Supporting Information

Assessment of single-photon ionization mass spectrometry for on-line monitoring of *in vitro* aerosol exposure experiments

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Characterization of the gas and aerosol flows

The influence of the flow rate of the aerosol stream and the position of the capillary were tested using a Collison nebulizer (CH Technologies, Westwood, NJ, USA) to generate aerosol at flows of 2–3 L/min. A solution of 45% glycerol, 45% propylene glycol, 8% water, and 2% nicotine was prepared.

No differences in velocity rates were observed in the SPI-MS spectrum. However, comparing a parallel and perpendicular position of the capillary with respect to the aerosol flow showed a reduction in signal when the sampling was performed perpendicular to the flow (depending on the substance and potentially its partitioning between the phases, resulting in selective sampling of the aerosol particles). Figure S1 shows the time series of nicotine, propylene glycol, and glycerol signals normalized to the total ion count. Almost no reduction in signal was detected for propylene glycol, while a reduction of 20%–30% was seen for glycerol.

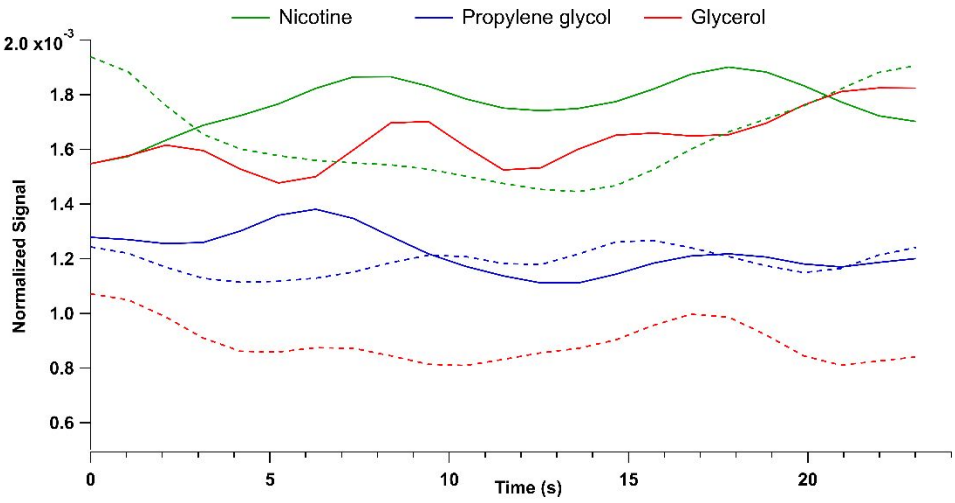

Figure S1. Capillary position respect to the aerosol flow. A Collison nebulizer was used to generate aerosol. The solid lines represent measurements parallel to the aerosol flow direction; the dotted lines represent measurements perpendicular to the aerosol flow direction.

Spectra of individual substances

Individual solutions of glycerol, propylene glycol, and nicotine were prepared at concentrations of 100 ppm for calibration (Figures S2-S4).

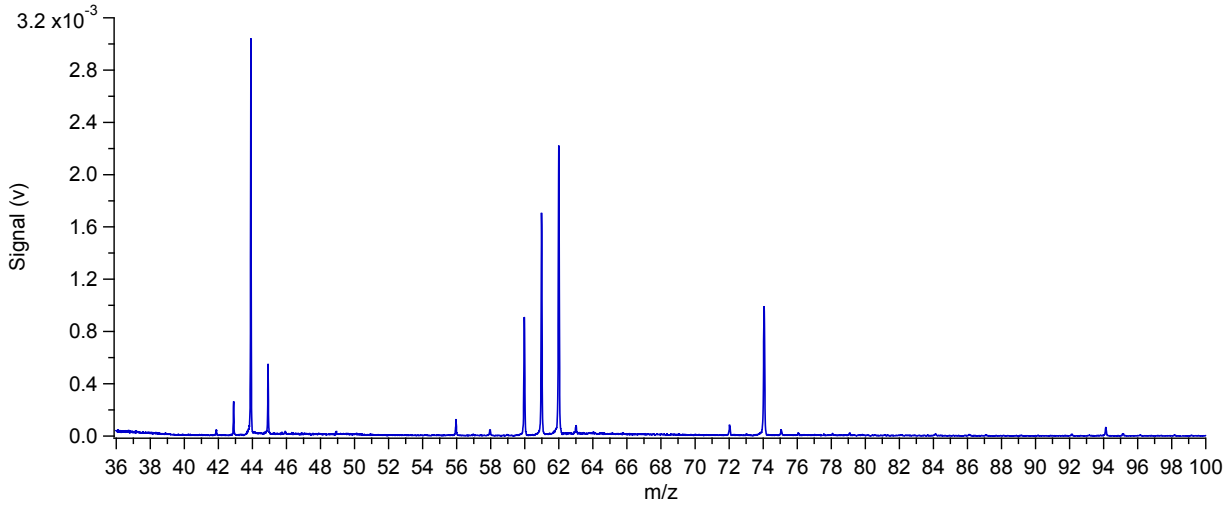

Figure S2. Glycerol spectrum. The main peaks are the fragments at 60, 61, and 62 m/z*. Glycerol products were also observed after heating the calibration solution, and included acetol ($C_3H_6O_2$, 74* m/z*), acetaldehyde (C_3H_6O, 44* m/z*), and acrolein (C_3H_4O, 56* m/z*).*

