Supplementary Information for Online Quantification of Nicotine in E-cigarette Aerosols by Vacuum Ultraviolet Photoionization Mass Spectrometry

Shaoxin Ye[a,b], Zuoying Wen[a]*, Kai Xie[a,b], Xuejun Gu[a], Jian Wang[c]*, Xiaofeng Tang[a]*, Weijun Zhang[a]

a. Anhui Institute of Optics and Fine Mechanics, Hefei Institutes of Physical Science, Chinese Academy of Sciences, Hefei 230031, China.

b. Science Island Branch, Graduate School, University of Science and Technology of China, Hefei 230026, China

c. Key Laboratory of Combustion and Pyrolysis, China Tobacco Anhui Industrial Co, Ltd, Hefei 230088, China

Table S1 GC-FID parameters used in measuring nicotine levels in e-cigarette aerosol according to the GB 41700-2022.

Lists	Parameters
Column	30 m, 0.32 mm ID, 0.25 µm (Agilent 19091J-413)
Injection mode	Split 20:1
Injection temperature	250 °C
Injection volume	1 µL
Carrier gas	Nitrogen, constant flow 1.8 mL/min
Makeup gas rate	20 mL/min
Air rate	450 mL/min
H_2 gas rate	40 mL/min
Oven	100 °C was held for 1 minute then ramped at a rate of 15 °C/min to 220 °C
FID temperature	275 °C
Run time	9 min

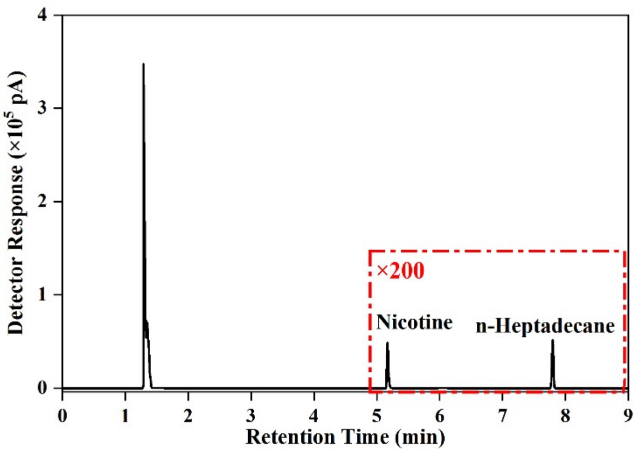

Fig. S1 A chromatogram of nicotine and n-heptadecane. The signal intensity is amplified 200 times for areas with retention times of 5 to 9 minutes to highlight the peaks of nicotine and n-heptadecane.

The chromatogram of nicotine and n-heptadecane measured by GC-FID is shown in Fig. S1. There are three distinct peaks in the spectrum, which are determined by single substance injection in turn. The peak at the retention time of 1.3 minutes is the signal of the solvent isopropanol. The signal of nicotine appears at a retention time of 5.2 minutes and the signal of n-heptadecane at 7.8 minutes.

