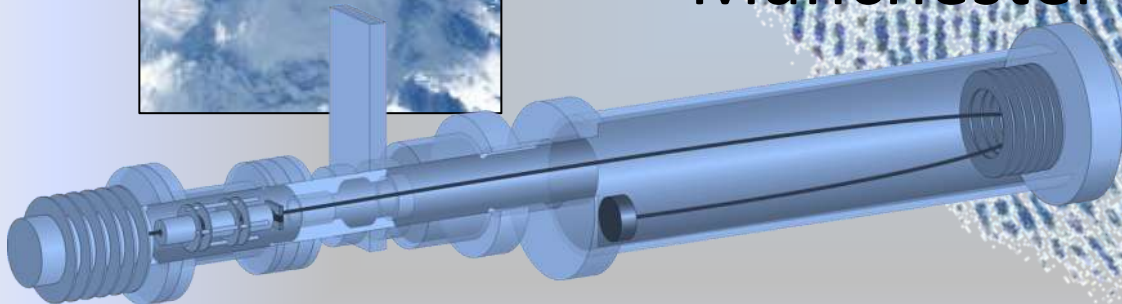
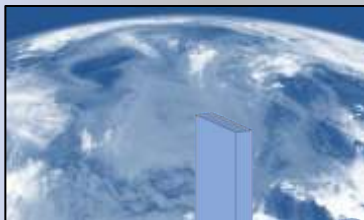




Leicester
PTR-MS OVOC
Measurements:

