Creation of output spreadsheet

Start with sample results

Script functions on the premise that input files have 5 sheets organized as: Result, Controls, Calibrants, Rbl, Method

For information on the tests run by SmartChem that are handled by the script and to view and update the lab-calculated MDL values, check “data/required/tests.xlsx”. Note that each test should only have 1 row in “tests.xlsx”.

Access lab-calculated MDL values at “GIWS1/Helen_Lab/SmartChem/SampleMDLs.xlsx”.

Determine the MDL

- If the test has a lab-calculated MDL recorded in tests.xlsx, use it
- If no lab-calculated MDL exists, calculate the MDL using the Controls sheet

$$Script\ calculated\ MDL = standard\ deviation\ of\ STND * 95\%\ CI\ student's\ t\ statistic$$

Extract the last run of each sample (the run with greatest dilution ratio)

Check how many duplicates were run for each sample (same SampleID, position, dilution)

Script makes sure that each run has 2 duplicates. If 2nd duplicate is missing, script creates a dummy duplicate (concentration = NA)

If more than 2 duplicates were run, script takes note and later flags as a “Multi-run sample”

Assign additional flags to each duplicate (see Final Flags)

Use the concentrations from the 2 duplicates to calculate

- mean
- difference and percent difference
- standard deviation and relative standard deviation

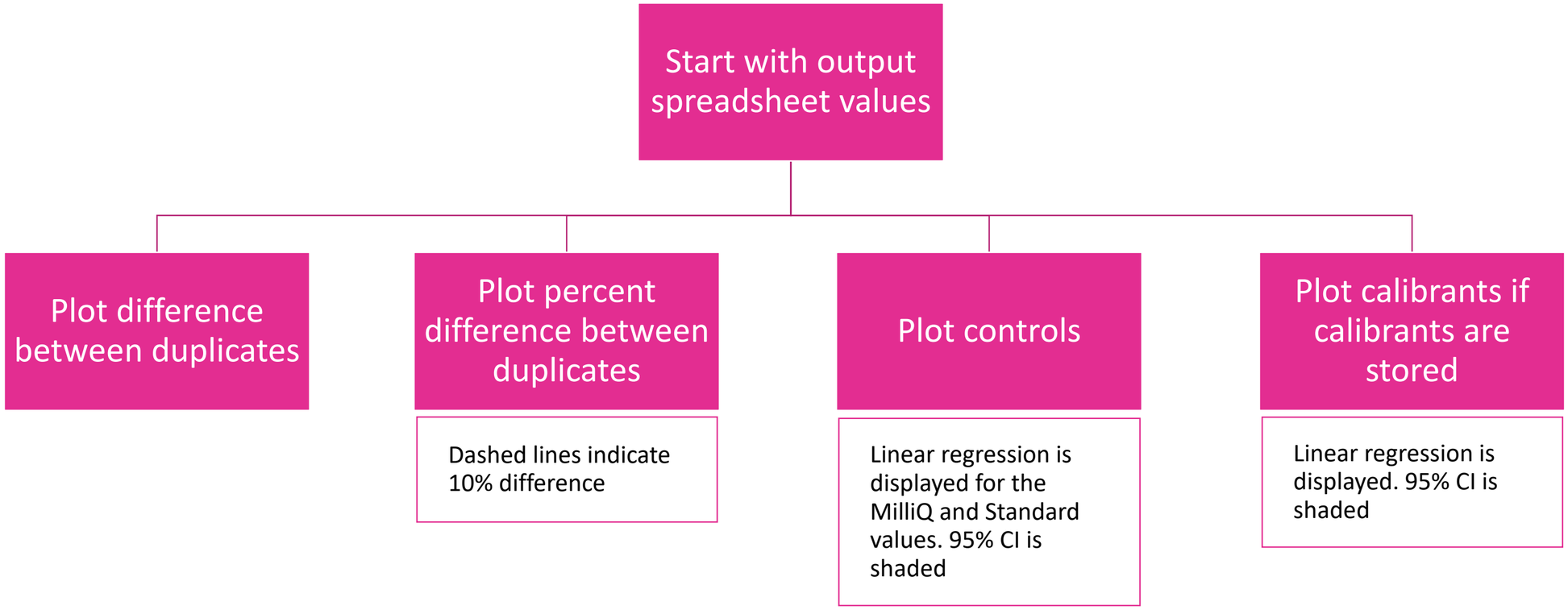
Assign flags to the newly calculated values (see Final Flags)

If either of the concentrations < 0, the mean is set to -111

If only 1 duplicate was run, the calculated difference, percent difference, standard deviation, and relative standard deviation are NA

Place all data together in one final output spreadsheet

Creation of output plots



Conversion of SC flags

SC flag	Expanded flag
LL	Linearity Low
LH	Linearity High
EPL	End-Point Limit
INV	Inversion
><	Out of Calibration Curve
SS	Short on Sample
SR	Short on Reagent
H	High

Final Flags

Flags for individual runs (columns: Flags Dup x)

