GeoThermalCloud_Utah

October 22, 2021

1 GeoThermalCloud: Geothermal Machine Learning Analysis: Utah

This notebook is a part of the GeoThermalCloud.jl: Machine Learning Framework for Geothermal Exploration.

```
<img src="https://raw.githubusercontent.com/SmartTensors/GeoThermalCloud.jl/master/logos/geothe
```

1.1 GeoThermalCloud installation

If **GeoThermalCloud** is not installed, first execute in the Julia REPL:

```
import Pkg
Pkg.add("GeoThermalCloud")
Pkg.add("NMFk")
Pkg.add("Mads")
Pkg.add("DelimitedFiles")
Pkg.add("JLD")
Pkg.add("Gadfly")
Pkg.add("Cairo")
Pkg.add("Fontconfig")
Pkg.add("Kriging")
Pkg.add("GMT")
Pkg.add("Images")
```

[1]:
```
import GeoThermalCloud
import NMFk
import Mads
import DelimitedFiles
import JLD
import Gadfly
import Cairo
import Fontconfig
import Kriging
import GMT
import Images
```

1.2 Load data

[2]:
```
Xdat, headers = DelimitedFiles.readdlm("utah/data/utah_geothermal_data.csv",␣
↪',', header=true);
```

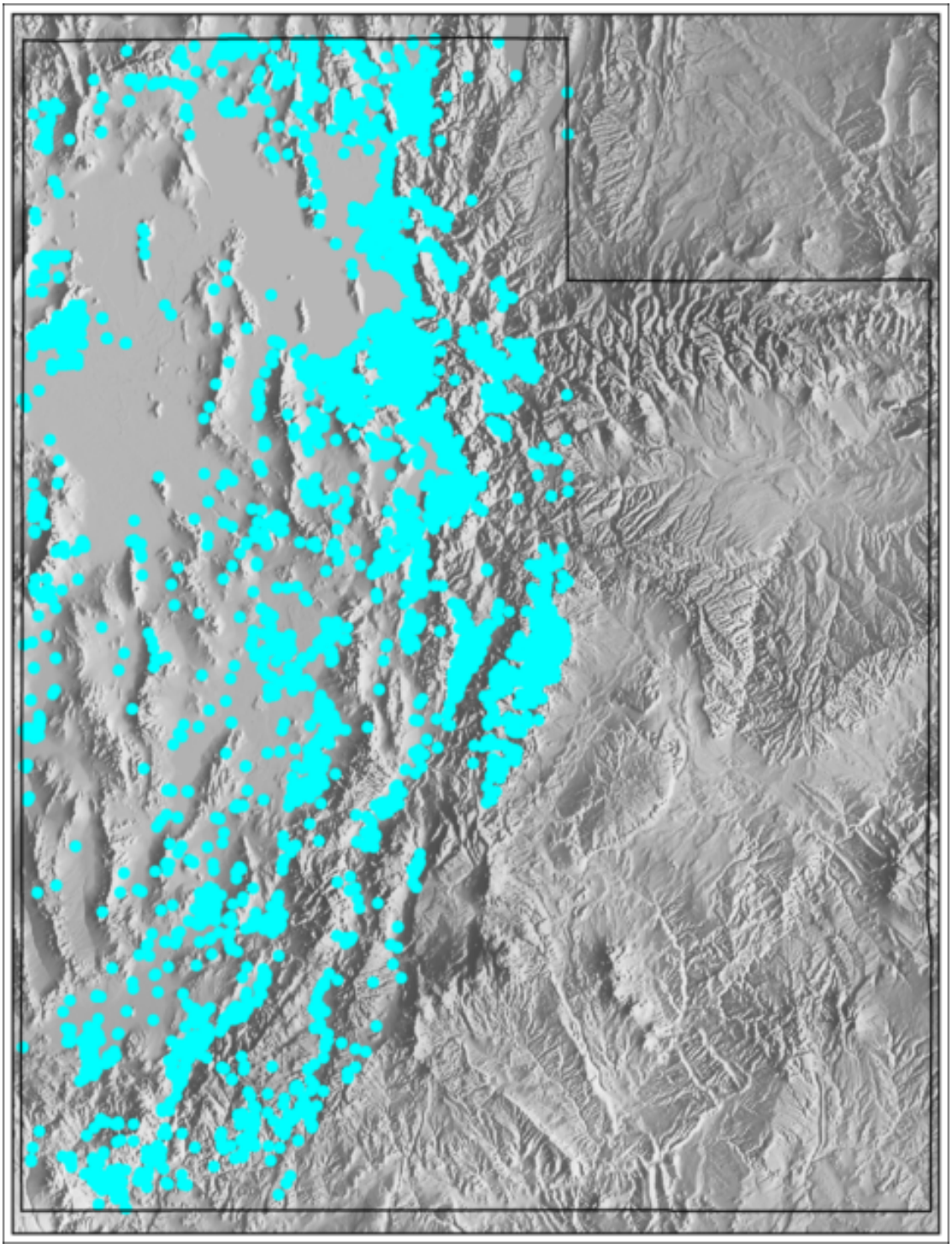
Set coordinates:

[3]:
```
xcoord = Array{Float32}(Xdat[:, 2])
ycoord = Array{Float32}(Xdat[:, 1]);
```

1.3 Data Locations

Plot data locations on a map:

[4]:
```
GMT.grdimage("utah/maps/utah.nc", proj=:Mercator, shade=(azimuth=100, norm="e0.
↪8"),
       color=GMT.makecpt(color=:grayC, transparency=10, range=(0,5000,500),␣
↪continuous=true),
       figsize=8, conf=(MAP_FRAME_TYPE="plain",␣
↪MAP_GRID_PEN_PRIMARY="thinnest,gray,.",
       MAP_GRID_CROSS_SIZE_SECONDARY=0.1, MAP_FRAME_PEN=0.5,␣
↪MAP_TICK_PEN_PRIMARY=0.1,
       MAP_TICK_LENGTH_PRIMARY=0.01), frame=(axis="lrtb"))
GMT.plot!(xcoord, ycoord, fill=:cyan, marker=:c, markersize=0.1, coast=(proj=:
↪Mercator,
   DCW=(country="US.UT", pen=(0.5,:black))),
   fmt=:png, savefig="utah/maps/locations");
Images.load("utah/maps/locations.png")
```



1.4 Define data attributes

We can use attribute names from the header in the input file.

However, the names are short.

For better understanding the variable names in the plots generated bellow, we are defining `short` and `long` attribute names:

[5]:
```
attributes = ["Temperature", "Quartz", "Chalcedony", "pH", "TDS", "Al", "B",␣
 ↪"Ba", "Be", "Br", "Ca", "Cl", "HCO3", "K", "Li", "Mg", "Na", " O18"]
attributes_long = ["Temperature (C)", "GTM quartz (C)", "GTM chalcedony (C)",␣
 ↪"pH ()", "TDS (ppm)", "Al (ppm)", "B (ppm)", "Ba (ppm)", "Be (ppm)", "Br␣
 ↪(ppm)", "Ca (ppm)", "Cl (ppm)", "HCO3 (ppm)", "K (ppm)", "Li (ppm)", "Mg␣
 ↪(ppm)", "Na (ppm)", " O18 (%)"];
```

1.5 Pre-processing

Set empty data entries to `NaN`:

[6]:
```
Xdat[Xdat .== ""] .= NaN;
```

Convert to `Float32`:

[7]:
```
X = convert.(Float32, Xdat[:,3:end]);
```

Rescale O18 data (‰):

[8]:
```
X[:,18] .+= 20;
```

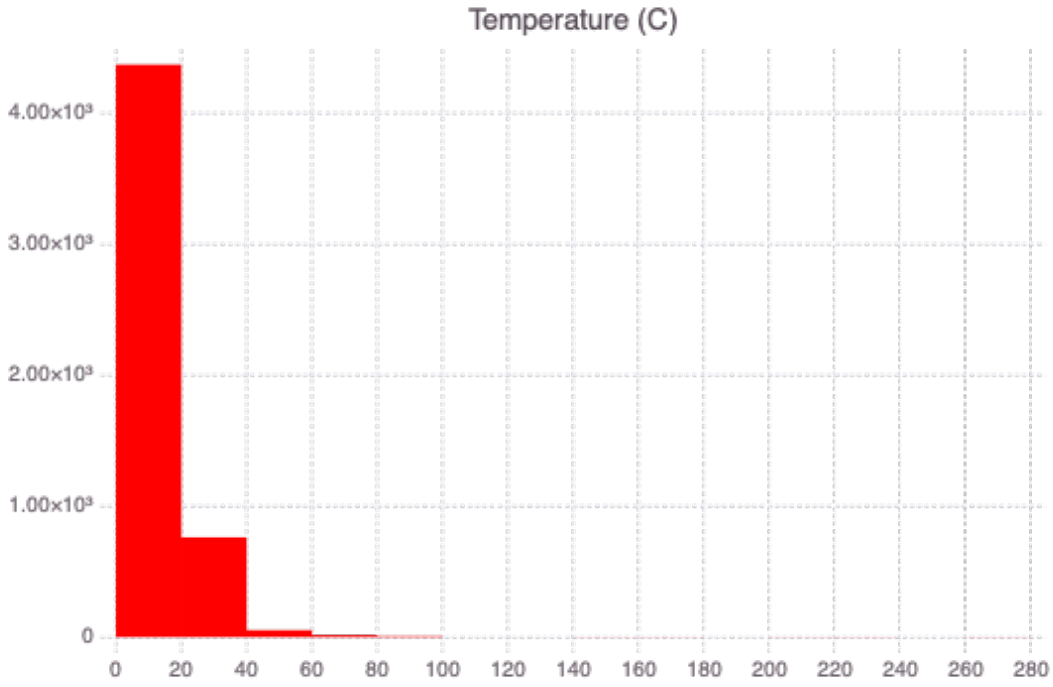
Set variables for the number of attributes and points:

[9]:
```
nattributes = length(attributes_long)
npoints = size(Xdat, 1)
```

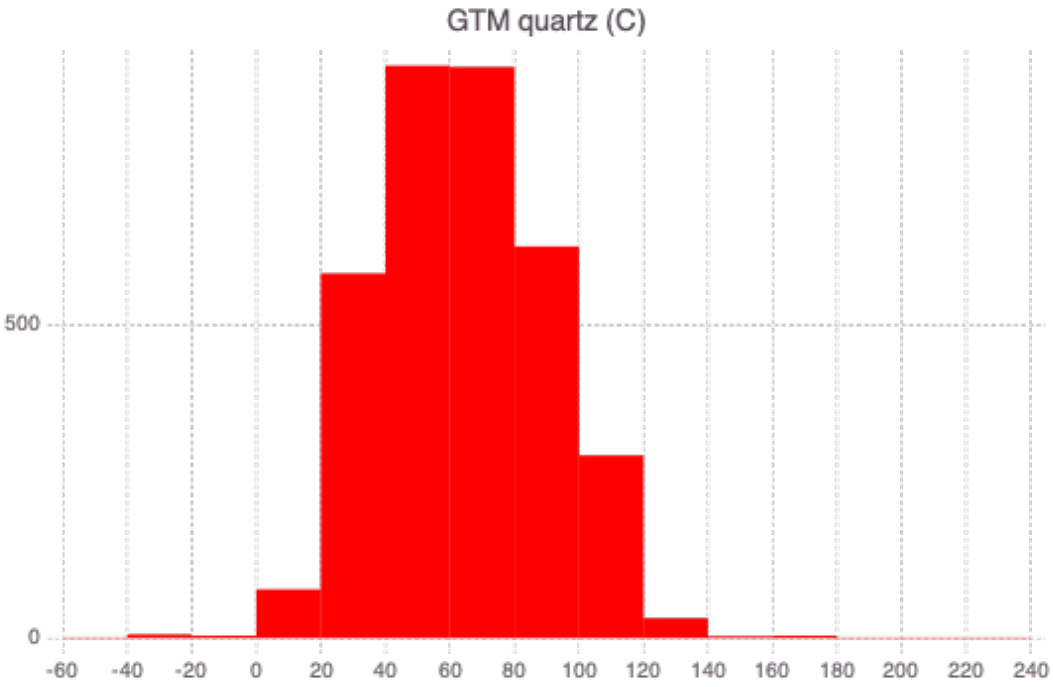
```
5218
```

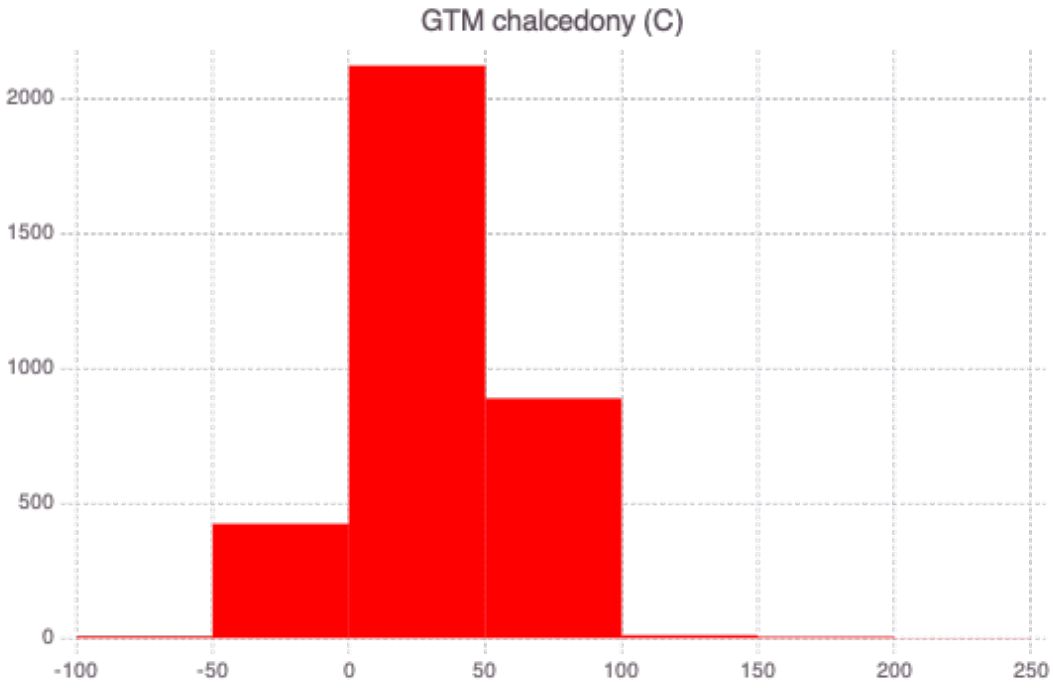
Plot histograms and compute data statistics:

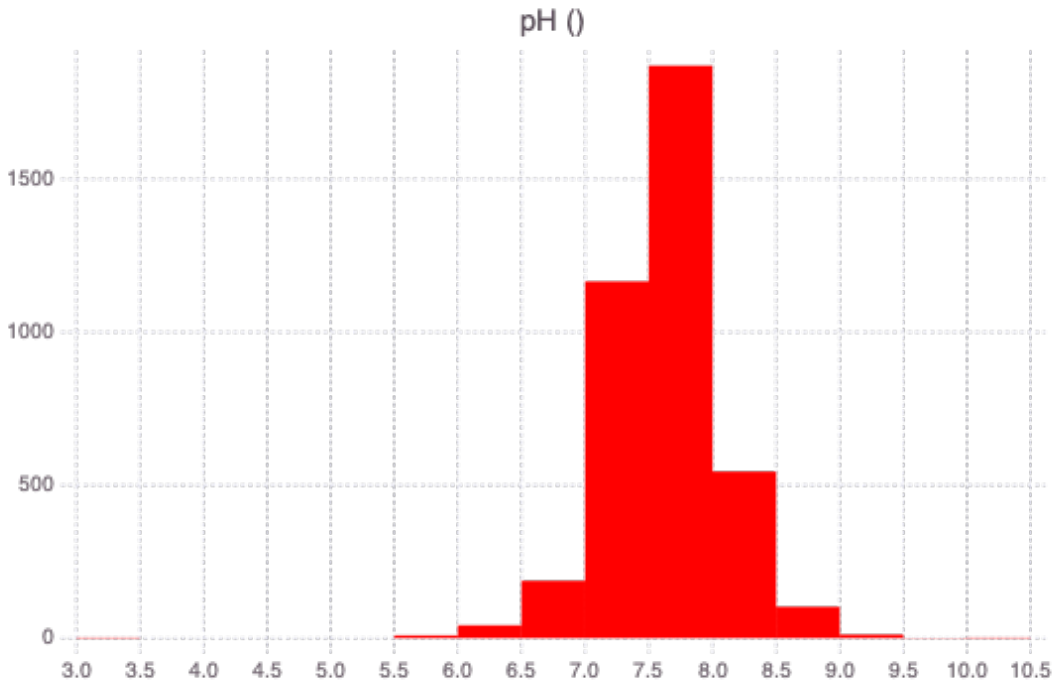
[10]:
```
NMFk.datanalytics(X, attributes_long; dims=2);
```



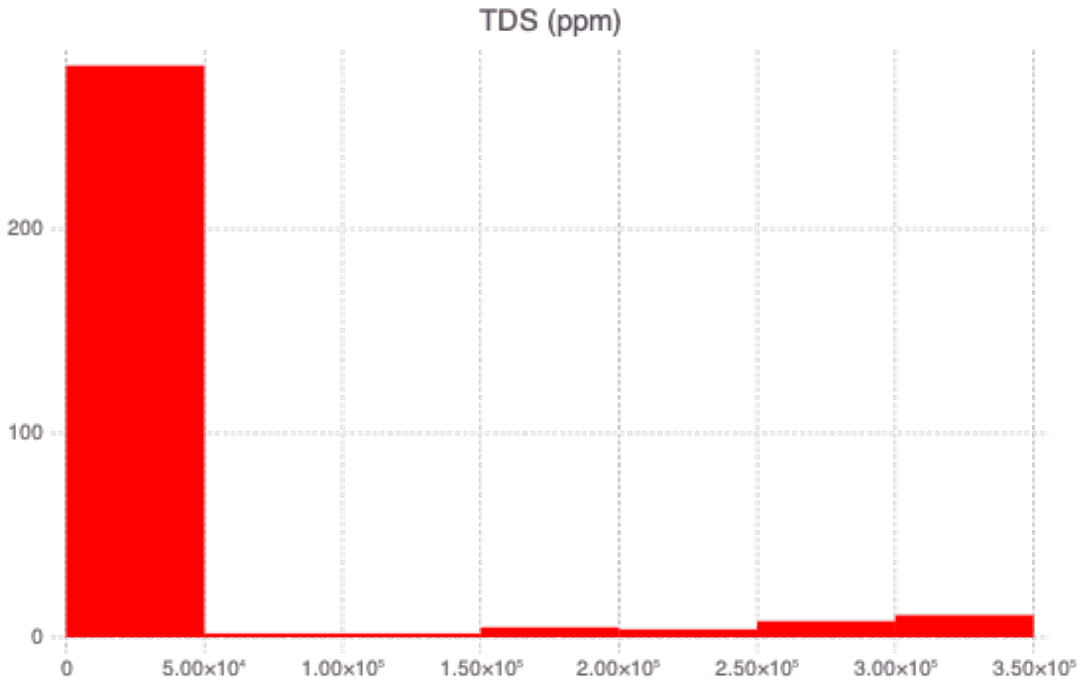

```
Info: Temperature (C)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

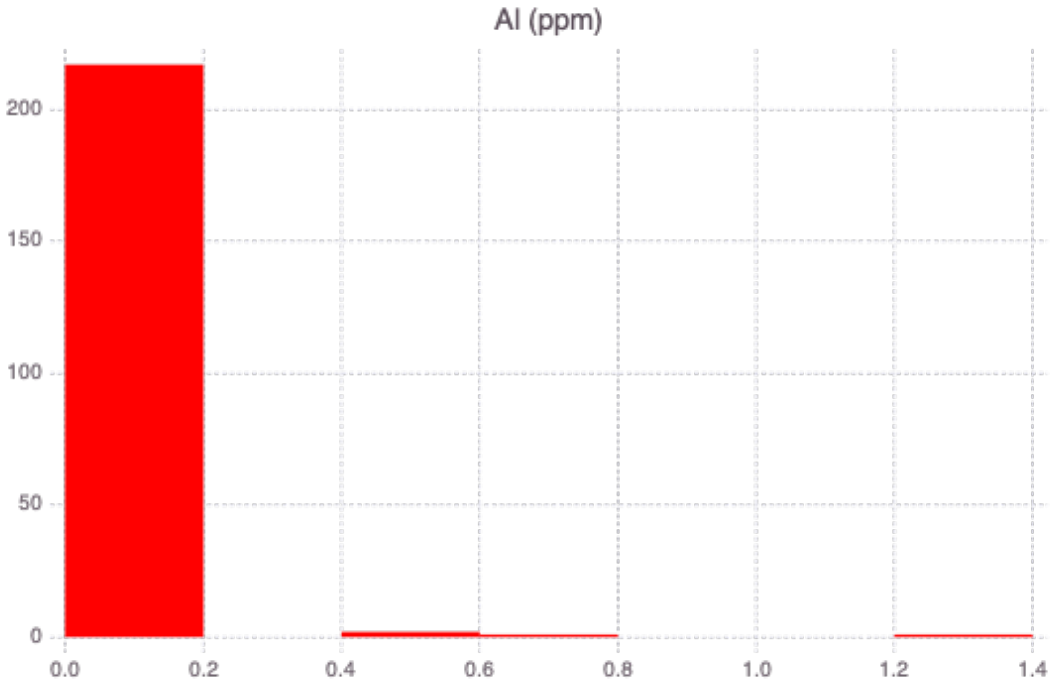


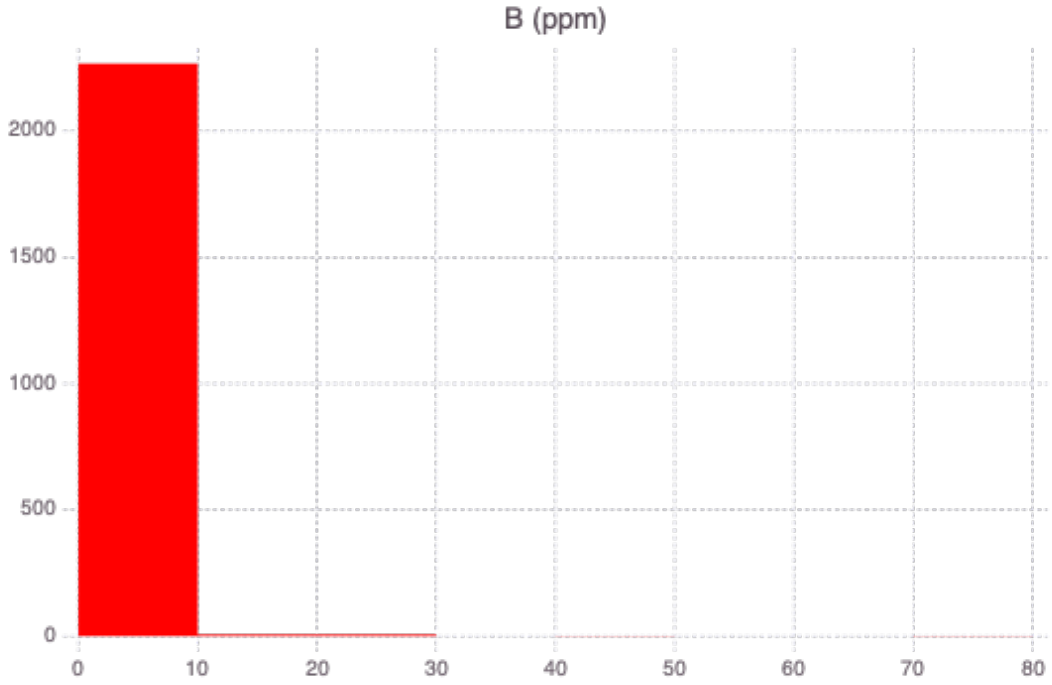

GTM chalcedony (C)
2000
1500
1000
500
0
-100
-50
0
50
100
150
200
250


pH ()
1500
1000
500
0
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5

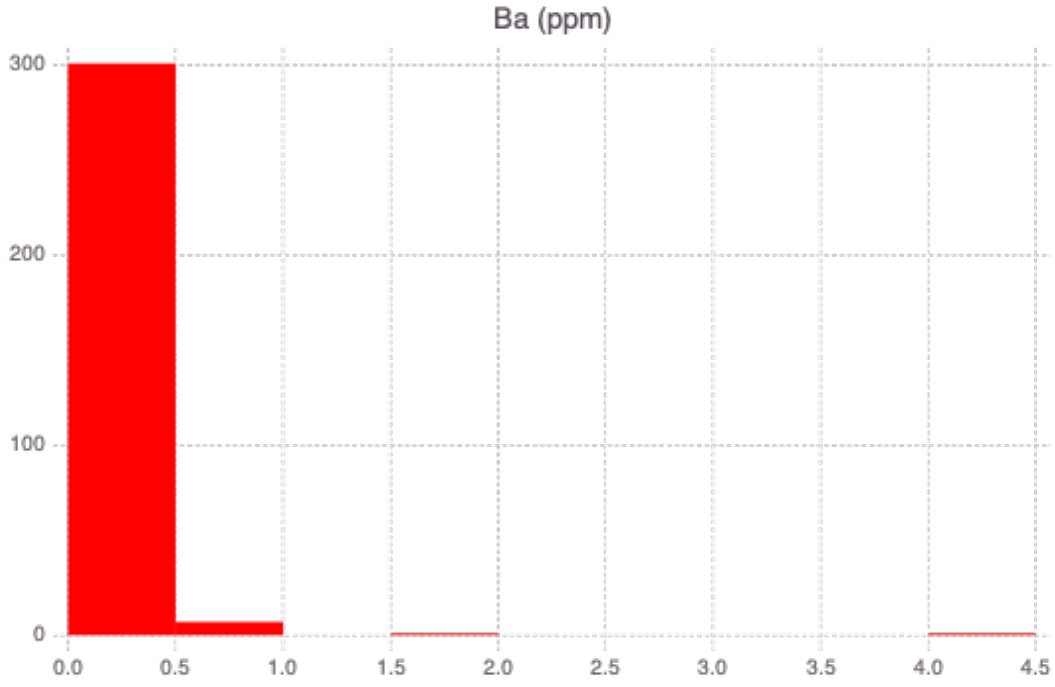
```
Temperature (C): Min 0.1 Max 261.0 StdDev 9.497179 Skewness 10.095466 Count 5214
GTM quartz (C): Min -50.870045 Max 222.28357 StdDev 26.329222 Skewness
0.24256101 Count 3460
GTM chalcedony (C): Min -81.64773 Max 208.67426 StdDev 27.450817 Skewness
0.3369881 Count 3460
  Info: GTM quartz (C)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: GTM chalcedony (C)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: pH ()
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

