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アプリケーションノート

A Step Change in High-Resolution Quantitative Performance Combining Novel StepWave, QuanTof, and MS^E Technology in the SYNAPT G2-S System

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Abstract

To successfully quantify compounds while acquiring high resolution full scan spectral data to allow unequivocal identification.

Benefits

By utilizing StepWave Technology within the SYNAPT G2-S platform, comprehensive untargeted identification and quantification of compounds can be carried out at the lowest levels in complex matrices while minimizing MS method development

Introduction

Routine quantitation has traditionally been reserved for tandem quadrupole instruments where the high level of selectivity enables scientists to detect very low levels while still providing a large dynamic range. ToF platforms, while providing the scientist with comprehensive amounts of data for untargeted quantitation, have often been limited not only in their detection levels when compared to tandem quadrupoles, but also in the range of concentrations that can be accurately determined in a single batch.

Both ToF platforms and tandem quadrupole instruments are limited to detecting whatever ions can be efficiently introduced via the source. Simply allowing more ions into the machine is never a guarantee that detection limits will be lowered.

The StepWave™ device allows significantly more ions to be introduced while utilizing a robust mechanism for elimination of neutral components and gas stream from the rest of the instrument. QuanTof Technology also provides a wide dynamic range to maximize both quantitative and qualitative performance with high resolution MS.

Results and Discussion

A SYNAPT® G2 coupled with an ACQUITY UPLC® System was used to chromatograph and detect Sulfadimethoxine. Calibration standards had been prepared by spiking separate solutions with increasing amounts of Sulfadimethoxine. These were then injected and analyzed in sequence. The entire sequence was repeated using the same solutions on a SYNAPT G2-S System, featuring high-sensitivity StepWave ion optics. The data was collected in UPLC®/MS^E mode. This allows both intact molecular ion and fragment ion information to be collected for all molecules in the sample. (No prior knowledge of the samples was required.) The data shown in Figure 2 demonstrates that the use of the StepWave in the SYNAPT G2-S instrument resulted in a six-fold increase in sensitivity (signal-tonoise) over that obtained with a SYNAPT G2 System.

Figure 1 shows that the quantitative performance standard, *i.e.* linear dynamic range and reproducibility, was not adversely affected by the use of StepWave Technology. In fact the StepWave enabled a 10x improvement in the limit of quantitation. The SYNAPT G2 achieved an LOQ of 250 femtograms and was linear up to 100 picograms demonstrating over 3.5 orders of dynamic range. The SYNAPT G2-S System with StepWave achieved a 10x lower detection limit, 25 femtograms, and more than 4 orders of linear dynamic range.

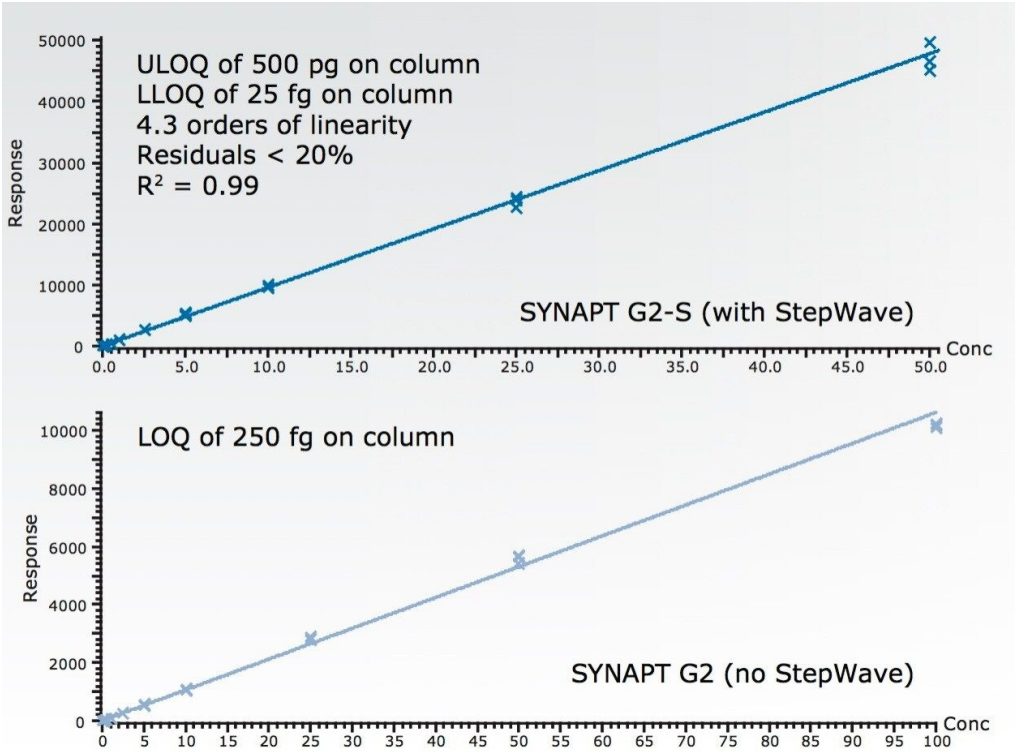

Figure 1. Increase in limit of quantitation by over 10X with StepWave Technology with over four orders of linearity provided by the high resolution QuanTof analyzer.

