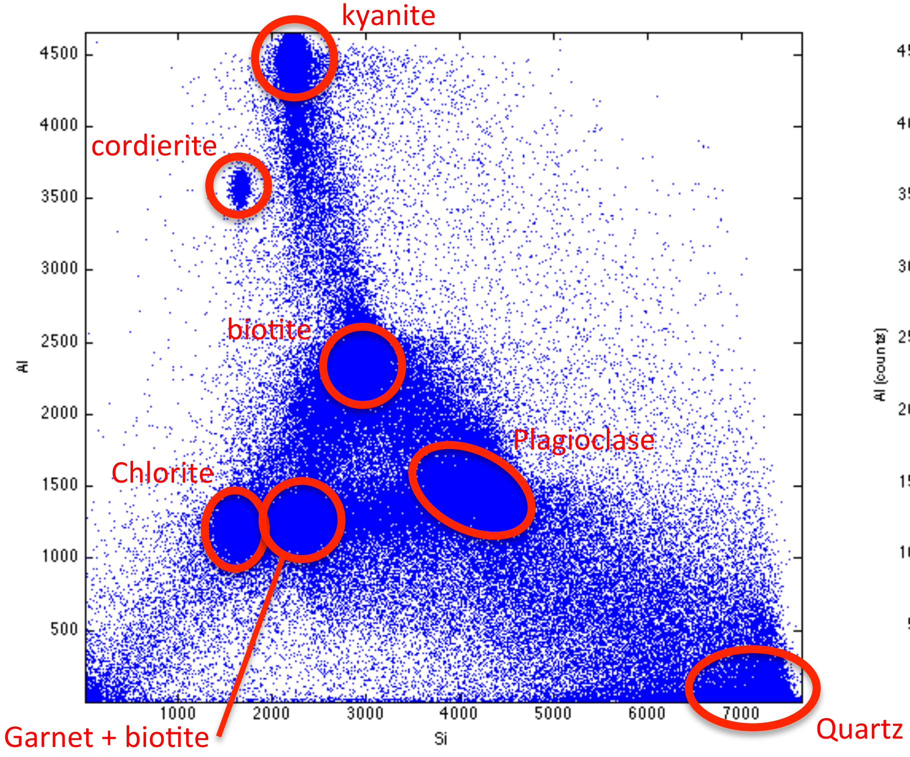


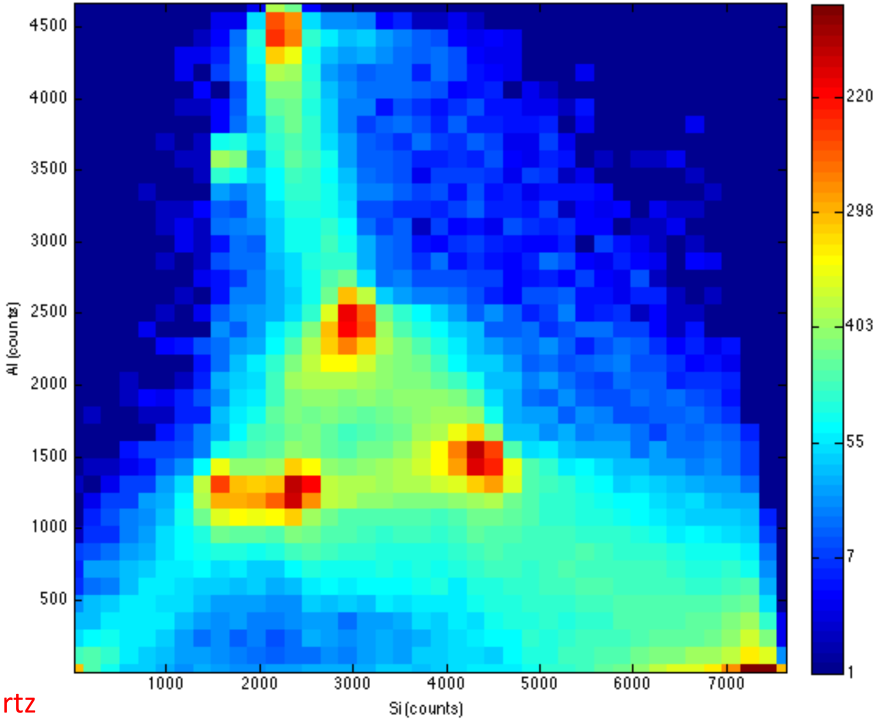


Manual classification with the Binary module

③ Close the density map

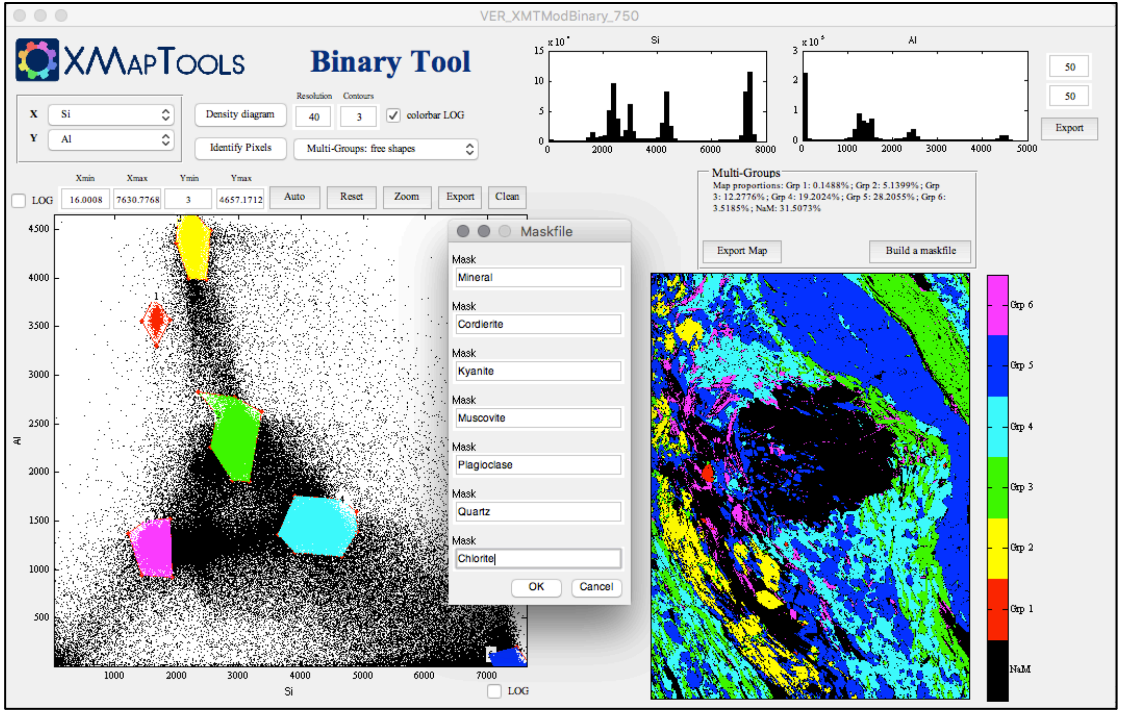
④ Identify the mineral(s) corresponding to each group of pixel

