

# ABSTRACT

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## Basic Information

**Abstract Number:** 2270-6

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**Session Title:** Strategies for the Automated Identification of Compounds from LC-MS/MS Data

**Event Type:** Organized Contributed Session

**Event Title:** Automated and Parameter-Free Peak Integration for LC/MS/MS Quantitation

**Presider(s):** Voyksner, Robert

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## Abstract Content

The continuing needs for high throughput quantitative analysis by LC/MS/MS have lead to the development of advanced technologies, including fast chromatography, sample pooling strategies, staggered injection or direct plasma injection, and parallel analysis with multiplexed sources have tremendously enhanced the throughput of data acquisition so much that the data processing has become the bottleneck of overall analytical procedures. This is a pressing issue to be solved for further improving quantitation throughput. This presentation will describe novel methodologies that enable parameter free peak integration for fast and accurate LC/MS/MS qunatitation. Currently most commercial instrument vendors offer automated procedures for the data processing. Unfortunately, these automation packages have not been widely used because they are not able to reliably integrate the LC/MS/MS peaks with low signal to noise ratio, asymmetric shape, and overlapped peaks due to inadequate separation, as is the case for chiral compounds or the existence of an interference peak. As a result, mass spectrometer operators need to individually develop processing method to optimize integration parameters. It is also necessary to inspect the integration results and perform manual integration selectively after the automated processing. We have developed a set of novel methodologies with unique calibration algorithm that not only performs noise filtering and baseline correction, but also calibrates LC/MS/MS peak shape variations. After this mathematical transformation, all peaks will have good peak shapes enabling accurate peak area integration and retention time calculation. The signal to noise ratio of the has also be dramatically improved. We have achieved automated peak integration with very noisy quantitation data and/or unresolved chromatographic peaks while providing significantly improved quantitative accuracy and precision.