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
```

```
Info: TensorLy is available
@ NTFk /Users/vvv/.julia/dev/NTFk/src/NTFkTensorly.jl:8
```

1.2 Load data

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

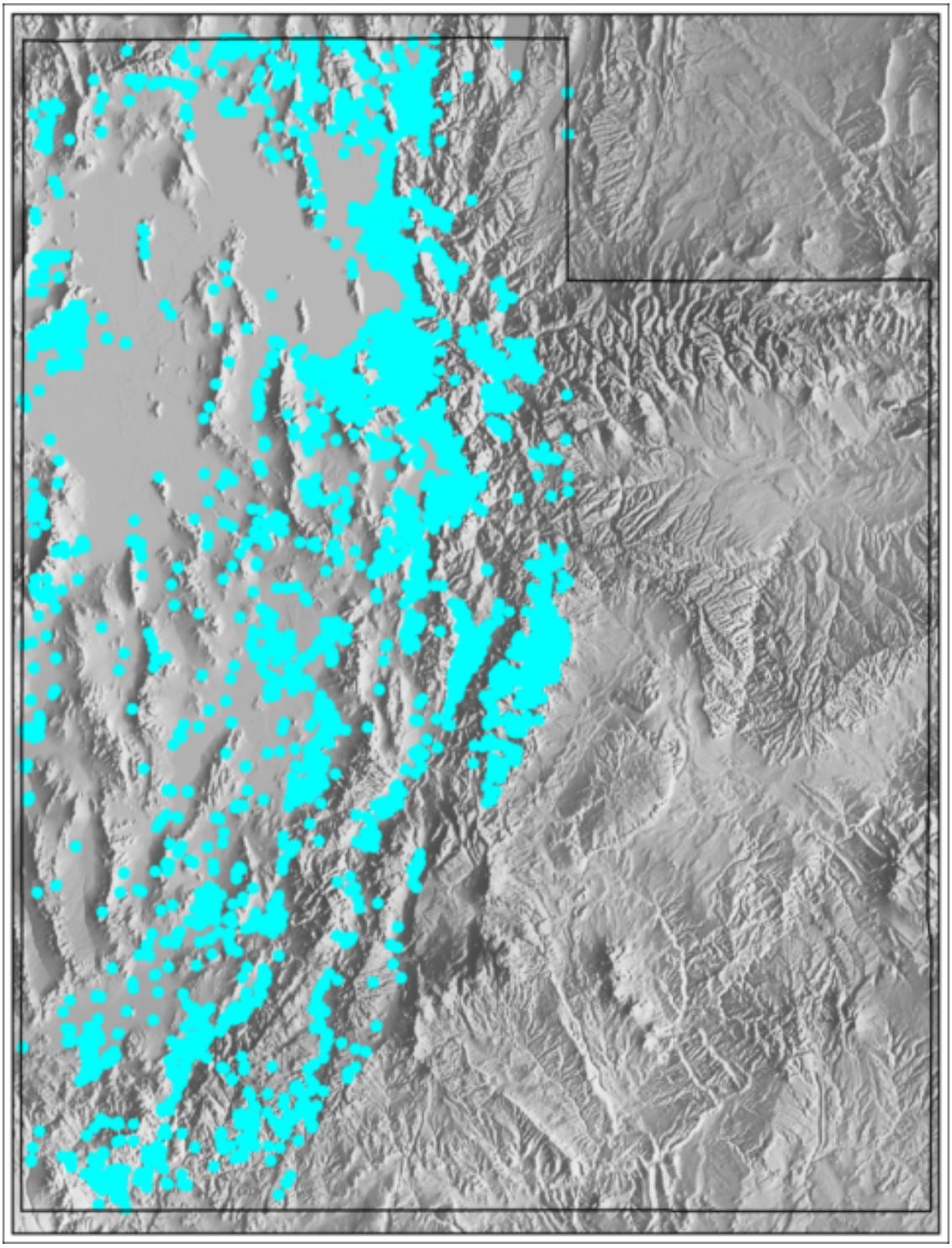
Set coordinates:

[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;
```

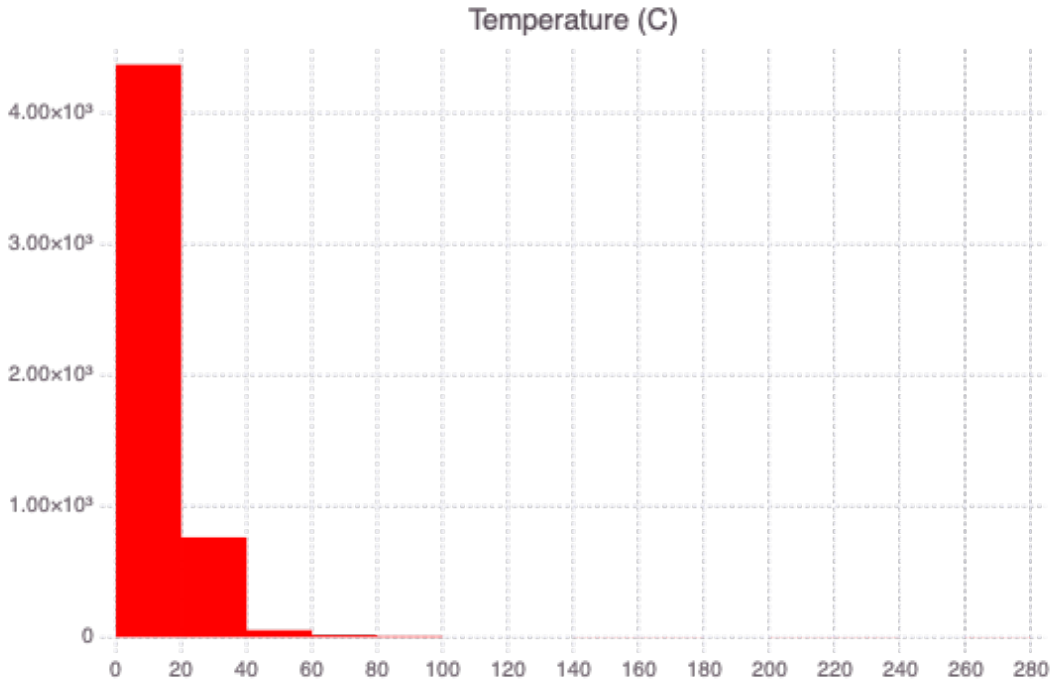
Set variables for the number of attributes and points:

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

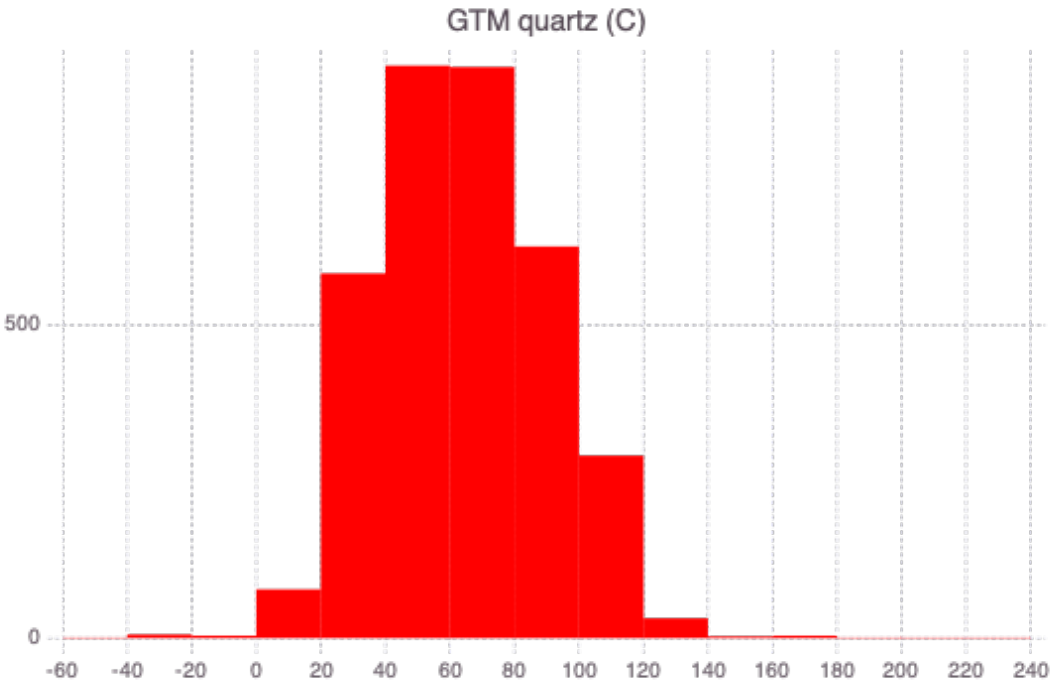
```
5218
```

Plot histograms and compute data statistics:

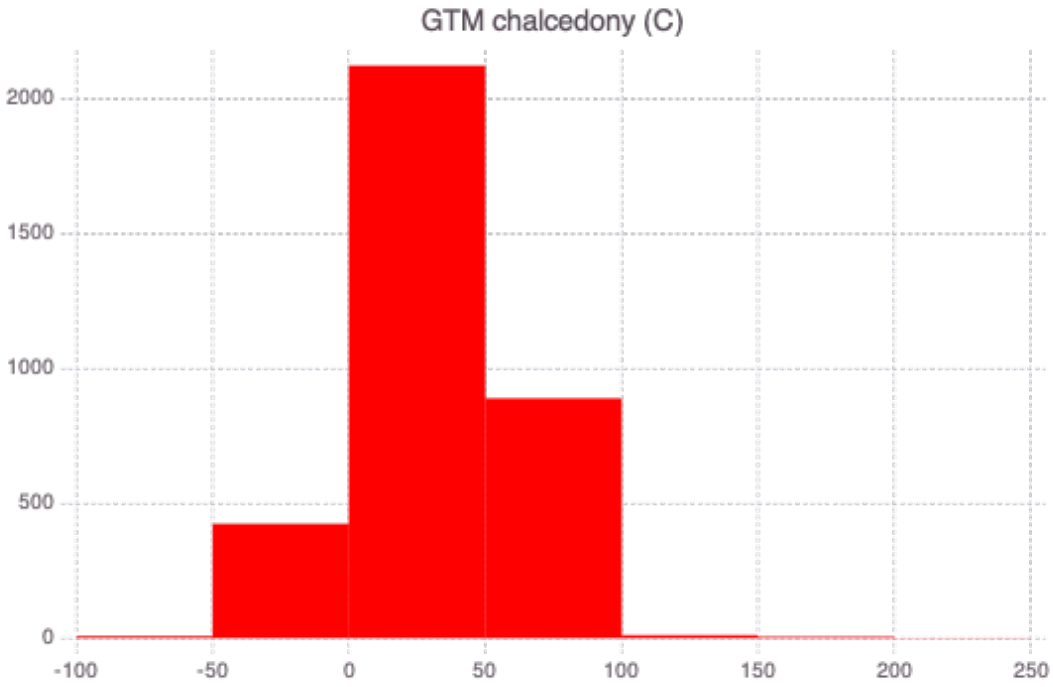
[10]:
```
NMFk.datanalytics(X, attributes_long; dims=2);
```



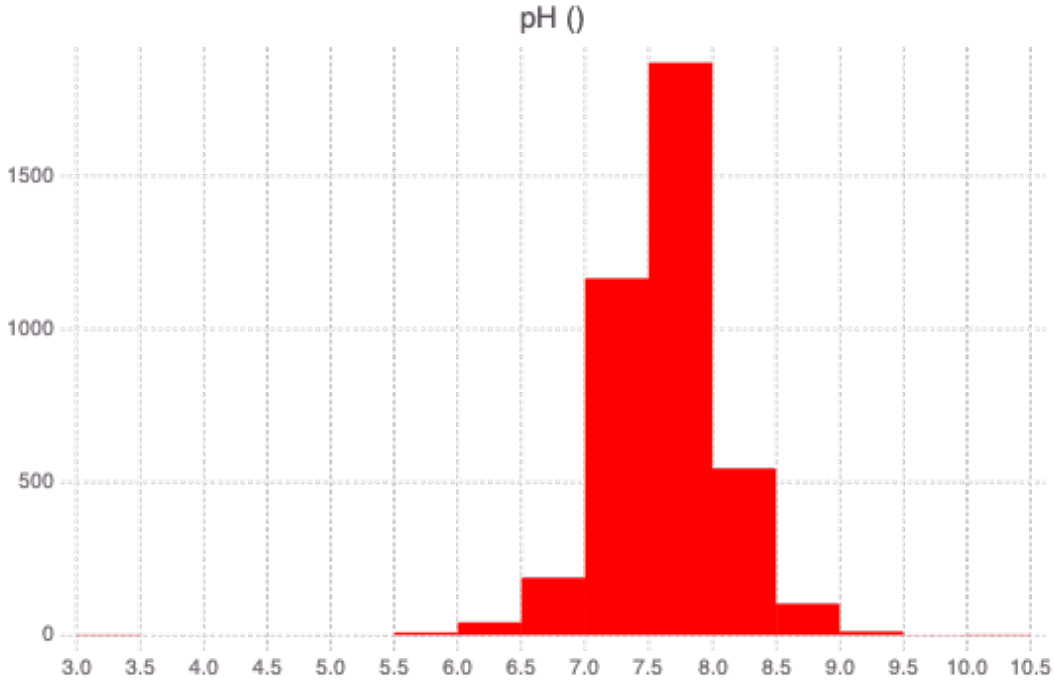

```
Info: Temperature (C)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



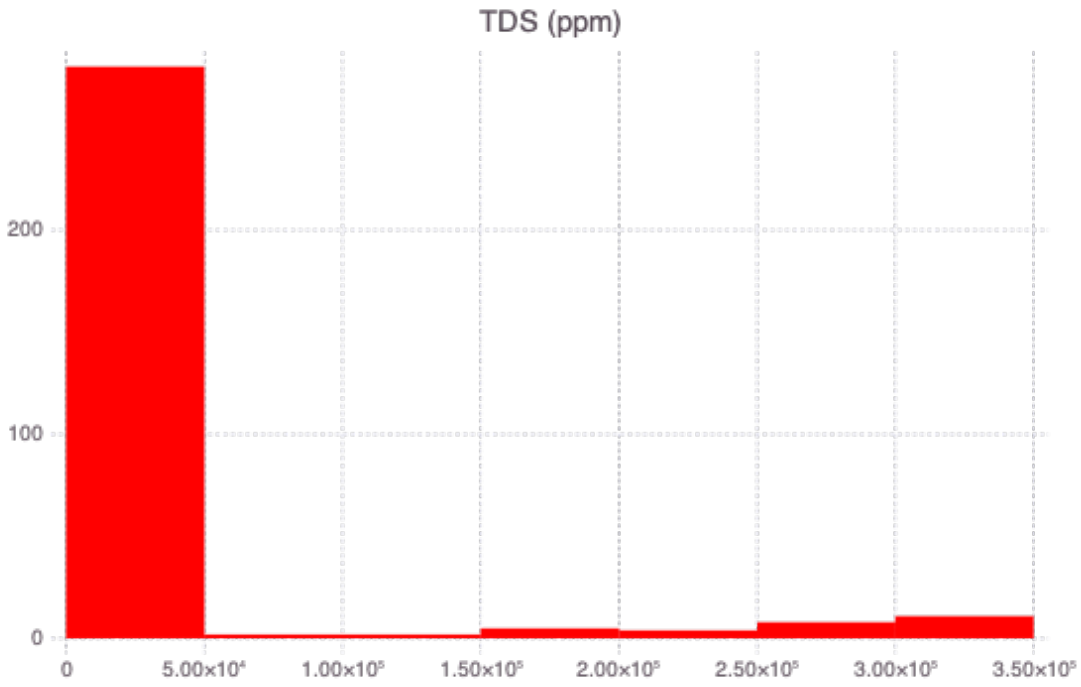
```
Temperature (C): Min 0.1 Max 261.0 StdDev 9.497179 Skewness 10.095466 Count 5214
  Info: GTM quartz (C)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



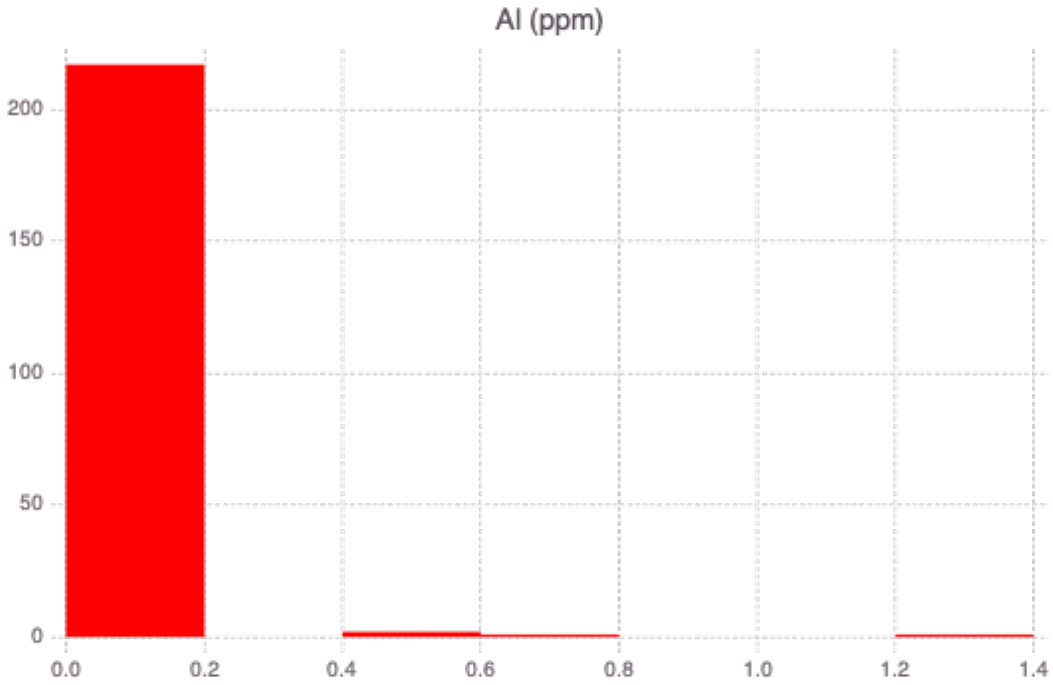

```
GTM quartz (C): Min -50.870045 Max 222.28357 StdDev 26.329222 Skewness
0.24256101 Count 3460
  Info: GTM chalcedony (C)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



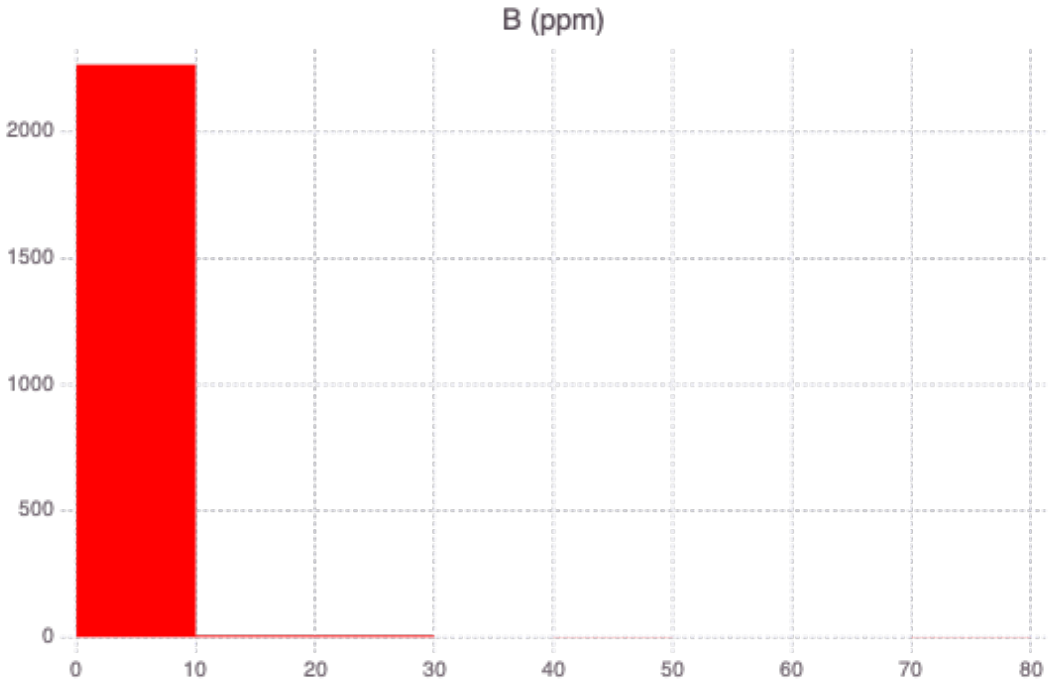

```
GTM chalcedony (C): Min -81.64773 Max 208.67426 StdDev 27.450817 Skewness
0.3369881 Count 3460
  Info: pH ()
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



