Axis 1

Ion mobility – mass spectrometry

Ion mobility and mass spectrometry

Ion mobility (IM) is a gas phase separation method based on the drift of ions through a buffer gas under the influence of an electric field. Interfaced to MS, IM adds an extra dimension, which is a function of charge (z), and collision cross section (Ω) of the ions. Travelling wave ion mobility (TWIM) is a type of IM based on low-voltage waves pushing the ions across a gas-filled ion guide. TWIM cell was incorporated a few years ago in commercially available hybrid quadrupole/time-of-flight mass spectrometer, Synapt G2 HDMS (**Figure 1**).
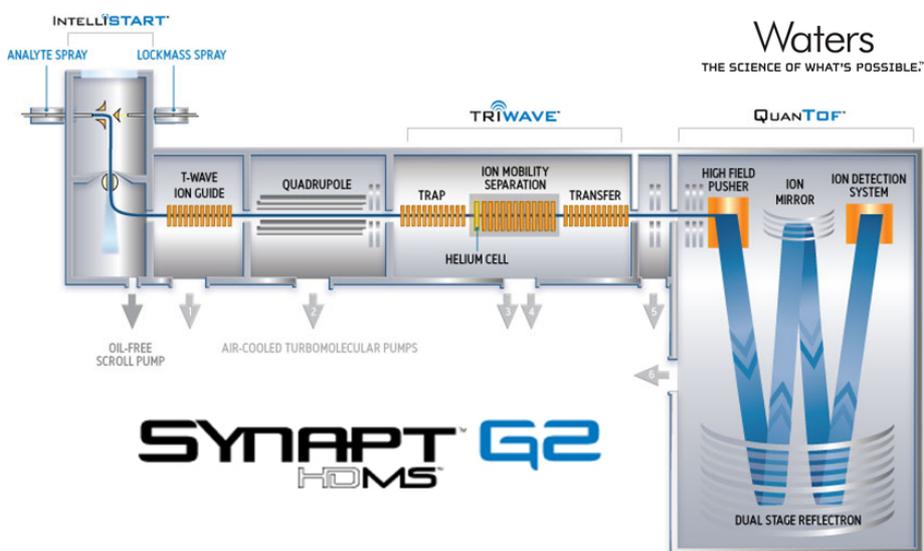

Figure 1. scheme of the Synapt G2 HDMS mass spectrometer (Waters)

One of the main research activity of the group is the development of new applications of the ion mobility - mass spectrometry (IM-MS). These last years the group published many articles showing the interest of this technique for the characterization of polymers, petroleum distillates or biological compounds such as peptides and lipids.

Differentiation of isomers
A strategy using the coupling IM-MS has been developed for stereoisomers, which present very close collision cross section difference. This strategy is based on cationization (with alkali cations or transition metals), formation of multimers and use of a third chiral molecule (**Figure 2**).
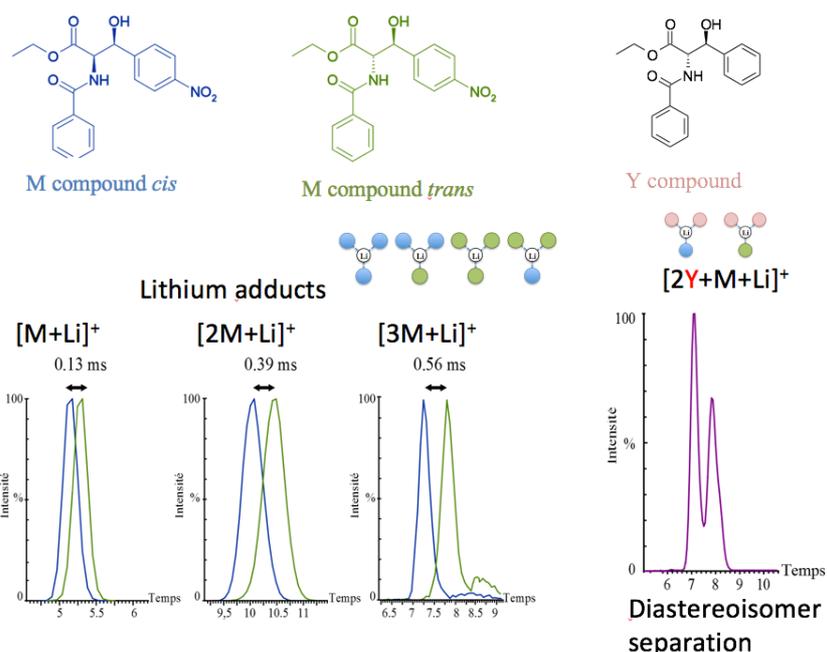
Figure 2. separation of diastereomers using IM-MS
Domalain, V.; Tognetti, V. ; Hubert-Roux, M.; Lange C. ; Joubert, L. ; Baudoux, J. ; Rouden, J. and Afonso, C.,
J. Am. Soc. Mass Spectrom., **2013**, 24, 1437-45.

Collision cross section determination

The measurement of the ion collision cross sections (CCS) can be performed after calibration of the TWIM instrument using standard species with known CCS. At present, these standard species do not cover well all charge states and CCS ranges. We are currently exploring the use of phosphoric acid cluster ions as possible standards for CCS calibration (**Figure 3**).
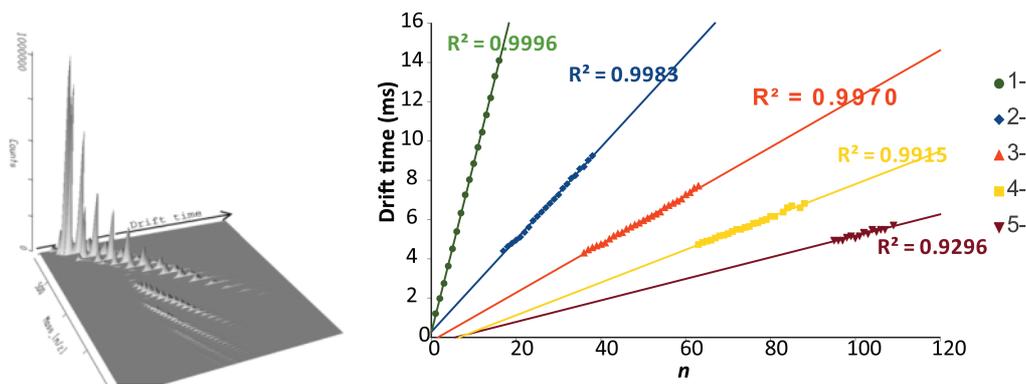

Figure 3. Ion mobility mass spectrometry of phosphoric acid cluster ions. $[(H_3PO_4)_n - zH]^{z-}$ are observed and show well defined trend lines according to charge states; for each given charge states z , drift times are correlated with the number of phosphoric acid molecules in the cluster ions. Lavanant, H. ; Tognetti, V. and Afonso, C., *J. Am. Soc. Mass Spectrom*., **2014**, 25, 572-80.