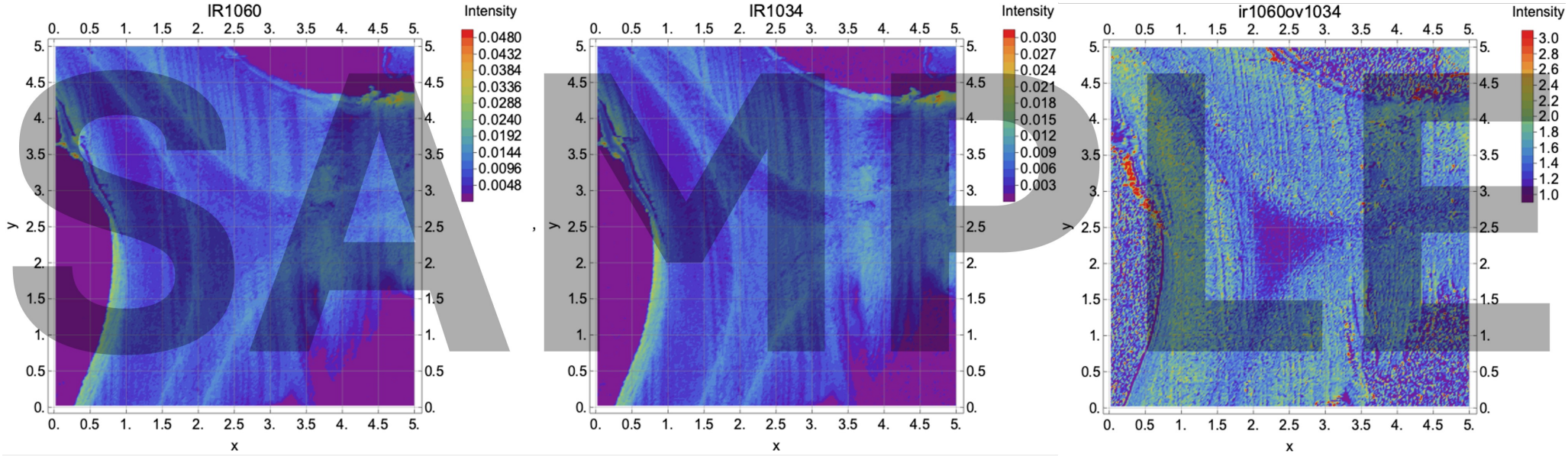
Mathematica code for AFM-IR Ratiomap (v2.1)

Contact: jongcheol1422@gmail.com



v2.1 updates

1. Defined a function that generate the 'ratio' table. You don't need to copy&paste a few lines that divide a table by another table manuall
   1-1. How to use? You need to run & save the results to a table with a proper name.

1.

b. Normalization - Ratio map

```
cut1 = 0;(*cut out outliers*)
cut2 = 1000; (*cut out outliers*)
```

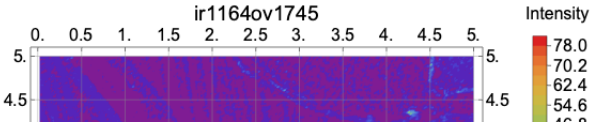
```
ratio[aa_, bb_] := Module[{},
  temp = Table[0, {i, 1, dim}, {j, 1, dim}];
  For[i = 1, i ≤ dim,
   For[j = 1, j ≤ dim,
    If[cut1 < aa[[i, j]] / bb[[i, j]] < cut2,
     temp[[i, j]] = aa[[i, j]] / bb[[i, j]];
    ];
    j++];
   i++]
 ]
```

1-1.

