GreatBasin

March 25, 2021

0.1 Geothermal machine learning analysis: Great Basin

This notebook is a part of the GTcloud.jl: GeoThermal Cloud for Machine Learning.

```
<img src="../../logos/geothermalcloud-small.png" alt="geothermalcloud" width=25%  max-width=125
```

Machine learning analyses are performed using the **SmartTensors** machine learning framework.

```
<img src="../../logos/SmartTensorsNewSmaller.png" alt="SmartTensors" width=25%  max-width=125px
```

This notebook demonstrates how the **NMFk** module of **SmartTensors** can be applied to perform unsupervised geothermal machine-learning analyses.

```
<img src="../../logos/nmfk-logo.png" alt="nmfk" width=25%  max-width=125px;/>
```

More information how the ML results are interpreted to provide geothermal insights is discussed in our research paper.

0.2 Introduction

- The Great Basin is the largest area of contiguous endorheic watersheds in North America
- It spans nearly all of Nevada, much of Oregon and Utah, and portions of California, Idaho, Wyoming, and Baja California, Mexico
- The Great Basin includes multiple geothermal reservoirs ranging from low- to high-temperature
- The Great Basin has huge potential geothermal potential
- Further explorations requires understanding of the local / regional spatial / temporal patterns in various geothermal-related attributes

- Here, we apply our unsupervised machine learning method **NMFk** to analyze the available geothermal and geochemical data to better understand the spatial distribution of the hydrothermal resources
- Our study area (below) includes 14,258 data points

```
<img src="../img/greatbasin_data_locs_alt.png" alt="greatbasin_data_locs_alt" width=50%  max-wi
```

0.3 Import required libraries for this work

If **NMFk** is not installed, first execute in the Julia REPL `import Pkg; Pkg.add("NMFk"); Pkg.add("DelimitedFiles"); Pkg.add("JLD"); Pkg.add("Gadfly"); Pkg.add("Cairo"); Pkg.add("Fontconfig"); Pkg.add("Mads")`.

[1]:
```
import Cairo
import NMFk
import DelimitedFiles
import JLD
import Gadfly
import Fontconfig
import Mads
import Revise
```

0.4 Load and pre-process the data

0.4.1 Setup the working directory containing the Great Basin data

[2]:
```
cd("../");
```

0.4.2 Load the data file

[3]:
```
Xdat, headers = DelimitedFiles.readdlm("data/gb_duplicatedRows.txt", ',',␣
 ↪header=true);
```

0.4.3 Define names of the data attributes (matrix columns)

[4]:
```
attributes = ["Temperature", "Quartz", "Chalcedony", "pH", "TDS", "Al", "B",␣
 ↪"Ba", "Be", "Br", "Ca", "Cl", "HCO3", "K", "Li", "Mg", "Na", "δ18O"]
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)", "δ18O (‰)"];
```

Short attribute names are used for coding.

Long attribute names are used for plotting and visualization.

0.4.4 Define location coordinates

[5]:
```
xcoord = Array{Float32}(Xdat[:, 2])
ycoord = Array{Float32}(Xdat[:, 1]);
```

0.4.5 Duplicates

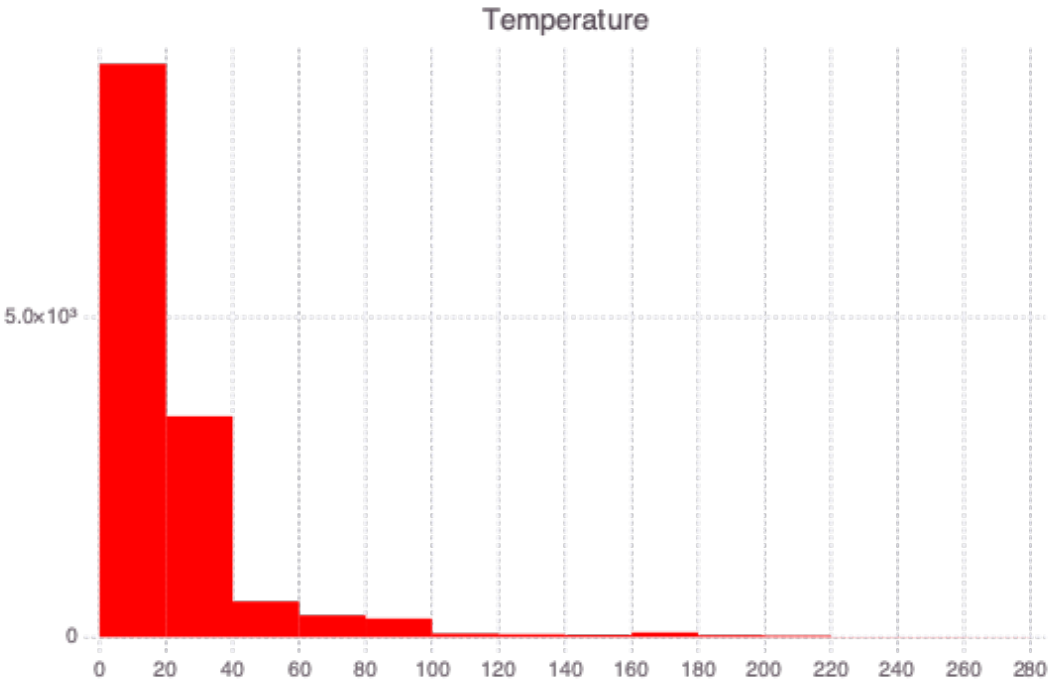
There 6 duplicate locations. However, this redundancy has been ignored.

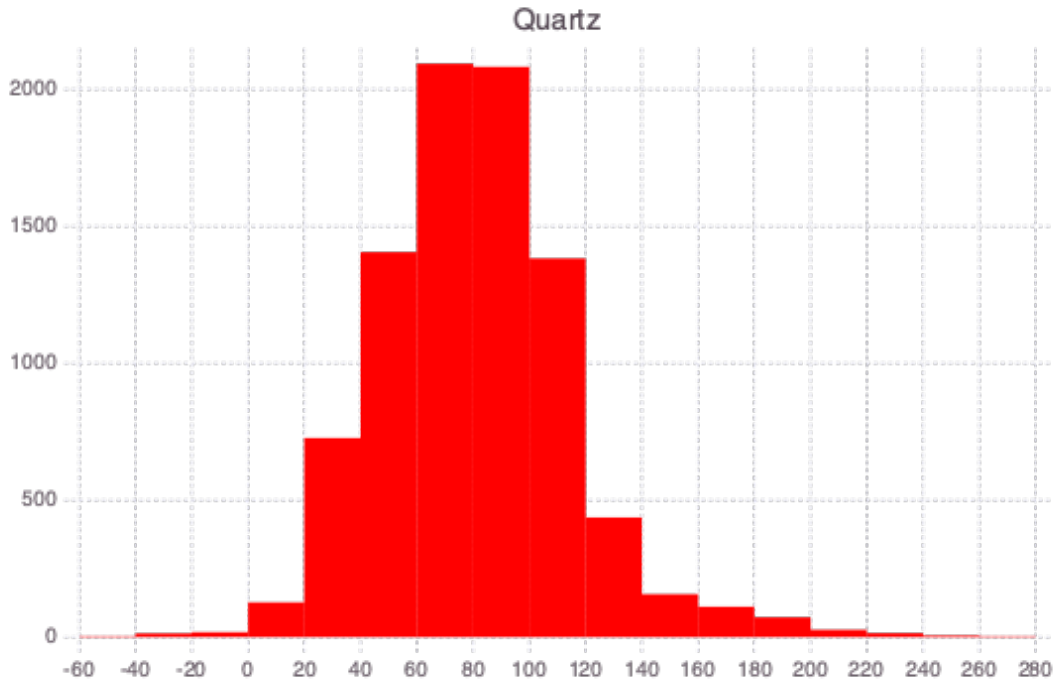
[6]:
```
length(xcoord) - size(unique([xcoord ycoord]; dims=1), 1)
```

[6]: 6

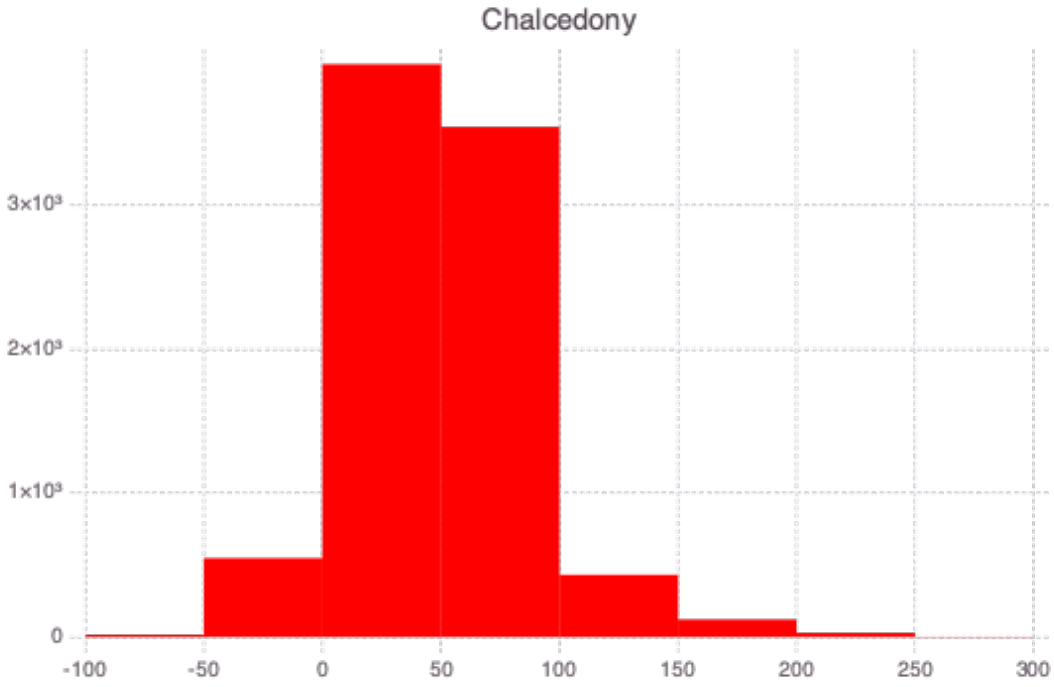
0.4.6 Pre-processing

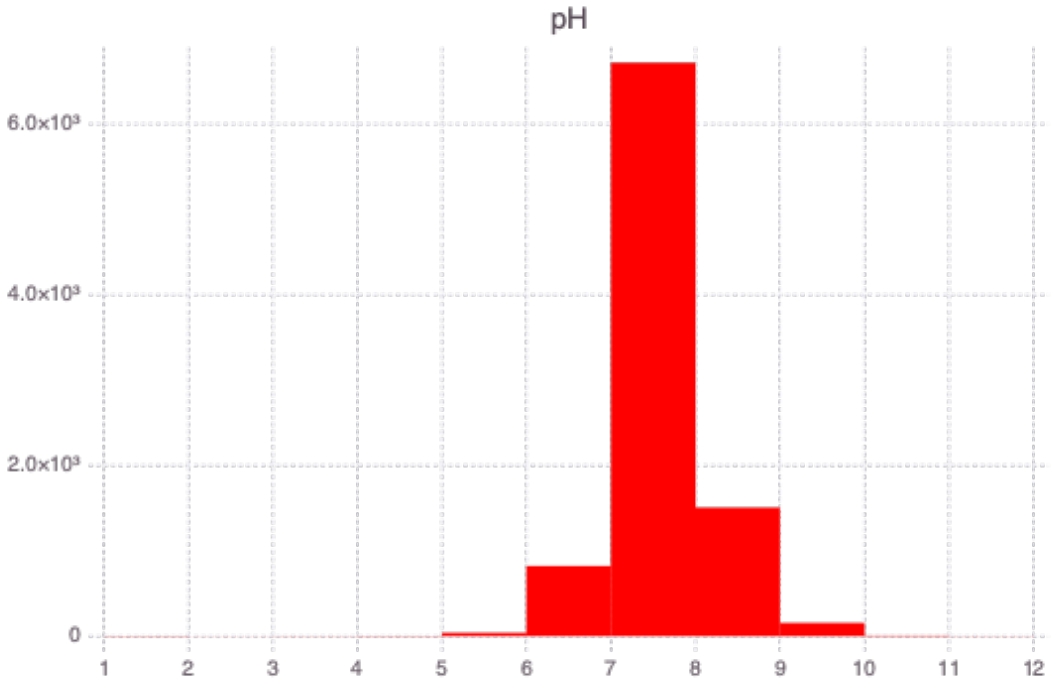
[7]:
```
Xdat[Xdat .== ""] .= NaN
X = convert.(Float32, Xdat[:,3:end])
X[:,16] .= abs.(X[:,16])
X[:,18] .+= 20 # rescale O18 data (%)

nattributes = length(attributes)
npoints = size(Xdat, 1)

NMFk.datanalytics(X, attributes; dims=2);
```





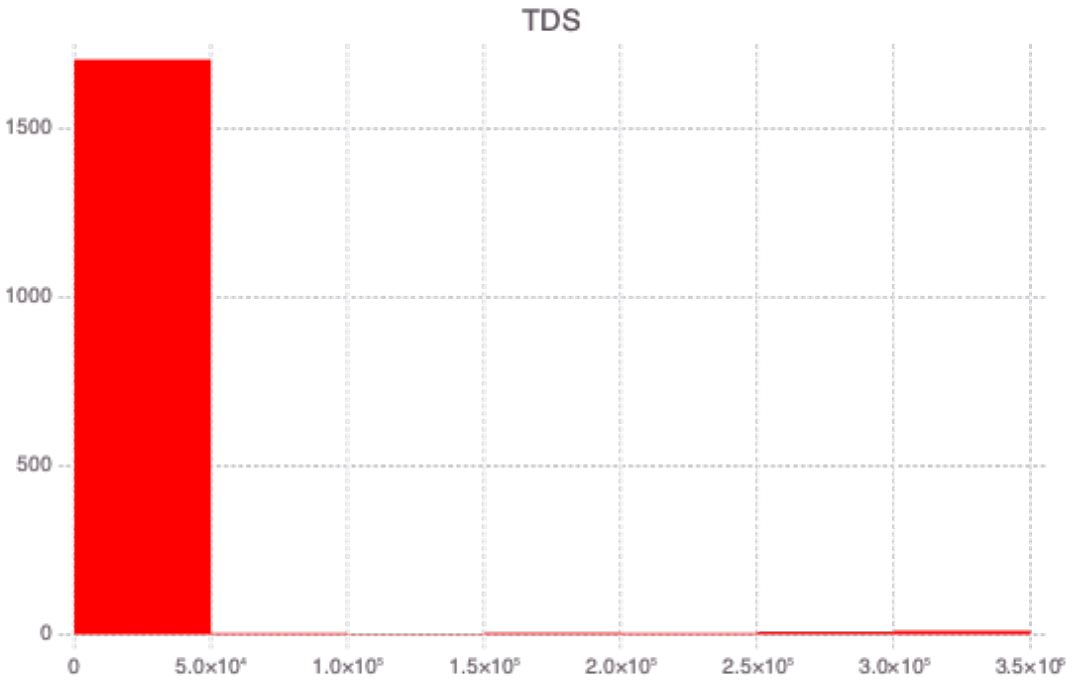

```
Temperature: Min 0.1 Max 275.0 StdDev 25.12217 Skewness 4.087667 Count 13894

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

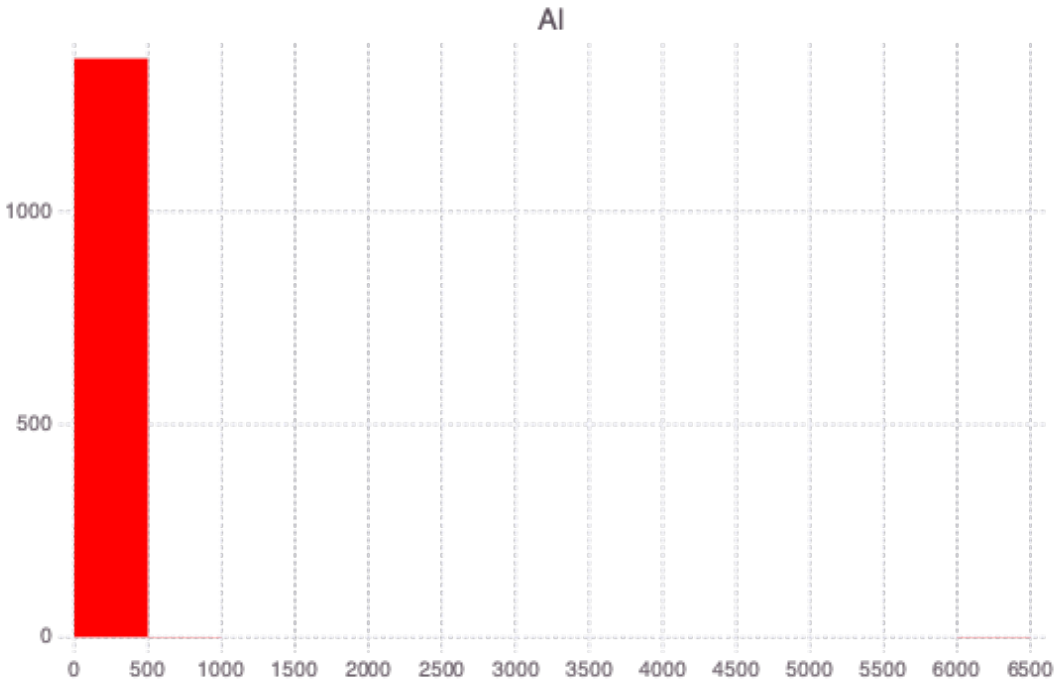

Chalcedony
3×10³
2×10³
1×10³
0
-100
-50
0
50
100
150
200
250
300


pH
6.0×10³
4.0×10³
2.0×10³
0
1
2
3
4
5
6
7
8
9
10
11
12

