

# Separation of Bile Acid Isomers with Differential Mobility Spectrometry

## Fast Separation of Bile Acids Isomers with the QTRAP® 6500+ System and SelexION® Technology

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Bile acids are involved in a wide range of biological functions including lipid resorption, immunological functions and metabolic regulation. They are part of a large family of molecules that consist of a four-ring steroid structure with various side chains.

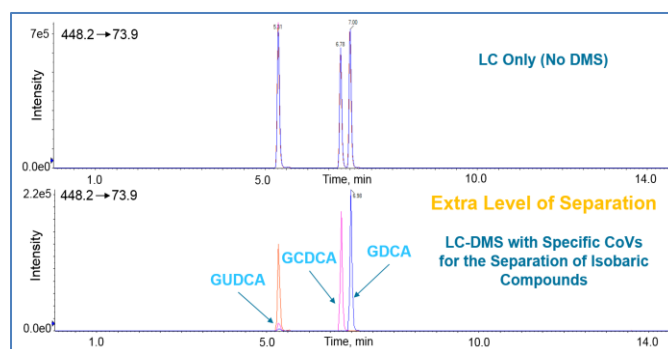
### The Challenge:

Through metabolic transformations, isomeric and isobaric variants of bile acids are generated, which makes the unequivocal identification and quantification of these individual chemical species difficult.

### The Solution:

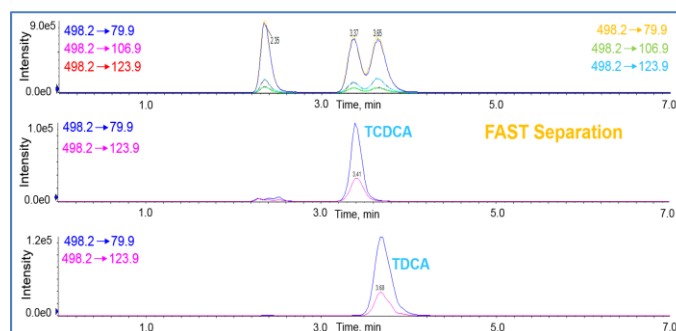
Here, differential ion mobility spectrometry (DMS, SelexION Technology) was used as a methodology for the separation of two groups of bile-acids isomers. SelexION technology is an ion mobility technology which separates molecules based on their dipole moment instead of  $m/z$ . This separation was used in conjunction with liquid chromatographic separation (LC-DMS-MS) as well as with fast isocratic separations to investigate bile acids. While the combination with chromatographic separation may improve selectivity for bile acid quantitation, the separation power of SelexION technology is sufficient for a clear separation of isomers, enhancing the selectivity of the measurement, and enables fast quantification with minimal LC separation.

### SelexION Technology is a Fast Separation Technique, for Analysis of Different Isomers of Bile Acids.



#### On-Column SelexION Separation of GDCA, GCDCA and GUDCA.

Without DMS (upper pane), only LC separation of these bile acids is possible. For all three isomeric compounds, the same transition is used (448.2 → 73.9). Adding the compound-specific Compensation Voltage (CoV) to the SRM table of transitions allows only the isomer with the corresponding CoV to enter the MS for detection hence separating different isomers (lower pane) allowing more confident detection.



**Fast Separation of Bile Acids with an Isocratic LC Method.** Without SelexION Technology, the two isobaric bile acids TDCA and TCDCA cannot be completely separated from each other. Confident identification and accurate quantitation would be difficult due to the overlap of the two LC peaks. Separation of these isobaric bile acids is possible by SelexION technology using the specific compensation voltages for these compounds.