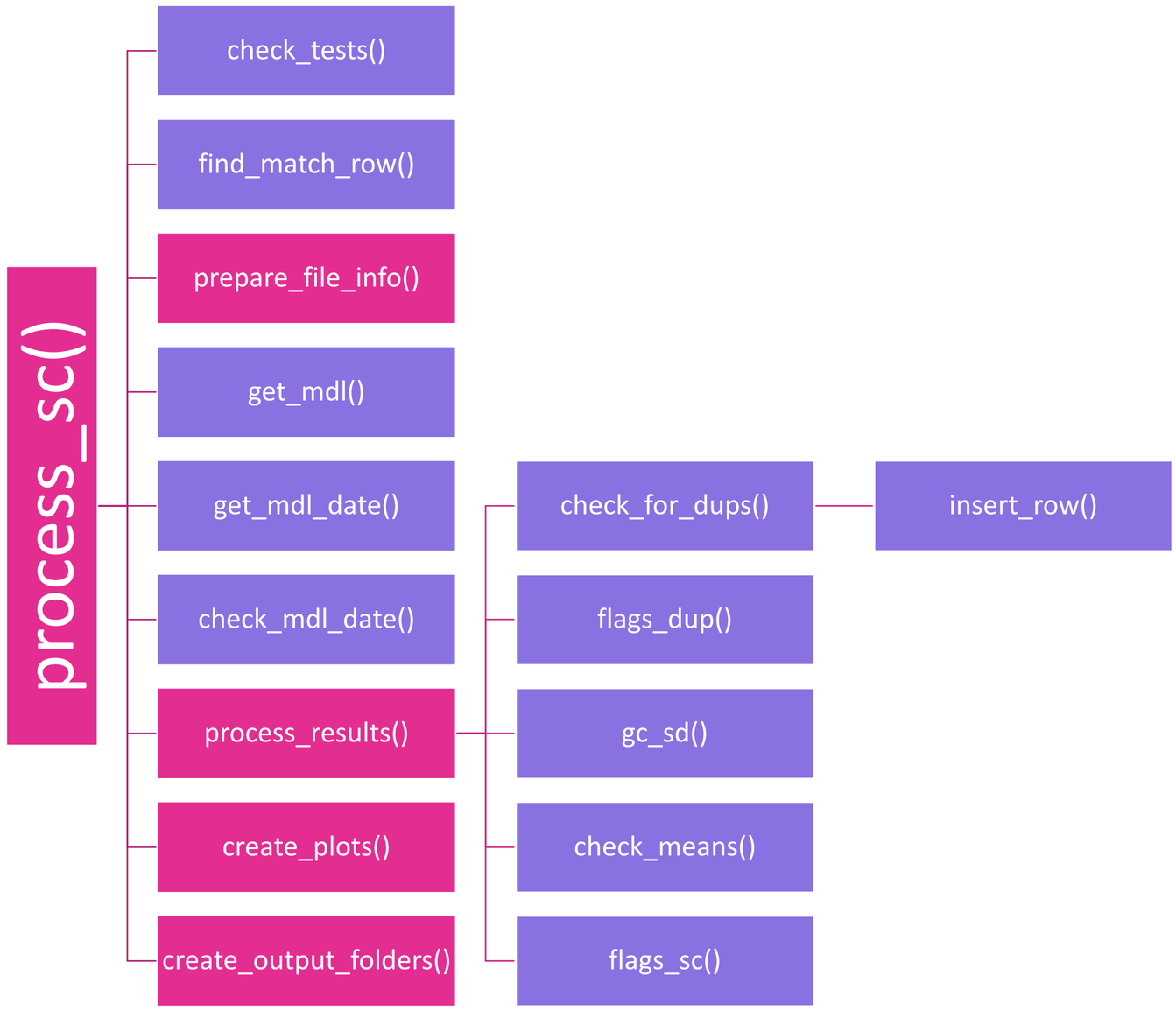
Flag	Meaning
Linearity Low	Abs value is low and outside of the calibration curve
Linearity High	Abs value is high and outside of the calibration curve
End-Point Limit	Sample sat longer than recommended while being read
Inversion	Negative absorbance
Out of Calibration Curve	Result plotted outside of the calibration curve
Short on Sample	Run could not complete due to insufficient sample
Short on Reagent	Run could not complete due to insufficient reagent
High	Sample was above the calibration curve
Run was not completed	Will apply only to _Dup rows. Indicates that _Dup row is missing in input
< 0 (actual value: xxx)	A negative concentration was recorded. Concentration value is stored in flag
< MDL	A concentration < MDL was recorded

Flags for comparison of duplicates (column: Flags)

Flag	Meaning
Perc difference > 10 & both conc above MDL	Percent difference is violated and both concentrations >= MDL
Perc difference > 10 & one or both conc below MDL	Percent difference is violated and one or both concentrations < MDL
Both conc below MDL	Percent difference not violated and concentrations < MDL
Rerun dilution	SC automatically reran this sample with a different dilution
Multi-run sample	User reran this sample with the same dilution

Callstack

For those who need to go into the code



function defined in sc_functions.R

function defined in sc_helper_functions.R