1164/1745 --> [S2- S1], great

```
ratio[rIR1164b, rIR1745]
ir1164ov1745 = temp;

IRmap[ir1164ov1745, 20]
```



2. Defined a new function for the Contour Plot. Now, you can freely control the color scheme range using 'IRmap2' function.
   2-2. How to use? 4 arguments. [table, min, max, bin]

2.

c. Imaging

0. inputs

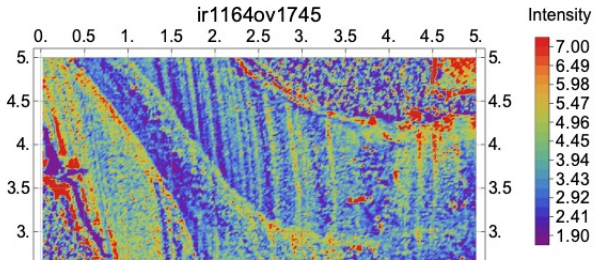
1. Define function - IRmap

```
(*Unnormalized*)
SetAttributes[IRmap, HoldFirst];
IRmap[temp_, cont_] := Module[{name1},
  name1 = SymbolName[Unevaluated[temp]];
  ListContourPlot[Evaluate[temp], PlotRange → All, Frame
   AspectRatio → ny / nx, ColorFunction → "Rainbow", Conto
   PlotLegends → Placed[BarLegend[Automatic, LegendMarke
```

```
(*Normalized*)
ClearAll[IRmap2, min, max, dd];
SetAttributes[IRmap2, HoldFirst];
IRmap2[temp_, min_, max_, dd_] := Module[{name2, leg},
  name2 = SymbolName[Unevaluated[temp]];
  leg = Round[Table[i, {i, min, max, (max - min) / dd}], 0.
  ListContourPlot[Evaluate[temp], PlotRange → All, Frame
   AspectRatio → ny/nx, GridLines → {Range[0, nx, dim / Lx *
   ColorFunction → Function[{z}, ColorData["Rainbow"][Re
   ColorFunctionScaling → False,
   Contours → leg, ContourStyle → None, (* Related to col
   PlotLegends → Placed[BarLegend[Automatic, LegendMa
   PlotLabel → Dynamic[name2]]
 ]
(*PlotLegends→Placed[BarLegend[{"Rainbow",{min,max}}
```

2-1.

```
IRmap2[ir1164ov1745, 1.9, 7, 20] (*wvn,min,max,bin*)
```



v2.1 updates

3. Make sure that the imported data files are properly assigned in the later step. To do that, Print function was added.

1. Data import

```
allFiles = FileNames["*.txt", "sample data"]; (*import .txt files in the directory name 'data'*)
allData = Import[#, "Data"] & /@ allFiles;
allData // Dimensions(*Check how many .txt files were imported*)
Print["Imported file names: ", allFiles](* Make sure to chekc the order of the file imported! *)
```

```
{6, 65 537, 1}

Imported file names: {sample data/1034.txt, sample data/1060.txt, sample data/1151.txt, sample data/r1034.txt, sample data/r1060.txt, sample data/r1151.txt}
```

3. Data name assignment

```
(*name each dataset for convenience*)
IR1034 = e[[1]];
IR1060 = e[[2]];
IR1151 = e[[3]];
rIR1034 = e[[4]];
rIR1060 = e[[5]];
rIR1151 = e[[6]];
```

Mathematica code for AFM-IR Ratiomap (v2)

