Supplementary Figure 1 Start **Open Raw File** and Set Scan Raw File **User Input** Range Count= End Start Scan to End Scan **Fetch Peak Lists** A and B Is No Yes Peak List B Count > 0? Detect Charge State, Monoisotopic Peak and All Isotopic **Envelope Peaks Determine Charge Averagine Fitting** Enter a Peptide Record in **Raw File List** Delete from peak

list B all Isotopic envelope peaks of determined peptide