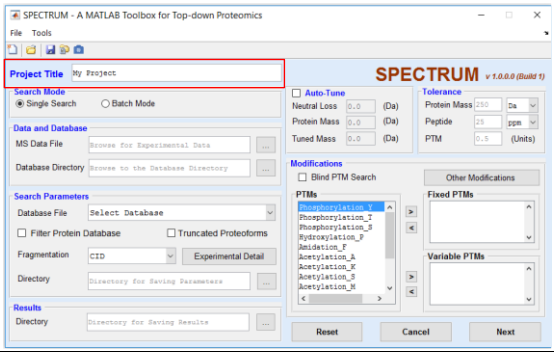
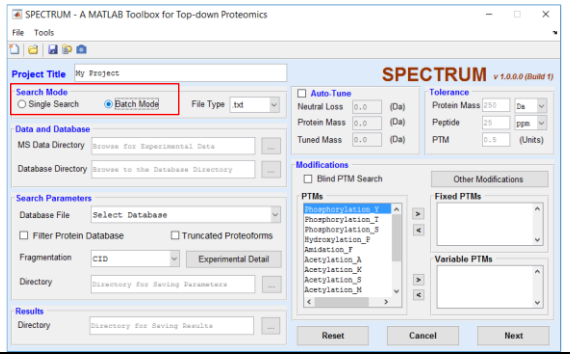
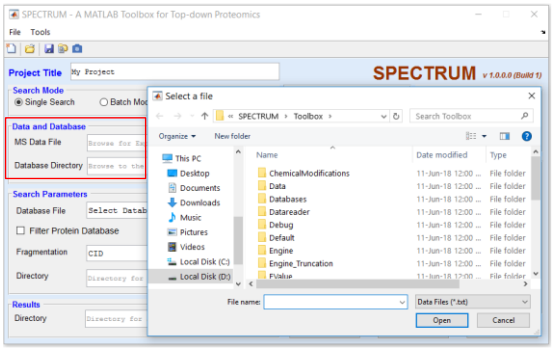
Step-by-Step Guidelines for using SPECTRUM



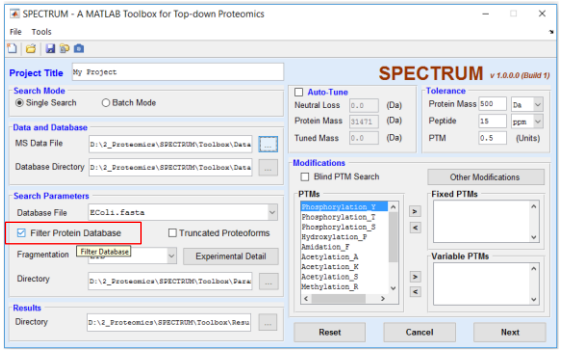
Step 1: Run the main GUI of the toolbox and input the 'Project Title'.



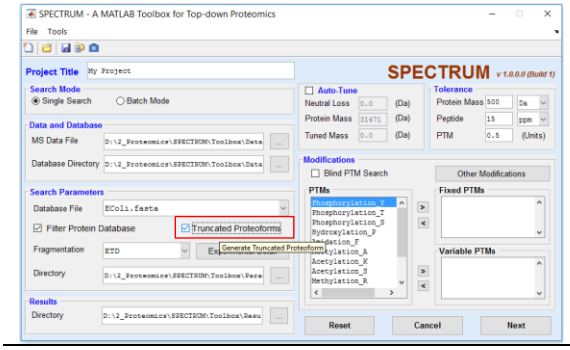
Step 2: Choose the processing mode as either 'Single Search' or 'Batch Mode'. For the batch run choose the 'File Type'.



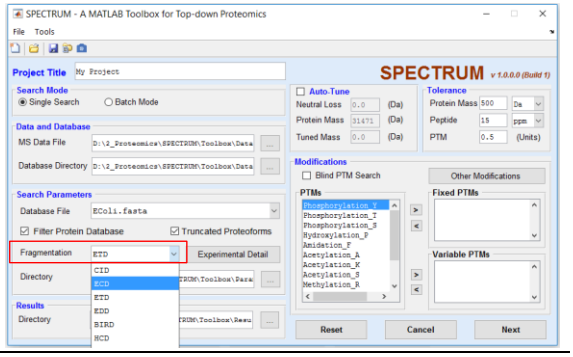
Step 3: Choose the directory for the Database, peak list file and output folder.



