In this analysis we will manually be performing a Tuning Correction using Unit Test\_10 as a basis for the analysis. Unit Test\_10 is a modified copy of unit test\_ 5. A reference pattern from unit test\_10 will be acquired (Is provided). Second, correction factors will be acquired using the excel file “180613MadixKoMSCorrectionsFactorExample\_NO\_HIDING” using the masses from sls sent from Ashi. The excel file “180613…” will be used as a guide. Third, a tuning correction polynomial from the two refence patterns (Internal & External) will be created. This will allow us to then create a mixed pattern refence file. Manual SLS will then be performed. The molecule concentrations will then be achieved (SC2RC) Scaled Concentration to Real Concentration scaling factor.

Root Directory:

* TuningCorrectorGasMixtureHypotheticalReferenceMeasuredVsSimulated
  + Will use as a refence to create polynomial fit for Tuning correction between Internal & External refence file
* Masses-Molecules\_SLS\_UnitTest\_Test\_10
  + Gives Masses and molecule names that will be used in SLS
* 180613MadixKoMSCorrectionsFactorExample\_NO\_HIDING
  + Will be used as a guide to create the correction factors for each molecule and their masses
* 180613MadixKoMSCorrectionsFactorExample\_NO\_HIDING\_PRACTICE
  + Will be used as a practice calculation using data provided in excel sheet.

1. This is a base file for the analysis.
   1. Unneeded files will be deleted
   2. test\_5.py will be copied and renamed to test\_10.py. It will then be modified to allow for the test to be solved using SLS
      1. allows for test 5 to be solved using SLS
2. Direct copy of “0”
   1. Will be used to acquire Ref Pattern from MSRESOLVE that has been preprocessed.
   2. This file is “Exported0ReferencePatternOriginalForCorrectionValues”
      1. “AcetaldehydeMeasured\_Scaled\_to\_100” will have the original reference pattern standardized to 100 manually.
         1. Masses under 4 will be filtered out
3. Direct copy of “1”
   1. Will be used to acquire correction factors for each molecule using file “180613MadixKo…” as a guide.
      1. Added “180613MadixKoMSCorrectionsFactorExample\_NO\_HIDING” from root directory and changed name to “180613MadixKo\_Test\_10”
   2. “Masses-Molecules\_SLS\_UnitTest\_Test\_10” gives the masses and molecules used for SLS.
   3. Copy of “AcetaldehydeMeasured” was made and named “AcetaldehydeMeasured\_Scaled\_to\_100”
      1. Intensities scaled to 100, all intensities under 4 removed, remaining intensities rounded to nearest whole number.
4. Direct copy of “2”
   1. Will be used to create a tuning correction polynomial fit using file “TuningCorrectorGasMixtureHypotheticalRef…” as a guide.
      1. Made copy of “TuningCorrectorGasMixtureHypotheticalRef…” from root directory and renamed it to “Created\_Polynomial\_Fit\_Test\_10”
         1. The polynomial fit will be created between the measured and Nist reference pattern.
            1. Nist pattern standardized to 100 in “ReferenceLiterature\_Standardized\_100”
         2. The polynomial fit will also be applied to the NIST ref patterns of “2-butenal, & 1butanal”
      2. “ExportedReferencePatternDesiredOriginal” will be used to acquire our original measured refence pattern.
         1. Will be copied & renamed to “MeasureRef\_Zeros\_Removed”
         2. Unneeded zeros will be removed
         3. Removed unneeded molecules, Kept: (Acetaldehyde, (E) 2-Butenal, Ethylene, Ethanol, Crotyl Alcohol)
      3. “ExportedReferencePatternExistingOriginal” will be used to acquire our Nist refence pattern.
         1. Will be copied & renamed to “NistRef\_Zeros\_Removed”
         2. Unneeded zeroes will be removed
   2. Mixed reference pattern will be made.
      1. “Mixed\_Ref.csv”
      2. Uses measured data of: Acetaldehyde, CO, CO2, Ethylene (Ethene), Ethanol, Crotyl Alcohol, H2, H2O
      3. Uses Nist-TuningCorrected (Nist with polynomial fit applied) data of: 1butanal
   3. Incorporating 1butanal tuning corrected into Madix&Ko to acquire new correction factors.
      1. “180613MadixKo\_Test\_10” renamed to “180613MadixKo\_Test\_10\_TC\_1butanal”
         1. This will incorporate the new Tuning corrected 1butanal, thus replacing the old 1butanal.
            1. 1butanal signals will be standardized to 100. Any less than 4 will be removed. The remaining signals will be rounded to the nearest whole number (This will be done using excel formulas in “Created\_Polynomial\_Fit\_Test\_10”)
5. Direct copy of 3. Will be used to perform sls
   1. SLS will be performed using molecules, masses, and correction factors from “Masses-Molecules\_SLS\_UnitTest\_Test\_10” & “180613MadixKo\_Test\_10\_TC\_1butanal”
      1. This will be documented in “Test\_10\_SLS.xlsx”
      2. Time 176.848 (Salmon Colored) will be used as well as Time 176.895 (Blue Colored)

A picture containing text, device

Description automatically generated

* + 1. Relationship Used: (C-1 \* Concentration = Signal) or (Signal \* C = Concentration)