### ELECTRONIC SUPPLEMENTARY INFORMATION

# **Remote Monitoring of Volatiles by Ion Mobility Spectrometry**

## with Wireless Data Transmission and Centralized Data Analysis

Hsuan-Ting Ou<sup>1</sup>, Krzysztof Buchowiecki<sup>1</sup>, Pawel L. Urban<sup>1,2\*</sup>

 <sup>1</sup> Department of Chemistry, National Tsing Hua University 101, Section 2, Kuang-Fu Rd., Hsinchu, 30013, Taiwan
<sup>2</sup> Frontier Research Center on Fundamental and Applied Sciences of Matters, National Tsing Hua University 101, Section 2, Kuang-Fu Rd., Hsinchu, 30013, Taiwan

\* Corresponding author:

P.L. Urban (urban@mx.nthu.edu.tw)

#### **ADDITIONAL TABLE**

Compound name	Formula	Monomer drift time / ms	Monomer reduced mobility / cm² V <sup>-1</sup> s <sup>-1</sup>	Reduced mobility from literature / cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup>	Dimer drift time / ms	Dimer reduced mobility / cm² V⁻¹ s⁻¹	Reduced mobility from literature / cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup>
pyrrolidine	$C_4H_9N$	7.31	2.01	2.08 <mark>(1)</mark>	7.73	1.90	n.a.
trimethylamine	$C_3H_9N$	7.22	2.03	2.07 <mark>(2)</mark>	8.31	1.77	n.a.
1,4-diaminobutane	$C_4H_4N_2$	7.32	2.01	1.98 (2)	8.60	1.71	n.a.
1,5-diaminopentane	$C_5H_{14}N_2$	7.66	1.92	1.91 (2)	9.42	1.56	n.a.
2,4-lutidine	C <sub>7</sub> H <sub>9</sub> N	7.98	1.84	1.84 (3)	10.23	1.44	1.37 (3)
(–)-nicotine	$C_{10}H_{14}N_2$	9.61	1.53	1.55 <mark>(</mark> 4)	13.22	1.11	n.a.

Table S1. Reduced mobilities of peaks recorded for six standard compounds.

References for Table S1:

- 1. Clement, R. E.; Siu, K. W. M.; Hill, H. H., *Instrumentation for Trace Organic Monitoring*; CRC Press: Boca Raton, 2018.
- Karpas, Z.; Litvin, O.; Cohen, G.; Mishin, J.; Atweh, E.; Burlakov, A. The Reduced Mobility of the Biogenic Amines: Trimethylamine, Putrescine, Cadaverine, Spermidine and Spermine. *Int. J. Ion Mobil. Spectrom.* 2011, 14, 3–6.
- 3. Eiceman, G. A.; Nazarov, E. G.; Stone, J. A. Chemical Standards in Ion Mobility Spectrometry. *Anal. Chim. Acta* **2003**, *493*, 185–194.
- 4. Ochoa, M. L.; Harrington, P. B. Detection of Methamphetamine in the Presence of Nicotine Using in Situ Chemical Derivatization and Ion Mobility Spectrometry. *Anal. Chem.* **2004**, *76*, 985–991.

### **ADDITIONAL FIGURES**



Figure S1. Schematic of the modified APCI source: (A) top-view; (B) side-view. Unit: mm



Figure S2. Schematic diagram showing gas flow in the portable IMS platform.



Figure S3. Technical drawing of the GPS module holder: (A) left side view; (B) side view; (C) front view; (D) side view. Unit: mm.



**Figure S4.** Temperature-time plot showing temperature variations around the drift tube. High voltage was always on. White part: cleaning fan and cooling fan were off. Pink part: cleaning fan and cooling fan were on (2-min interval).



S-7



**Figure S6.** System optimization based on the dimer peak of 2,4-lutidine (drift time:  $10.23\pm0.01$ , n = 3); (A) Drift gas flow rate; (B) sample flow rate. Default values: sample flow rate,  $1.2 \text{ Lmin}^{-1}$ ; drift gas flow rate,  $0.746 \text{ Lmin}^{-1}$ .



Figure S7. Verification of carryover using the spectra recorded to produce the PCA result shown in Figure 4. The amounts of analytes: 30 nmol 2,4-lutidine; 200 nmol pyrrolidine; 600 nmol nicotine; 80 nmol 1,4-diaminobutane; 600 nmol 1,5-diaminopentane; 200 nmol trimethylamine.



**Figure S8.** Calibration plots (n = 3): (A) pyrrolidine; (B) trimethylamine; (C) 1,4-diaminobutane; (D) 1,5-diaminopentane; (E) 2,4-lutidine; (F) (–)-nicotine. See **Table 1** for the calibration equations.



Figure S9. Spectra revealing food decomposition process: (A) chicken breast; (B) Mozambique tilapia; (C) white shrimp.



Figure S10. Comparison of spectra of TMA and real samples: (A) chicken breast; (B) Mozambique tilapia; (C) white shrimp.