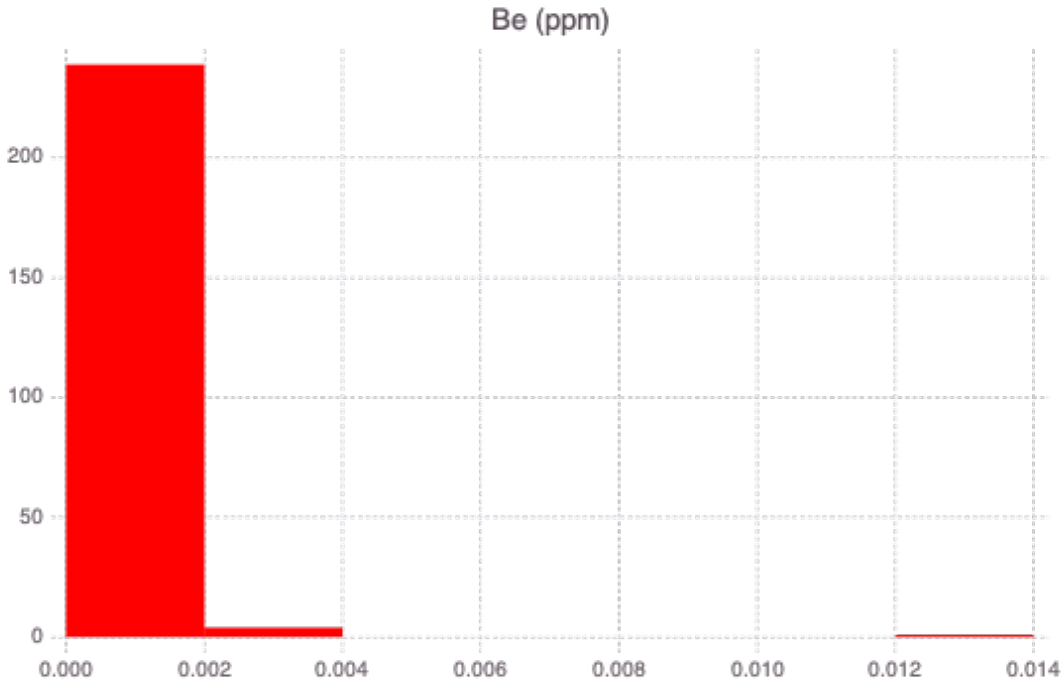


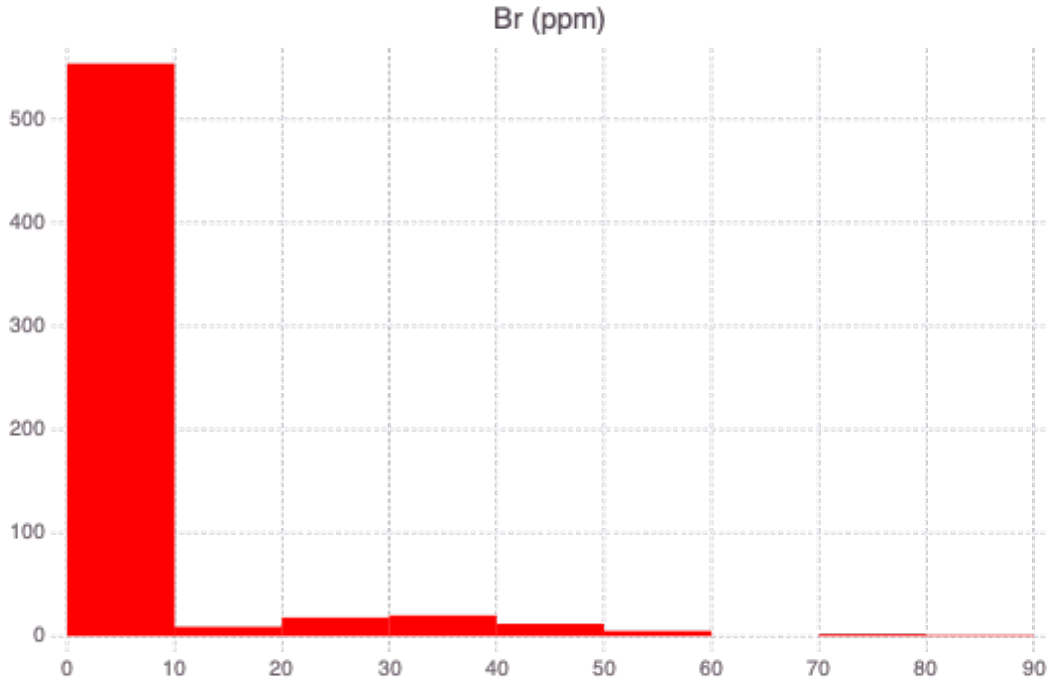

Al (ppm)
200
150
100
50
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4


B (ppm)
2000
1500
1000
500
0
0
10
20
30
40
50
60
70
80

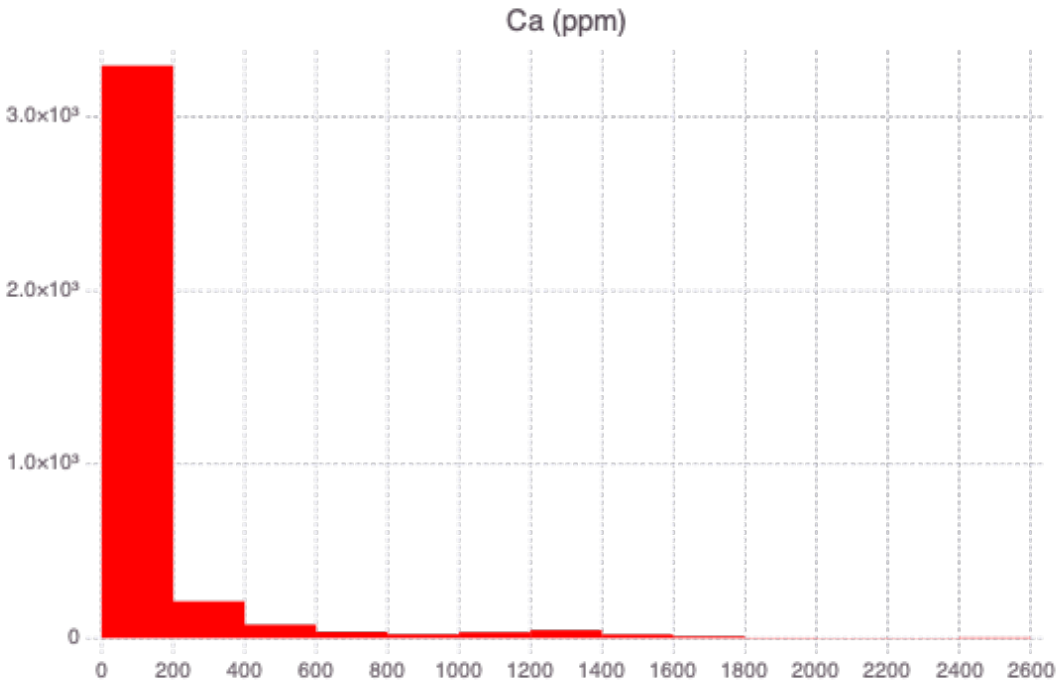
```
pH (): Min 3.4 Max 10.2 StdDev 0.44822767 Skewness -0.45681924 Count 3941
TDS (ppm): Min 122.0 Max 329000.0 StdDev 78777.95 Skewness 2.9479313 Count 312
Al (ppm): Min 0.0 Max 1.251 StdDev 0.10527698 Skewness 9.031239 Count 221
  Info: TDS (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: Al (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: B (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

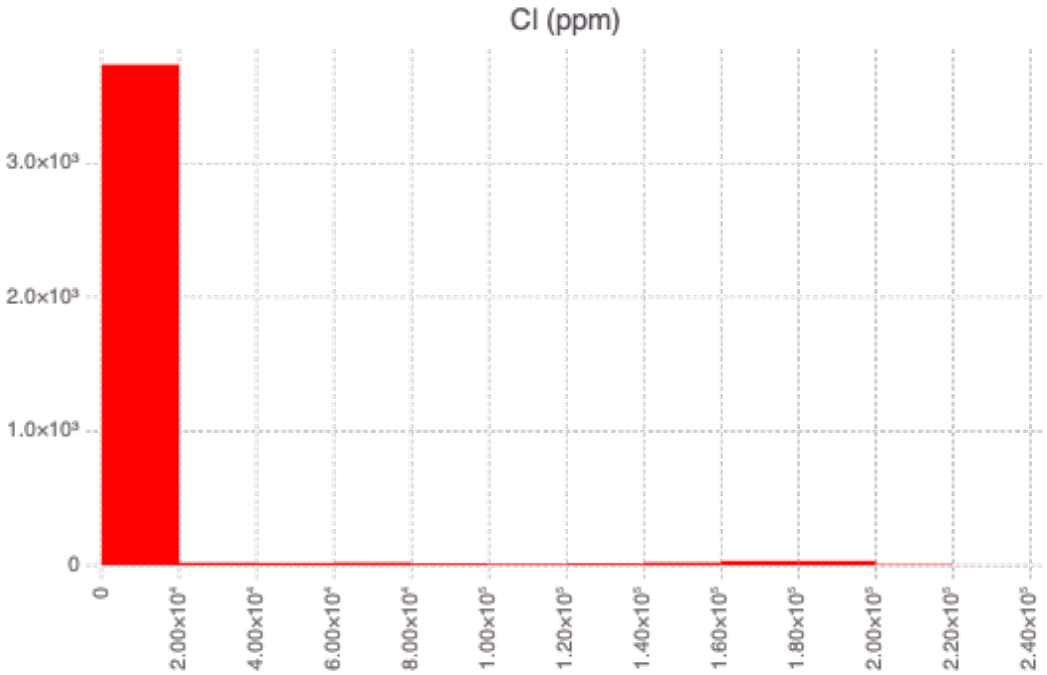


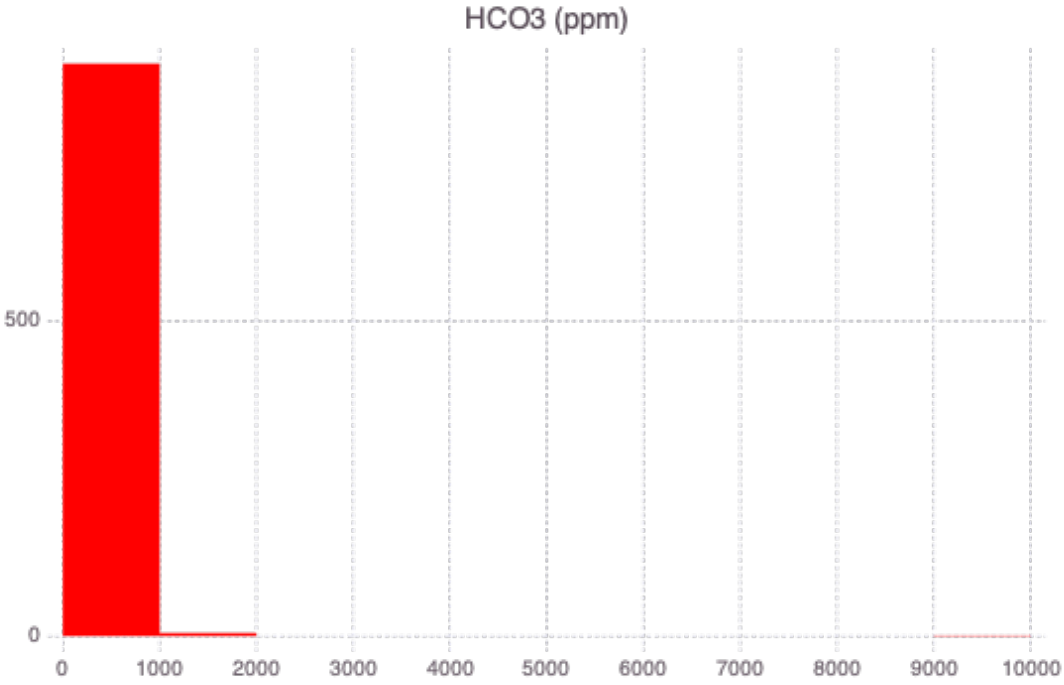

Be (ppm)
200
150
100
50
0
0.000
0.002
0.004
0.006
0.008
0.010
0.012
0.014


Br (ppm)
500
400
300
200
100
0
0
10
20
30
40
50
60
70
80
90

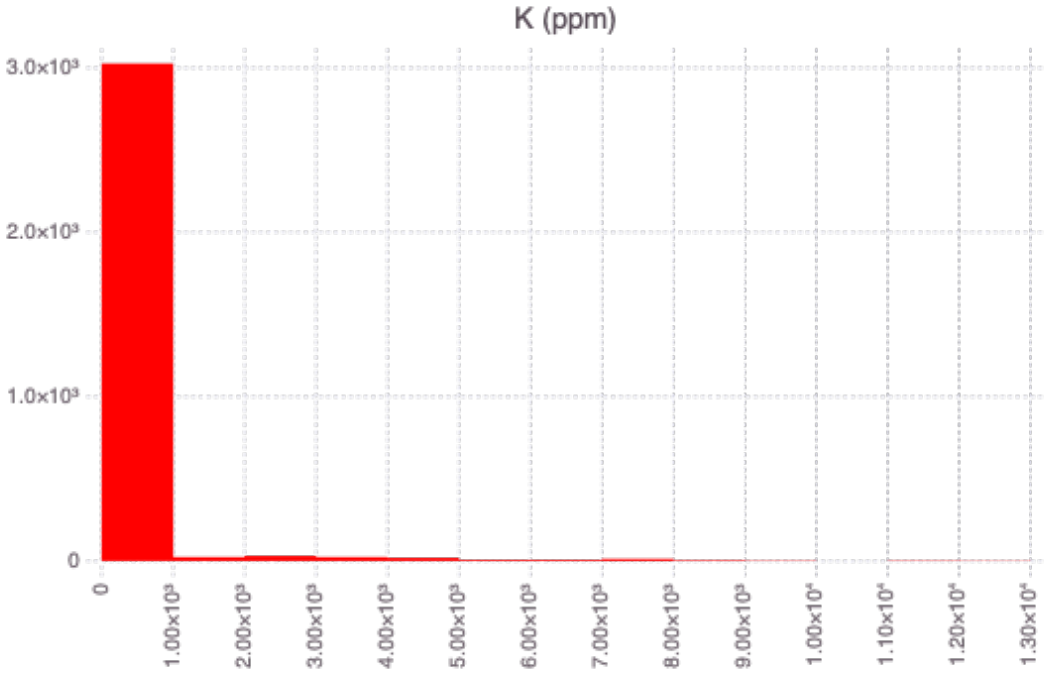
```
B (ppm): Min 0.0 Max 76.5 StdDev 2.6950865 Skewness 15.190172 Count 2284
Ba (ppm): Min 0.002 Max 4.5 StdDev 0.2898333 Skewness 11.825817 Count 310
Be (ppm): Min 5.3333333e-5 Max 0.013 StdDev 0.00089295243 Skewness 10.968073
Count 244
  Info: Ba (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: Be (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: Br (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

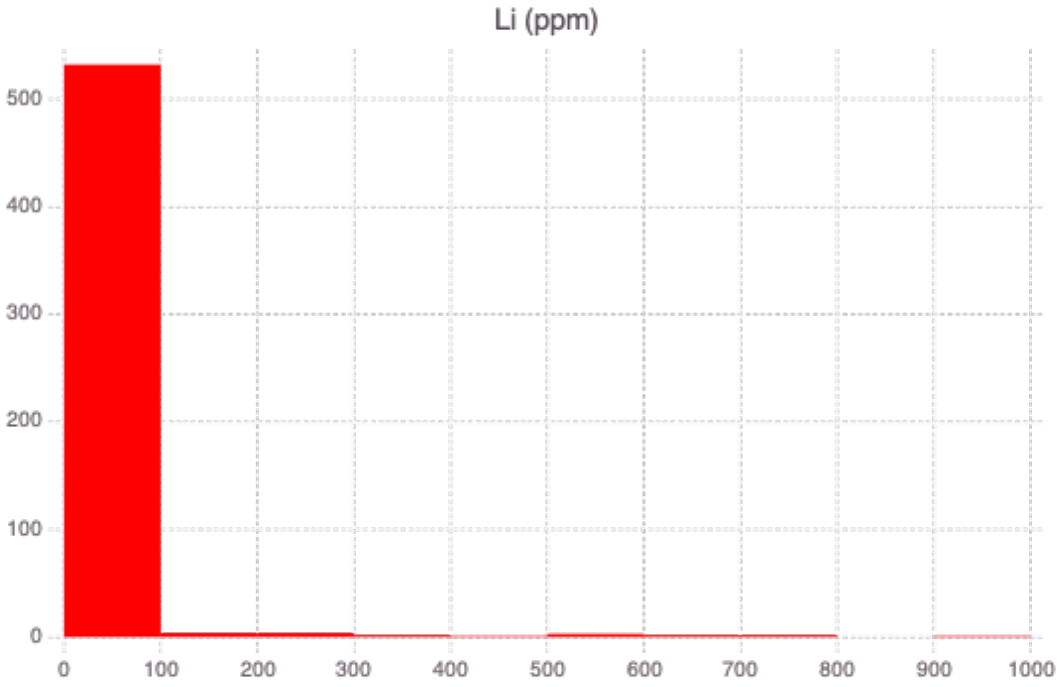


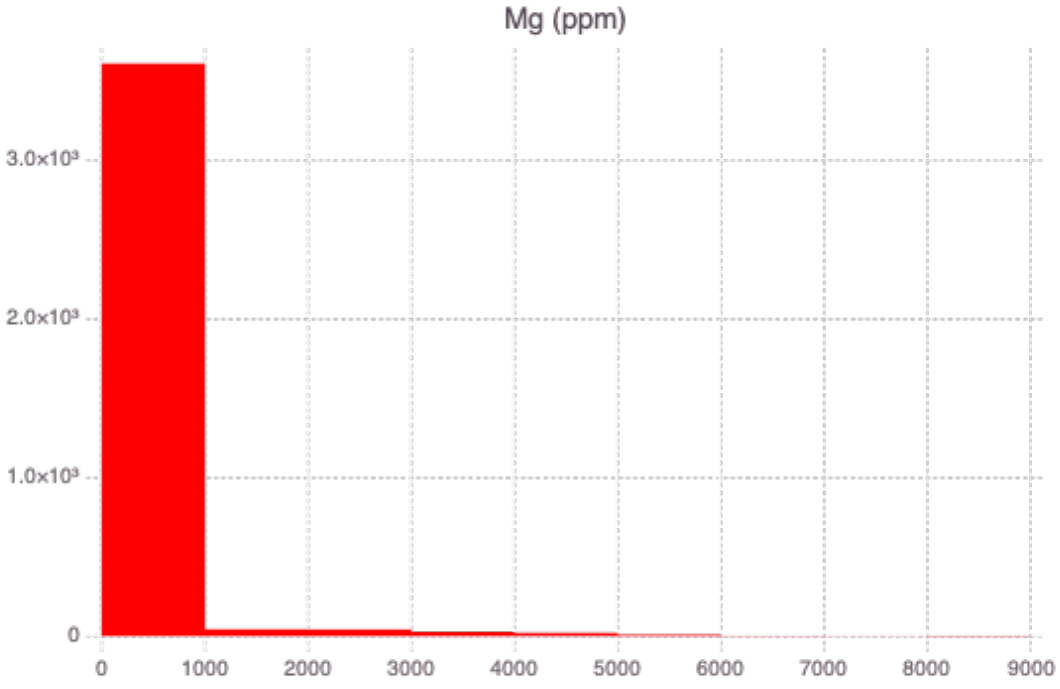

Cl (ppm)
3.0x10³
2.0x10³
1.0x10³
0
0
2.00x10⁴
4.00x10⁴
6.00x10⁴
8.00x10⁴
1.00x10⁵
1.20x10⁵
1.40x10⁵
1.60x10⁵
1.80x10⁵
2.00x10⁵
2.20x10⁵
2.40x10⁵


HCO3 (ppm)
500
0
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000

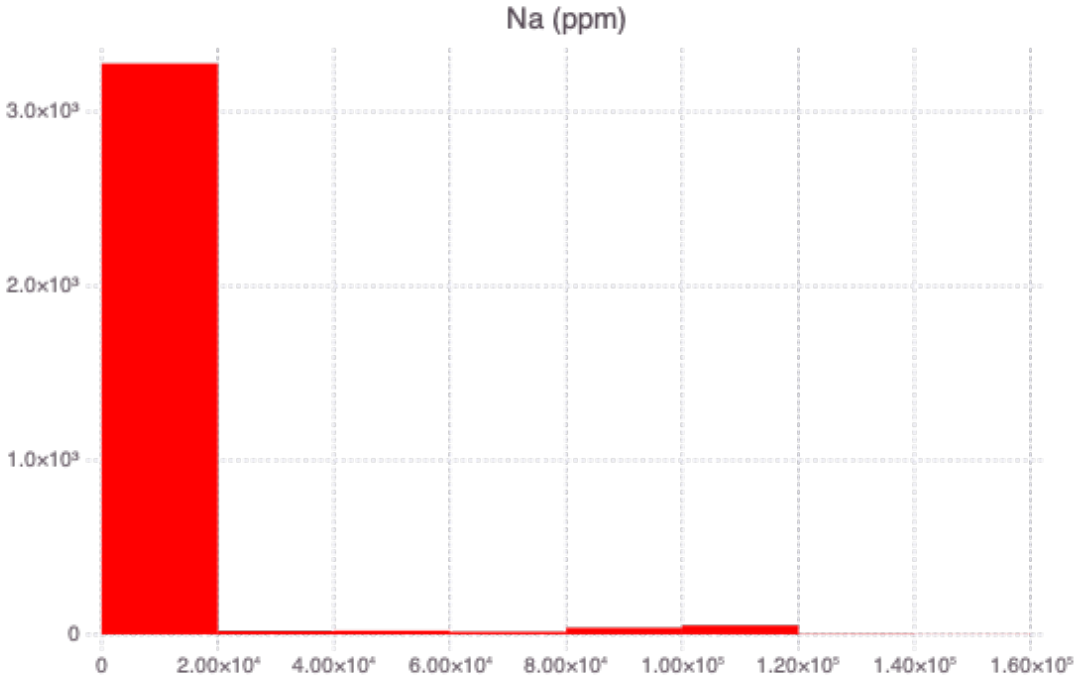
```
Br (ppm): Min 0.0 Max 84.0 StdDev 11.680384 Skewness 3.435088 Count 621
Ca (ppm): Min 0.6 Max 2566.6667 StdDev 262.82578 Skewness 4.424904 Count 3772
Cl (ppm): Min 0.6 Max 240000.0 StdDev 28681.555 Skewness 5.21565 Count 3923
  Info: Ca (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: Cl (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: HCO3 (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

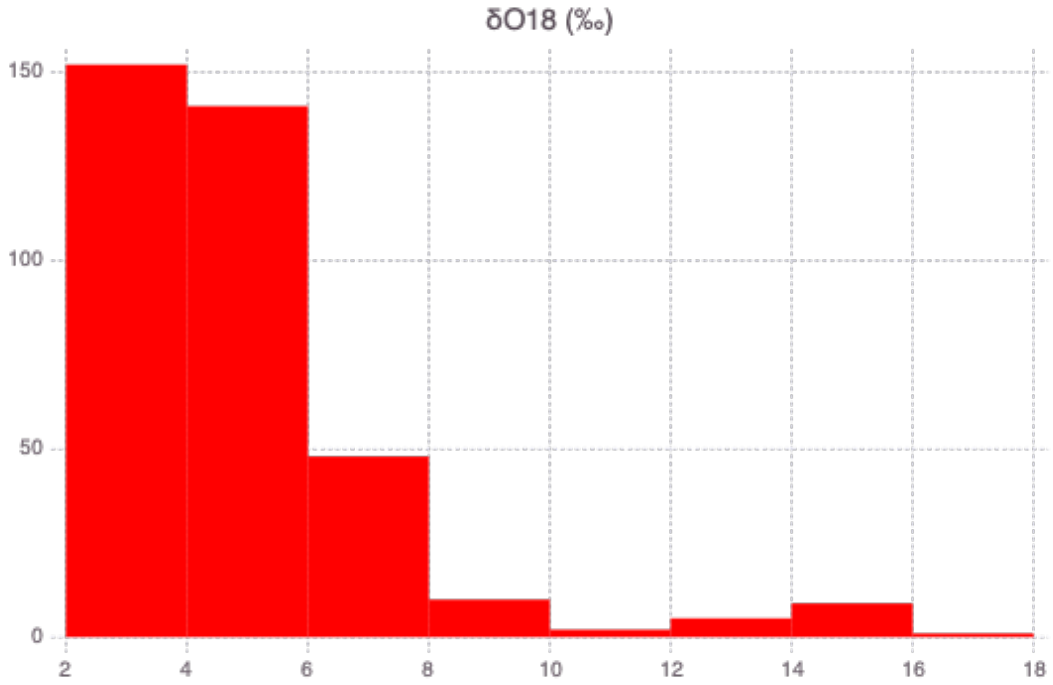



Li (ppm)
500
400
300
200
100
0
0
100
200
300
400
500
600
700
800
900
1000


Mg (ppm)
3.0×10³
2.0×10³
1.0×10³
0
0
1000
2000
3000
4000
5000
6000
7000
8000
9000

```
HCO3 (ppm): Min 37.0 Max 9217.0 StdDev 329.8163 Skewness 22.165213 Count 915
K (ppm): Min 0.0 Max 13000.0 StdDev 1063.7937 Skewness 6.380783 Count 3177
Li (ppm): Min 0.0 Max 970.0 StdDev 90.79041 Skewness 6.6990304 Count 551
  Info: K (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: Li (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: Mg (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```






```
Mg (ppm): Min 0.0 Max 8500.0 StdDev 663.7361 Skewness 6.581147 Count 3760
Na (ppm): Min 0.5 Max 160000.0 StdDev 17983.25 Skewness 4.946034 Count 3437
  Info: Na (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info:  O18 (‰)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 O18 (‰): Min 2.1499996 Max 16.36 StdDev 2.4535506 Skewness 2.5710073 Count 368
Name Min Max StdDev Count (non-NaN's)
Temperature (C) 0.1 261.0 9.497179 10.095466 5214
GTM quartz (C) -50.870045 222.28357 26.329222 0.24256101 3460
GTM chalcedony (C) -81.64773 208.67426 27.450817 0.3369881 3460
pH () 3.4 10.2 0.44822767 -0.45681924 3941
TDS (ppm) 122.0 329000.0 78777.95 2.9479313 312
Al (ppm) 0.0 1.251 0.10527698 9.031239 221
B (ppm) 0.0 76.5 2.6950865 15.190172 2284
Ba (ppm) 0.002 4.5 0.2898333 11.825817 310
Be (ppm) 5.3333333e-5 0.013 0.00089295243 10.968073 244
Br (ppm) 0.0 84.0 11.680384 3.435088 621
Ca (ppm) 0.6 2566.6667 262.82578 4.424904 3772
Cl (ppm) 0.6 240000.0 28681.555 5.21565 3923
HCO3 (ppm) 37.0 9217.0 329.8163 22.165213 915
K (ppm) 0.0 13000.0 1063.7937 6.380783 3177
Li (ppm) 0.0 970.0 90.79041 6.6990304 551
Mg (ppm) 0.0 8500.0 663.7361 6.581147 3760
```

```
Na (ppm) 0.5 160000.0 17983.25 4.946034 3437
 O18 (‰) 2.1499996 16.36 2.4535506 2.5710073 368
  Info: Attributes
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:70
```

Note that the data entries for `TDS`, `Al`, and `O18` are heavily missing.

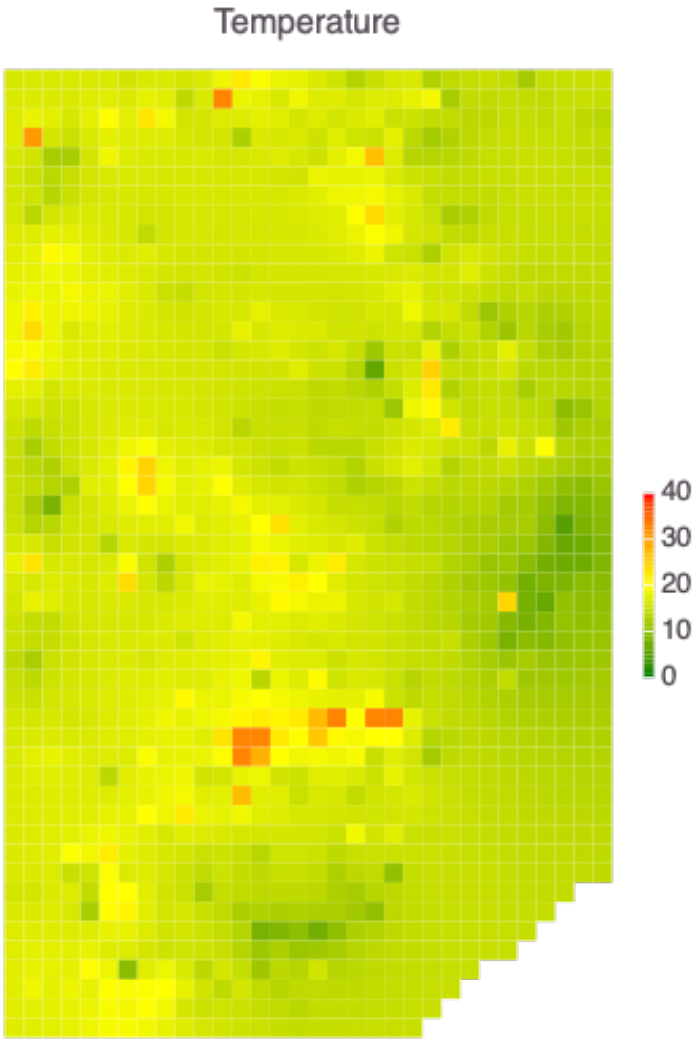
Even though the dataset is very sparse, our ML methods can analyze the inputs.

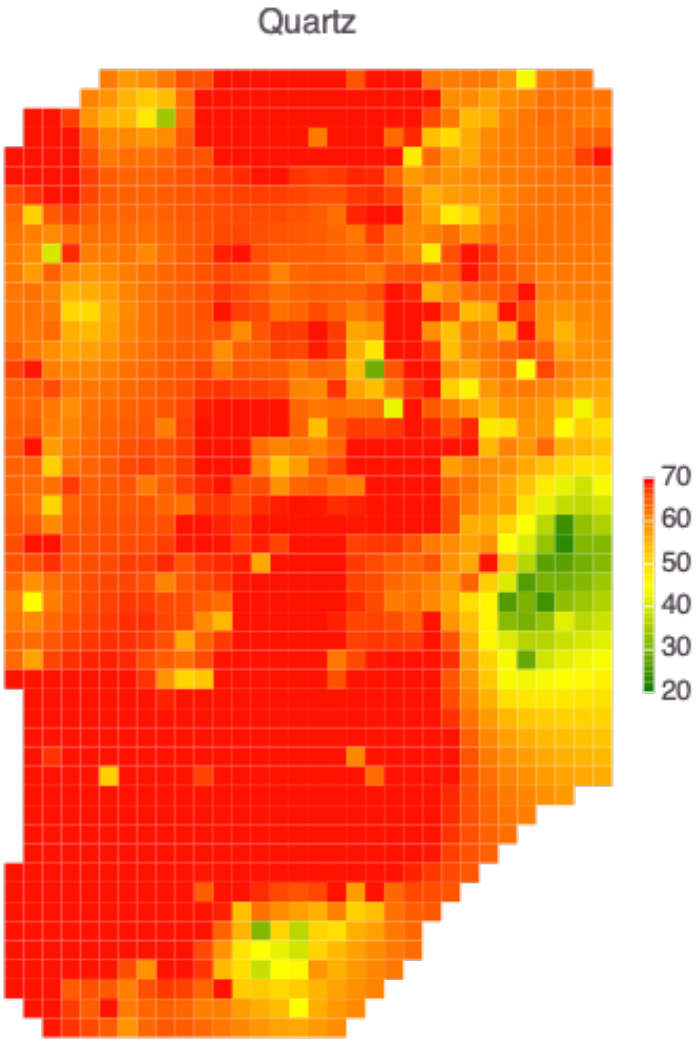
Most of the commonly used ML methods cannot process datasets that are sparse.

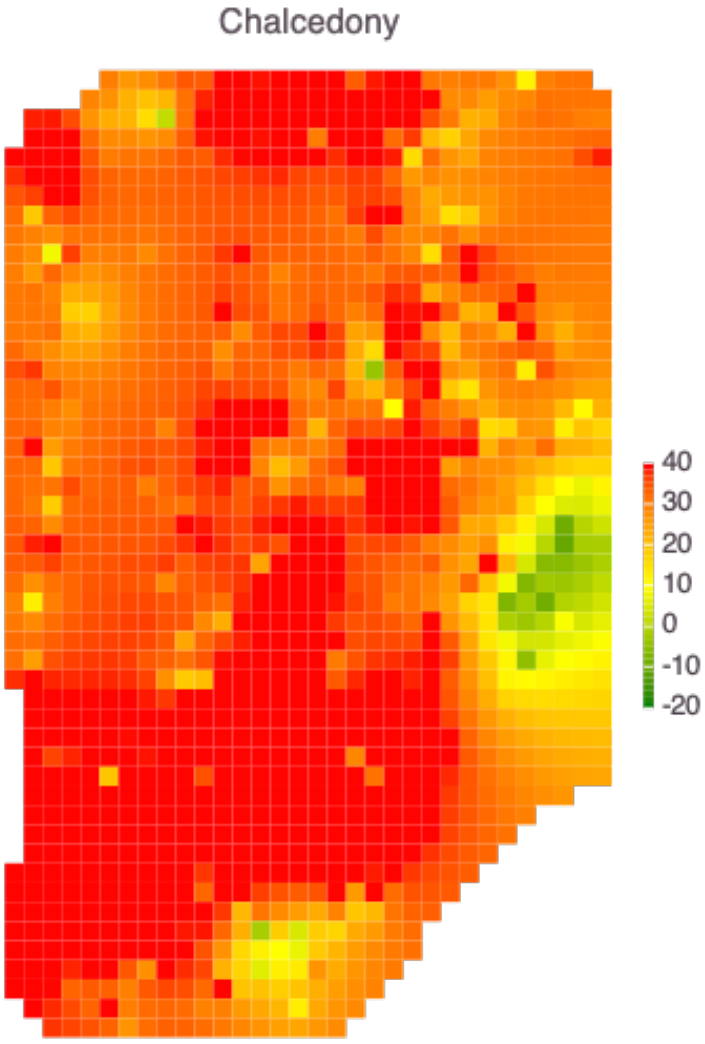
Furthermore, different attributes in the Great Basin dataset cover different areas.