```
Quartz: Min -50.870045 Max 273.2438 StdDev 34.105637 Skewness 0.6946969 Count
8683
Chalcedony: Min -81.64773 Max 271.23828 StdDev 36.418324 Skewness 0.8679946
Count 8683
```

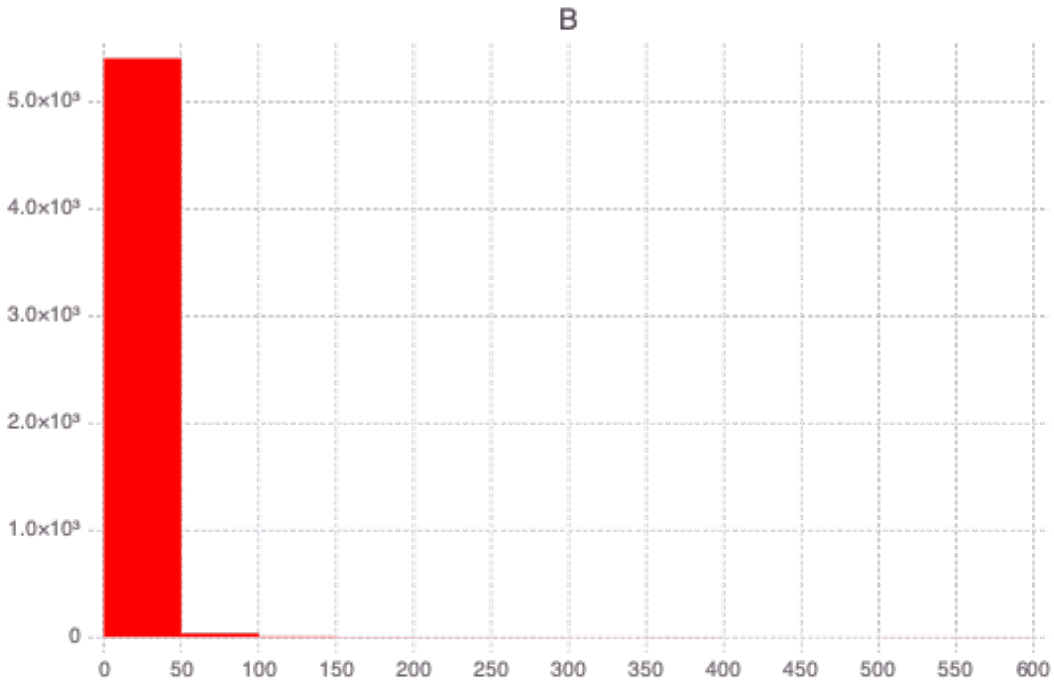
```
  Info: Chalcedony
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
  Info: pH
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

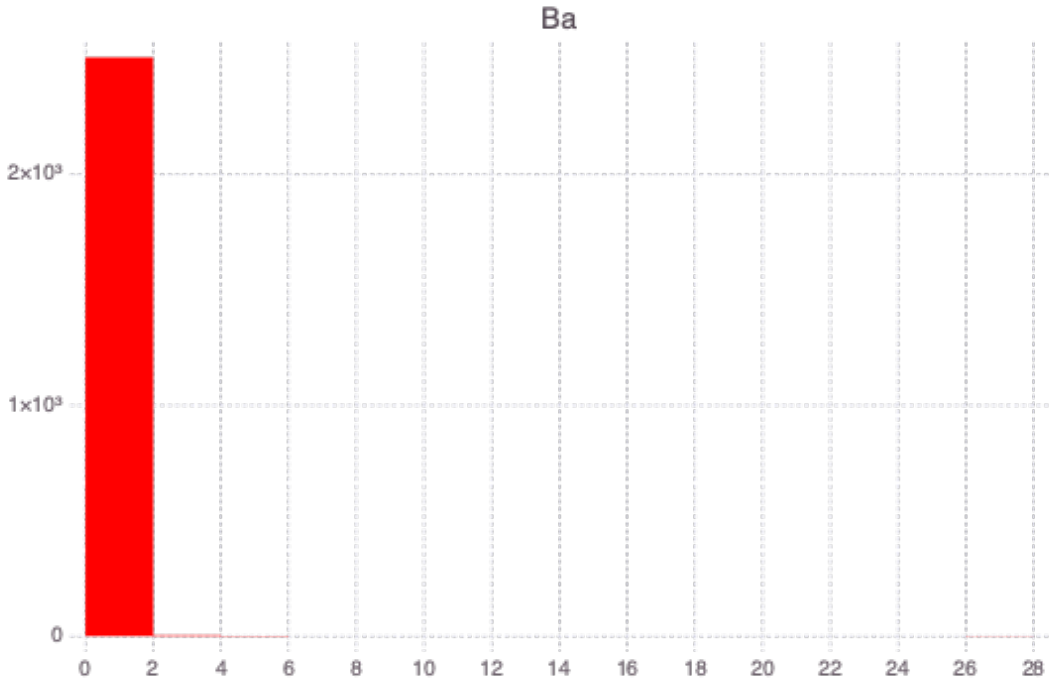





```
pH: Min 1.0 Max 11.7 StdDev 0.55800503 Skewness -0.5521828 Count 9261
TDS: Min 0.0 Max 329000.0 StdDev 34939.605 Skewness 7.7629066 Count 1740
```

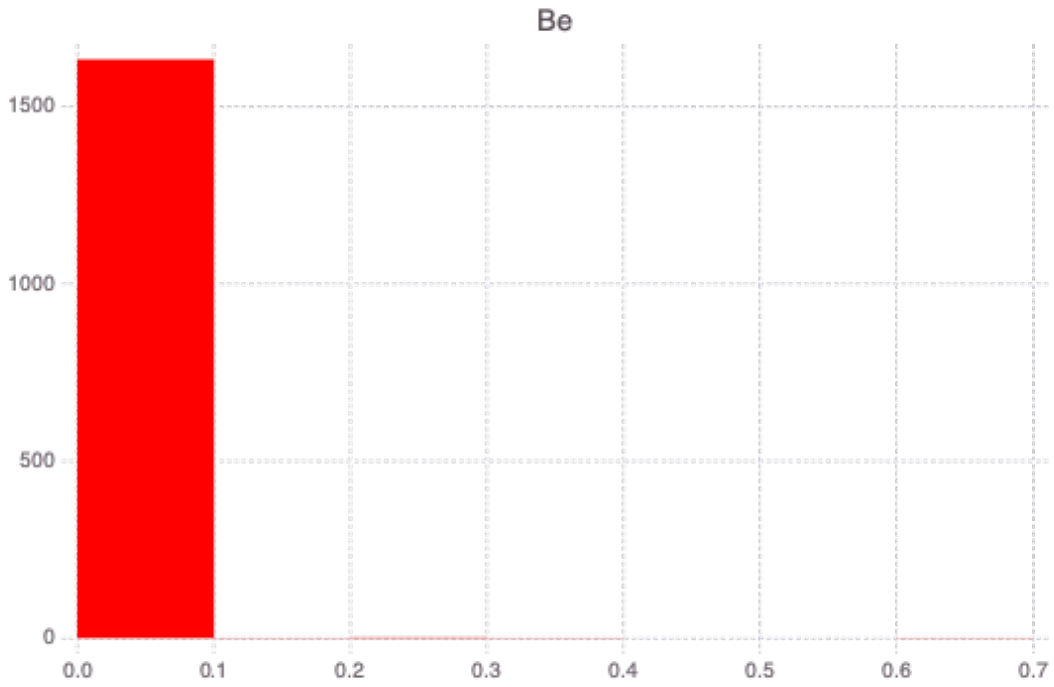
```
 Info: TDS
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 Info: Al
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

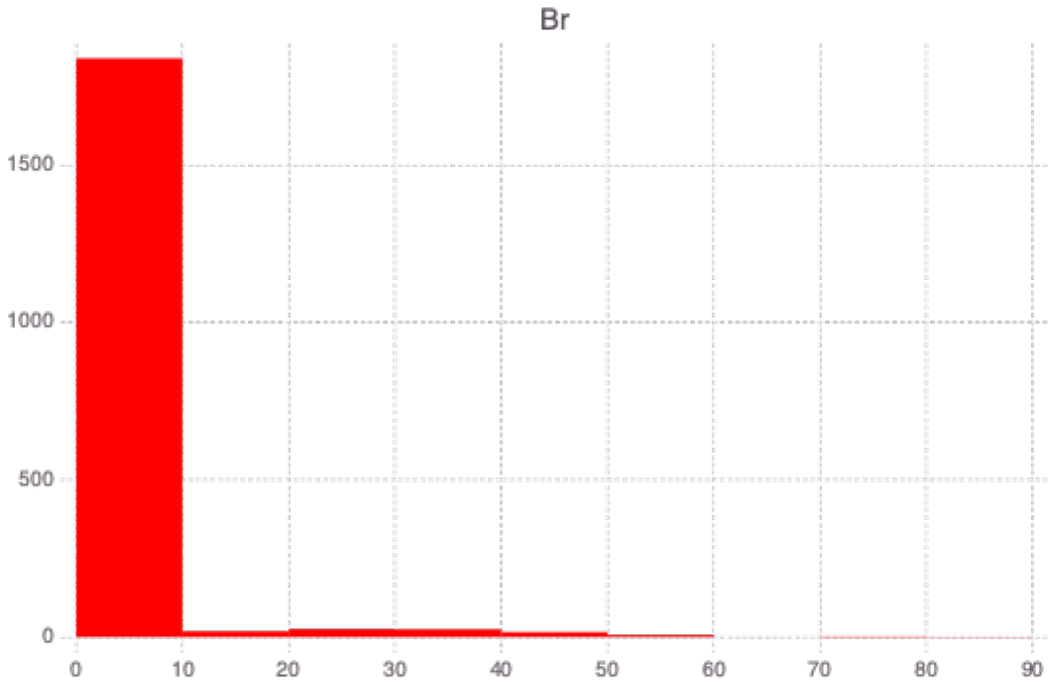

B
5.0x10³
4.0x10³
3.0x10³
2.0x10³
1.0x10³
0
0
50
100
150
200
250
300
350
400
450
500
550
600

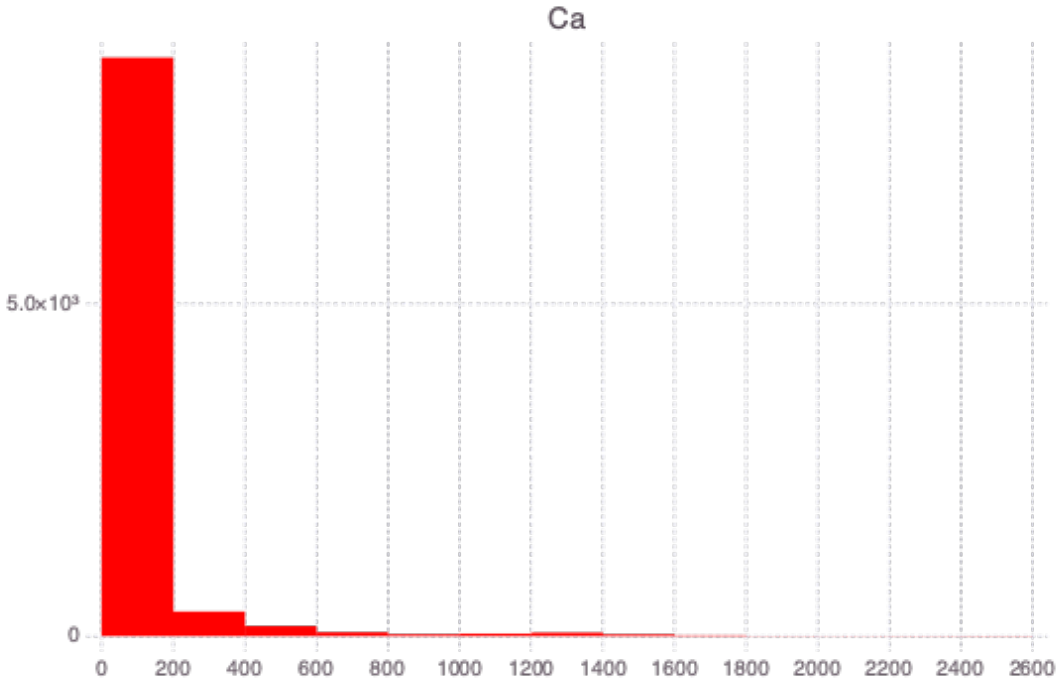

Ba
2x10³
1x10³
0
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28

```
Al: Min 0.0 Max 6400.0 StdDev 175.44391 Skewness 35.600906 Count 1362
B: Min 0.0 Max 590.0 StdDev 19.017153 Skewness 19.091574 Count 5462
```

```
 Info: B
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 Info: Ba
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