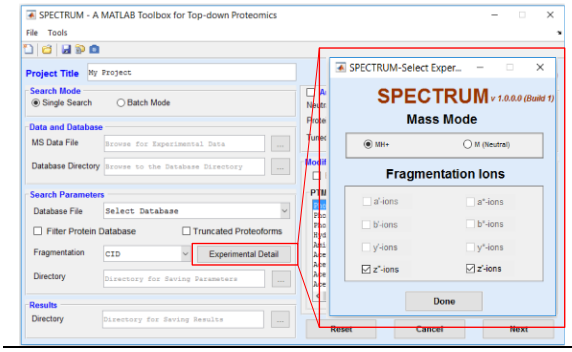
Step 4: Select whether to 'Filter Protein Database' for intact protein mass and tune the whole protein molecular weight.



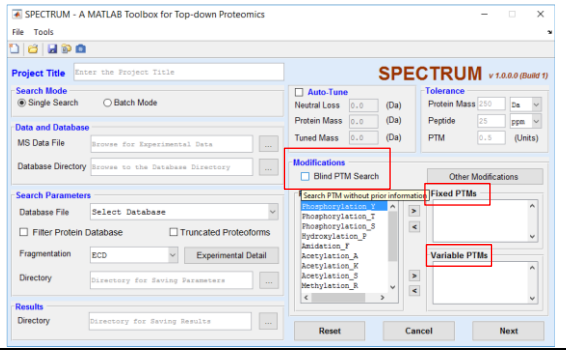
Step 5: Select whether to allow for 'Truncated Proteoforms'.



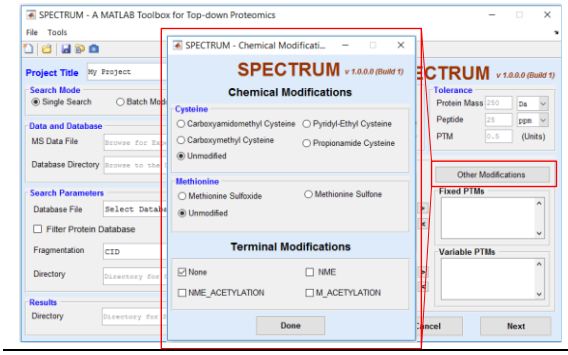
Step 6: Select the 'Fragmentation' type.



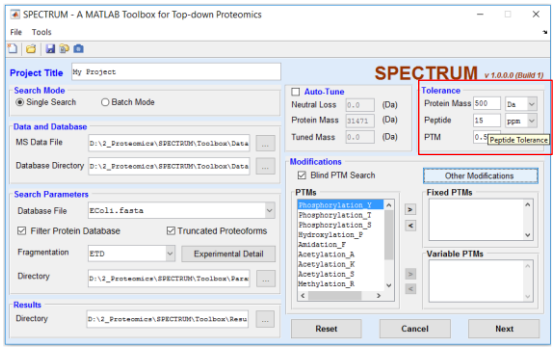
Step 7: Select 'Experimental Detail' to include special ions in protein search. Select 'Mass Mode' of experimental data.