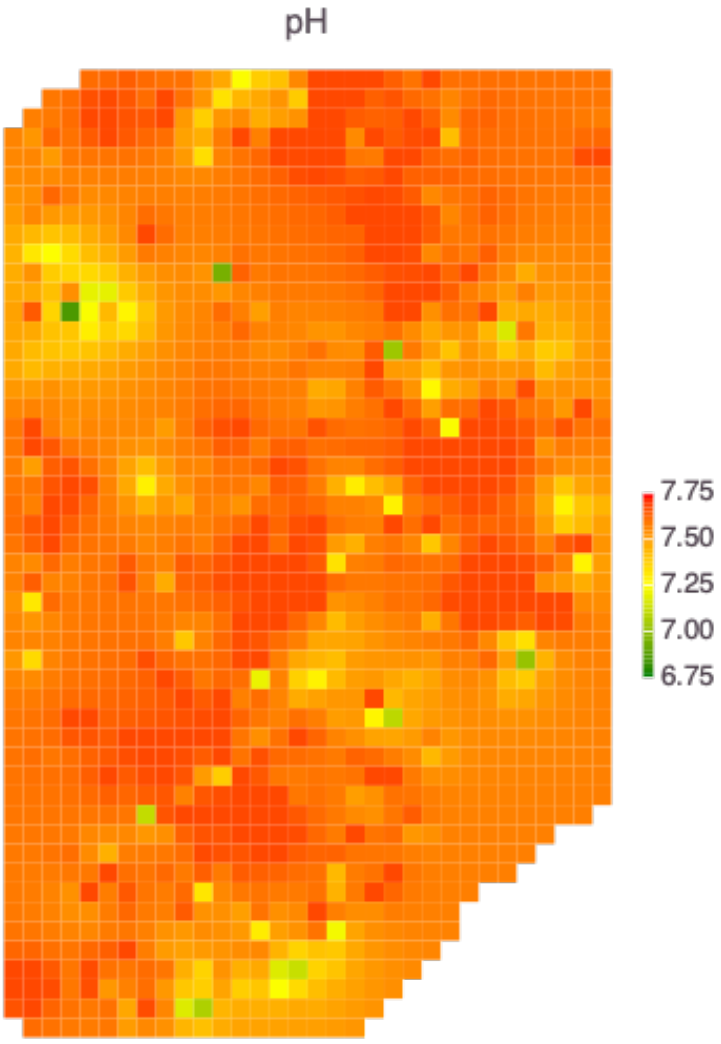
This is demonstrated in the maps generated below.

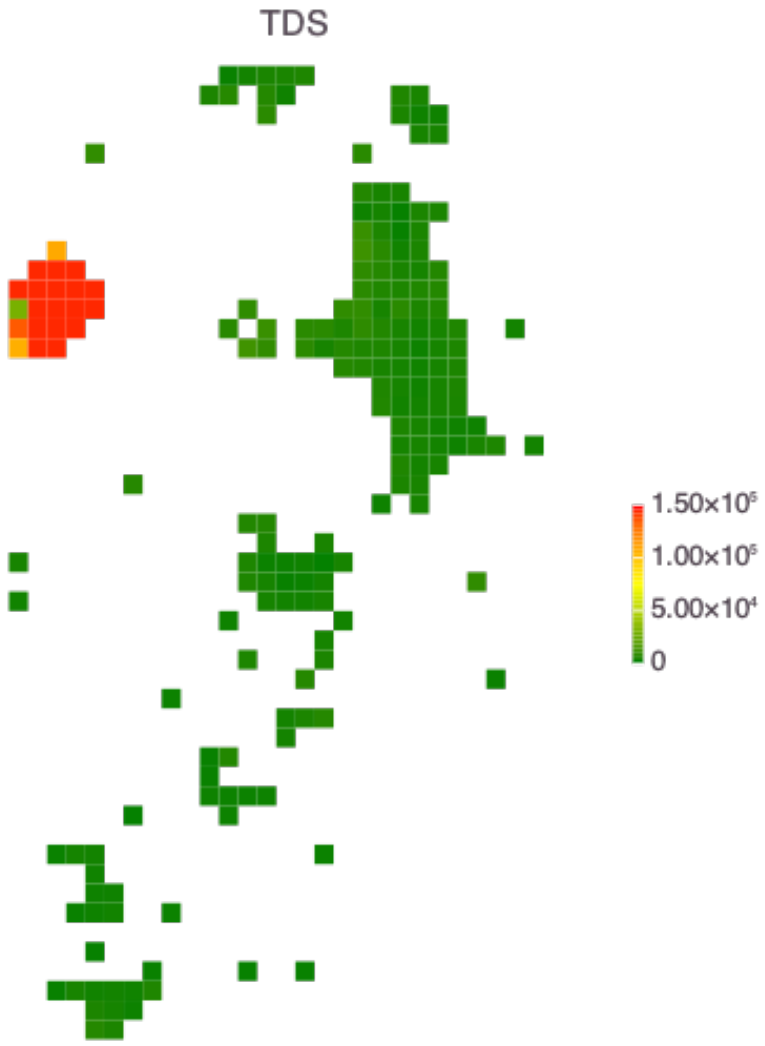
[11]:
```
coord = permutedims([xcoord ycoord])

xgrid, ygrid = NMFk.griddata(xcoord, ycoord; stepvalue=0.1)

for i = 1:nattributes
        inversedistancefield = Array{Float64}(undef, length(xgrid),␣
 ↪length(ygrid))
        v = X[:,i]
        iz = .!isnan.(v)
        icoord = coord[:,iz]
        v = v[iz]
        for (i, x) in enumerate(xgrid), (j, y) in enumerate(ygrid)
                inversedistancefield[i, j] = Kriging.
 ↪inversedistance(permutedims([x y]), icoord, v, 2; cutoff=1000)[1]
        end
        imax = NMFk.maximumnan(inversedistancefield)
        imin = NMFk.minimumnan(inversedistancefield)
        NMFk.plotmatrix(rotl90(inversedistancefield); quiet=false,␣
 ↪filename="utah/maps/Attribute_$(attributes[i])_map_inversedistance.png",␣
 ↪title="$(attributes[i])", maxvalue=imin + (imax - imin)/ 2)
end
```

