

## **AUTOMATED PEPTIDE ANALYSIS OF BODY FLUIDS WITH MALDI TOF AND HYBRID TANDEM MASS SPECTROMETRY**

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Automation is the key to high productivity in the analytical laboratory. High sample throughput as well as on-line LC-MS and LC-MS/MS are common requirements in today's research. For single compounds and simple mixtures bench top MS systems are standard tools for the research scientist. For complex mixtures high resolution MS often in combination with MS/MS is mandatory <sup>1</sup>. The complexity of mixtures even raises when body fluids are analyzed.

For this approach we took a sample from a peptide bank established from large amounts of human blood ultrafiltrate <sup>2</sup>. These samples are usually very heterogeneous and complex over a wide molecular mass range (hundreds up to thousands of compounds from < 1 kDa to approximately 30 kDa). To automatically obtain structural information on the different compounds of these complex mixtures a list of the nominal molecular masses is the only required information prior to the experiment on the hybrid tandem MS system.

Initial sample information was generated using a MALDI-TOF mass spectrometer operating in linear mode. A list of molecular weights obtained by this method was then used to set up the subsequent experiment on the sector field ion trap tandem mass spectrometer. Without any other information than the singly charged mass of the different compounds, the hybrid tandem mass spectrometer performed a multiple set of data dependant measurements. These steps include the intensity check of the differently charged molecular ions for the selection of the most abundant one for the subsequent MS/MS experiment.

We will demonstrate the power of the hybrid tandem mass spectrometer for this type of experiments for a single mixture containing more than 200 peptides/proteins of various molecular weights up to 5 kDa. For this example we have automatically analyzed 20 compounds out of this mixture. The resolution power of the sector field part of the mass spectrometer was set to have unit resolution on the largest precursor ion available in the MALDI TOF spectrum.

[1] Muenster, Pesch, Horning, presented at the 44th ASMS, Dallas, Tx, USA

[2] Schulz-Knappe, P. et al., J. Chromatogr. A, 776(1), 1997, 125-32

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