AN IMPROVED CALIBRATION APPROACH FOR TRAVELLING WAVE ION MOBILITY SPECTROMETRY: ROBUST, HIGH-PRECISION COLLISION CROSS SECTION CORRECTIONS

Keith Richardson1, David Lapidge1, Kevin Gill1, Supriya Dixit1, Jakuti Upendra3, Brandon Ruotolo4

1Waterston Corporation, Atkinson Road, Wilmington, DE, USA, 2Department of Chemistry, University of Michigan, 3Ann Arbor, MI, USA, 4AB Sciex, 5Waters Corporation, Manchester, UK

OVERVIEW

PURPOSE: Development of significantly improved methods for calibration of travelling wave ion mobility (TWIM) spectrometry data

METHODS: United TWIM Theory and ion optical simulations. Calibration of experimental data for a wide range of collision cross sections (CCS) and conditions.

RESULTS: CCS calibrations of significantly improved precision and accuracy were produced over a broad range of collision cross sections.

CONCLUSIONS: We have shown that a single mixture containing a single native protein ion results in very accurate and robust CCS calibrations utilizing only two and three parameters.

We introduce new TWIM CCS calibration functions that allow significant improvements in precision and accuracy over a wide range of collision cross sections and conditions. These calibration functions utilize only two and three parameters to provide significant improvement in the calibration of TWIM spectrometry data.

INTRODUCTION

Travelling Wave Ion Mobility, since its introduction in 2004, has developed into a ubiquitous separation tool, impacting a broad range of LC-MS applications. TWIM separations using a series of DC waves operating in a gas-filled ion tube have the advantage of being rapid, compact, and low cost. TWIM is sensitive to changes in temperature, pressure, humidity, and the presence of water vapor. Ion mobility is a dimensionless parameter that can be used to classify molecules and ions. TWIM is capable of separating ions of the same mass but different charge state, and can be used to obtain CCS values for a wide range of ions. TWIM is a powerful separation tool, impacting a broad range of applications.

METHODS

We performed calibration studies in a lab-scale TWIM instrument, using mixtures containing a single native protein and a large number of standard small molecules. We evaluated the performance of different calibration methods over a range of TWIM conditions and conditions.

RESULTS

The results of the new calibration methods were compared to those of the traditional calibration methods, and showed improved precision and accuracy over a wide range of collision cross sections and conditions. The improved calibration methods were shown to be significantly more robust than the traditional methods.

CONCLUSIONS

We have shown that a single mixture containing a single native protein ion results in very accurate and robust CCS calibrations utilizing only two and three parameters. These methods are optimized for the TWIM spectrometry platform and can be used for a wide range of applications. The improved Methods: We introduced new TWIM CCS calibration functions that allow significant improvements in precision and accuracy over a wide range of collision cross sections and conditions. These calibration functions utilize only two and three parameters to provide significant improvement in the calibration of TWIM spectrometry data.

RESULTS

The new calibration functions were compared to traditional calibration methods, and showed improved precision and accuracy over a wide range of collision cross sections and conditions. The improved calibration methods were shown to be significantly more robust than the traditional methods.

CONCLUSIONS

We have shown that a single mixture containing a single native protein ion results in very accurate and robust CCS calibrations utilizing only two and three parameters. These methods are optimized for the TWIM spectrometry platform and can be used for a wide range of applications. The improved calibration functions are capable of improving the precision and accuracy of CCS measurements over a broad range of collision cross sections and conditions.

We have shown that a single mixture containing a single native protein ion results in very accurate and robust CCS calibrations utilizing only two and three parameters. These methods are optimized for the TWIM spectrometry platform and can be used for a wide range of applications. The improved calibration functions are capable of improving the precision and accuracy of CCS measurements over a broad range of collision cross sections and conditions. The results of these new calibration methods were compared to those of the traditional calibration methods, and showed improved precision and accuracy over a wide range of collision cross sections and conditions. The improved calibration methods were shown to be significantly more robust than the traditional methods.

CONCLUSIONS

We have shown that a single mixture containing a single native protein ion results in very accurate and robust CCS calibrations utilizing only two and three parameters. These methods are optimized for the TWIM spectrometry platform and can be used for a wide range of applications. The improved calibration functions are capable of improving the precision and accuracy of CCS measurements over a broad range of collision cross sections and conditions.

We have shown that a single mixture containing a single native protein ion results in very accurate and robust CCS calibrations utilizing only two and three parameters. These methods are optimized for the TWIM spectrometry platform and can be used for a wide range of applications. The improved calibration functions are capable of improving the precision and accuracy of CCS measurements over a broad range of collision cross sections and conditions.

We have shown that a single mixture containing a single native protein ion results in very accurate and robust CCS calibrations utilizing only two and three parameters. These methods are optimized for the TWIM spectrometry platform and can be used for a wide range of applications. The improved calibration functions are capable of improving the precision and accuracy of CCS measurements over a broad range of collision cross sections and conditions.