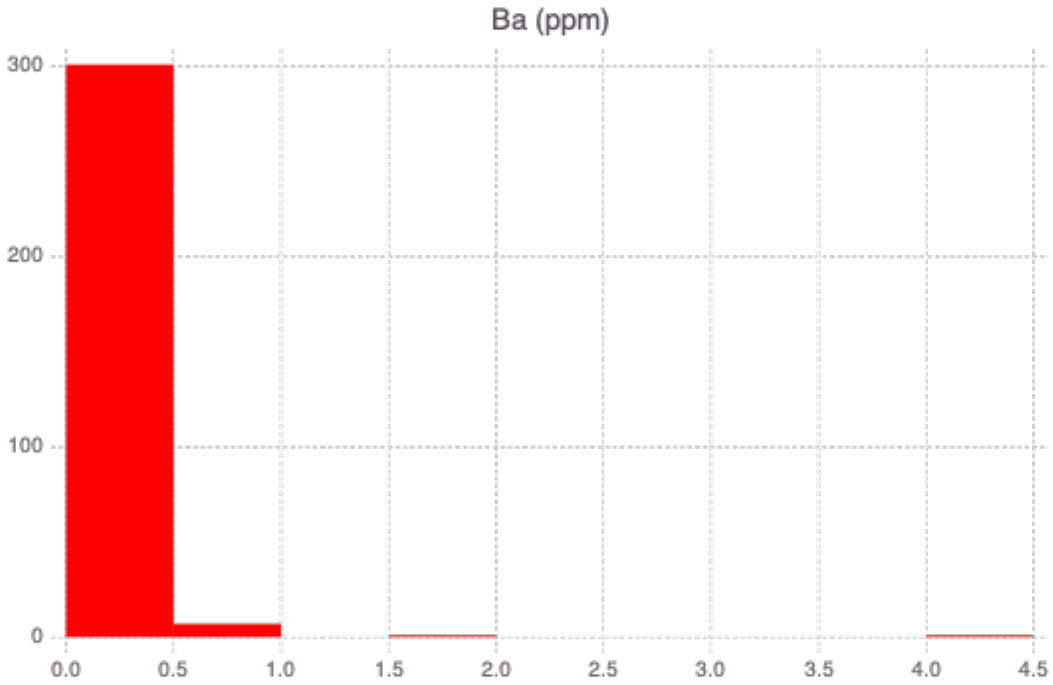

```
pH (): Min 3.4 Max 10.2 StdDev 0.44822767 Skewness -0.45681924 Count 3941
  Info: TDS (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



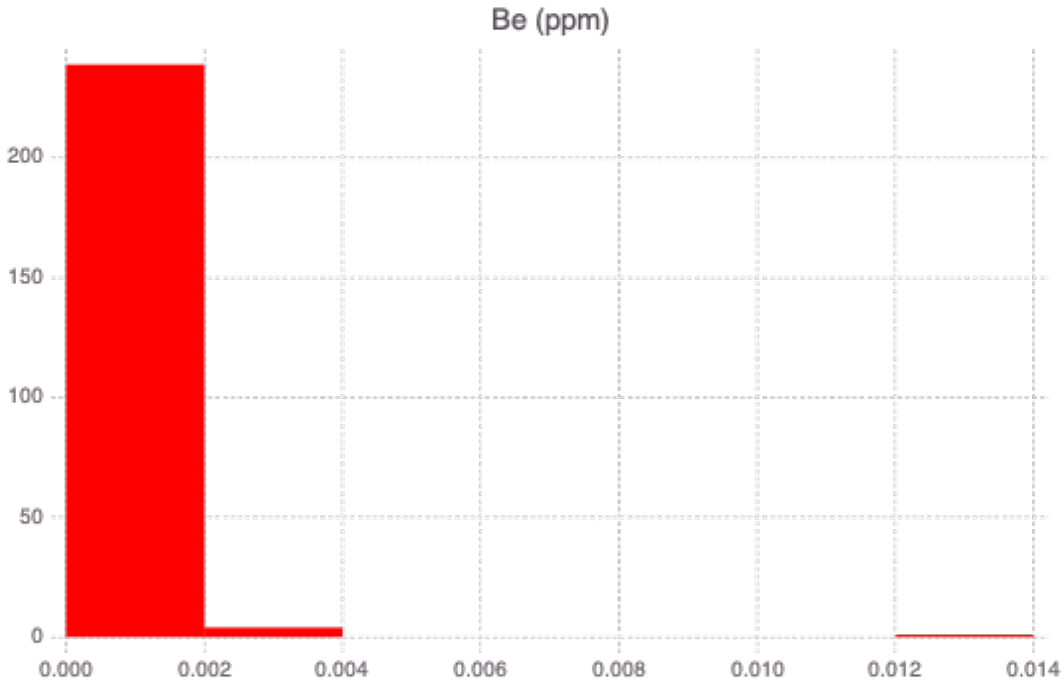

```
TDS (ppm): Min 122.0 Max 329000.0 StdDev 78777.95 Skewness 2.9479313 Count 312
  Info: Al (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



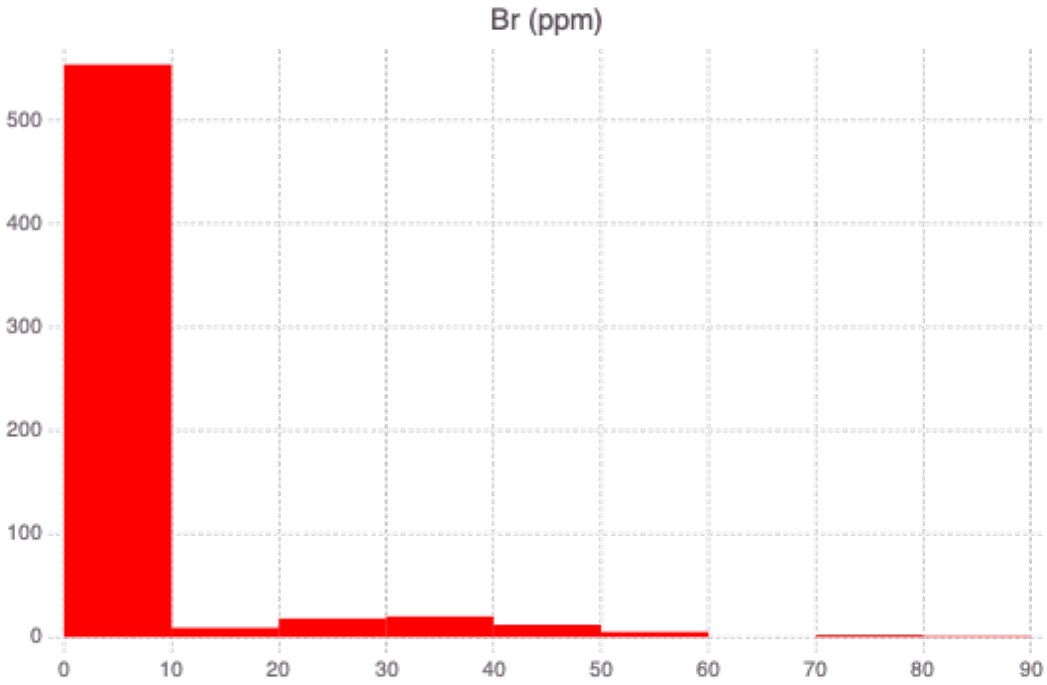

```
Al (ppm): Min 0.0 Max 1.251 StdDev 0.10527698 Skewness 9.031239 Count 221
  Info: B (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



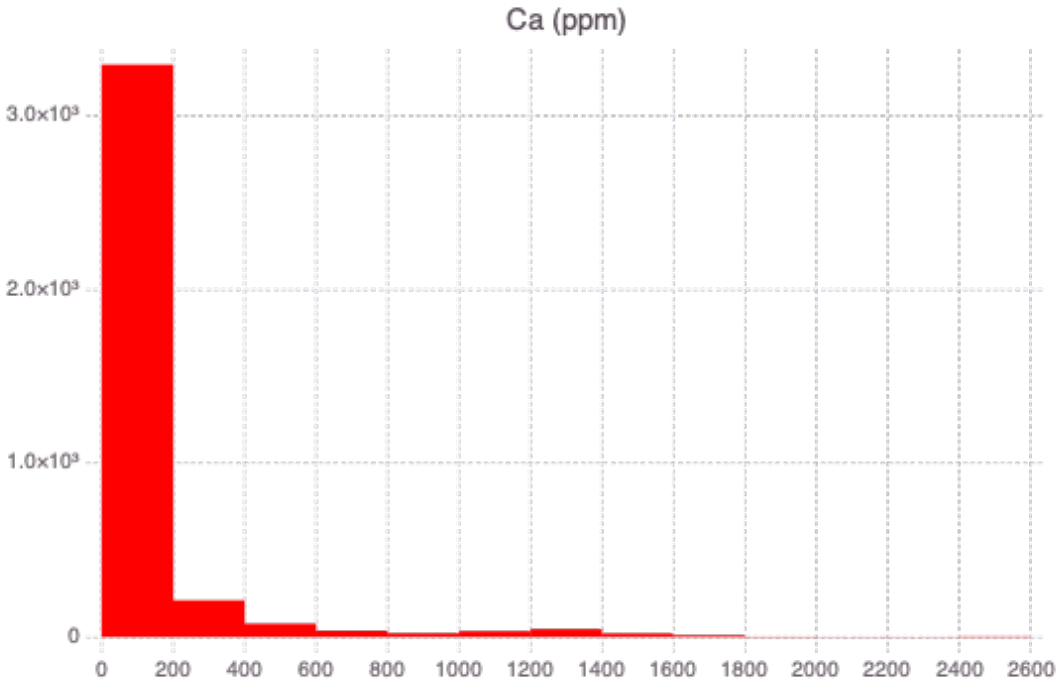

```
B (ppm): Min 0.0 Max 76.5 StdDev 2.6950865 Skewness 15.190172 Count 2284
  Info: Ba (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



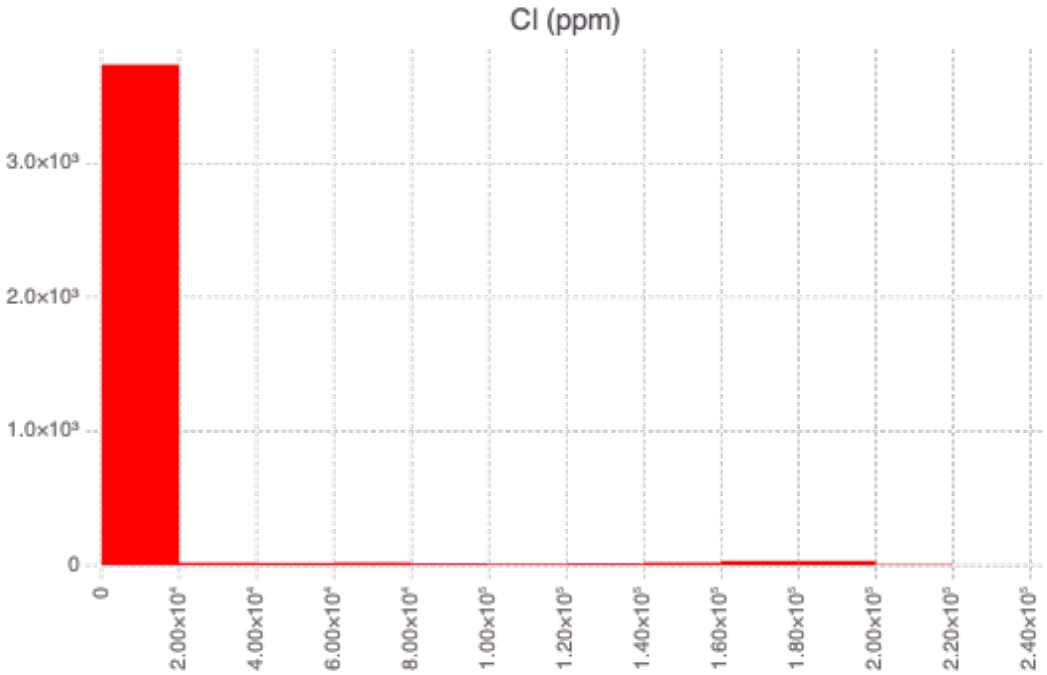

```
Ba (ppm): Min 0.002 Max 4.5 StdDev 0.2898333 Skewness 11.825817 Count 310
  Info: Be (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



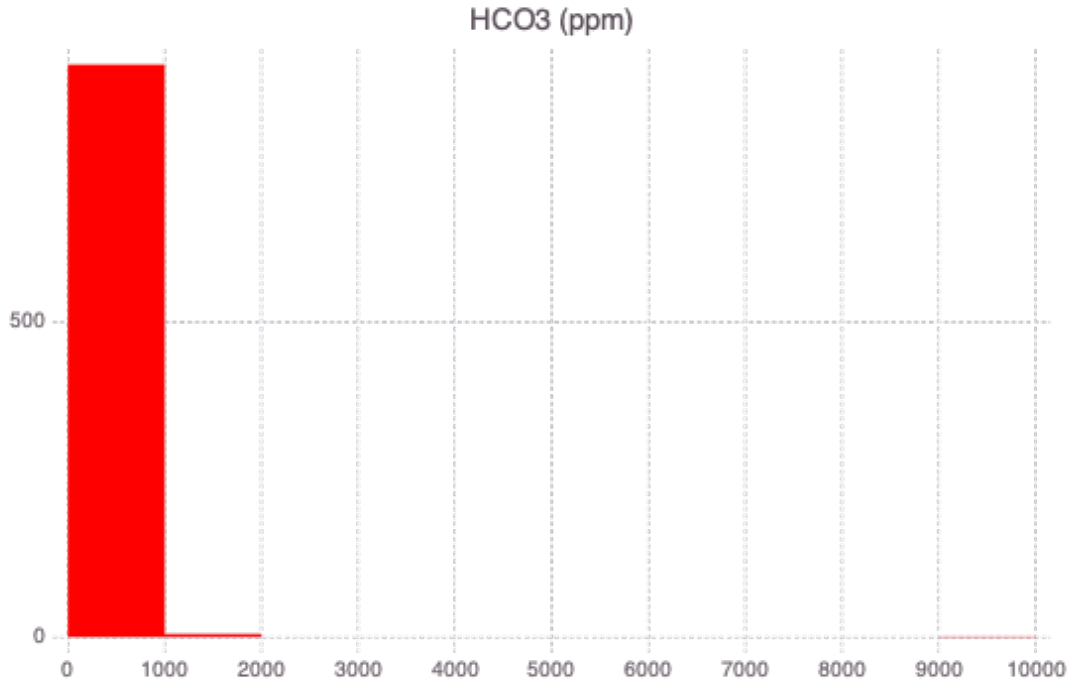

```
Be (ppm): Min 5.3333333e-5 Max 0.013 StdDev 0.00089295243 Skewness 10.968073
Count 244
  Info: Br (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



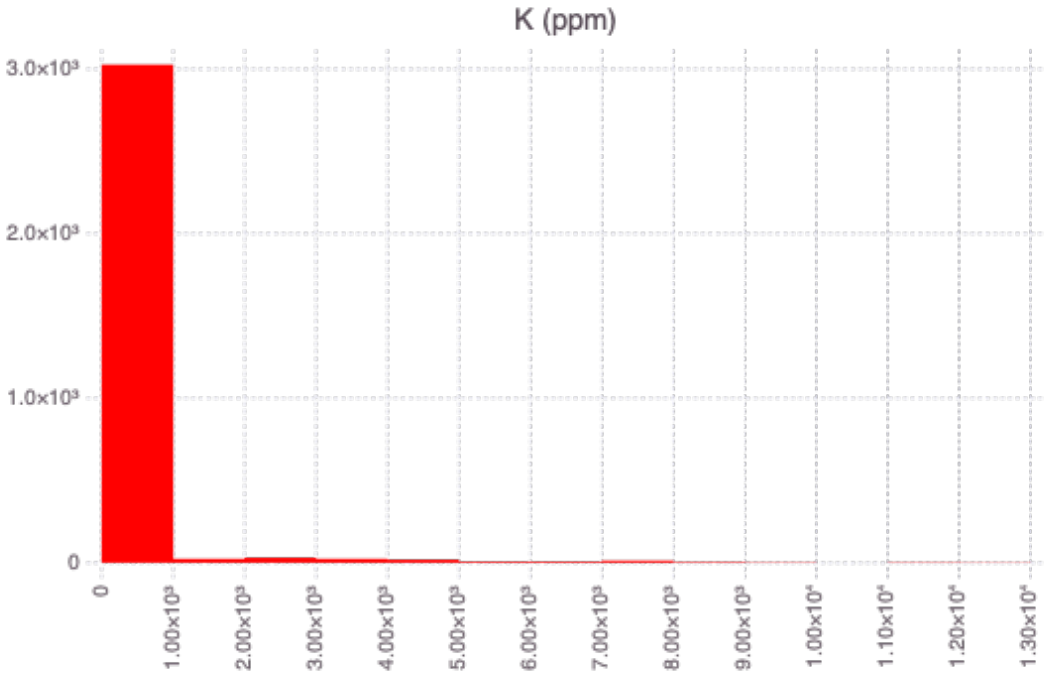

```
Br (ppm): Min 0.0 Max 84.0 StdDev 11.680384 Skewness 3.435088 Count 621
  Info: Ca (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

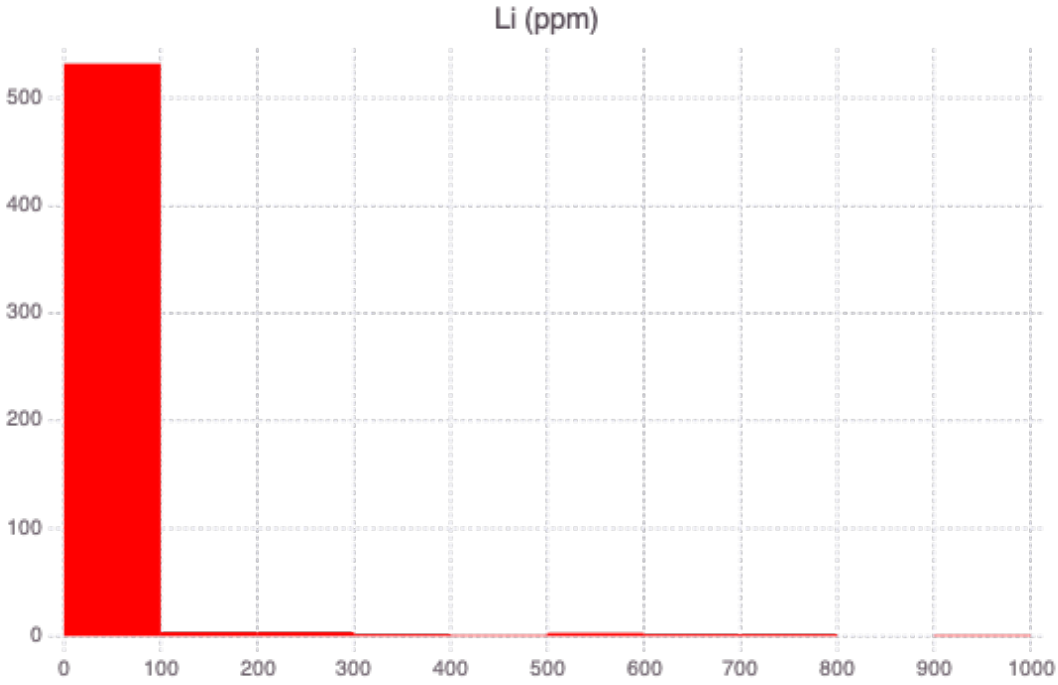


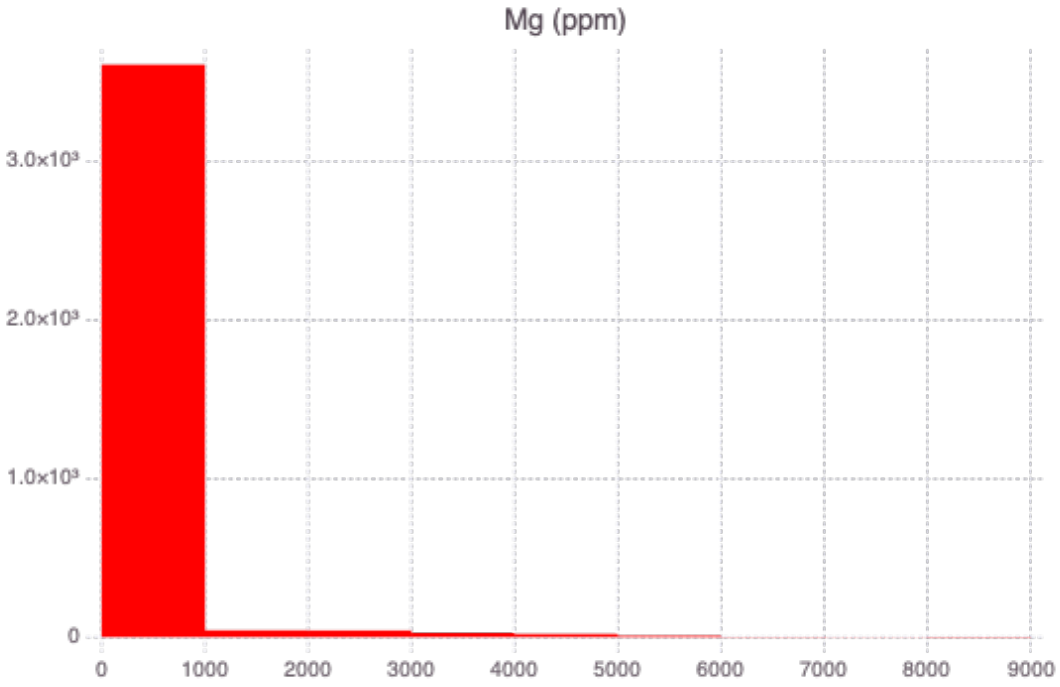

```
Ca (ppm): Min 0.6 Max 2566.6667 StdDev 262.82578 Skewness 4.424904 Count 3772
  Info: Cl (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```



