Research Report for SALT research group (DRAFT REPORT)

ICPOMS data processing tool GitHub:

[Github](https://github.com/HemingYHM/ICPMS)

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1. **Scope**

* The ICPMS data processing tool aims to automate the data processing process for the elemental analysis project and act as a tool to facilitate ICPMS data exploration.
* The data processing tool includes a second part that act as a data exploration tool to plot the samples vs. the calibration curve for visualization.
* In addition to these features, we are currently planning to give more freedom to the user to access and modify the intermediate tables for the integrity of the data as well as data processing procedure.

1. **Background and Motivation**

* The goal is to follow the data processing procedure for ICP MS in order to derive the original table.

1. **Necessary Inputs**

* ICP-MS Device Input as a csv format
* **A table with numbers and numbers

  Description automatically generated**

1. **Instructions for use**

* For now since its in development, functions are run in the interactive python notebook, however, they will be compiled into a compact program toward the end of the semester.

1. **//Naming Conventions (Standards vs. Samples)**

**For standards:**

* The user has to strictly put the number before ppm in order for the program to successfully parse the table
* Example: .1ppm NiCr -> the .1 standard

0 ppm NiCr -> the 0 standard

Be sure to include the 0 !!!!

**For samples**

* Unlike the previous work, the ICPMS has no strictly policy on naming for samples, however, since our graph and data are generated **on demand**, you have to keep the names consistent.
* For reference, here is the ICPOES naming
  + Each sample(SA ID column) follows the following format:
    - 10 (Letter) (1..9) ([01…99])(01…99)(Letter) (Date)
      * 10: Project Number 10
      * Letter: Type of Sample {D: Digestion, S: Salt, L: Dilution, B: Blank}
      * 1..9: The Type of salt that will be indicated {1: FLiNak, 2: FLiBe, 3: Other.. to be named}
      * [01…99]: For indexing purposes in data storage. Corresponds to the blank.
      * 01…99: This number will always be double digits so if it's the first 9 in the iteration the numbers will be 01, 02, 03... etc. This is used for if the amount of salt, or another aspect, is different than what has been made before. It is to differentiate the samples if they are all FLiNaK with the sample blank.
      * Letter: Finally, the last part of this will be for duplicating the sample. This will allow for keeping track if the sample is duplicated. No matter what start off labeling the first sample with an A, and if another almost exact one is produced it will be labeled B, next one C, etc
      * Finally the date: yyyy/mm/dd
    - Example**: 10B1[01]01A20221108**

1. **Future Work**

* Fixing the graphs to include the 0 ppms(Currently not included)
* Better intermediate table outputs
* Prettier/interactive graphs
* Subset graphs on user selected standard values(as well as data tables)