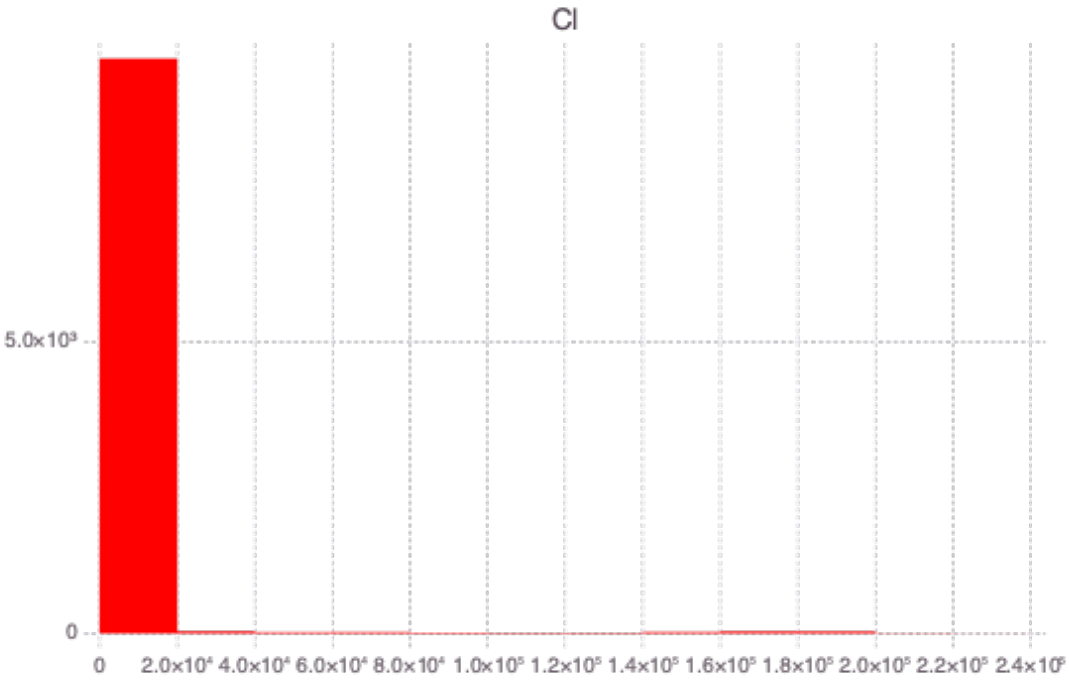


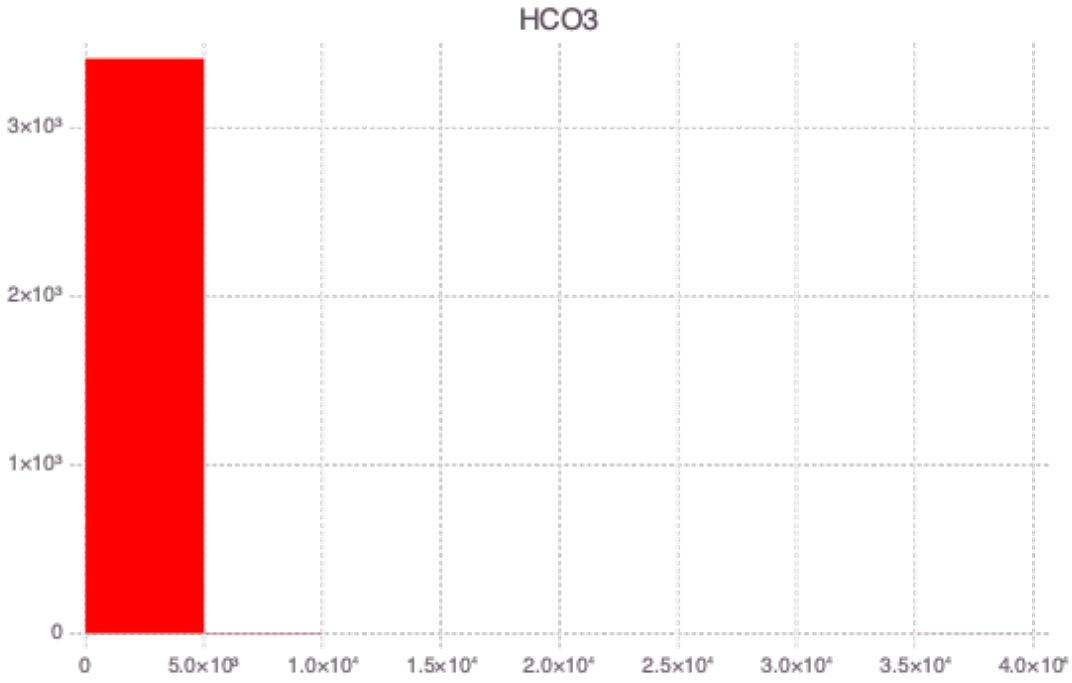

Br
1500
1000
500
0
0
10
20
30
40
50
60
70
80
90

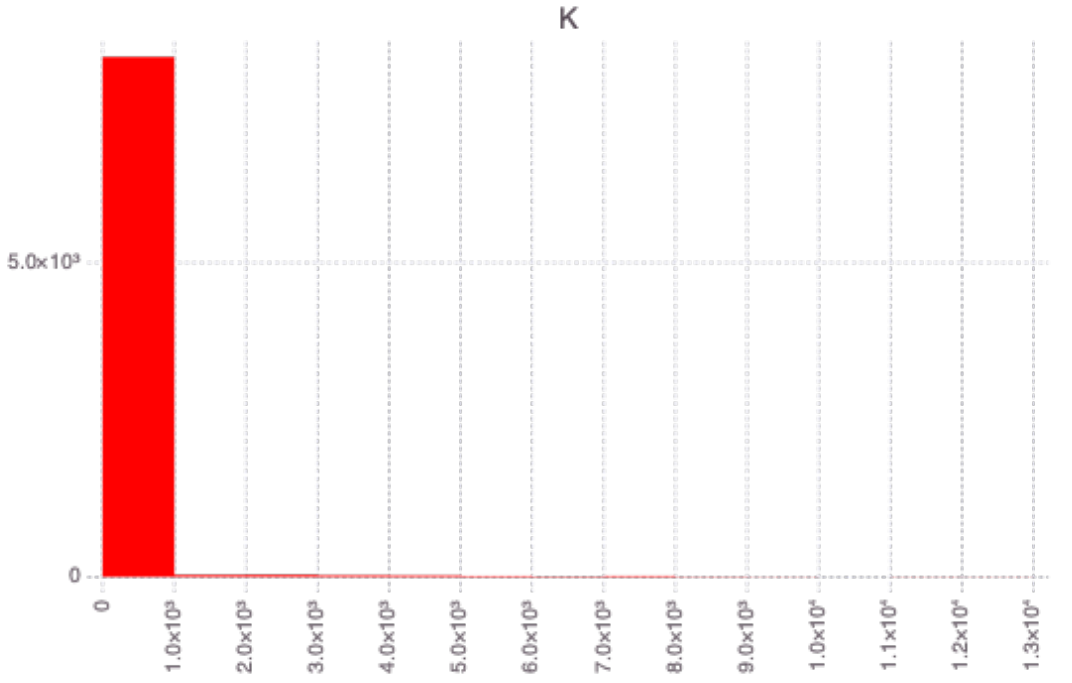

Ca
5.0×10³
0
0
200
400
600
800
1000
1200
1400
1600
1800
2000
2200
2400
2600

```
Ba: Min 0.0 Max 27.430857 StdDev 0.58066297 Skewness 41.943157 Count 2516
Be: Min 0.0 Max 0.7 StdDev 0.020862982 Skewness 26.046818 Count 1640
Br: Min 0.0 Max 84.0 StdDev 7.721104 Skewness 5.398518 Count 1935
```

```
 Info: Be
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 Info: Br
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 Info: Ca
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

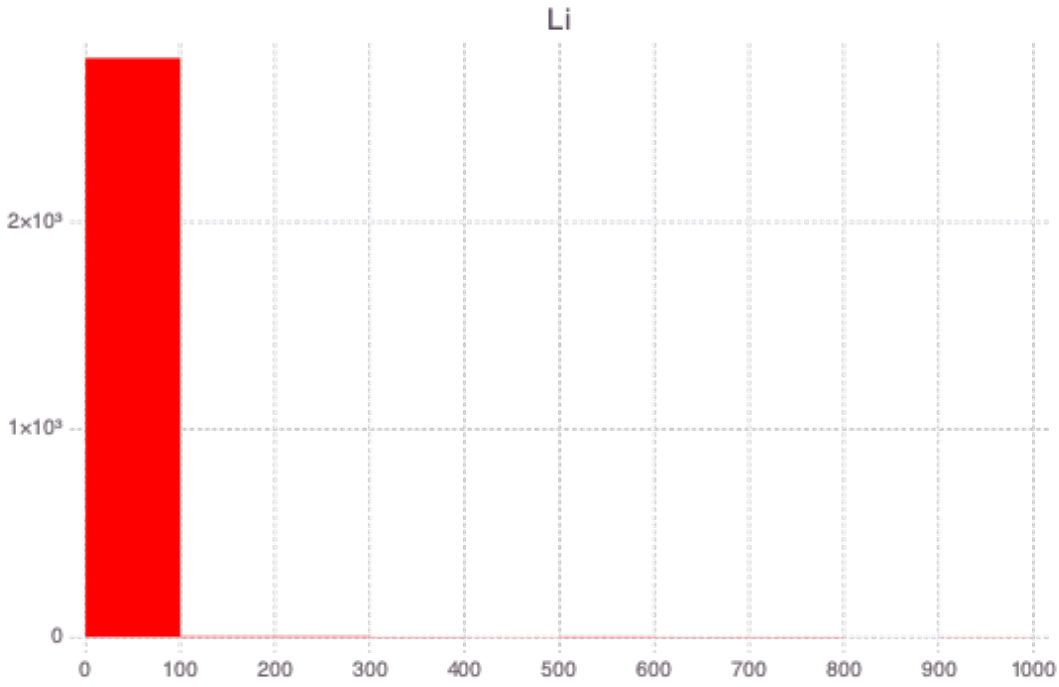


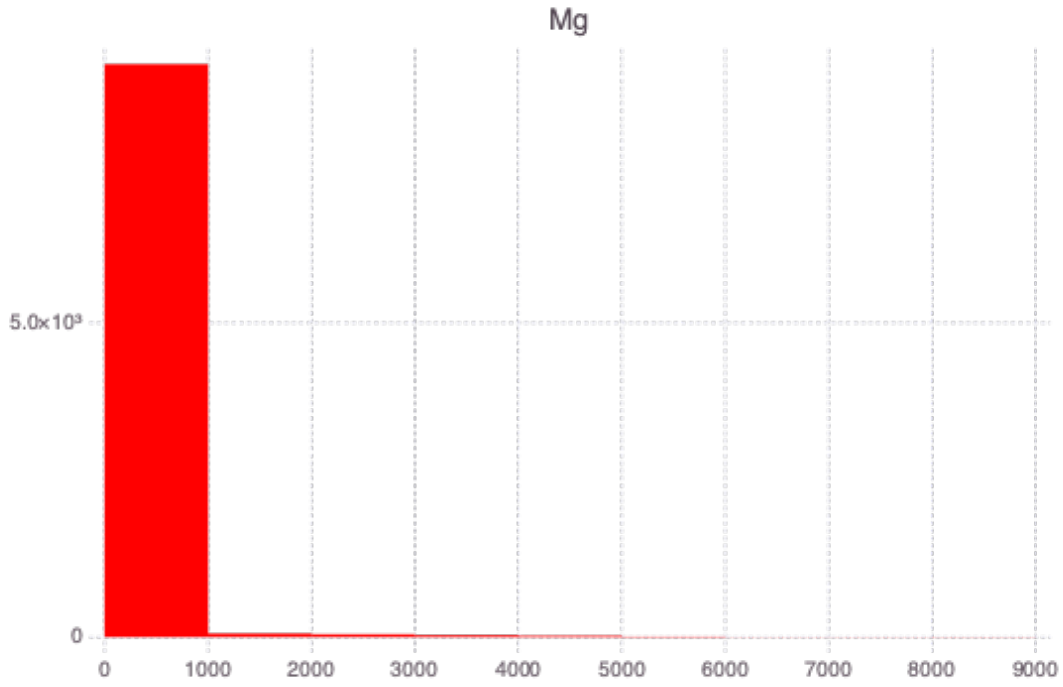

HCO3
3×10³
2×10³
1×10³
0
0
5.0×10³
1.0×10⁴
1.5×10⁴
2.0×10⁴
2.5×10⁴
3.0×10⁴
3.5×10⁴
4.0×10⁴


K
5.0×10³
0
0
1.0×10³
2.0×10³
3.0×10³
4.0×10³
5.0×10³
6.0×10³
7.0×10³
8.0×10³
9.0×10³
1.0×10⁴
1.1×10⁴
1.2×10⁴
1.3×10⁴

```
Ca: Min 0.0 Max 2566.6667 StdDev 191.38284 Skewness 5.880362 Count 9468
Cl: Min 0.0 Max 240000.0 StdDev 19115.326 Skewness 8.088112 Count 10091
HCO3: Min 0.0 Max 37000.0 StdDev 740.00256 Skewness 37.66232 Count 3413
```

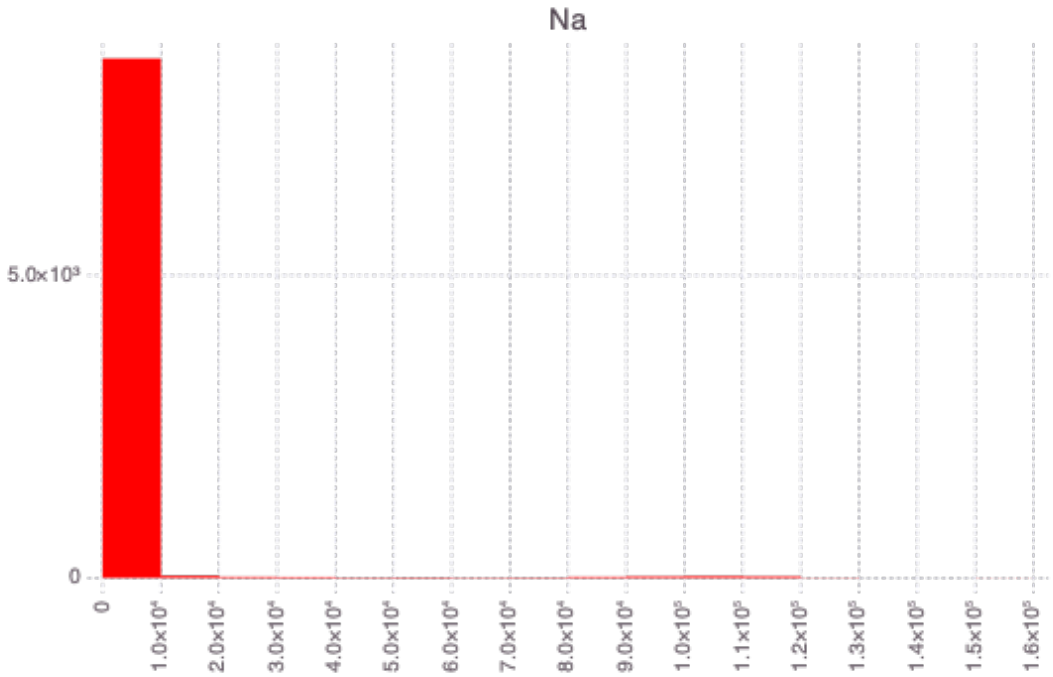
```
┌ Info: Cl
└ @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
┌ Info: HCO3
└ @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
┌ Info: K
└ @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

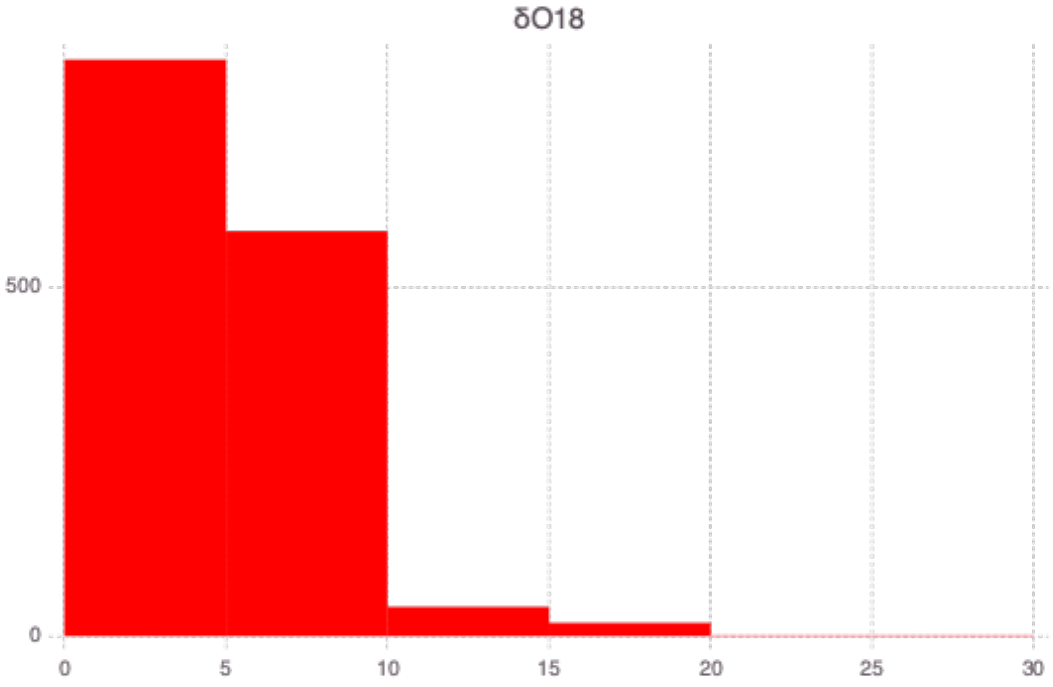





```
K: Min 0.0 Max 13000.0 StdDev 692.70734 Skewness 9.866844 Count 8446
Li: Min 0.0 Max 970.0 StdDev 41.178646 Skewness 15.181558 Count 2809
```

```
 Info: Li
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 Info: Mg
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```


Na
5.0x10³
0
0
1.0x10⁴
2.0x10⁴
3.0x10⁴
4.0x10⁴
5.0x10⁴
6.0x10⁴
7.0x10⁴
8.0x10⁴
9.0x10⁴
1.0x10⁵
1.1x10⁵
1.2x10⁵
1.3x10⁵
1.4x10⁵
1.5x10⁵
1.6x10⁵


δO18
500
0
0
5
10
15
20
25
30

```
Mg: Min 0.0 Max 8500.0 StdDev 454.54953 Skewness 9.703973 Count 9296
Na: Min 0.0 Max 160000.0 StdDev 12159.811 Skewness 7.597518 Count 8814
 O18: Min 0.79999924 Max 27.85 StdDev 2.772077 Skewness 2.0067368 Count 1471
Name Min Max StdDev Count (non-NaN's)
Temperature 0.1 275.0 25.12217 4.087667 13894
Quartz -50.870045 273.2438 34.105637 0.6946969 8683
Chalcedony -81.64773 271.23828 36.418324 0.8679946 8683
pH 1.0 11.7 0.55800503 -0.5521828 9261
TDS 0.0 329000.0 34939.605 7.7629066 1740
Al 0.0 6400.0 175.44391 35.600906 1362
B 0.0 590.0 19.017153 19.091574 5462
Ba 0.0 27.430857 0.58066297 41.943157 2516
Be 0.0 0.7 0.020862982 26.046818 1640
Br 0.0 84.0 7.721104 5.398518 1935
Ca 0.0 2566.6667 191.38284 5.880362 9468
Cl 0.0 240000.0 19115.326 8.088112 10091
HCO3 0.0 37000.0 740.00256 37.66232 3413
K 0.0 13000.0 692.70734 9.866844 8446
Li 0.0 970.0 41.178646 15.181558 2809
Mg 0.0 8500.0 454.54953 9.703973 9296
Na 0.0 160000.0 12159.811 7.597518 8814
 O18 0.79999924 27.85 2.772077 2.0067368 1471

  Info: Na
  @ 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
```

It is important to note that a lot of the attribute data are missing.

Attribute name	Minimum	Mean	Maximum	Missing (%)
Groundwater temperature (℃)	0.1	23.7	275	2.6
Quartz geothermometer (℃)	-50.8	81	273	39.1
Chalcedony geothermometer (℃)	-81.6	50.3	271	39.1
pH	1	7.5	11.7	35
TDS (total dissolved solid) (PPM)	0	5770	329000	87.8
Al^{3+} (PPM)	0	7.3	6400	90.5
B^{+} (PPM)	0	3.1	590	61.7
Ba^{2+} (PPM)	0	0.1	27.4	82.4
Be^{2+} (PPM)	0	0	0.7	88.5
Br^{-} (PPM)	0	2	84	86.4
Ca^{2+} (PPM)	0	97	2570	33.6
Cl^{-} (PPM)	0	2870	240000	29.2
HCO_3^{-} (PPM)	0	278	37000	76.1
K^{+} (PPM)	0	101	13000	40.8
Li^{+} (PPM)	0	4.95	970	80.3
Mg^{2+} (PPM)	0	86.8	8500	34.8
Na^{+} (PPM)	0	1960	160000	38.2
$\delta^{18}O$ (‰)	-19.2	-14.6	7.8	89.7

Close to complete records are available only for `Temperature`.

Data 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.

0.4.7 Log-transformation

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

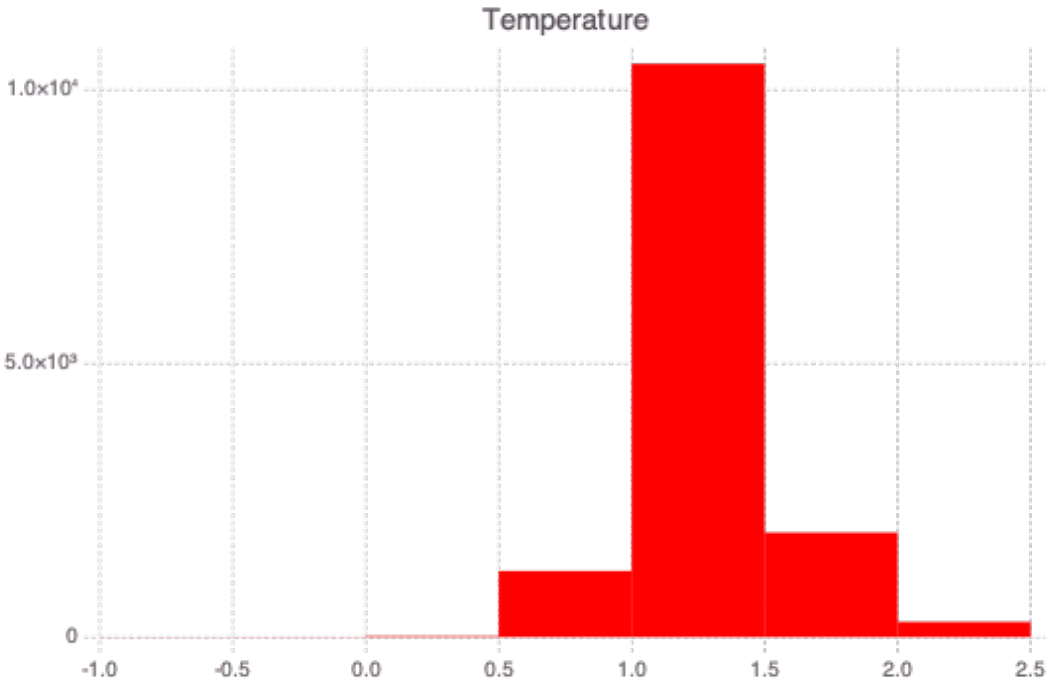
All attributes execpt for `Quartz`, `Chalcedony` and `pH` are log-transformed.

[8]:
```
logv = [true, false, false, false,  true, true, true, true, true, true, true,␣
 ↪true, true, true, true, true, true, true]
[attributes logv]
```

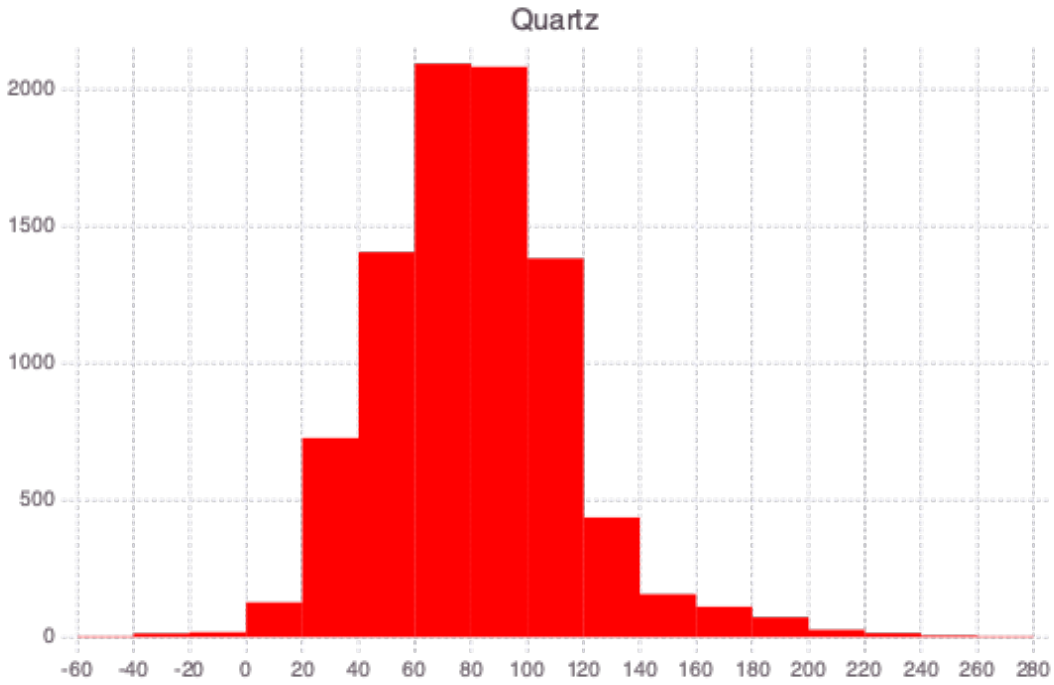
[8]:
```
18×2 Array{Any,2}:
 "Temperature"   true
 "Quartz"       false
 "Chalcedony"   false
 "pH"           false
 "TDS"           true
 "Al"            true
 "B"             true
 "Ba"            true
 "Be"            true
 "Br"            true
```

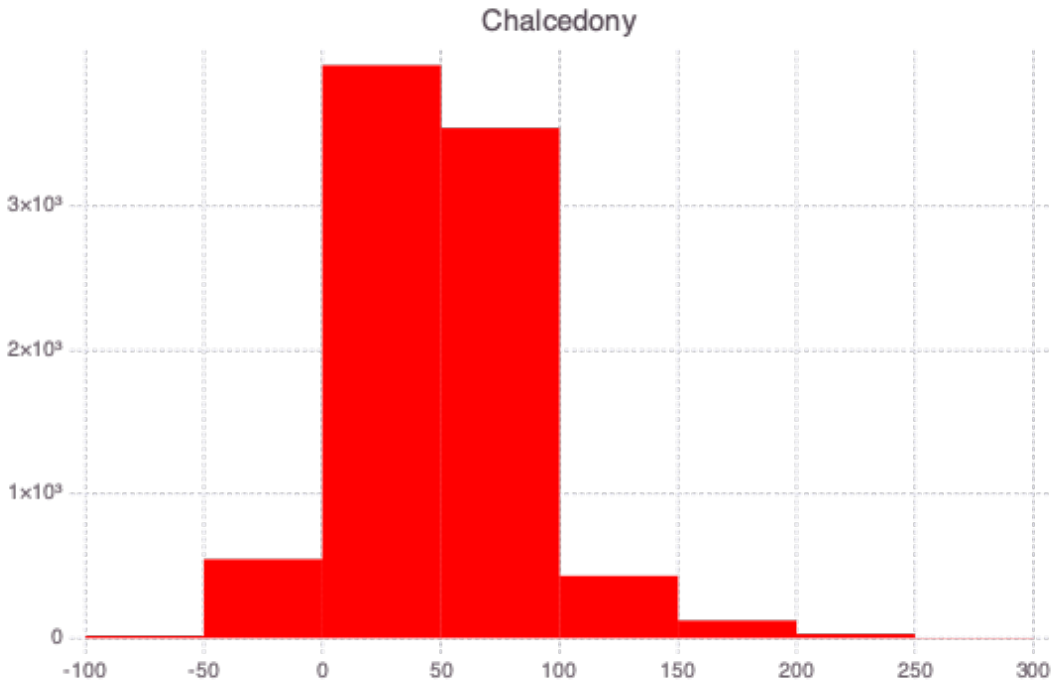
```
"Ca"            true
"Cl"            true
"HCO3"          true
"K"             true
"Li"            true
"Mg"            true
"Na"            true
" O18"         true
```

[9]:
```
NMFk.datanalytics(X, attributes; dims=2, logv=logv);
```



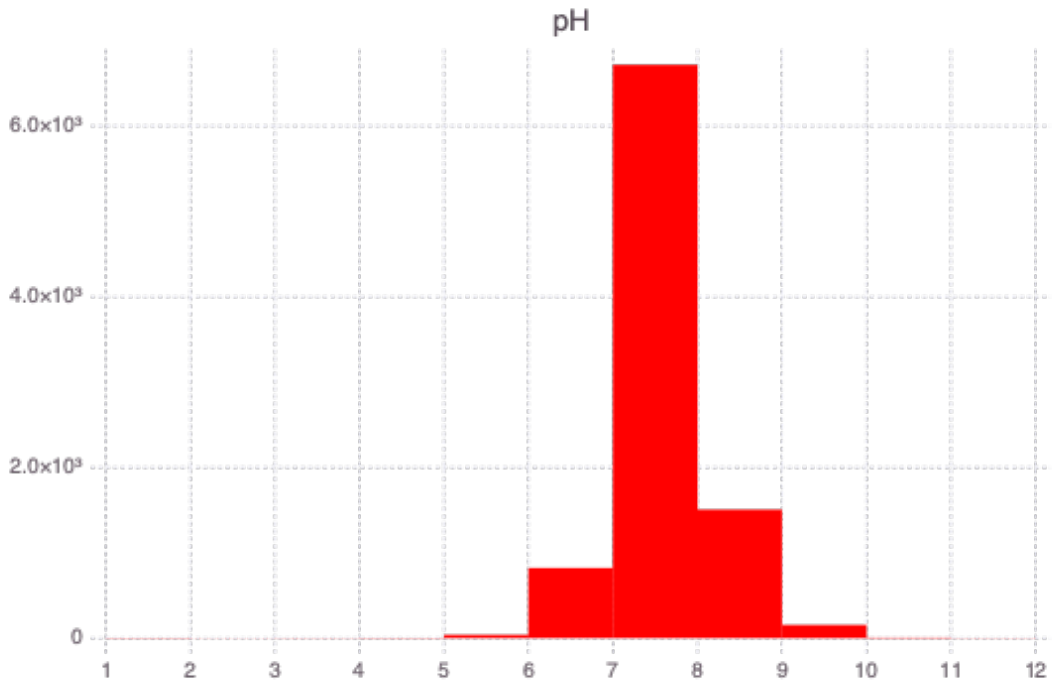