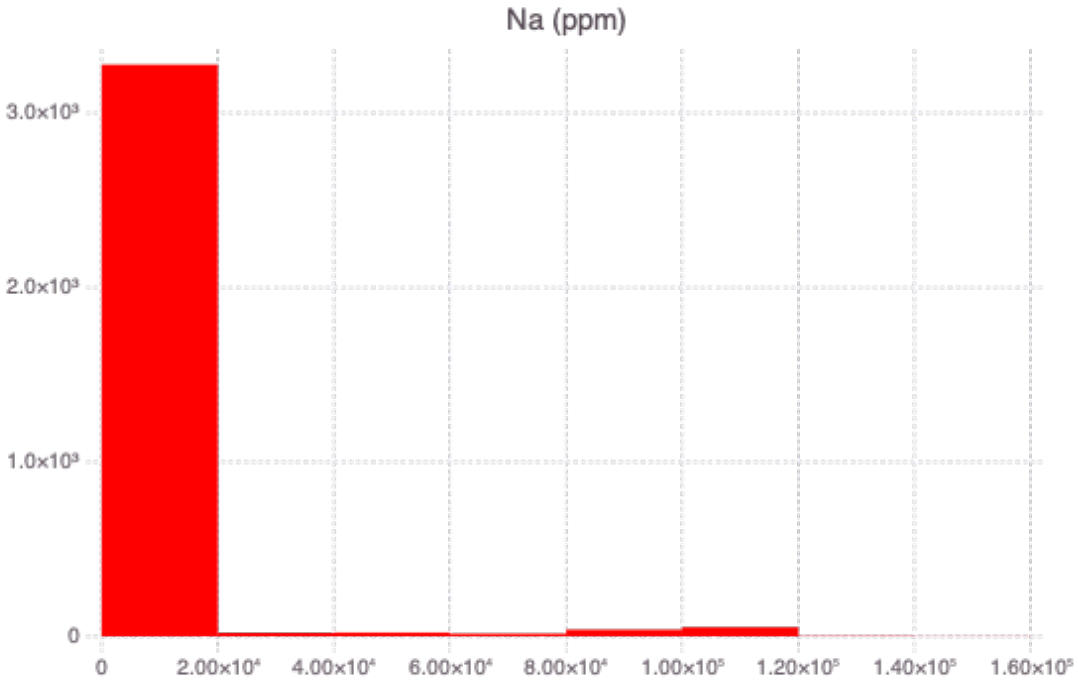

```
Cl (ppm): Min 0.6 Max 240000.0 StdDev 28681.555 Skewness 5.21565 Count 3923
  Info: HCO3 (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

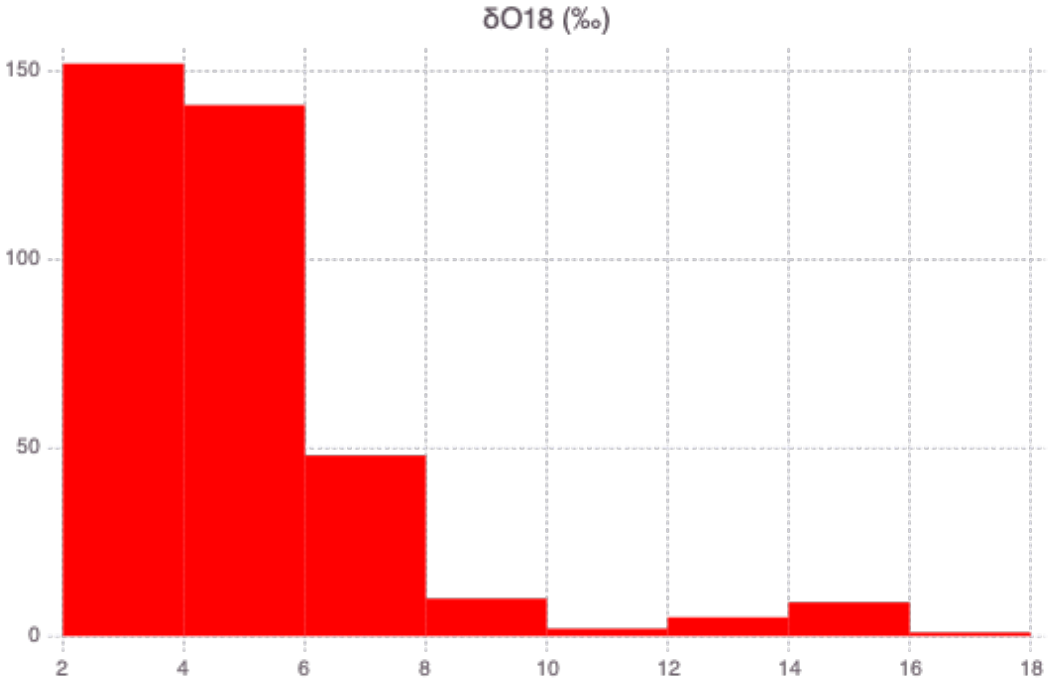

K (ppm)
3.0x10³
2.0x10³
1.0x10³
0
0
1.00x10³
2.00x10³
3.00x10³
4.00x10³
5.00x10³
6.00x10³
7.00x10³
8.00x10³
9.00x10³
1.00x10⁴
1.10x10⁴
1.20x10⁴
1.30x10⁴


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




```
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
```


Na (ppm)
3.0×10³
2.0×10³
1.0×10³
0
0
2.00×10⁴
4.00×10⁴
6.00×10⁴
8.00×10⁴
1.00×10⁵
1.20×10⁵
1.40×10⁵
1.60×10⁵


δO18 (‰)
150
100
50
0
2
4
6
8
10
12
14
16
18

```
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
 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: Na (ppm)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info:  O18 (‰)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  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.

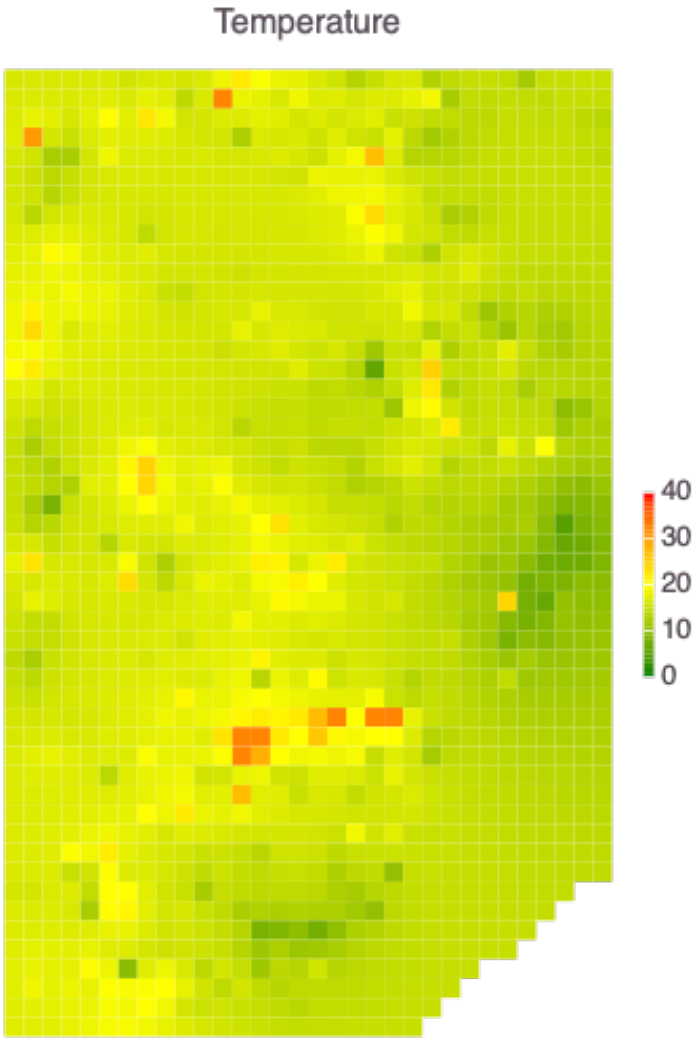
Most of the commonly used ML methods cannot process datasets that are sparse.

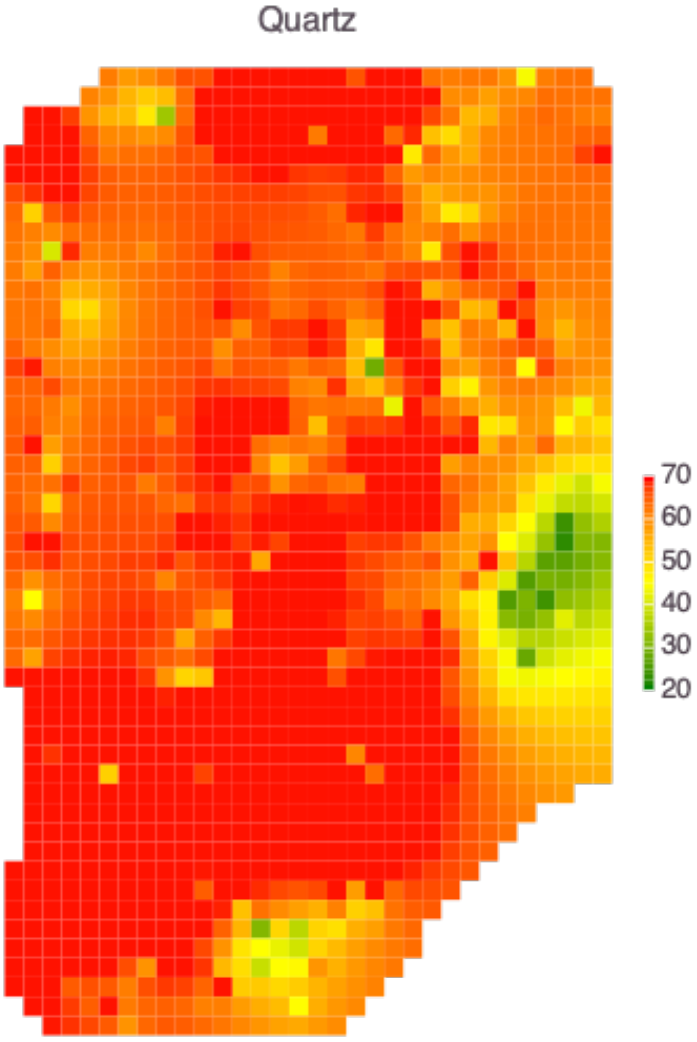
Furthermore, different attributes in the Great Basin dataset cover different areas.

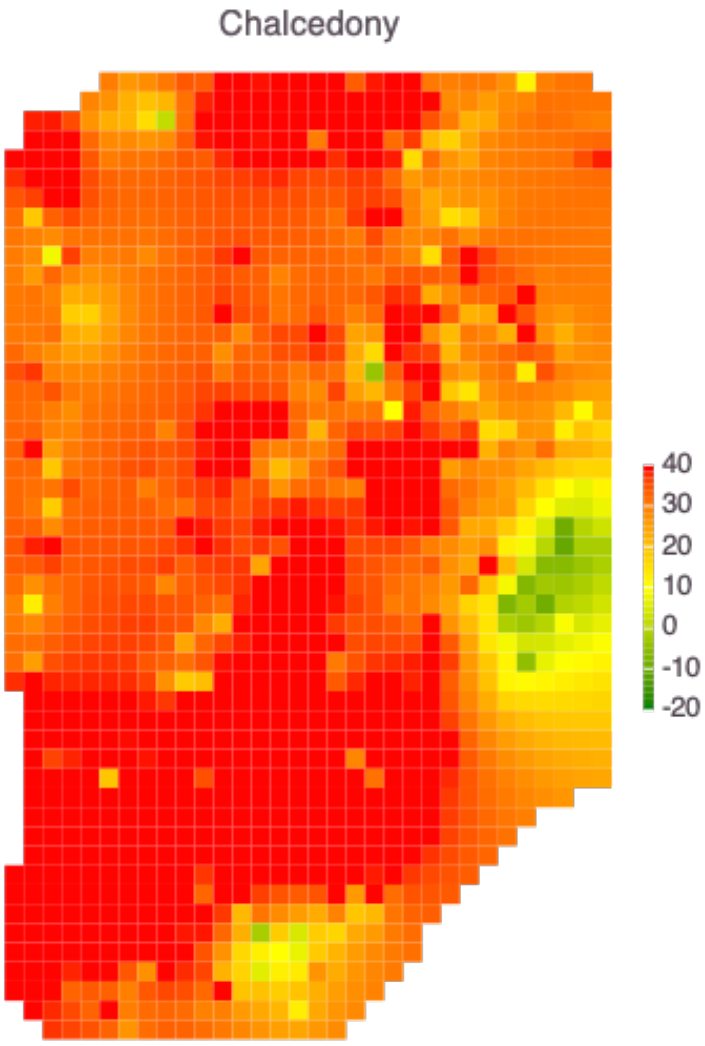
This is demonstrated in the maps generated below.

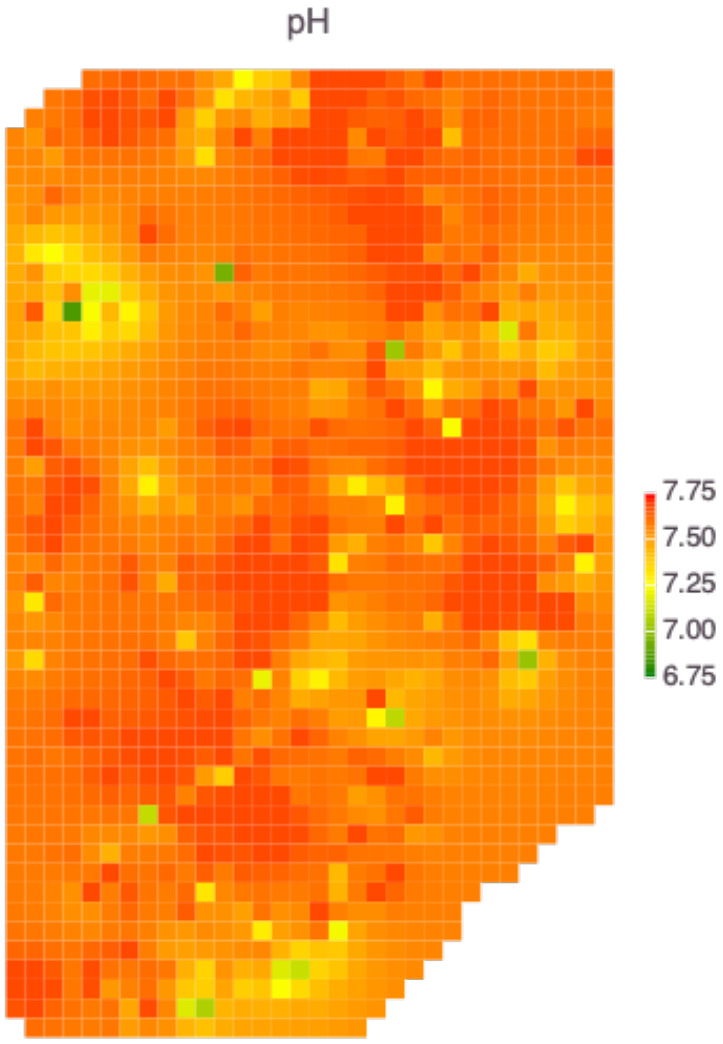
[11]:
```
coord = permutedims([xcoord ycoord])

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]
```