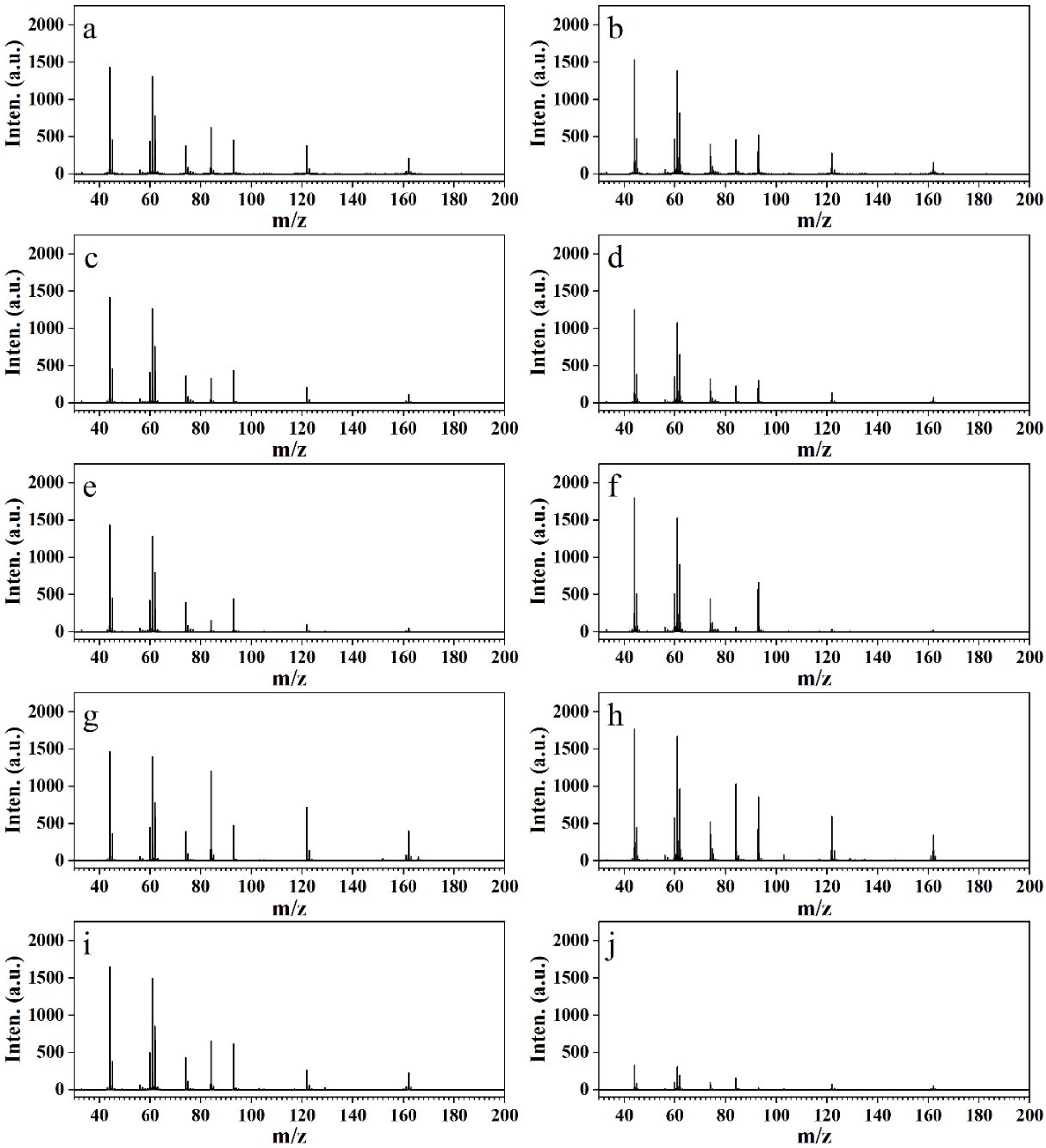

Fig. S2 The photoionization mass spectra of aerosol particles generated by (a) 6% nicotine e-liquid, (b) 4.5% nicotine e-liquid, (c) 3.5% nicotine e-liquid, (d) 2.5% nicotine e-liquid, (e) 1.5% nicotine e-liquid, (f) 0.5% nicotine e-liquid, (g) e-cigarette R, (h) e-cigarette Y, (i) e-cigarette V, and (j) e-cigarette K.

The photoionization mass spectra of aerosol particles generated from a set of concentrations of e-liquid and four kinds of commercial e-cigarettes are shown in Fig. S2. The peaks of all photoionization mass spectrometry are mainly concentrated in substances such as nicotine (m/z = 162, 84), glycerol (m/z = 74, 62, 61, 60, 44), propylene glycol (m/z = 76, 61, 45, 44), and benzoic acid (m/z = 122).