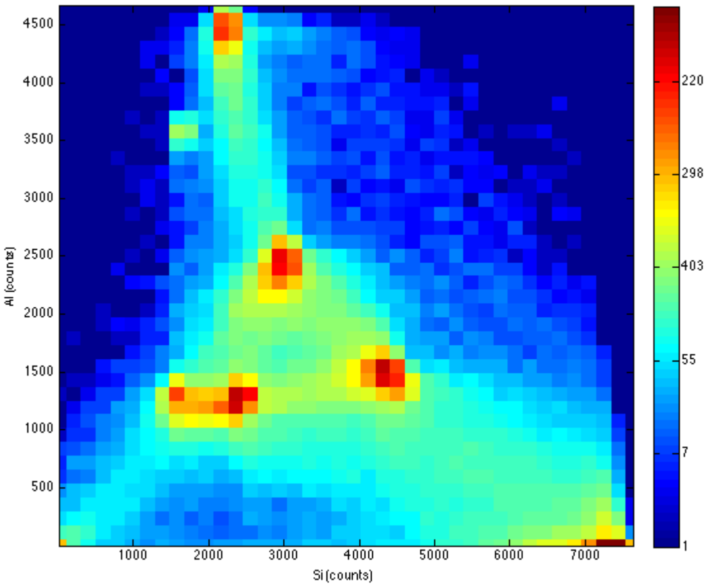




Manual classification with the Binary module

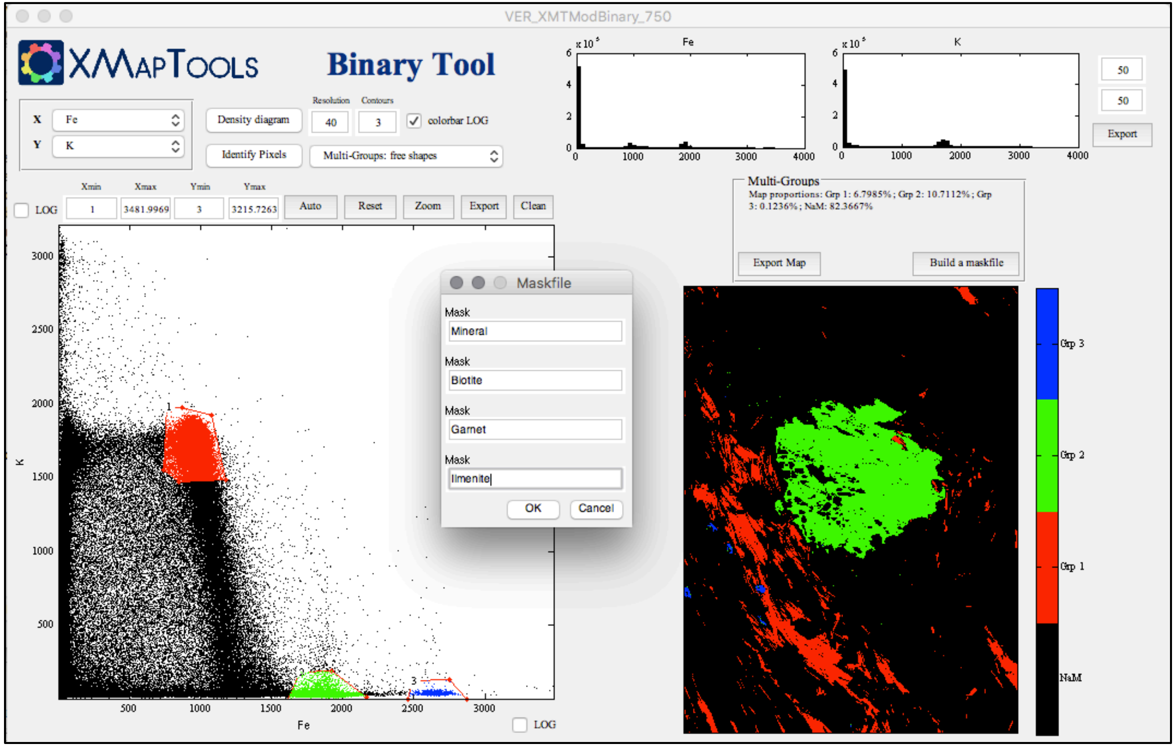
③ Use the tool identify pixels (multi-groups free shapes to select the pixels of the phases: (1) cordierite, (2) kyanite, (3) muscovite, (4) plagioclase, (5) quartz and (6) chlorite and save the corresponding maskfile (*name: Manual_Crd-Ky-Ms-Pl-Qz-Chl.txt*)





MANUAL CLASSIFICATION WITH THE BINARY MODULE

④ Plot a diagram *Fe vs K* and export a maskfile containing (1) biotite, (2) garnet and (3) ilmenite (*Manual_Bi-Grt-Ilm.txt*)

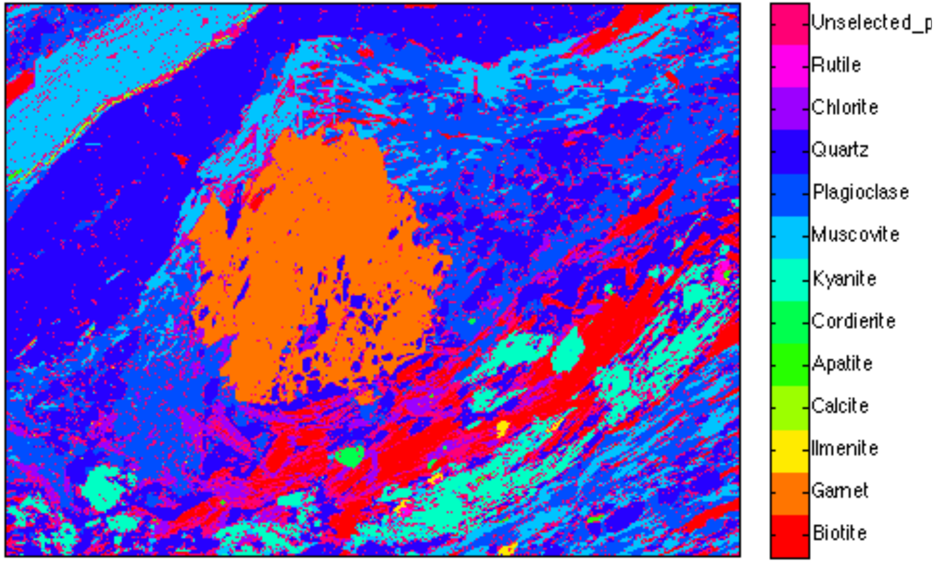


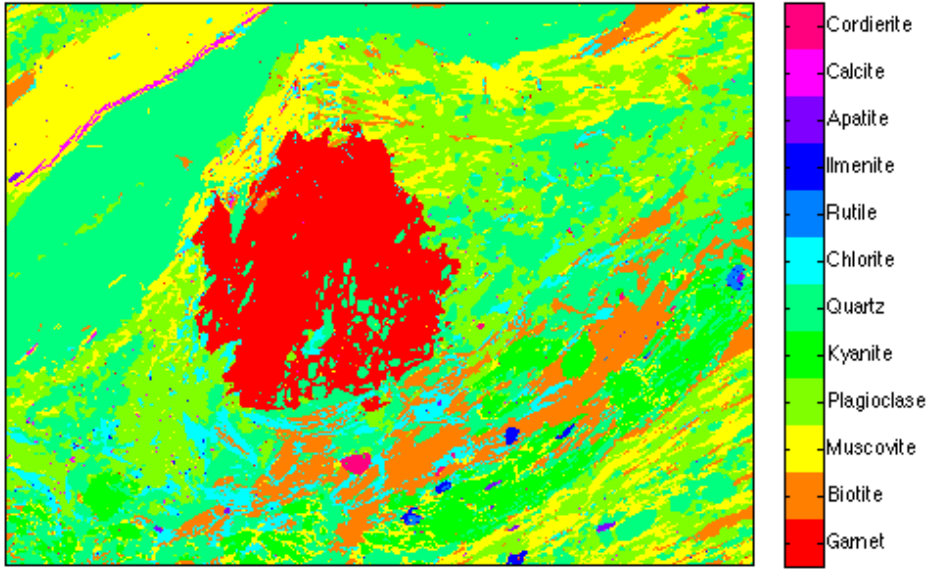
Manual classification with the Binary module

⑤ Plot a diagram *Zr vs Ca* and export a maskfile containing (1) calcite and (2) apatite (*Manual_Clc-Ap-Ilm.txt*)

⑥ Plot a diagram *Ti vs Ca* and export a maskfile containing the pixels of rutile (*Manual_Rt.txt*)