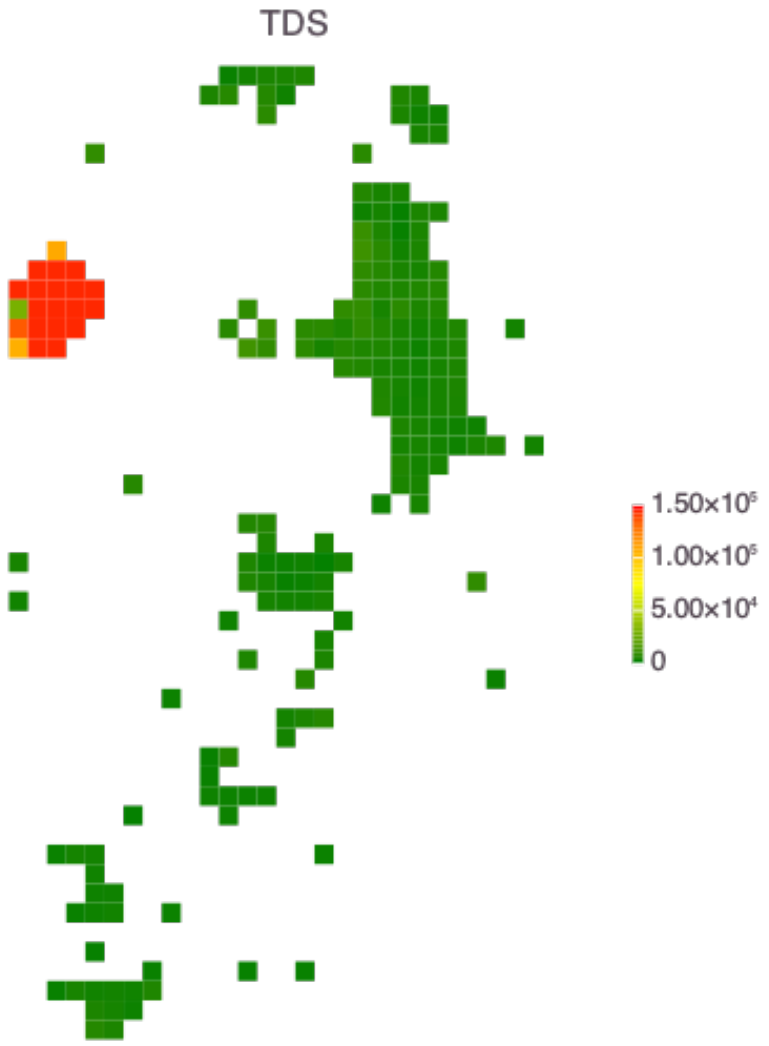
```
        for (i, x) in enumerate(xgrid), (j, y) in enumerate(ygrid)
                inversedistancefield[i, j] = Kriging.
↪inversedistance(permutedims([x y]), icoord, v, 2; cutoff=1000)[1]
        end
        imax = NMFk.maximumnan(inversedistancefield)
        imin = NMFk.minimumnan(inversedistancefield)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

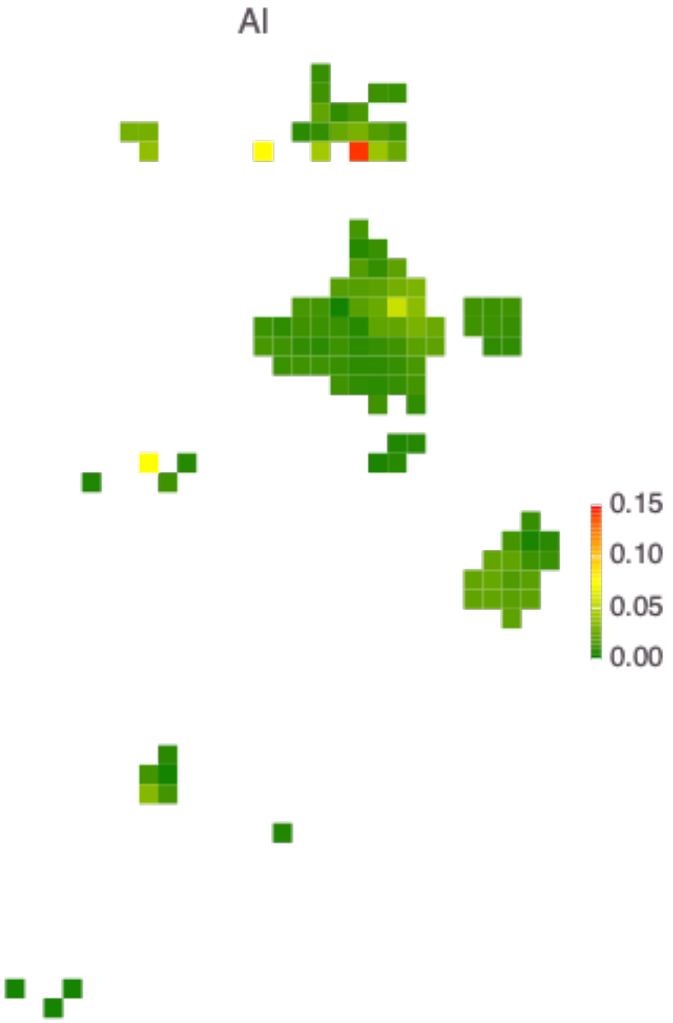


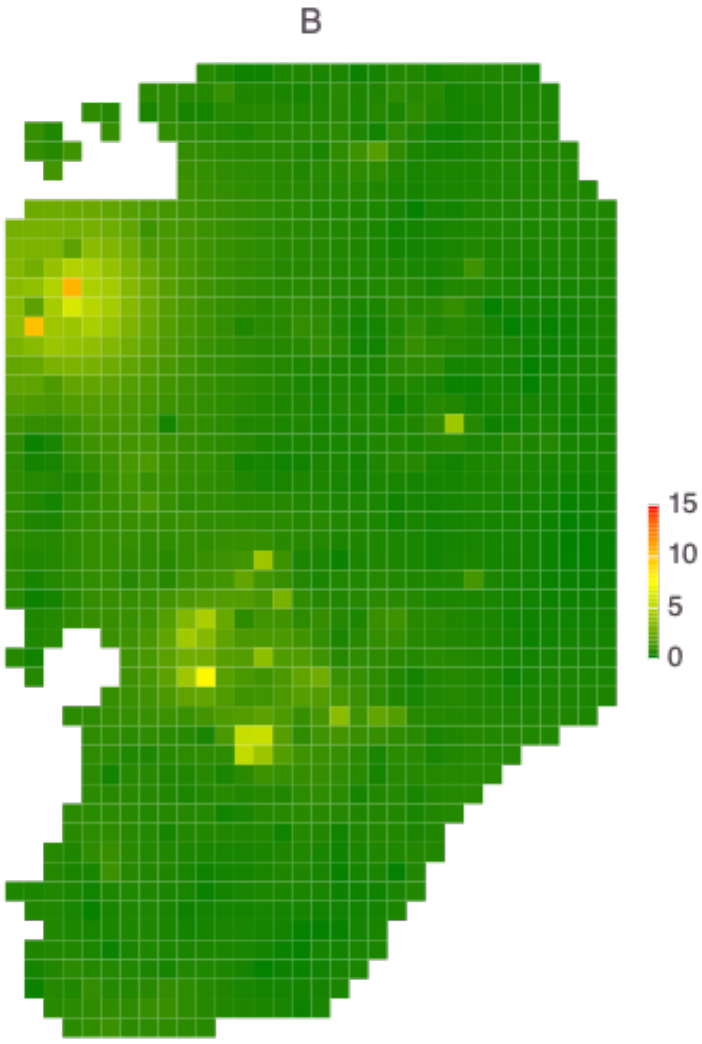

Quartz
70
60
50
40
30
20

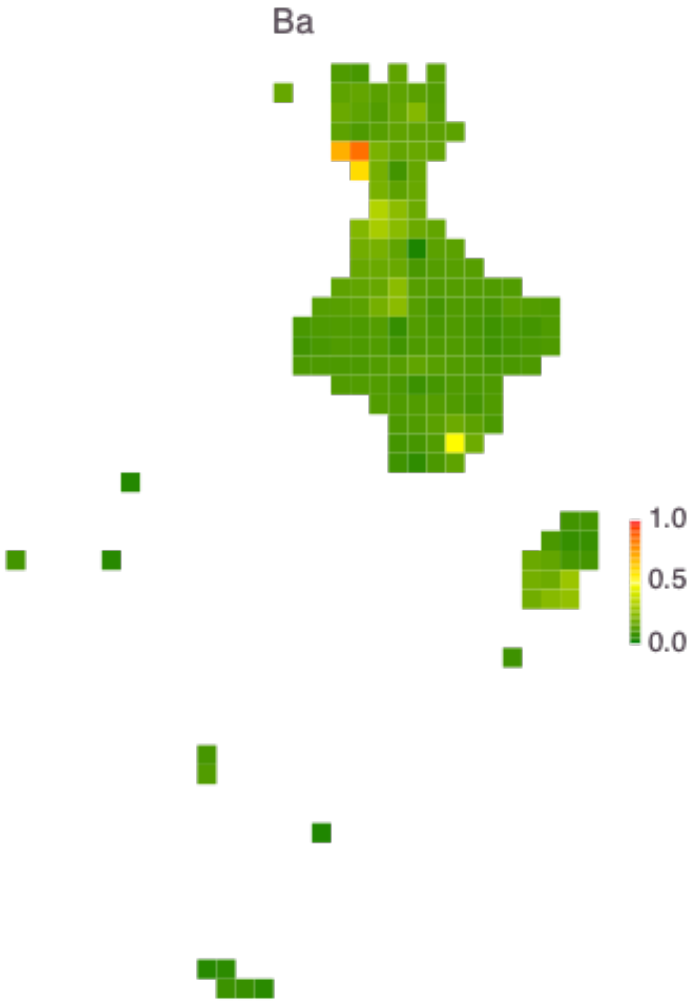

Chalcedony
40
30
20
10
0
-10
-20

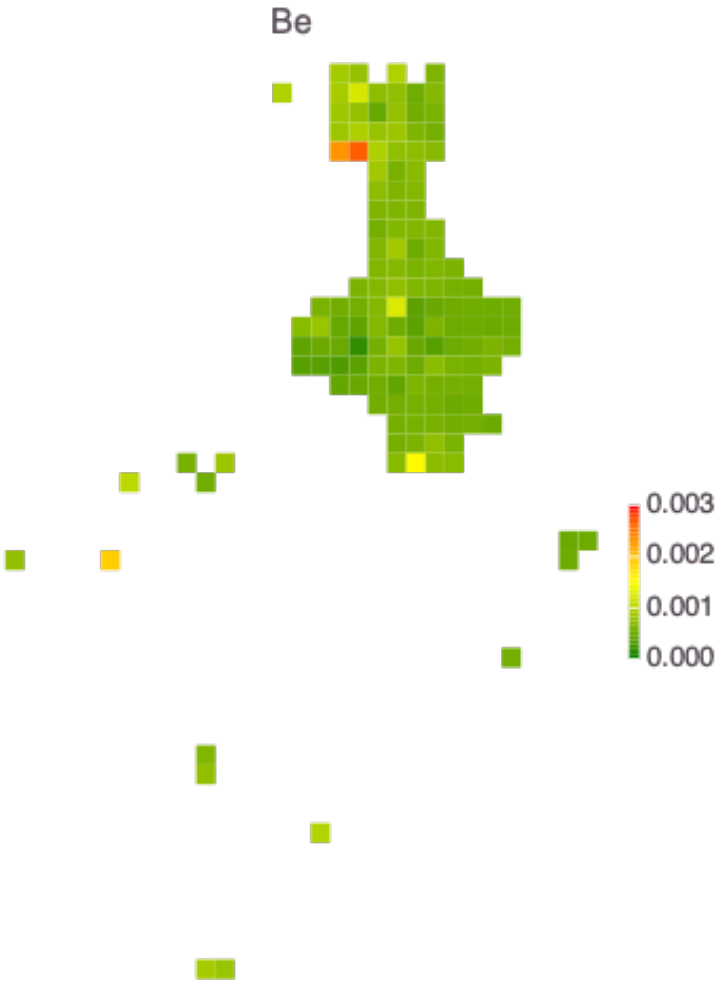

pH
7.75
7.50
7.25
7.00
6.75

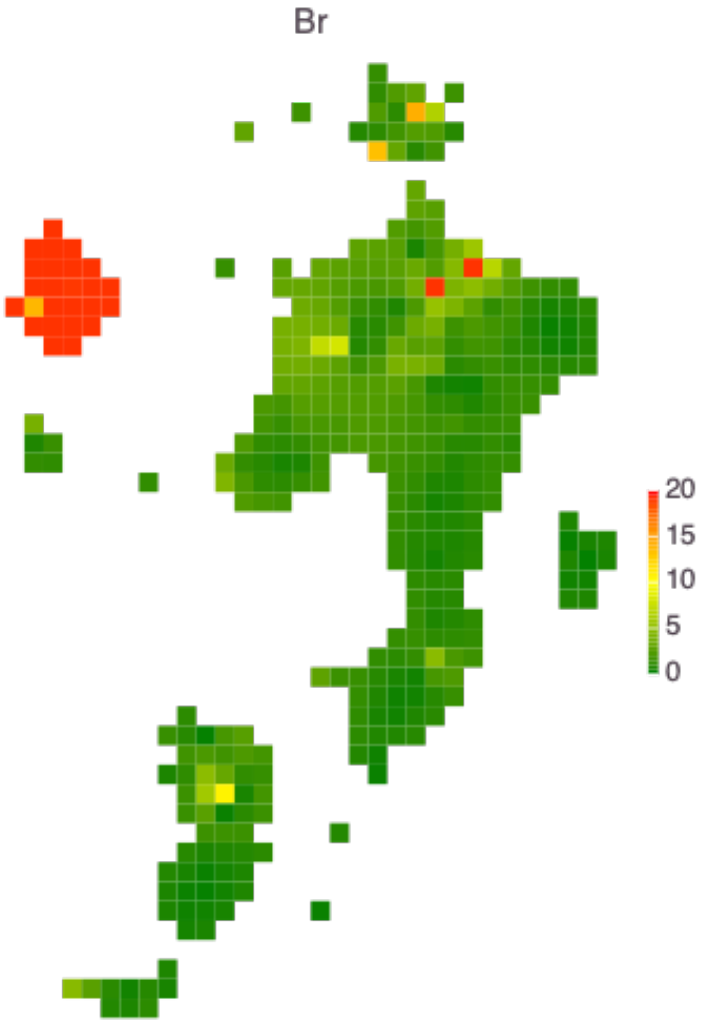

TDS
1.50×10⁵
1.00×10⁵
5.00×10⁴
0

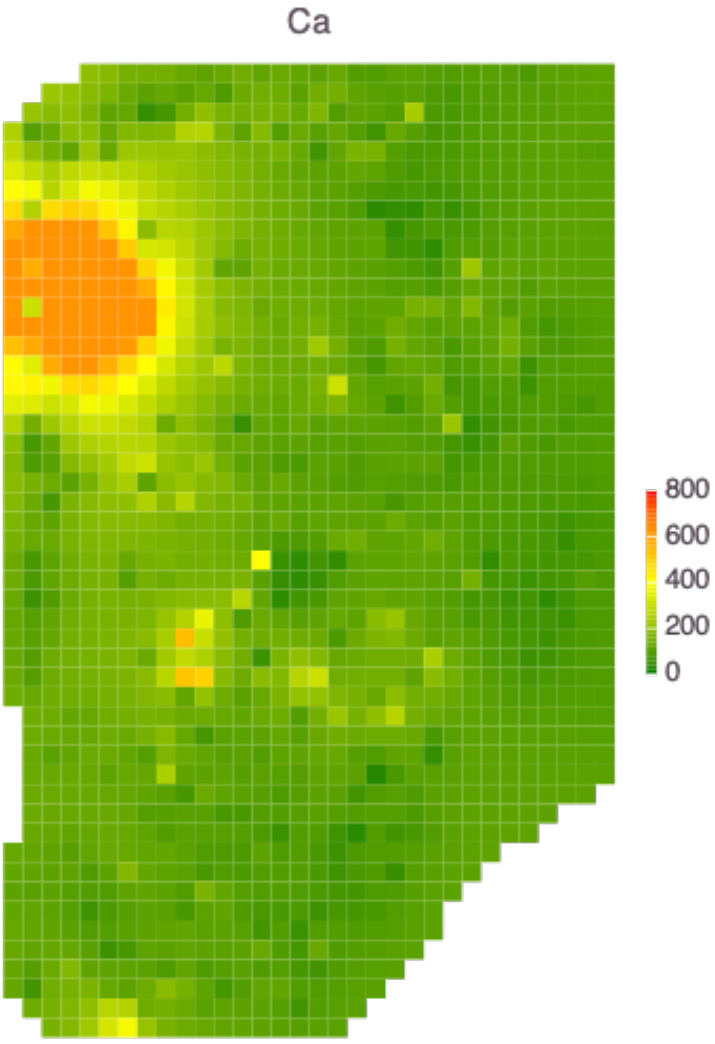

Al
0.15
0.10
0.05
0.00

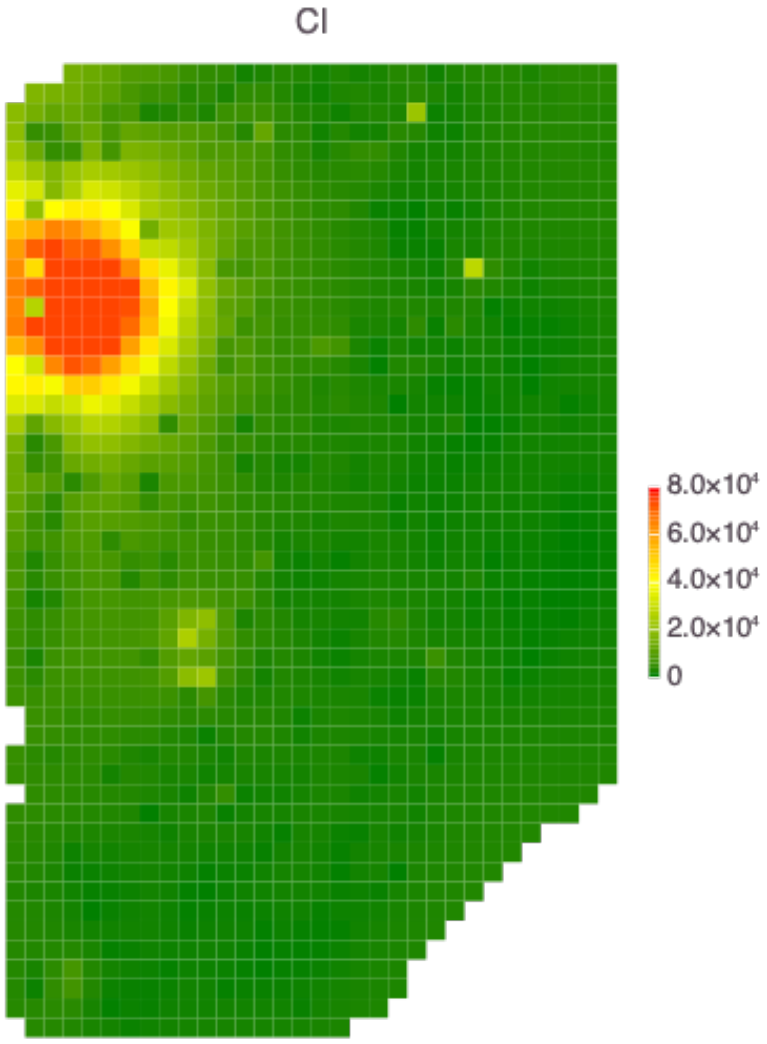

B
15
10
5
0

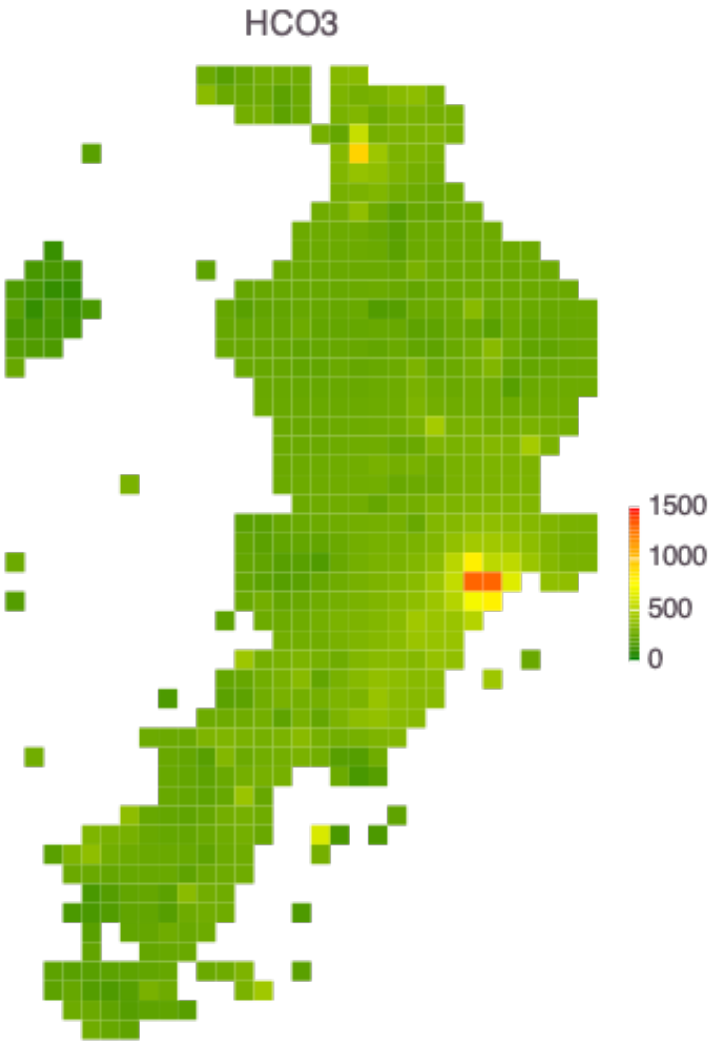

Ba
1.0
0.5
0.0

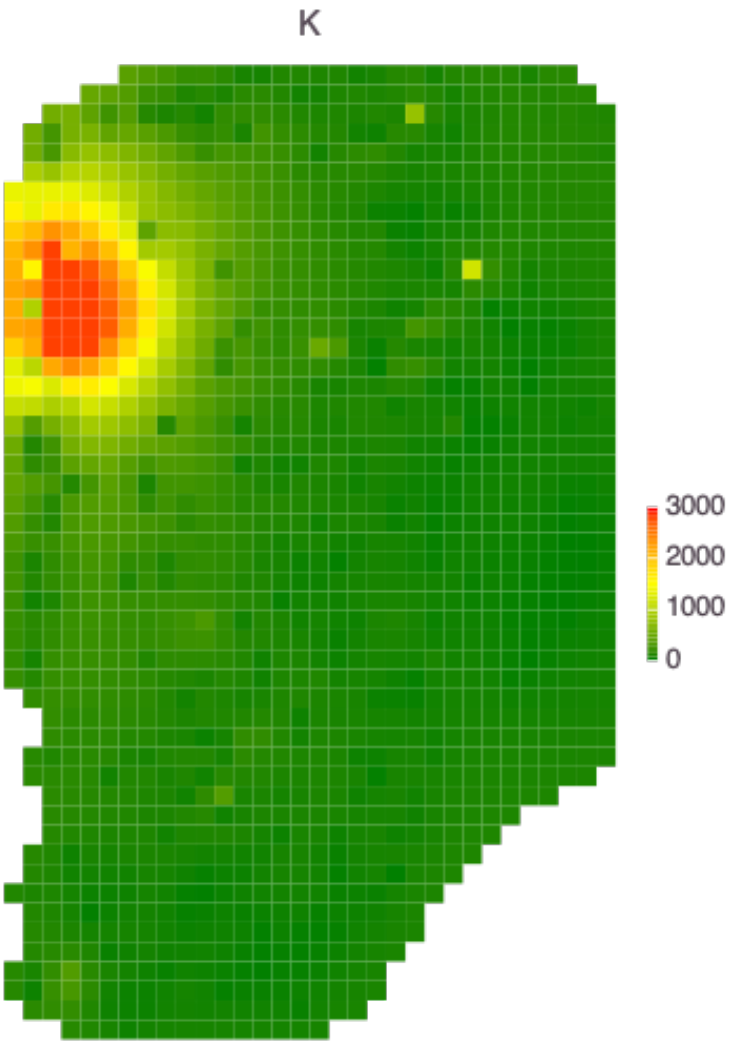

Be
0.003
0.002
0.001
0.000

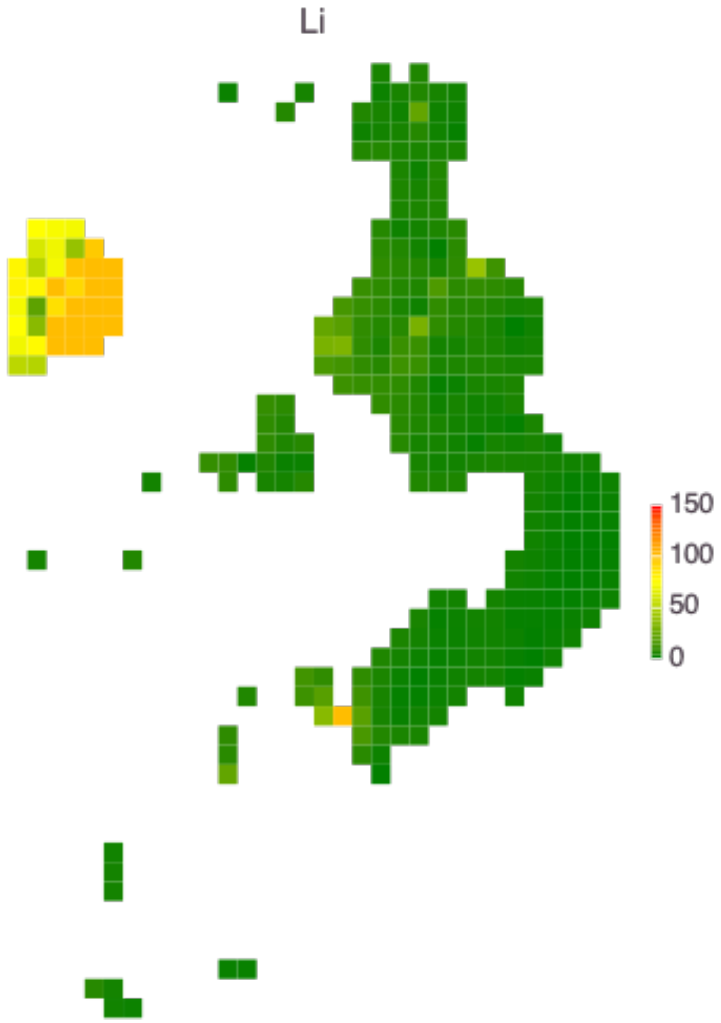

Br
20
15
10
5
0

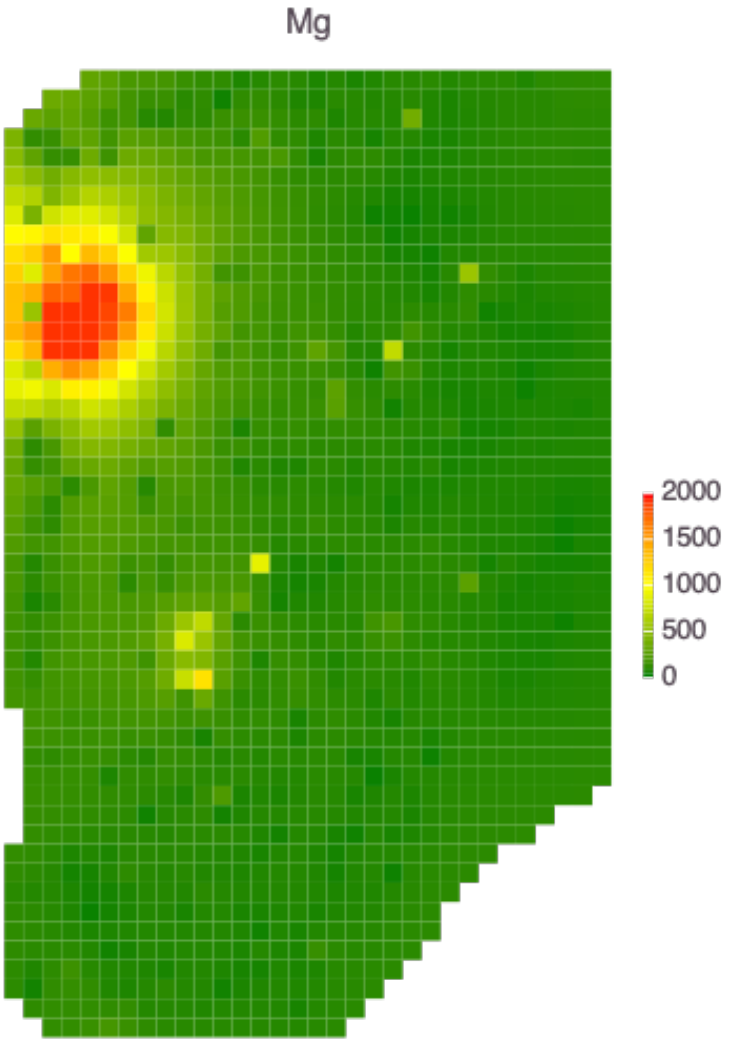

Ca
800
600
400
200
0

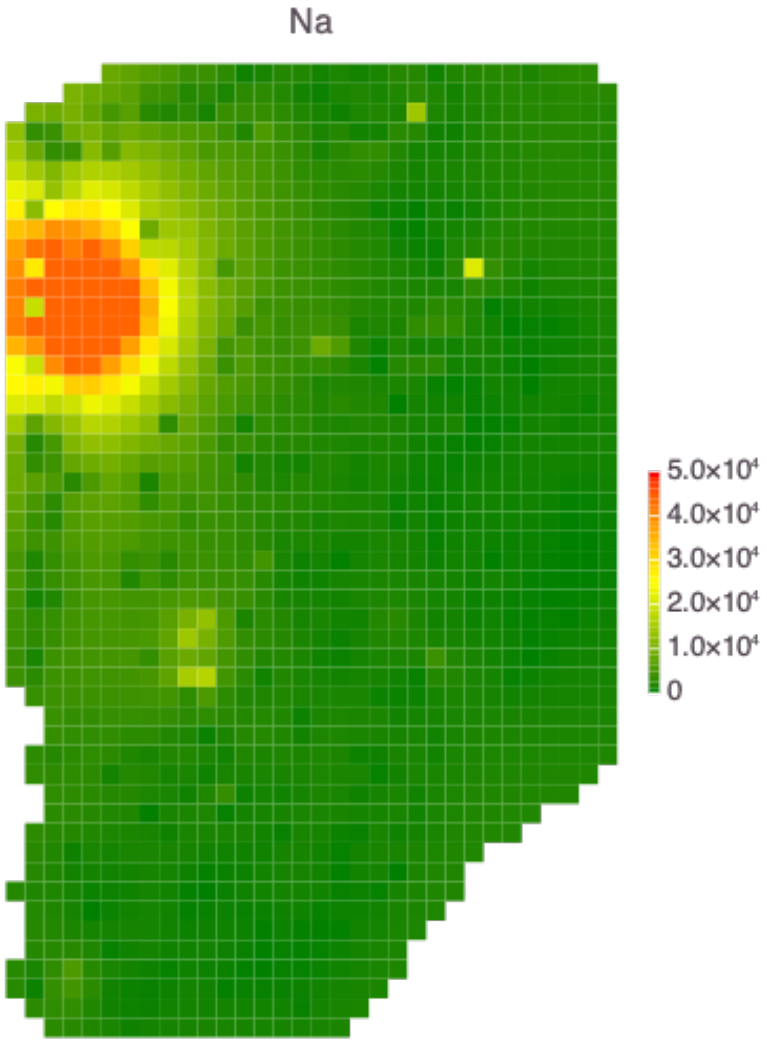

Cl
8.0×10⁴
6.0×10⁴
4.0×10⁴
2.0×10⁴
0

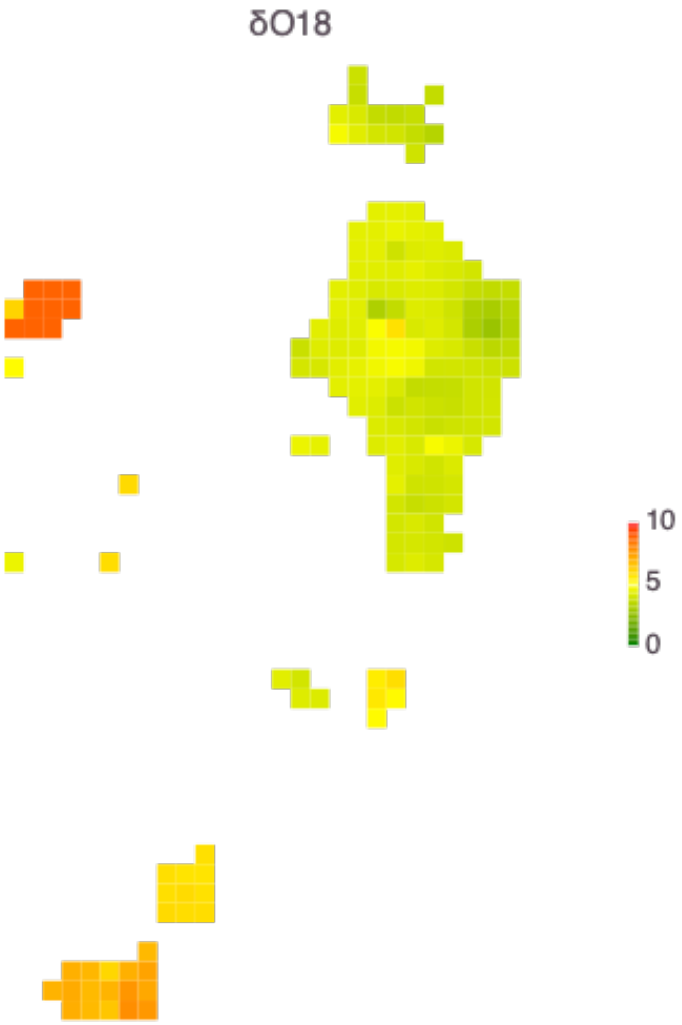

HCO3
1500
1000
500
0


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.

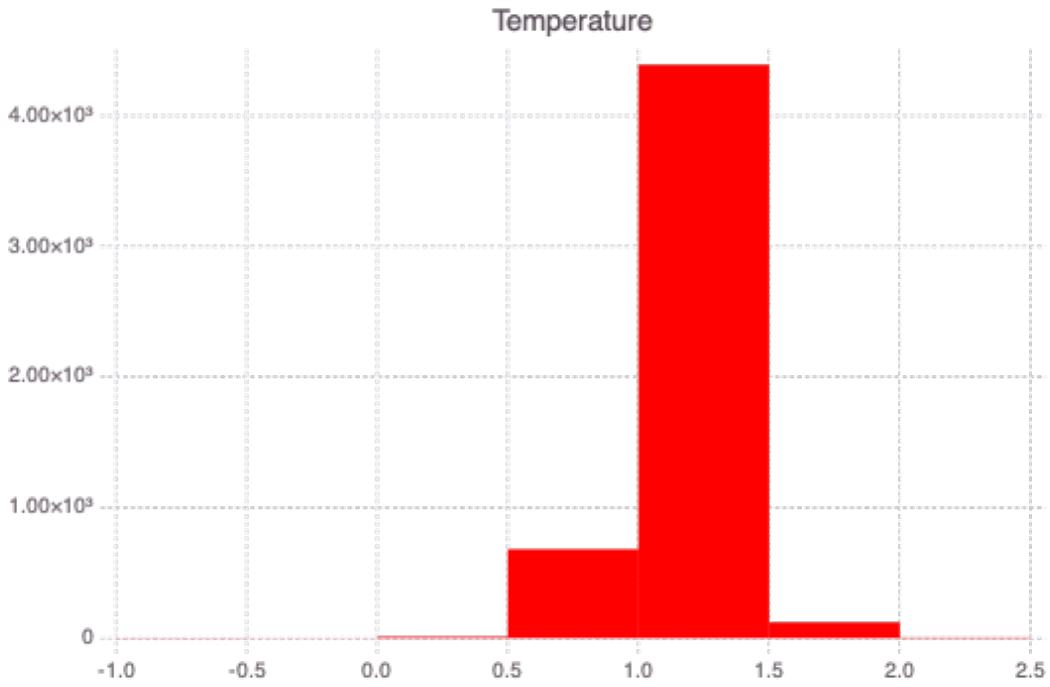
All attributes except for `Quartz`, `Chalcedony` and `pH` are log-transformed (`Quartz` and `Chalcedony` have negative values).

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

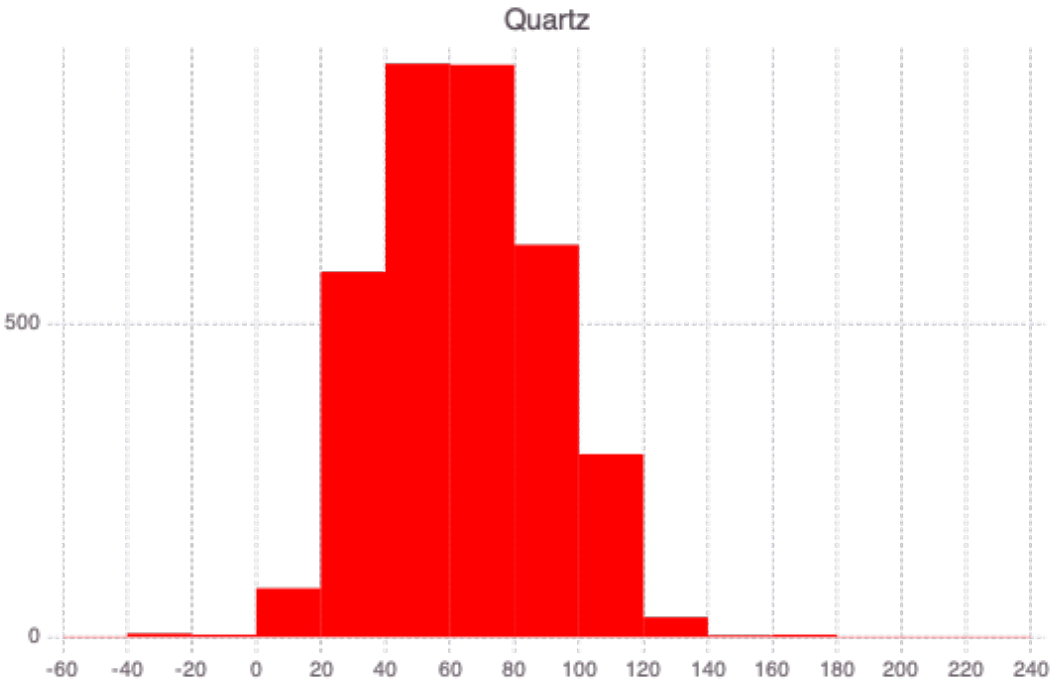
```
18×2 Matrix{Any}:
 "Temperature"   true
```

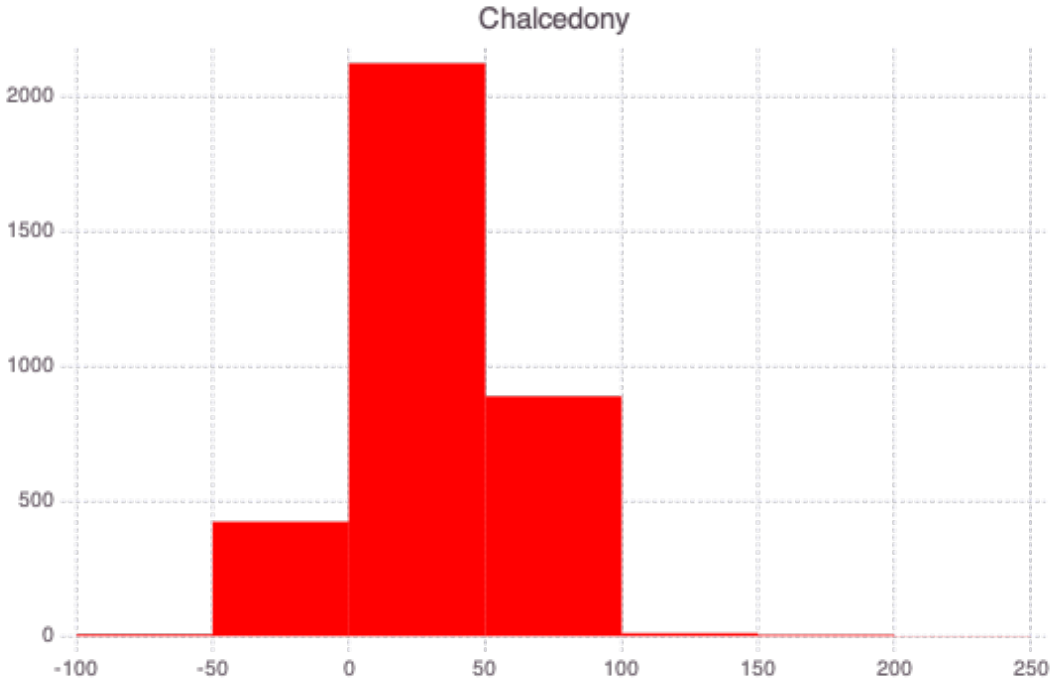
```
"Quartz"       false
"Chalcedony"   false
"pH"           false
"TDS"           true
"Al"            true
"B"             true
"Ba"            true
"Be"            true
"Br"            true
"Ca"            true
"Cl"            true
"HCO3"          true
"K"             true
"Li"            true
"Mg"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