```
Info: Temperature: log10-transformed
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```

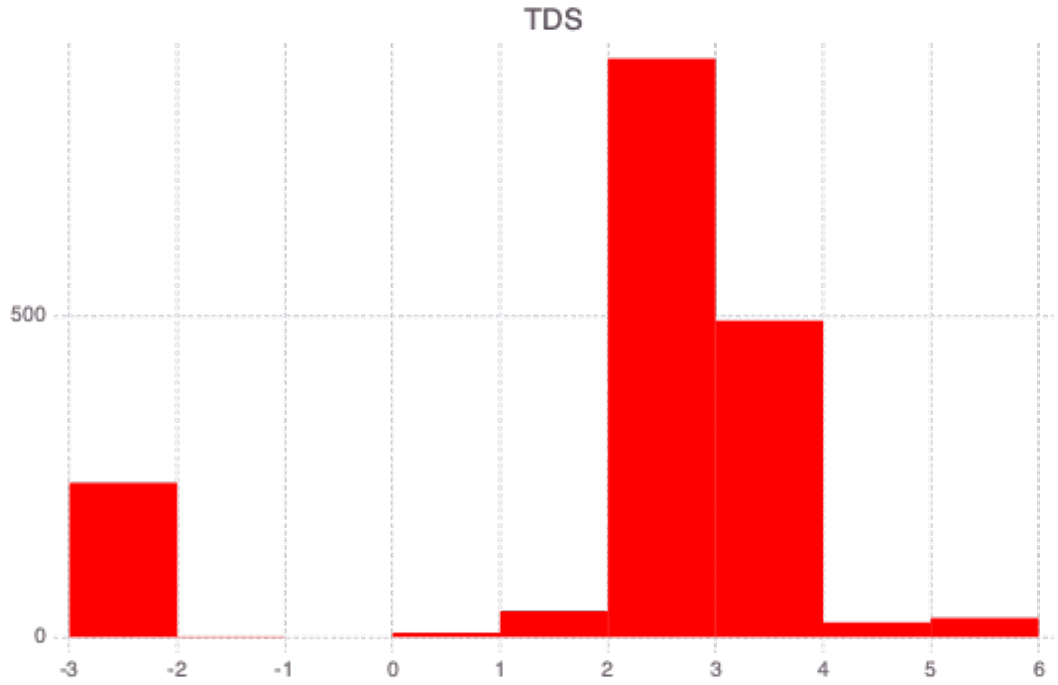

Quartz
2000
1500
1000
500
0
-60
-40
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280


Chalcedony
3×10³
2×10³
1×10³
0
-100
-50
0
50
100
150
200
250
300

```
Temperature: Min -1.0 Max 2.4393327 StdDev 0.28062904 Skewness 0.8823397 Count
13894
Quartz: Min -50.870045 Max 273.2438 StdDev 34.105637 Skewness 0.6946969 Count
8683
```

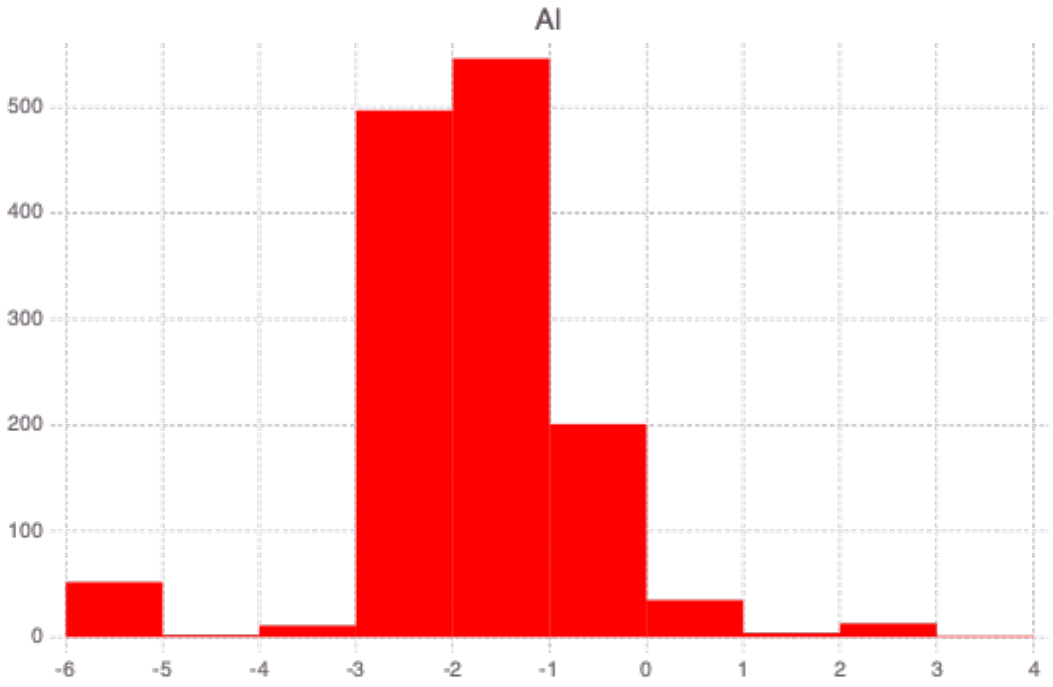
```
 Info: Quartz
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 Info: Chalcedony
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
```

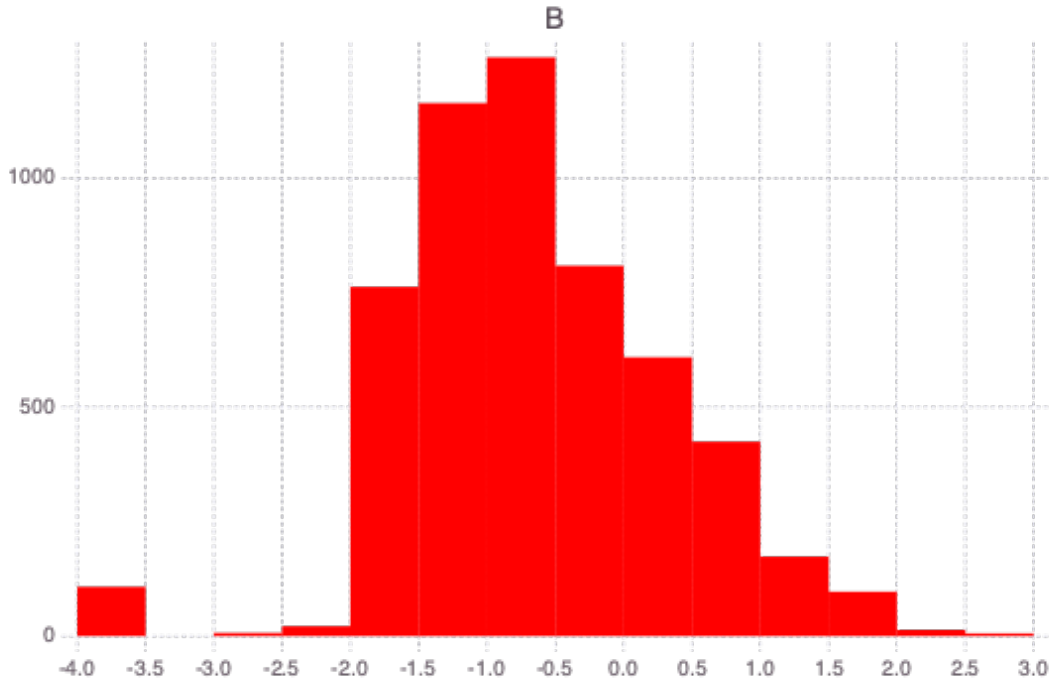




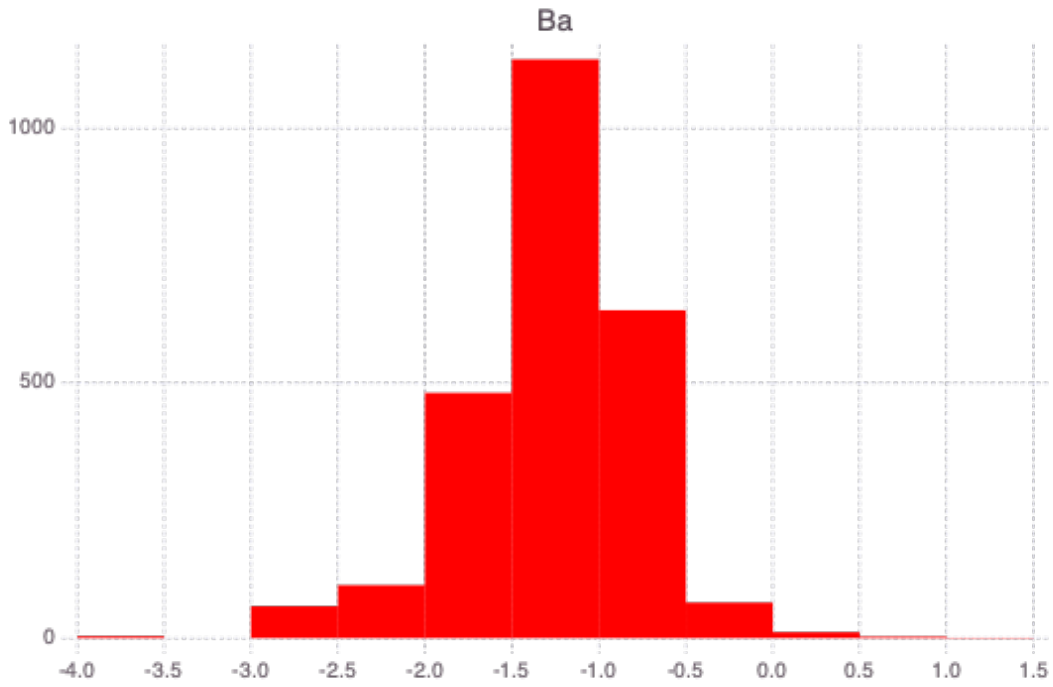

```
Chalcedony: Min -81.64773 Max 271.23828 StdDev 36.418324 Skewness 0.8679946
Count 8683
pH: Min 1.0 Max 11.7 StdDev 0.55800503 Skewness -0.5521828 Count 9261
```

```
 Info: pH
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 Info: TDS: log10-transformed
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```

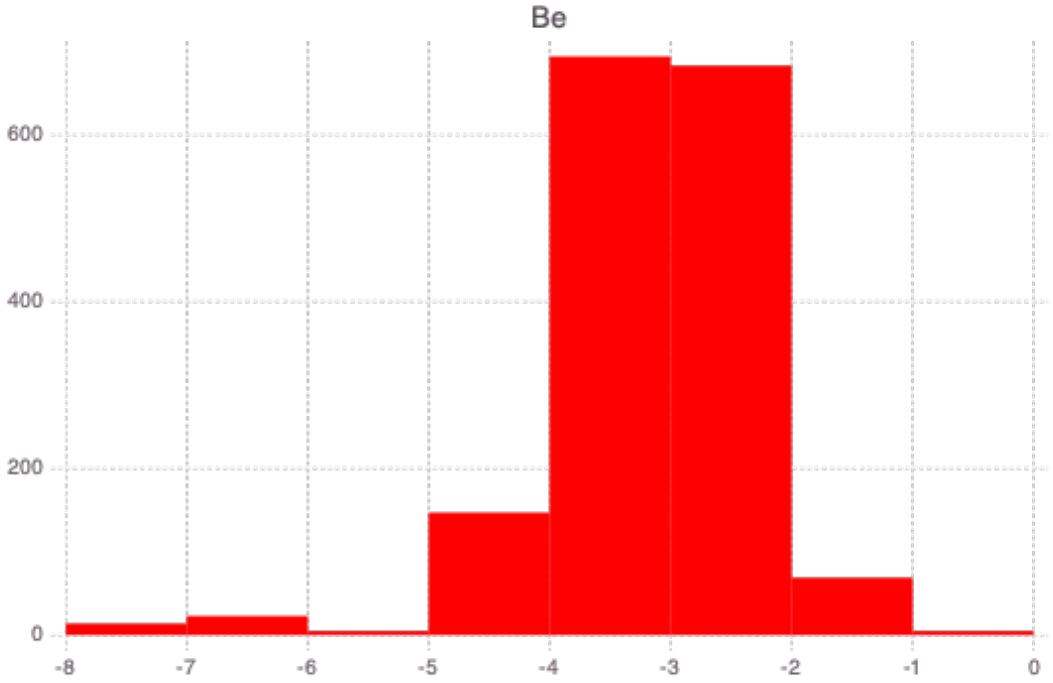

Al
500
400
300
200
100
0
-6
-5
-4
-3
-2
-1
0
1
2
3
4

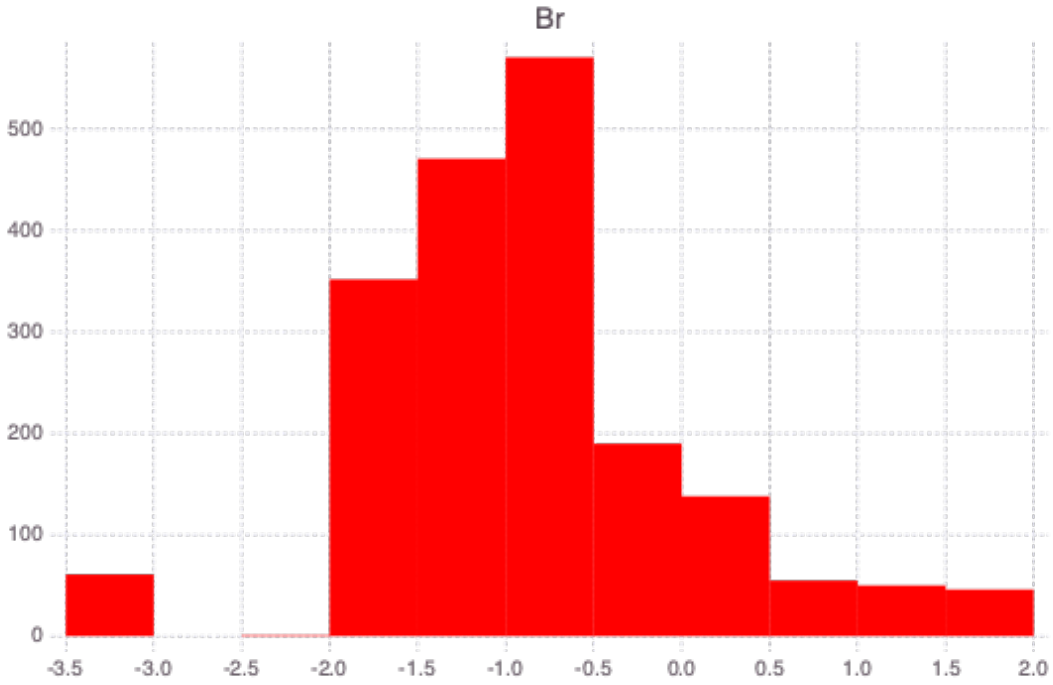

B
1000
500
0
-4.0
-3.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0

