ION MOBILITY MASS SPECTROMETRY AS A TOOL FOR STRUCTURAL INVESTIGATION OF HIGH M/Z SPECIES

A TOOL FOR STRUCTURAL INVESTIGATION

INTRODUCTION

The travelling wave device described here is similar to that described by Kirchner in US Patent 5,206,506 (1993). The travelling wave used in the IMS T-Wave for (Argon) and the pressure in the IMS T-Wave was 0.5 mbar leased form the trap in 500µs wide packets. The gas pressure deliver the mobility separated ions into the oa-ToF analyser. The transfer T-Wave is used to are released in a packet into the IMS T-Wave in which the mobility separation is occurring. The transfer T-Wave was used to deliver the mobility separated ions into the oa-ToF analyser. All the species produced upon MS/MS fragmentation into cross sectional areas and fragmentation pathways which would otherwise be impossible by MS or MS/MS alone.

WHAT CAN ALSO BE OBSERVED IS THAT THERE ARE 2 DISTINCT DRIFT TIME POPULATIONS FOR THE 1.1MER (744Da), Region A and Region B. When the mass spectra are extracted from these regions, Figure 7, there are two different charge state envelopes, which both deconvolute to the mass of the 1.1mer (744Da). The two different populations could be a result of the monomer being expelled from a different position within the GroEL 14mer, with one mechanism of ejection being favoured over another.

Figure 8 shows the effect of increasing the injection energy of the intact GroEL ions into the Trap T-Wave. As the energy is increased, the drift-time for the intact GroEL increases. This effect is most likely as a result of an increase in the size of the GroEL complex due to activation which would be expected to occur prior to fragmentation.

Haemoglobin

Under native conditions haemoglobin is in the form of a tetramer made up of 2 alpha (Mr = 15,169) and 2 beta chains (Mr = 15,887) and four haem groups (Mr = 615). Upon injection of the intact GroEL (744kDa) possesses relatively few charges and appears very high in the m/z range, between 1200-2500. Trimeric (mixed alpha 2/alpha, beta 2/beta, beta 2/alpha, beta 3) species are also observed in the m/z range 5000-7000. The haem group is also observed at m/z 615. All the species produced upon MS/MS fragmentation have well defined drift times as observed in Figure 9.

CONCLUSION

• A novel quadrupole/ion mobility/oa-ToF mass spectrometer was used to mobility separate and analyse large m/z species
• Mobility separation of up to 5 charge states series of CaCl2 clusters up to m/z 20,000 has been shown
• Ion mobility separation of the MS and MS/MS ions of large biomolecule species has been demonstrated
• Mobility separation of the GroEL 13mer has potentially provided new information on the fragmentation mechanism.

This additional dimension allows us to gain insights into cross sectional areas and fragmentation pathways which would otherwise be impossible by MS or MS/MS alone.

REFERENCES


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