

## 4.7

### **NOVEL CAPABILITIES OF A HYBRID QUADRUPOLE LINEAR ION TRAP MASS SPECTROMETER FOR THE STUDY OF PROTEOMICS AND METABOLISM**

Christie Hunter

Applied Biosystems, Foster City, CA, USA

Often times when approaching a scientific experiment, significant information is available about the sample to enable specific questions to be asked. For performing these hypothesis-driven experiments, the direct combination of triple quadrupole and ion trapping capabilities in a hybrid quadrupole linear ion trap instrument provides for powerful workflows. The unique specificity of the precursor ion (PI), neutral loss (NL) and multiple reaction monitoring (MRM) triple quadrupole scans can be automatically linked to high sensitivity ion trap MS/MS scans on an LC time scale. In addition, the ability to switch rapidly between positive ion and negative ion while performing these scans provides the maximum flexibility for method design. Novel strategies will be presented for the discovery and identification of metabolites and post-translationally modified (PTMs) peptides in biological samples.

When studying the metabolism, many of the metabolites of the parent drug can be predicted while other metabolites are unexpected. The ability to use a range of different survey scans to detect a potential metabolite to be sent for MS/MS during an LCMS run allows for the identification of more metabolites. A strategy for identifying as many metabolites as possible is presented and utilizes many of the unique features of this hybrid mass spectrometer.

Because of the complexity of biological samples, the identification of post-translationally modified peptides is often difficult due to their low abundance in the sample and requires a more targeted strategy. Using precursor ion scanning to specifically detect phosphorylated peptides, the modification state of a protein kinase is investigated quantitatively.