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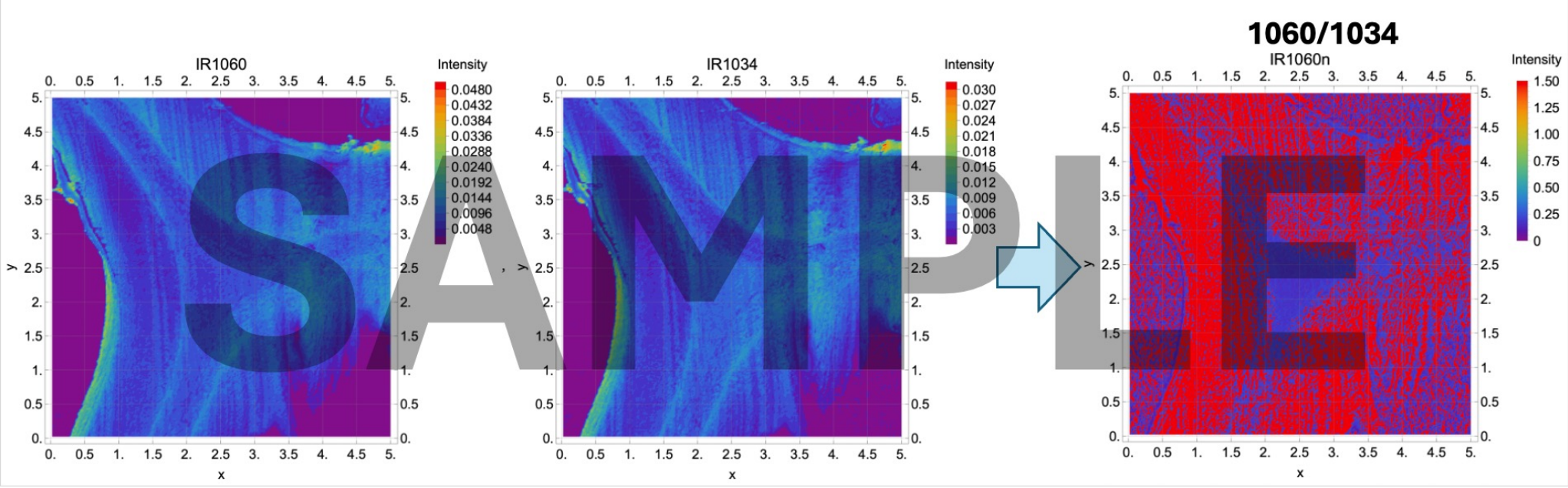
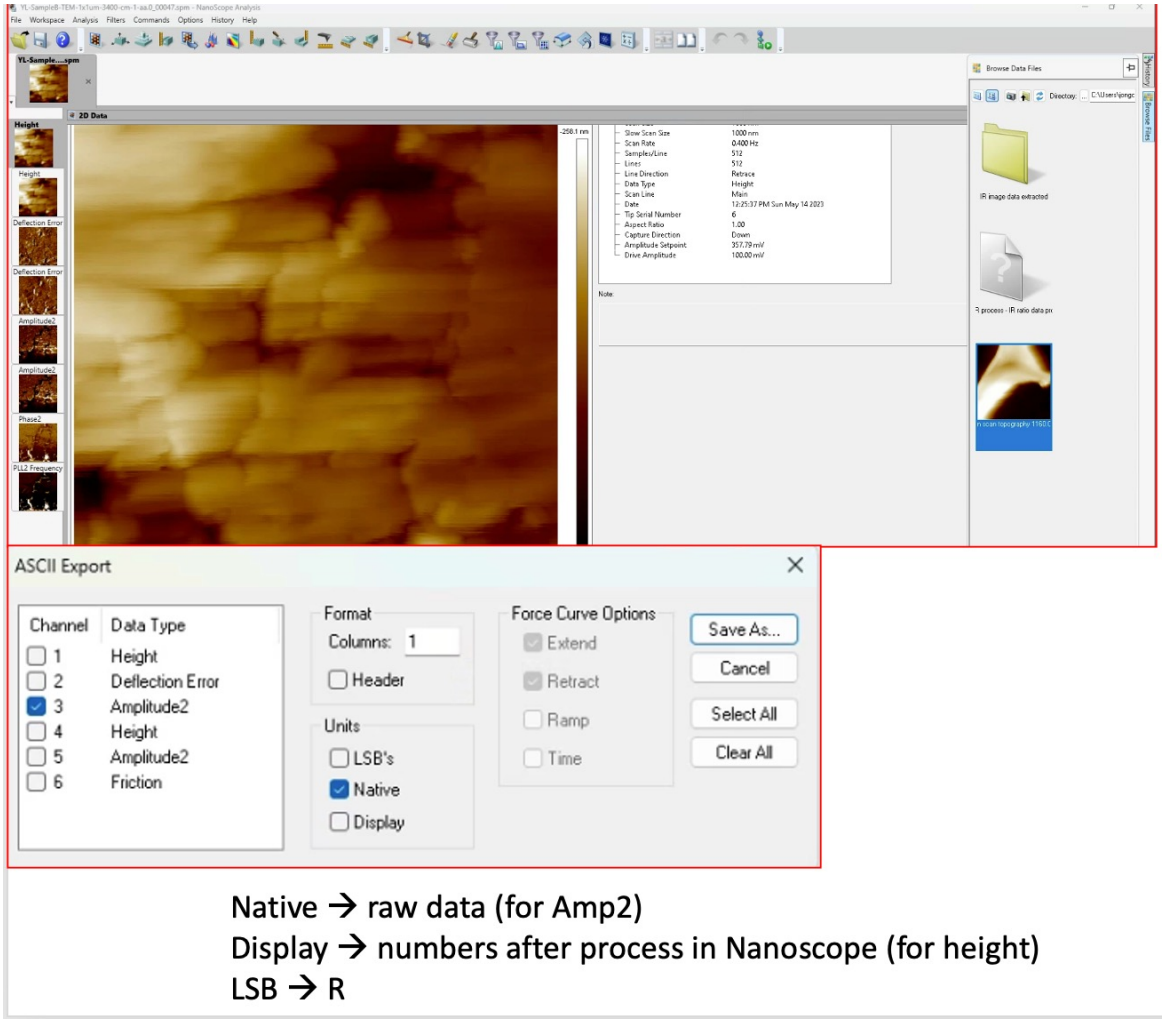
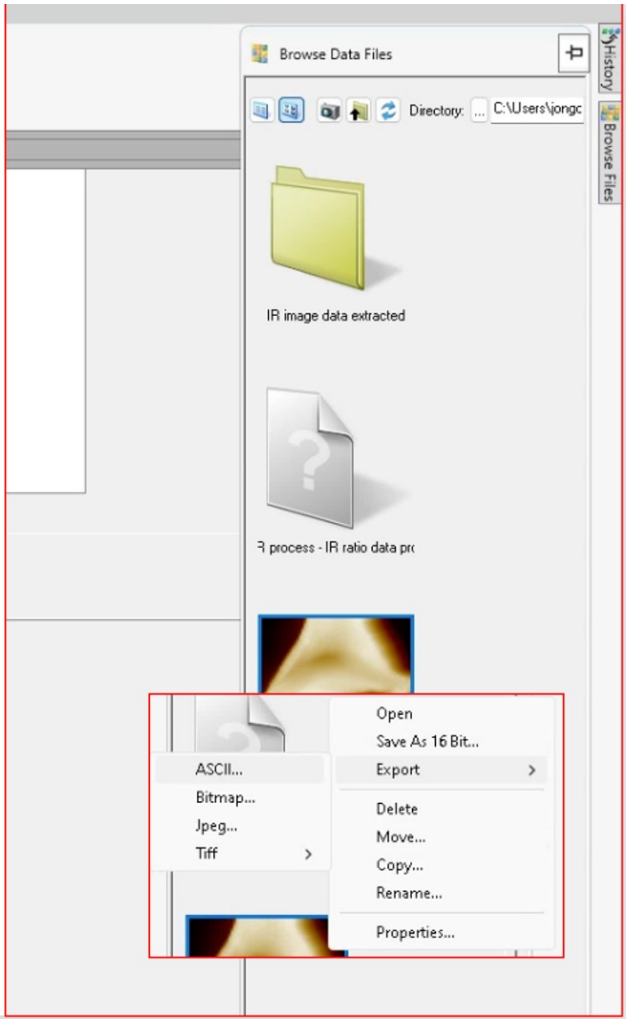


