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# The Use of Collision Cross Section (CCS) Measurements in Food and Environmental Analysis

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## TECHNOLOGY BENEFITS

- Precursor ion (with isotopes), fragment ion information, and CCS values acquired in a single analysis for all components.
- CCS values are unaffected by sample matrix and can be measured from very low intensity MS ions.
- CCS provides complimentary orthogonal identification information.
- CCS measurements in parallel with traditional parameters (such as exact mass) increase targeted screening specificity.

## WATERS SOLUTIONS

ACQUITY UPLC® I-Class System

Ion Mobility-Mass Spectrometry (IM-MS) Systems

UNIFI® Scientific Information System

## KEY WORDS

ion mobility, CCS, screening, food, environmental

## INTRODUCTION

The use of Waters® UltraPerformance Liquid Chromatography (UPLC®) in combination with high resolution mass spectrometry has increased significantly in food and environmental laboratories in recent times, offering unique advantages for screening and profiling complex mixtures. Waters' introduction of ion mobility mass spectrometry (IM-MS), which combines high resolution mass spectrometry and high efficiency ion mobility based measurements and separations has taken the quality, volume, and specificity of information that can be obtained from food and environmental samples to a new level. One of the benefits of IM-MS enabled solutions is the ability to measure collision cross section (CCS) values of ions.

## DISCUSSION

A collision cross section (CCS) value is a robust and precise physicochemical property of an ion which is related to its chemical structure and three-dimensional conformation, as shown in Figure 1, where the shadow of a rotating three-dimensional ion represents the average collision cross section.

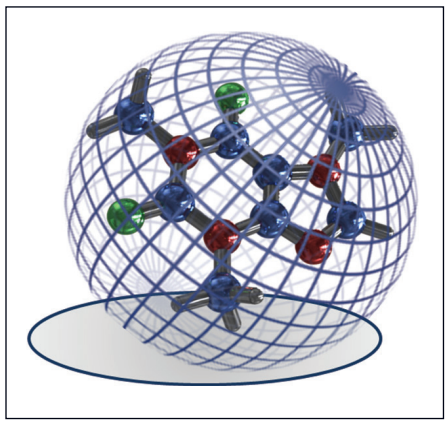

*Figure 1. Illustration of rotating three-dimensional conformation of an ion and average collision cross section (shadow).*

CCS values can be measured routinely using Waters, IM-MS systems. Ion mobility spectrometry (IMS) is a rapid, orthogonal, gas phase separation technique that gives another dimension of separation within an LC timeframe allowing compounds to be differentiated based on size, shape, and charge. In addition, precursor ion (with isotopes), fragment ion information, and CCS values can be acquired in a single analysis for all components.

The use of CCS measurements in parallel with traditional parameters such as exact mass can increase targeted and non-targeted screening specificity. CCS values can be added into a Scientific Library within UNIFI and integrated into a routine screening workflow to allow them to be utilized to screen and confirm the presence of food and environmental contaminants, nutrients, flavor compounds, or any other molecules of interest. By utilizing CCS as an additional 'data filter' can also help to remove false positive and most importantly false negative identifications. Measurement and use of CCS values can also aid method development by reducing the burden of costly retention time confirmation using expensive standards for compounds where the CCS value has previously been determined.

