# A Software for Top-Down Spectral Deconvolution and Protein Identification

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## BACKGROUND

In the last two years, due to advances in protein separation and mass spectrometry, top-down mass spectrometry moved from analyzing single proteins to analyzing complex samples and identifying hundreds and even thousands of proteins. However, computational tools for database search of top-down spectra against protein databases are still in infancy.

## TECHNOLOGY DESCRIPTION

UC San Diego researchers have developed MS-Align+, a fast algorithm for top-down protein identification based on spectral alignment that enables searches for unexpected post-translational modifications (PTMs). The first step in top-down spectral interpretation is usually spectral deconvolution, which converts a complex top-down spectrum to a list of monoisotopic masses (a deconvoluted spectrum). Every protein (possibly with modifications) can be scored against a top-down deconvoluted spectrum, resulting in a protein-spectrum-match (PrSM). MS-Align+ shares the spectral alignment approach with MS-TopDown, but greatly improves on speed, statistical analysis (providing E-values of PrSMs), and the number of identified PrSMs (e.g., by finding spectral alignments between spectra and truncated proteins).

## ADVANTAGES

UC San Diego researchers compared MS-Align+ with various tools for top-down protein identification on two data sets from Saccharomyces cerevisiae (SC) and Salmonella typhimurium (ST). The results demonstrate that MS-Align+ significantly increase the number of identified spectra as compared to MASCOT and OMSSA on both data sets. While MS-Align+ and ProSightPC have similar performance on the ST data set, MS-Align+ outperforms ProSightPC on the more complex SC data set.

## RELATED MATERIALS

▶ Liu X, Sirotkin Y, Shen Y, Anderson G, Tsai YS, Ting YS, Goodlett DR, Smith RD, Bafna V, Pevzner PA. Protein Identification Using Top-Down Spectra. Mol Cell Proteomics. 2011 Oct 25. [Epub ahead of print.]

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## OTHER INFORMATION

**KEYWORDS**
protein identification, mass spectrometry, top-down MS, MS-Align +

**CATEGORIZED AS**
▶ Research Tools
▶ Other

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