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SYNAPT G2 HIGH-DEFINTION MASS SPECTROMETRY: SEPARATION AND COLLISION CROSS-SECTION DETERMINATION OF LEUCINE AND ISOLEUCINE BY TRAVELLING WAVE ION MOBILITY MASS SPECTROMETRY

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INTRODUCTION

Here we demonstrate the use of travelling wave ion mobility mass spectrometry with the SYNAPT™ G2 High Definition Mass Spectrometry™ (HDMS™) platform to separate the two amino acid structural isomers isoleucine and leucine, which differ in a collision cross-section (CCS; (Ω)) by less than 3 Å^2.

Distinguishing between isoleucine and leucine has only previously been demonstrated on instruments such as magnetic sectors or MALDI Tof-Tof mass spectrometers that are capable of performing high energy Collision Induced Dissociation (CID).

Following separation of these isomers, the T-Wave™ collision cross-section values were automatically generated with DriftScope™ Informatics (v2.1). This new capability allows one to automatically generate a T-Wave ion mobility calibration function, and derive CCS values for such compounds.

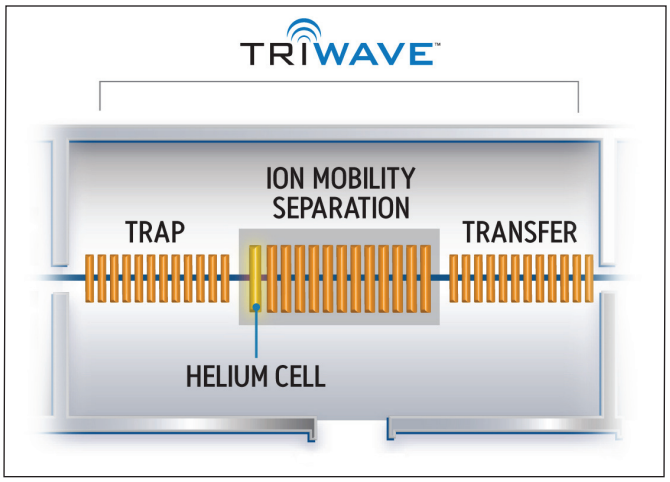

Figure 1. Schematic of the second-generation Triwave™ Technology of SYNAPT G2. The enhanced IM resolution is achieved through both the increased length and pressure of the IMS T-Wave region.

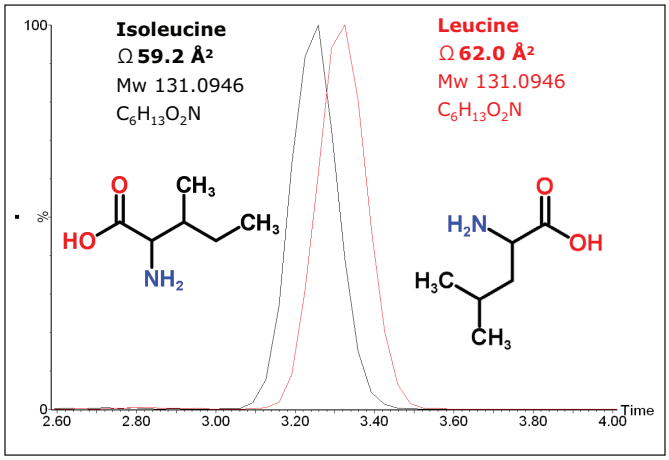

Figure 2. T-Wave ion mobility drift time (msec) chromatograms for isoleucine and leucine and their respective T-Wave derived collision cross-sections (Ω).

EXPERIMENTAL

SYNAPT G2 is an innovative hybrid quadrupole IMS oa-Tof mass spectrometer incorporating second-generation Triwave Technology (Figure 1), which provides significantly enhanced ion mobility resolution (over 40 (Ω/ΔΩ)). The increased pressures of the drift gas (e.g. N_2) and overall length of the IMS T-Wave provide an ion mobility resolution increase of up to a factor of 4 compared to traditional Triwave Technology, while maintaining high transmission efficiency via the novel Helium-filled entry cell. The T-Wave ion mobility calibration was carried out using previously determined collision cross-section values for polyglycine (from http://www.indiana.edu/~clemmer).

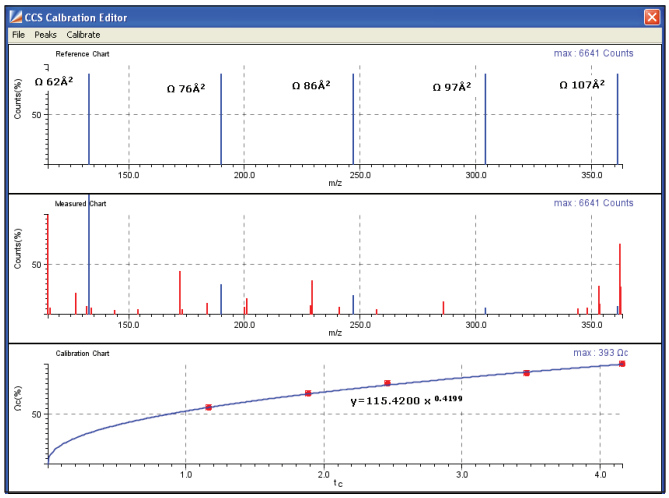

Figure 3. DriftScope Software's (v2.1) automated T-Wave ion mobility collision cross-section calibration editor. Data displayed are polyglycine.

An automated T-Wave ion mobility calibration can be carried out using DriftScope Software (v2.1) (Figure 3). The top panel shows the ion mobility calibration compound (polyglycine) with annotated collision cross-sections. The second panel shows a polyglycine mass spectra with automated peak selection. The third panel shows a charge and reduced-mass corrected collision cross-section vs. drift time plot, fitted with a power relationship, which can be used to derive CCS values for unknown compounds.

CONCLUSIONS

It is possible to distinguish between the structural isomers of leucine and isoleucine by travelling wave ion mobility MS where the absolute collision cross-section measurements of structural isomers differ by less than 3 Å^2.

DriftScope Informatics enable routine collision cross-section determination of such compounds with the use of an automated T-Wave ion mobility calibration editor.

SYNAPT G2 with HDMS now enables such structural studies to be performed with enhanced specificity (enhanced IM resolution (over 40 (Ω/ΔΩ)) and speed (DriftScope Informatics).

Reference:

1. The travelling wave device described here is similar to that described by Kirchner in US Patent 5,206,506 (1993).

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