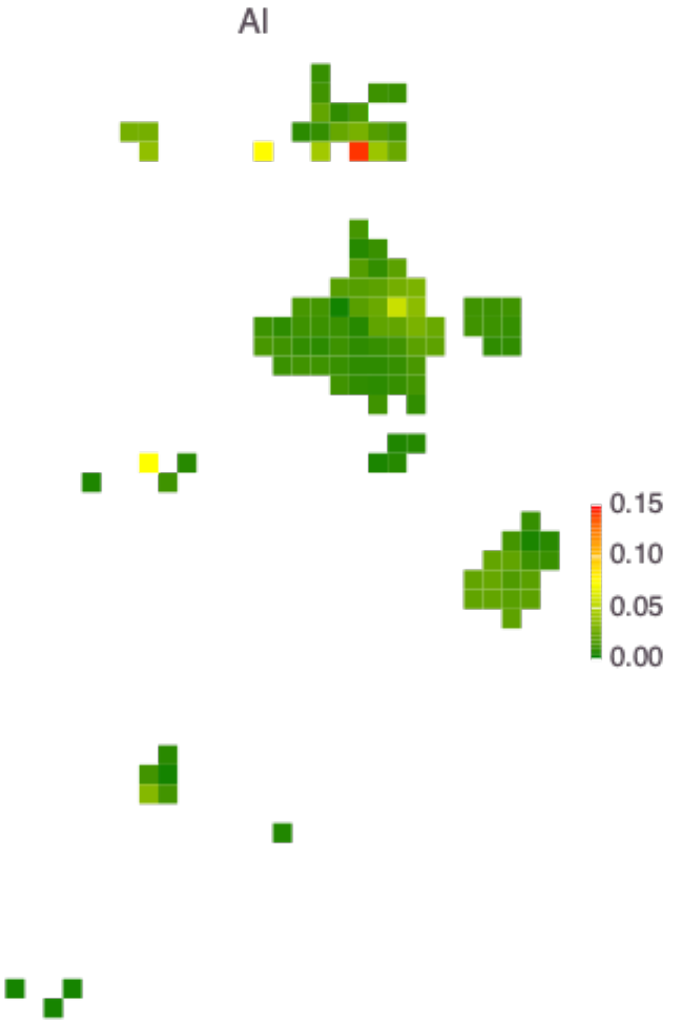

Temperature
40
30
20
10
0

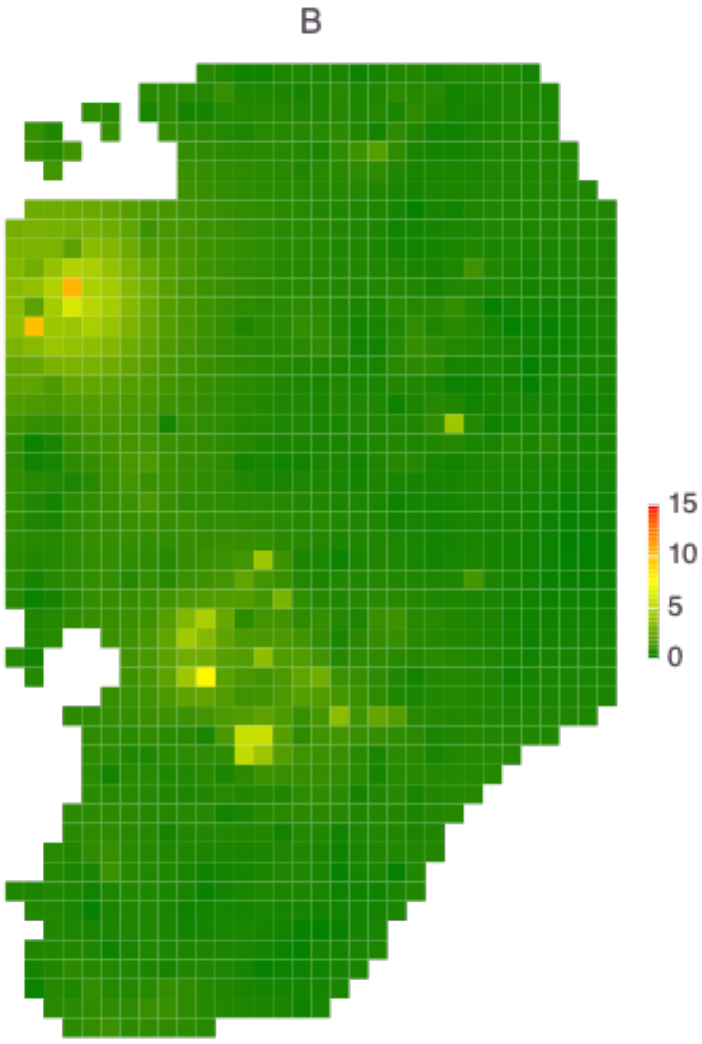

Quartz
70
60
50
40
30
20

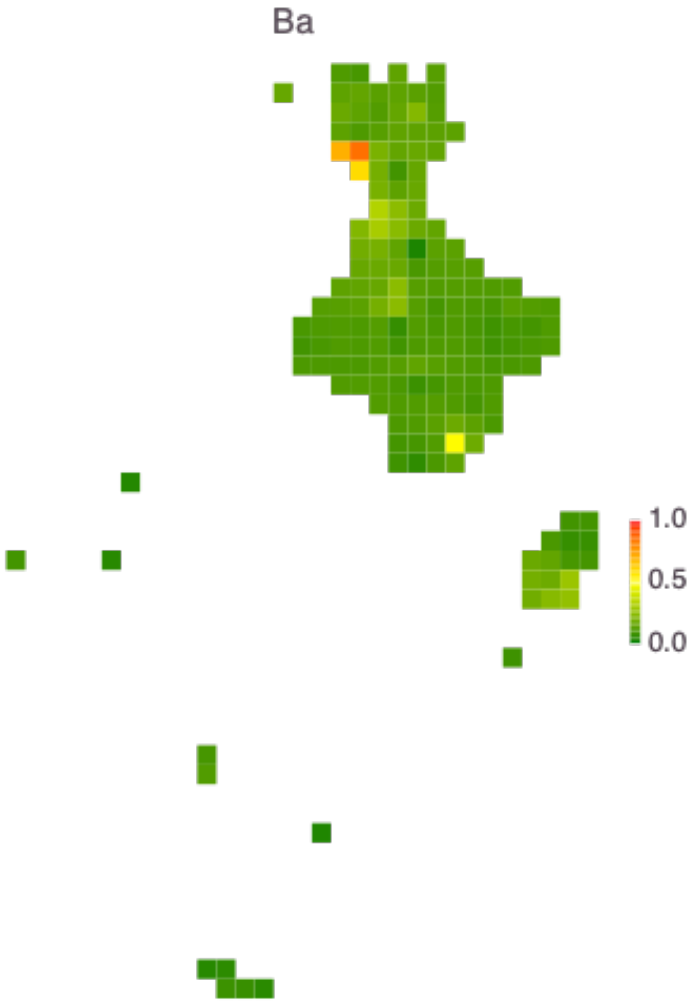

Chalcedony
40
30
20
10
0
-10
-20

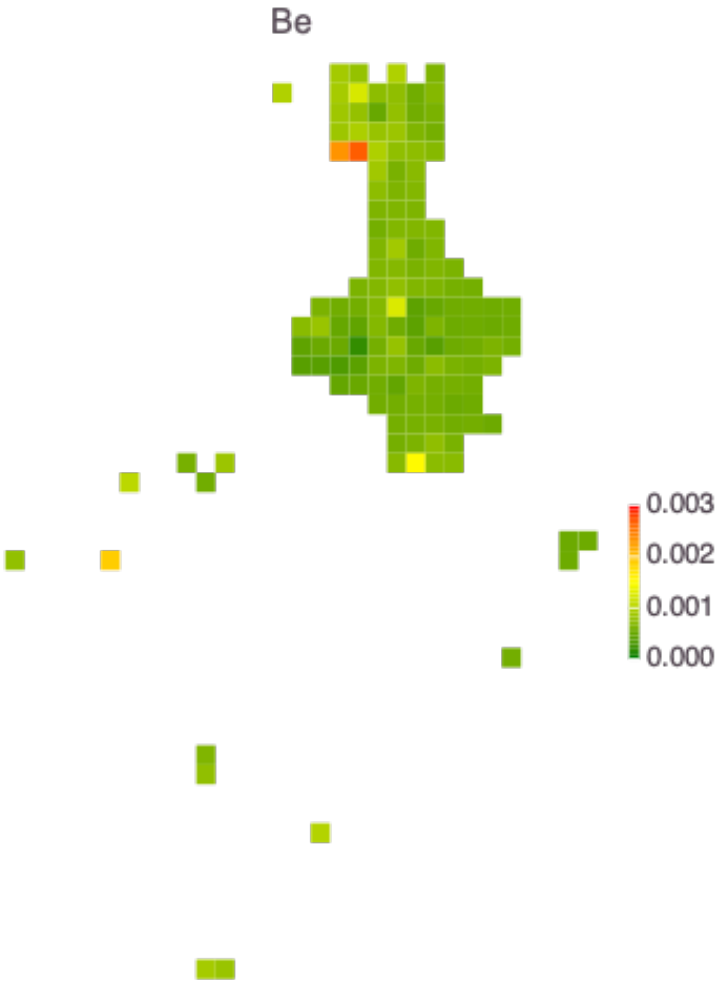

pH
7.75
7.50
7.25
7.00
6.75

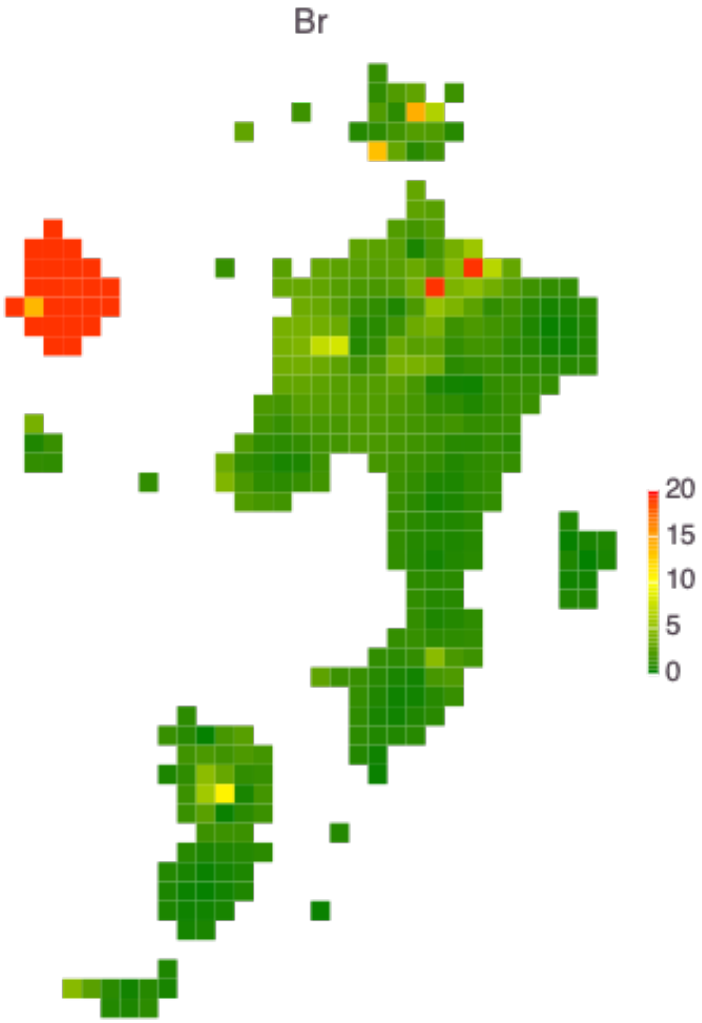

TDS
1.50×10⁵
1.00×10⁵
5.00×10⁴
0

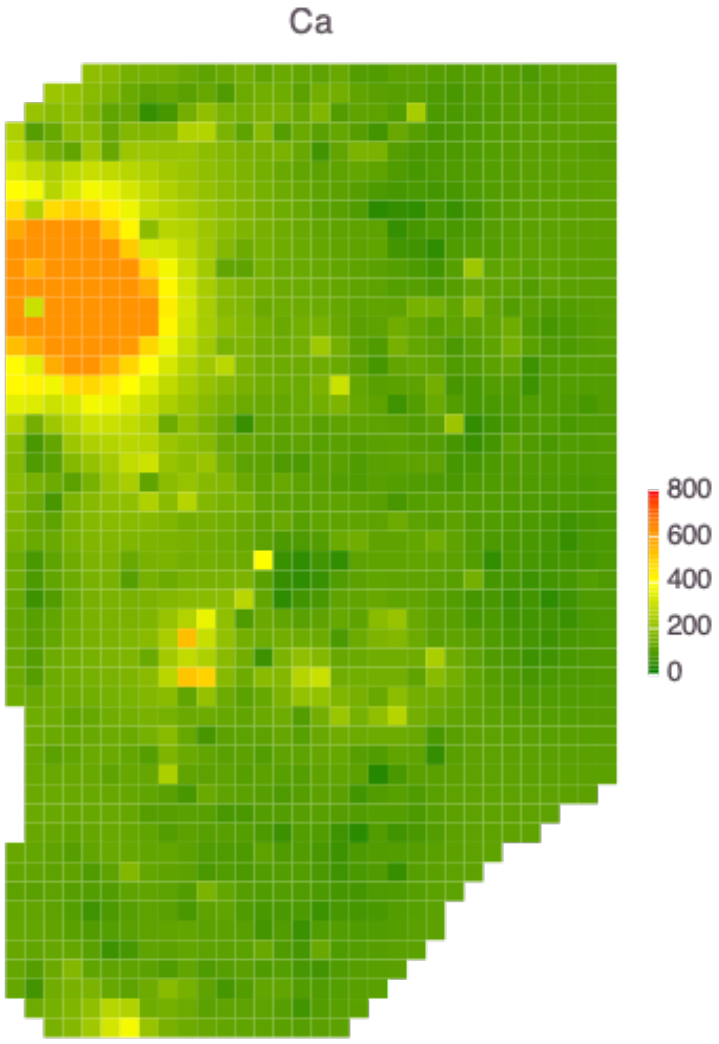

Al
0.15
0.10
0.05
0.00

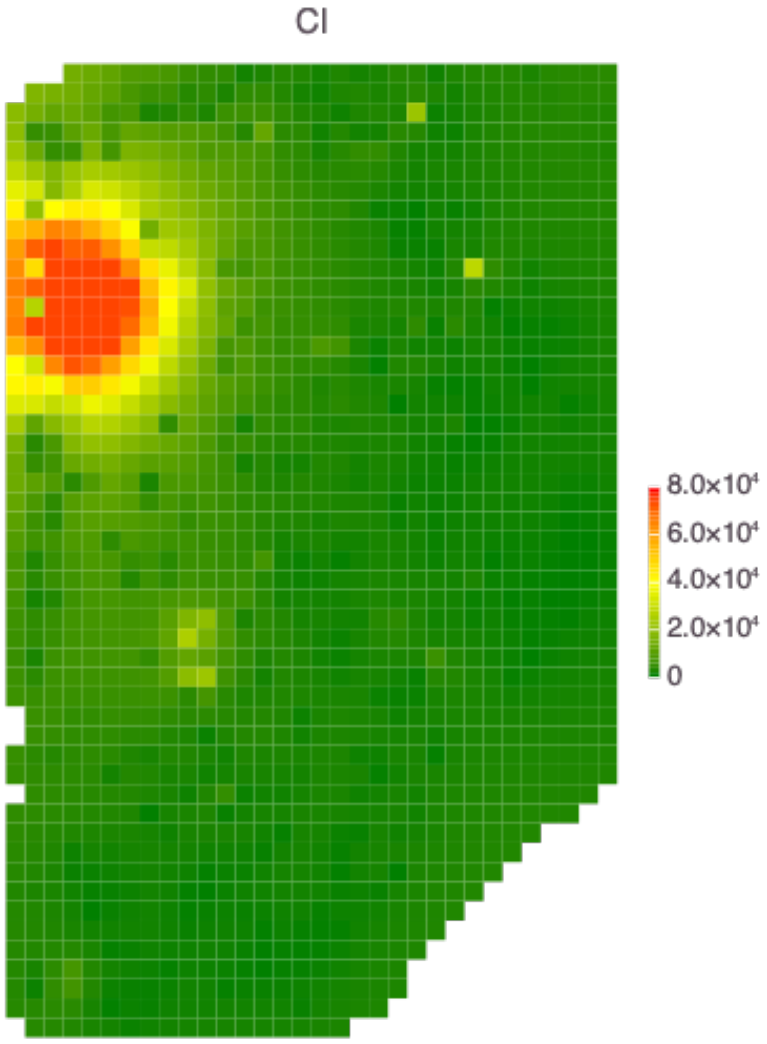

B
15
10
5
0

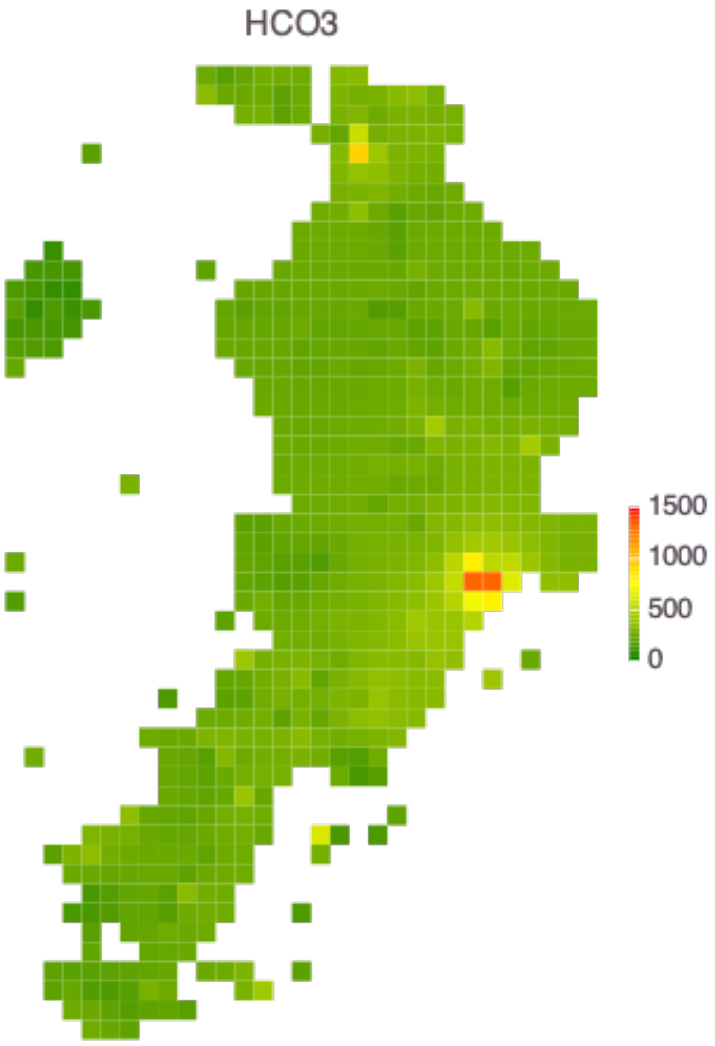

Ba
1.0
0.5
0.0

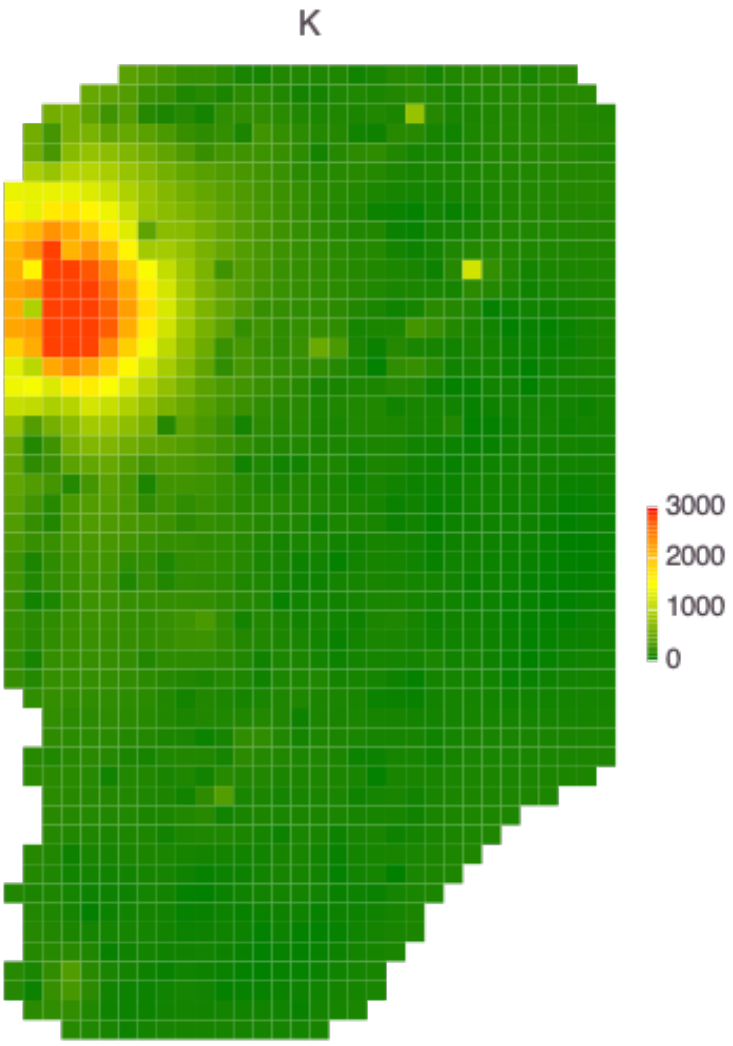

Be
0.003
0.002
0.001
0.000

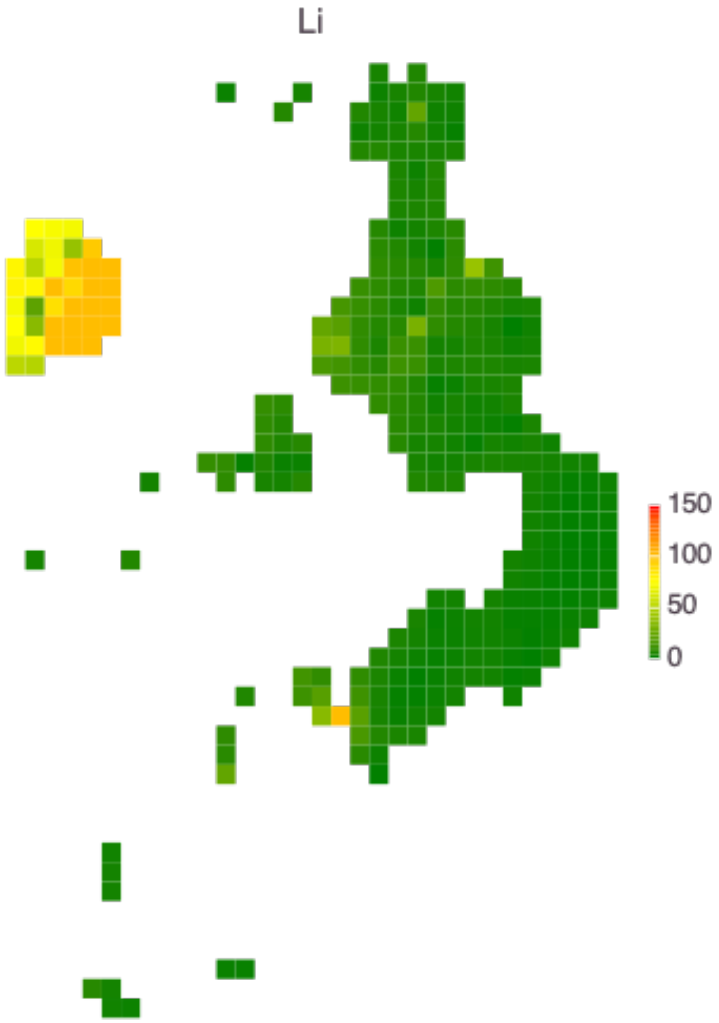

Br
20
15
10
5
0

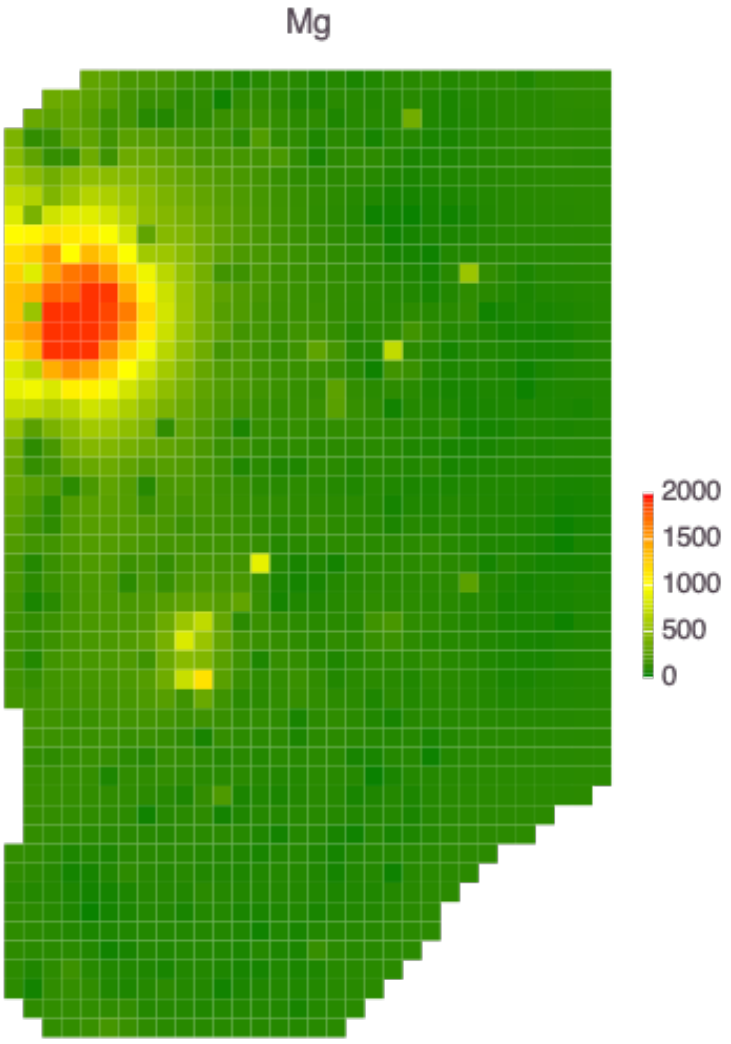

Ca
800
600
400
200
0

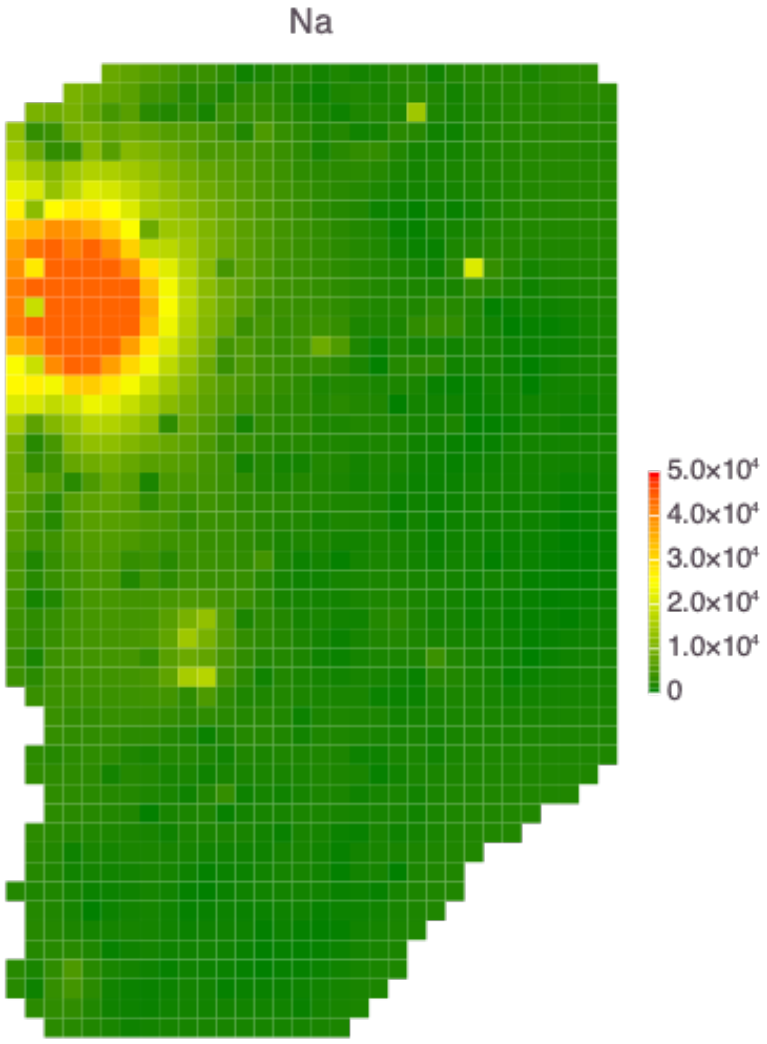

Cl
8.0×10⁴
6.0×10⁴
4.0×10⁴
2.0×10⁴
0

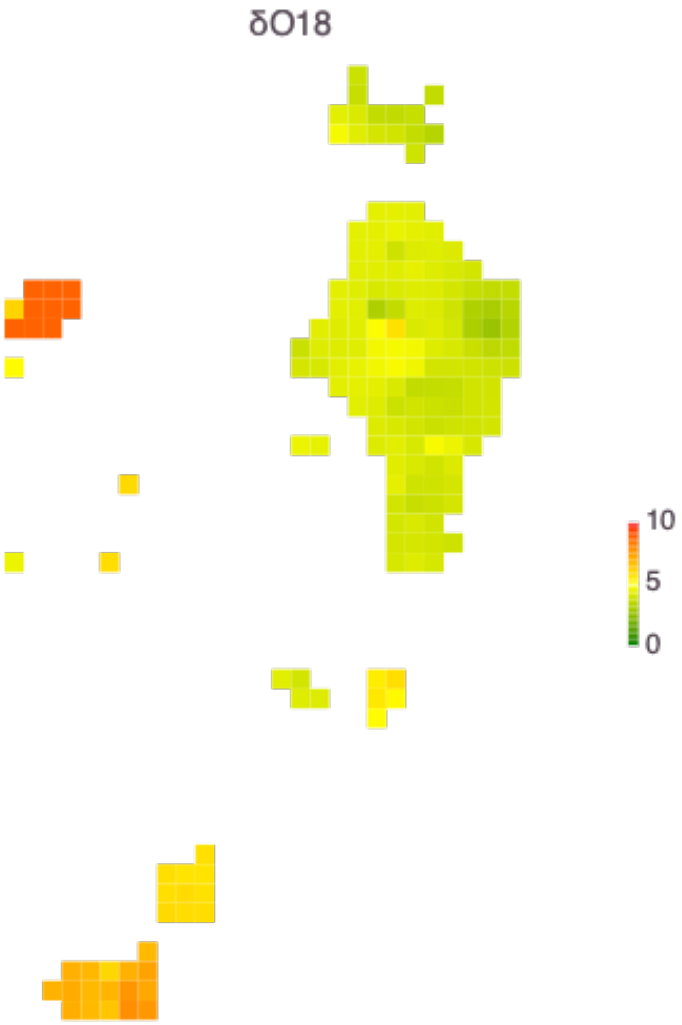

HCO3
1500
1000
500
0


K
3000
2000
1000
0


Li
150
100
50
0


Mg
2000
1500
1000
500
0


Na
5.0×10⁴
4.0×10⁴
3.0×10⁴
2.0×10⁴
1.0×10⁴
0



1.6 Log-transformation

Attribute values are log-transformed to better capture the order of magnitude variability.

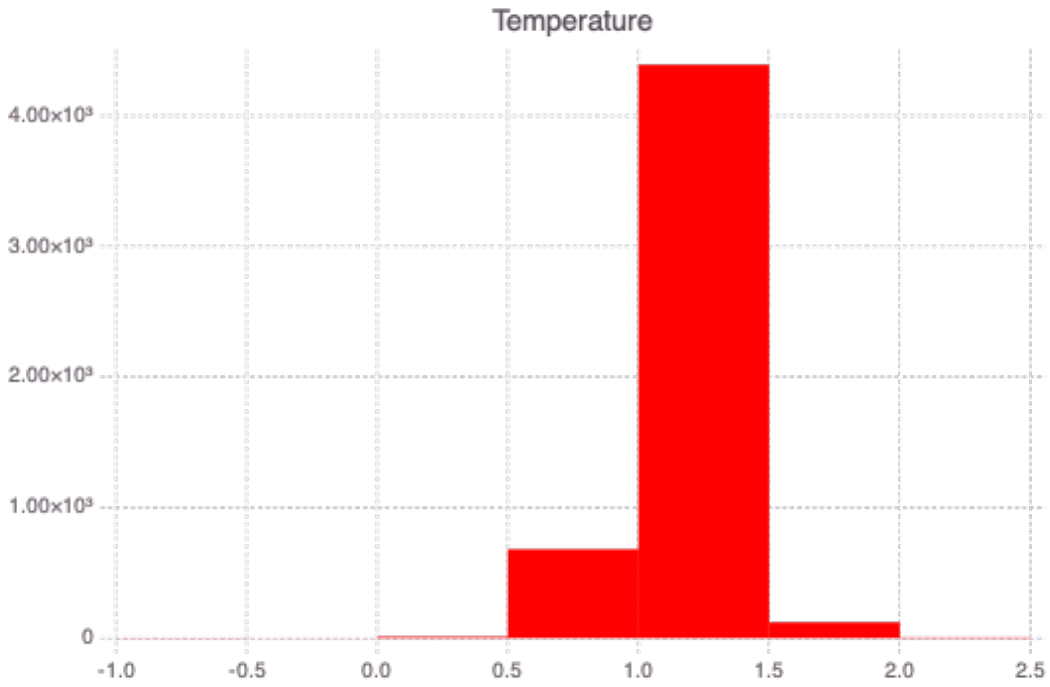
All attributes except for `Quartz`, `Chalcedony` and `pH` are log-transformed (`Quartz` and `Chalcedony` have negative values).

[12]:
```
logv = [true, false, false, false,  true, true, true, true, true, true, true,␣
 ↪true, true, true, true, true, true, true]
[attributes logv]
```

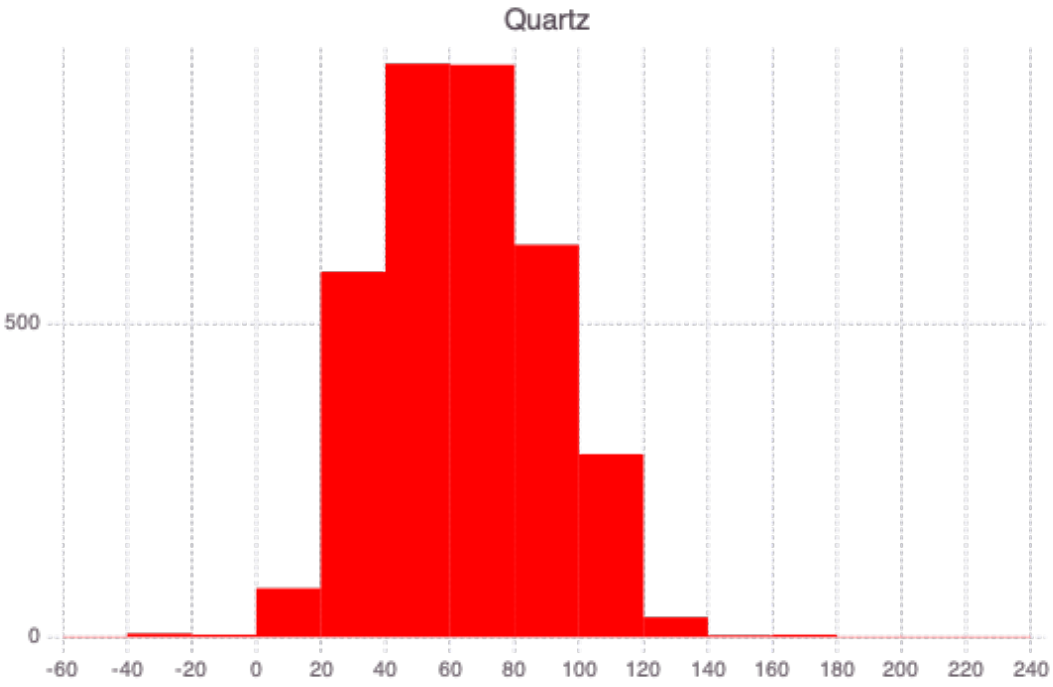
```
18×2 Matrix{Any}:
 "Temperature"   true
```

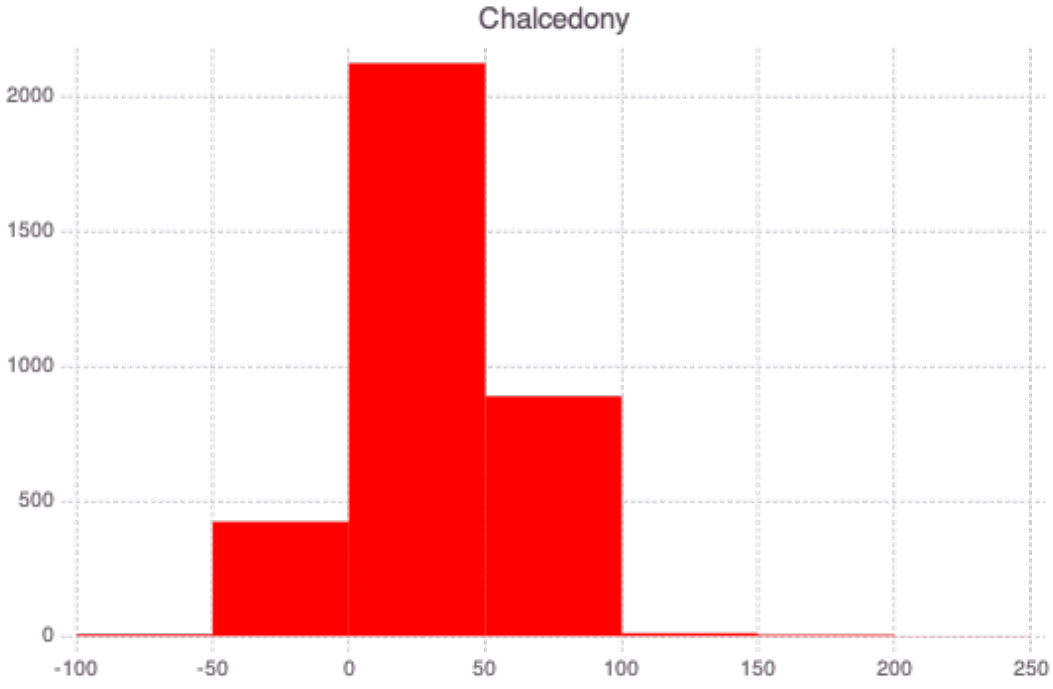
```
"Quartz"       false
"Chalcedony"   false
"pH"           false
"TDS"           true
"Al"            true
"B"             true
"Ba"            true
"Be"            true
"Br"            true
"Ca"            true
"Cl"            true
"HCO3"          true
"K"             true
"Li"            true
"Mg"            true
"Na"            true
" O18"         true
```

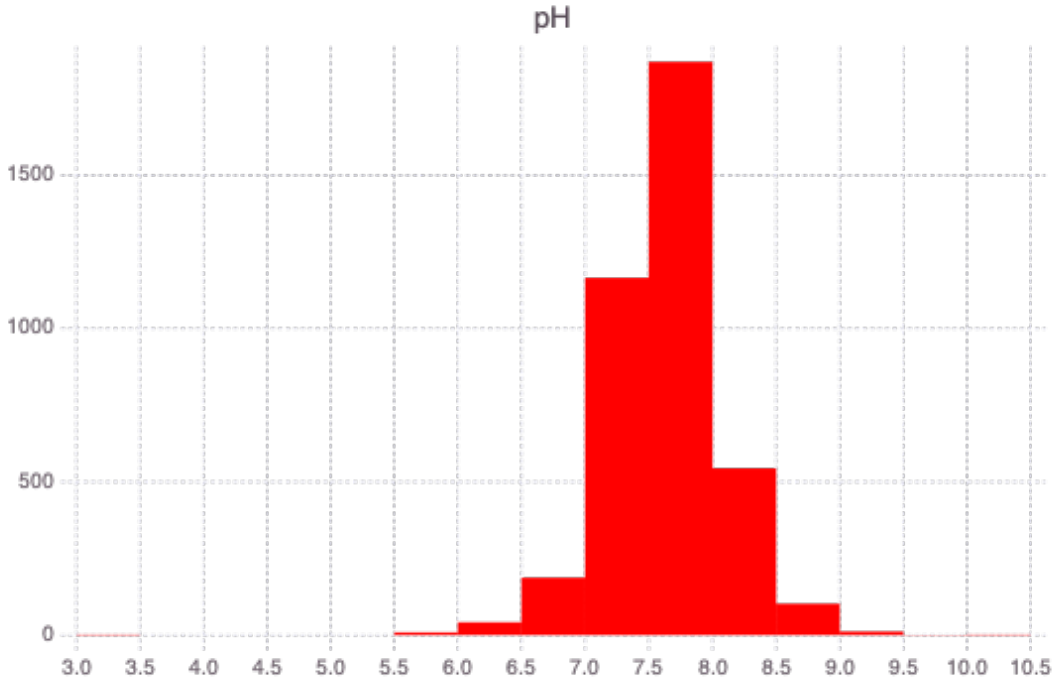
[13]:
```
NMFk.datanalytics(X, attributes; dims=2, logv=logv);
```



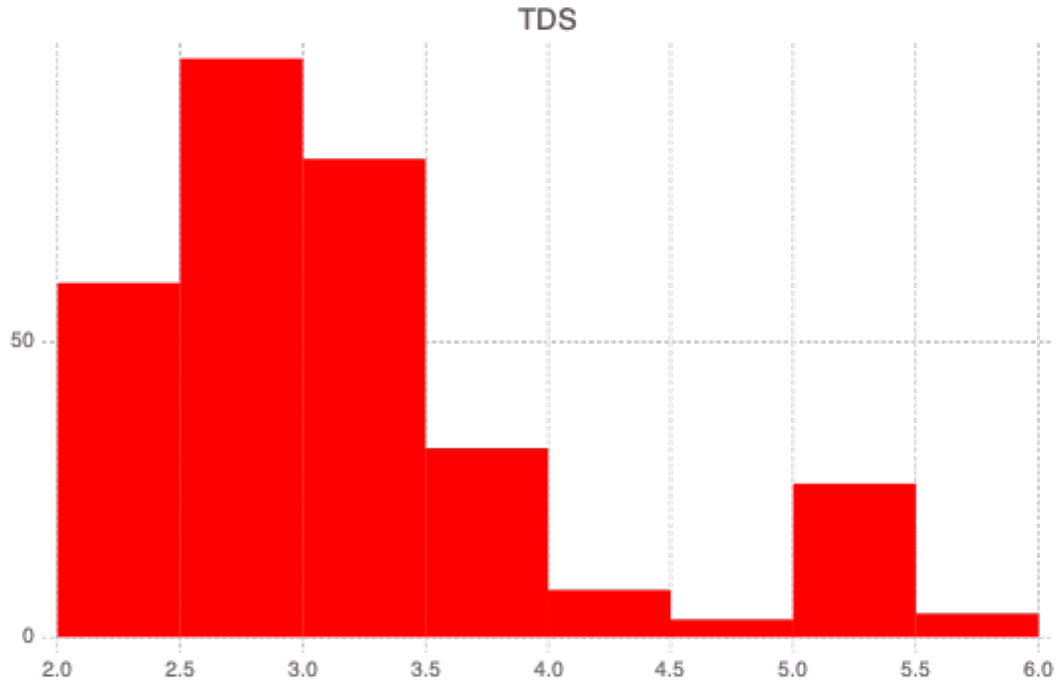

```
Info: Temperature: log10-transformed
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```

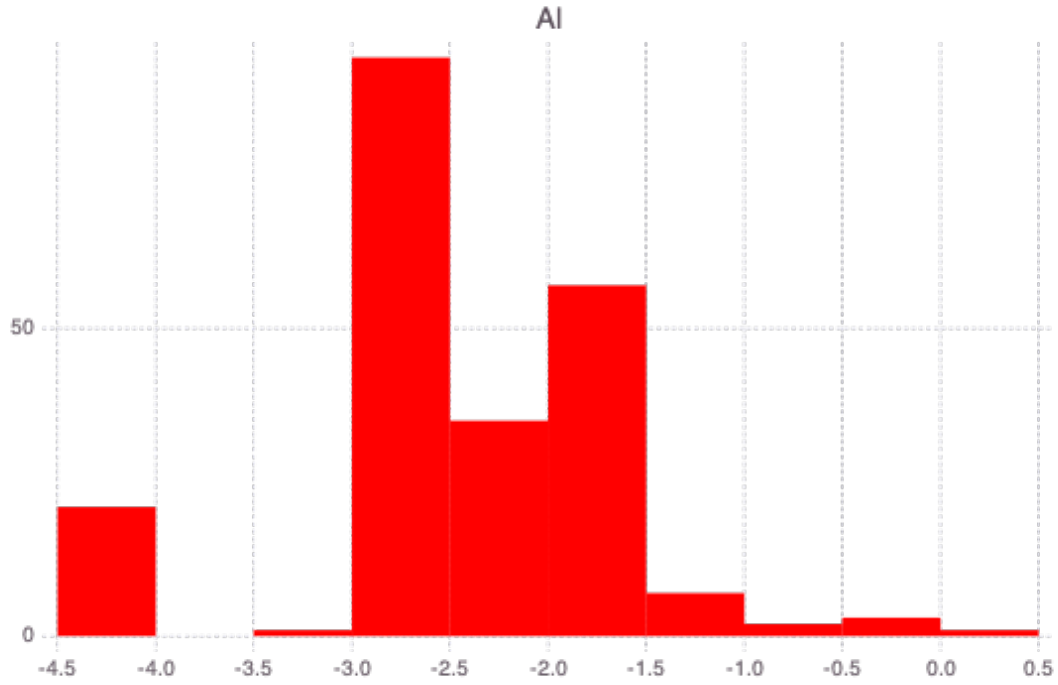

Quartz
500
0
-60
-40
-20
0
20
40
60
80
100
120
140
160
180
200
220
240

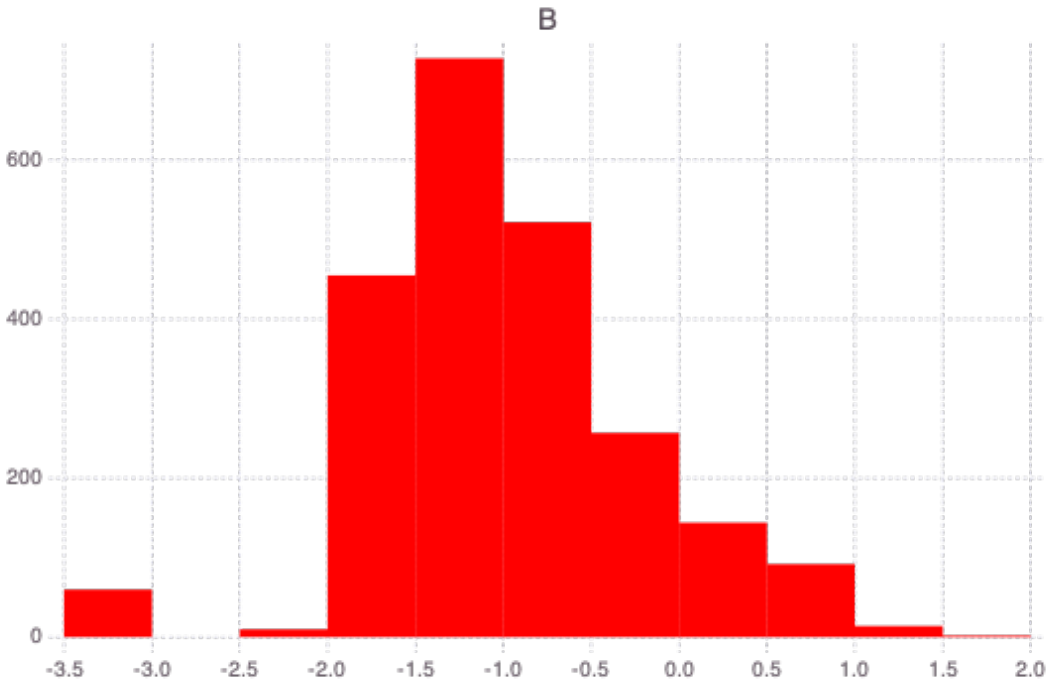

Chalcedony
2000
1500
1000
500
0
-100
-50
0
50
100
150
200
250



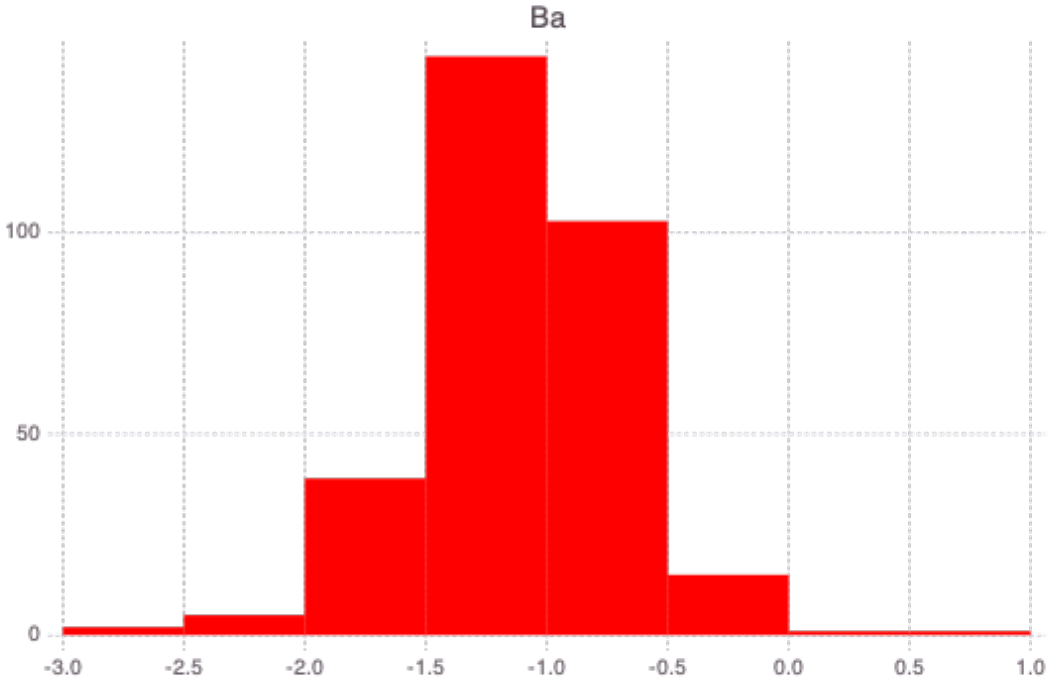

```
Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count
5214
Quartz: Min -50.870045 Max 222.28357 StdDev 26.329222 Skewness 0.24256101 Count
3460
Chalcedony: Min -81.64773 Max 208.67426 StdDev 27.450817 Skewness 0.3369881
Count 3460
  Info: Quartz
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: Chalcedony
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: pH
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