BUNIAACIC

Manchester CAS

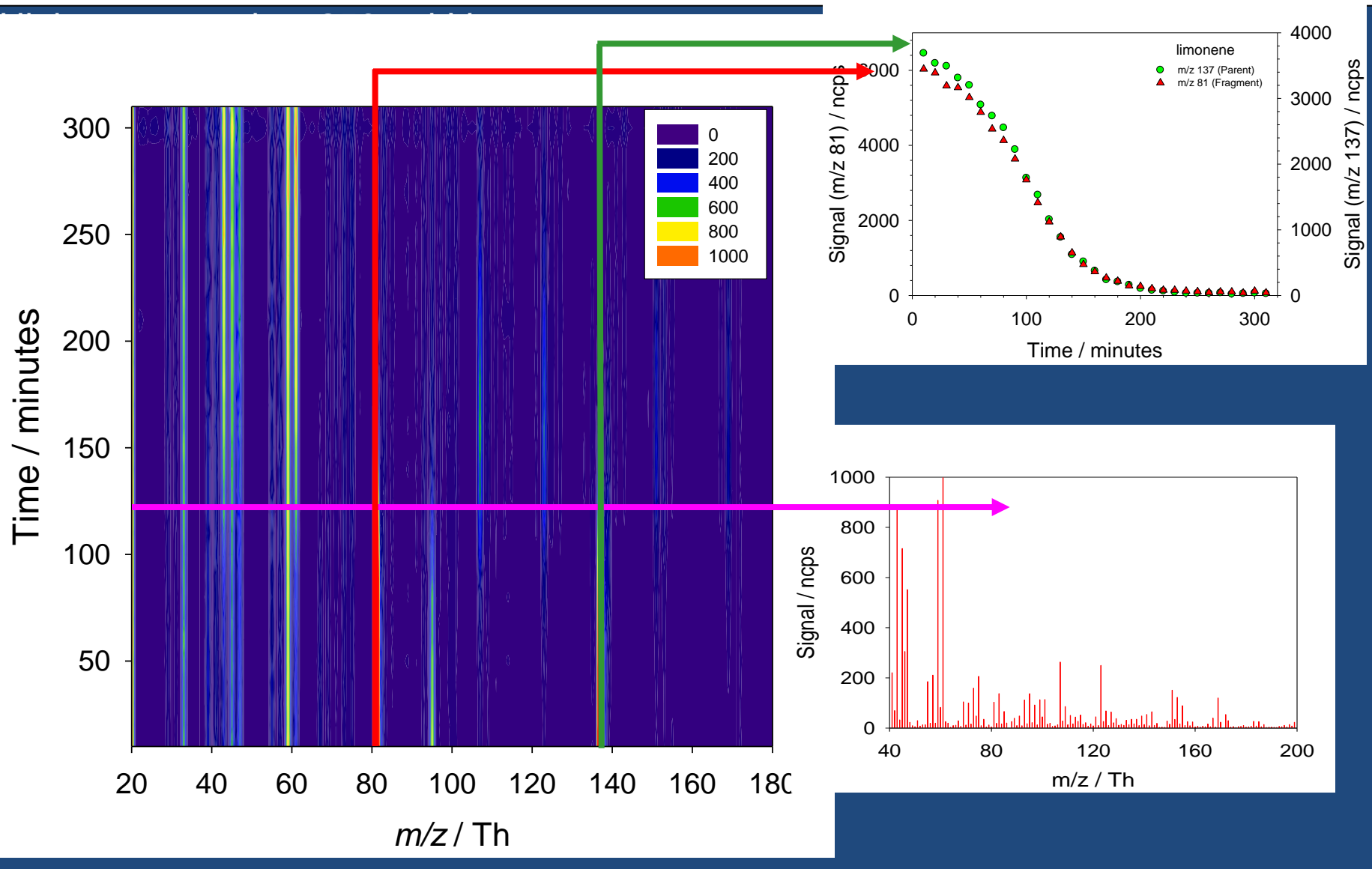


Iain White
Kevin Wyche
Paul S. Monks

OVERVIEW

- Overview of the Work at UoL
- Case studies and examples
 - From last time: Chamber studies, ambient air monitoring in London
- RF funnel development

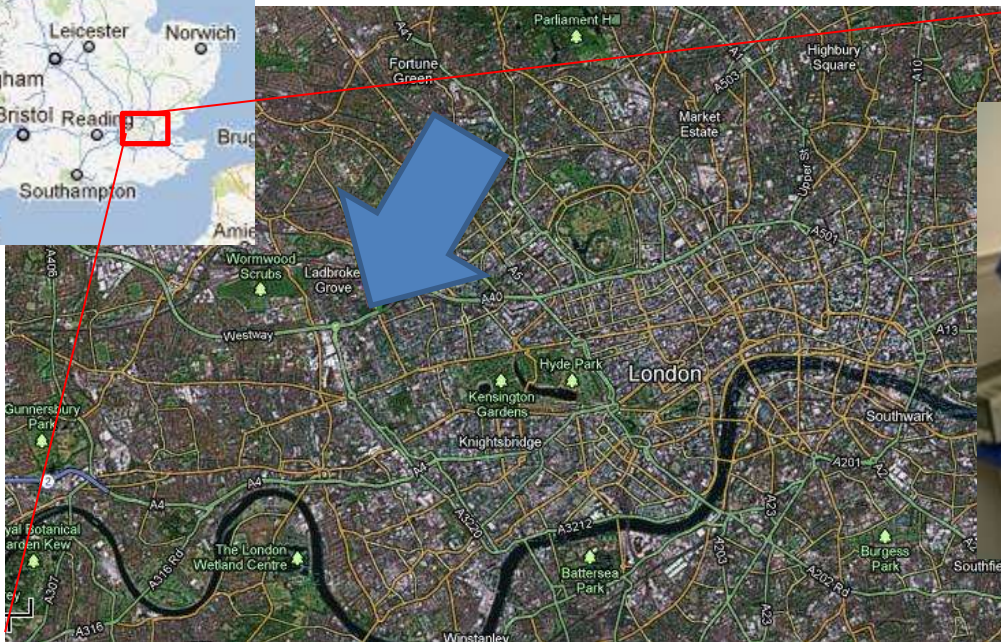
Eg. From last time: Limonene Photo-oxidation



