

USER REQUIREMENT SPECIFICATIONS FOR TANDEM MASS SPECTROMETER





LEIDS UNIVERSITAIR MEDISCH CENTRUM

USER REQUIREMENT SPECIFICATIONS
Advanced tandem mass spectrometer

Advanced mass spectrometer for PTM analysis in complex peptide/protein mixtures

Afdeling Center for Proteomics and Metabolomics

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Approval			

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1 Introduction

1. This is the User Requirement Specification (URS) for a tandem mass spectrometer. This tandem mass spectrometer will be used to comprehensively characterize (HLA-)peptidomes and glycoproteomes by an array of advanced combined fragmentation techniques. In addition the mass spectrometer will be used for relative (SILAC, multiplex, label free) and absolute quantification (PRM) of complex peptide samples. Maximization of identifications of complex PTM modified peptides/proteins is of key importance.

2 Aim

The aim of this specification is to describe the specific requirements for the tandem mass spectrometer.

3 User Requirement Specifications

3.1 General:

- Rebuilding of the existing facility is not necessary in order to place the instrument.
- Preferable dimensions within 1 x 1.5 meters
- Is already been put into operation in other comparable laboratories.

3.2 Technical specifications

- Capability to generate MS_n spectra up to 20 Hz
- Multiple stages of fragmentation, i.e. MS_n up to n=5
- Accurate mass measurement (< 1-10 ppm) of fragment ions with high mass resolution (>50.000 @ m/z 200)
- Ion source compatible with nanoHPLC and CE
- Collision Induced Dissociation (CID)
- Higher energy collisional dissociation (HCD)
- Electron transfer dissociation (ETD)
- Electron transfer dissociation in combination with high collision energy dissociation (ETHCD). As shown by the Heck lab.
- HCD fragmentation of multiple selected CID generated fragment ions
- Accurate quantitation by multinotch MS₃ of TMT labeled peptides. As shown by the Gygi lab.
- Flexible usage of different fragmentation combinations (e.g. ETHCD and HCD-CID MS_n)
- Data independent data acquisition (DIA)
- Parallel reaction monitoring (PRM)
- Middle and top-down analysis.
- Middle and top-down analysis software
- Product ion dependent scanning
- Data dependent neutral loss scanning
- Neutral loss ion exclusion experiments
- Parallelization of different scan modes
- Flexible workflow programming for method adjustment/optimization
- All the above mentioned requirements in the same device.

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3.3 Safety

- CE compliant

3.4 Documentation

- Instruction manuals
- Product Specification sheet
- The system should meet the regulatory compliance:
 - EMC Directive 2004/108/EC
 - Low Voltage Safety Compliance
 - FCC Compliance Statement
 - WEEE Directive 2012/19/EU

3.5 Maintenance

- Prevention maintenance is included in service agreement
- Available (by telephone or internet) for troubleshooting during office hours
- Time to response is ≤ 3 working days
- Software updates

- This User Requirement Specification should be approved and signed by the supplier before purchase and is part of the purchase-order.