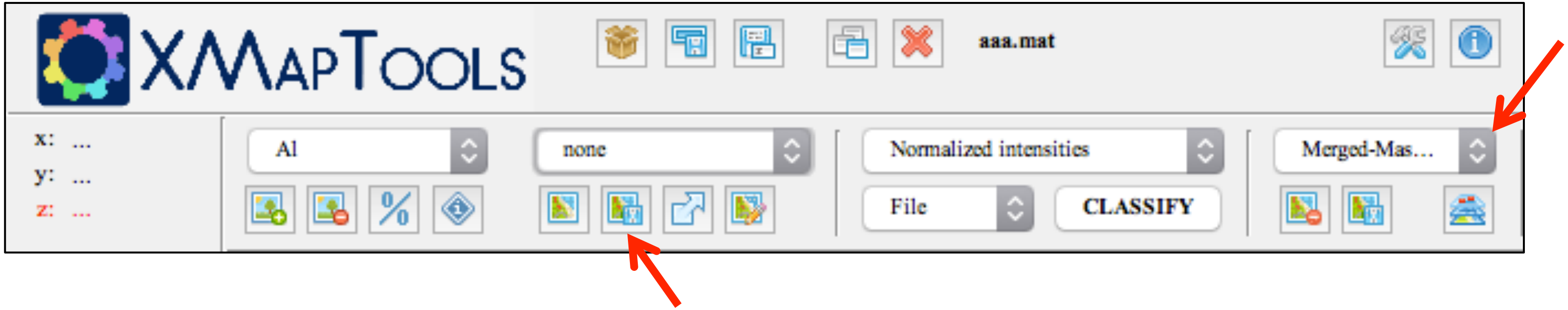
⑦ Go back to XMapTools and import the maskfiles *Manual_Crd-Ky-Ms-Pl-Qz-Chl.tx, Manual_Bi-Grt-Ilm.txt, Manual_Clc-Ap-Ilm.txt* and *Manual_Rt.txt*





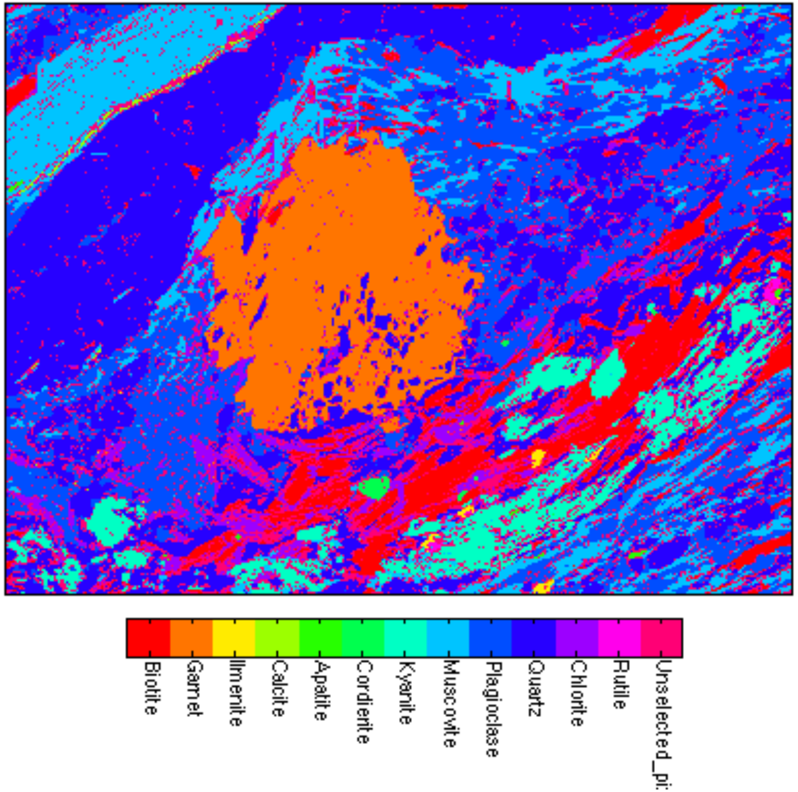
Manual classification with the Binary module

⑧ Export the phase proportions of the semi-automated and manual maskfiles

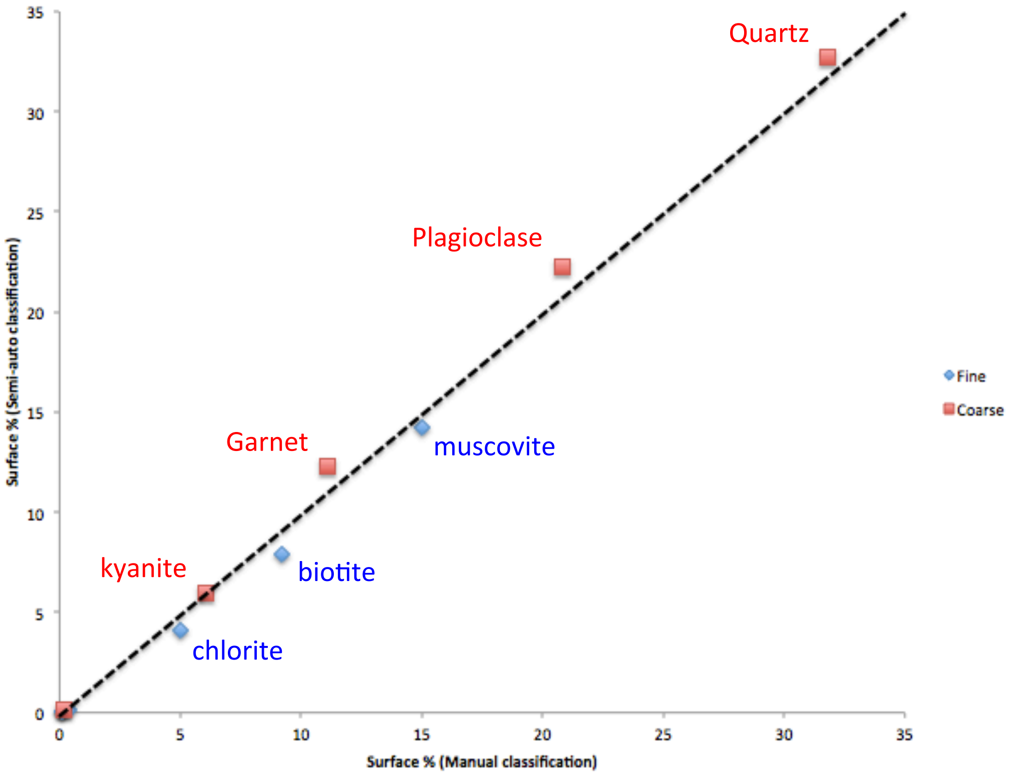


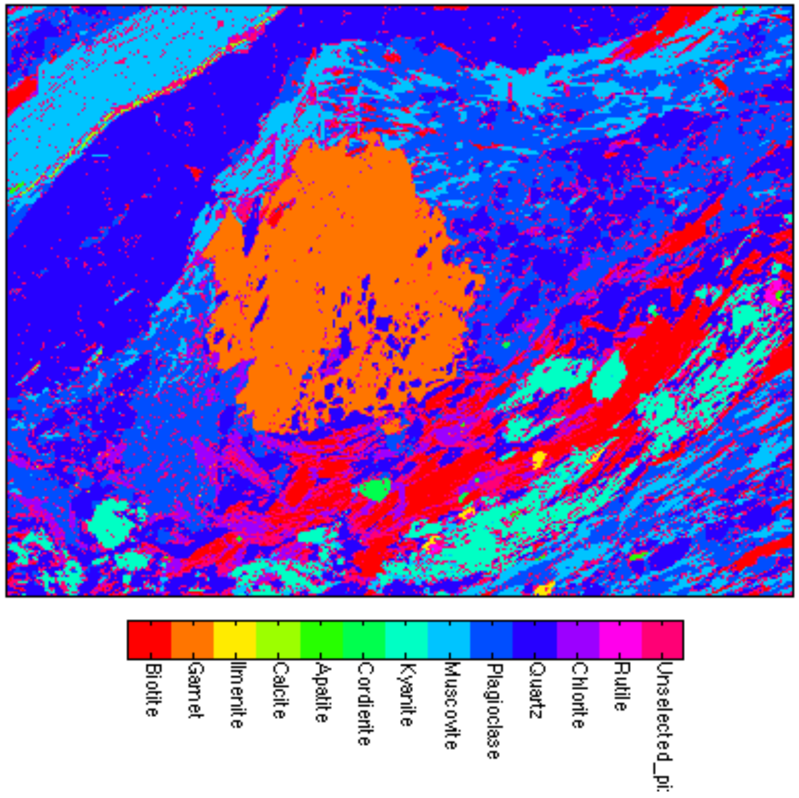
Manual classification with the Binary module