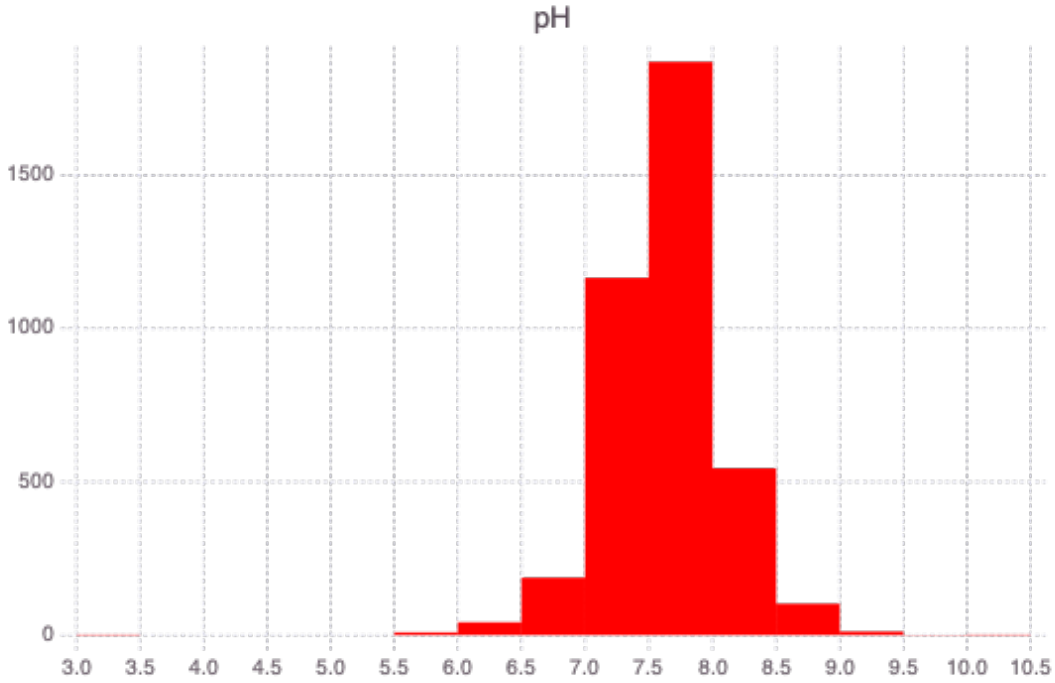
[13]:
```
NMFk.datanalytics(X, attributes; dims=2, logv=logv);
```



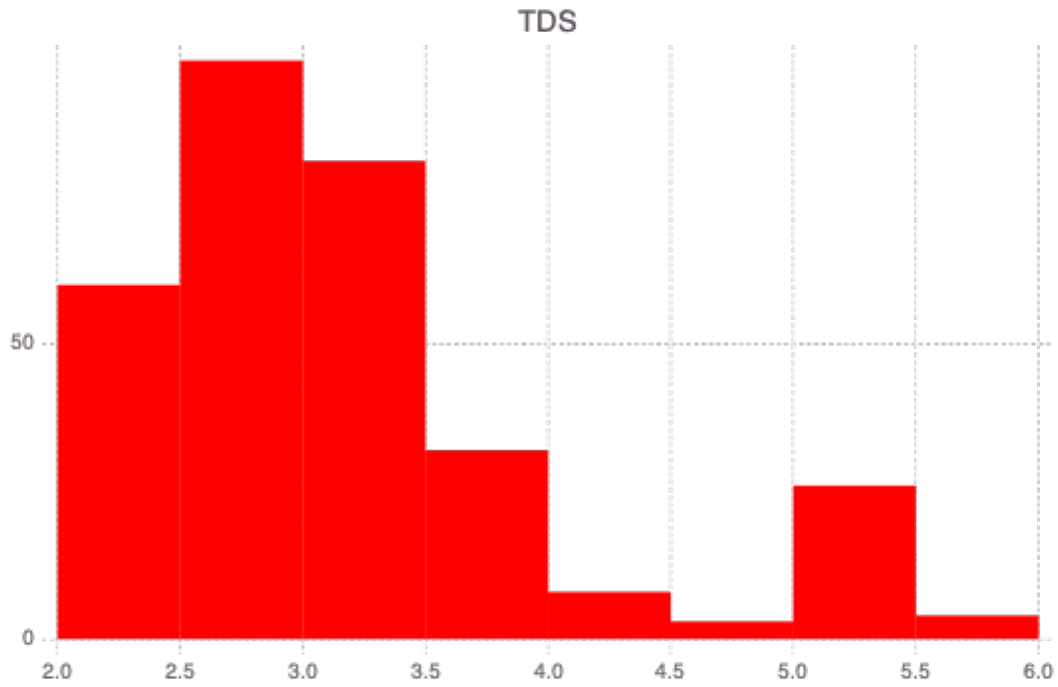

```
Info: Temperature: log10-transformed
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```


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

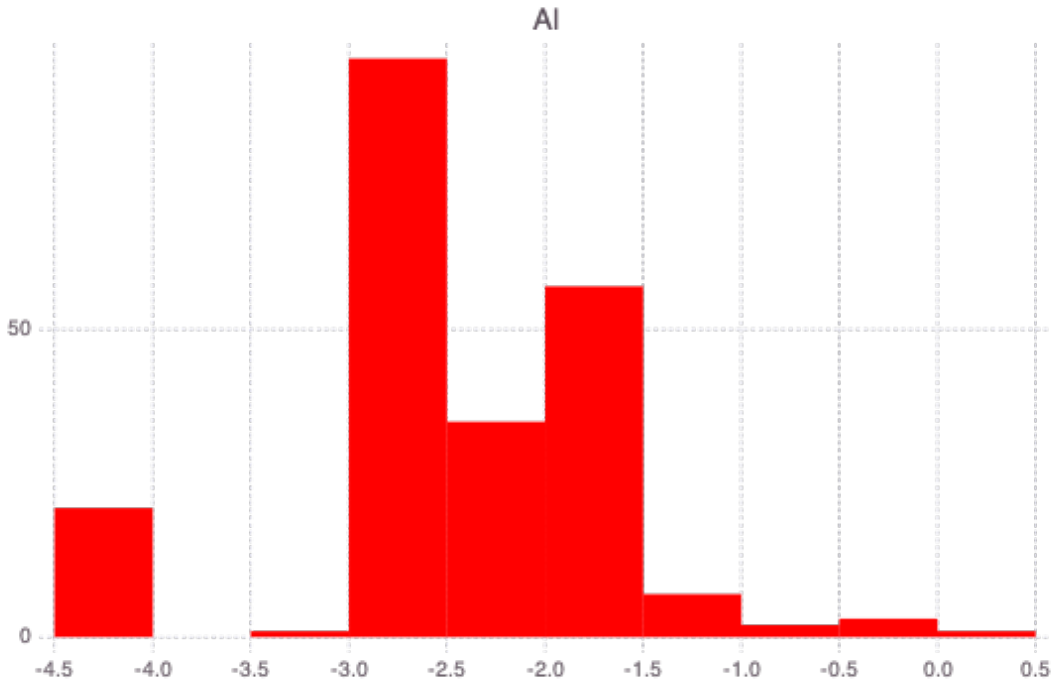

Chalcedony
2000
1500
1000
500
0
-100
-50
0
50
100
150
200
250

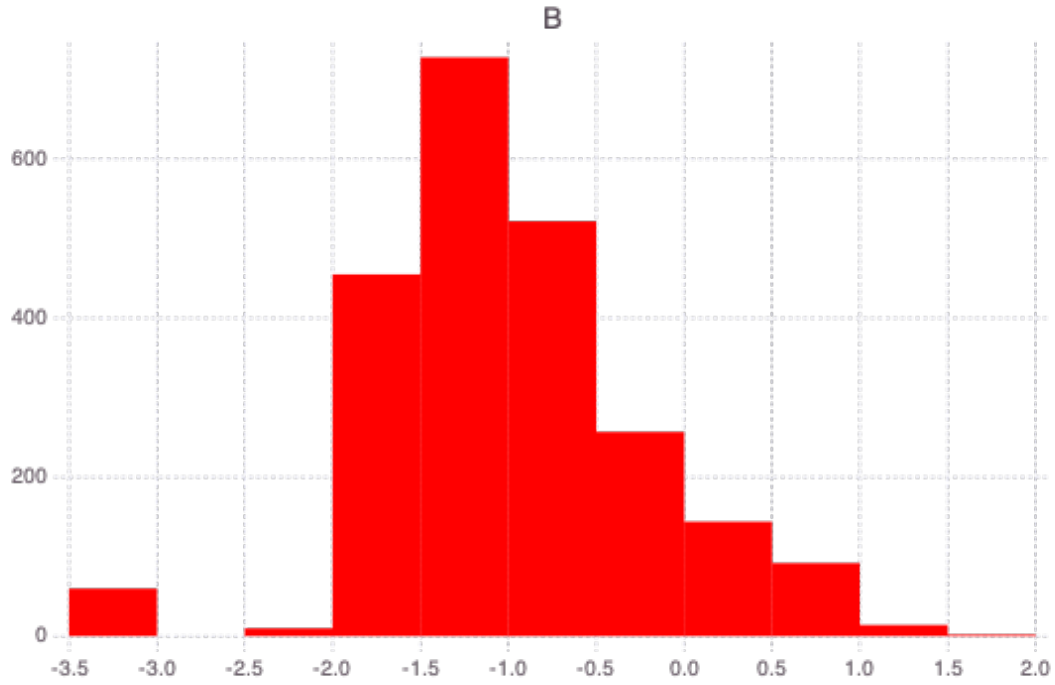



```
Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count
5214
Quartz: Min -50.870045 Max 222.28357 StdDev 26.329222 Skewness 0.24256101 Count
3460
Chalcedony: Min -81.64773 Max 208.67426 StdDev 27.450817 Skewness 0.3369881
Count 3460
  Info: Quartz
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54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

