In this analysis we will manually be performing SLS with Implicit SLS on using Unit Test\_11 as a basis for the analysis. Unit Test\_11 is a modified copy of unit test\_ 10. A reference pattern from unit test\_11 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\_11
  + 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
      1. test\_10.py will be copied and renamed to test\_11.py. It will then be modified to allow for the test to be solved using Implicit SLS
         1. MSRESOLVE.G.implicitSLScorrection = True
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\_11”
   2. “Masses-Molecules\_SLS\_UnitTest\_Test\_11” 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\_11”
         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\_11” renamed to “180613MadixKo\_Test\_11\_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\_11”)
      2. 180613MadixKo\_Test\_11\_TC\_1butanal\_SLS\_Implicit
         1. This will incorporate the new Tuning corrected 1butanal, thus replacing the old 1butanal.
            1. 1butanal signals will be standardized to 100. All molecule intensities from the mixed reference pattern, even those less than 4, will be inputted into this Madix and Ko file.
5. Direct copy of 3. Will be used to perform sls
   1. SLS will be performed (without Manual SLS Implicit) using molecules, masses, and correction factors from “Masses-Molecules\_SLS\_UnitTest\_Test\_11” & “180613MadixKo\_Test\_11\_TC\_1butanal”
      1. This will be documented in “Test\_11\_SLS.xlsx”
      2. Time used: 176.848
   2. SLS will be performed (With SLS Implicit) using molecules, masses, and correction factors from “Masses-Molecules\_SLS\_UnitTest\_Test\_11” & “180613MadixKo\_Test\_11\_TC\_1butanal\_SLS\_Implicit”
      1. This will be documented in “Test\_11\_SLS\_Implicit.xlsx”
      2. Time used: 176.848

A picture containing text, device

Description automatically generated

* + 1. Relationship Used: (C-1 \* Concentration = Signal) or (Signal \* C = Concentration)
    2. Once SLS is performed, remaining molecule concentrations will be solved using the left-over signals from SLS. This is known as SLS Implicit. Once the left over concentrations are solved for, they will be added back to the final solved molecule concentration.