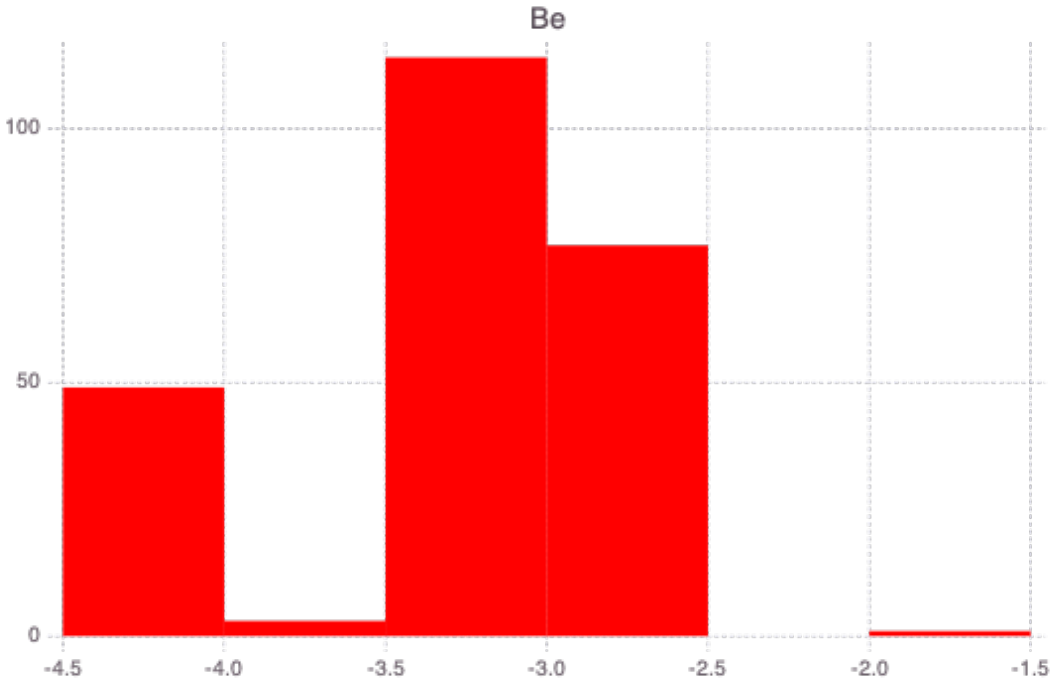

TDS
50
0
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0

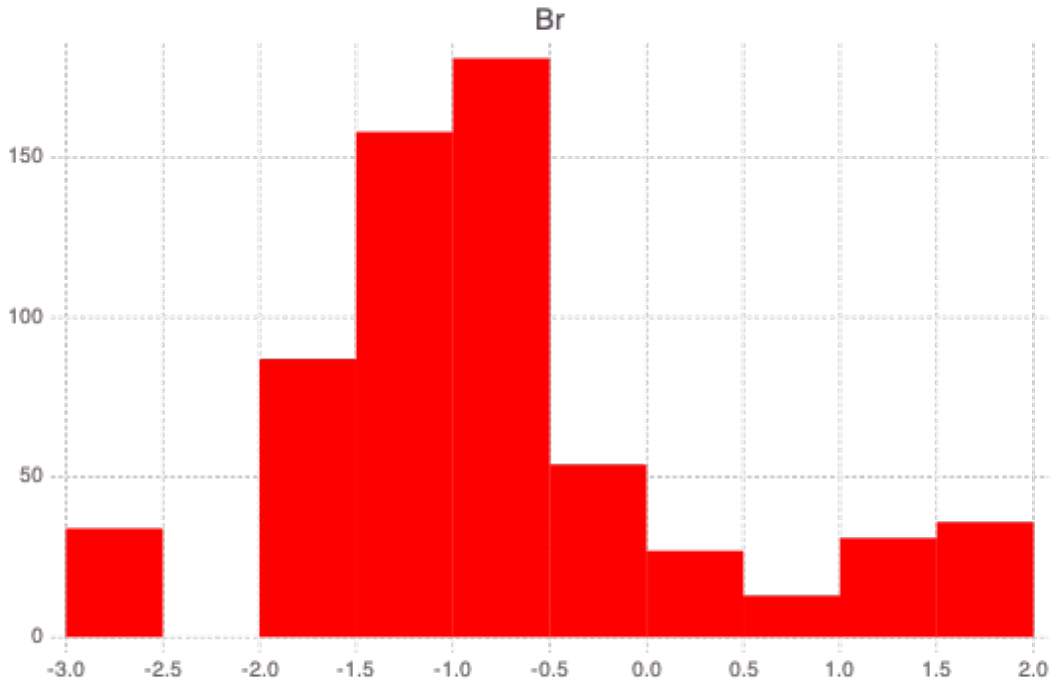

AI
50
0
-4.5
-4.0
-3.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5



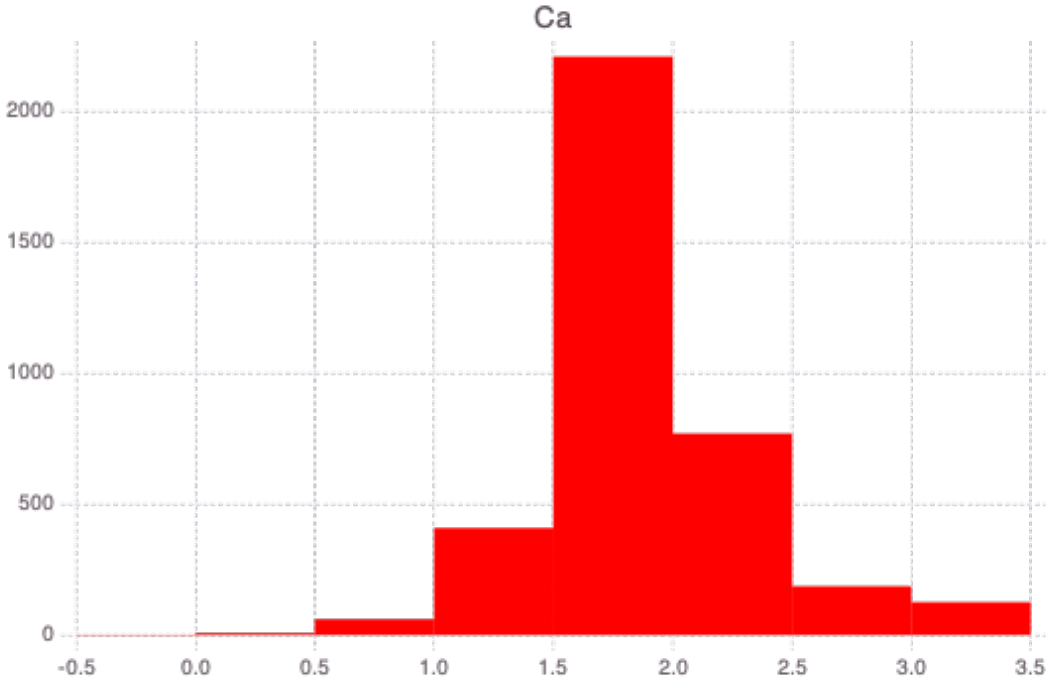

```
pH: Min 3.4 Max 10.2 StdDev 0.44822767 Skewness -0.45681924 Count 3941
TDS: Min 2.0863597 Max 5.5171957 StdDev 0.8672777 Skewness 1.4807001 Count 312
Al: Min -4.3979397 Max 0.09725732 StdDev 0.8454361 Skewness -0.37494856 Count
221
  Info: TDS: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  Info: Al: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  Info: B: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```

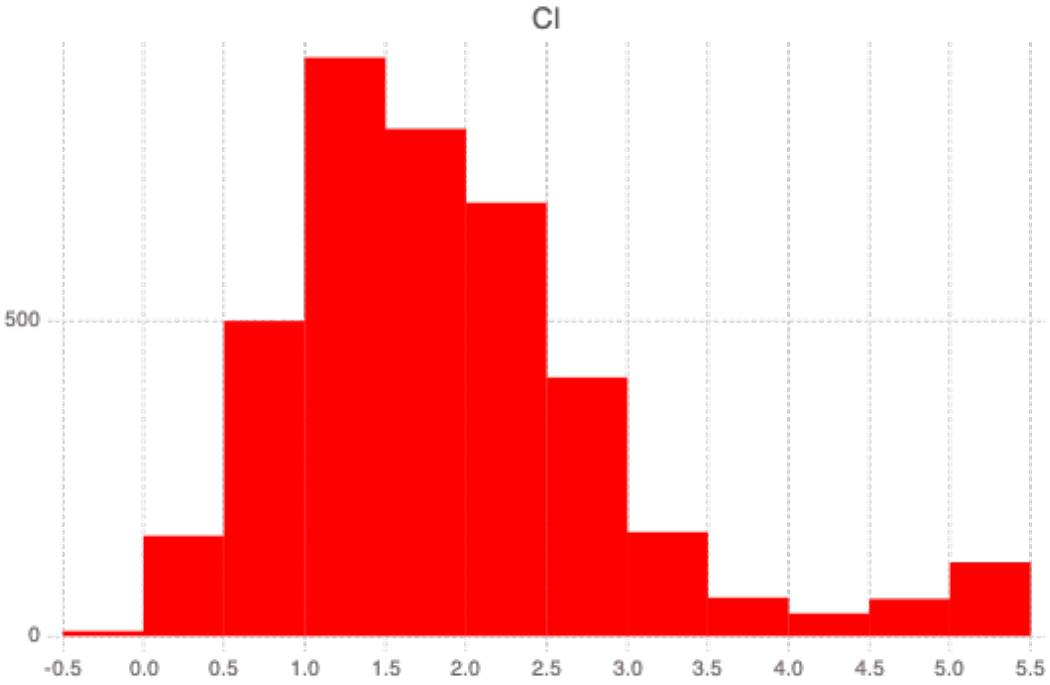

Ba
100
50
0
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0


Be
100
50
0
-4.5
-4.0
-3.5
-3.0
-2.5
-2.0
-1.5

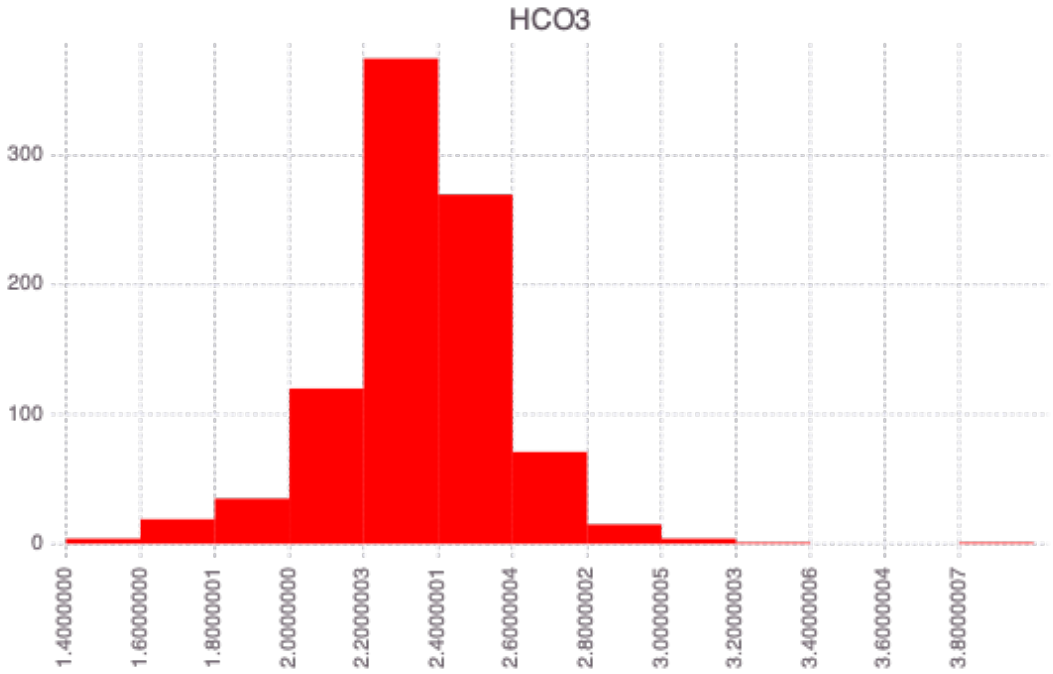


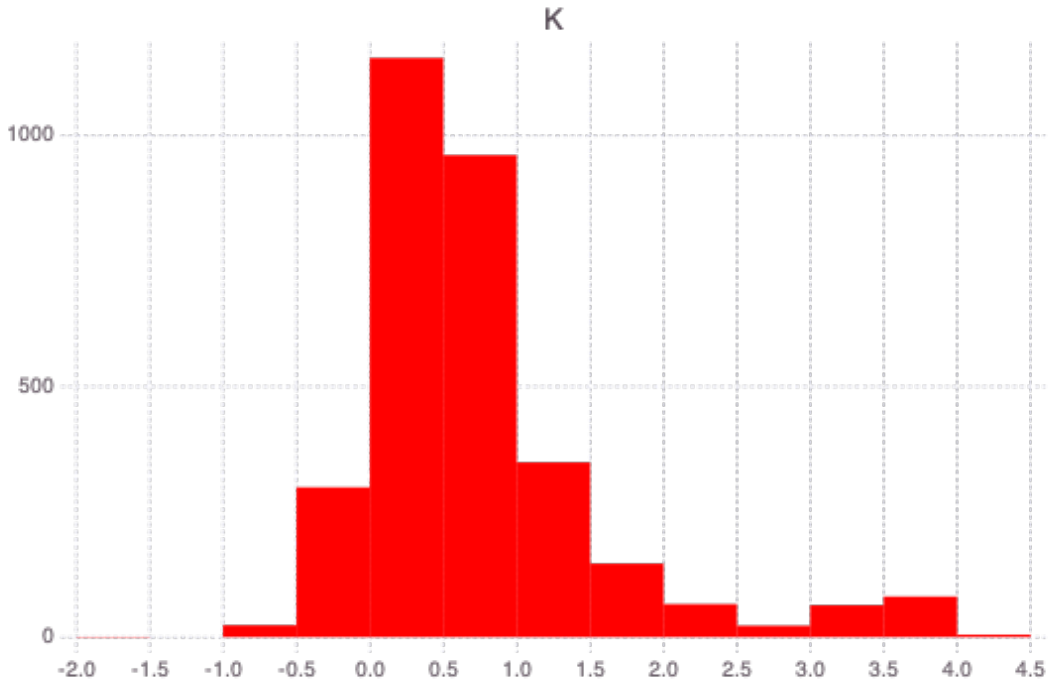

```
B: Min -3.30103 Max 1.8836614 StdDev 0.77384454 Skewness 0.08153698 Count 2284
Ba: Min -2.69897 Max 0.6532125 StdDev 0.40884706 Skewness -0.013896148 Count 310
Be: Min -4.273001 Max -1.8860567 StdDev 0.46150032 Skewness -0.83869493 Count
244
  Info: Ba: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  Info: Be: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  Info: Br: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```

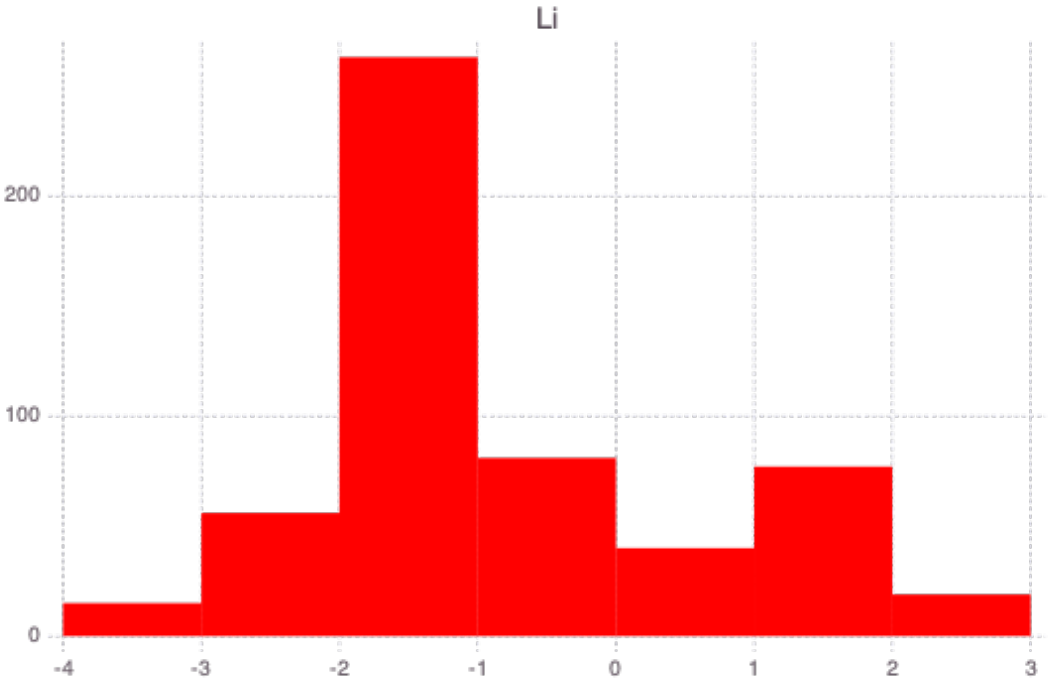

Ca
2000
1500
1000
500
0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5


Cl
500
0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5

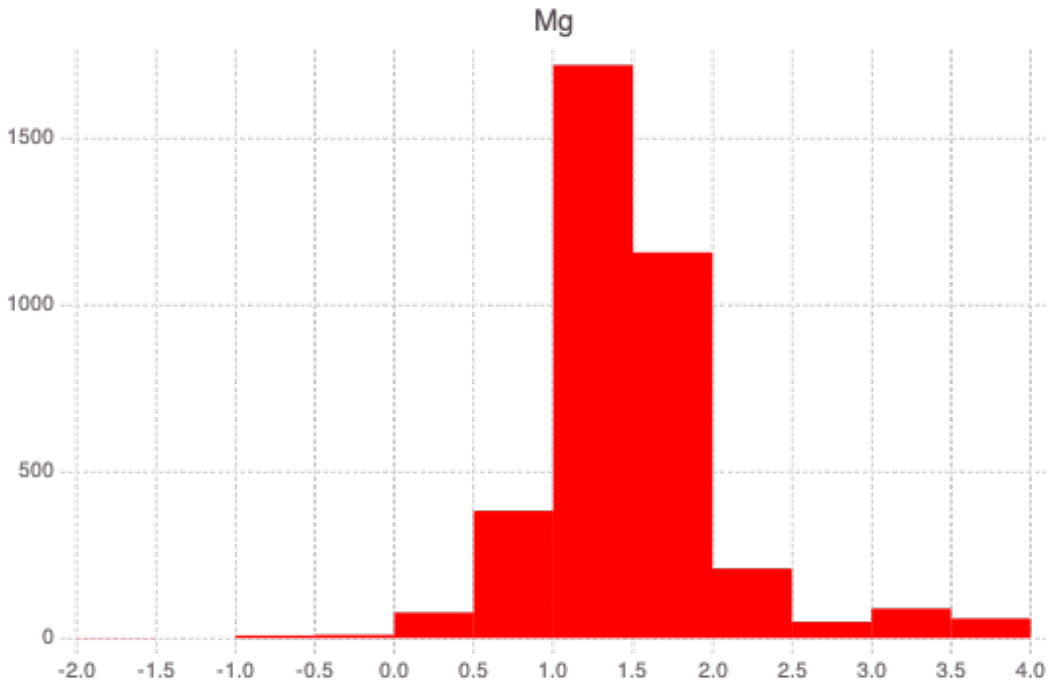
```
Br: Min -3.0 Max 1.9242793 StdDev 1.0616237 Skewness 0.5956521 Count 621
Ca: Min -0.22184873 Max 3.4093695 StdDev 0.43120933 Skewness 0.5738154 Count
3772
  Info: Ca: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  Info: Cl: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```

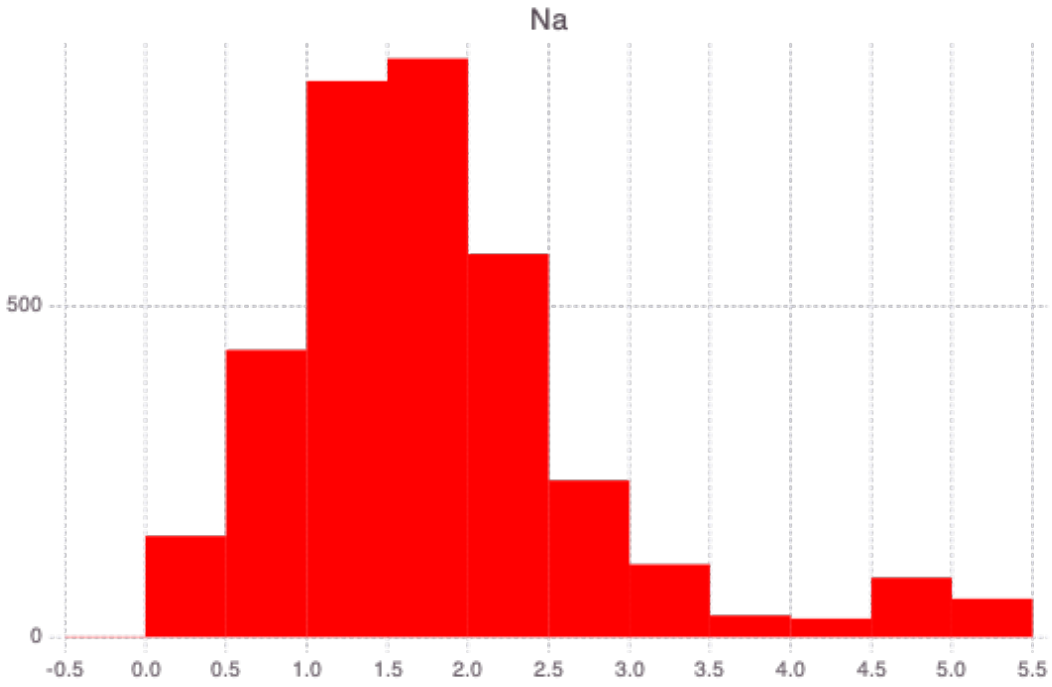


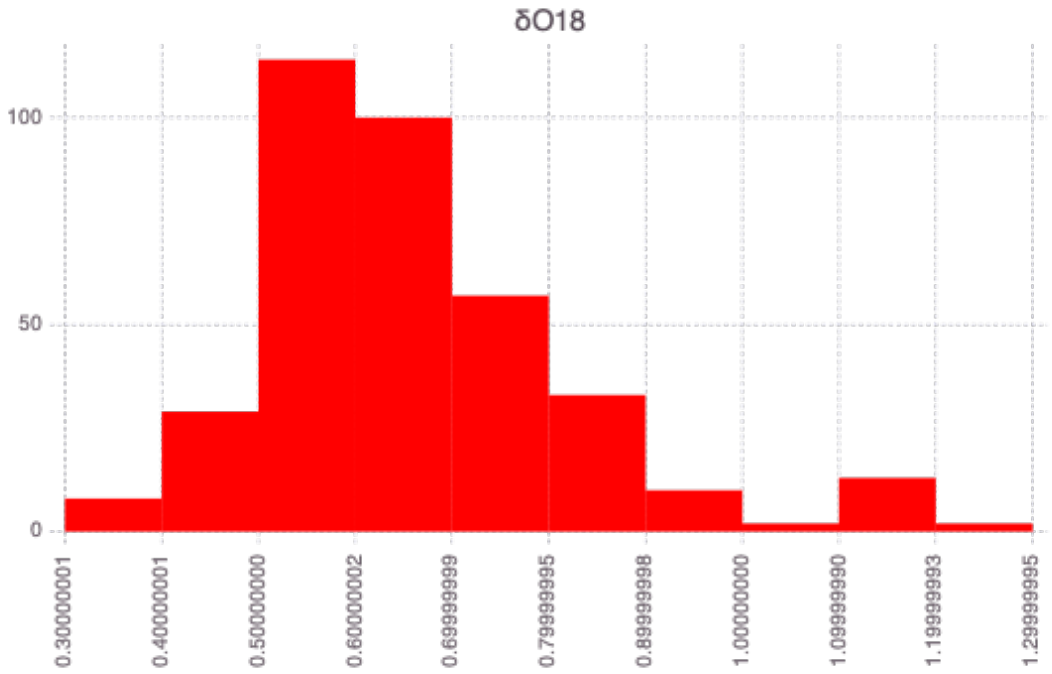

K
1000
500
0
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5


Li
200
100
0
-4
-3
-2
-1
0
1
2
3

```
Cl: Min -0.22184873 Max 5.3802114 StdDev 1.0519629 Skewness 1.1927316 Count 3923
HCO3: Min 1.5682018 Max 3.9645896 StdDev 0.22752158 Skewness 0.051133487 Count
915
K: Min -2.0 Max 4.1139436 StdDev 0.8480291 Skewness 1.8444492 Count 3177
  Info: HCO3: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  Info: K: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  Info: Li: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```




Na
500
0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5


δO18
100
50
0
0.30000001
0.40000001
0.50000000
0.60000002
0.69999999
0.79999995
0.89999998
1.00000000
1.09999990
1.19999993
1.29999995

```
Li: Min -3.9586072 Max 2.9867718 StdDev 1.4681796 Skewness 0.6889145 Count 551
Mg: Min -2.0 Max 3.929419 StdDev 0.5826601 Skewness 1.142913 Count 3760
Na: Min -0.30103 Max 5.20412 StdDev 0.985548 Skewness 1.3556563 Count 3437
 Info: Mg: log10-transformed
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
 Info: Na: log10-transformed
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
 Info:  O18: log10-transformed
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
O18: Min 0.33243838 Max 1.2137833 StdDev 0.16311567 Skewness 1.1355046 Count
368
Name Min Max StdDev Count (non-NaN's)
Temperature -1.0 2.4166405 0.19028741 -0.5570712 5214
Quartz -50.870045 222.28357 26.329222 0.24256101 3460
Chalcedony -81.64773 208.67426 27.450817 0.3369881 3460
pH 3.4 10.2 0.44822767 -0.45681924 3941
TDS 2.0863597 5.5171957 0.8672777 1.4807001 312
Al -4.3979397 0.09725732 0.8454361 -0.37494856 221
B -3.30103 1.8836614 0.77384454 0.08153698 2284
Ba -2.69897 0.6532125 0.40884706 -0.013896148 310
Be -4.273001 -1.8860567 0.46150032 -0.83869493 244
Br -3.0 1.9242793 1.0616237 0.5956521 621
Ca -0.22184873 3.4093695 0.43120933 0.5738154 3772
Cl -0.22184873 5.3802114 1.0519629 1.1927316 3923
HCO3 1.5682018 3.9645896 0.22752158 0.051133487 915
K -2.0 4.1139436 0.8480291 1.8444492 3177
Li -3.9586072 2.9867718 1.4681796 0.6889145 551
Mg -2.0 3.929419 0.5826601 1.142913 3760
Na -0.30103 5.20412 0.985548 1.3556563 3437
O18 0.33243838 1.2137833 0.16311567 1.1355046 368
 Info: Attributes
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:70
```

1.7 Normalize the data

[14]:
```
Xnl, xlmin, xlmax, zflag = NMFk.normalizematrix_col(X; logv=logv);
```

1.8 Define the number of signatures to be explored

[15]:
```
nkrange = 2:10
```

```
2:10
```

1.9 Define a directory where outputs should be stored

[16]:
```
resultdir = "utah/results";
```

1.10 Define the number of NMF iterations (NMF random initial guess runs):

[17]:
```
nruns = 100;
```

1.11 Run NMFk on normalized data

[18]:
```
# W, H, fitquality, robustness, aic, kopt = NMFk.execute(Xnl, nkrange, nruns;␣
 ↪cutoff=0.3, resultdir=resultdir, casefilename="nmfk-nl", load=true)
W, H, fitquality, robustness, aic, kopt = NMFk.load(nkrange, nruns; cutoff=0.3,␣
 ↪resultdir=resultdir, casefilename="nmfk-nl");
```

```
Signals:  2 Fit:      186.979 Silhouette:    0.5600511 AIC:    -193490.6 Signal
order: [1, 2]
Signals:  3 Fit:     116.1197 Silhouette:    0.3400365 AIC:    -202059.3 Signal
order: [1, 2, 3]
Signals:  4 Fit:     81.67226 Silhouette: -0.004722083 AIC:      -205653 Signal
order: [1, 2, 3, 4]
Signals:  5 Fit:     55.85581 Silhouette:   0.03561851 AIC:    -210367.2 Signal
order: [1, 2, 3, 4, 5]
Signals:  6 Fit:     37.37445 Silhouette:   0.08498218 AIC:    -215954.6 Signal
order: [1, 2, 3, 4, 5, 6]
Signals:  7 Fit:     22.77074 Silhouette:  -0.06623857 AIC:    -225288.2 Signal
order: [1, 2, 3, 4, 5, 6, 7]
Signals:  8 Fit:     14.94362 Silhouette:    0.0637157 AIC:    -231651.2 Signal
order: [1, 2, 3, 4, 5, 6, 7, 8]
Signals:  9 Fit:     9.241436 Silhouette:   -0.1125796 AIC:    -240388.3 Signal
order: [1, 2, 3, 4, 5, 6, 7, 8, 9]
Signals: 10 Fit:     6.104004 Silhouette:  -0.01305462 AIC:      -246494 Signal
order: [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
 Info: Optimal solution: 3 signals
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkIO.jl:30
```

1.12 Get the acceptable solutions within the present range of number of signatures:

[19]:
```
NMFk.getks(nkrange, robustness[nkrange], 0.3)
```

```
2-element Vector{Int64}:
 2
 3
```

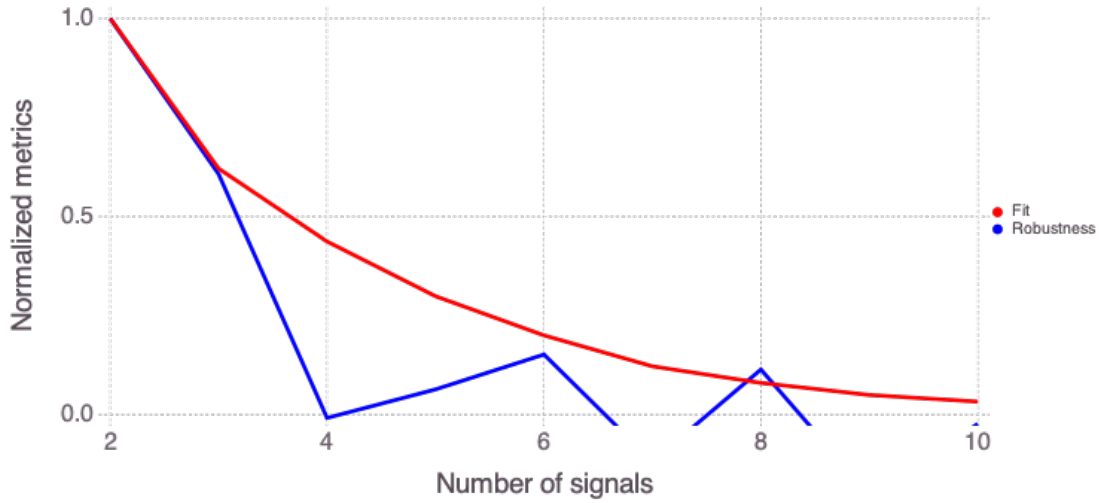
1.13 Get the optimal number of signatures:

[20]:
```
NMFk.getk(nkrange, robustness[nkrange], 0.3)
```

```
3
```

1.14 Plot the fit and robustness of the solution

[21]:
```
resultdirpost = "utah/results-postprocessing-nl-$(nruns)"
figuredirpost = "utah/figures-postprocessing-nl-$(nruns)"
NMFk.plot_feature_selecton(nkrange, fitquality, robustness;␣
 ↪figuredir=figuredirpost)
```



1.15 Analysis of the optimal solution

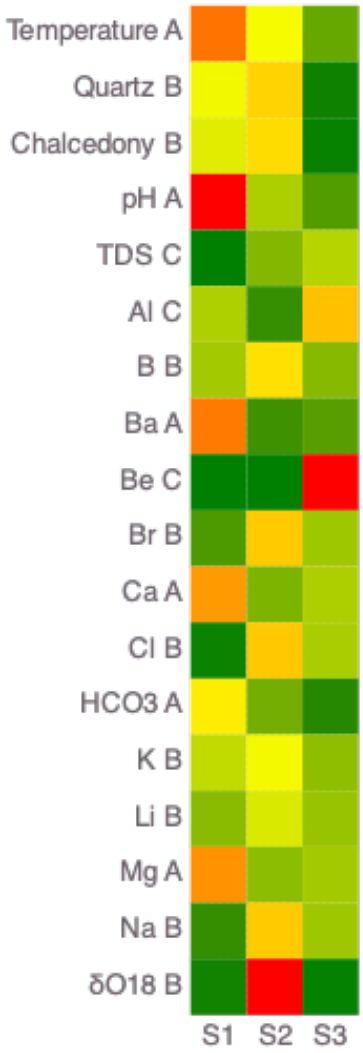
[22]:
```
Sorder, Wclusters, Hclusters = NMFk.clusterresults(NMFk.getk(nkrange,␣
 ↪robustness[nkrange], 0.3), W, H, string.(collect(1:npoints)), attributes;␣
 ↪lon=xcoord, lat=ycoord, resultdir=resultdirpost, figuredir=figuredirpost,␣
 ↪ordersignal=:Wcount, Hcasefilename="attributes", Wcasefilename="locations",␣
 ↪biplotcolor=:WH, sortmag=false, biplotlabel=:H, point_size_nolabel=2Gadfly.
 ↪pt, point_size_label=4Gadfly.pt)
```

```
 Info: Number of signals: 3
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:205
 Info: Attributes (signals=3)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:209
 Warning: type
Clustering.KmeansResult{Core.Array{Core.Float32,2},Core.Float32,Core.Int64} not
present in workspace; reconstructing
 @ JLD /Users/vvv/.julia/packages/JLD/JHrZe/src/jld_types.jl:697
 Info: Robust k-means analysis results are loaded from file utah/results-
postprocessing-nl-100/Hmatrix-3-3_18-1000.jld!
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:67
```

```
6×2 Matrix{Any}:
 "pH"           1.0
 "Temperature"  0.858848
 "Ba"           0.84477
 "Mg"           0.788068
 "Ca"           0.76783
 "HCO3"         0.549396
```

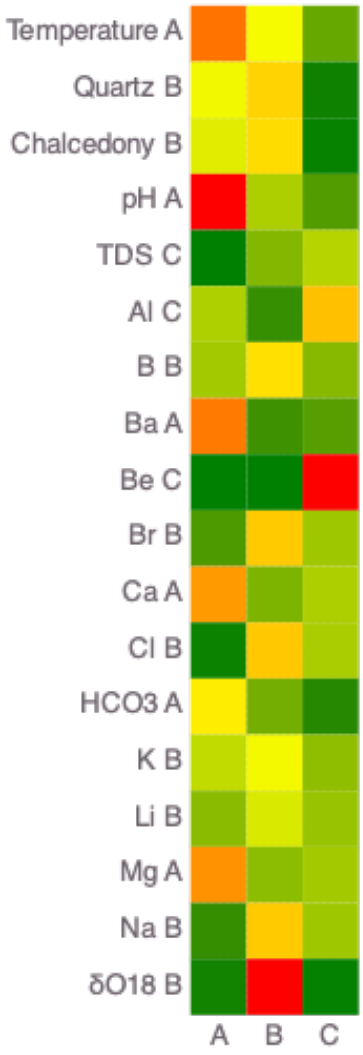
```
9×2 Matrix{Any}:
 " O18"        1.0
 "Cl"          0.651079
 "Na"          0.643991
 "Br"          0.642053
 "Quartz"      0.620207
 "Chalcedony"  0.596872
 "B"           0.586983
 "K"           0.475275
 "Li"          0.414782
```

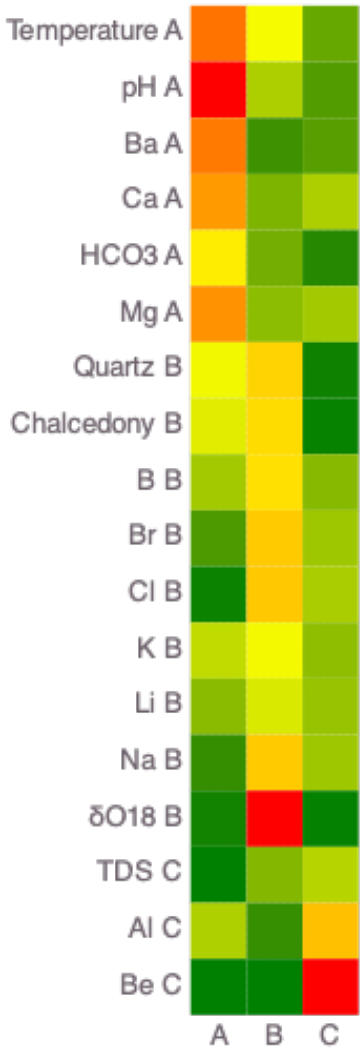
```
3×2 Matrix{Any}:
 "Be"   1.0
 "Al"   0.672723
 "TDS"  0.332944
```