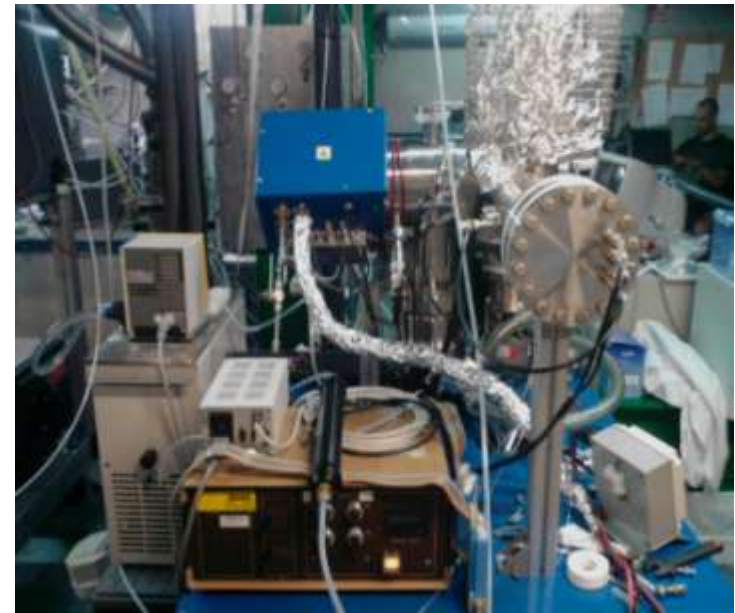
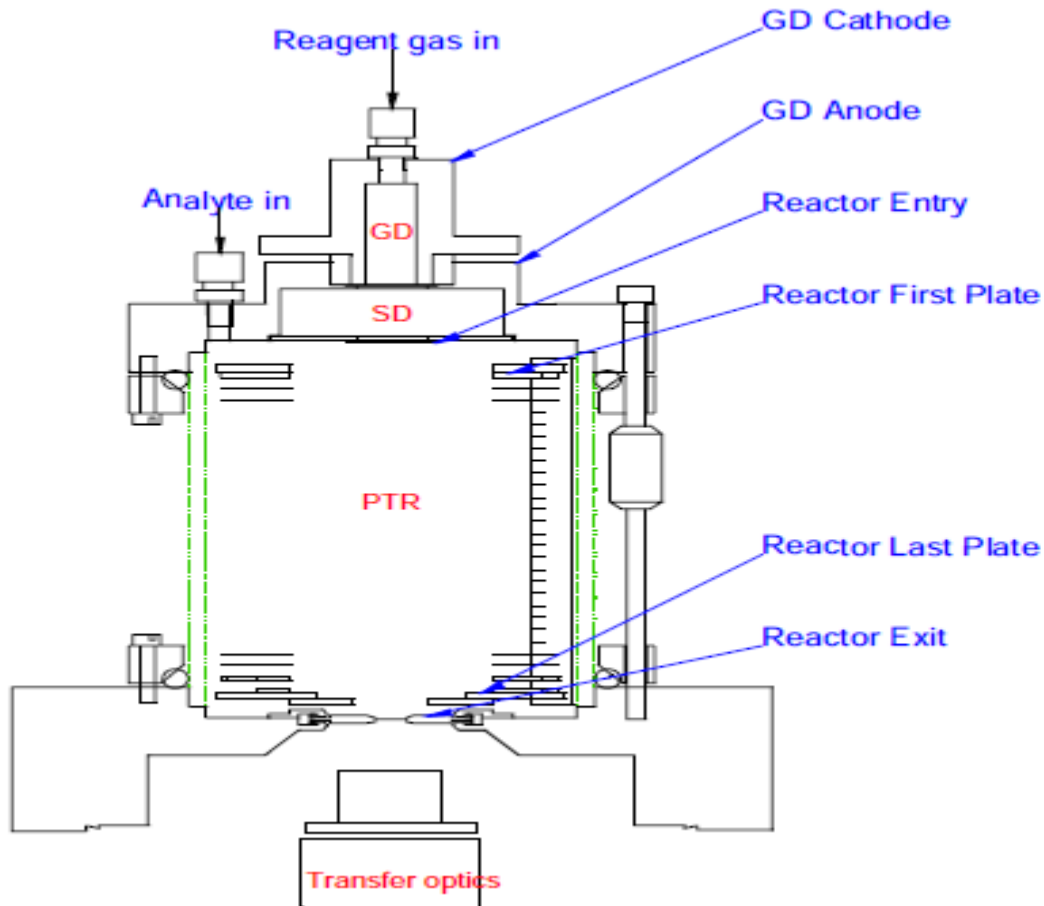
- Deconvolute and **speciate** complex spectra produced from mixtures of gases representing biogenic and anthropogenic systems using multivariate statistical techniques
- **Identify** and **Quantify** OVOC products invoking knowledge of PTR ion chemistry using values obtained from DFT and through intercomparison with atmospheric chemistry models



