

Application of TIMScore to De Novo Search Engine, DeepNovo in PaSER

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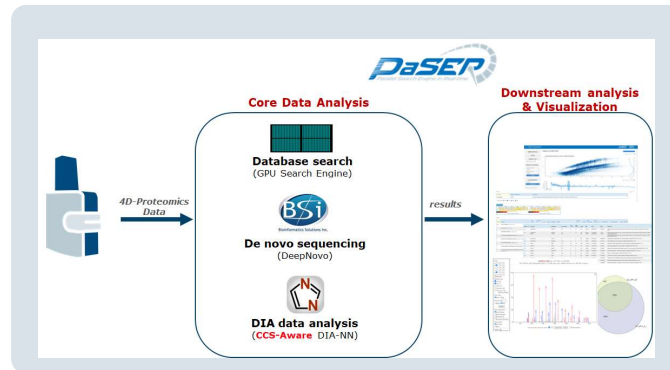
Introduction

We have recently integrated a de novo peptide sequencing tool, DeepNovo, into PaSER (Parallel Search Engine in Real-time) to sequence peptides in real-time by using deep learning and dynamic programming. To address the de novo peptide candidate ambiguity problem for a given spectrum, we have extended previously developed CCS-aware search scoring function, TIMScore, to de novo search results.

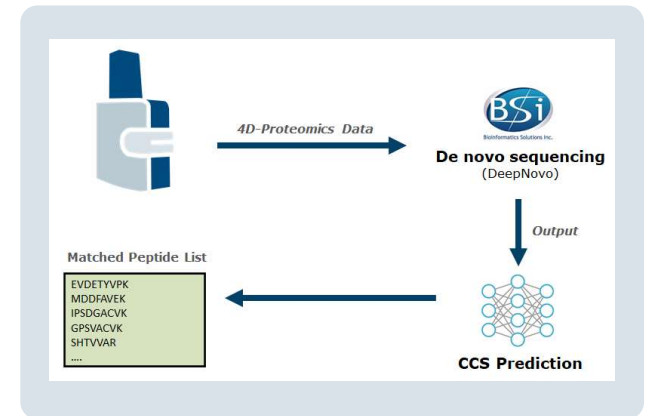
Methods

We developed a CCS prediction module and integrated it into the PaSER platform to dynamically generate predicted ion mobility values on the fly for de novo search. Similar to how TIMScore has been used for the database search, the search engine feeds the top five peptide candidates for each spectrum to the CCS prediction model to generate ion mobility values. Then, PaSER calculates TIMScore for each candidate. The program evaluates the ambiguity of the peptide candidates and applies TIMScore to attempt to clarify true peptide candidates.

PaSER Data Analysis Platform Overview



CCA-Aware De Novo Sequencing Strategy



DeepNovo Sequencing Results

- timsTOF Pro
- HeLa 200ng
- 90 min
- DeepNovo Sequencing

Total PSMs	Ambiguous Spectra	Percent
277,199	109,281	39%

Ambiguous spectra: 1st and 2nd peptide candidates have the same de novo score (Alc-score)

Apply TIMScore to De Novo Sequencing Ambiguity Problem

