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HIGH CONFIDENT PROTEIN IDENTIFICATION FROM ETD AND ECD SPECTRA WITH A NEW MASS LIST PREPROCESSOR

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Due to the nature of the ECD or ETD fragmentation mechanism, the spectra contain some peaks that are directly related to the parent ion peaks: the remnants and neutral losses thereof, the reduced charge species. The removal of these irrelevant peaks has shown to increase the confidence of identification for database searches.

A simple tool has been developed that uses the charge state information of the ECD or ETD precursor ions in high resolution FTMS spectra. For high resolution FTMS instruments like LTQ FT or LTQ Orbitrap, the charge state of the precursor ions can be easily determined and from that information all the non-fragment peaks can be calculated. We have developed a spectrum preprocessor tool that removes all non-fragment masses from the spectrum mass list before submitted to database searches using Sequest and Mascot. This spectrum preprocessor tool was implemented in Proteome Discoverer 1.0 software. The search results for all identified peptides show a significant increase in the peptide score and – even more importantly – a large number of false positive identifications are eliminated in comparison to the search without the preprocessor.