- PTR-ToF-MS deployed in central London as part of the *ClearfLo* project.
- VOCs measured in near real-time over a 5 week period between January and February 2012

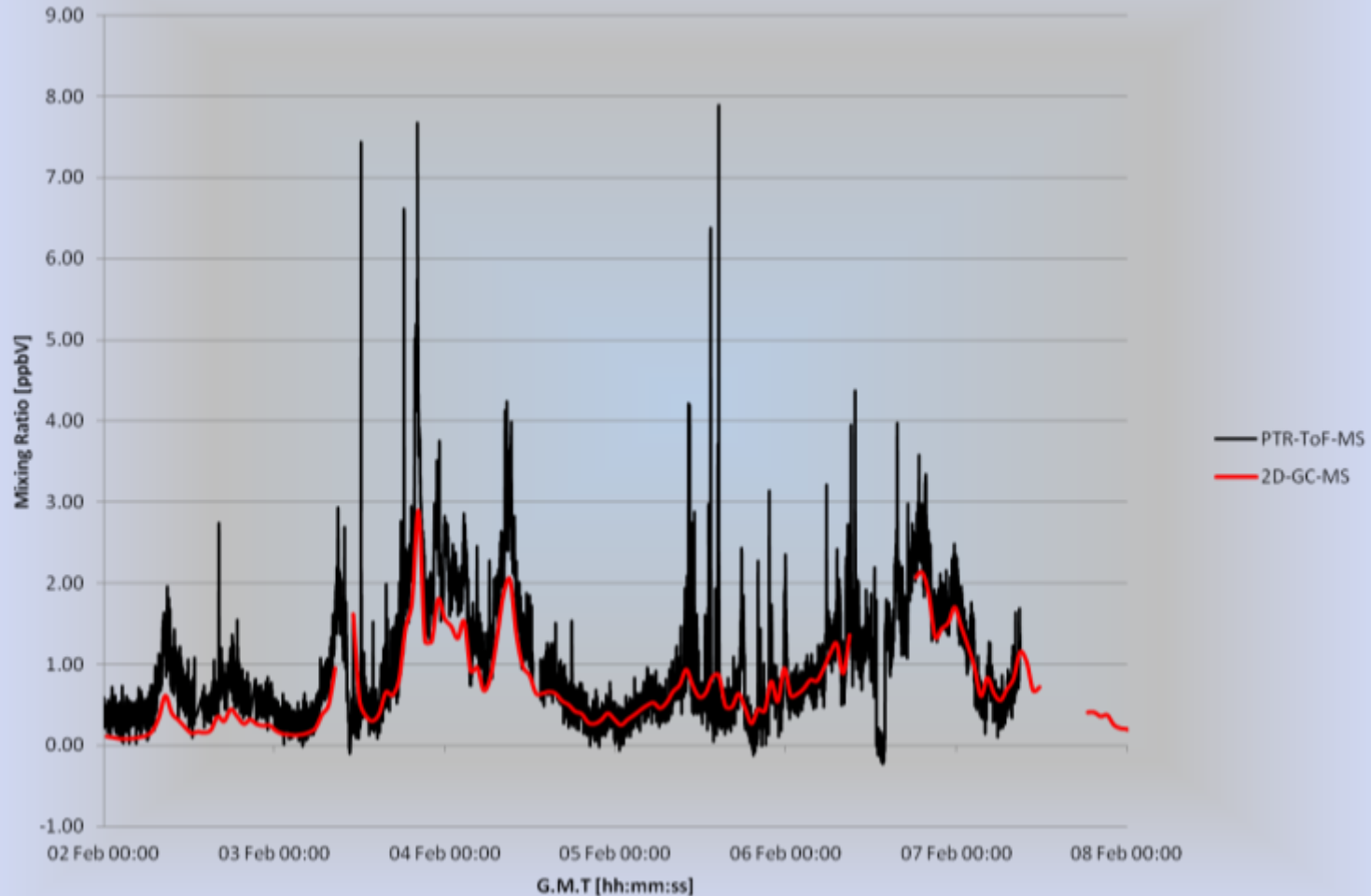


Leicester Field Instrument



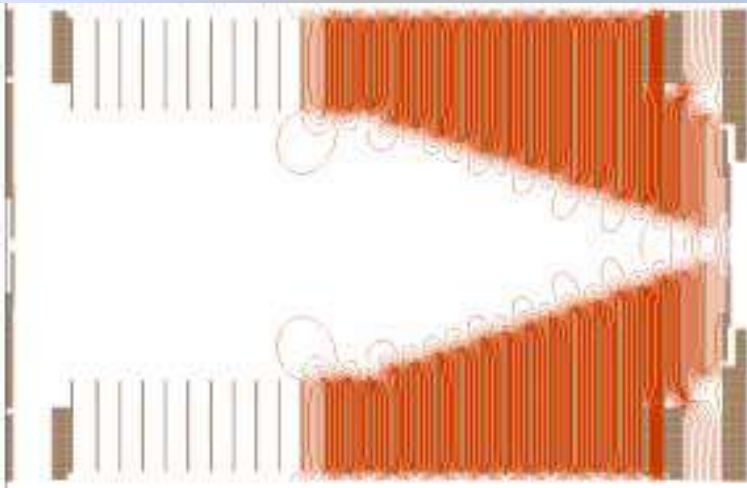
•PTR-ToF-MS Field Instrument

PTR-MS (20s av.) vs York 2D-GCMS measurements of Toluene

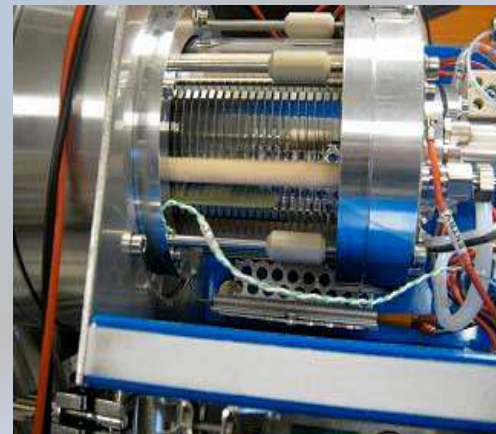


RF Funnel

- The funnel consists of a series of ring electrodes where the internal diameter tapers down to an exit
- The RF and DC electric potentials are applied to these electrodes and the ions are 'guided' into the flight tube
- 2 orders of magnitude improvement on sensitivity



RF component modelled



RF Funnel attached to instrument

RF-Ion Funnel PTR-ToF-MS

- Barber et al. Anal. Chem., 84 (12), 5387-5391, 2012

dx.doi.org | ACSJCA | JCA1001465/W Unicode | research.3f (R3.1.5.2: HF01:3738 | 2.0 alpha 39) 2012/05/23 16:28:00 | PROD-JCAVA | eq_1540693 | 5/25/2012 05:32:42 | 5