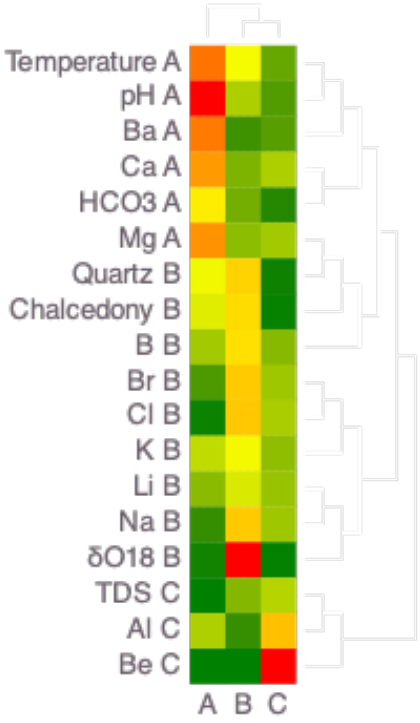


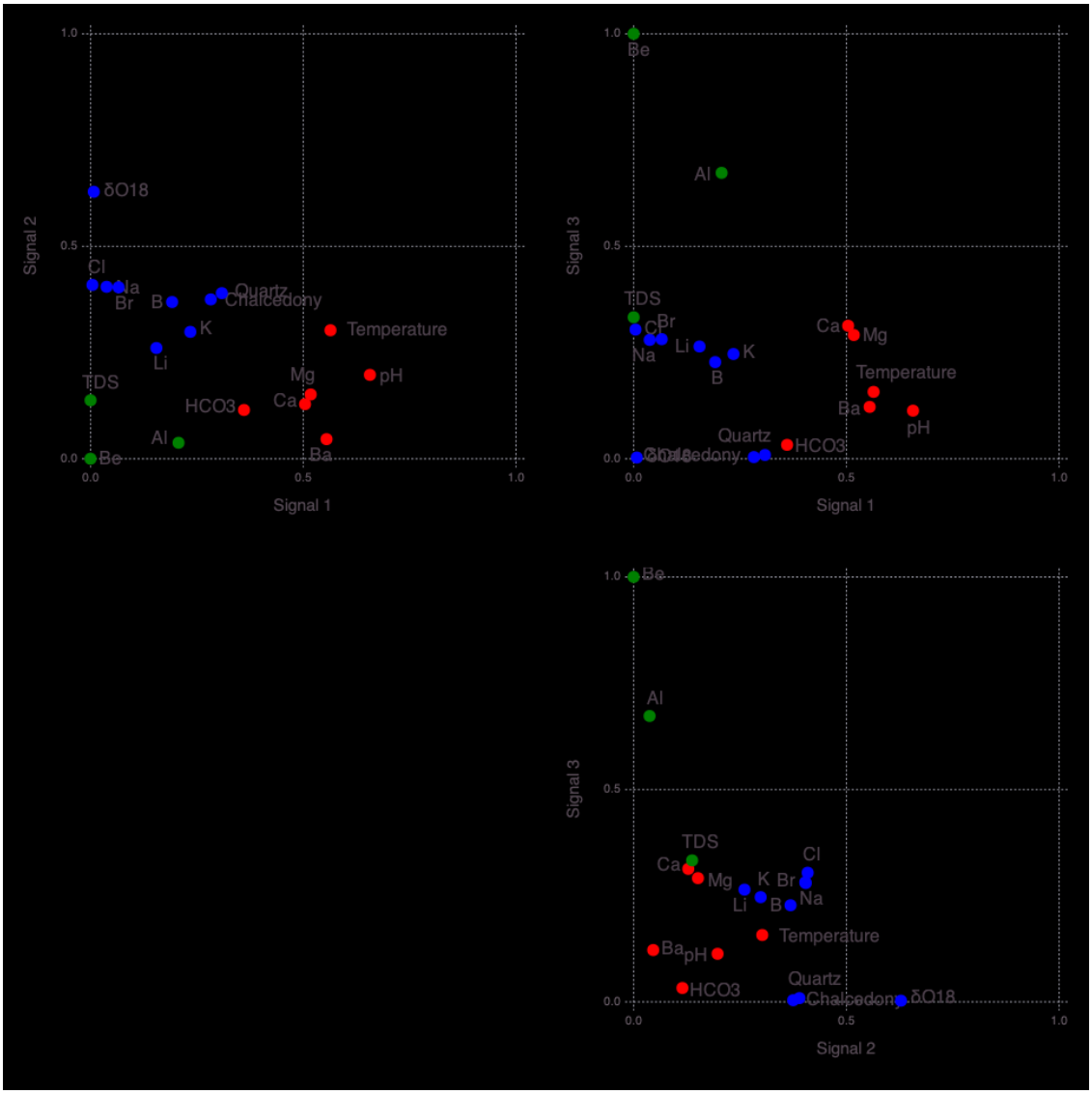

```
  Warning: Procedure to find unique signals could not identify a solution …
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
  Warning: Procedure to find unique signals could not identify a solution …
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
  Warning: Procedure to find unique signals could not identify a solution …
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
  Warning: type
Clustering.KmeansResult{Core.Array{Core.Float32,2},Core.Float32,Core.Int64} not
present in workspace; reconstructing
  @ JLD /Users/vvv/.julia/packages/JLD/JHrZe/src/jld_types.jl:697
  Info: Robust k-means analysis results are loaded from file utah/results-
postprocessing-nl-100/Wmatrix-3-3_5218-1000.jld!
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:67
```

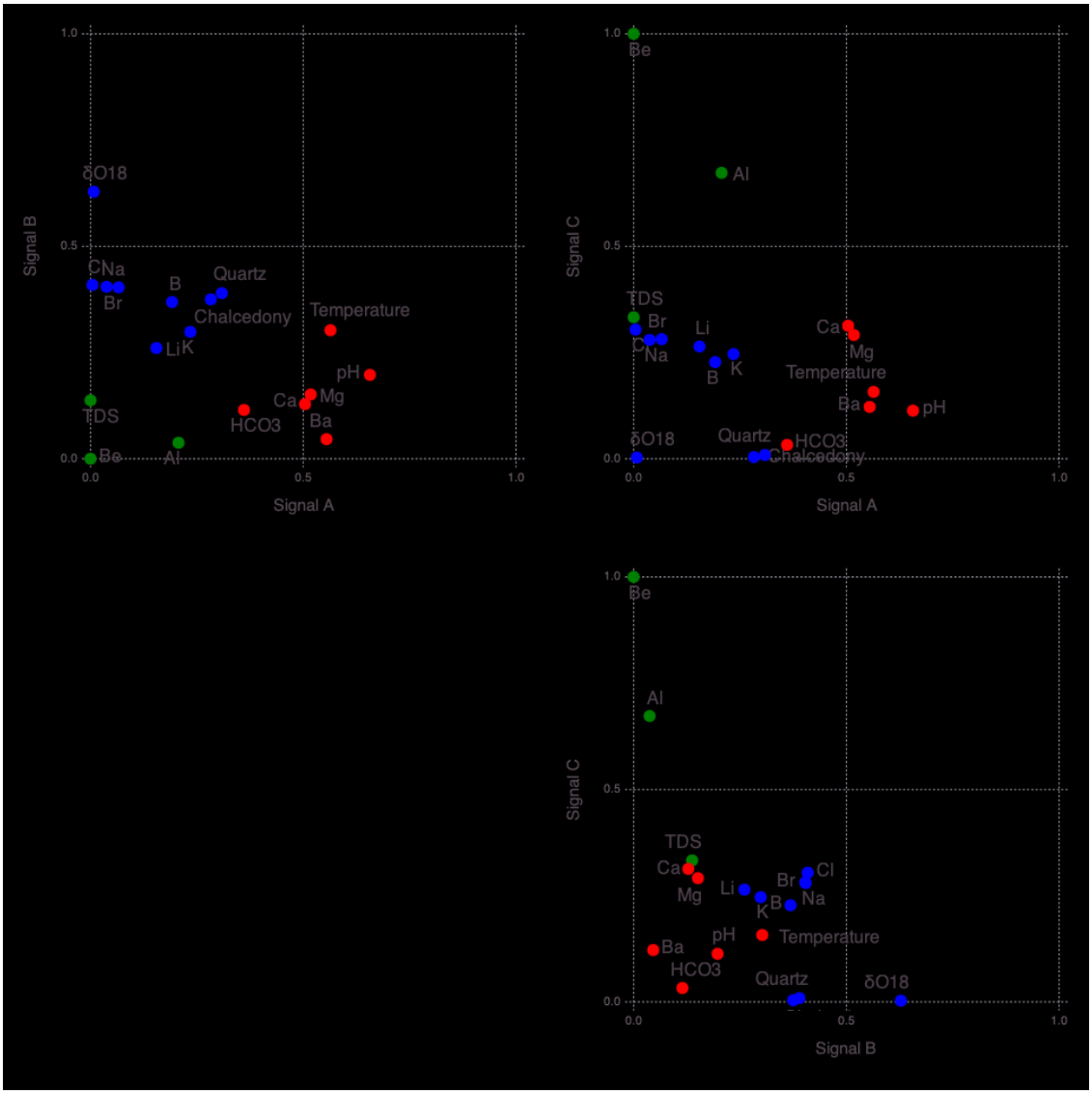
```
Warning: Procedure to find unique signals could not identify a solution …
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
Warning: Procedure to find unique signals could not identify a solution …
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
Warning: Procedure to find unique signals could not identify a solution …
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
Info: Signal B -> A Count: 6
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:316
Info: Signal A -> B Count: 9
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:316
Info: Signal C -> C Count: 3
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:316
Info: Signal A (S1) (k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:333
Info: Signal B (S2) (k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:333
Info: Signal C (S3) (k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:333
```


Temperature A
Quartz B
Chalcedony B
pH A
TDS C
Al C
B B
Ba A
Be C
Br B
Ca A
Cl B
HCO3 A
K B
Li B
Mg A
Na B
δO18 B
A
B
C


Temperature A
pH A
Ba A
Ca A
HCO3 A
Mg A
Quartz B
Chalcedony B
B B
Br B
Cl B
K B
Li B
Na B
δO18 B
TDS C
Al C
Be C
A
B
C


Temperature A
pH A
Ba A
Ca A
HCO3 A
Mg A
Quartz B
Chalcedony B
B B
Br B
Cl B
K B
Li B
Na B
δO18 B
TDS C
Al C
Be C
A B C

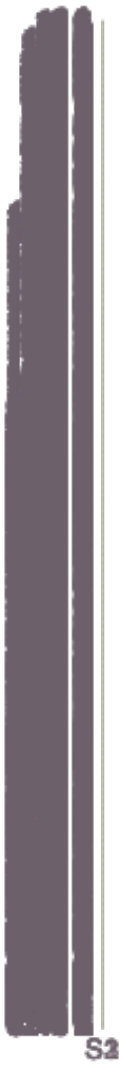

Signal 2
Signal 1
δO18
Cl
Na
Br
B
Quartz
Chalcedony
K
Temperature
Li
Mg
pH
TDS
HCO3
Ca
Al
Ba
Be
Signal 3
Signal 1
Be
Al
TDS
Cl
Br
Na
Li
K
B
Ca
Mg
Temperature
Ba
pH
Quartz
HCO3
Signal 3
Signal 2
Be
Al
TDS
Ca
Cl
Mg
K
Br
Li
B
Na
Temperature
Ba
pH
HCO3
Quartz
Chalcedony
δO18




```
2131×2 Matrix{Any}:
 "4816"  1.0
 "4655"  0.970208
 "4826"  0.958804
 "2260"  0.955817
 "4015"  0.938536
 "3257"  0.93743
 "4889"  0.929527
 "1797"  0.924136
 "3405"  0.924069
 "2566"  0.905143
```

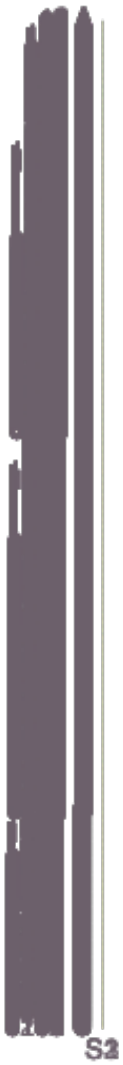
```
 "350"   0.492666
 "341"   0.491852
 "2730"  0.487104
 "3987"  0.47064
 "483"   0.466211
 "2909"  0.464978
 "476"   0.46367
 "2931"  0.435235
 "452"   0.359449
1966×2 Matrix{Any}:
 "4430"  1.0
 "2992"  0.972819
 "2309"  0.920633
 "4913"  0.90427
 "4056"  0.88218
 "564"   0.868838
 "4978"  0.866204
 "4319"  0.857647
 "4788"  0.855117
 "2468"  0.831267

 "375"   0.203084
 "159"   0.202853
 "3798"  0.198906
 "5112"  0.1978
 "738"   0.19415
 "3317"  0.193811
 "747"   0.189873
 "10"    0.181605
 "4954"  0.163099
1121×2 Matrix{Any}:
 "5013"  1.0
 "5118"  0.985958
 "5064"  0.978501
 "5068"  0.974911
 "5126"  0.969774
 "2554"  0.952582
 "5049"  0.948387
 "5048"  0.914722
 "5006"  0.910949
 "5095"  0.910366

 "4154"  0.174466
 "4710"  0.174457
 "3376"  0.172963
 "1412"  0.170218
 "3662"  0.161509
```

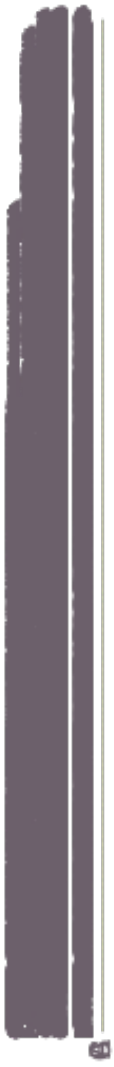
```
"4300"  0.160252
"2742"  0.148677
"4289"  0.144853
"2028"  0.129906
```

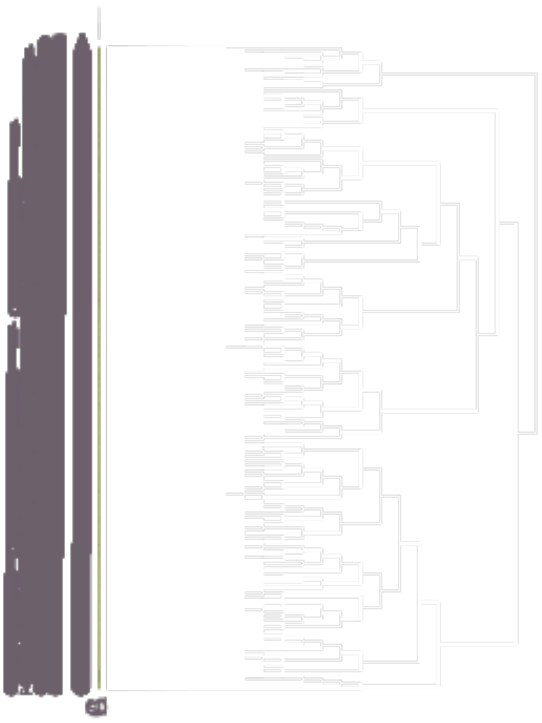


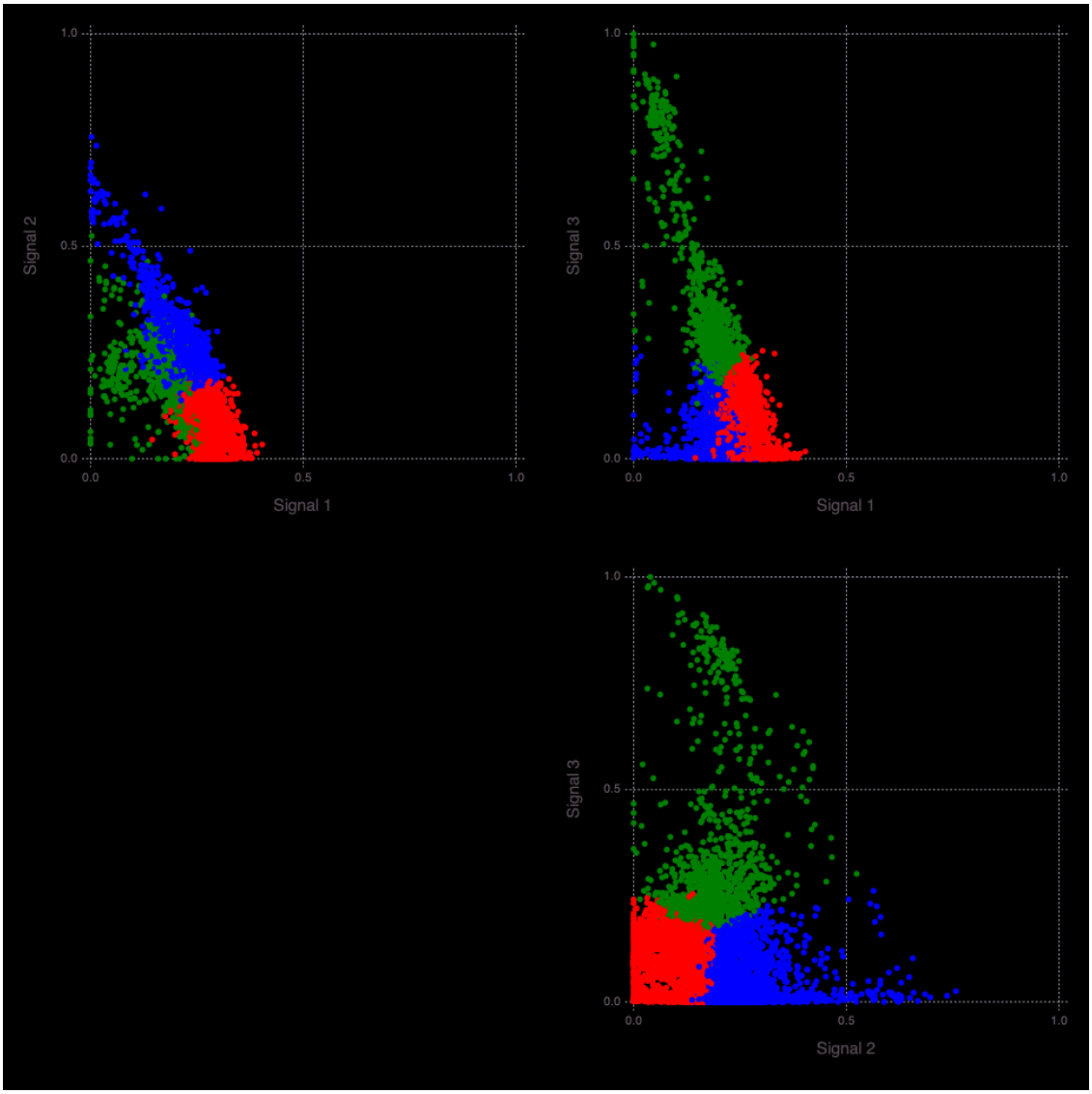

```
Info: Locations (signals=3)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:391
Info: Signal A (S1) Count: 2131
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:404
Info: Signal B (S2) Count: 1966
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:404
Info: Signal C (S3) Count: 1121
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:404
Info: Signal A -> A Count: 2131
```

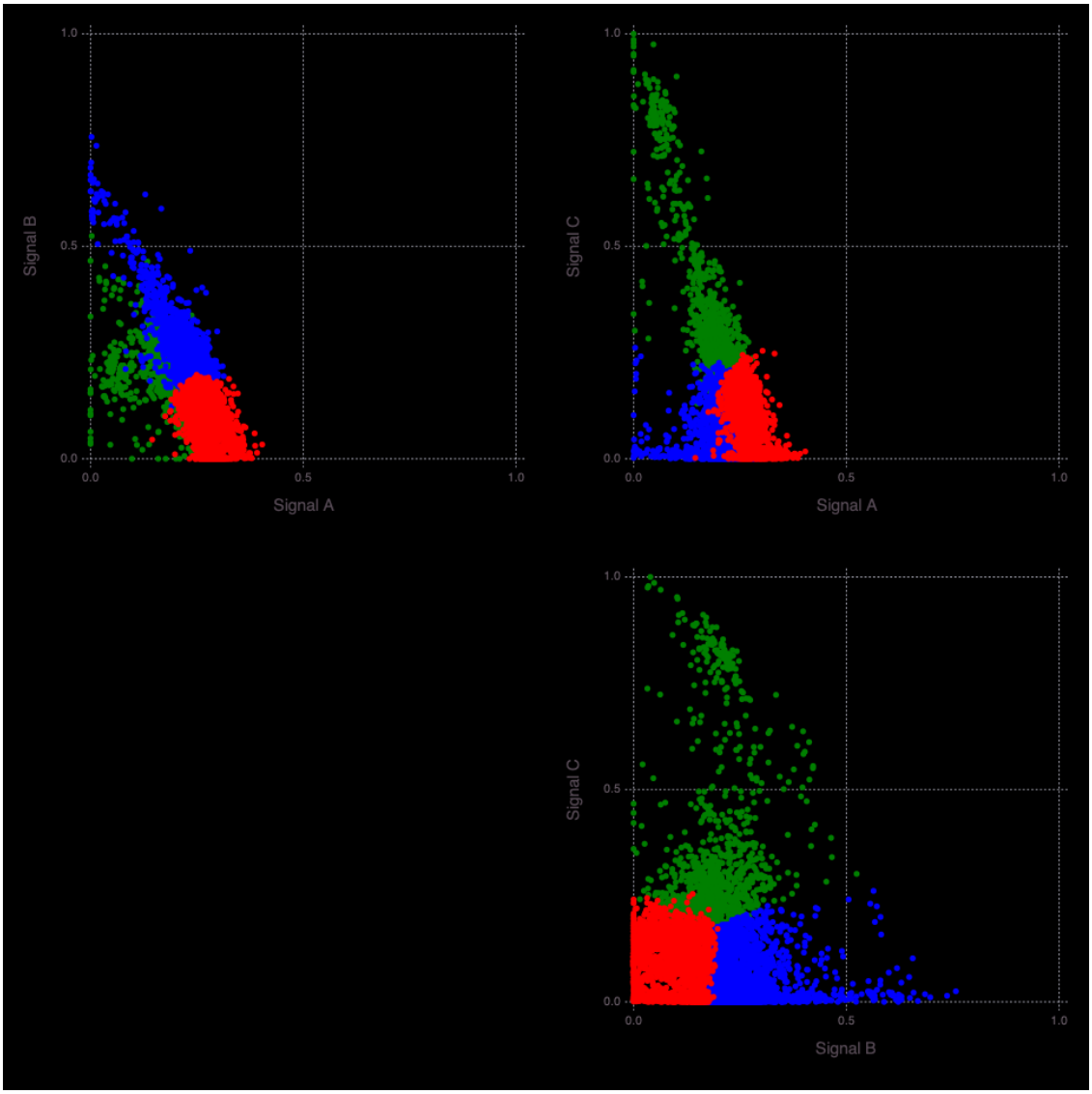
```
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:414
Info: Signal B -> B Count: 1966
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:414
Info: Signal C -> C Count: 1121
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:414
Info: Signal A (remapped k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:429
Info: Signal B (remapped k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:429
Info: Signal C (remapped k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:429
```

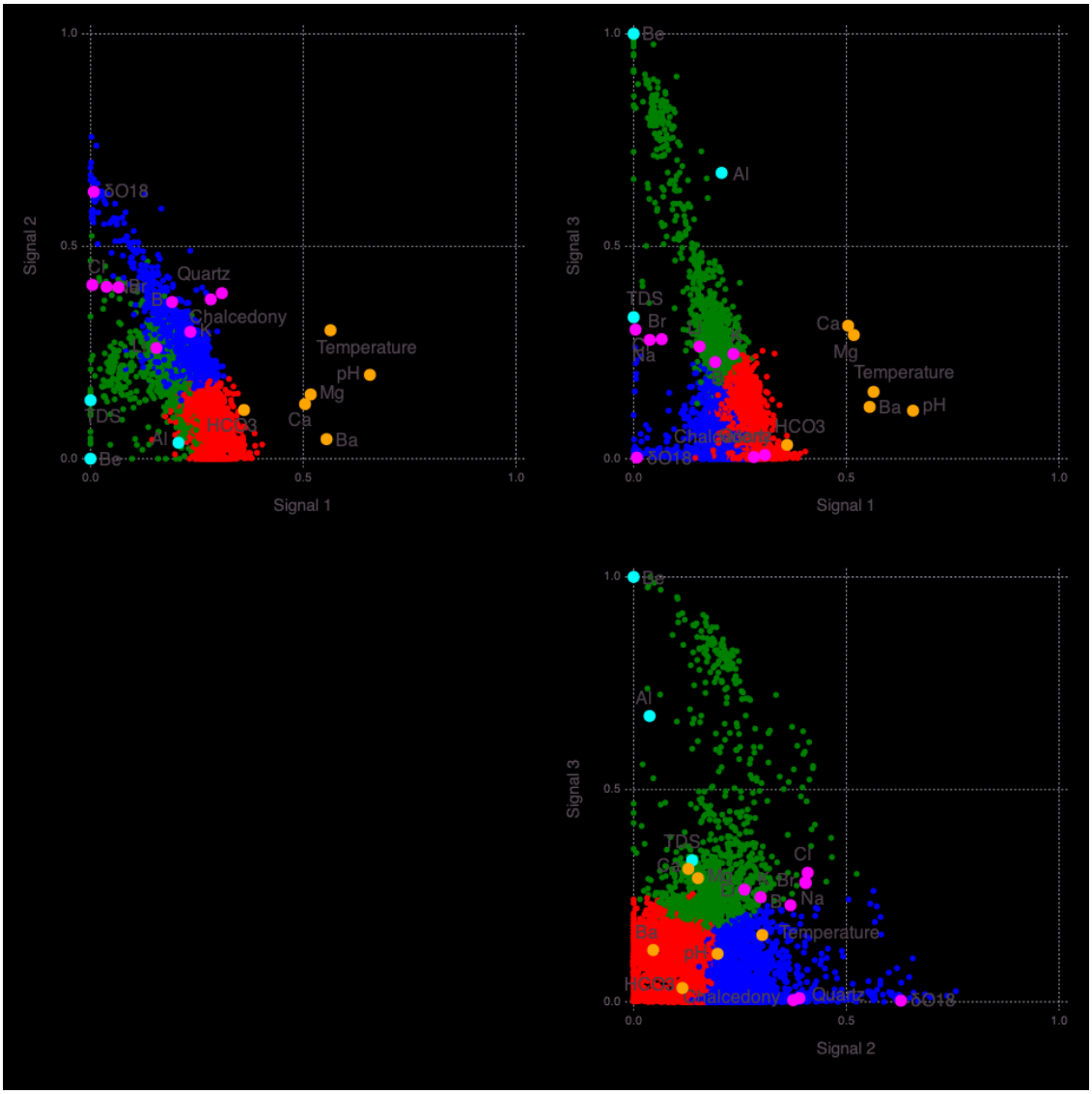


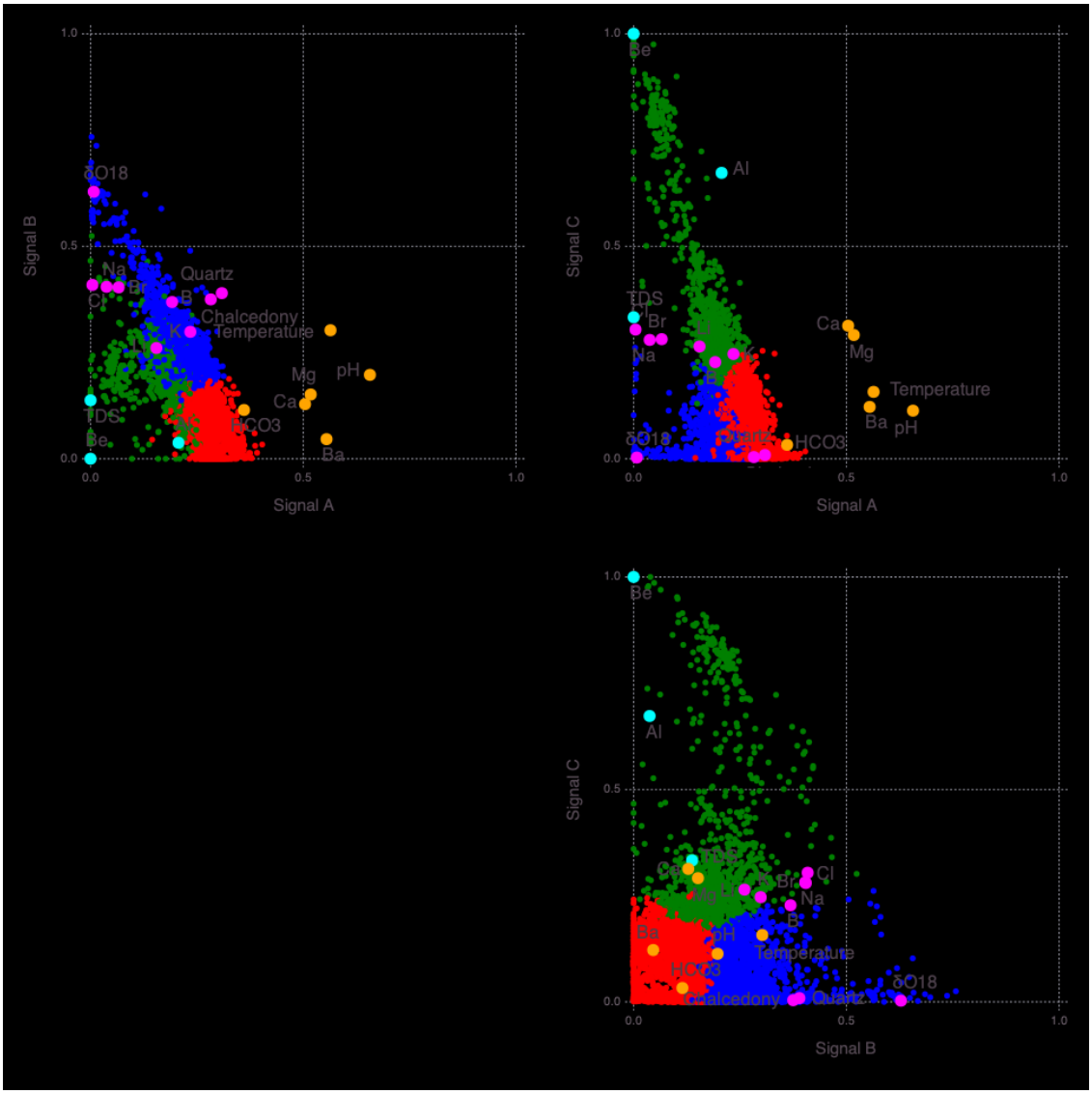





1.0
0.5
0.0
Signal 2
0.0
0.5
1.0
Signal 1
1.0
0.5
0.0
Signal 3
0.0
0.5
1.0
Signal 1
1.0
0.5
0.0
Signal 3
0.0
0.5
1.0
Signal 2