	Semi-auto	Manual
Biotite:	9.21	7.87
Garnet:	11.12	12.29
Ilmenite:	0.21	0.14
Calcite:	0.4	0.15
Apatite:	0.13	0.09
Cordierite:	0.16	0.17
Kyanite:	6.06	5.96
Muscovite:	14.99	14.23
Plagioclase:	20.79	22.25
Quartz:	31.82	32.68
Chlorite:	5.02	4.08
Rutile:	0.1	0.09



MANUAL CLASSIFICATION WITH THE BINARY MODULE





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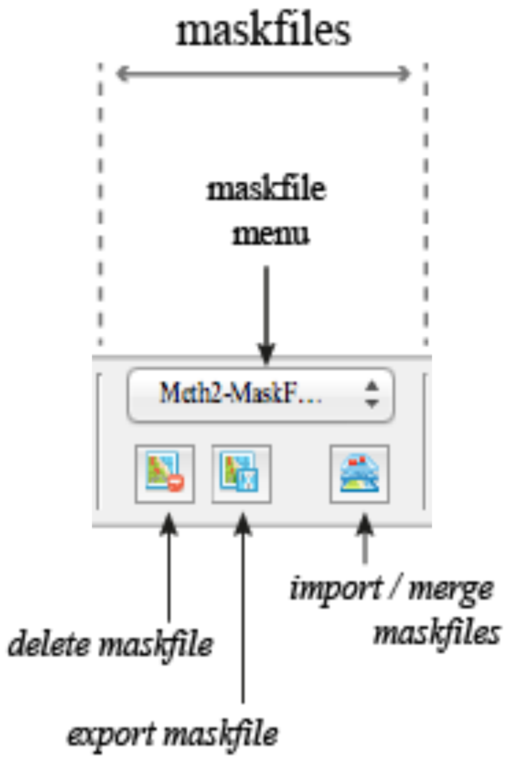
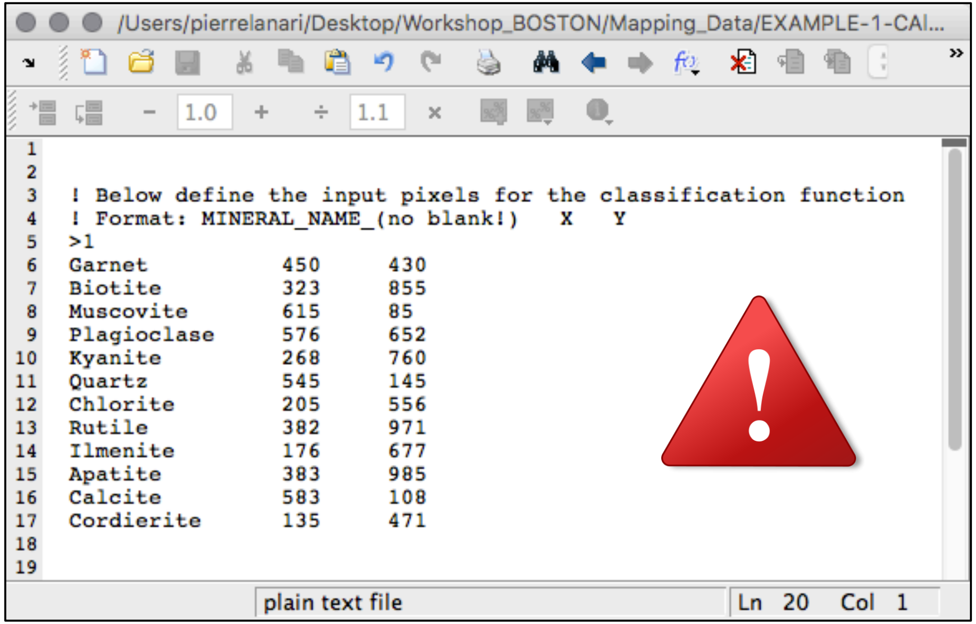


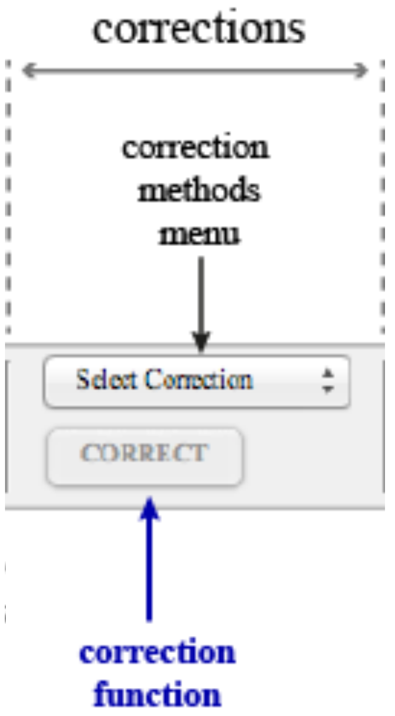
⑨ Keep the maskfile from the semi-automated classification and delete the other maskfiles



Key steps

- Import the maps into XMapTools
- Identify the mineral phases
- Automated classification
- Manual classification using the Binary module
- Corrections

CORRECTIONS (X-RAY WORKSPACE)



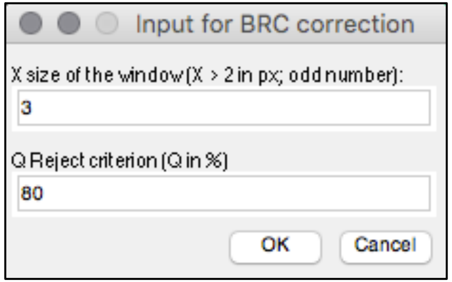
Abbreviation	Name	Button string	Correction mode	Requirements
BRC	Border-removing correction	APPLY	No	existing mask file
TRC	Topo-related correction	SET	Yes (External GUI)	TOPO map
MPC	Map position correction	ACTIVATE	Yes	Standards analyses
SPC	Standard position correction	ACTIVATE	Yes	Standards analyses
IDC	Intensity drift correction	APPLY	No	Phase selected
BA1	Background correction (using maps)	APPLY	No	Background maps
RM1	Clean pixels (area; all maps)	SELECT	Yes	...

Table 3.1 – *Corrections available in XMapTools, modes and requirements*

- **BRC filters mixing pixels out**
- IDC corrects time-related intensity drift
- TRC corrects TOPO-related intensity variations

CORRECTIONS (X-RAY WORKSPACE): BRC

① Select “BRC” in the correction menu and press “APPLY”



Considering a mask i.e., a matrix with ones where the pixels are allocated to the selected phase, and a given pixel:

$$px(i,j) \tag{3.1}$$

with

$$((X-1)/2) < i < i_{max} - ((X-1)/2) \tag{3.2}$$

and

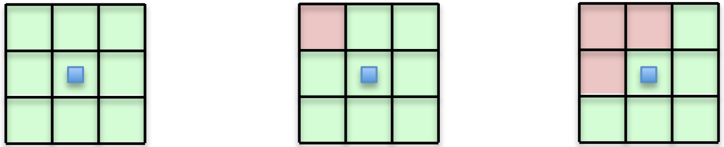
$$((X-1)/2) < j < j_{max} - ((X-1)/2) \tag{3.3}$$