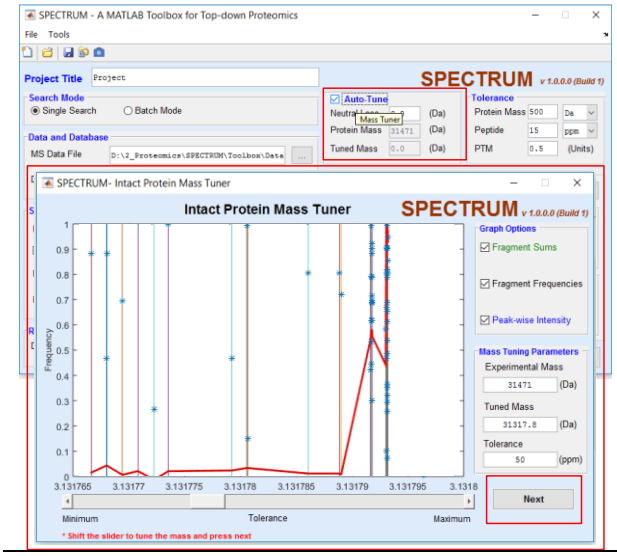
Step 8: Select the desired 'Fixed' and 'Variable' post translational modifications or search for 'Blind PTMs'.



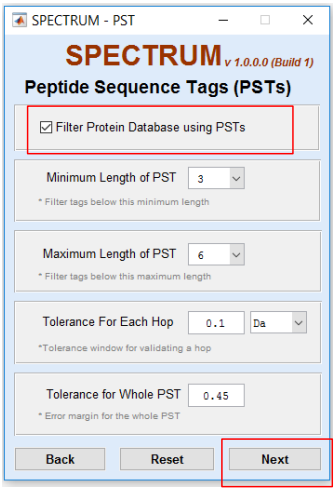
Step 9: Select cystine and methionine 'Chemical Modifications' along with desired 'Terminal Modifications'.



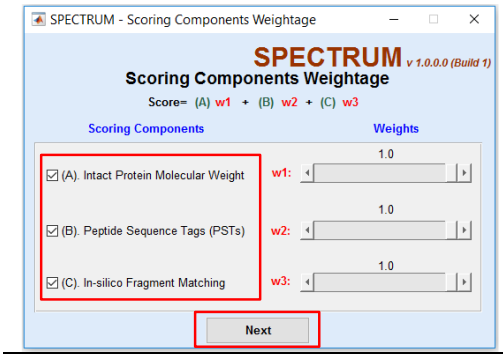
Step 10: Set the fragments and molecular weight 'Tolerance' with desired tolerance measurement.

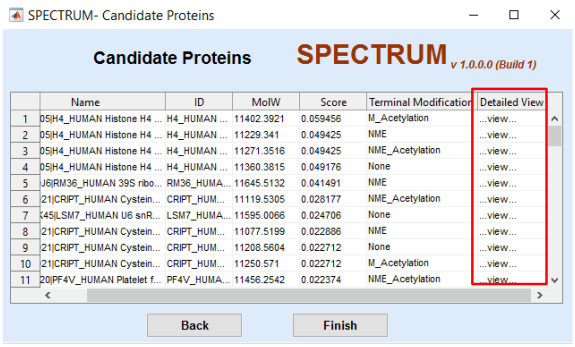


Step 11: Once the toolbox is run, if selected for molecular weight tuning the molecular weight estimation toolbox will open. Using this, the whole protein molecular weight can be estimated with the desired tolerance.



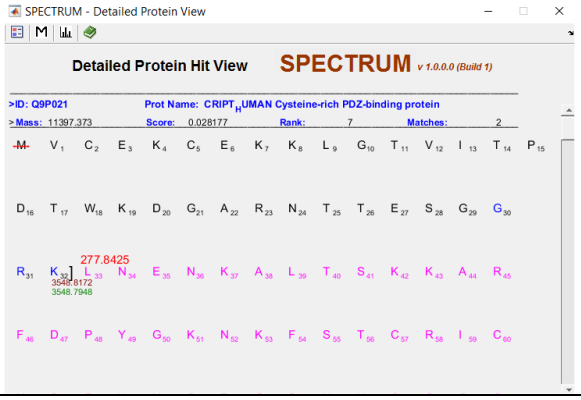
Step 12: In the PST GUI add the length of sequence tag, 'Tolerance For Each Hop' and 'Tolerance For Whole PST' to check for and score PST's in the given peak list file.





Step 13: Select the weight of each component towards final scoring

Step 14: This GUI will show summary result. To see detailed results for a protein, select 'Detailed View'.



Step 15: Detailed View of the protein selected in Step 14.