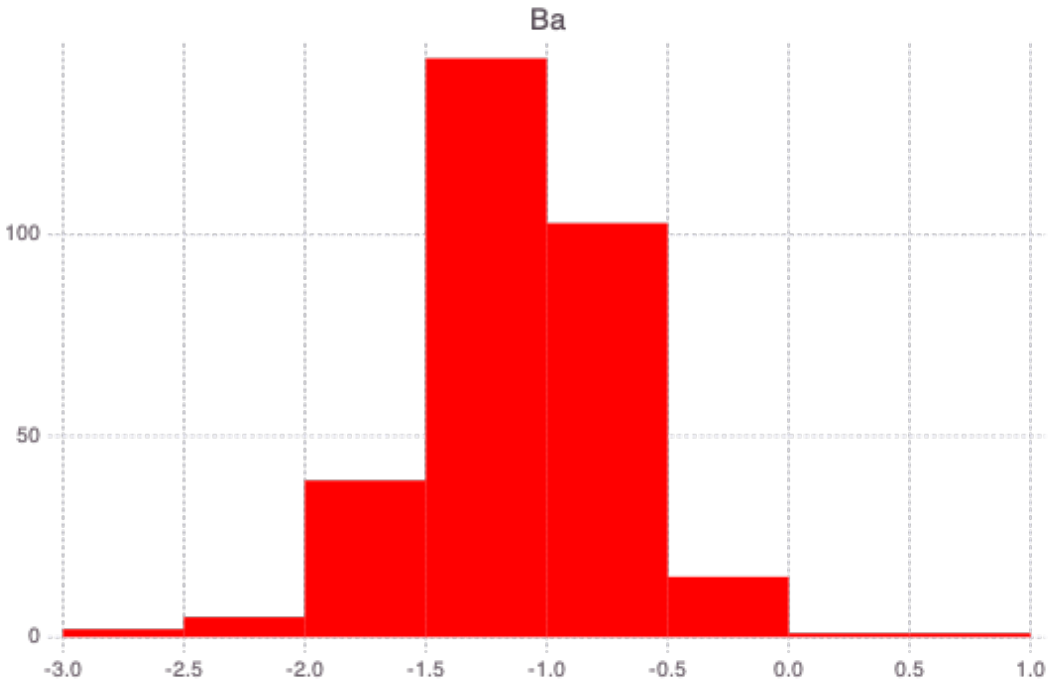



```
pH: Min 3.4 Max 10.2 StdDev 0.44822767 Skewness -0.45681924 Count 3941
  Info: TDS: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```

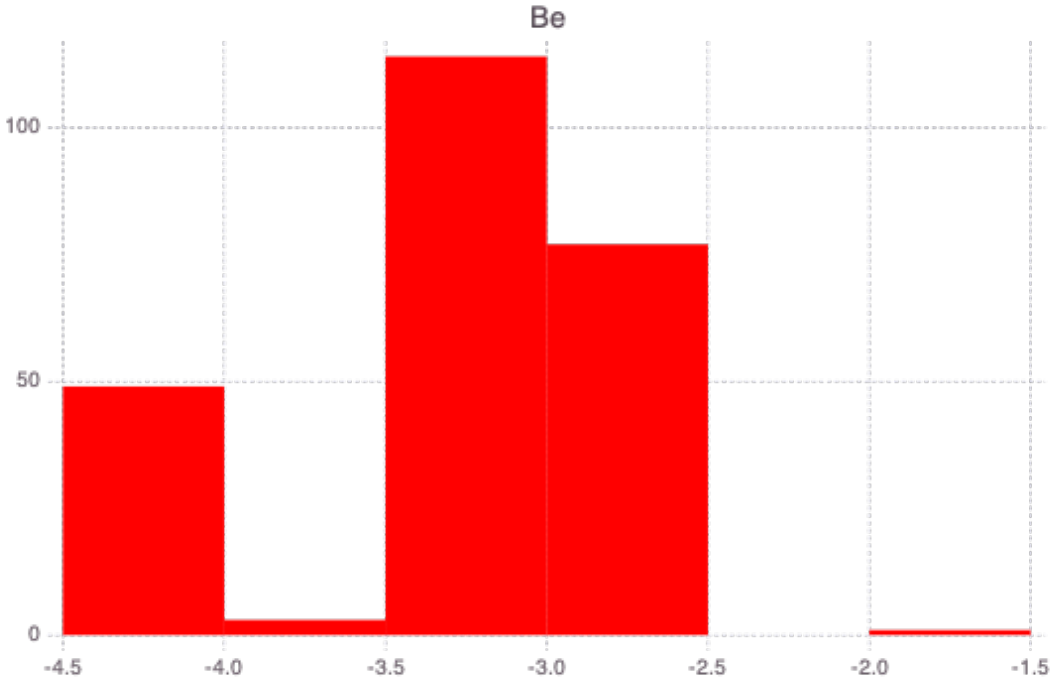

Al
50
0
-4.5
-4.0
-3.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5

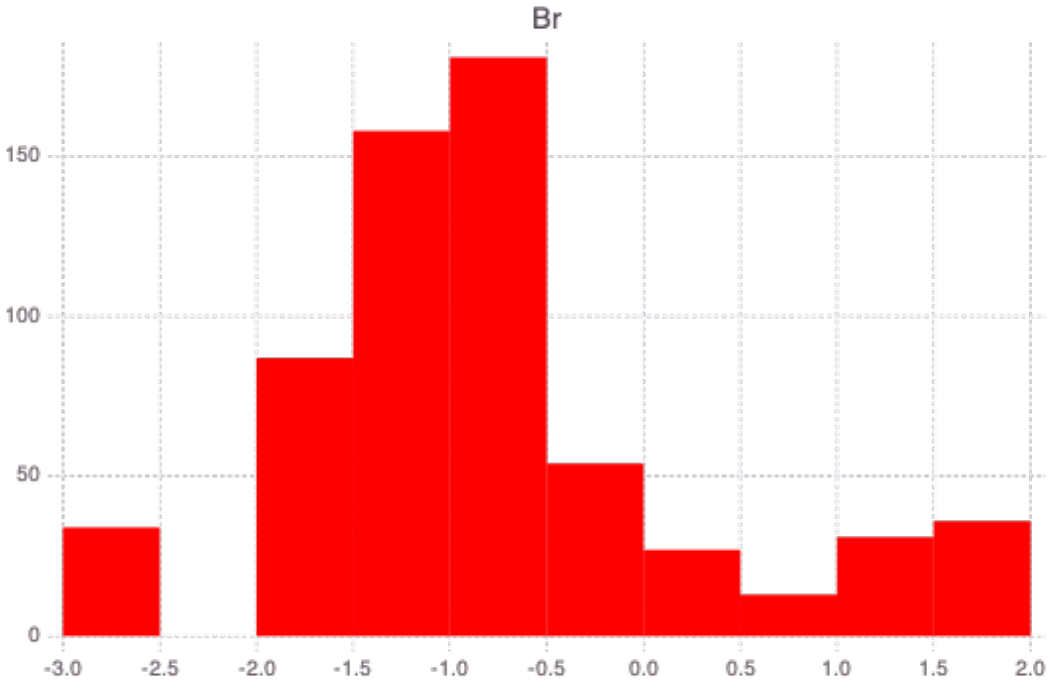

B
600
400
200
0
-3.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0

```
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: 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
```

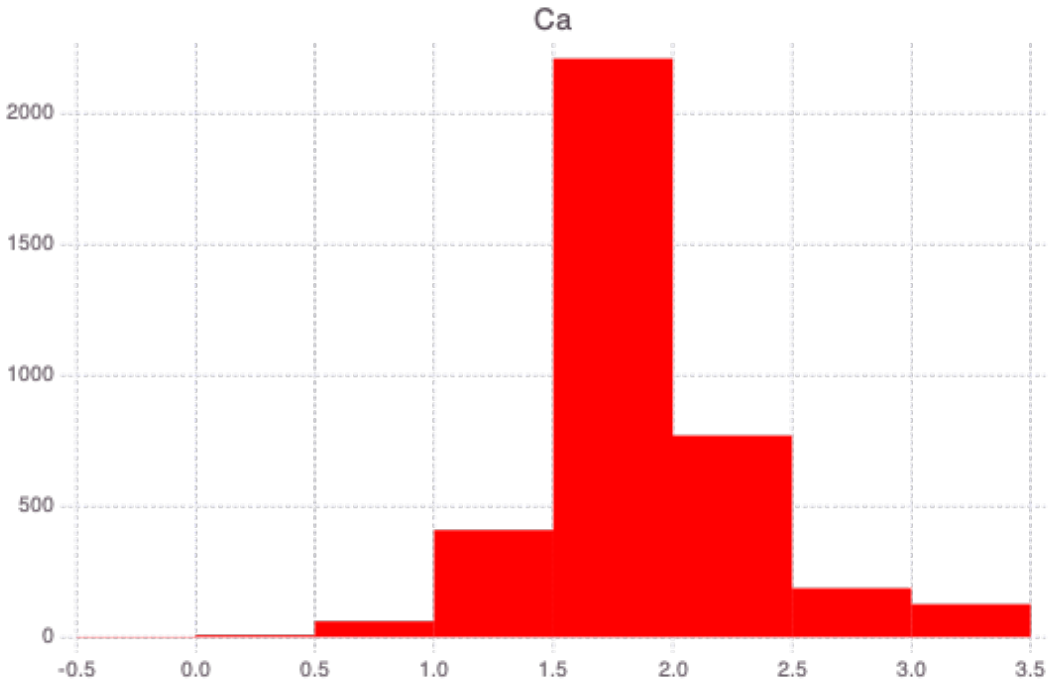



```
B: Min -3.30103 Max 1.8836614 StdDev 0.77384454 Skewness 0.08153698 Count 2284
  Info: Ba: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```

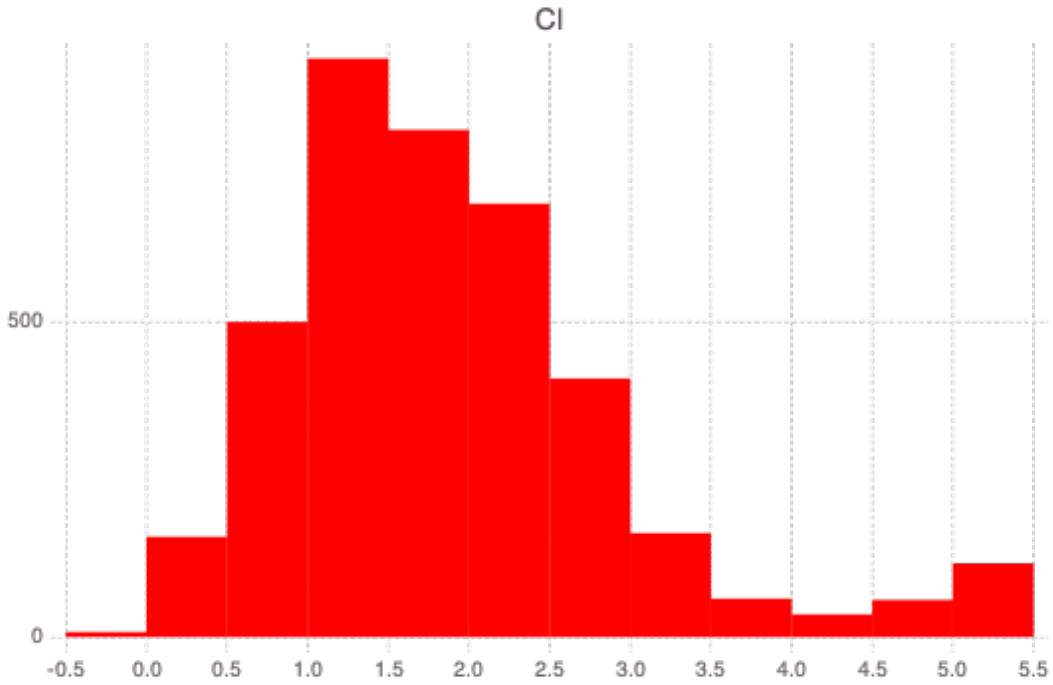

Be
100
50
0
-4.5
-4.0
-3.5
-3.0
-2.5
-2.0
-1.5

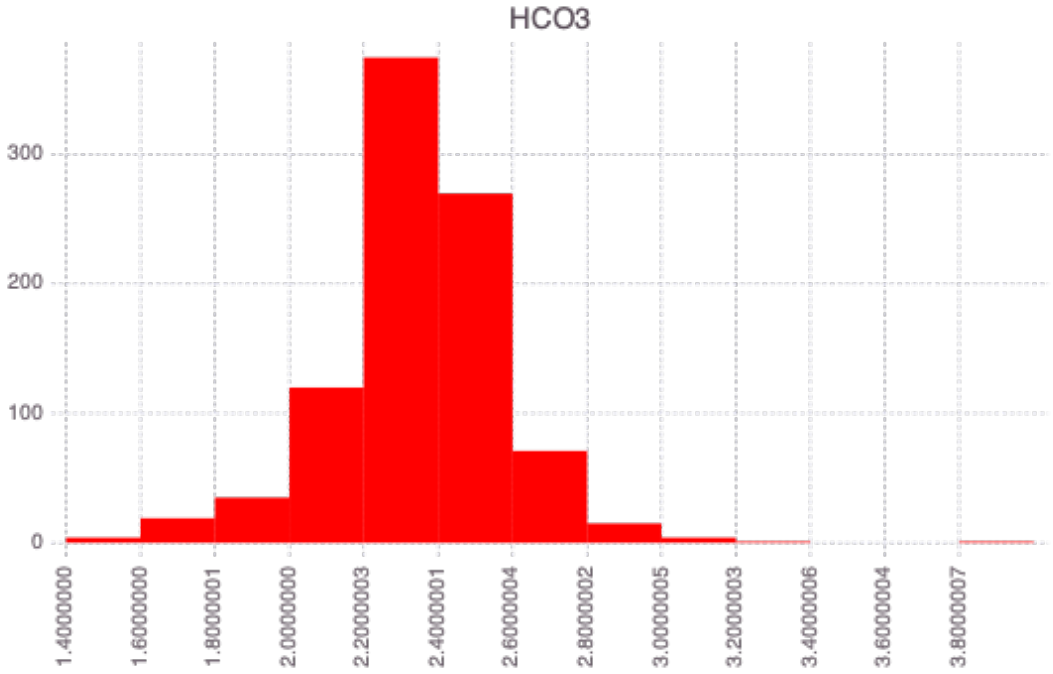

Br
150
100
50
0
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0

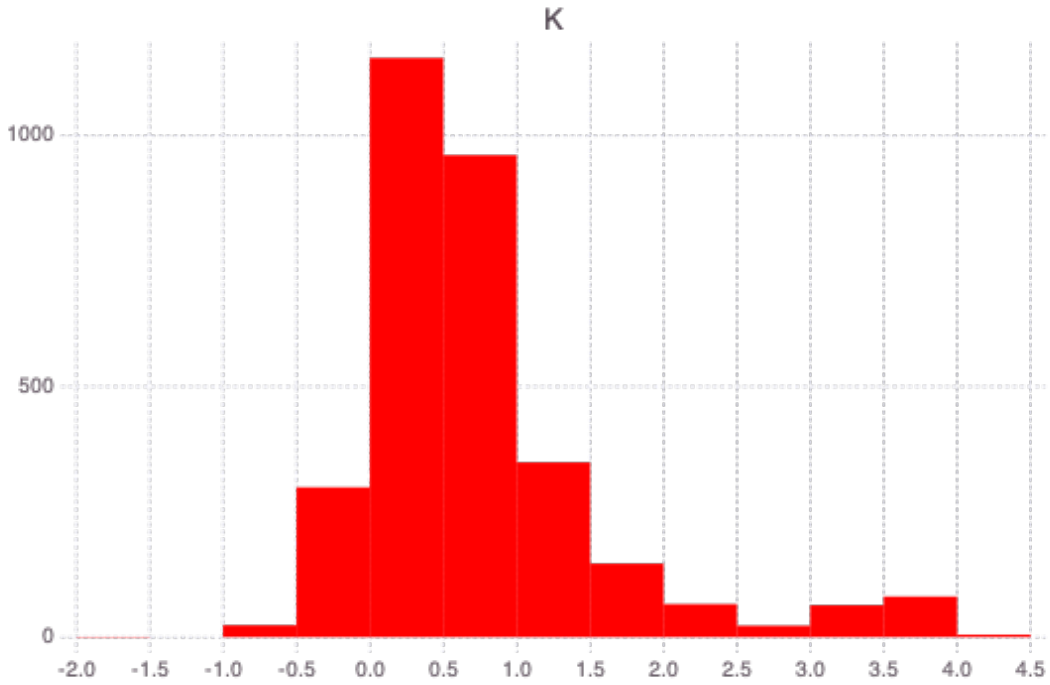
```
Ba: Min -2.69897 Max 0.6532125 StdDev 0.40884706 Skewness -0.013896148 Count 310
Be: Min -4.273001 Max -1.8860567 StdDev 0.46150032 Skewness -0.83869493 Count
244
 Info: Be: log10-transformed
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
 Info: Br: log10-transformed
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51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



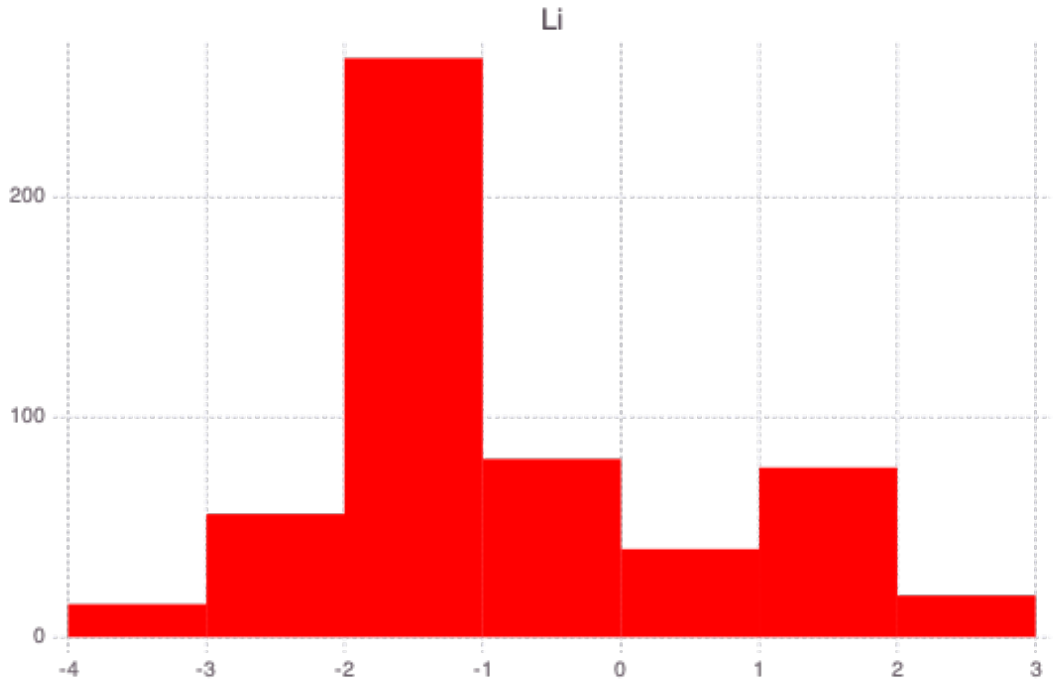

```
Br: Min -3.0 Max 1.9242793 StdDev 1.0616237 Skewness 0.5956521 Count 621
 Info: Ca: log10-transformed
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```


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

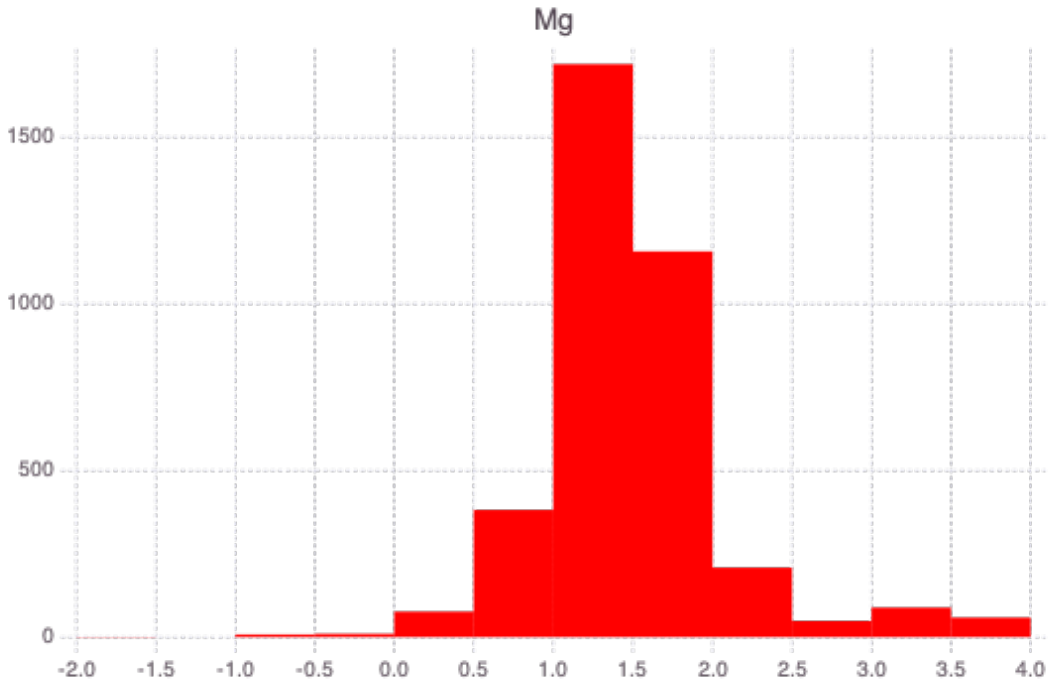

HCO3
300
200
100
0
1.4000000
1.6000000
1.8000001
2.0000000
2.2000003
2.4000001
2.6000004
2.8000002
3.0000005
3.2000003
3.4000006
3.6000004
3.8000007

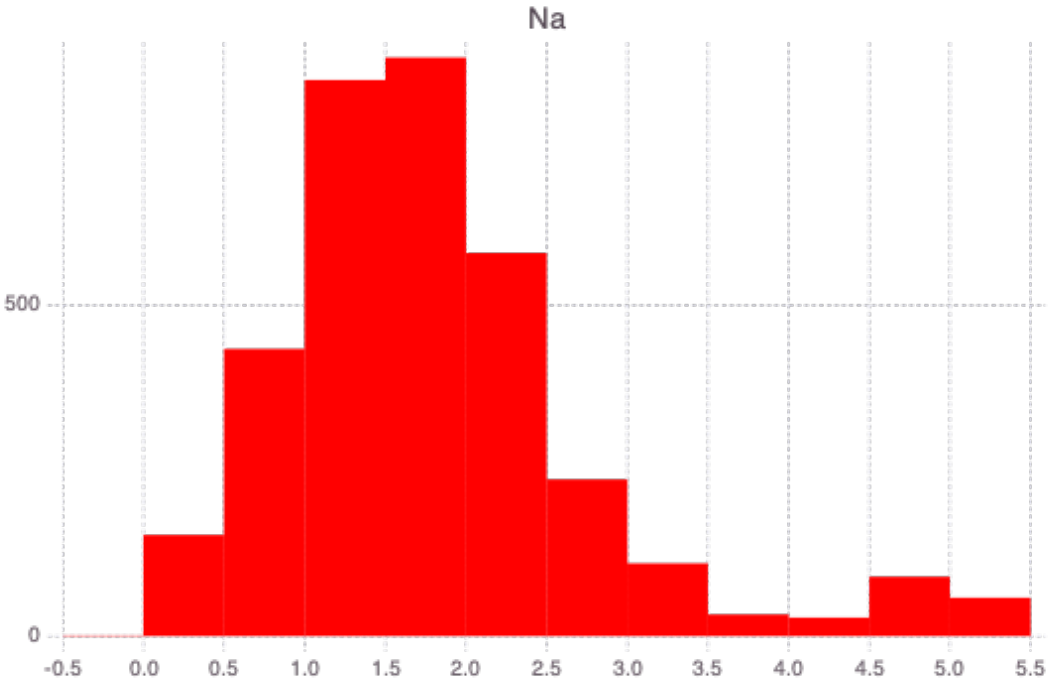



```
Ca: Min -0.22184873 Max 3.4093695 StdDev 0.43120933 Skewness 0.5738154 Count
3772
Cl: Min -0.22184873 Max 5.3802114 StdDev 1.0519629 Skewness 1.1927316 Count 3923
HCO3: Min 1.5682018 Max 3.9645896 StdDev 0.22752158 Skewness 0.051133487 Count
915
  Info: Cl: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  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
```