This pixel is removed by the BRC function ($BRC(i,j) = 0$) if

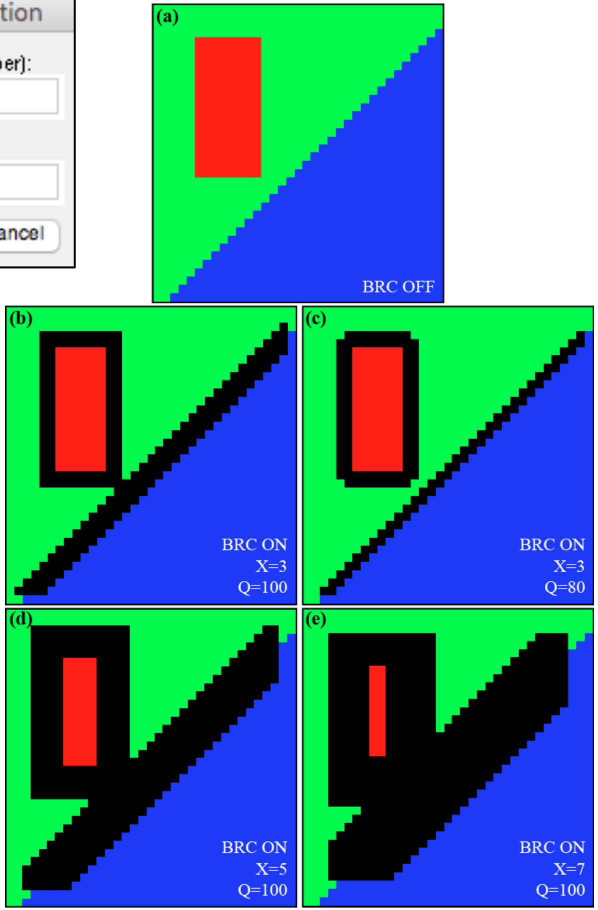
$$\sum_{1}^{X^2} (px(i-(X-1)/2 : i+(X-1)/2, j-(X-1)/2 : j+(X-1)/2)) < X^2 \frac{Q}{100} \tag{3.4}$$

with X the size of the scanning window in pixel (odd number >= 3) and Q the reject criterion in %. This filtering procedure is applied to all the pixels of all the masks.

The equation (3.4) implies that *BRC* may not filter the pixels located at the rim of the map. The width of this rim is exactly $(X-1)/2$ pixels.



100 %   88 %   66 %



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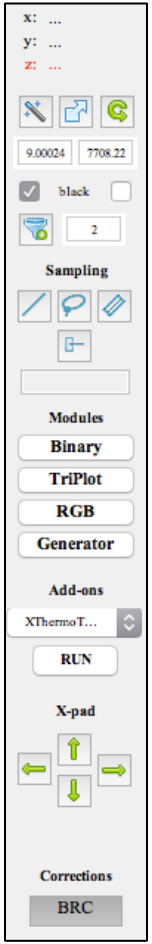
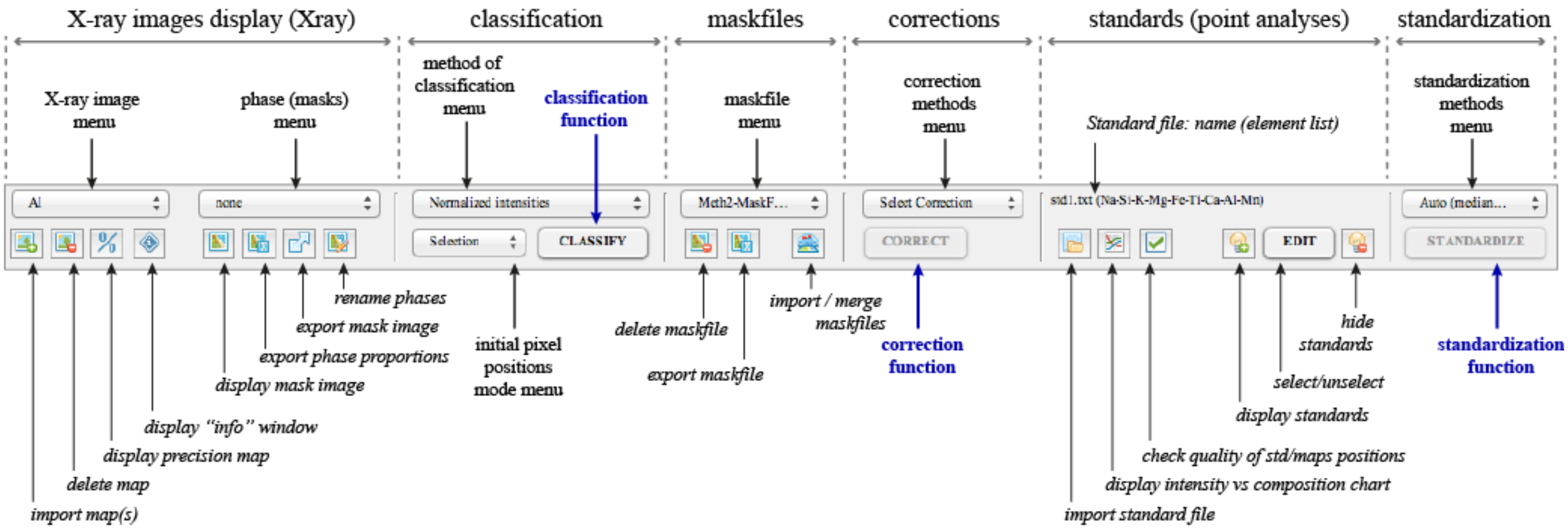
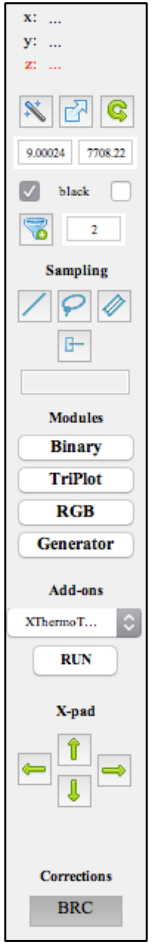


You can activate or deactivate the BRC correction using the button BRC on the left hand-side. Once BRC is activated, the correction is applied for most of the operations and plots performed in the workspace *X-ray*





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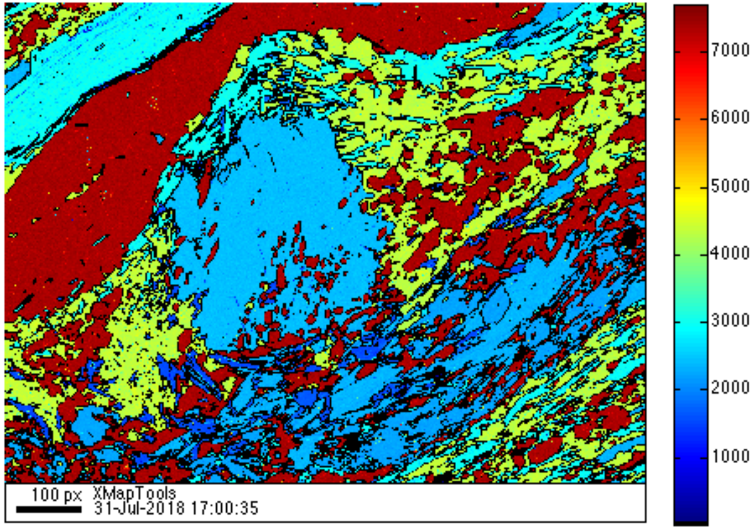
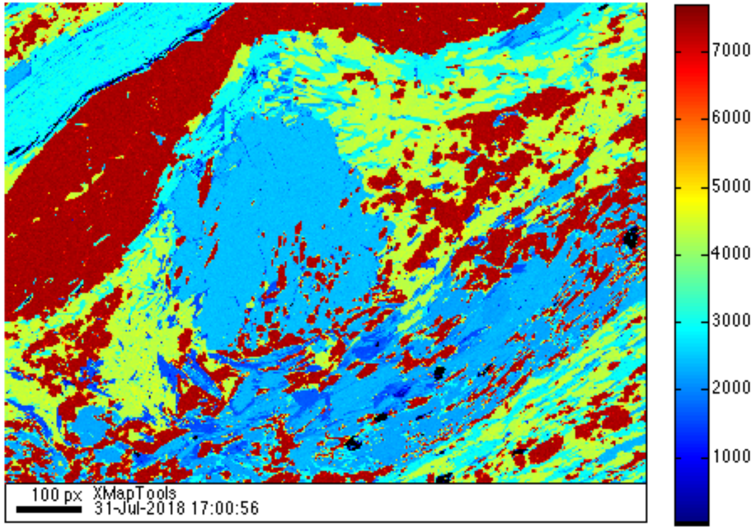
② Compare the map of silicon with the BRC active and without





