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Meeting abstract

Prediction of peptide drift time in ion mobility-mass spectrometry

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Background

Understanding the proteome, the structure and function of each protein, and the interactions among proteins will give clues to search useful targets and biomarkers for pharmaceutical design. Peptide drift time prediction in IMMS will improve the confidence of peptide identification by limiting the peptide search space during MS/MS database searching and therefore reducing false discovery rate (FDR) of protein identification. A peptide drift time prediction method was proposed here using an artificial neural networks (ANN) regression model. We test our proposed model on three peptide datasets with different charge state assignment (see Table 1). The results can be found in Figure 1, where a higher prediction performance was achieved, over 0.9 for CI and C2, as well as 0.75 for C3.

Conclusion

In this study, an ANN regression model was developed to predict peptide drift time in IMMS. Three peptide datasets with different peptide charge states were used to train the predictor to capture the differences of drift time among the varied peptides. The high performance of predictor indicated the capacity of our proposed method. In addition, a simple net architecture, which consisted of an input layer with four neurons, a hidden layer with four nodes and an output layer with one neuron, make our

Table 1: Experimental datasets with different charge state assignment

Dataset	Charge state assignment	Number of peptides
C1	+1	212
C2	+2	306
C3	+3	77

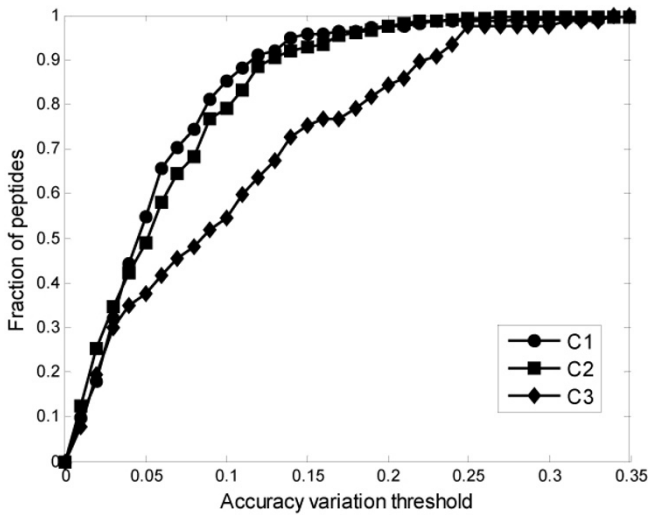

Figure 1
Fraction of peptides vs. prediction accuracy variation threshold. The diagram shows the number of peptides which can be predicted in different accuracy variation levels.

model more effective for application of protein identification.

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