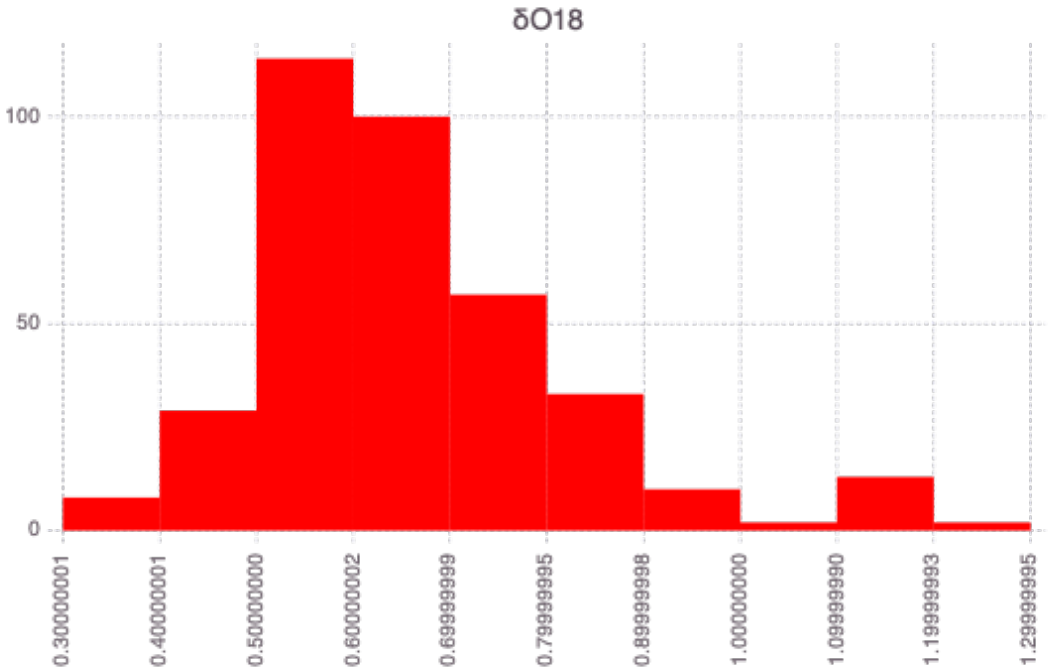



```
K: Min -2.0 Max 4.1139436 StdDev 0.8480291 Skewness 1.8444492 Count 3177
  Info: Li: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```


Mg
1500
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


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

```
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
 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
```




```
Na: Min -0.30103 Max 5.20412 StdDev 0.985548 Skewness 1.3556563 Count 3437
 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:  O18: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  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 = NMFk.execute(Xnl, nkrange, nruns;␣
 ↪cutoff=0.3, resultdir=resultdir, casefilename="nmfk-nl", load=true)
W, H, fitquality, robustness, aic = 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
```

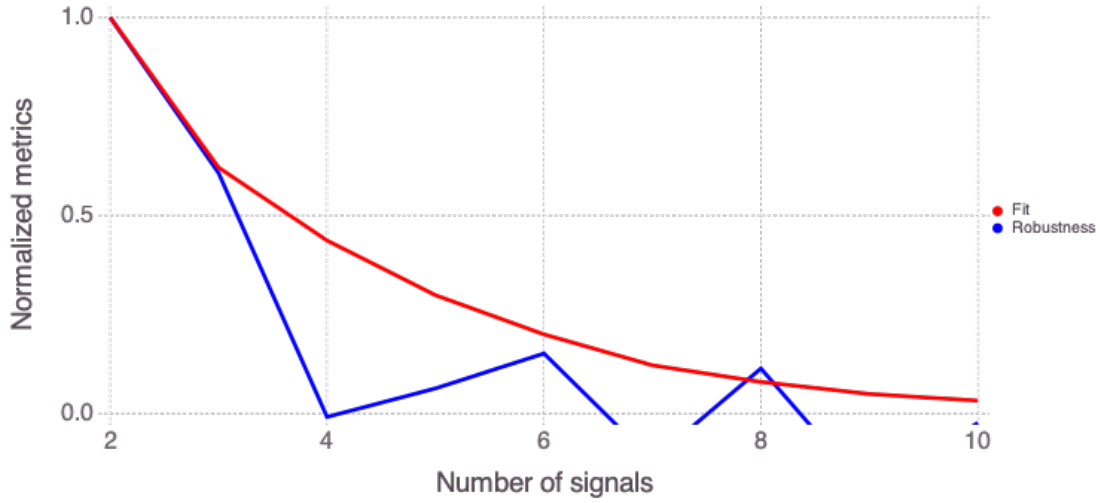
1.13 Get the optimal number of signatures:

[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)
```

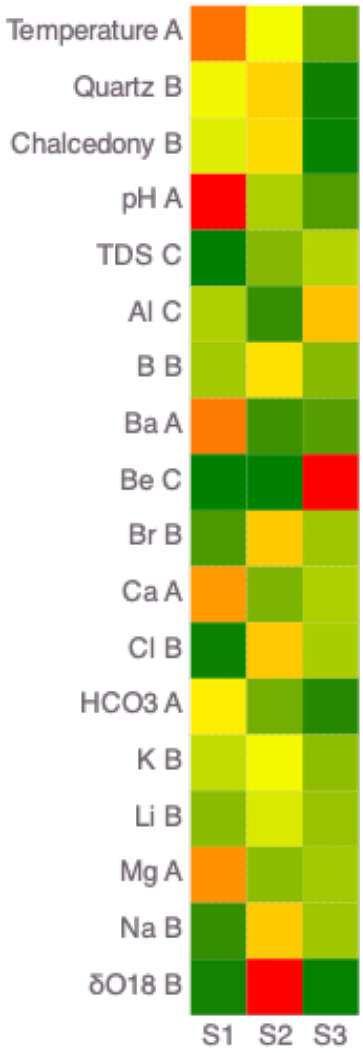
```
 Info: Number of signals: 3
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:205
 Info: Attributes (signals=3)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:209
 Warning: type
Clustering.KmeansResult{Core.Array{Core.Float32,2},Core.Float32,Core.Int64} not
present in workspace; 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
 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

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

```
 "HCO3"          0.549396
```

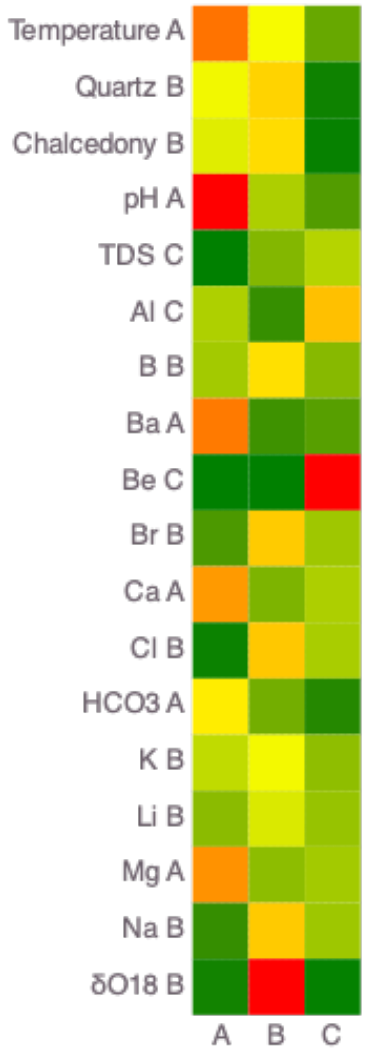
```
 Info: Signal B -> A Count: 6
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:316
 Info: Signal A -> B Count: 9
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:316
 Info: Signal C -> C Count: 3
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:316
 Info: Signal A (S1) (k-means clustering)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:333
```

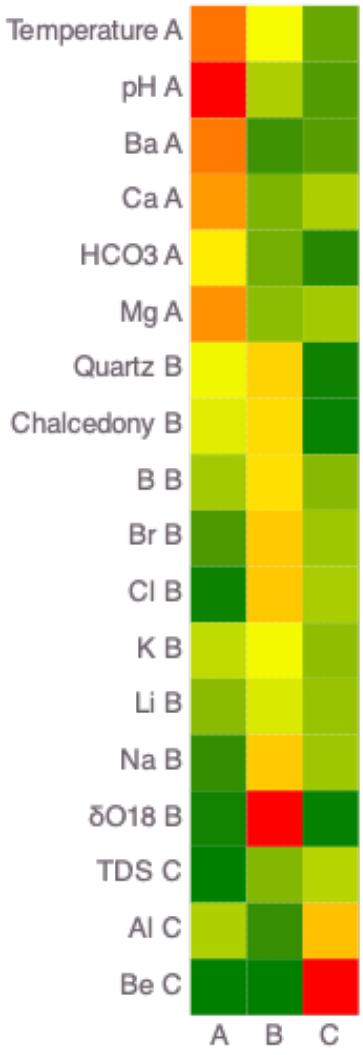
```
9×2 Matrix{Any}:
 " O18"         1.0
 "Cl"           0.651079
 "Na"           0.643991
 "Br"           0.642053
 "Quartz"       0.620207
 "Chalcedony"   0.596872
 "B"            0.586983
 "K"            0.475275
 "Li"           0.414782
```

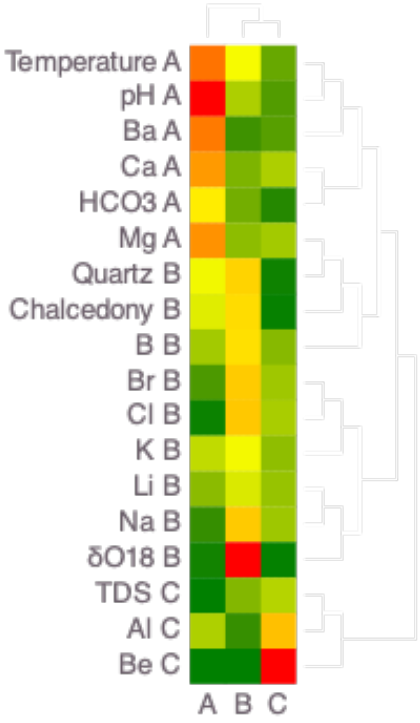
```
3×2 Matrix{Any}:
 "Be"   1.0
 "Al"   0.672723
 "TDS"  0.332944
```

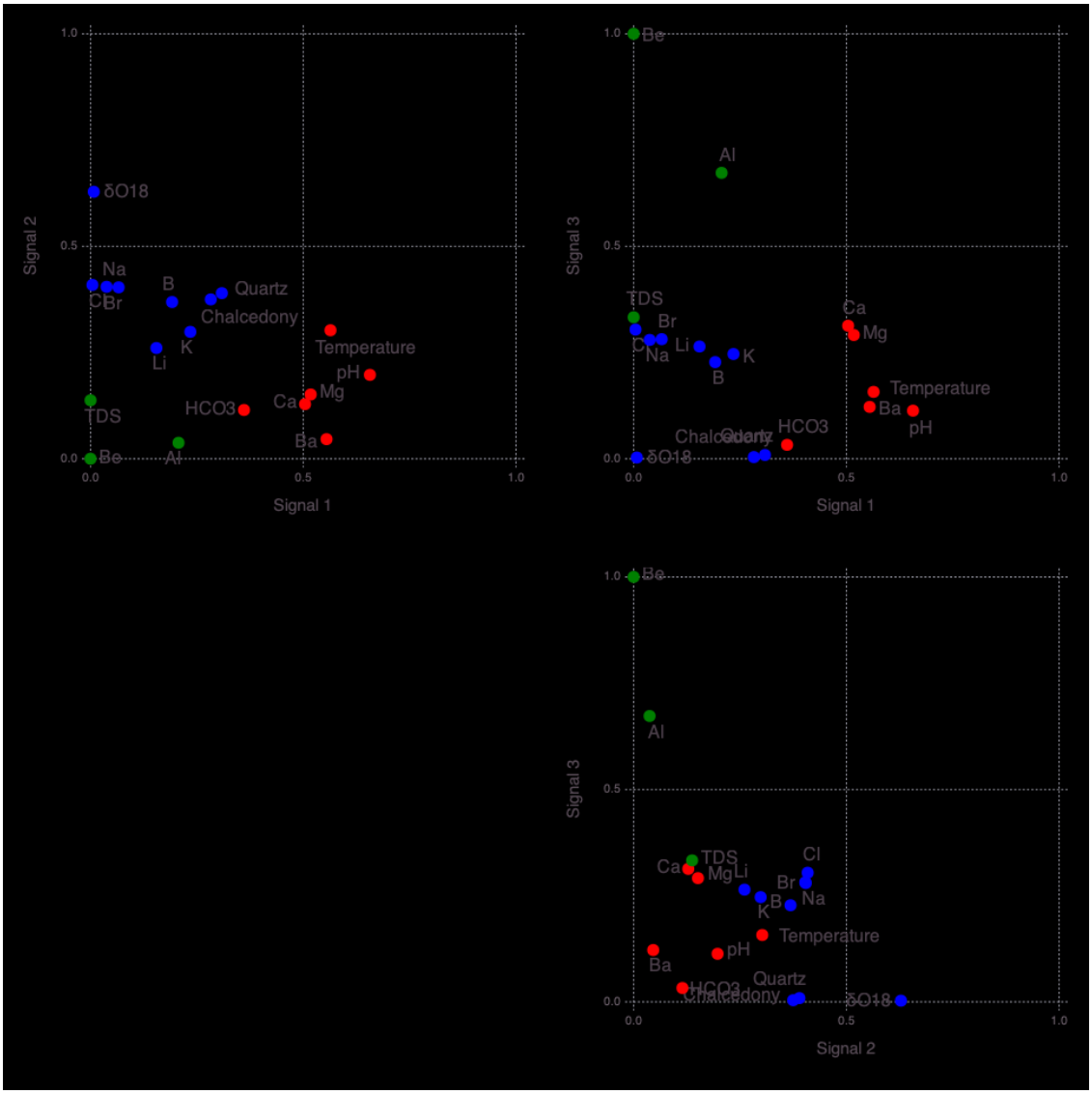


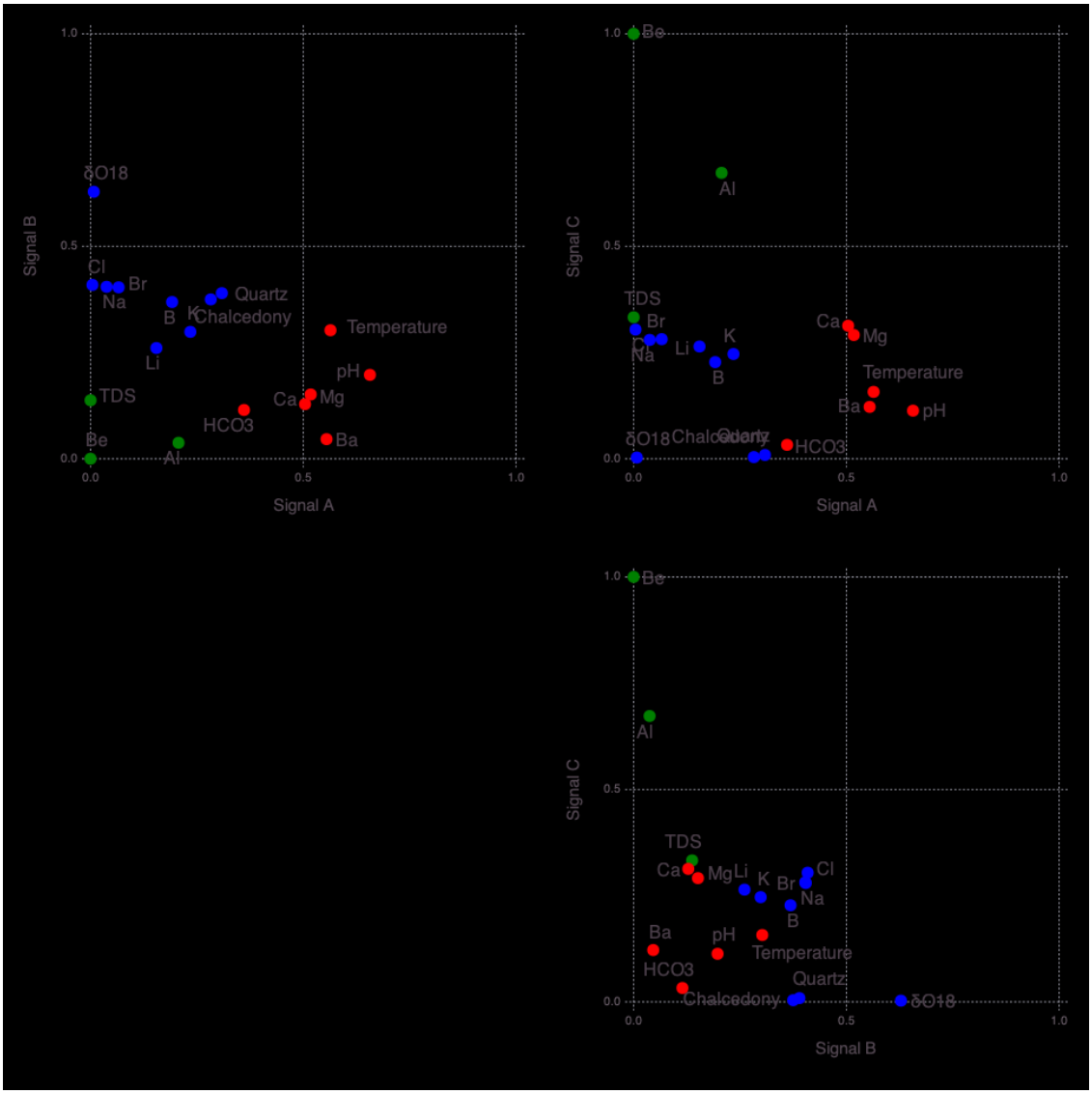

```
Info: Signal B (S2) (k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:333
Info: Signal C (S3) (k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:333
```


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

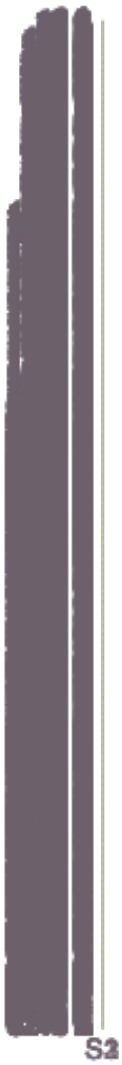

Signal 2
Signal 1
δO18
Na
Cl
Br
B
Quartz
Chalcedony
K
Li
Temperature
pH
Mg
Ca
HCO3
TDS
Ba
Be
Al
Signal 3
Signal 1
Be
Al
TDS
Br
Cl
Na
Li
K
B
Ca
Mg
Temperature
Ba
pH
HCO3
Chalcedony
Quartz
δO18
Signal 3
Signal 2
Be
Al
TDS
Ca
Mg
Li
Cl
Br
B
Na
K
Temperature
pH
Ba
Quartz
HCO3
Chalcedony
δO18




```
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
```

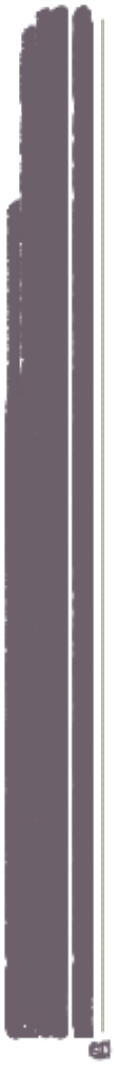
```
 "350"   0.492666
 "341"   0.491852
 "2730"  0.487104
 "3987"  0.47064
 "483"   0.466211
 "2909"  0.464978
 "476"   0.46367
 "2931"  0.435235
 "452"   0.359449
1966×2 Matrix{Any}:
 "4430"  1.0
 "2992"  0.972819
 "2309"  0.920633
 "4913"  0.90427
 "4056"  0.88218
 "564"   0.868838
 "4978"  0.866204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

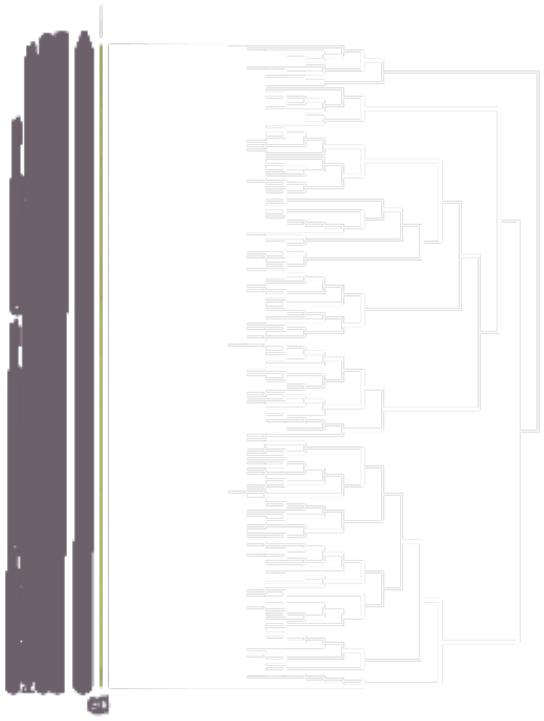
```
"4300"  0.160252
"2742"  0.148677
"4289"  0.144853
"2028"  0.129906
```