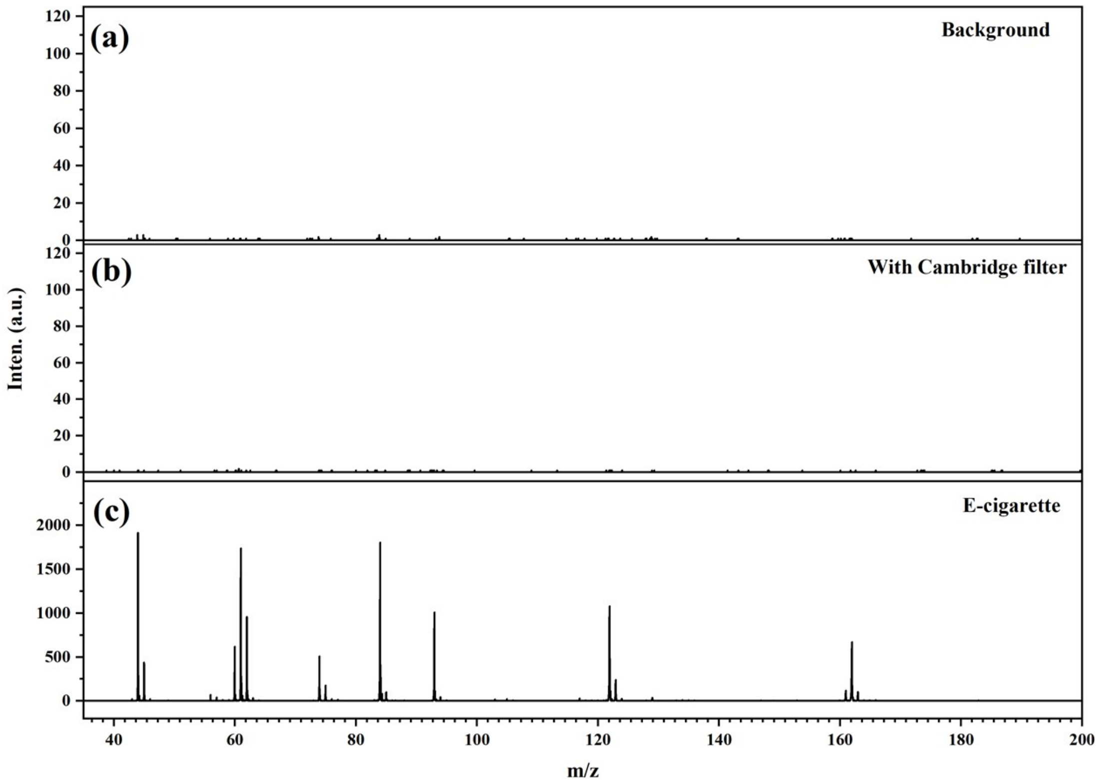

Fig. S3 (a) Photoionization mass spectrum of the background of the VUV-AMS, (b) photoionization mass spectrum of the e-cigarette aerosols after passing the Cambridge filter, (c) photoionization mass spectrum of e-cigarette F aerosol particles.

The photoionization mass spectrum of the background was detected by VUV-AMS without sample injection, which shows low signals. The photoionization mass spectrum of the gas-phase matters in e-cigarette aerosols was obtained by passing through Cambridge filters to remove particulate matter, which proves the ADL in VUV-AMS filters out the gas in e-cigarette aerosols very well. The ordinates of Fig S3(a) and Fig S3(b) are enlarged by 20 times compared with the ordinate of Fig S3(c) to show a clean background with rare gas-phase interference.

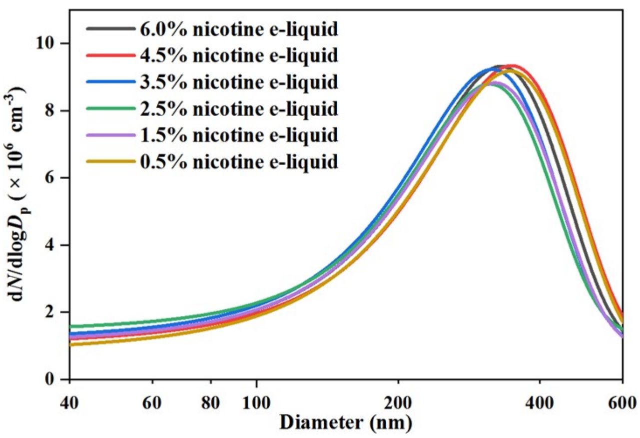

Fig. S4 The particle size distribution of aerosols produced by e-liquids with different nicotine concentrations. The horizontal axis is logarithmic, and the vertical axis represents the logarithmic distribution of the mass concentration per unit volume of particles.

The particle size distribution of aerosols produced by e-liquids with different nicotine concentrations is presented in Fig. S4. The median particle sizes of aerosol particles produced by 0.5% to 6% nicotine e-cigarette liquid are 350 nm, 320 nm, 315 nm, 318 nm, 350 nm, and 330 nm, respectively. According to the dilution of 50 times, the calculated particle number concentrations are 2.6×10^8, 2.7×10^8, 2.6×10^8, 2.5×10^8, 2.5×10^8, and 2.6×10^8 particles/cm^3.

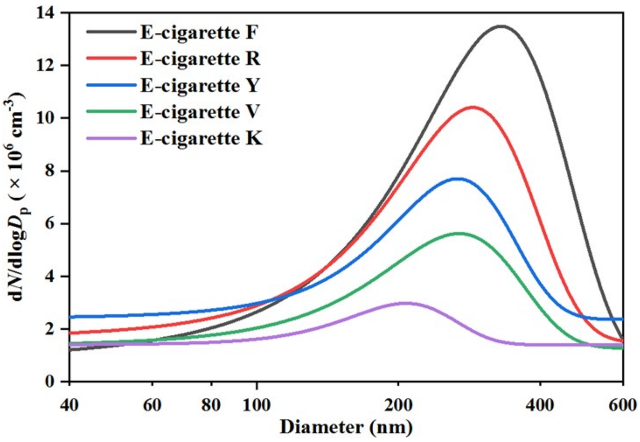

Fig. S5 The particle size distribution of aerosols generated by five different commercial e-cigarettes.

The median particle sizes of aerosol particles produced by e-cigarettes F, R, Y, V, and K are 333 nm, 289 nm, 268 nm, 270 nm, and 206 nm, respectively. According to the dilution of 50 times, the calculated particle number concentrations are 3.3×10^8, 2.8×10^8, 2.4×10^8, 1.8×10^8, and 1.5×10^8 particles/cm^3.