ExtentOfSLSUniqueSolvable() Algorithm

1. If specified, the truncatedProvided reference data will be multiplied by the molecular likelihoods. The intensities of any mass fragments containing only intensities less than the majorPeakThreshold=30% will be set to zero. Create a truncatedProvidedRefDataas1sand0s with the altered truncatedProvided reference intensity array where 1 represents the location of a non-zero intensity and 0, the intensity at the location of a zero.
2. Use the truncatedProvidedRefDataas1sand0s to create a parallel array only containing the location of any unique fragments. This will be called uniqueMassFragmentsInTruncatedProvidedRefIntensityArray.
3. A 1-D array containing the sums of the 1s (non-zero reference intensities) across all molecules for each mass fragment in the truncatedProvidedRefDataas1sand0s will be created. If any value within that array is non-zero, the molecule is solvable by SLS. An N number of truncated mass fragmentation patterns (reducedFragmentationPatterns)specified by keep\_N\_ExtentOfSLSUniqueSolvableCombinations) will be stored in extentOfSLSUniqueSolvableFragements as sorted by their count of solvable molecules and the also an intensity based term for the objective function.. *z = (zs,zI) so z is 2D.*
   1. There are two options for second part of the objective function , *zI*,which is the intensity part: 1) sum of the square roots of the maximum unique peaks and 2) significance sum.
      1. If all the molecules are solvable by SLS-Unique, option 1 will be used. We will take the square root of intensity of the maximum intensity unique fragment for each molecule, and sum these square roots(summed across all the molecules), creating a scalar. This is used because the significance factor does not account for entirely unique fragments without any overlap. The significance factor for an entirely unique fragment is equal to zero. By using the sum of the square roots of the maximum unique peaks, larger peaks are favored over smaller ones and can be ranked according to the magnitude of their peaks.
      2. Else the significance factors sum is used. This finds the significance factor for each intensity in the array (which is a function of the other values in each mass fragment row/column) and sums them all together. Since fragments do overlap in this else statement, the significance sum is used to rank the mass fragment combinations.
      3. The count of solved molecules (the solvability part of the objective function) and the other sum term (the intensity part of the objective function) value will be stored in a tuple and passed to the store and pop function.
      4. The top mass fragment combination in the list of extentOfSLSUniqueSolvableFragements will be returned to the user in the form of a reference file. The other fragment combinations will be printed to another file (one combination per row, followed by the objective function for each combination).
4. FUTURE WORK:
   1. In the future, when calculating zI, the molecules that can be solved should be subtracted and the significance sum only used for the remaining molecules.
   2. With the above step of the future work completed, an ExtentOfSLSCommonSolvable() will be created to determine the best mass fragments for the SLS Common method .