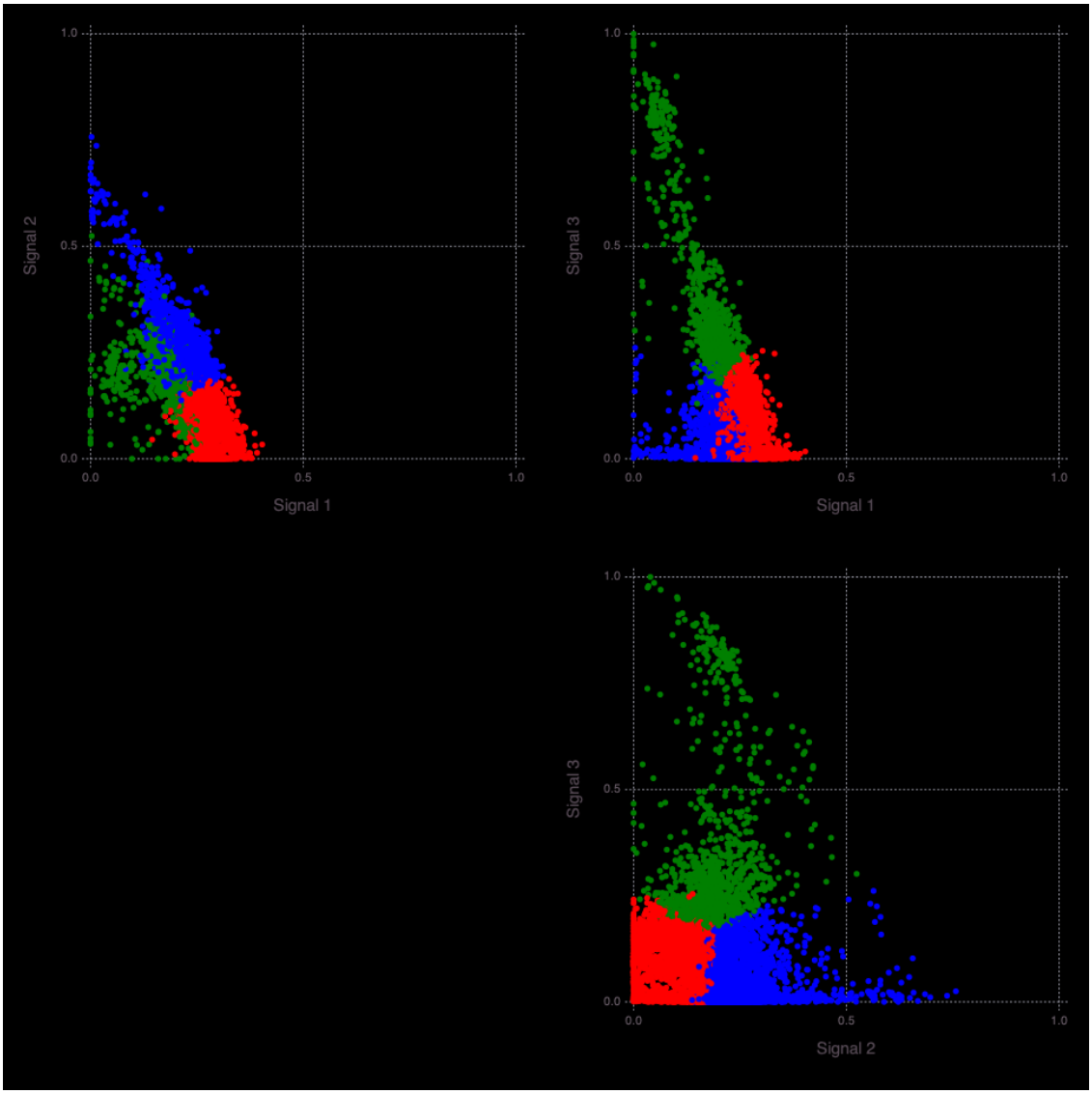


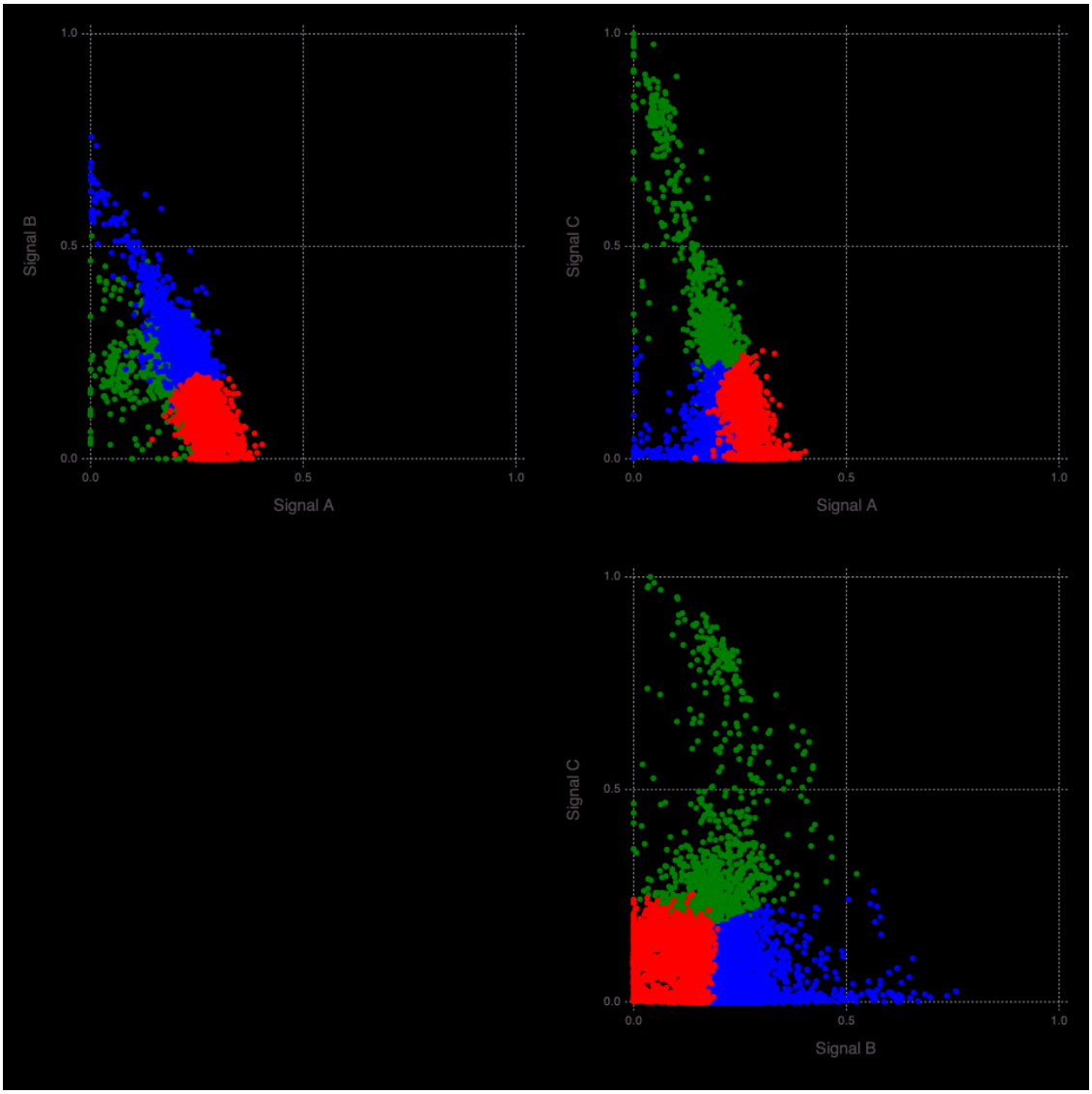

```
Info: Locations (signals=3)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:391
Info: Signal A (S1) Count: 2131
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:404
Info: Signal B (S2) Count: 1966
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:404
Info: Signal C (S3) Count: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

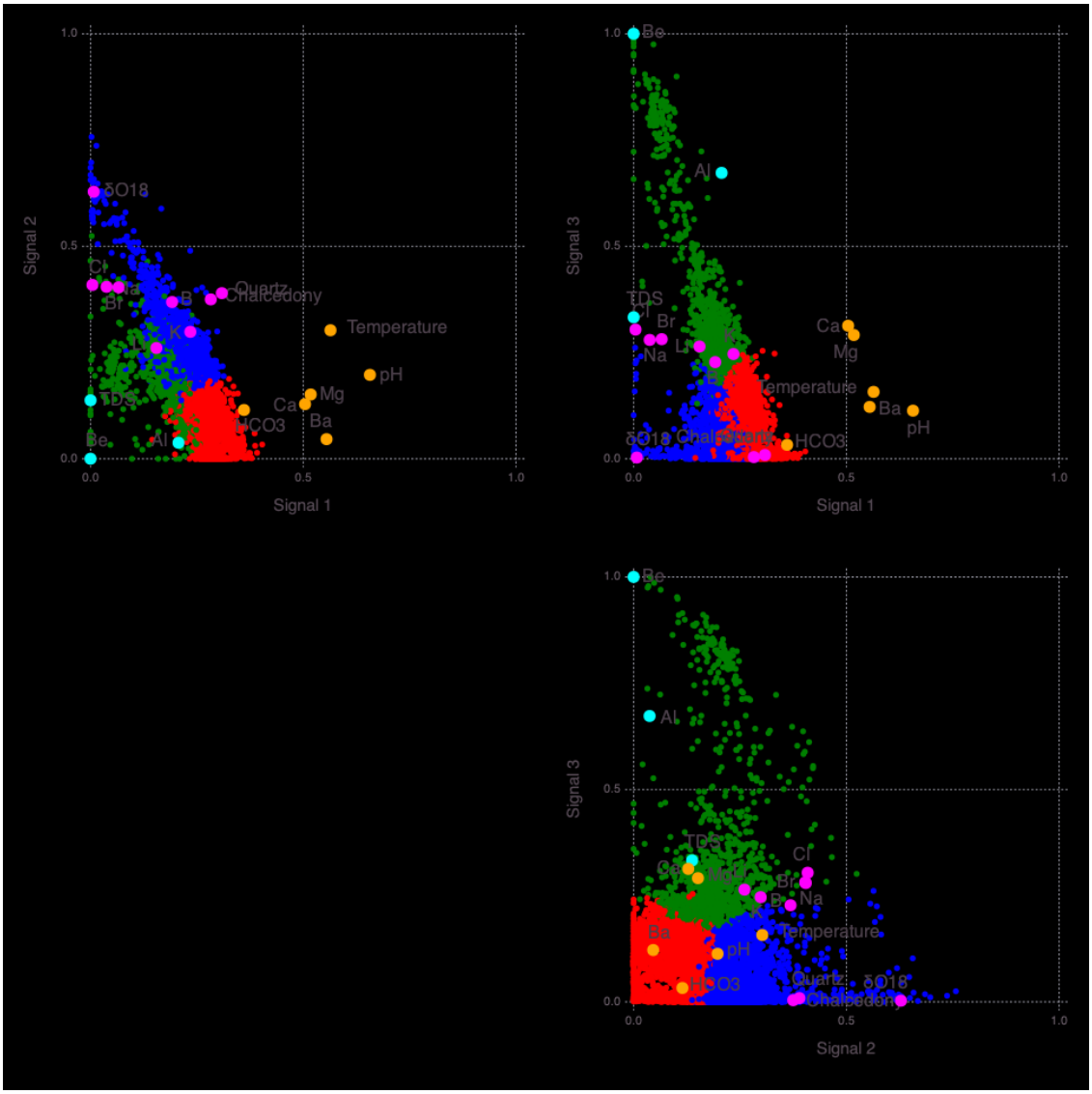
```
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:414
Info: Signal B -> B Count: 1966
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:414
Info: Signal C -> C Count: 1121
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:414
Info: Signal A (remapped k-means clustering)
@ NMFk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

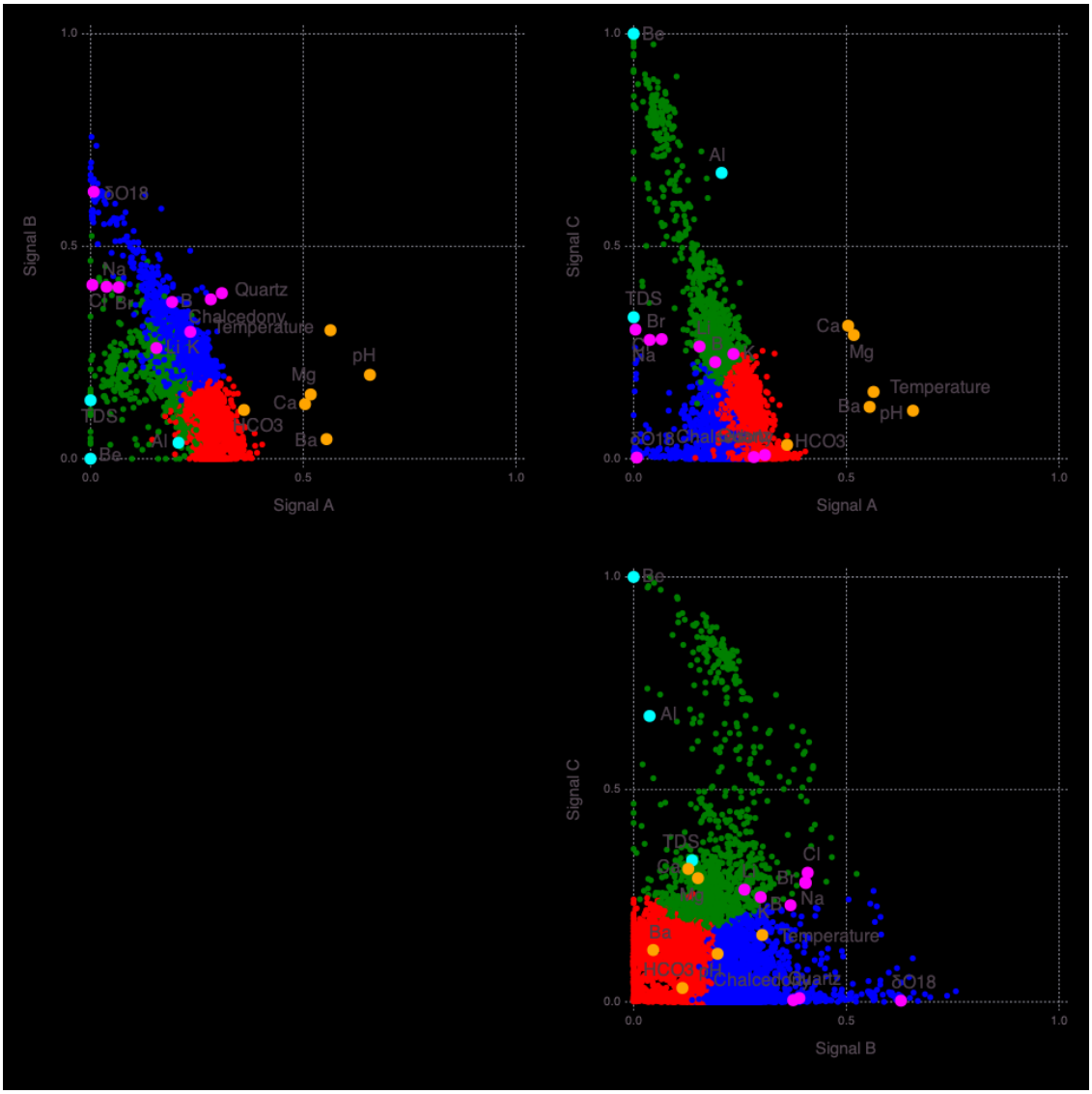





1.0
0.5
0.0
Signal 2
0.0
0.5
1.0
Signal 1
1.0
0.5
0.0
Signal 3
0.0
0.5
1.0
Signal 1
1.0
0.5
0.0
Signal 3
0.0
0.5
1.0
Signal 2


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


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




```
([[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

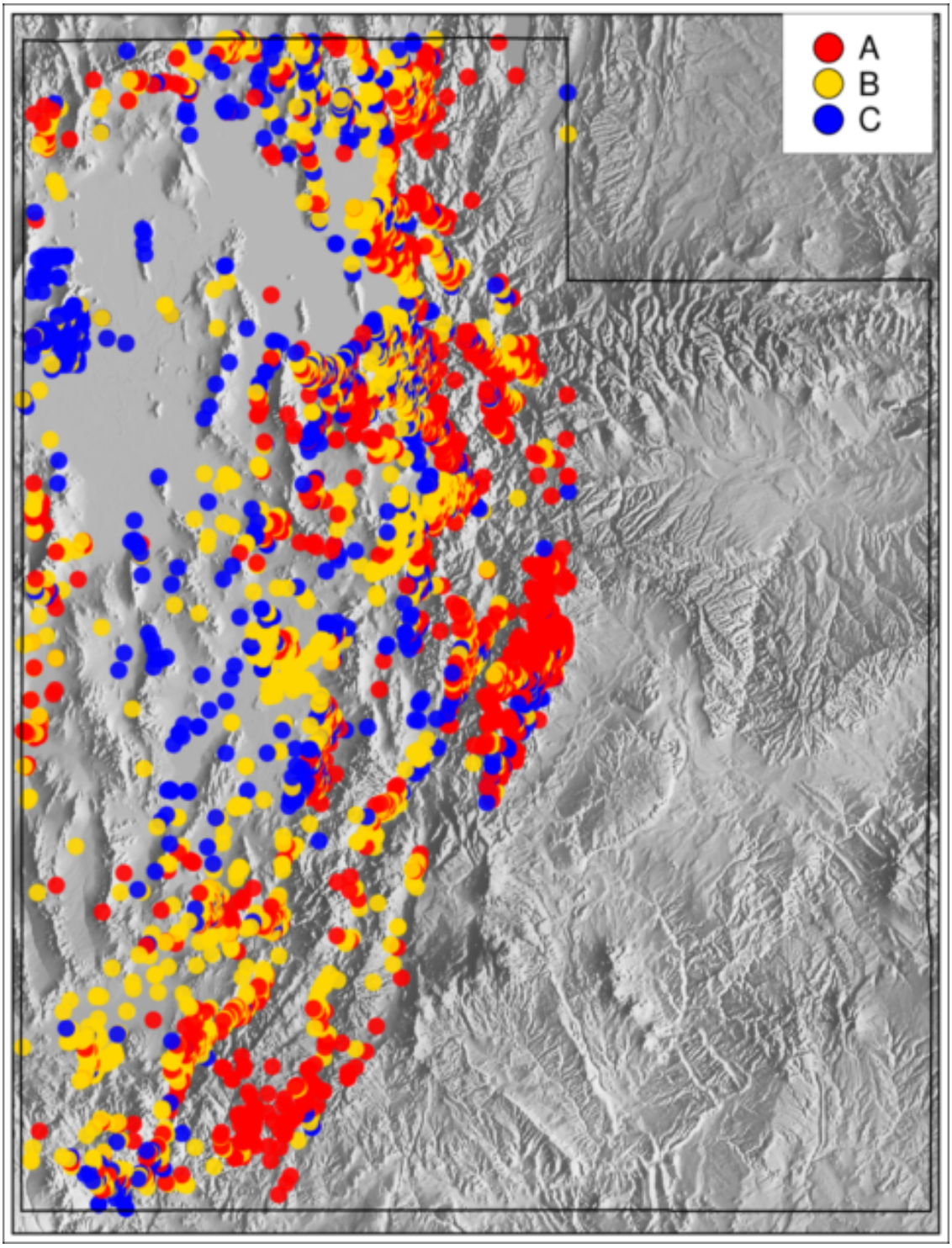
[24]:
```
locations, lhs = DelimitedFiles.readdlm("utah/results-postprocessing-nl-100/
 ↪locations-3.csv", ',', header=true)
clusters = sort(unique(locations[:,end]))
for i=1:size(clusters,1)
        locations[locations .== clusters[i]] .= Integer(i)
end
locations = convert.(Float32, locations)
```

```
5218×7 Matrix{Float32}:
    1.0  -111.06   39.4341  0.6627    0.0234368   0.124347    1.0
    2.0  -111.066  39.4233  0.670377  0.0287214   0.14722     1.0
    3.0  -111.053  39.4658  0.615474  8.88704f-7  0.203825    1.0
    4.0  -111.07   39.4286  0.669782  0.0108548   0.0435491   1.0
    5.0  -111.112  39.3211  0.640001  0.152409    0.00993296  1.0
    6.0  -111.056  39.4947  0.763099  5.00038f-5  0.0934381   1.0
    7.0  -111.056  39.4947  0.760624  0.0         0.0882335   1.0
    8.0  -111.057  39.4947  0.69465   0.0         0.175217    1.0
    9.0  -111.116  39.328   0.855406  0.0417626   0.00724127  1.0
   10.0  -111.113  39.3455  0.528689  0.181605    0.00429201  2.0

 5210.0  -113.908  41.6355  0.575887  0.313012    0.12041     2.0
 5211.0  -113.908  41.6369  0.497084  0.331514    0.00821709  2.0
 5212.0  -113.909  41.6333  0.569316  0.312737    0.110429    2.0
 5213.0  -113.935  41.5866  0.785556  0.214434    0.00475439  1.0
 5214.0  -113.919  41.6333  0.607505  0.337506    0.103709    2.0
```

```
 5215.0  -113.955  41.563   0.626563  0.314026    0.00605548  2.0
 5216.0  -113.936  41.6496  0.723449  0.206588    0.00947504  1.0
 5217.0  -113.926  41.7227  0.644214  0.224996    0.0861631   1.0
 5218.0  -113.984  41.6888  0.70402   0.208866    0.0225921   1.0
```

[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!(locations[:,2], locations[:,3], marker=:c, markersize=:0.15,
    color=(:red, :gold, :blue), zcolor=locations[:,end], 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")
```

```
   **** WARNING: .setopacityalpha is deprecated (as of 9.53.0) and will be
removed in a future release
   **** See .setfillconstantalpha/.setalphaisshape for the improved solution
   **** WARNING: .setopacityalpha is deprecated (as of 9.53.0) and will be
removed in a future release
   **** See .setfillconstantalpha/.setalphaisshape for the improved solution
pslegend [WARNING]: Representation of font type not recognized. Using default.
```


A
B
C