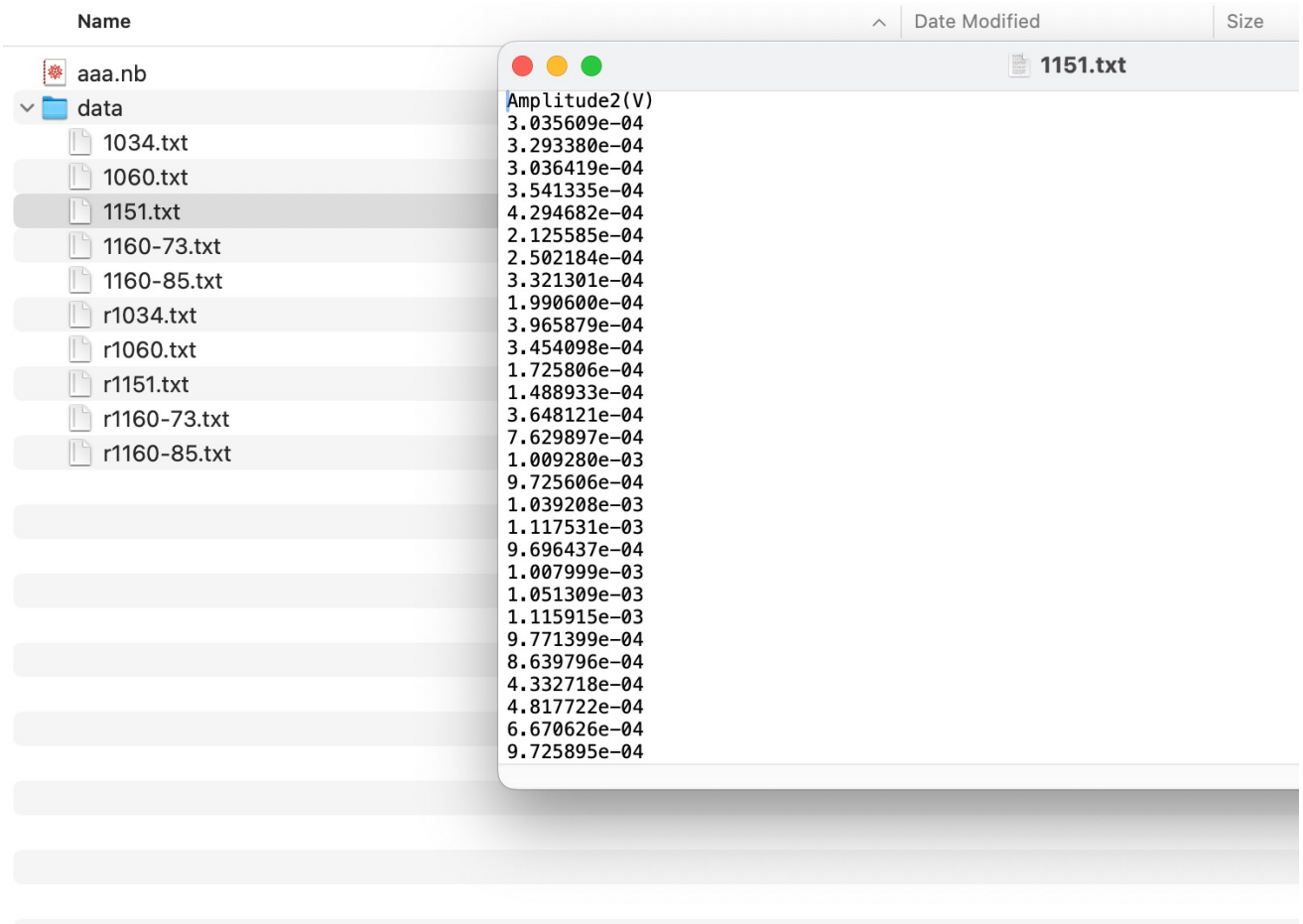
How to expoert Data from Bruker – Nanoscope software.