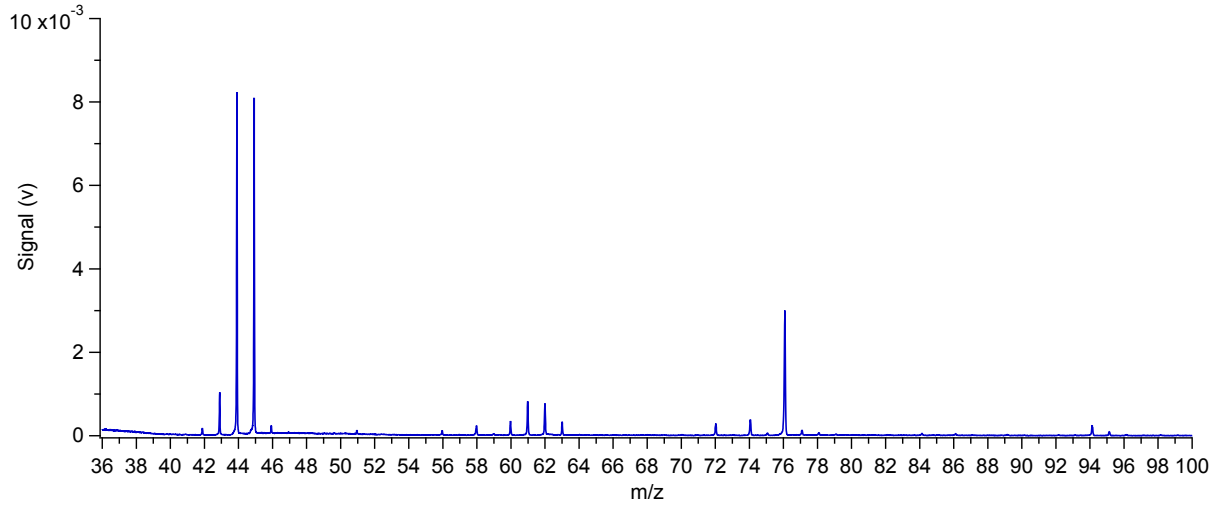

Figure S3. Propylene glycol spectrum. Propylene glycol was detected at its nominal mass at 76 m/z*. Acetaldehyde (C_3H_6O, 44* m/z*) was one of the main products of propylene decomposition after heating the calibration solution.*

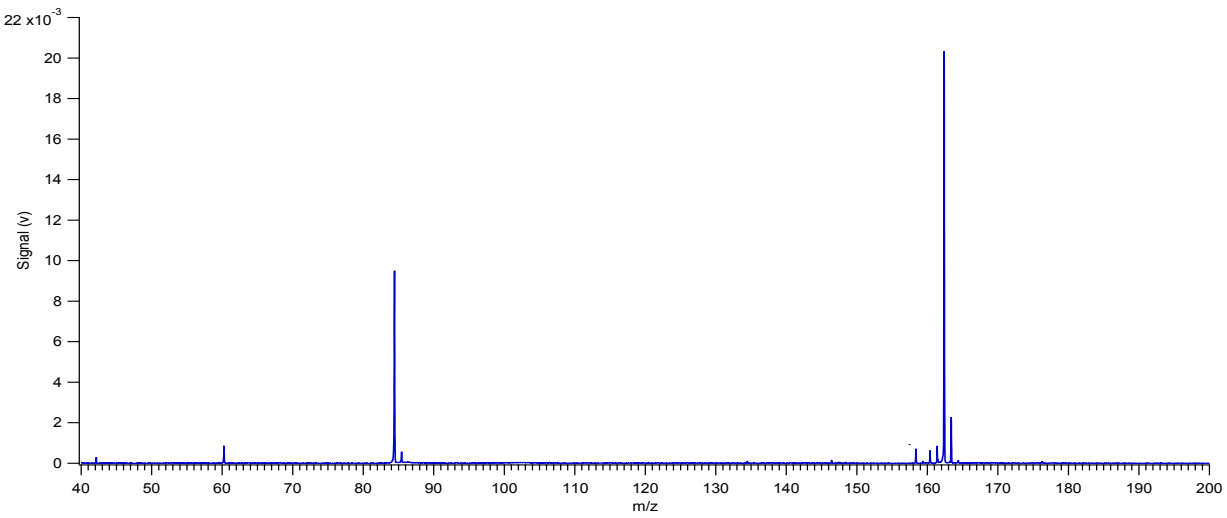

Figure S4. Nicotine spectrum. The main peaks are nicotine ($C_{10}H_{14}N_2$, 162 m/z*) and its fragment cyclopentanone (C_5H_8O, 84* m/z*).*

Temperature measurement

The temperature at the tip of the sampling capillary was measured using a thermocouple (Figure S5) and a thermal camera (Fluke Ti400) (Figure S6). The temperature in the sampling line was 200°C, but the actual temperature at the tip of the sampling line was around 60°C.

