

## **Improving the proteoform inference from bottom-up proteomic data using protein identifications from MS1 spectra**

### **Bioinformatics**

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Protein inference is one of the crucial steps in proteome characterization using a bottom-up approach. Multiple algorithms to solve the problem are focused on extensive analysis of shared peptides identified from fragmentation mass spectra (MS/MS). However, many proteoforms of a particular protein have typically the identical lists of identified peptides due to the problem of proteome undersampling in bottom-up approach, and, thus, cannot be distinguished by existing protein inference methods. Here, we propose the use of peptide feature information extracted from MS1 spectra to assist in identification of proteoforms otherwise indistinguishable from MS/MS only spectra. The proposed method was integrated with a protein inference algorithm based on the parsimony principle and built-in in the post-search utility Scavenger. The results demonstrate increasing accuracy and efficiency of proteoform identifications for the well characterized datasets including the one with known proteoforms from ABRF iPRG-2016 study.