Native → raw data (for Amp2)
Display → numbers after process in Nanoscope (for height)
LSB → R

Check if the txt files are below. First line is the value name. spl x spl values are in one column. Ver. 2



Cells with light yellow background → You need to input proper numbers about your data information.

Explanations are in (*exp*)

Ver.2 (nx x ny data in one column, in .txt)

In[62]:=
```
$Version
ClearAll["Global`*"]
SetDirectory[NotebookDirectory[]];(*Mathematica file in the proper location*)
```

Out[62]= 12.3.0 for Mac OS X x86 (64-bit) (May 10, 2021)

a. Data import and process

0. Data information

In[65]:=
```
Lx = 5;(*um-scanned area *)
Ly = 5;(*um-scanned area *)
dim = 256;(*sample per line *)
nx = dim;
ny = dim;
```

1. Data import

In[70]:=
```
allFiles = FileNames["*.txt", "sample data"];(*import .txt files in the directory name 'data'*)
allData = Import[#, "Data"] & /@ allFiles;
allData // Dimensions(*Check how many .txt files were imported*)
```

Out[71]= {10, 65 537, 1}

In[72]:=
```
allData2 = Table[i, {i, 1, Length[allData]}];
For[i = 1, i ≤ Length[allData],
 allData2[[i]] = Drop[allData[[i]], 1]; (*Drop the first line (names)*)
 i++]
allData // Dimensions
```