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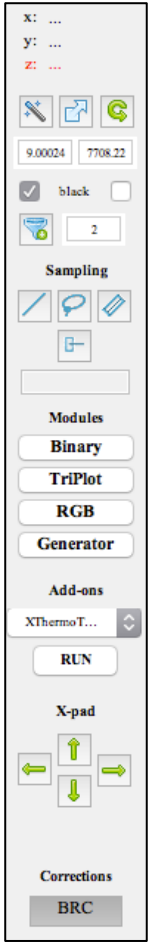

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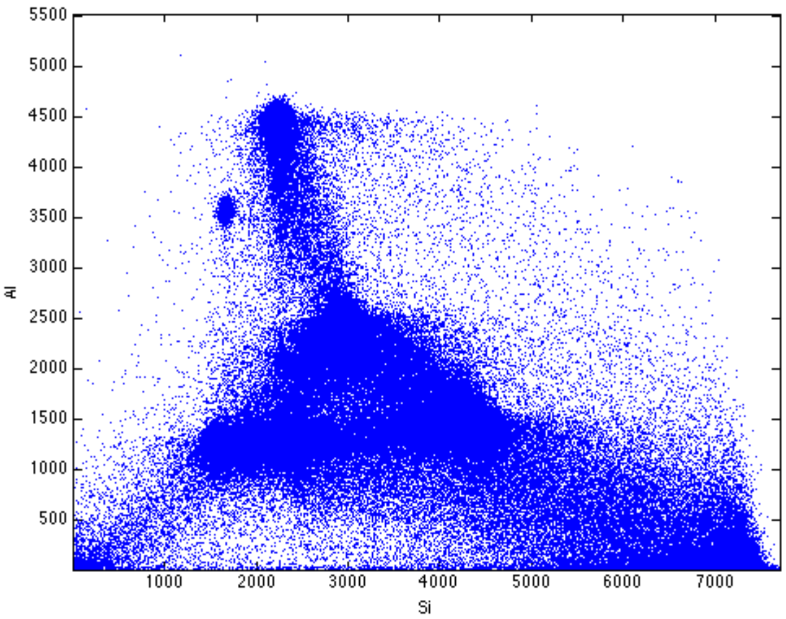
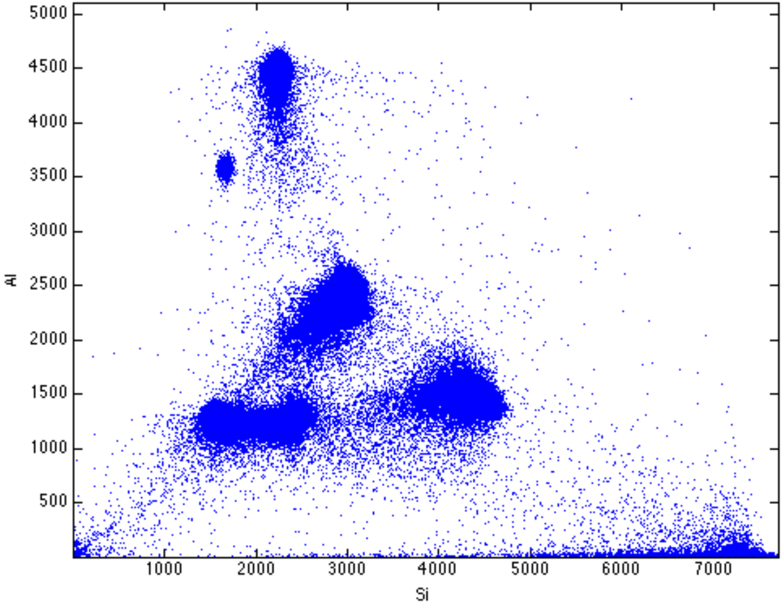
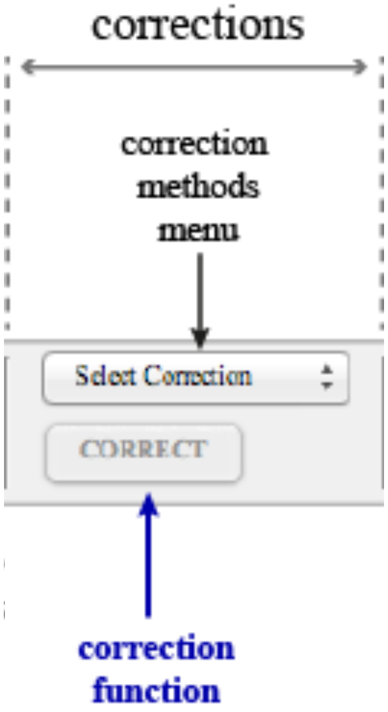
③ Plot a binary diagram *Si vs Al* containing all the pixels





CORRECTIONS (X-RAY WORKSPACE)



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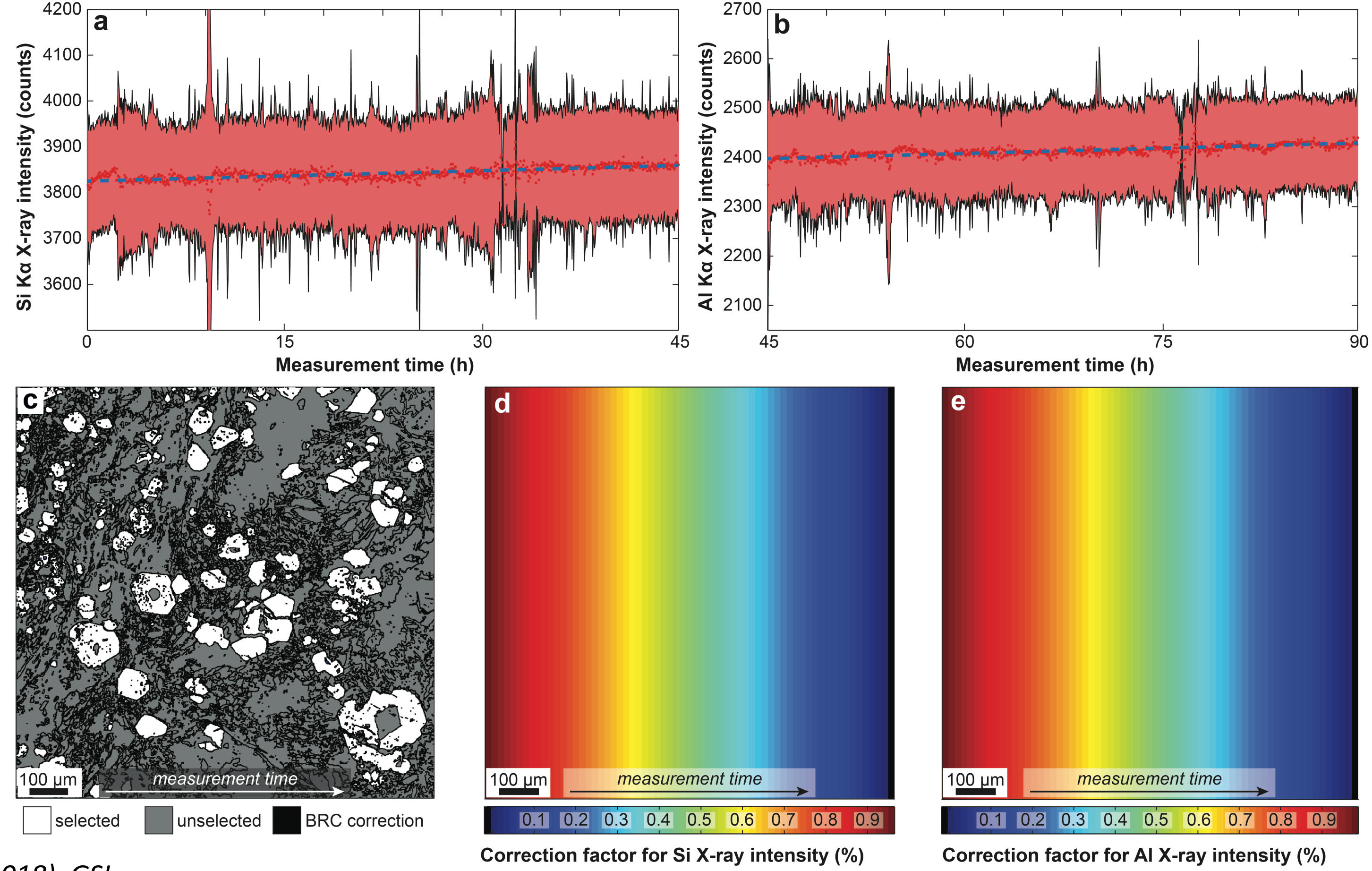
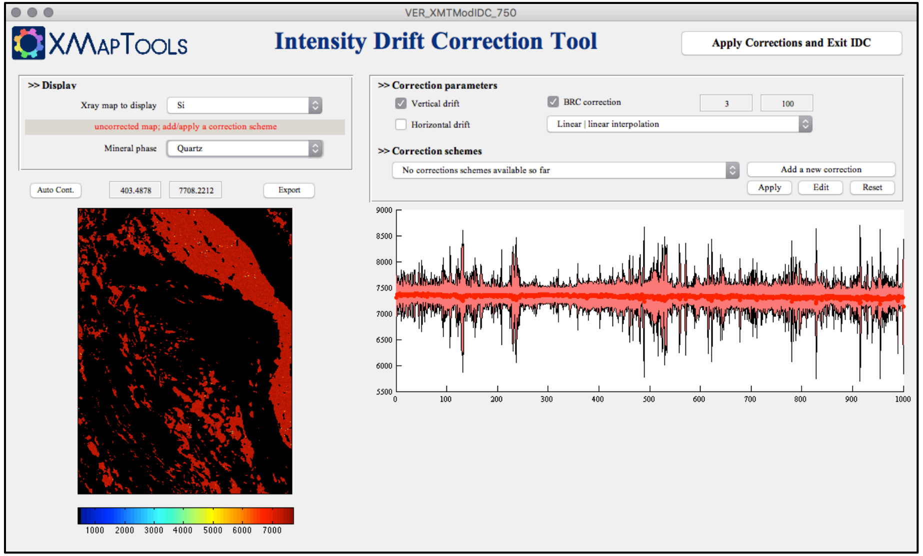


