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Post-Translational modifications and the effects on protein identification through mass spectrometry

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Mass Spectrometry is an effective tool for protein identification. A typical process for protein identification is to break down a protein into smaller peptides and to determine the mass of each of these peptides. These peptide masses are then compared against a database of proteins, to identify the protein which composes these peptides. Most proteins undergo co- and /or post-translational modifications such as glycosylation, phosphorylation etc after they are synthesized. Post translational modifications (PTMs), cause the masses of the peptides to be different than they are in the database, causing the computer programs to predict them incorrectly. While developing a program to accurately predict proteins using Mass Spectrometry, consideration must be given to such PTMs that may occur. The aim of the project was to modify a program currently in development, to allow the users to select some PTMs for consideration. The major challenge was to account for the PTMs without introducing large amounts of error into the system. In order to avoid the possibility of the program matching the mass of selected PTMs to false positive hits, the users will be instructed to only select a small number (less than 5) of PTMs. The actual program will be able to include an infinite number of PTMs, but the prototype only includes 47. There still needs to be some testing done as to which method of scoring gives the best confidence of the predictions. However, taking PTMs into account will definitely allow for a more successful identification of a larger number of proteins.