```
TDS: Min -2.6989698 Max 5.5171957 StdDev 2.0129914 Skewness -1.7111415 Count
1740
Al: Min -5.8860564 Max 3.80618 StdDev 1.2161667 Skewness -0.44271475 Count 1362

  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
```



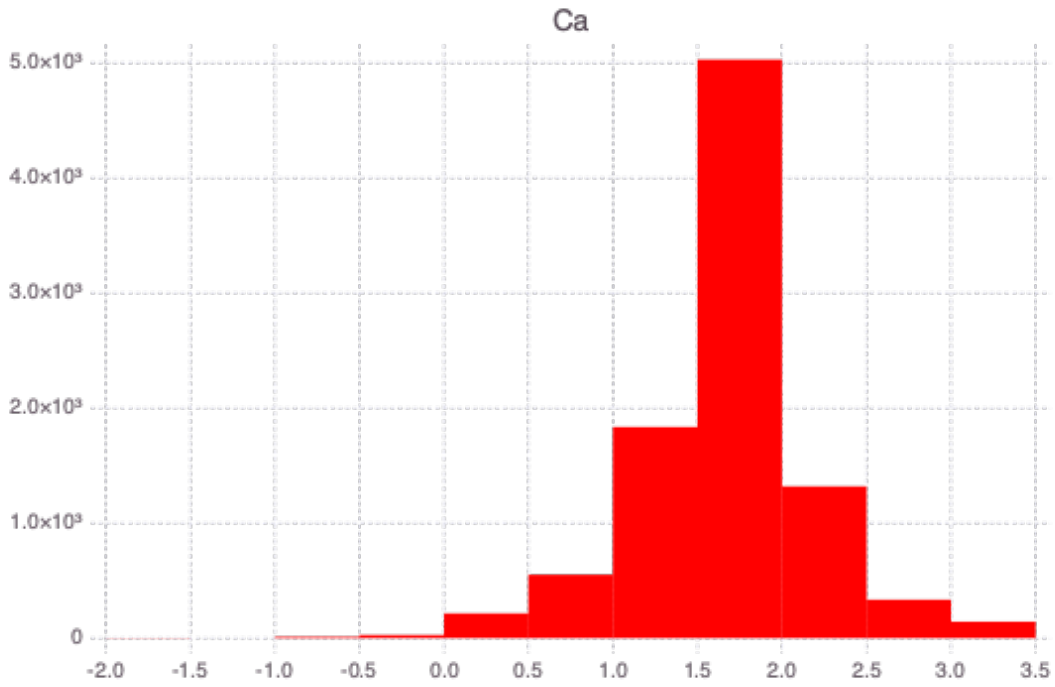

```
B: Min -4.0 Max 2.770852 StdDev 0.99189556 Skewness -0.15991572 Count 5462

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


Be
600
400
200
0
-8
-7
-6
-5
-4
-3
-2
-1
0


Br
500
400
300
200
100
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

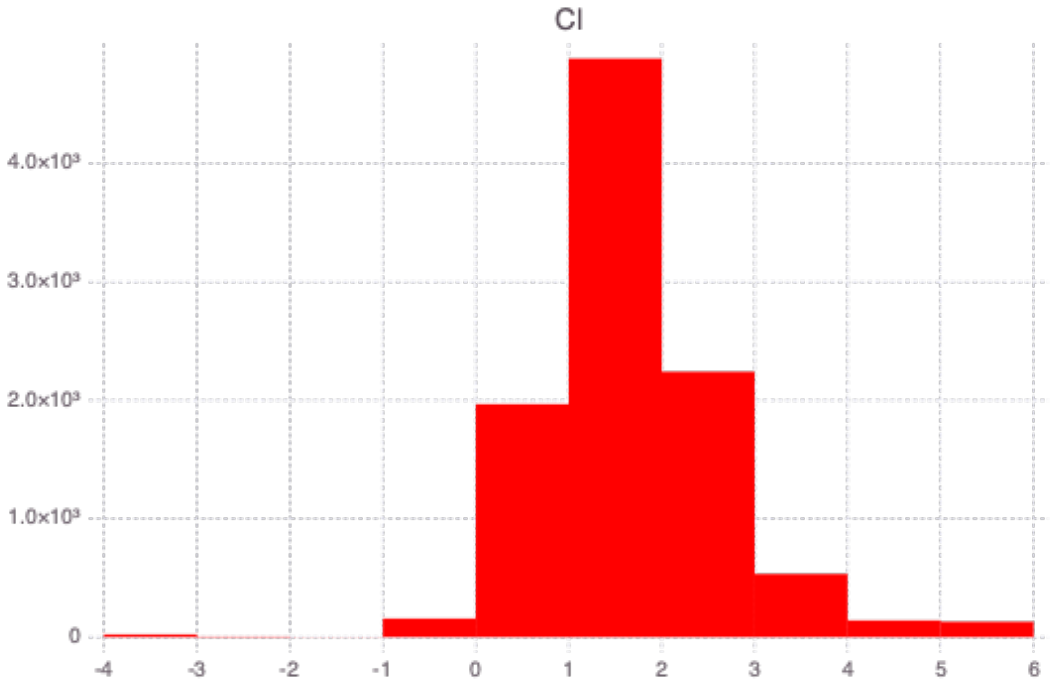
```
Ba: Min -4.0 Max 1.4382393 StdDev 0.492002 Skewness -0.63361335 Count 2516
Be: Min -8.0 Max -0.15490197 StdDev 0.8196359 Skewness -2.5543597 Count 1640
```

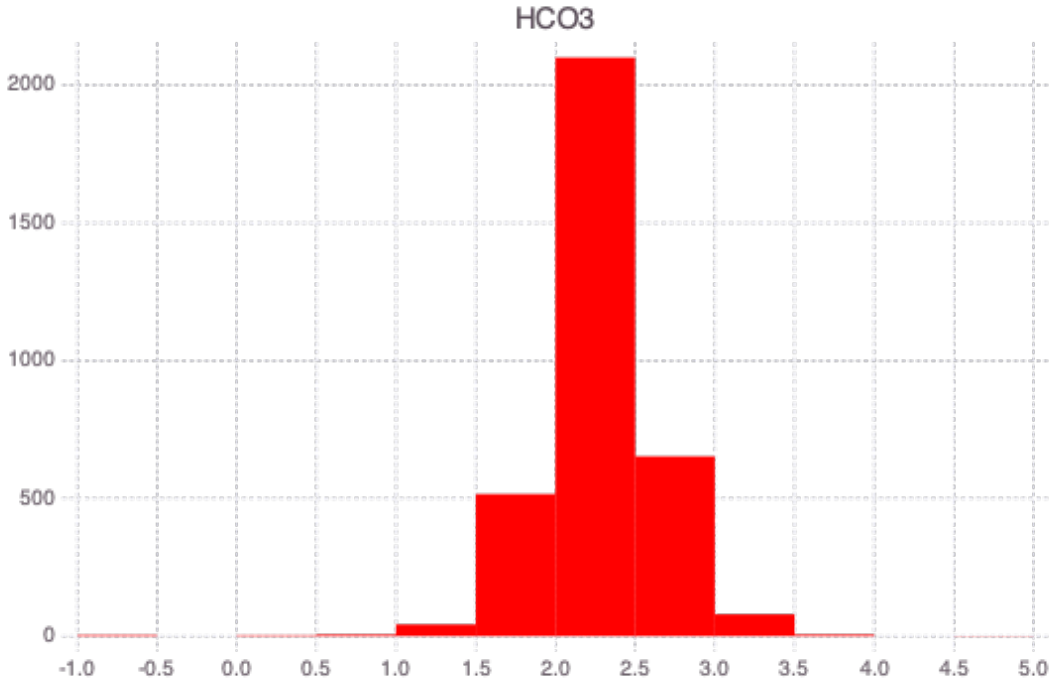
```
  Info: Be: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
  Info: Br: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```




```
Br: Min -3.102373 Max 1.9242793 StdDev 0.90064573 Skewness 0.497394 Count 1935
```

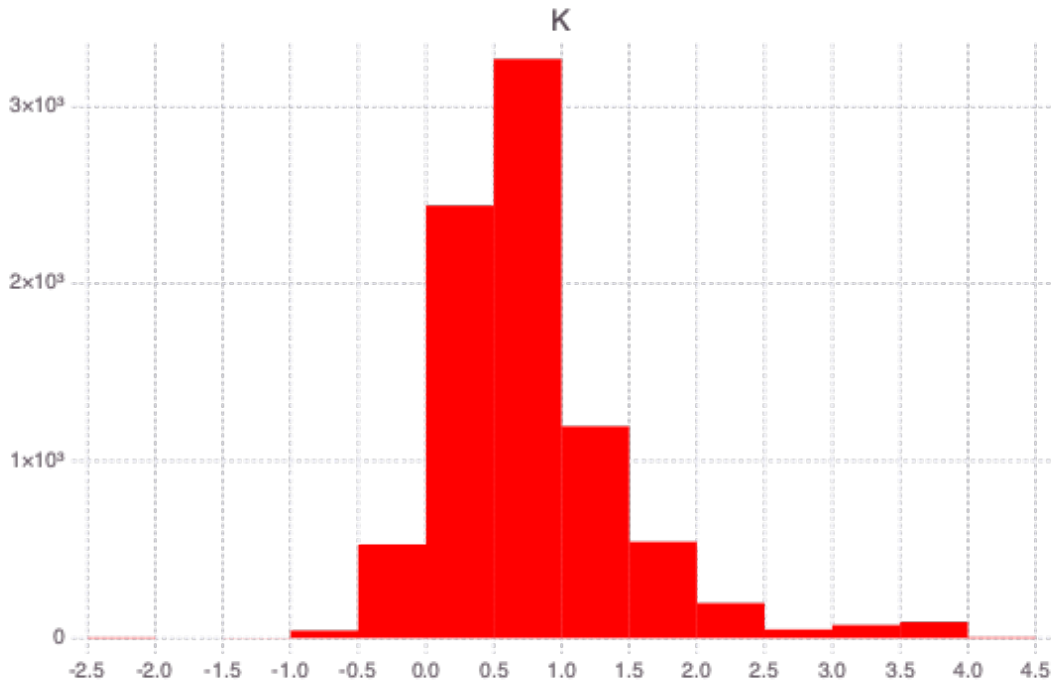
```
  Info: Ca: log10-transformed
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
```


Cl
4.0x10³
3.0x10³
2.0x10³
1.0x10³
0
-4
-3
-2
-1
0
1
2
3
4
5
6


HCO3
2000
1500
1000
500
0
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0

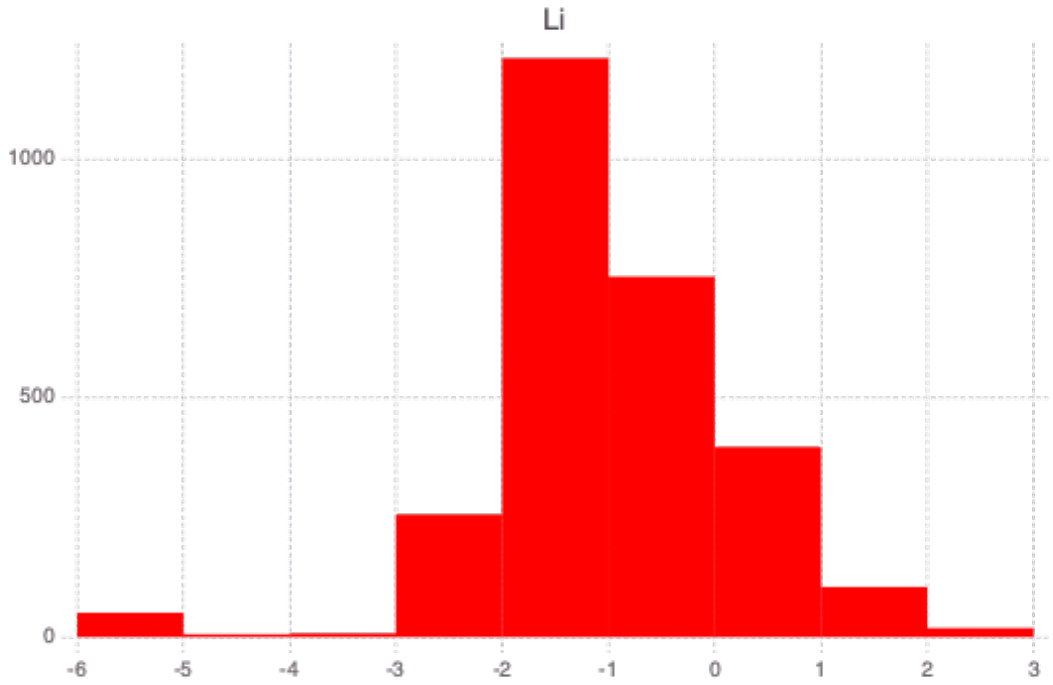
```
Ca: Min -2.0 Max 3.4093695 StdDev 0.51392627 Skewness -0.4936186 Count 9468
Cl: Min -4.0 Max 5.3802114 StdDev 0.99255455 Skewness 0.45536557 Count 10091
```

```
  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
```

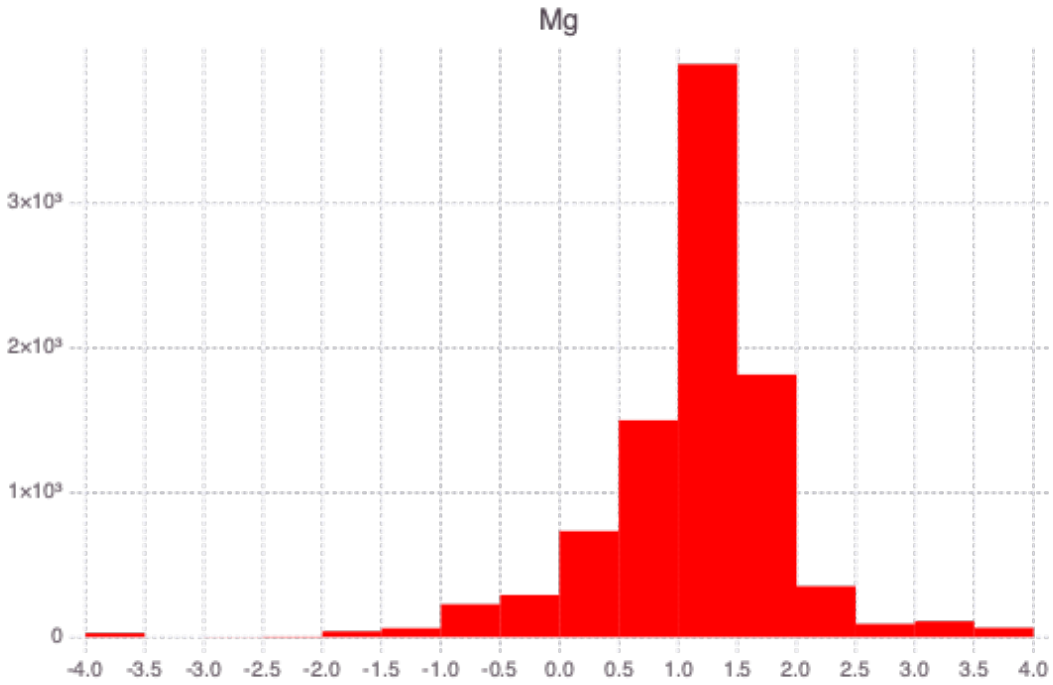


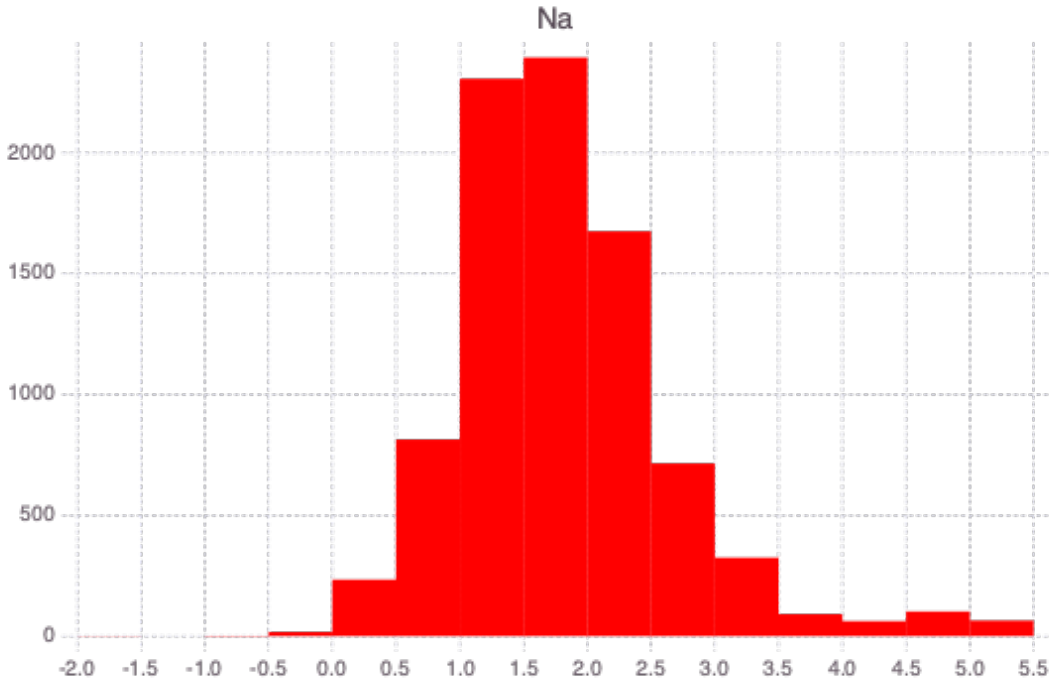