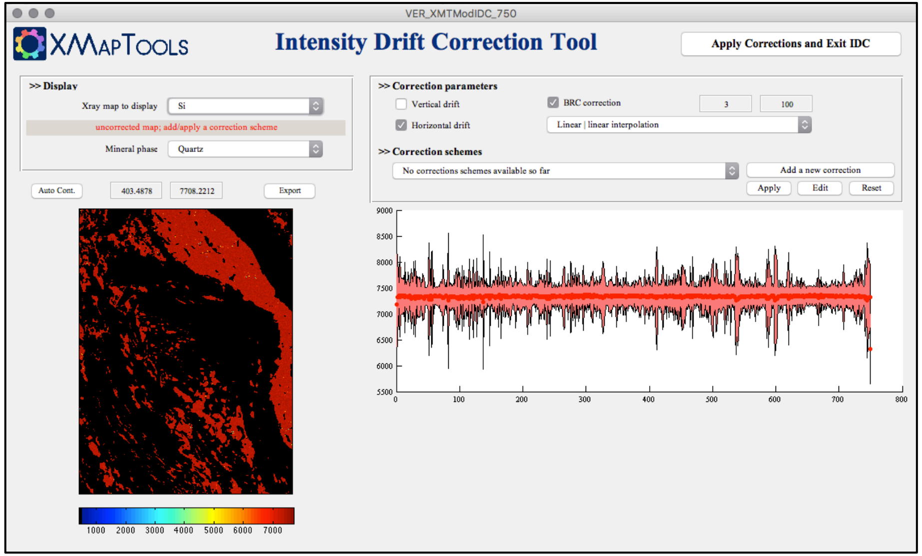
Lanari et al. (2018), GSL

CORRECTIONS (X-RAY WORKSPACE): IDC

① Select "IDC" in the correction menu and press "RUN"

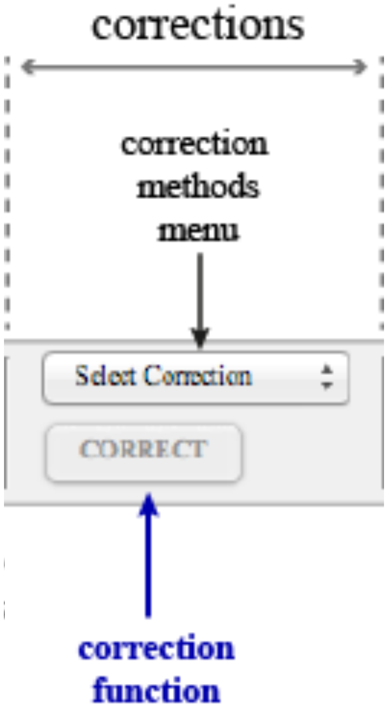
② Display the map "Si" and the phase "Quartz". Check for vertical and horizontal drift





③ Close the IDC module

CORRECTIONS (X-RAY WORKSPACE)



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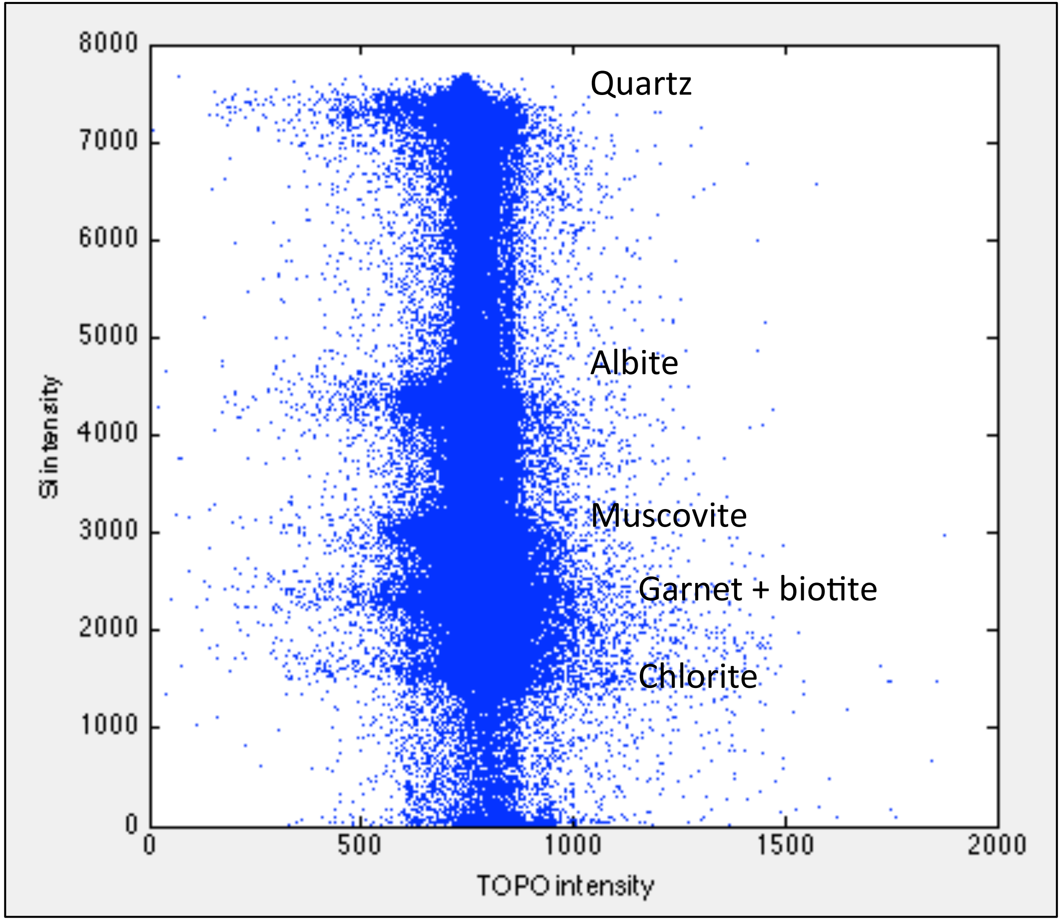
CORRECTIONS (X-RAY WORKSPACE): IDC