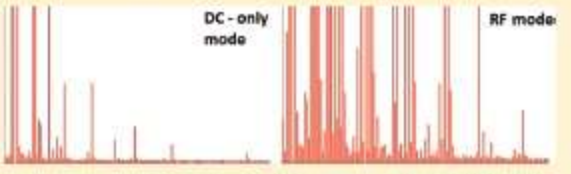
analytical chemistry Article
pubs.acs.org/ac

1 Increased Sensitivity in Proton Transfer Reaction Mass Spectrometry 2 by Incorporation of a Radio Frequency Ion Funnel

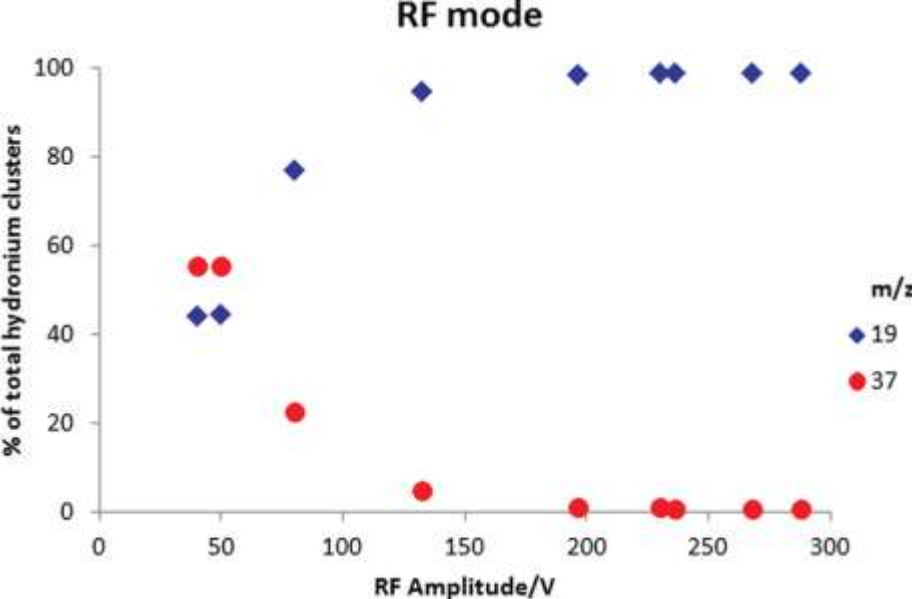
3 Shane Barber,[†] Robert S. Blake,[†] Iain R. White,[†] Paul S. Monks,[†] Fraser Reich,[‡] Steve Mullock,[‡]
4 and Andrew M. Ellis^{*†}

5 [†]Department of Chemistry, University of Leicester, University Road, Leicester LE1 7RH, U.K.
6 [‡]Kore Technology Limited, Cambridgeshire Business Park, Ely, Cambridgeshire CB7 4EA, U.K.

7 **ABSTRACT:** A drift tube capable of simultaneously function-
8 ing as an ion funnel is demonstrated in proton transfer
9 reaction mass spectrometry (PTR-MS) for the first time. The
10 ion funnel enables a much higher proportion of ions to exit the
11 drift tube and enter the mass spectrometer than would
12 otherwise be the case. An increase in the detection sensitivity
13 for volatile organic compounds of between 1 and 2 orders of
14 magnitude is delivered, as demonstrated using several compounds. Other aspects of analytical performance explored in this study
15 include the effective E/N (ratio of electric field to number density of the gas) and dynamic range over which the drift tube is
16 operated. The dual-purpose drift tube/ion funnel can be coupled to various types of mass spectrometers to increase the detection
17 sensitivity and may therefore offer considerable benefits in PTR-MS work.