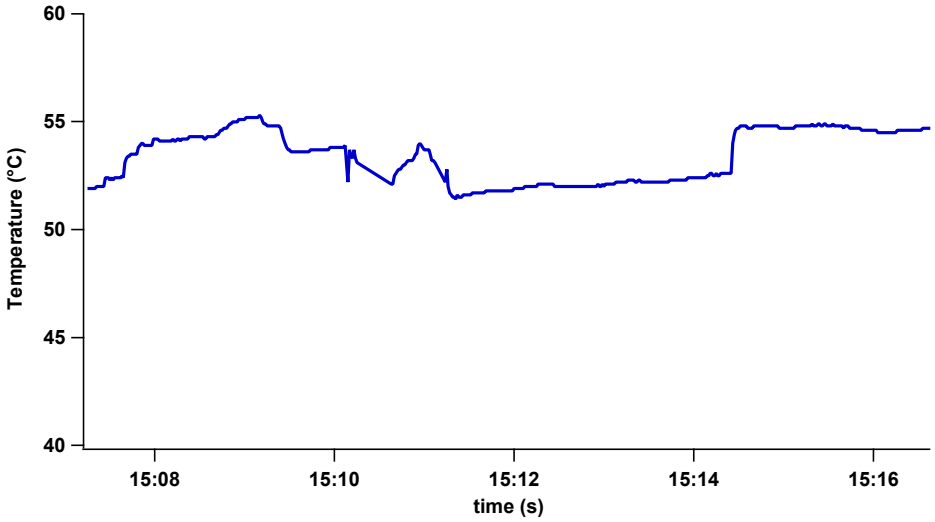

Figure S5. Thermocouple measurements of the capillary temperature over time.

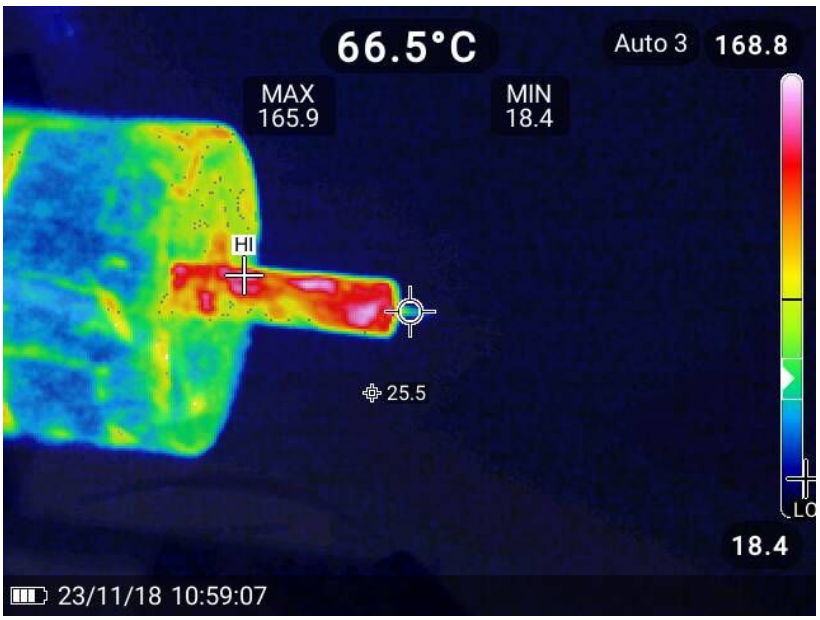

Figure S6. Thermal camera measurements showing the temperature field around the capillary.

Concentrations of glycerol, propylene glycol, and nicotine

Table S1. Concentrations of aerosol constituents in the dilution line and in the quartz crystal microbalance port under the second testing protocol (values from Figure 8).

	Dilution line					
	Glycerol (µg/puff)		Propylene glycol (µg/puff)		Nicotine (µg/puff)	
Delivery line	Average	Standard deviation	Average	Standard deviation	Average	Standard deviation
1	1,380	431.166	2,570	694.603	70.1	10.39
2	838	298.878	1,540	415.897	44.1	12.27
3	360	72.8483	514	262.1	14.4	5.98
4	185	142.601	388	285.624	10	8.64
5	114	66.533	84	28.31	5.15	5.14
6	36.3	12.42	77.3	21.5202	1.34	0.16
	Quartz crystal microbalance port					
1	1,540	384.562	3,030	645.63	77.3	7.55
2	1,050	381.098	1,670	597.55	45.5	14.92
3	363	28.81	503	47.07	12.1	0.59
4	175	22.53	299	123.955	7.08	3.31
5	91.5	19.09	119	71.16	2.55	2.06
6	533	7	84.2	6.74	1.5	1.03

Vapor pressure of propylene glycol, nicotine, and glycerol

Table S2. Vapor pressure of propylene glycol, nicotine, and glycerol at 25°C (pubchem.ncbi.nlm.nih.gov).

Substance	Vapor pressure (mmHg, 25°C)
Propylene glycol	0.13
Nicotine	0.038
Glycerol	$1.68 \cdot 10^{-4}$