```
HCO3: Min -1.0 Max 4.5682015 StdDev 0.36140293 Skewness -0.94632554 Count 3413
```

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



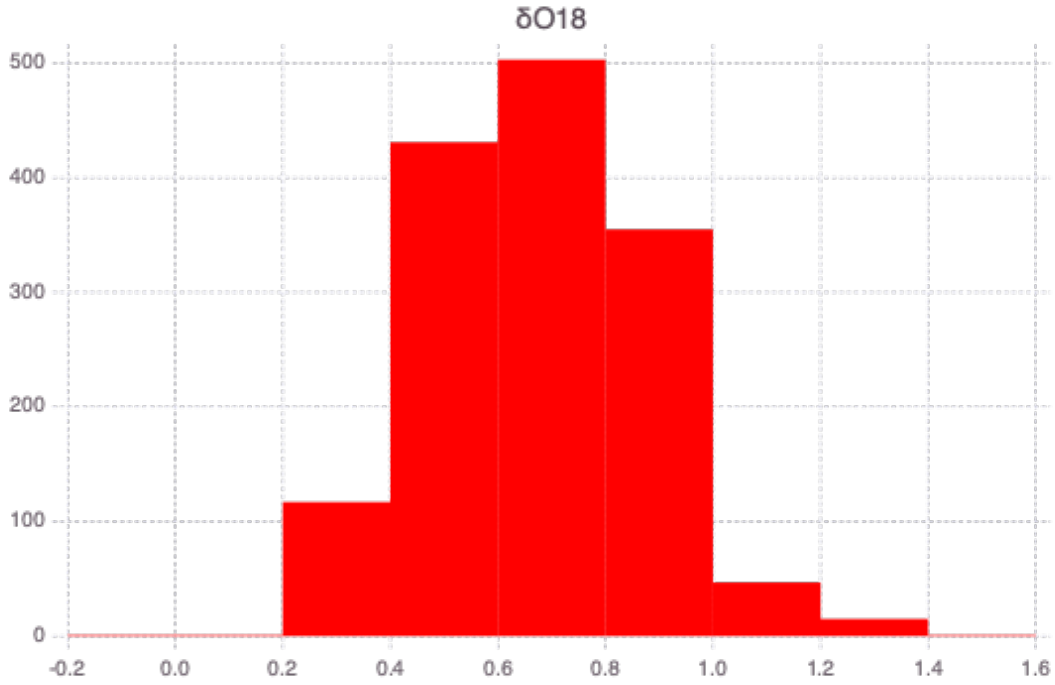

```
K: Min -2.09691 Max 4.1139436 StdDev 0.686127 Skewness 1.5732428 Count 8446

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


Mg
3×10³
2×10³
1×10³
0
-4.0 -3.5 -3.0 -2.5 -2.0 -1.5 -1.0 -0.5 0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0


Na
2000
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 4.5 5.0 5.5

```
Li: Min -6.0 Max 2.9867718 StdDev 1.2346249 Skewness -0.6840743 Count 2809
Mg: Min -3.69897 Max 3.929419 StdDev 0.79547274 Skewness -1.0883808 Count 9296
```

```
 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 -1.6989701 Max 5.20412 StdDev 0.8328025 Skewness 1.1553397 Count 8814
 O18: Min -0.096910425 Max 1.4448252 StdDev 0.20046535 Skewness 0.21996279 Count
1471
Name Min Max StdDev Count (non-NaN's)
Temperature -1.0 2.4393327 0.28062904 0.8823397 13894
Quartz -50.870045 273.2438 34.105637 0.6946969 8683
Chalcedony -81.64773 271.23828 36.418324 0.8679946 8683
pH 1.0 11.7 0.55800503 -0.5521828 9261
TDS -2.6989698 5.5171957 2.0129914 -1.7111415 1740
Al -5.8860564 3.80618 1.2161667 -0.44271475 1362
B -4.0 2.770852 0.99189556 -0.15991572 5462
Ba -4.0 1.4382393 0.492002 -0.63361335 2516
Be -8.0 -0.15490197 0.8196359 -2.5543597 1640
Br -3.102373 1.9242793 0.90064573 0.497394 1935
Ca -2.0 3.4093695 0.51392627 -0.4936186 9468
Cl -4.0 5.3802114 0.99255455 0.45536557 10091
```

```
HCO3 -1.0 4.5682015 0.36140293 -0.94632554 3413
K -2.09691 4.1139436 0.686127 1.5732428 8446
Li -6.0 2.9867718 1.2346249 -0.6840743 2809
Mg -3.69897 3.929419 0.79547274 -1.0883808 9296
Na -1.6989701 5.20412 0.8328025 1.1553397 8814
 O18 -0.096910425 1.4448252 0.20046535 0.21996279 1471
```

```
 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
```

Define and normalize the data matrix

[10]:
```
Xnl, xlmin, xlmax, zflag = NMFk.normalizematrix_col(X; logv=logv);
```

0.4.8 Define a range for number of signatures to be explored

[11]:
```
nkrange = 2:10;
```

0.4.9 Define directory with exsiting model runs

[12]:
```
resultdir = "results";
```

Define the number of NMF runs to be exectuted The higher the NMF runs, the better. In addition, convergence has been already explored using different numbers of NMF runs.

[13]:
```
nruns = 640;
```

0.5 Perform ML analyses

The **NMFk** algorithm factorizes the normalized data matrix `Xn` into `W` and `H` matrices. For more information, check out the **NMFk** website

[14]:
```
W, H, fitquality, robustness, aic = NMFk.execute(Xnl, nkrange, nruns;␣
 ↪resultdir=resultdir, casefilename="nmfk-nl", load=true)
W, H, fitquality, robustness, aic = NMFk.load(nkrange, nruns;␣
 ↪resultdir=resultdir, casefilename="nmfk-nl");
```

```
Signals:  2 Fit:     490.2203 Silhouette:     0.886031 AIC:    -531856.6
Signals:  3 Fit:     315.1114 Silhouette:     0.498339 AIC:    -551467.8
Signals:  4 Fit:      224.617 Silhouette:  -0.01242121 AIC:    -559810.1
Signals:  5 Fit:     157.1487 Silhouette:  0.004662591 AIC:    -570187.6
Signals:  6 Fit:     118.4444 Silhouette:   -0.1862046 AIC:    -572450.7
Signals:  7 Fit:      85.8435 Silhouette:  -0.09372894 AIC:    -578982.6
Signals:  8 Fit:      62.9881 Silhouette:    -0.113508 AIC:    -584169.8
Signals:  9 Fit:     45.59955 Silhouette:  -0.05323793 AIC:    -590824.9
Signals: 10 Fit:     33.40136 Silhouette:  -0.08453866 AIC:    -596199.8
Signals:  2 Fit:     490.2203 Silhouette:     0.886031 AIC:    -531856.6
Signals:  3 Fit:     315.1114 Silhouette:     0.498339 AIC:    -551467.8
```

```
Signals:  4 Fit:      224.617 Silhouette:  -0.01242121 AIC:    -559810.1
Signals:  5 Fit:     157.1487 Silhouette:  0.004662591 AIC:    -570187.6
Signals:  6 Fit:     118.4444 Silhouette:   -0.1862046 AIC:    -572450.7
Signals:  7 Fit:      85.8435 Silhouette:  -0.09372894 AIC:    -578982.6
Signals:  8 Fit:      62.9881 Silhouette:    -0.113508 AIC:    -584169.8
Signals:  9 Fit:     45.59955 Silhouette:  -0.05323793 AIC:    -590824.9
Signals: 10 Fit:     33.40136 Silhouette:  -0.08453866 AIC:    -596199.8
Signals:  2 Fit:     490.2203 Silhouette:     0.886031 AIC:    -531856.6
Signals:  3 Fit:     315.1114 Silhouette:     0.498339 AIC:    -551467.8
Signals:  4 Fit:      224.617 Silhouette:  -0.01242121 AIC:    -559810.1
Signals:  5 Fit:     157.1487 Silhouette:  0.004662591 AIC:    -570187.6
Signals:  6 Fit:     118.4444 Silhouette:   -0.1862046 AIC:    -572450.7
Signals:  7 Fit:      85.8435 Silhouette:  -0.09372894 AIC:    -578982.6
Signals:  8 Fit:      62.9881 Silhouette:    -0.113508 AIC:    -584169.8
Signals:  9 Fit:     45.59955 Silhouette:  -0.05323793 AIC:    -590824.9
Signals: 10 Fit:     33.40136 Silhouette:  -0.08453866 AIC:    -596199.8
```

```
Info: Results
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkExecute.jl:15
Info: Optimal solution: 3 signals
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkExecute.jl:20
Info: Optimal solution: 3 signals
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkIO.jl:30
```

Here, the **NMFk** results are loaded from a prior ML run.

As seen from the output above, the NMFk analyses identified that the optimal number of geothermal signatures in the dataset **3**.

Solutions with a number of signatures less than **3** are underfitting.

Solutions with a number of signatures greater than **3** are overfitting and unacceptable.

The set of acceptable solutions are defined as follows:

[15]:
```
NMFk.getks(nkrange, robustness[nkrange])
```

[15]:
```
2-element Array{Int64,1}:
 2
 3
```

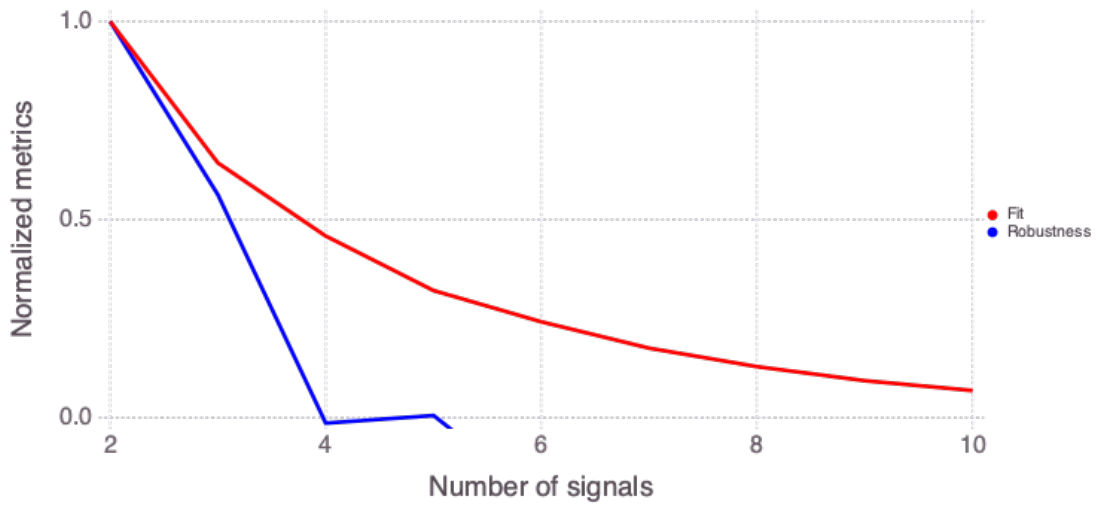
The acceptable solutions contain 2 and 3 signatures.

0.5.1 Post-processing NMFk results

Number of signatures Plot representing solution quality (fit) and silhouette width (robustness) for different number of signatures `k`:

[16]:
```
resultdirpost = "results-postprocessing-nl-$(nruns)"
figuredirpost = "figures-postprocessing-nl-$(nruns)";
```

[17]:
```
NMFk.plot_feature_selecton(nkrange, fitquality, robustness;␣
↪figuredir=figuredirpost)
```



The plot above also demonstrates that the accceptable solutions contain 2 and 3 signatures. Note, any solution is accepted, if the robustness >0.25.

Analysis of the optimal solution The ML solution with the optimal number of signatures (3) is further analyzed as follows:

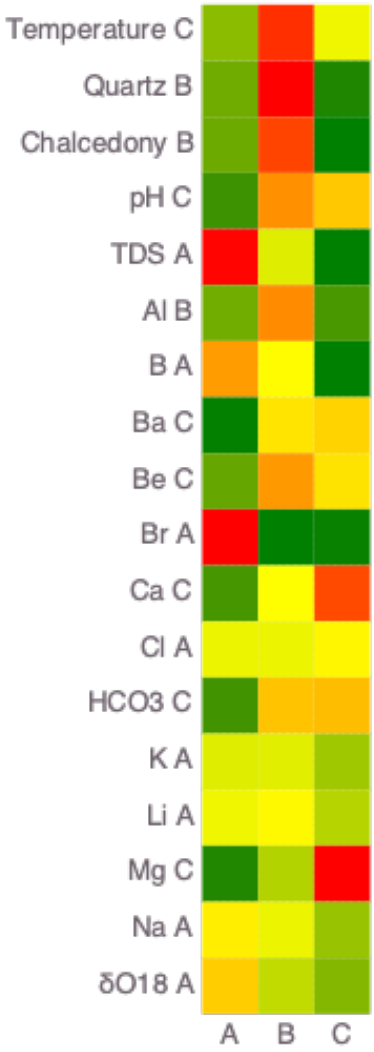
[18]:
```
Sorder, Wclusters, Hclusters = NMFk.clusterresults(NMFk.getk(nkrange,␣
↪robustness[nkrange]), W, H, string.(collect(1:npoints)), attributes;␣
↪lon=xcoord, lat=ycoord, resultdir=resultdirpost, figuredir=figuredirpost,␣
↪ordersignal=:Wcount, Hcasefilename="attributes", Wcasefilename="locations",␣
↪biplotcolor=:WH, sortmag=false, biplotlabel=:H, point_size_nolabel=2Gadfly.
↪pt, point_size_label=4Gadfly.pt)
```

```
Signal importance (high->low): [2, 1, 3]
```

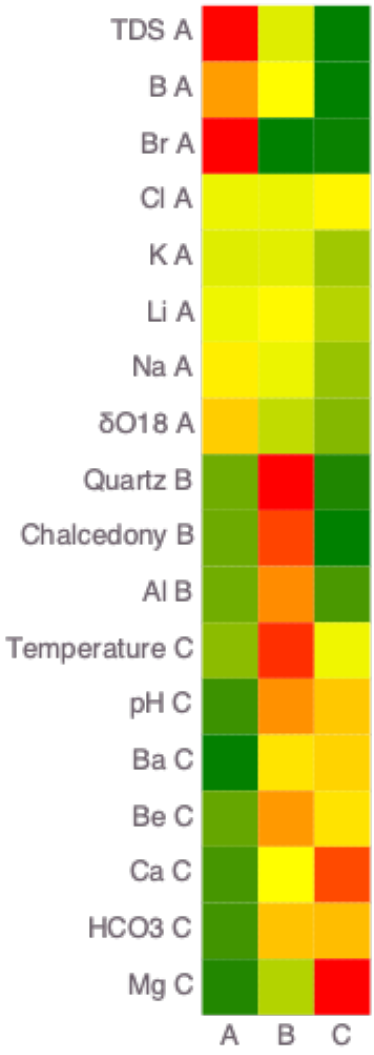
```
 Info: Number of signals: 3
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:154
 Info: Attributes (signals=3)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:158
 Warning: type
Clustering.KmeansResult{Core.Array{Core.Float32,2},Core.Float32,Core.Int64} not
present in workspace; reconstructing
 @ JLD /Users/vvv/.julia/packages/JLD/nQ9iW/src/jld_types.jl:697
 Info: Robust k-means analysis results are loaded from file results-
postprocessing-nl-640/Hmatrix-3-3_18-1000.jld!
```

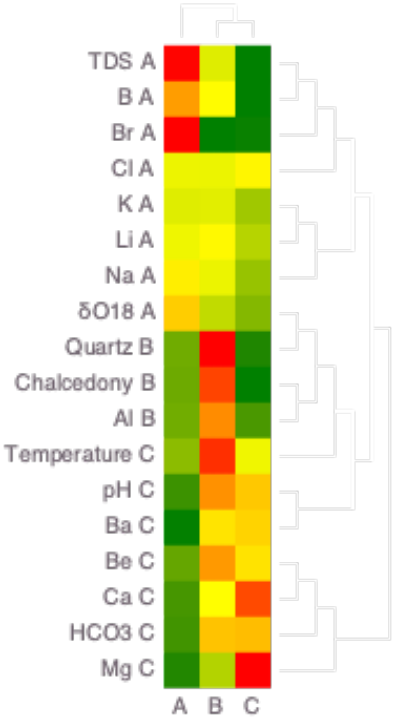
```
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:67
  Warning: Procedure to find unique signals could not identify a solution …
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
  Warning: Procedure to find unique signals could not identify a solution …
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
  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/nQ9iW/src/jld_types.jl:697
  Info: Robust k-means analysis results are loaded from file results-
postprocessing-nl-640/Wmatrix-3-3_14258-1000.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

8×2 Array{Any,2}:
 "Br"    1.0
 "TDS"   0.998519
 "B"     0.761876
 " O18"  0.63782
 "Na"    0.548602
 "Li"    0.463867
 "Cl"    0.457713
 "K"     0.427433

  Info: Signal A -> A Count: 8
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:265
  Info: Signal C -> B Count: 3
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:265
  Info: Signal B -> C Count: 7
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:265
  Info: Signal A (S3) (k-means clustering)
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:282

3×2 Array{Any,2}:
 "Quartz"      1.0
 "Chalcedony"  0.945545
 "Al"          0.802297

7×2 Array{Any,2}:
 "Mg"           1.0
 "Ca"           0.935713
 "HCO3"         0.679563
 "pH"           0.651626
 "Ba"           0.622107
 "Be"           0.578012
```