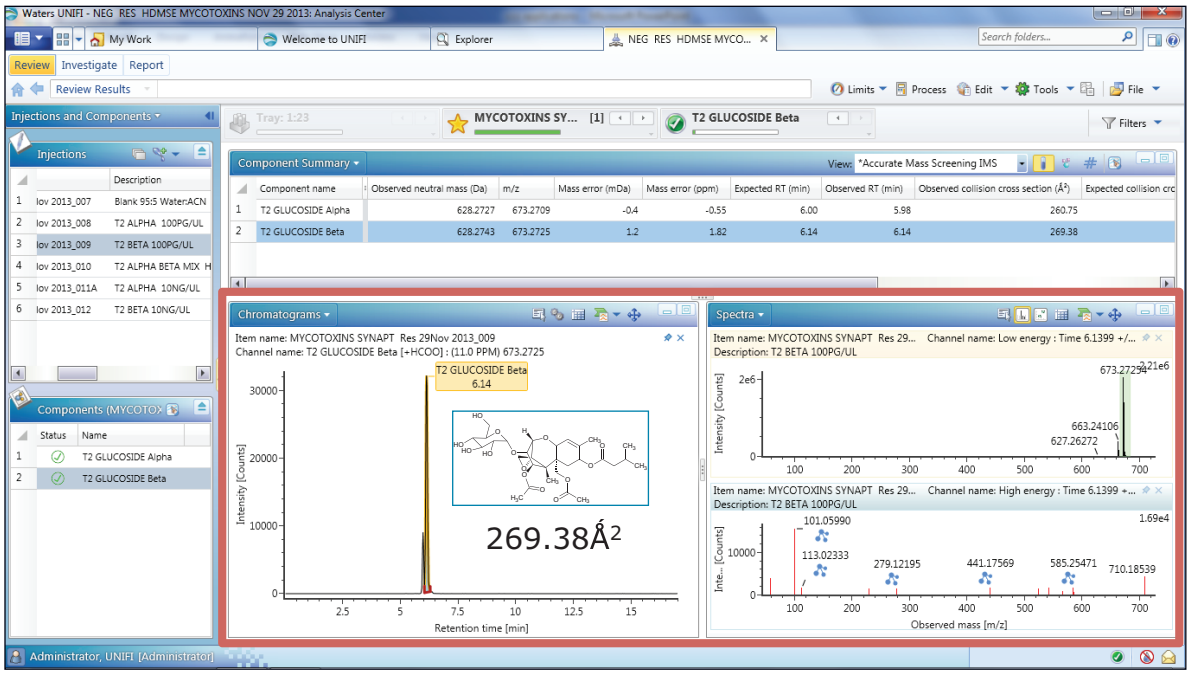


*Figure 2. UNIFI Software screenshot showing CCS value for a masked mycotoxin compound T2 β-glucoside together with the corresponding exact mass precursor ion and ion mobility product ion spectra.*

One of the major challenges for food and environmental analysts is the variety of sample matrices encountered and overcoming the subsequent analytical matrix effects. Typical matrix effects are variations in chromatographic retention times that occur when switching between different matrices, or due to column degradation, suppression and/or enhancement of the detected MS signal. CCS values are unaffected by sample matrix so in addition to retention time, precursor ion and fragment, they can be measured from very low intensity MS ions where only mono isotopic information is available.

Examples showing the use of CCS measurement can be found here:

- Collision Cross Section: A New Identification Point for a "Catch All" Non-Targeted Screening Approach
- Use of Ion Mobility Spectral Cleanup and Collision Cross Section Values to Increase Confidence and Efficiency in Pesticide Residues Screening Strategies
- Utility of the ACQUITY UPLC I-Class System and Ion Mobility in a Routine Workflow to Understand the Challenge of Analyzing Fluoroquinolone Antibiotic Residues
- Discovery of Pesticide Protomers Using Routine Ion Mobility Screening
- Profiling of Flavonoid Isomers in Highly Complex Citrus Juice Samples Using UPLC Ion Mobility Time of Flight Mass Spectrometry
- Determination and Characterization of Perfluoroalkyl and Polyfluoroalkyl Substances (PFAS's) in Environmental Samples Using UPLC Ion Mobility MS


## SUMMARY

A collision cross section (CCS) value is a robust and precise physicochemical property of an ion which can be measured routinely using Waters Ion Mobility - Mass Spectrometry (IM-MS) systems. CCS values are reproducible and unaffected by sample matrix, making them invaluable in screening and profiling experiments in food and environmental laboratories.


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