Signal B
Signal A
Signal C
Signal A
Signal C
Signal B
0.0
0.5
1.0


Signal 2
Signal 1
δO18
Cl
Br
Quartz
Chalcedony
Temperature
pH
Mg
TDS
Ca
Ba
Al
HCO3
Be
Signal 3
Signal 1
Be
Al
TDS
Br
Na
Ca
Mg
Temperature
Ba
pH
HCO3
Chalcedony
δO18
Signal 3
Signal 2
Be
Al
TDS
Cl
Ca
Mg
Br
Na
Temperature
Ba
pH
HCO3
Chalcedony
Quartz
δO18




```
([[1, 2, 3]], [['A', 'A', 'A', 'A', 'A', 'A', 'A', 'A', 'A', 'B'  …  'A', 'B',␣
↪'B', 'B', 'A', 'B', 'B', 'A', 'A', 'A']], [['A', 'B', 'B', 'A', 'C', 'C', 'B',␣
↪'A', 'C', 'B', 'A', 'B', 'A', 'B', 'B', 'A', 'B', 'B']])
```

1.16 Associations of the data attributes with the extracted signatures

[23]:
```
Mads.display("utah/results-postprocessing-nl-100/attributes-3-groups.txt")
```

```
Signal A (S1)
pH              1.0
Temperature     0.859
Ba              0.845
```

```
Mg              0.788
Ca              0.768
HCO3            0.549

Signal B (S2)
 O18           1.0
Cl              0.651
Na              0.644
Br              0.642
Quartz          0.62
Chalcedony      0.597
B               0.587
K               0.475
Li              0.415

Signal C (S3)
Be              1.0
Al              0.673
TDS             0.333
```

1.17 Associations of the data locations with the extracted signatures

[24]:
```
ldata, lhs = DelimitedFiles.readdlm("utah/results-postprocessing-nl-100/
 ↪locations-3.csv", ',', header=true)
signallabels = unique(sort(ldata[:,end]))
zcolor = Vector{Int64}(undef, length(ldata[:,1]))
for i = 1:length(clusters)
        ci = ldata[:,end] .== signallabels[i]
        println("Signal $(signallabels[i])")
        si = sortperm(ldata[ci,2+i]; rev=true)
        display([ldata[ci,1:3] ldata[ci,3+i]][si,:][1:10,:])
        zcolor[ci] .= i
end
```

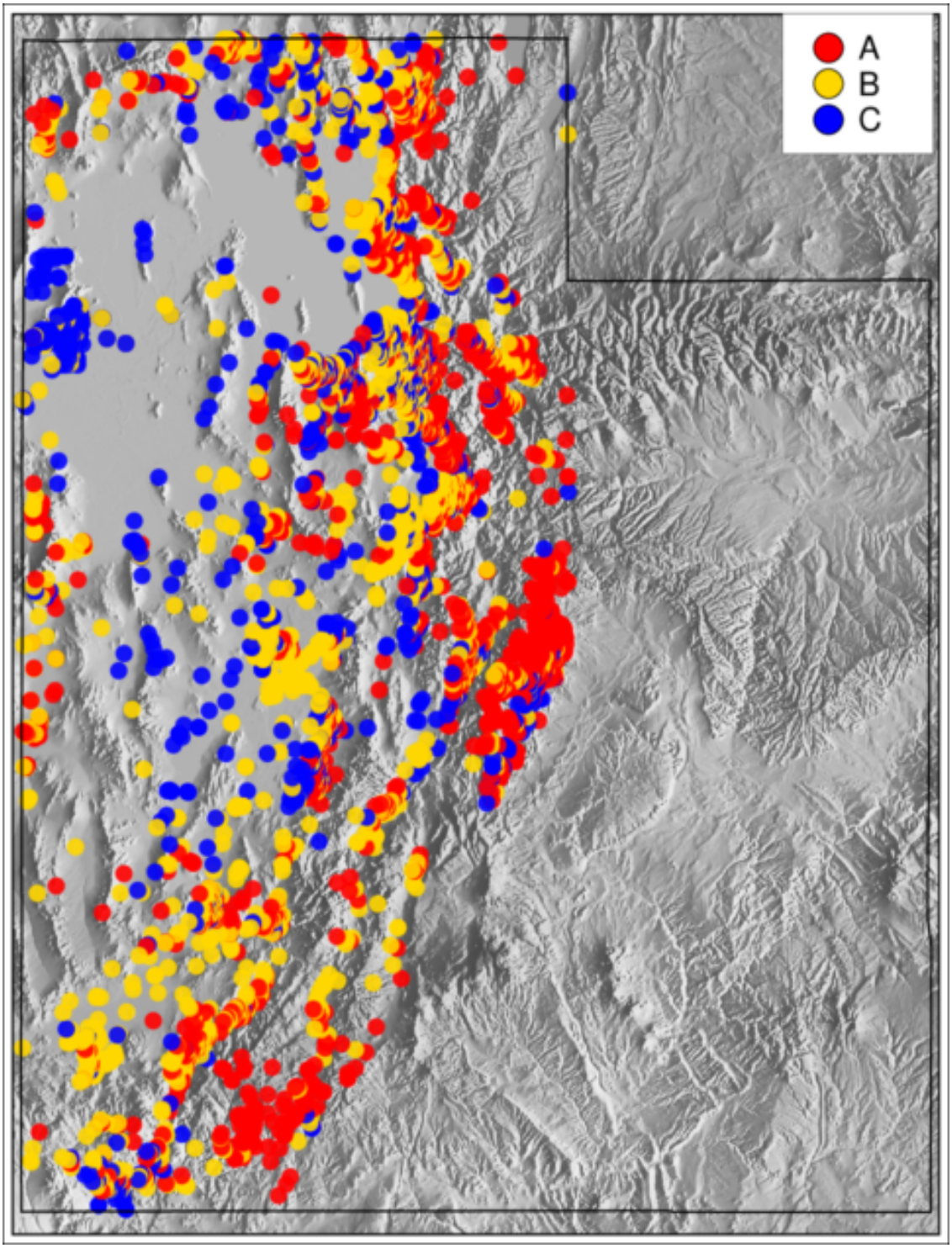
```
10×4 Matrix{Any}:
 4816  -112.863  41.9985  1.0
 4684  -112.352  41.9921  0.609925
 4826  -112.882  41.9907  0.958804
 4735  -112.512  41.9874  0.664952
 4739  -112.534  41.986   0.579875
 4664  -112.304  41.9847  0.60673
 2510  -111.424  41.9844  0.633779
 4830  -112.892  41.9796  0.797651
 4841  -112.916  41.9796  0.849636
 4851  -112.931  41.9794  0.796321

10×4 Matrix{Any}:
```

```
 4330  -112.221  41.298   0.256844
 4336  -112.222  41.301   0.287342
 5047  -113.776  40.7324  0.284777
 1428  -111.769  40.123   0.255764
 1278  -111.732  40.0933  0.261085
 1011  -111.62   40.133   0.263974
 4062  -113.198  38.1853  0.395614
 1436  -111.769  40.1366  0.291657
 1144  -111.698  40.078   0.304277
 2586  -112.063  40.2983  0.244356

10×4 Matrix{Any}:
 4977  -113.607  40.841   0.301232
 4563  -112.277  41.6733  0.340562
 5103  -113.794  40.8641  0.385976
 4801  -113.228  40.8558  0.282822
 4959  -113.581  40.7563  0.417108
 5019  -113.734  40.781   0.555066
 5109  -113.83   40.7844  0.549928
 4909  -113.476  40.7352  0.406015
 4802  -113.228  40.856   0.366626
 5129  -113.888  40.7569  0.523086

Signal A
Signal B
Signal C
```

[25]:
```
GMT.grdimage("utah/maps/utah.nc", shade=(azimuth=100, norm="e0.8"), proj=:
 ↪Mercator,
    color=GMT.makecpt(color=:grayC, transparency=10, range=(0,5000,500),␣
 ↪continuous=true),
    figsize=8, conf=(MAP_FRAME_TYPE="plain",␣
 ↪MAP_GRID_PEN_PRIMARY="thinnest,gray,.", MAP_GRID_CROSS_SIZE_SECONDARY=0.1,␣
 ↪MAP_FRAME_PEN=0.5, MAP_TICK_PEN_PRIMARY=0.1, MAP_TICK_LENGTH_PRIMARY=0.01,␣
 ↪FORMAT_GEO_MAP="ddd", FONT_ANNOT_PRIMARY=0.1, FONT_ANNOT_SECONDARY=0.1),␣
 ↪frame=(axis="lrtb"))
GMT.legend!(box=(pen=false, fill=:white),
            pos=(inside=true, anchor=:T, width=1.30, justify=:CM, offset=(-0.7,␣
 ↪-0.6)),
            GMT.text_record([
                "S 0.10i c 0.10i red  0.25p 0.2i A"
                "S 0.10i c 0.10i gold 0.25p 0.2i B"
                "S 0.10i c 0.10i blue 0.25p 0.2i C"]),
            par=(:FONT_ANNOT_PRIMARY, "8p,Arial"))
GMT.scatter!(ldata[:,2], ldata[:,3], marker=:c, markersize=:0.15,
    color=(:red, :gold, :blue), zcolor=zcolor, alpha=10,
    coast=(proj=:Mercator,
    DCW=(country="US.UT", pen=(0.5,:black))),
```

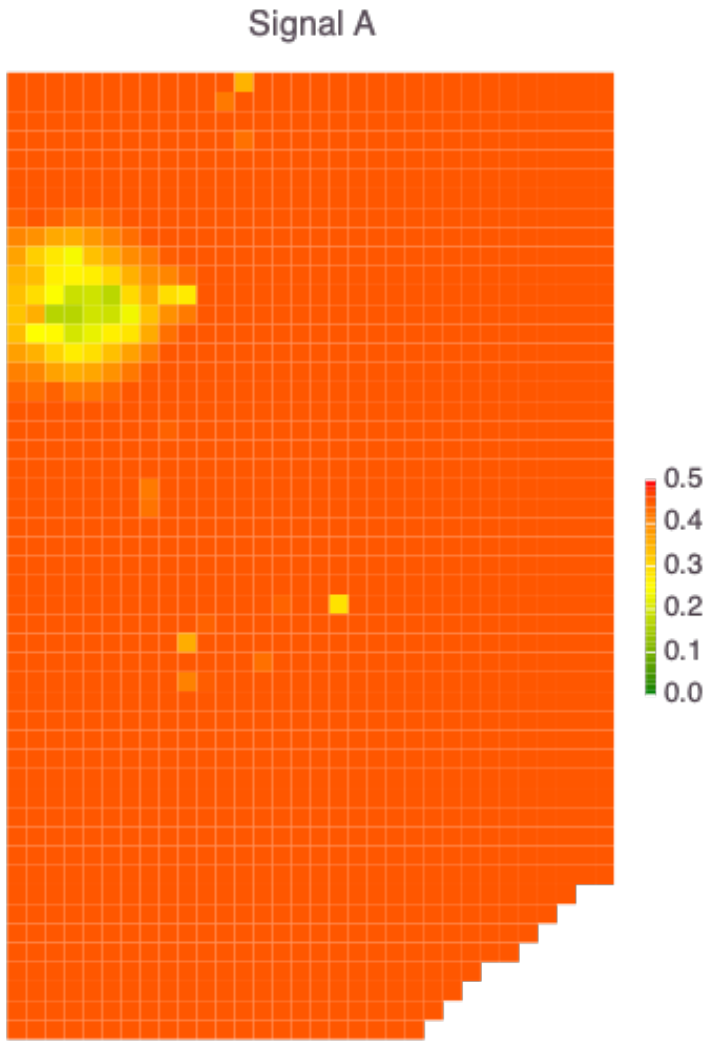
```
    fmt=:png, savefig="utah/maps/signatures-3")
Images.load("utah/maps/signatures-3.png")
```

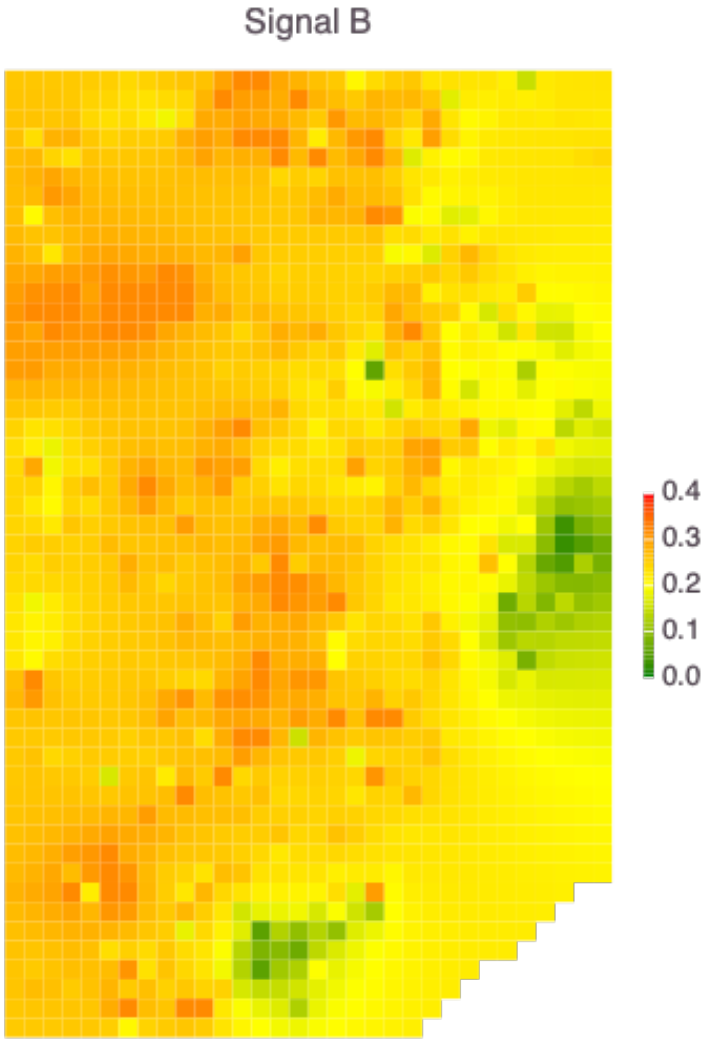
```
pslegend [WARNING]: Representation of font type not recognized. Using default.
```

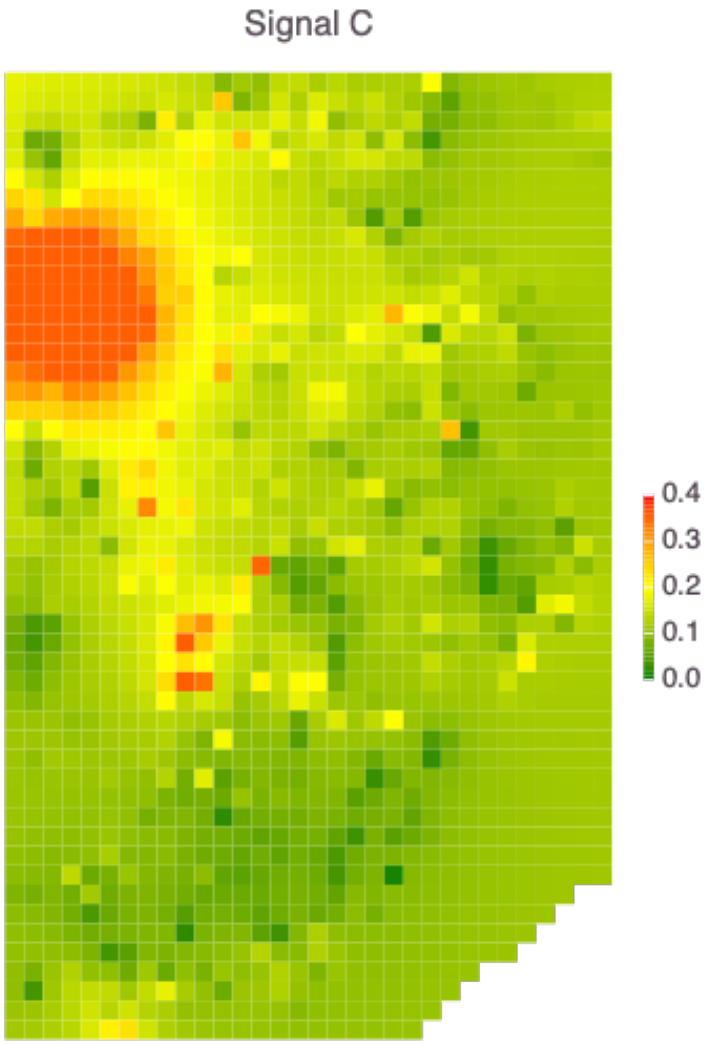


1.18 Spatial distribution of the extracted geothermal features (signals)

[26]:
```
for i in Sorder[1]
        inversedistancefield = Array{Float64}(undef, length(xgrid),␣
↪length(ygrid))
        v = W[kopt][:,i] ./ maximum(W[kopt][:,i])
        iz = .!isnan.(v)
        icoord = coord[:,iz]
        v = v[iz]
        for (i, x) in enumerate(xgrid), (j, y) in enumerate(ygrid)
                        inversedistancefield[i, j] = Kriging.
↪inversedistance(permutedims([x y]), icoord, v, 2; cutoff=1000)[1]
        end
        imax = NMFk.maximumnan(inversedistancefield)
        imin = NMFk.minimumnan(inversedistancefield)
        NMFk.plotmatrix(rotl90(inversedistancefield); quiet=false,␣
↪filename="utah/maps/Signal_$(signallabels[i])_map_inversedistance_prediction.
↪png", title="Signal $(signallabels[i])", maxvalue=imin + (imax - imin)/ 2)
end
```


Signal A
0.5
0.4
0.3
0.2
0.1
0.0


Signal B
0.4
0.3
0.2
0.1
0.0

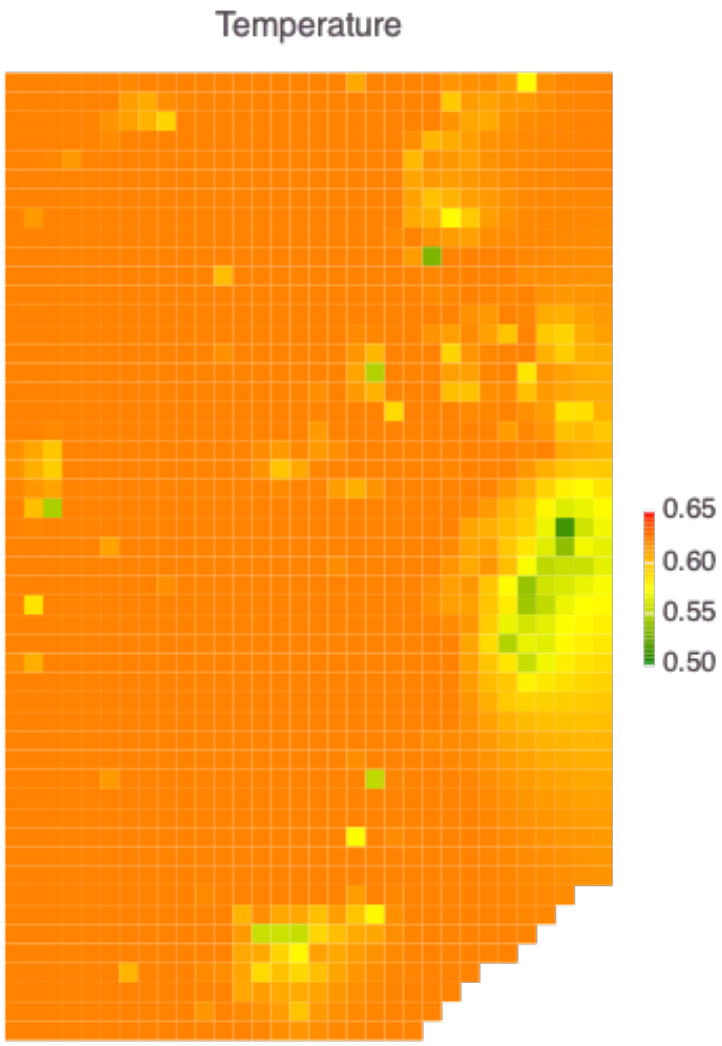


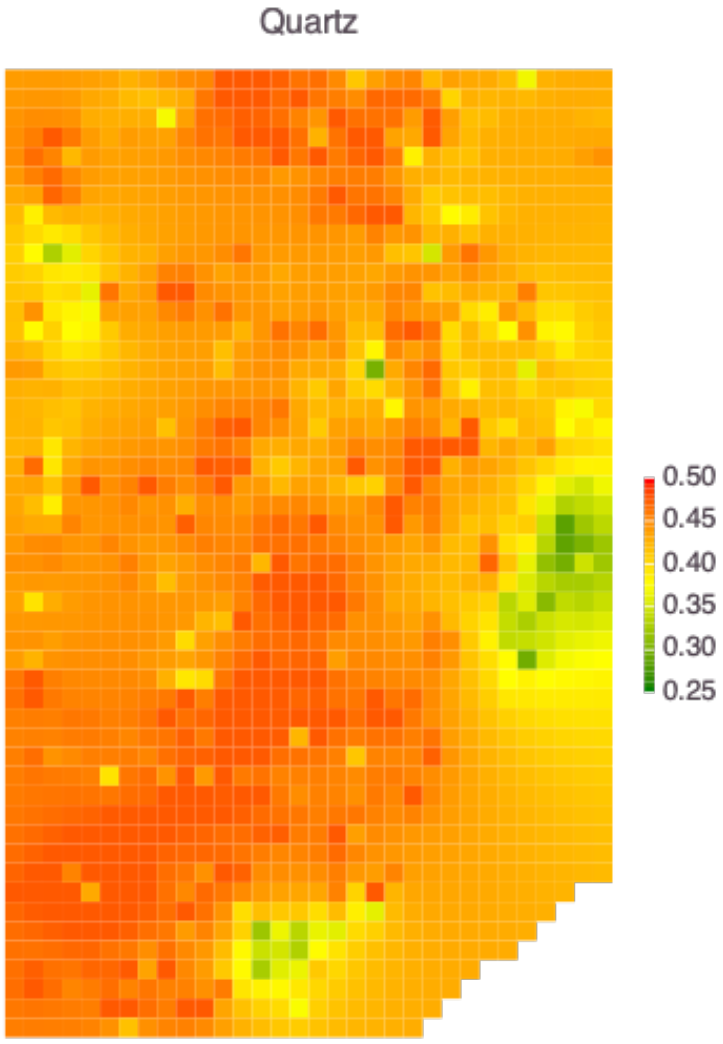
1.19 Map of NMFk predicted geothermal attributes

Our ML "fills in" the gaps in our knowledge:

[27]:
```
Xe = W[kopt]  * H[kopt]

for i = 1:nattributes
                inversedistancefield = Array{Float64}(undef, length(xgrid),␣
↪length(ygrid))
                v = Xe[:,i]
                iz = .!isnan.(v)
```

```
                icoord = coord[:,iz]
                v = v[iz]
                for (i, x) in enumerate(xgrid), (j, y) in enumerate(ygrid)
                                inversedistancefield[i, j] = Kriging.
 ↪inversedistance(permutedims([x y]), icoord, v, 2; cutoff=1000)[1]
                end
                imax = NMFk.maximumnan(inversedistancefield)
                imin = NMFk.minimumnan(inversedistancefield)
                NMFk.plotmatrix(rotl90(inversedistancefield); quiet=false,␣
 ↪filename="utah/maps/
 ↪Attribute_$(attributes[i])_map_inversedistance_prediction.png",␣
 ↪title="$(attributes[i])", maxvalue=imin + (imax - imin)/ 2)
end
```




Quartz
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0.35
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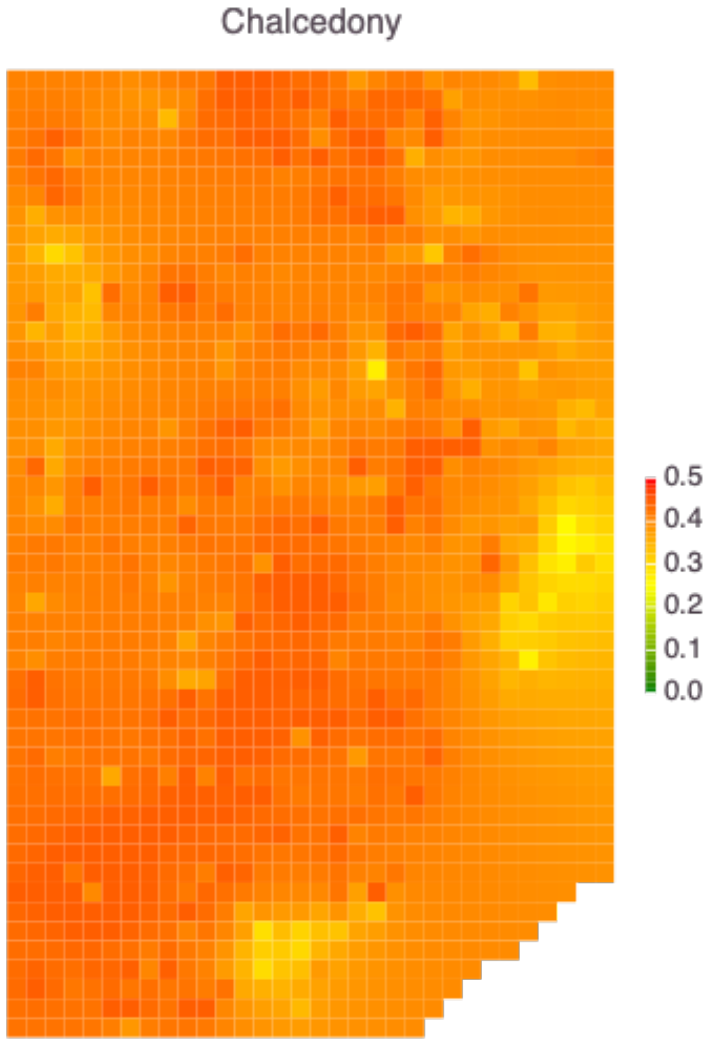
0.25


Chalcedony
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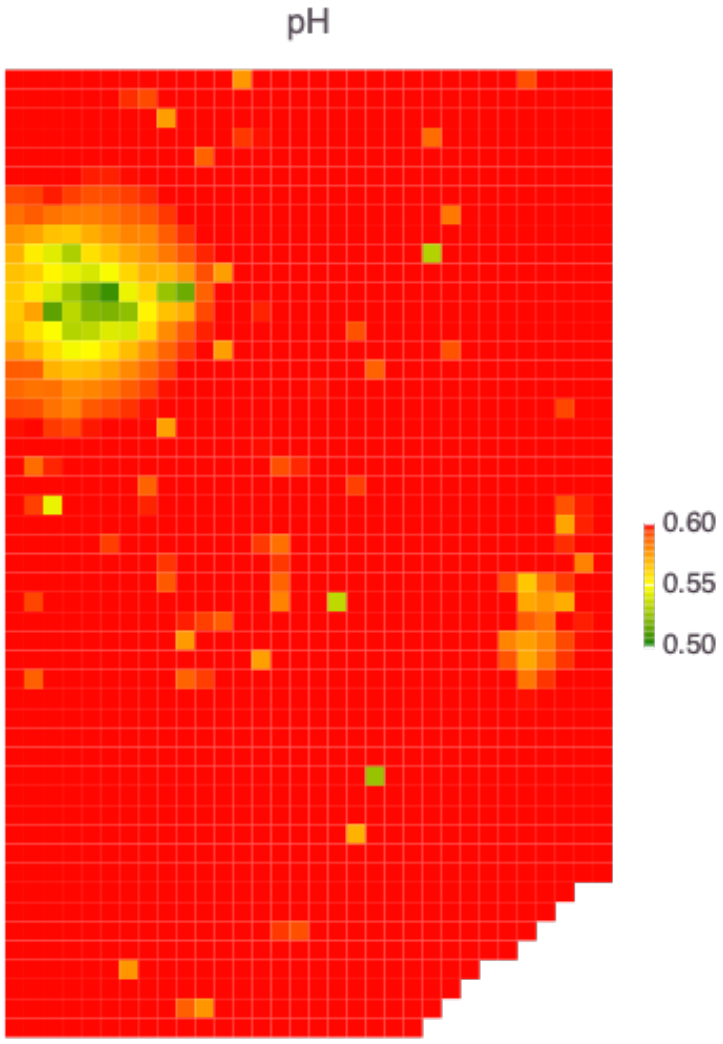
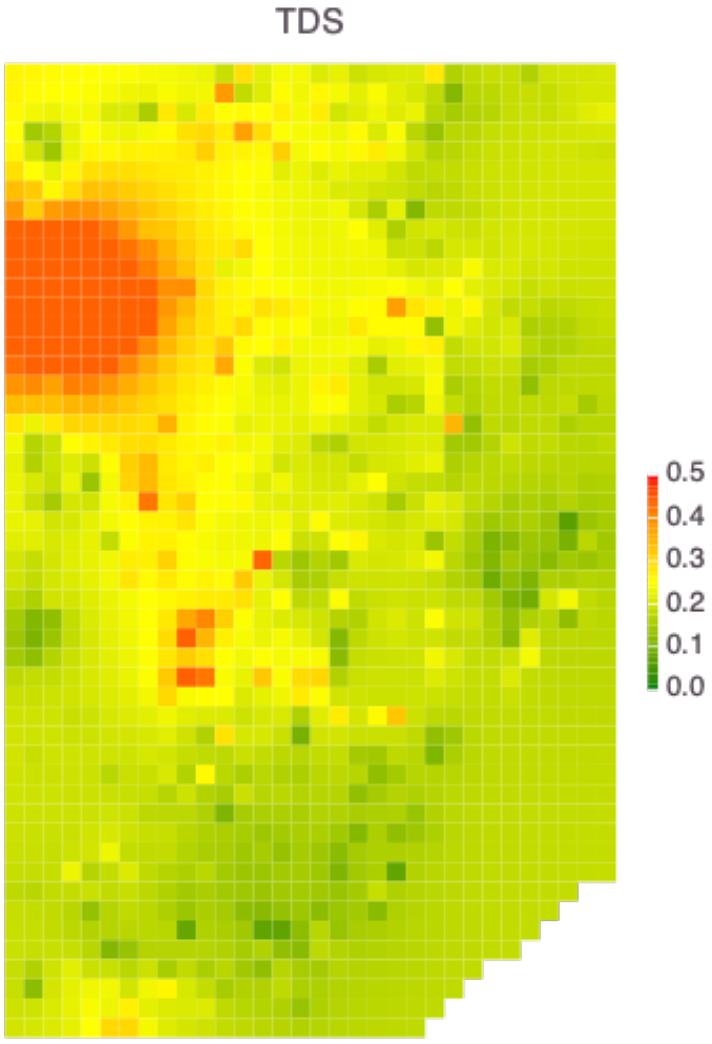
0.0


pH
0.60
0.55
0.50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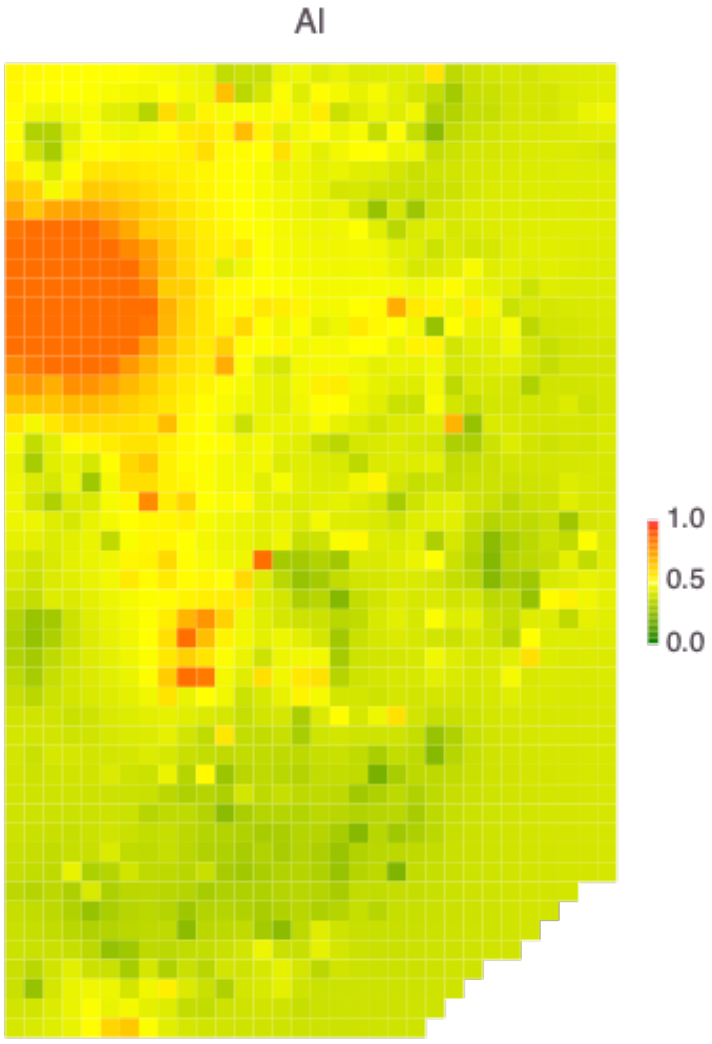
0.0


