Master 2014

Ms. Archana Abiram

Performance Evaluation and Optimization of Orbitrap Mass Analyzer.

ABSTRACT - Masterthesis

The purpose of this thesis is the selection of data acquisition parameters based on the transients behavior for targeted Selected Ion Monitoring (tSIM) to enable efficient and accurate acquisition of mass spectra, such that multiply charged single ions are observed in the acquired mass spectra. Performing these experiments on the two available versions of the Orbitrap mass analyzer which are the standard Orbitrap mass analyzer (D30) embedded into the Q Exactive mass spectrometer and the high field Orbitrap mass analyzer (D20) embedded into the Q Exactive HF mass spectrometer. This detection of multiply charged single ions is done for the exact determination of the FT - signal response per charge.

This study was conducted in Thermo Fisher scientific GmbH, Bremen, using the Q Exactive instrument and Q Exactive HF instrument. The proteomic samples used for the study included ubiquitin and insulin.

Comparison is done between the experimental mass spectra obtained from these two instruments at different transient lengths and depending on the results the limit of detection of these mass analyzers are determined. Between the two existing Orbitrap mass analyzer, a better suitable Orbitrap mass analyzer for performing tSIM experiments is determined and proposals to enhance the quality of the detected signals in the corresponding mass spectra are discussed. Therefore evaluating the performance of the D30 and D20 Orbitrap and optimizing their parameters for data acquisition in tSIM.