Laboratory 5: spICPMS Data Processing Instructions

Dissolved gold standards analysis

1. On the **"Raw Data"** tab in the green cells, compute the average of the data for each concentration level of the 5 dissolved gold standards. Make sure to select the entire column of data for each sample in the computation.
2. Transfer the average values to the corresponding cells in yellow on the **"Dissolved Au_CalStd"** page. The slope and intercept should automatically populate, along with the plot with the linear fit and the R^2 value.

Au Nanoparticle (60 nm) – For Transfer Efficiency

1. Data processing will be done in the **"spICPMS_AuTE_Unknown Samples"** tab.
2. Fill in the **Dwell time** and **Flowrate** values as recorded from the lab session.
3. Copy the column of measured values from the **"Raw Data"** tab into the **"Background Intensity"** column under the Transport Efficiency Determination.
4. Using the "Sort" tool (in the "Data" section in Excel), sort the column of intensity data from highest to lowest value.
5. Complete the **Dissolved Ions** section in yellow:
    a. **"Cal Slope"** – Copy the value of the slope from the **"Dissolved Au_CalStd"** page.
    b. **"Mean Background"** – Take the average of the entire column of values in the "Background Intensity" column.
    c. **"Std Dev Background"** – Take the standard deviation (STDEV or STDEV.S) of the entire column of values in the "Background Intensity" column.
    d. **"Ion/Particle Cutoff"** – Compute the threshold signal for ions versus particles as "Mean Background" + 5×"Std Dev Background."
6. Separate background and spike signals as follows:
    a. Inspect the data in the **"Background Intensity"** column. Cut all values higher than the "Ion/Particle Cutoff" value and paste into the **"Spike Intensity"** column.
    b. The **"Ion/Particle Cutoff"** value will be lower after moving the data. Go into the "Background Intensity" column again to transfer values higher than the new cutoff value to the "Spike Intensity" column.
    c. Repeat until there are no values in "Background Intensity" higher than the cutoff.
7. **"Particle Intensity"** column:
    a. Subtract the "Mean Background" value from the "Spike Intensity."
    b. Check the bottom of the column to remove any rows that may have auto-filled past the bottom of the "Spike Intensity" column.
8. Complete the **Nanoparticles** section in pink:
    a. **"Particle Frequency"** – Use the Excel "COUNT()" function to count the entries in the "Particle Intensity" column, and divide by the "Measurement Duration." This is $\boldsymbol{q_p}$ in the formulas from **ISO/TS 19590:2017**.
    b. **"Detected Particles/L"** – The formula is already included in the spreadsheet template, including unit conversions required when the other cells are inputted with the units specified in the template.
    c. **"Transport Efficiency"** – Calculate as $\boldsymbol{\eta_n}$ using the formula from **ISO/TS 19590:2017**. Make sure that you apply or remove unit conversions as necessary, if there are any discrepancies between units on the input values in the spreadsheet versus the formula from the standard.
    d. **"Molar mass ratio"** – The molar mass ratio is 1 (i.e., 100%) for the Au content in

the Au nanoparticles, which do not contain any other elements besides Au.

e. **"Density (g/mL)"** – The density is 19.3 g/mL for Au.

9. **"Particle Mass"** column:
   a. Calculate as $\boldsymbol{m_p}$ using the formula from **ISO/TS 19590:2017**. Make sure that you apply or remove unit conversions as necessary, if there are any discrepancies between units on the input values in the spreadsheet versus the formula from the standard.
   b. Check the bottom of the column to remove any rows that may have auto-filled past the bottom of the "Spike Intensity" column.
10. **"Particle Diameter"** column:
   a. Calculate as $\boldsymbol{d_p}$ using the formula from **ISO/TS 19590:2017**. Make sure that you apply or remove unit conversions as necessary, if there are any discrepancies between units on the input values in the spreadsheet versus the formula from the standard.
   b. Check the bottom of the column to remove any rows that may have auto-filled past the bottom of the "Spike Intensity" column.
11. **"# Average Diameter"** (highlighted in yellow) – Take the average of the entire column of values in the "Particle Diameter" column.
12. Prepare the results for a **Histogram Plot** of the size distribution.
   a. SAVE YOUR FILE. The histogram may take some time to compute.
   b. Select the "Data Analysis" tool from the "Data" section in Excel. If it does not appear, Go to "File" → "Options" in Excel, then "Add-ins". Next to "Manage: Excel Add-ins" at the bottom, click "Go…" Check the box for **"Analysis ToolPak"** if it is not already enabled.
   c. Select **"Histogram"** and complete the following sections:
      i. **"Input Range"** – Select the column of "Particle Diameter" data (only the numerical values, not the "Particle Diameter" text in the heading)
      ii. **"Bin Range"** – Select the column of values in Column A under "Size Bins for Histograms" (only the numerical values).
      iii. Leave **"Labels"** unchecked.
      iv. Select **"New Worksheet Ply"** for the Output options. You do not need to type anything into the box next to it.
      v. Click **OK** to run.
      vi. A new sheet should appear with the results. Copy the "Frequency" column into the highlighted column on the **"Au60nm_TE"** tab. The histogram plot should automatically populate with the results.

Other Au Nanoparticle Samples

- The data processing for the other 3 samples is performed in exactly the same way, **except you will use the Transfer Efficiency value from Step 8(c) instead of calculating it.**
- Note the AuMix sample has 3 minutes measurement time (hence 3 times more data points).
- While some formulas can be copy-pasted from before if set up properly, **you will always need to reselect the data column for each sample** when computing the mean, standard deviation, counting particles, etc., since each sample has a different number of measurements, particles, etc.