Al
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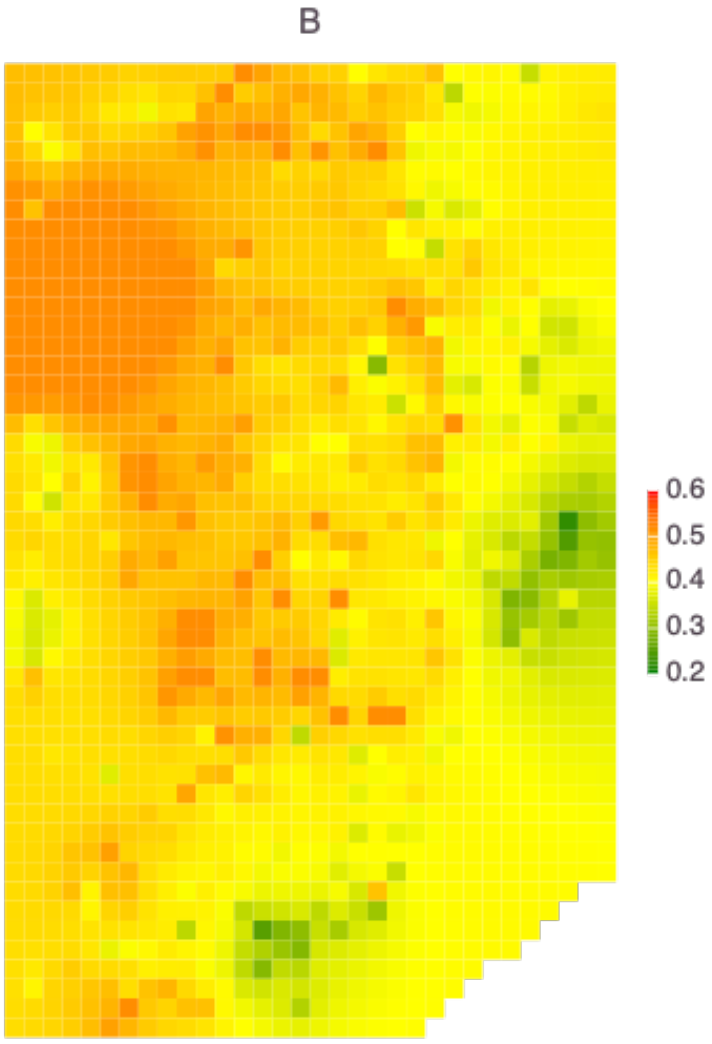
0.5
0.0


B
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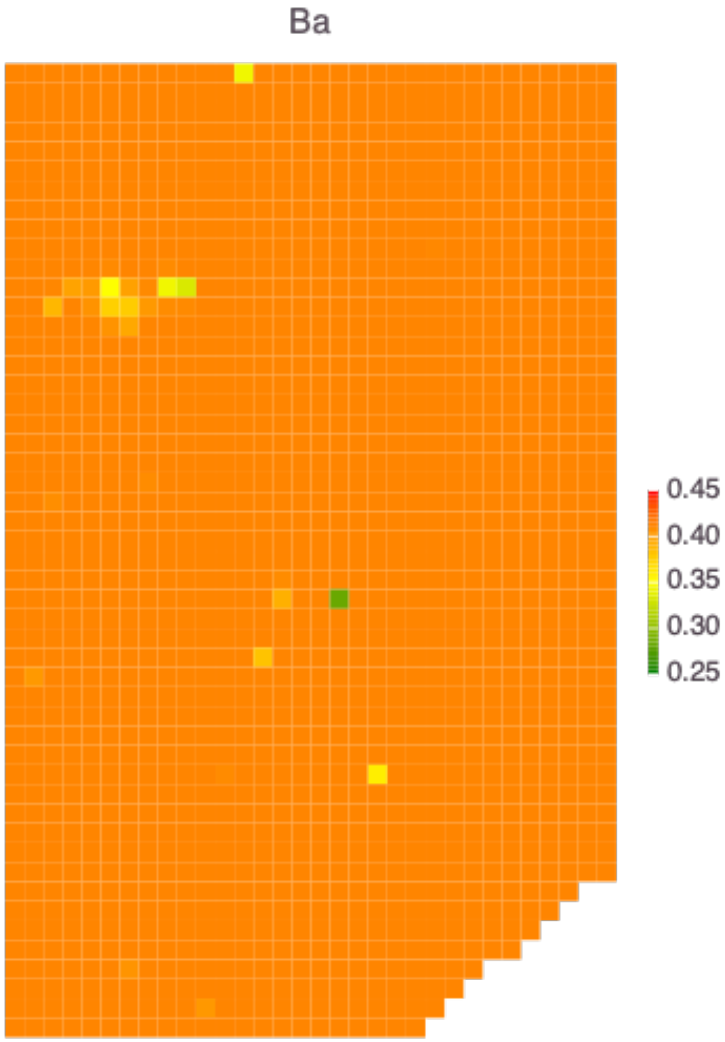
0.5
0.4
0.3
0.2


Ba
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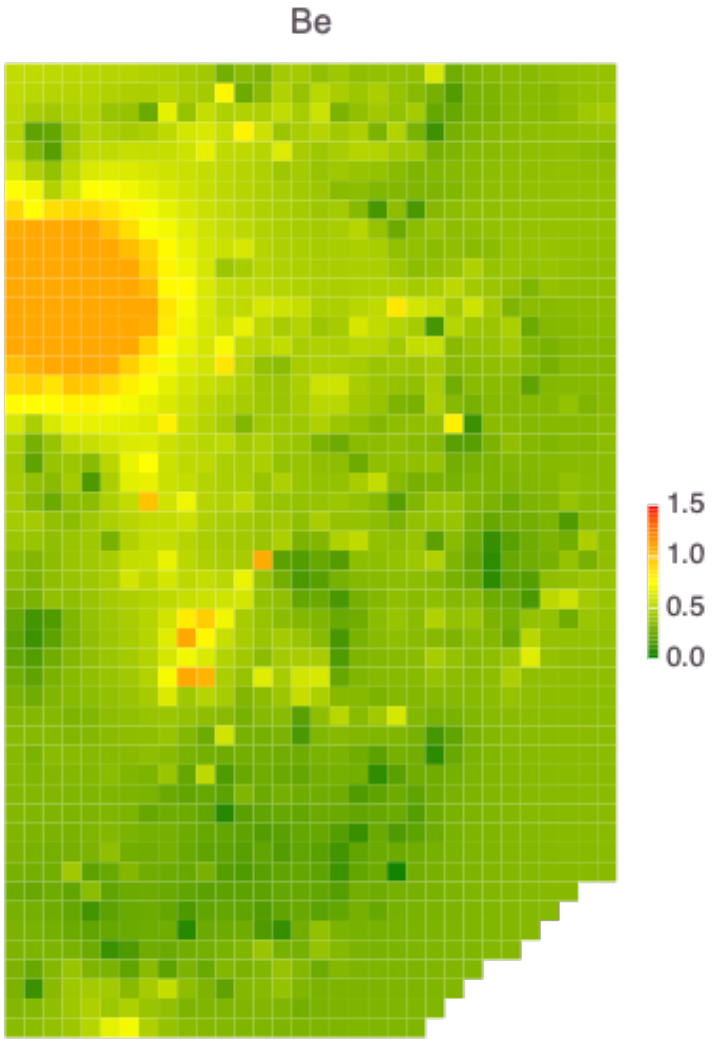
0.25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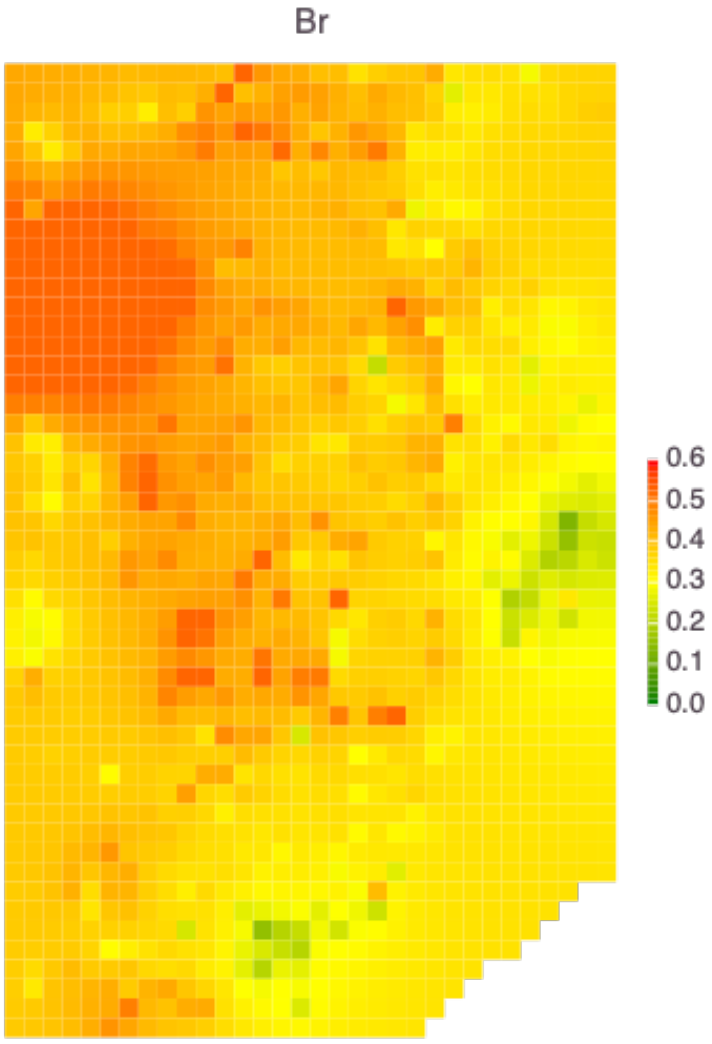
0.5
0.0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0.4
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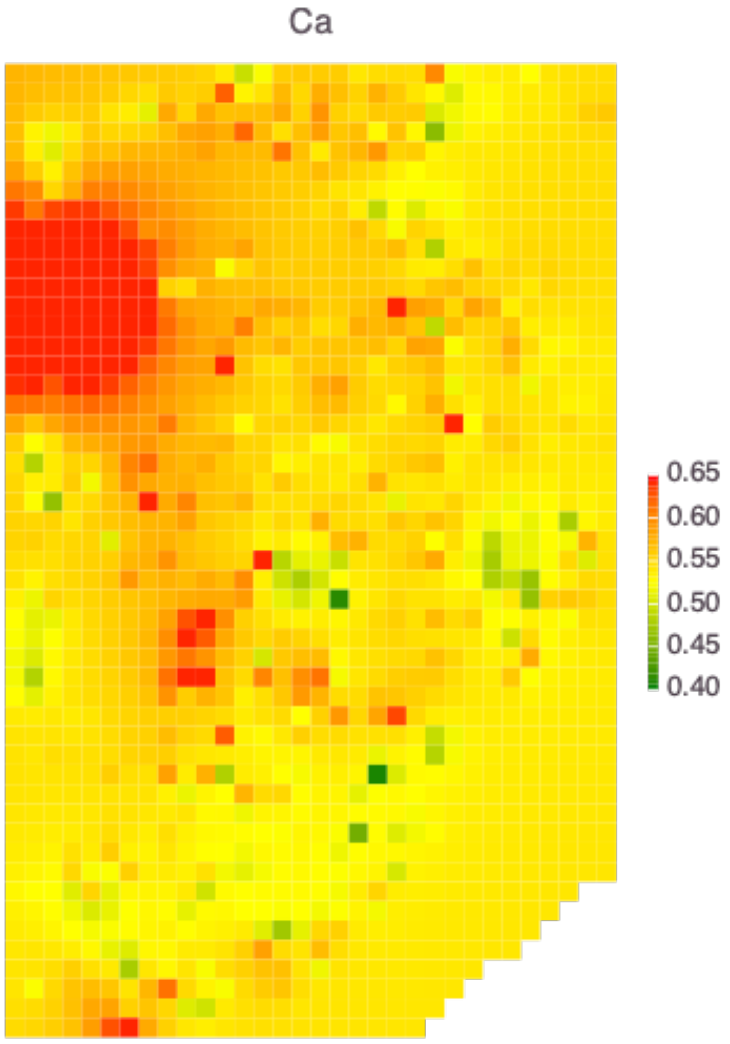
0.2
0.1
0.0


Ca
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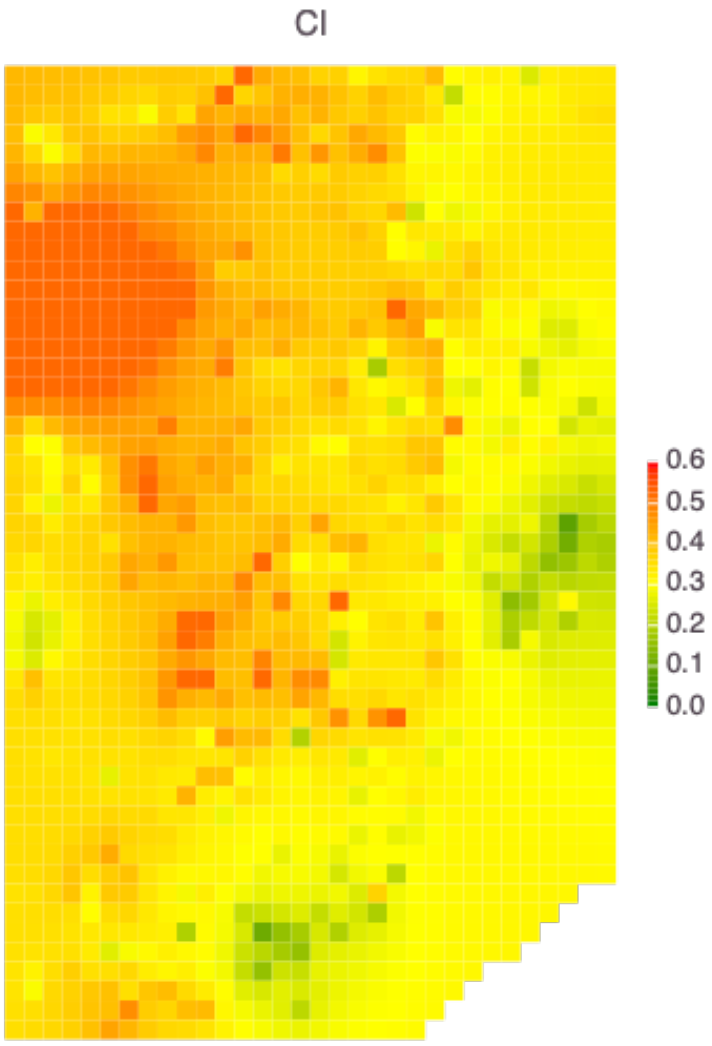
0.40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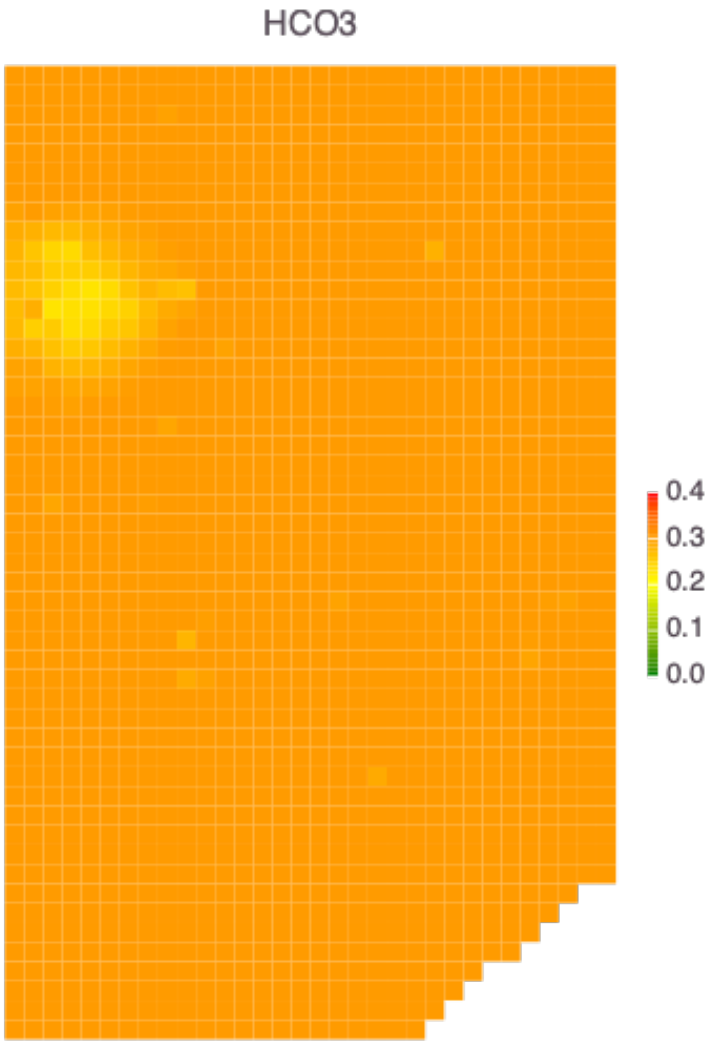
HCO3
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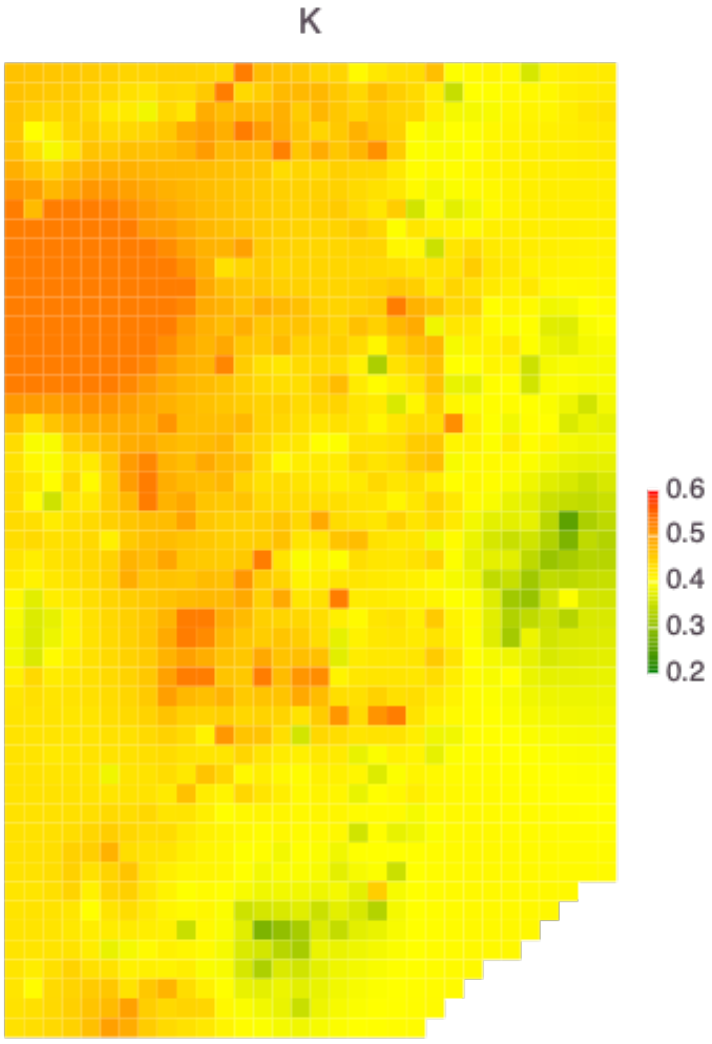
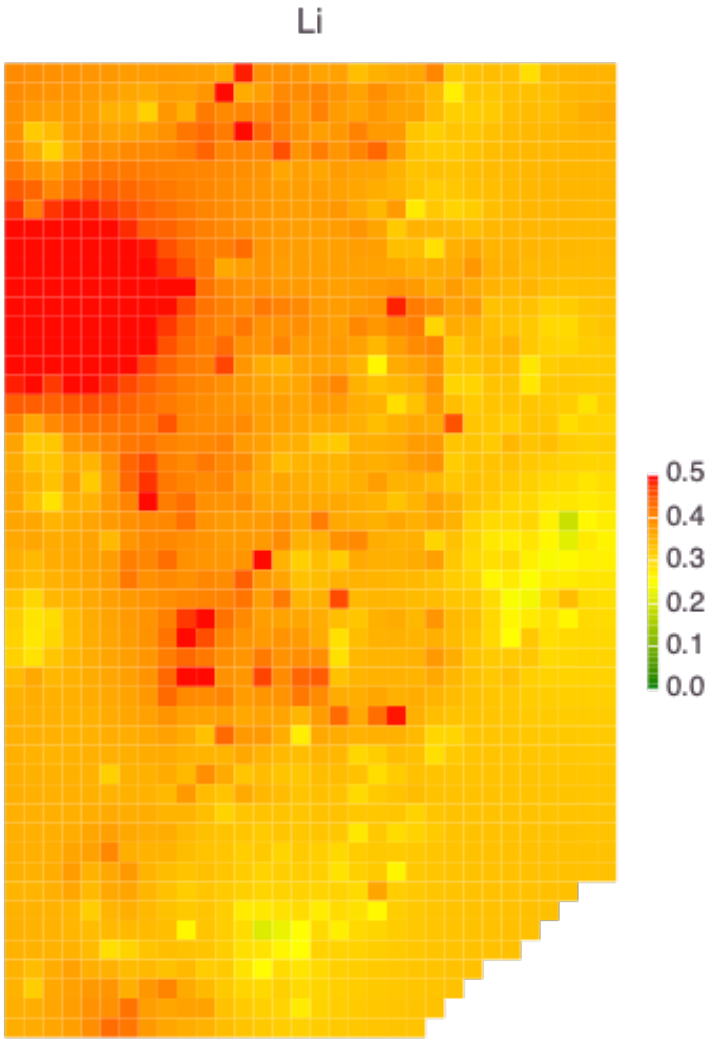
0.1
0.0


K
0.6
0.5
0.4
0.3
0.2


Li
0.5
0.4
0.3
0.2
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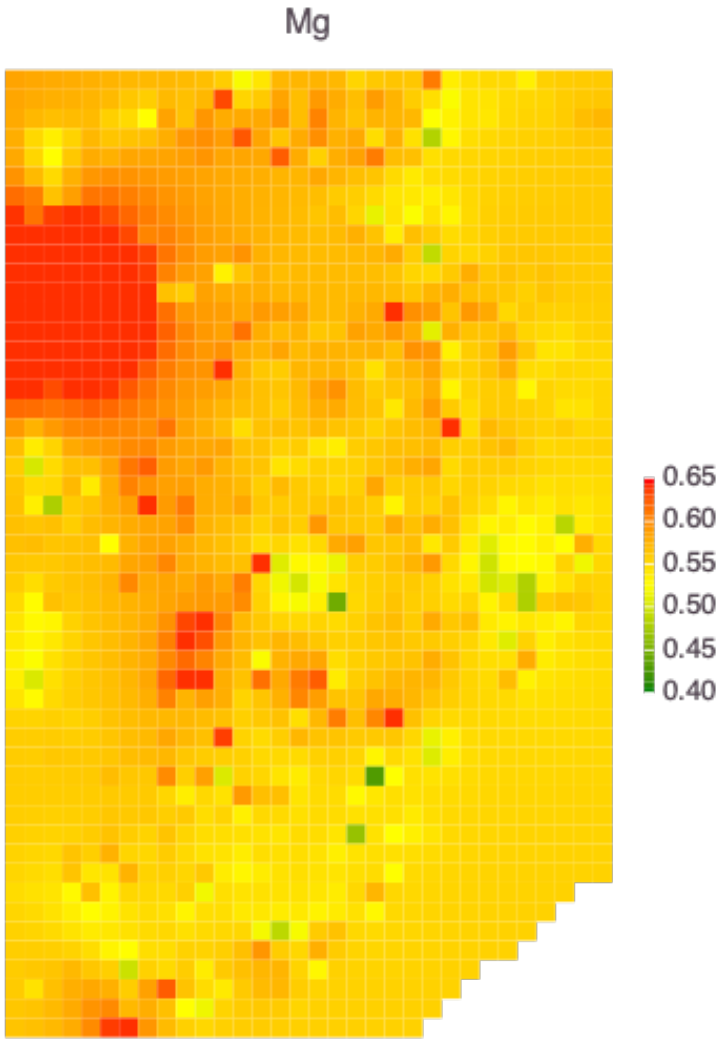
Mg
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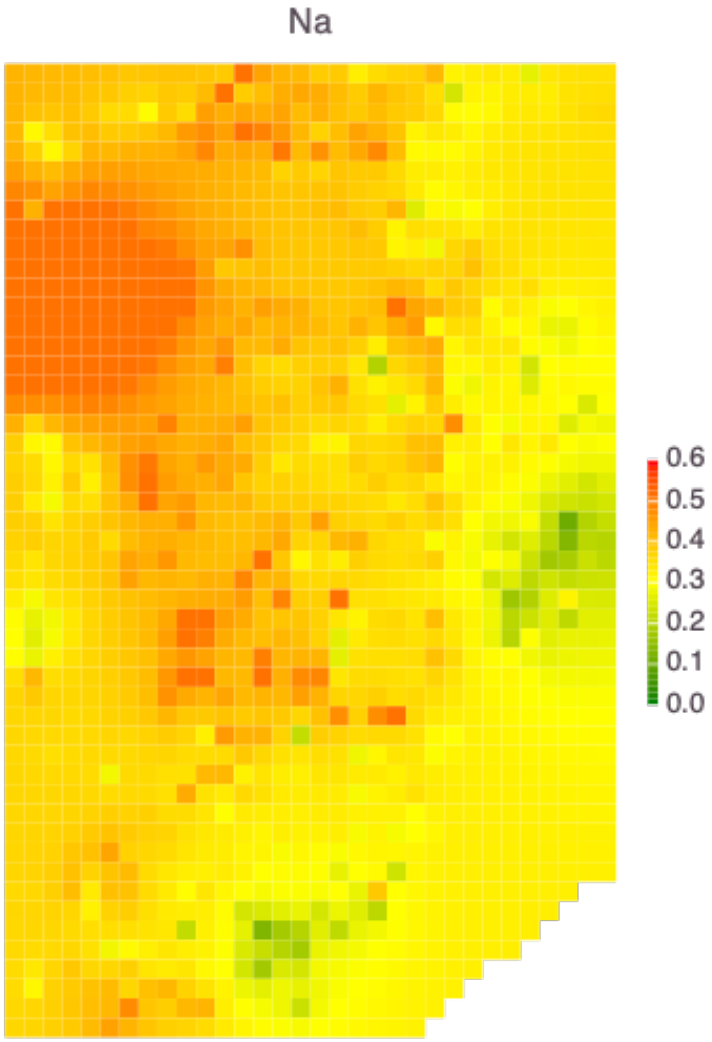
0.55
0.50
0.45
0.40


Na
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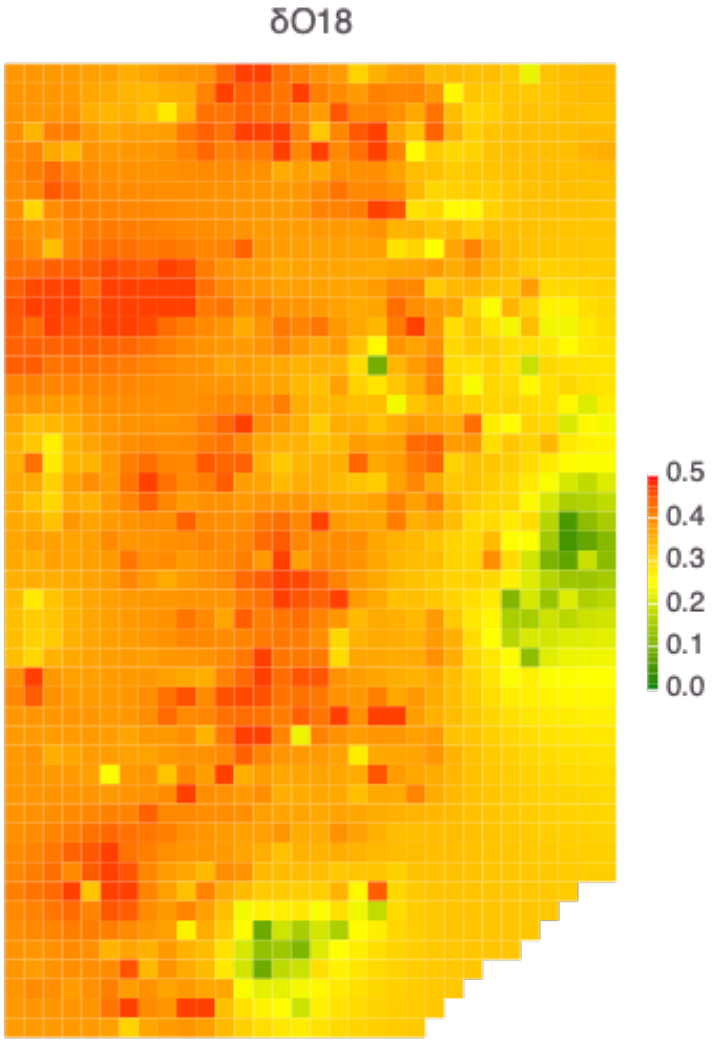
0.4
0.3
0.2
0.1
0.0


δO18
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0.2
0.1
0.0