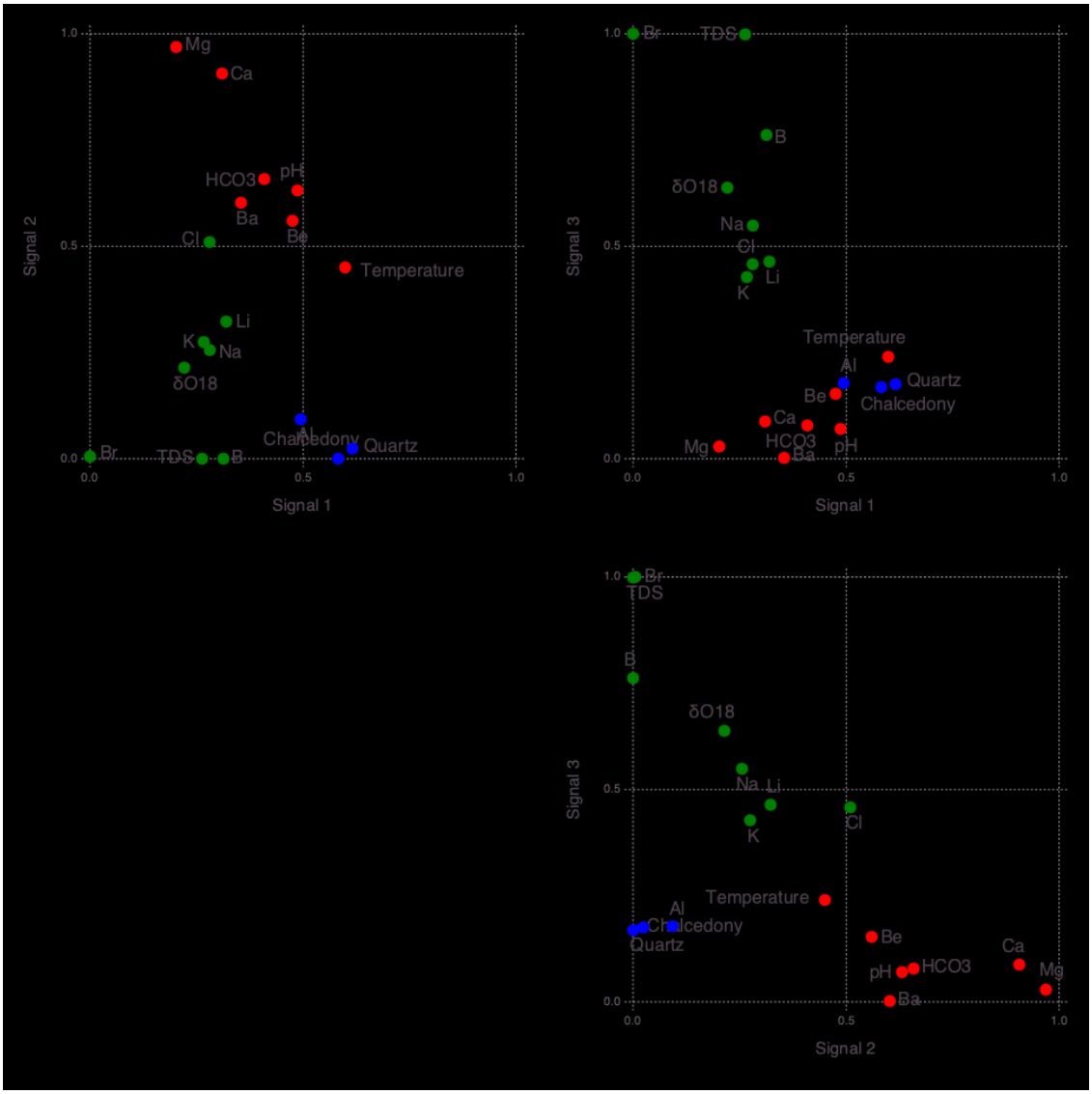
```
"Temperature"  0.464707
```

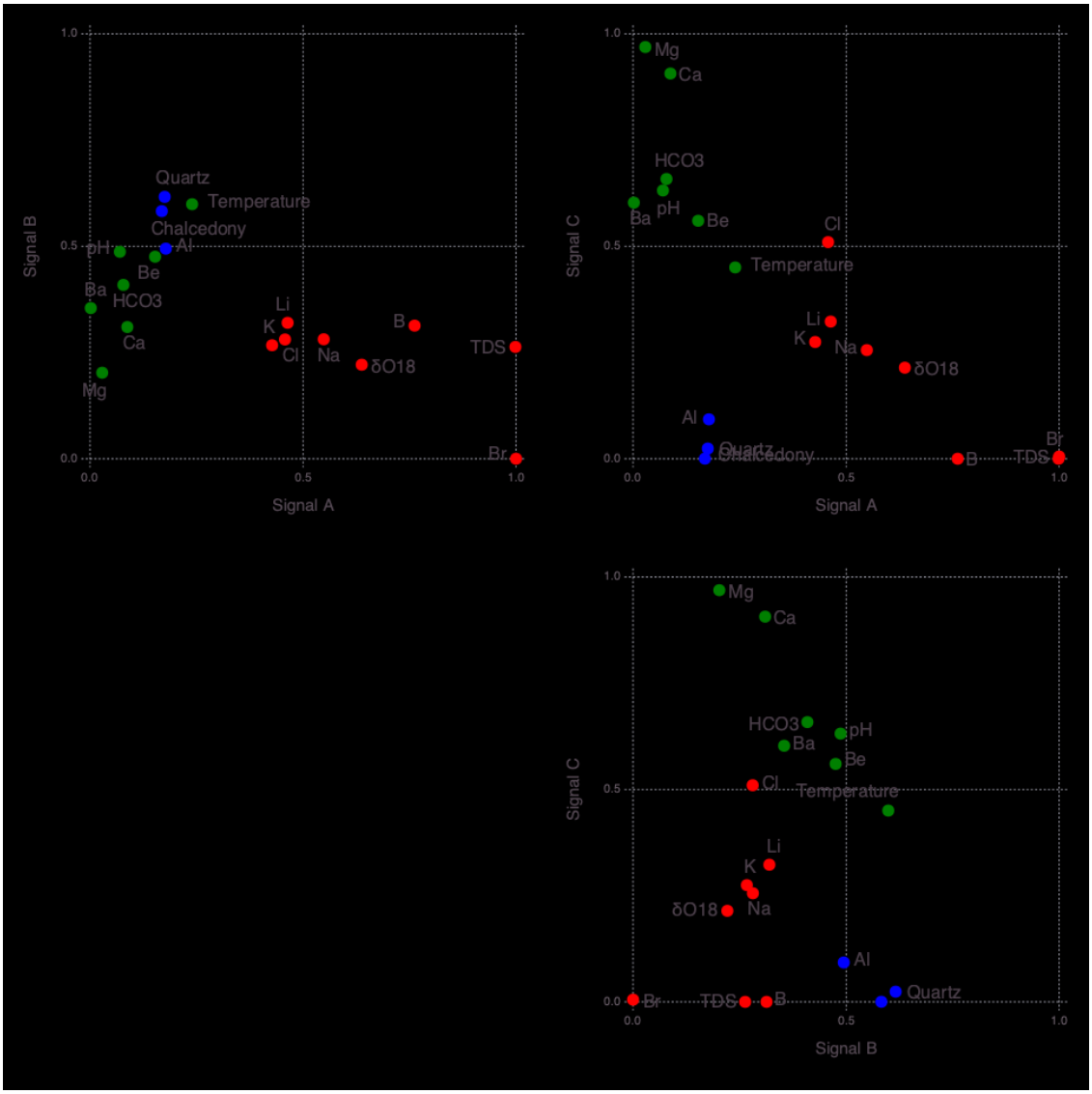



```
Info: Signal B (S1) (k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:282
Info: Signal C (S2) (k-means clustering)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:282
```


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


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

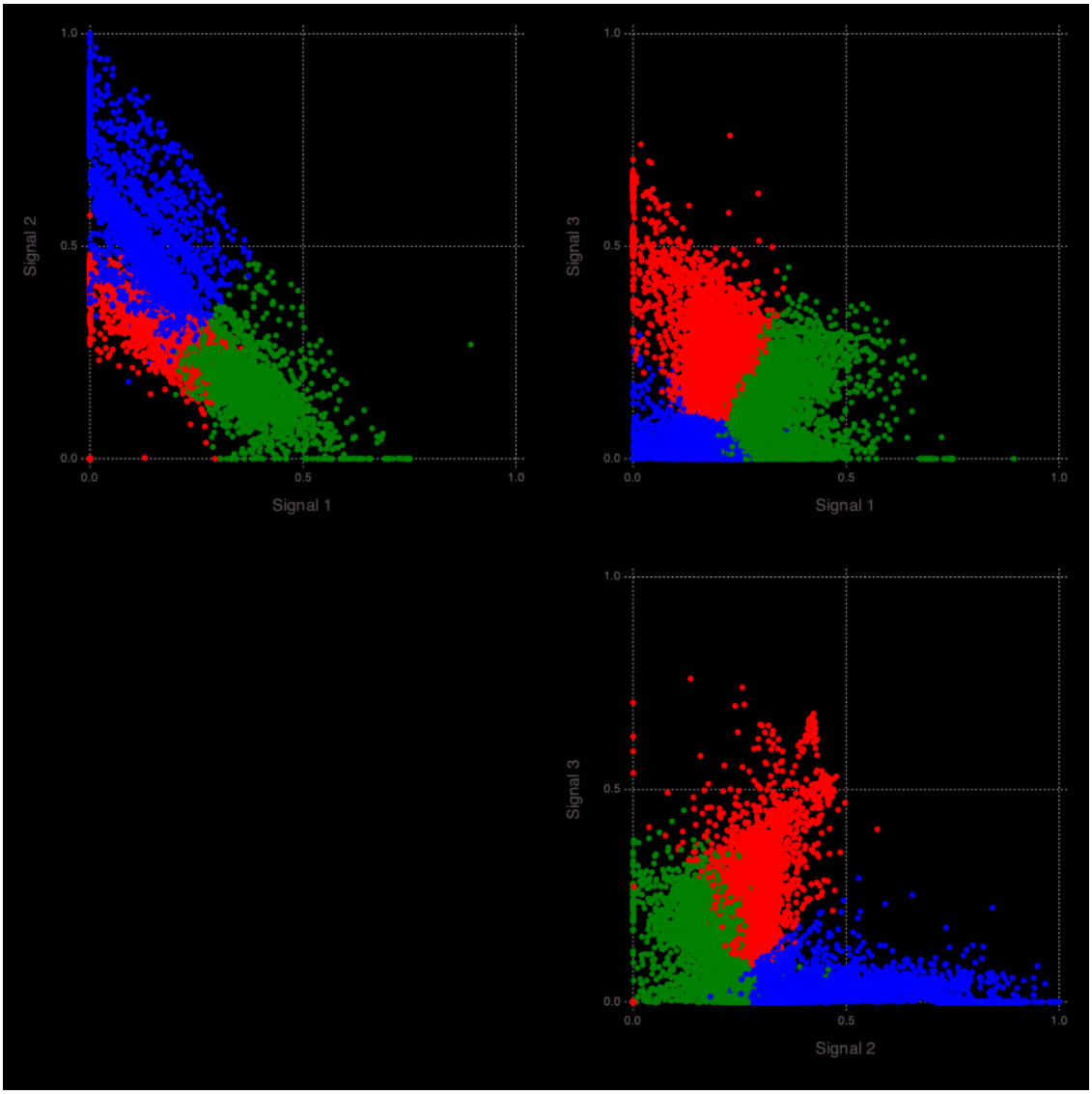

Signal 1
Signal 2
Signal 3
Mg
Ca
HCO3
pH
Ba
Be
Cl
Temperature
Li
K
Na
δO18
Al
Chalcedony
Quartz
Br
TDS
B
Ca
Mg
Ba
0.0
0.5
1.0




```
6256×2 Array{Any,2}:
 "8740"   1.0
 "4307"   0.973089
 "13597"  0.926034
 "6745"   0.920183
 "6743"   0.915929
 "6995"   0.892192
 "6902"   0.88208
 "7159"   0.880767
 "7013"   0.879407
 "6947"   0.87884
 "6998"   0.877846
```

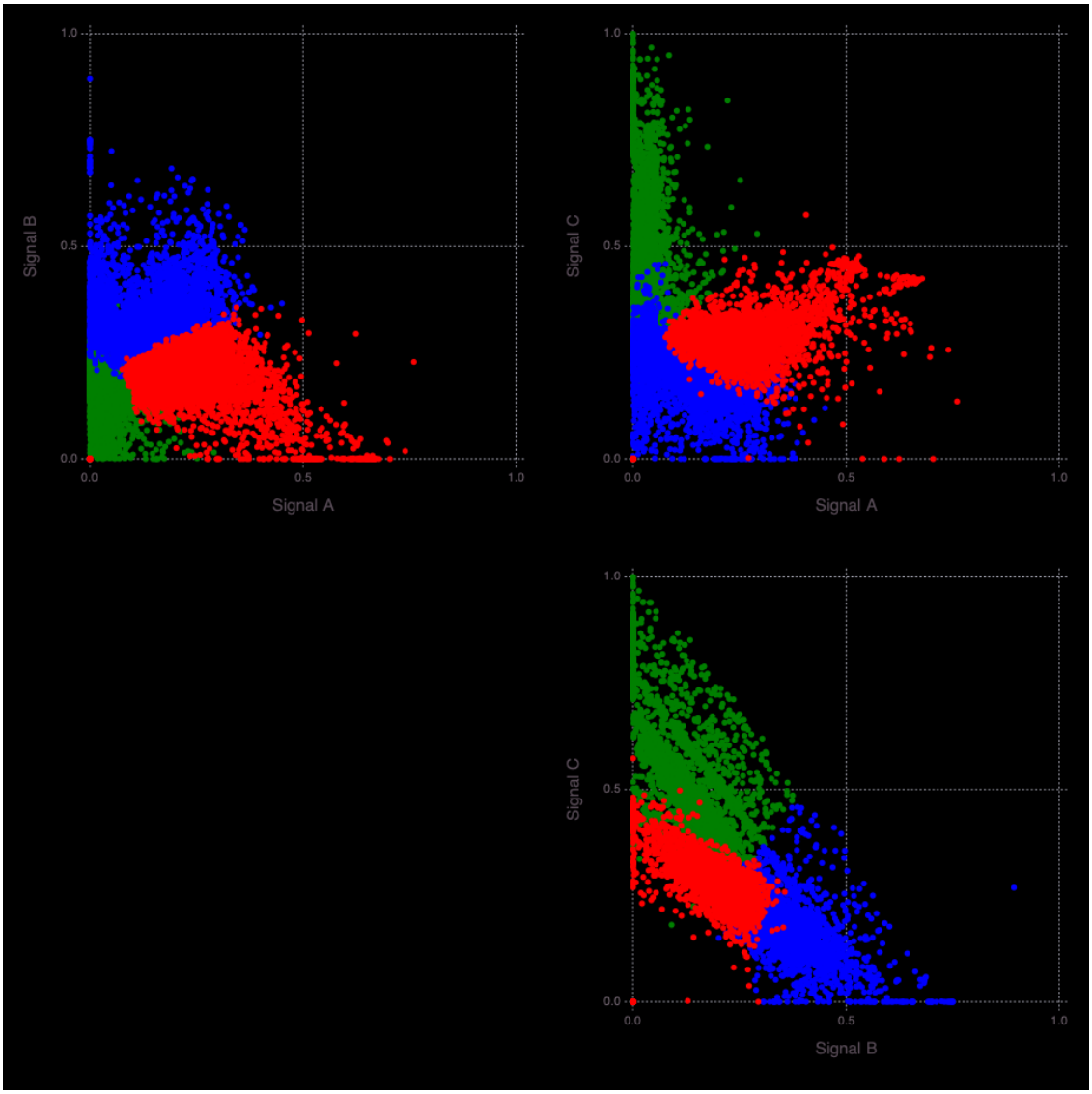
```
 "7000"   0.875902
 "6985"   0.874451

 "13228"  0.0
 "13282"  0.0
 "13373"  0.0
 "13389"  0.0
 "13397"  0.0
 "13434"  0.0
 "13439"  0.0
 "13441"  0.0
 "13456"  0.0
 "13460"  0.0
 "13517"  0.0
 "13882"  0.0
5201×2 Array{Any,2}:
 "3910"   1.0
 "10796"  0.839622
 "10799"  0.839453
 "10784"  0.836072
 "10797"  0.833352
 "10786"  0.829575
 "10800"  0.825416
 "10785"  0.817501
 "12799"  0.810014
 "10883"  0.795935
 "10882"  0.785195
 "10877"  0.784725
 "10876"  0.78121

 "903"    0.243983
 "10531"  0.243834
 "983"    0.243368
 "3502"   0.241069
 "108"    0.240825
 "12996"  0.240369
 "1819"   0.240354
 "487"    0.233168
 "514"    0.225323
 "14122"  0.225207
 "3356"   0.221252
 "7392"   0.215268
 Info: Locations (signals=3)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:340
 Info: Signal A (S3) Count: 6256
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:353
 Info: Signal B (S1) Count: 5201
```

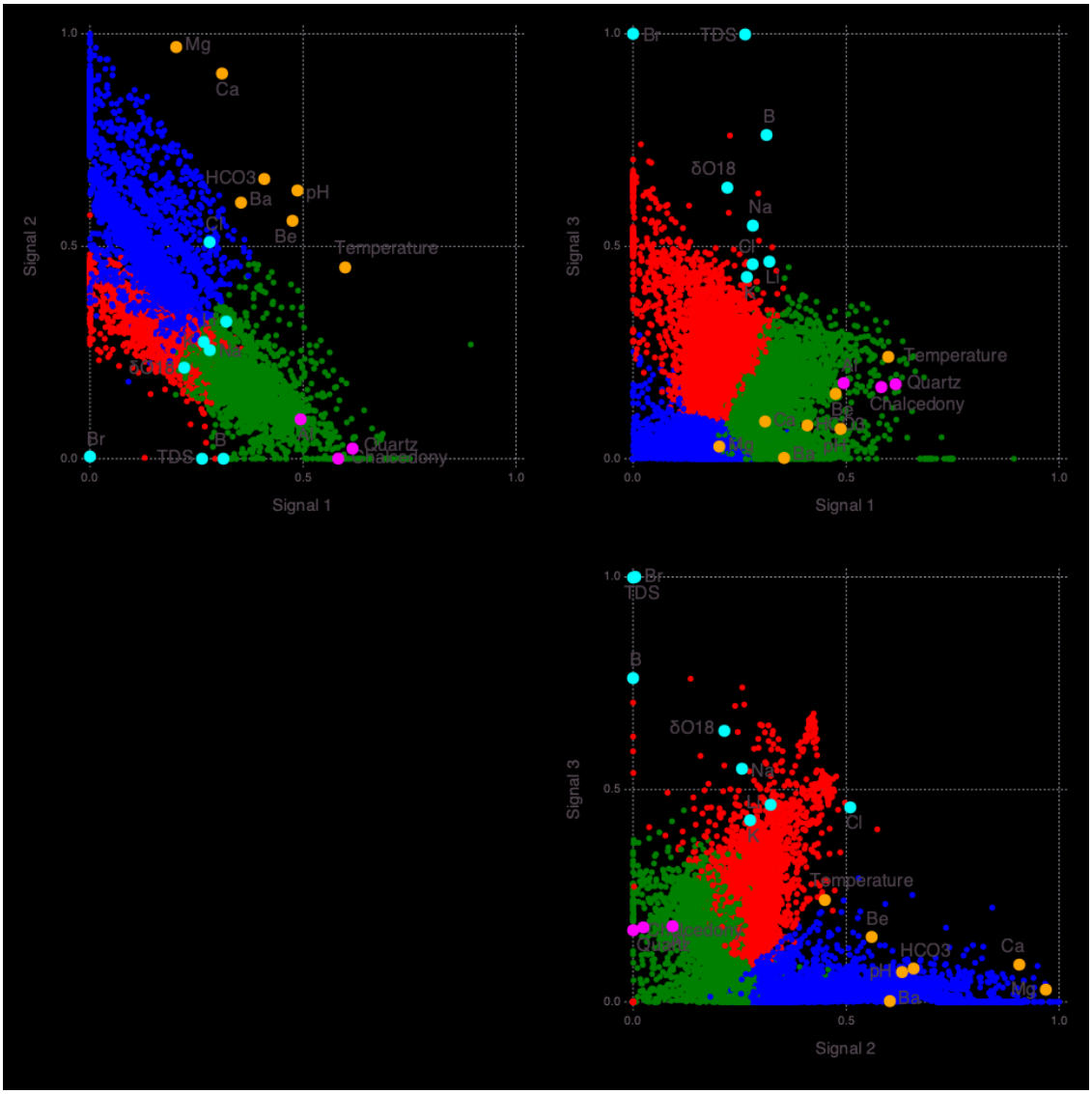
```
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:353
 Info: Signal C (S2) Count: 2801
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:353
 Info: Signal A -> A Count: 6256
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:363
 Info: Signal B -> B Count: 5201
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:363
 Info: Signal C -> C Count: 2801
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:363
 Info: Signal A (remapped k-means clustering)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:378
 Info: Signal B (remapped k-means clustering)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:378
 Info: Signal C (remapped k-means clustering)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:378

2801×2 Array{Any,2}:
 "11813"  1.0
 "12933"  0.995532
 "10102"  0.985685
 "7816"   0.979038
 "11102"  0.976738
 "11533"  0.967216
 "12897"  0.960254
 "11808"  0.95469
 "10483"  0.949177
 "9907"   0.944174
 "12909"  0.941319
 "11535"  0.939949
 "11817"  0.939765

 "9942"   0.272538
 "14153"  0.27231
 "2717"   0.270224
 "7956"   0.268112
 "233"    0.264453
 "3219"   0.263445
 "484"    0.255068
 "16"     0.253433
 "8652"   0.233033
 "499"    0.229715
 "7334"   0.224784
 "470"    0.181262
```