① Load the TOPO map

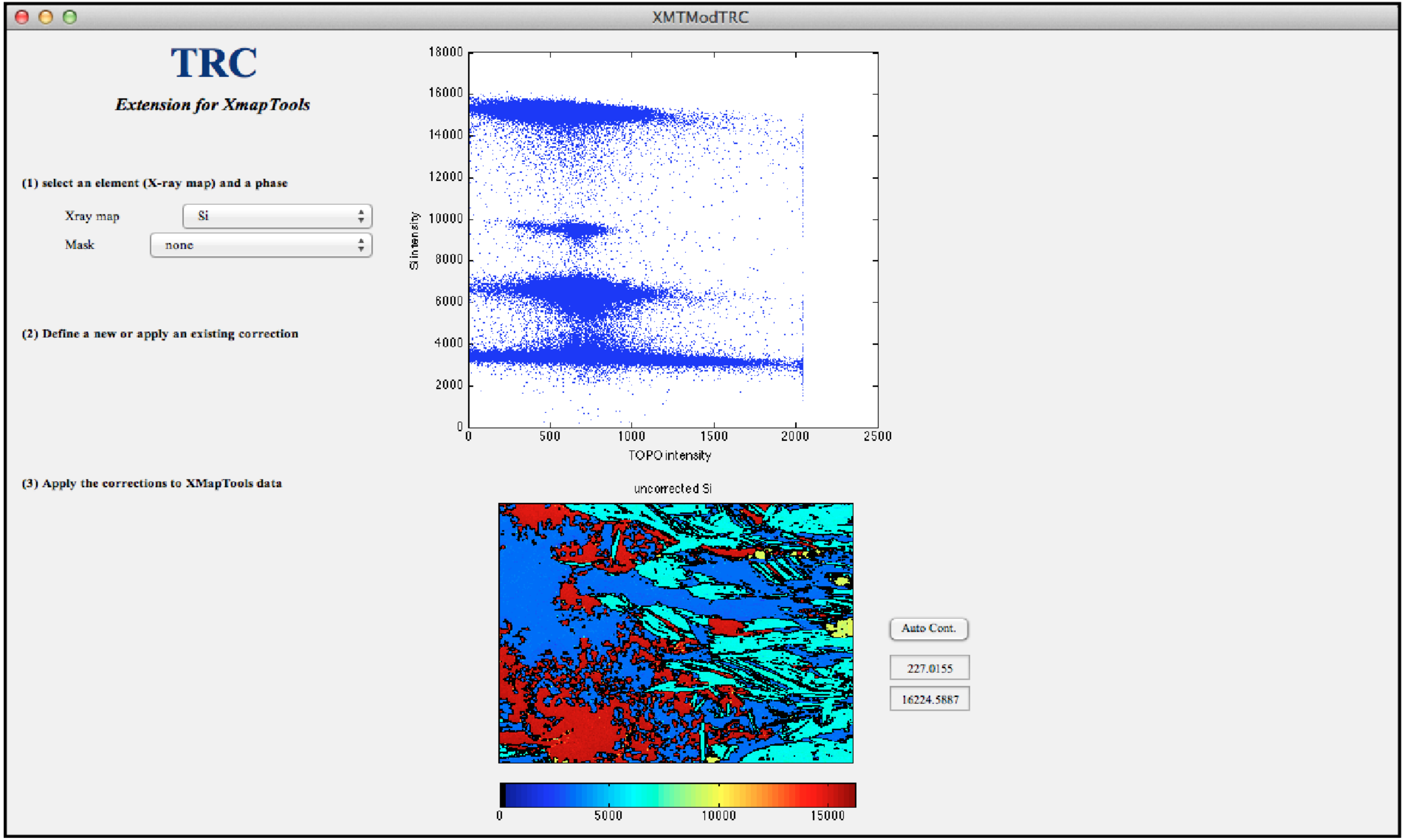
② Activate the BRC

③ Select "TRC" in the correction menu and press "RUN"

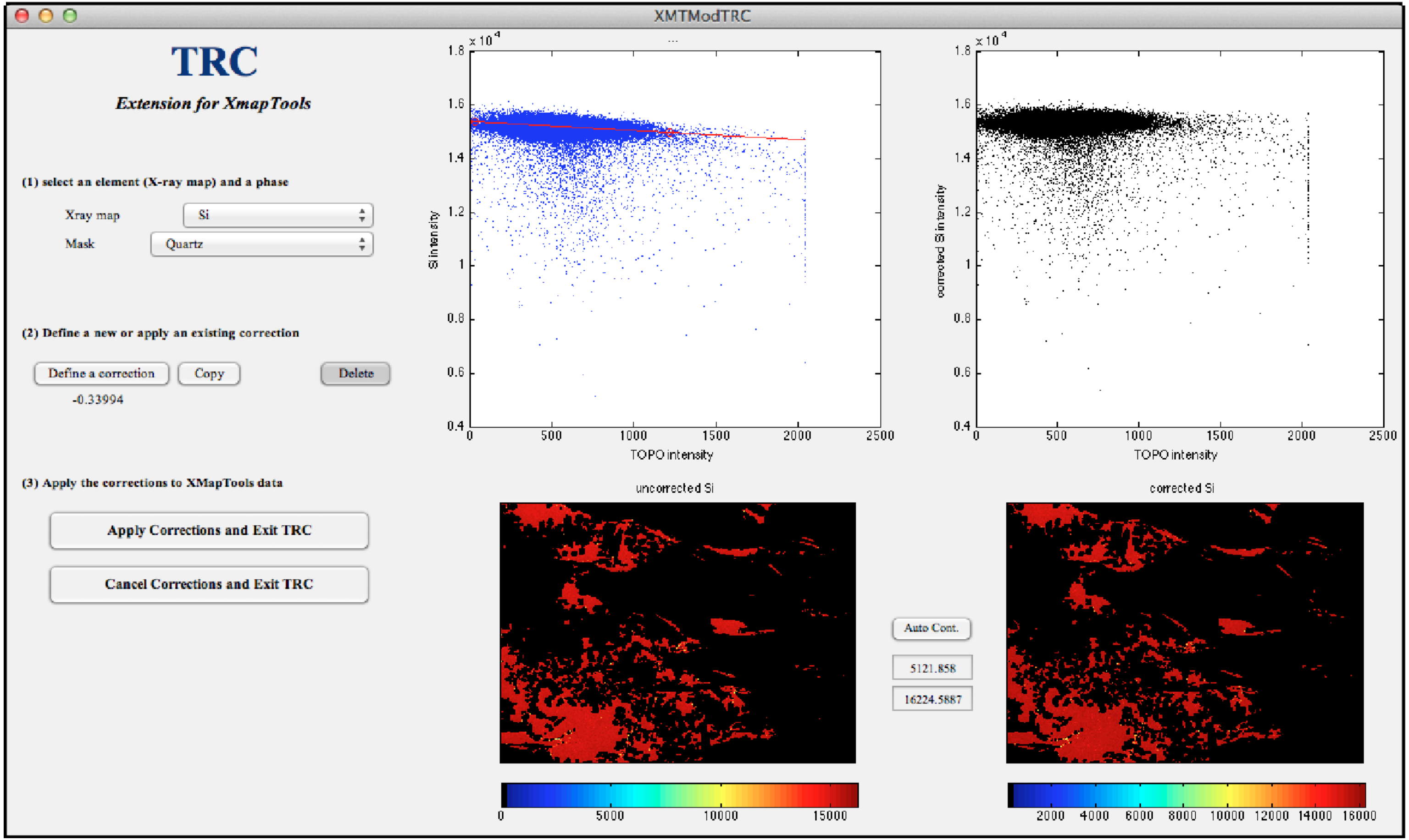
④ Select the element "Si" and "none" in the phase menu



CORRECTIONS (X-RAY WORKSPACE): IDC



CORRECTIONS (X-RAY WORKSPACE): IDC



CORRECTIONS (X-RAY WORKSPACE): IDC

① Load the TOPO map

② Activate the BRC

③ Select “TRC” in the correction menu and press “RUN”

④ Select the element “Si” and “none” in the phase menu

⑤ Check the other elements

⑥ Close the TRC module

Questions / Discussion