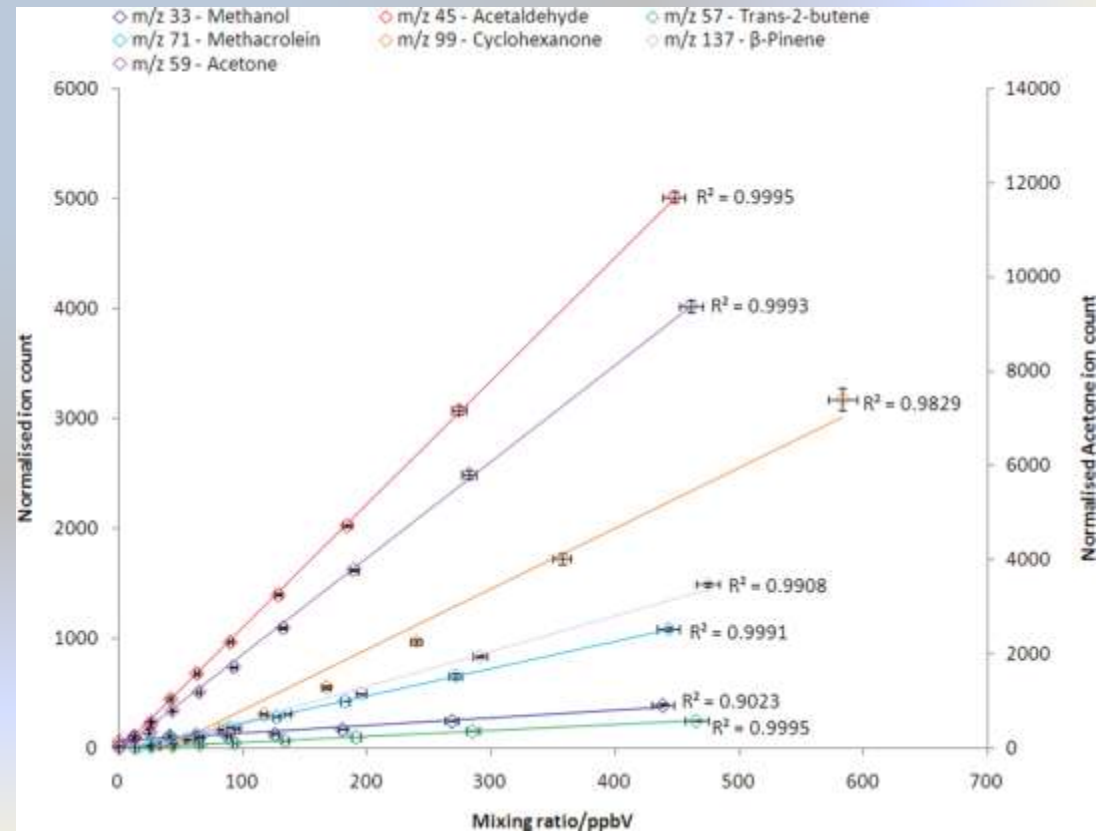


18 **I**ntroduced in the mid 1990s, proton transfer reaction mass
19 spectrometry (PTR-MS) has become an increasingly
20 important technique for the detection and monitoring of
21 volatile organic compounds (VOCs) in air.^{1–5} It possesses a
flight mass spectrometry (TOF-MS) is particularly promising
because it is a multichannel device capable of detecting all ions
simultaneously. Moreover, with suitably folded ion trajectories,
as seen in the standard reflectron, and other mass analyzer



- RF amplitude optimised

- Dynamic range quantified
- (Up to 3 orders of magnitude increase in sensitivity?)
- RF field interacts with (more polarisable) analytes



- Approach centred towards biogenic VOC oxidation product measurement:
 - Building library of fragmentation patterns for biogenics and oxidation products
 - Drift tube optimised: high yield in drift tube, hotter than conventional PTR-MS, soft ionisation conditions with low 'mass spec' energy and CID.
- Back to back measurements with PTR-ToF and PTR-ToF fitted with Ion funnel to be deployed during next IOP in London

β -caryophyllene Oxidation Products

Compound Identification