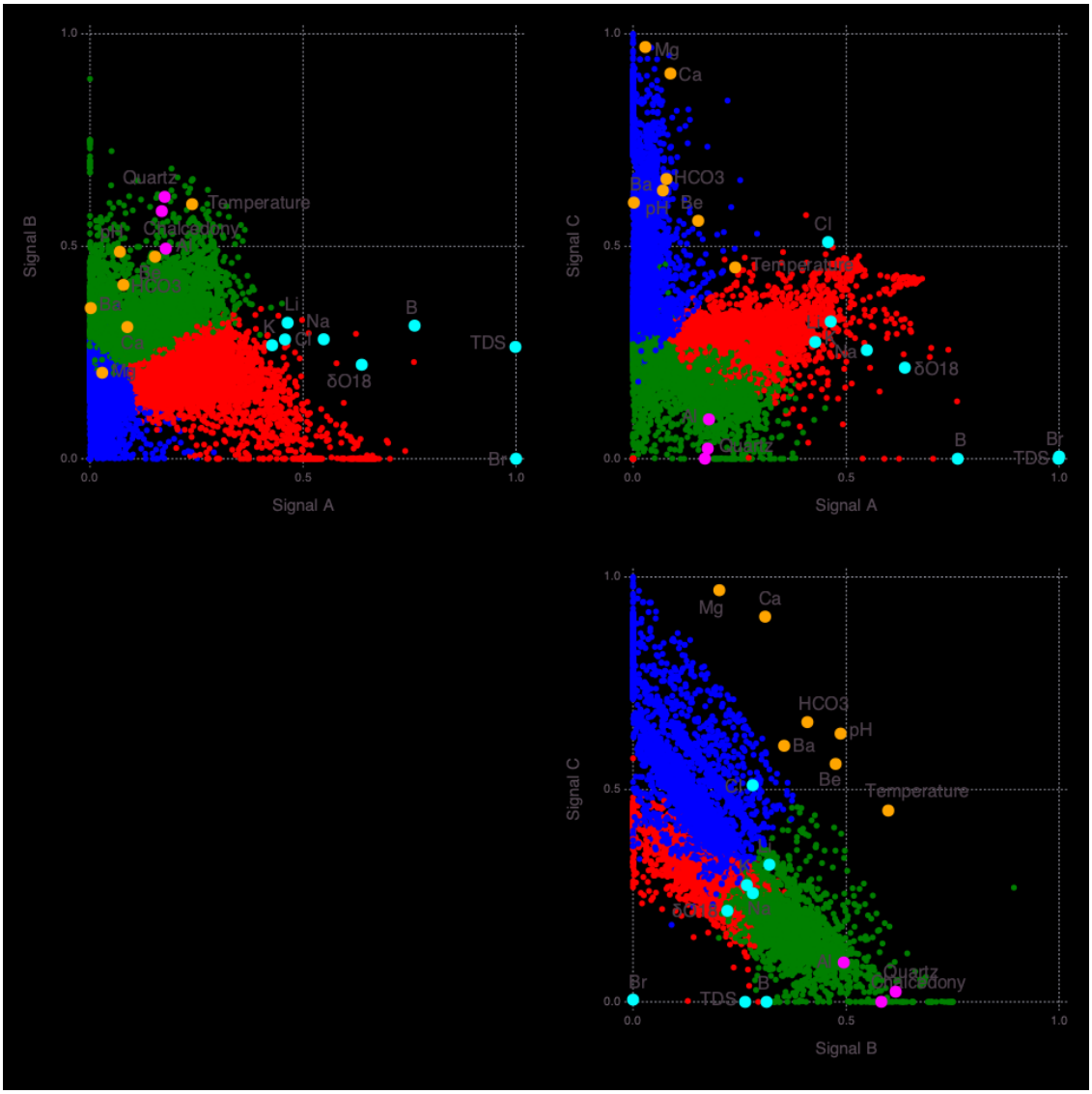



```
ArgumentError("Distance matrix should be symmetric.")
```

```
  Warning: Dendogram ploting failed!
  @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:431
```


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


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

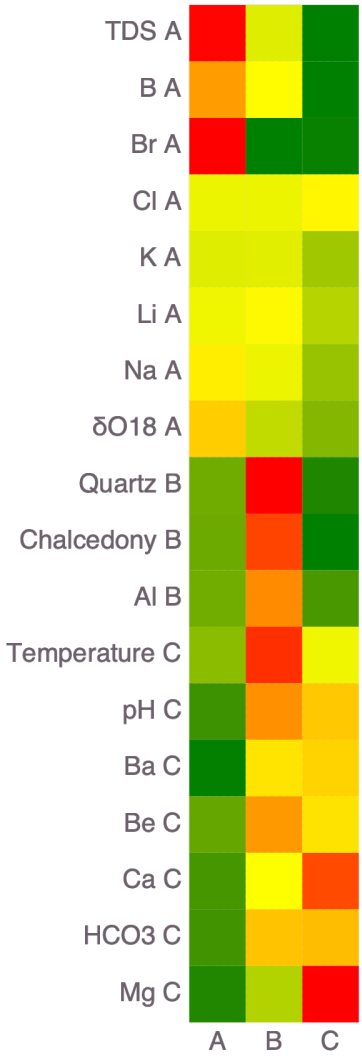


[18]: ([[3, 1, 2]], [['A', 'A', 'A', 'A', 'C', 'A', 'A', 'A', 'C', 'B' … 'A', 'A', 'B', 'A', 'A', 'B', 'A', 'B', 'B', 'A']], [['C', 'B', 'B', 'C', 'A', 'B', 'A', 'C', 'C', 'A', 'C', 'A', 'C', 'A', 'A', 'C', 'A', 'A']])

The geothermal attributes are clustered into **3** groups:

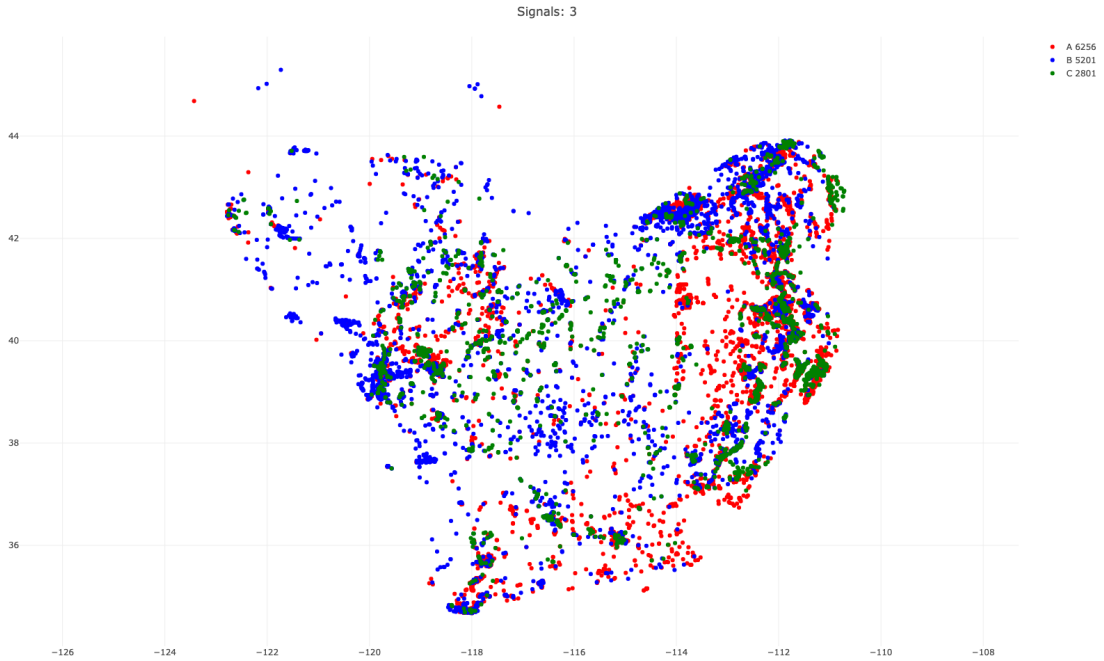
```
<iframe src="../results-postprocessing-nl-640/attributes-3-groups.txt" frameborder="0" height="
  width="95%"></iframe>
```

This grouping is based on analyses of the attribute matrix `W`:



The well locations are also clustered into **3** groups. The grouping is based on analyses of the location matrix `H`.

A spatial map of the locations is obtained:



The map ../figures-postprocessing-nl-640/locations-3-map.html provides interactive visualization of the extracted location groups (the html file can be also openned with any browser).

```
<iframe src="../figures-postprocessing-nl-640/locations-3-map.html" frameborder="0" height="800
```

0.5.2 Discussion of NMFk results

Our ML algorithm extracted **3** signatures in the analyzed dataset.

Signature **B** is detected at 5201 locations shown in the map above.

At these locations, `Temperature`, `Quartz`, `Chalcedony` and `Al` appear to be elevated. There is general correlations between `Temperature`, `Quartz`, `Chalcedony` and `Al` observations at these locations. All these locations can be identified as geothermal resources with high prospectivity.

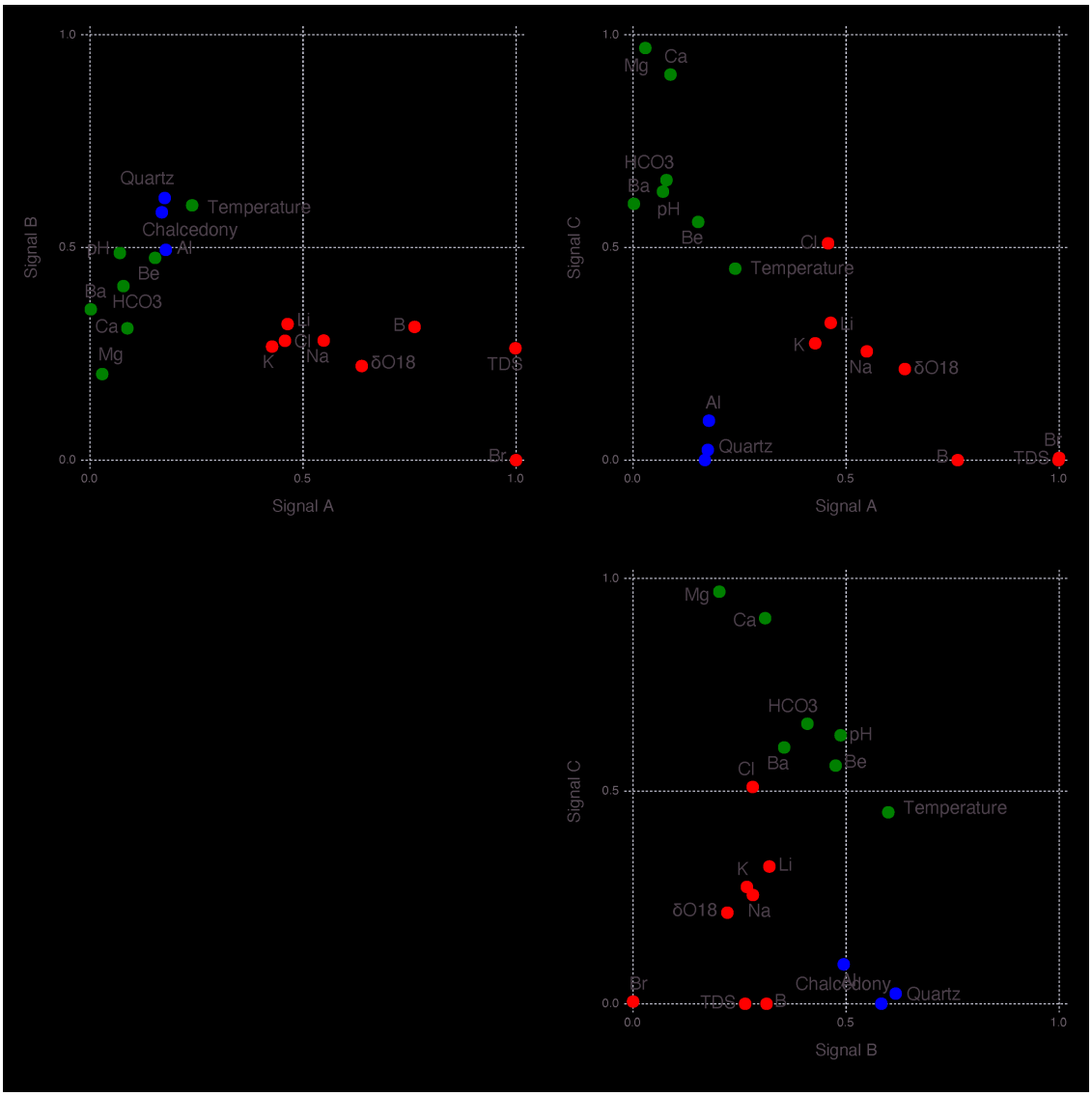
Signature **C** is detected at 2801 locations shown in the map above.

At these locations, `Temperature` is also elevated. However, `Quartz`, `Chalcedony` and `Al` are low. However, `Ca` and `Mg` are elevated as well. All these locations can be identified as geothermal resources with lower prospectivity. Additional analyses and data acquisition activities are needed to define their prospectivity.

Signature **A** is detected at 6256 locations shown in the map above.

At these locations, `TDS`, `B` and `Br` are elevated. However, the `Temperature` is low. These locations can be identified as geothermal resources with low prospectivity.

Biplots are also generated by the scripts presented above to map the interelations between the attributes as defined by the extraced **3** signatures which can be viewed also as basis vectors. The interpretation of the biplots is consistent with the way eigen-analysis (SVD/PCA) biplots are also interpreted.



It clear from the figure above, that `Temperature`, `Quartz`, `Chalcedony` and `Al` are generally collocated.

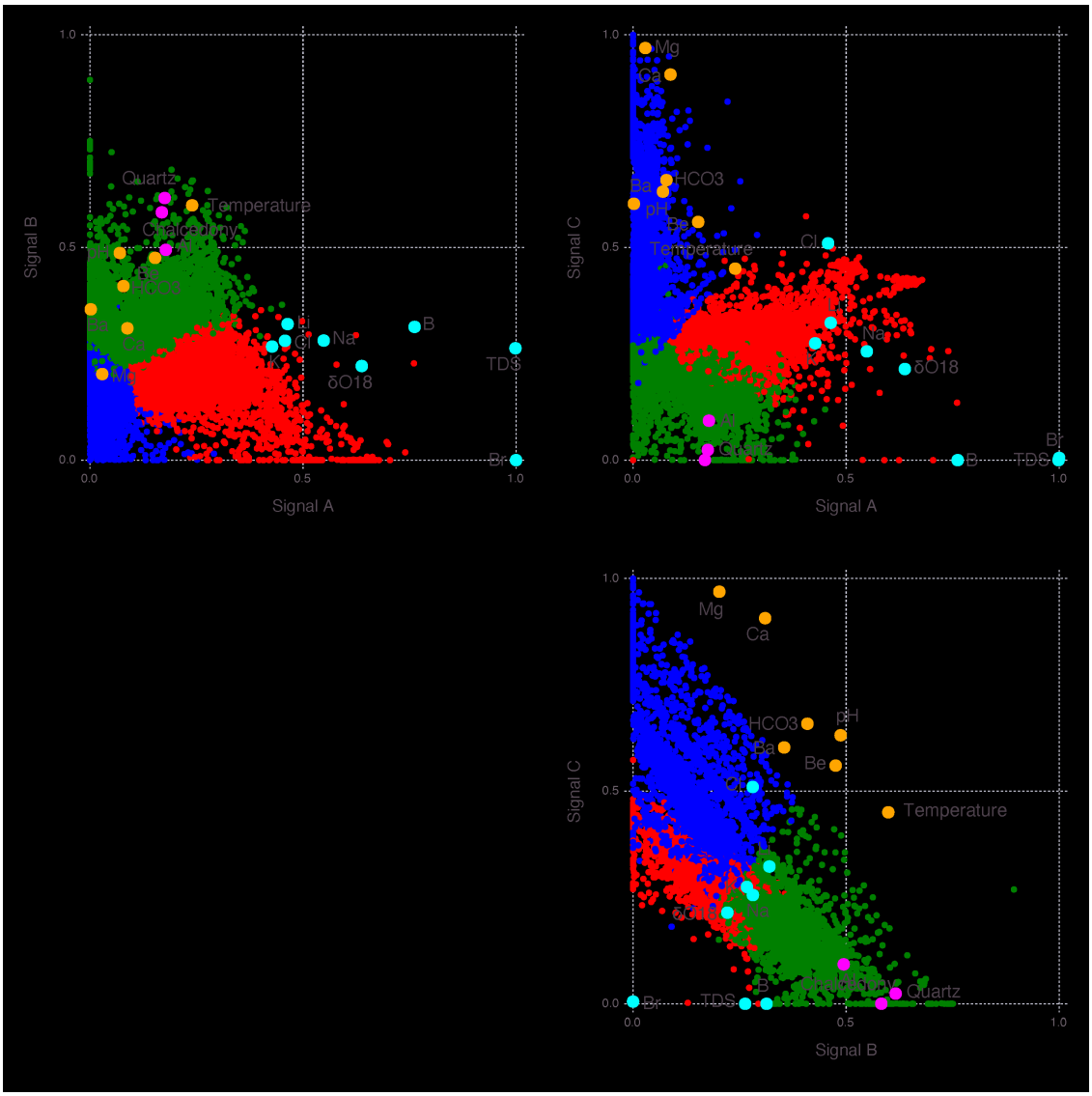
`Ca` and `Mg` are also collocated.

Similarly, `K`, `Li` and `Na` are also collocated.

The coloring of the dots represents the ML clustering of the attributes into **3** groups.

The figure demonstrates that ML algorithm successfully identified attributes which have generally similar spatial patterns.

The biplots can also map the locations at which the data are collected as shown in the figure below.



The coloring of the dots represents the ML clustering of the attributes and locations into **3** groups each (**6** groups in total).

The biplots above show how the attribute data is applied to label the locations so that they are optimally grouped into **3** locations clusters.