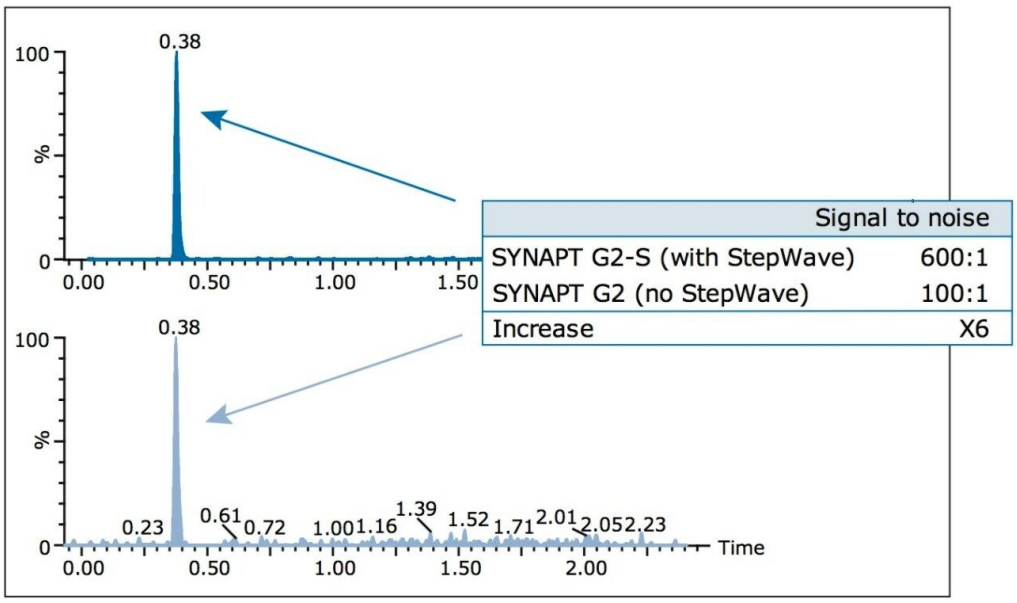

Figure 2. Increase in signal:noise with the combined ability of StepWave to maximize ion sampling efficiency while eliminating neutral contaminants.

Due to the 'data independent' MS^E acquisition mode employed in this analysis, it is possible to unequivocally identify the components in the sample using high resolution molecular and fragment ion spectral data from every delectable component. For example, Figure 3 shows the high and low energy spectra obtained for one of the Sulfadimethoxine peak at 2.5 pg on column injections.

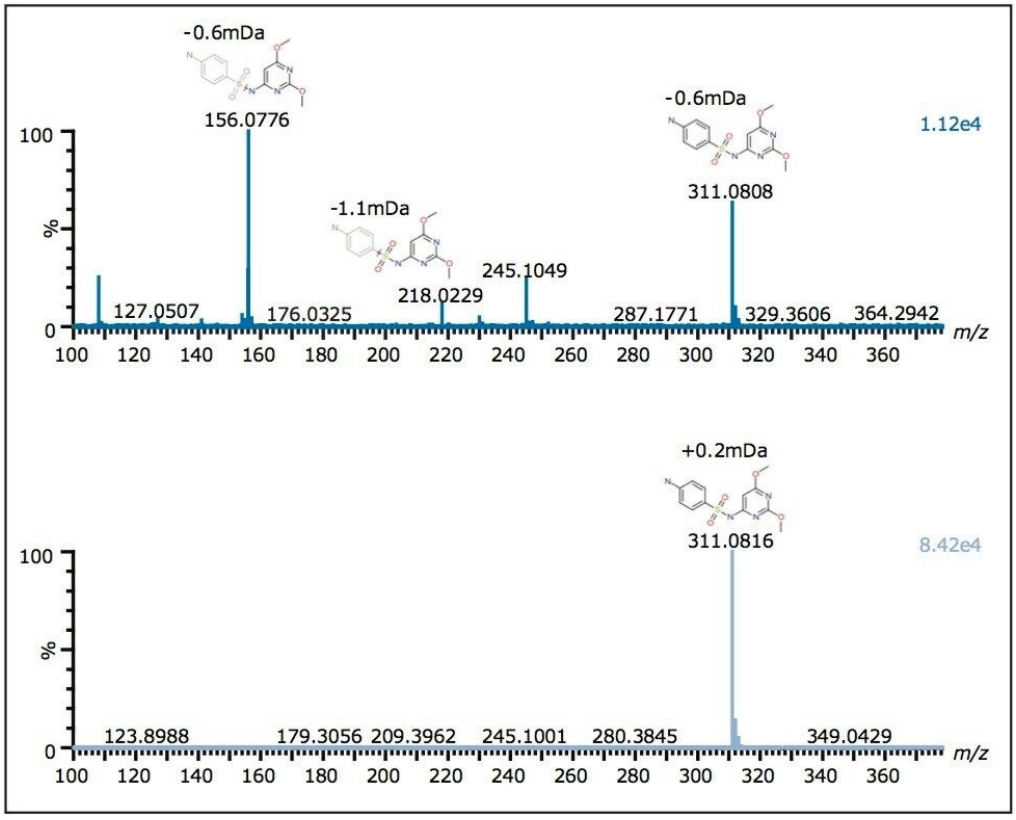

Figure 3. Exact mass molecular ion (lower spectrum) and fragment ion (upper spectrum) data from the UPLC/MS^E analysis enabling rapid, unequivocal structural identification of Sulfadimethoxine with MassFragment™ Software.

Conclusion

The data collected demonstrates excellent sensitivity and linearity together with high mass resolution and exact mass accuracy. The StepWave successfully enables the SYNAPT G2-S platform to meet the quantitative performance required by today’ s scientists while still allowing the capacity to collect high resolution molecular and fragment ion spectral data for hundreds of compounds. High resolution ToF data reduces the need for method development as there is no requirement for MRM discovery or optimization, which can be a labor-intensive process for applications where many analytes are targeted. Unbiased full scan data also enables archived data to be interrogated at any point in the future for new compounds of interest.

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