Electronic Supplementary Information

for

Paper cone spray ionization mass spectrometry (PCSI MS) for simple and rapid analysis of raw solid samples

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Contents

I. Experimental Section.

Chemicals and Materials. Information of pharmaceutical tablets used in this study is summarized in Table S1. Eye-of-round ground beef, infant formula, and green tea leaves were purchased from a local grocery store. Low-nitrogen parchment weighing papers with the thickness of 0.02 mm and the weight of 20 g/m^2 (Cat. No. KA22-13) were obtained from Korea Ace Scientific Co. (Seoul, Korea). Grade 1, grade 2, and glass microfiber filter papers and a Grade 31 ET chromatography paper were purchased from Whatman (Maidstone, England). Various solvents including methanol, ethanol, isopropanol, hexane were obtained from Fisher scientific (Fairlawn, NJ, USA).

Paper cone spray tips and sample preparation. A triangular-pyramidal-shaped paper cone tip was prepared by folding a circular-sector-shaped paper (a quadrant with a radius of 1.5 cm). The volume of the prepared paper cone tip was about 77 μL. For pharmaceutical tablet analysis, a tablet was first crushed by using a pestle and motar, and the resulting powders (1.0 to 5.0 mg) were loaded to a paper cone tip. Other solid samples (ground beef, green tea leaves, and infant formula) were directly added to a paper cone tip without any pretreatment.

PCSI MS. For PCSI MS analysis, a paper cone tip with a desired solid sample was located in front of a MS inlet by fixing it with an alligator clip connected to a high voltage power supply [Figure 1(b)]. The paper cone tip was located 5 mm away from the mass inlet and at 30 degrees to the horizontal. After positioning the paper cone tip, 20 to 50 μL of spraying solvent was added to the paper cone tip. A high voltage was applied to the paper cone tip either immediately after or 30 to 60 seconds after spraying solvent was added. Mass spectrometric analysis was performed using a Thermo Finnigan LCQ Deca XP MAX quadrupole ion trap mass spectrometer (Thermo Scientific Inc., San Jose, CA, USA). The voltage used for PCSI MS was ± 3 - 4 kV. Capillary voltage and temperature were set to 35 V and 250 °C, respectively.

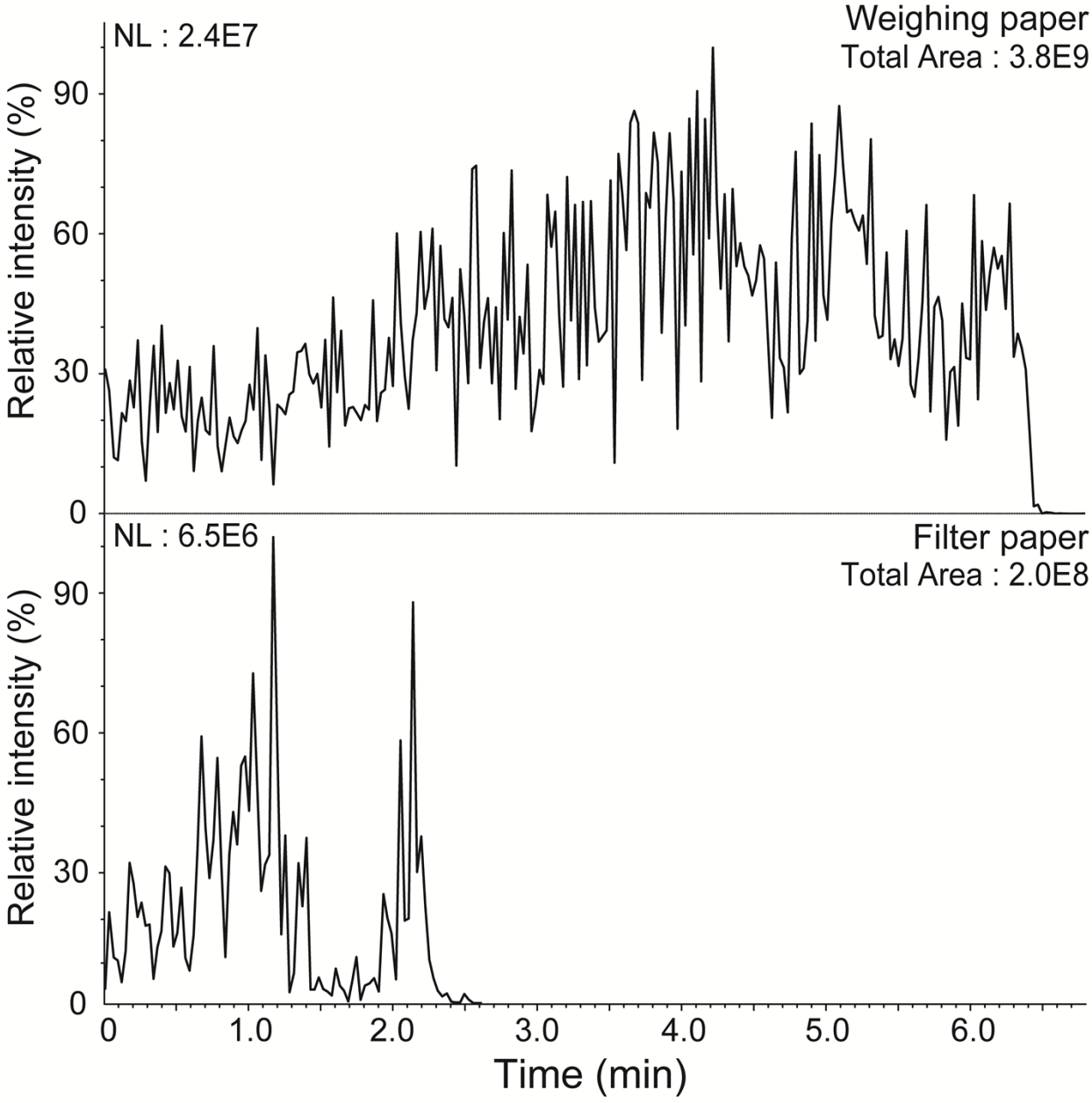
II. Supplementary Table

Supplementary Table S1. Information of pharmaceutical tablets analyzed in this study.

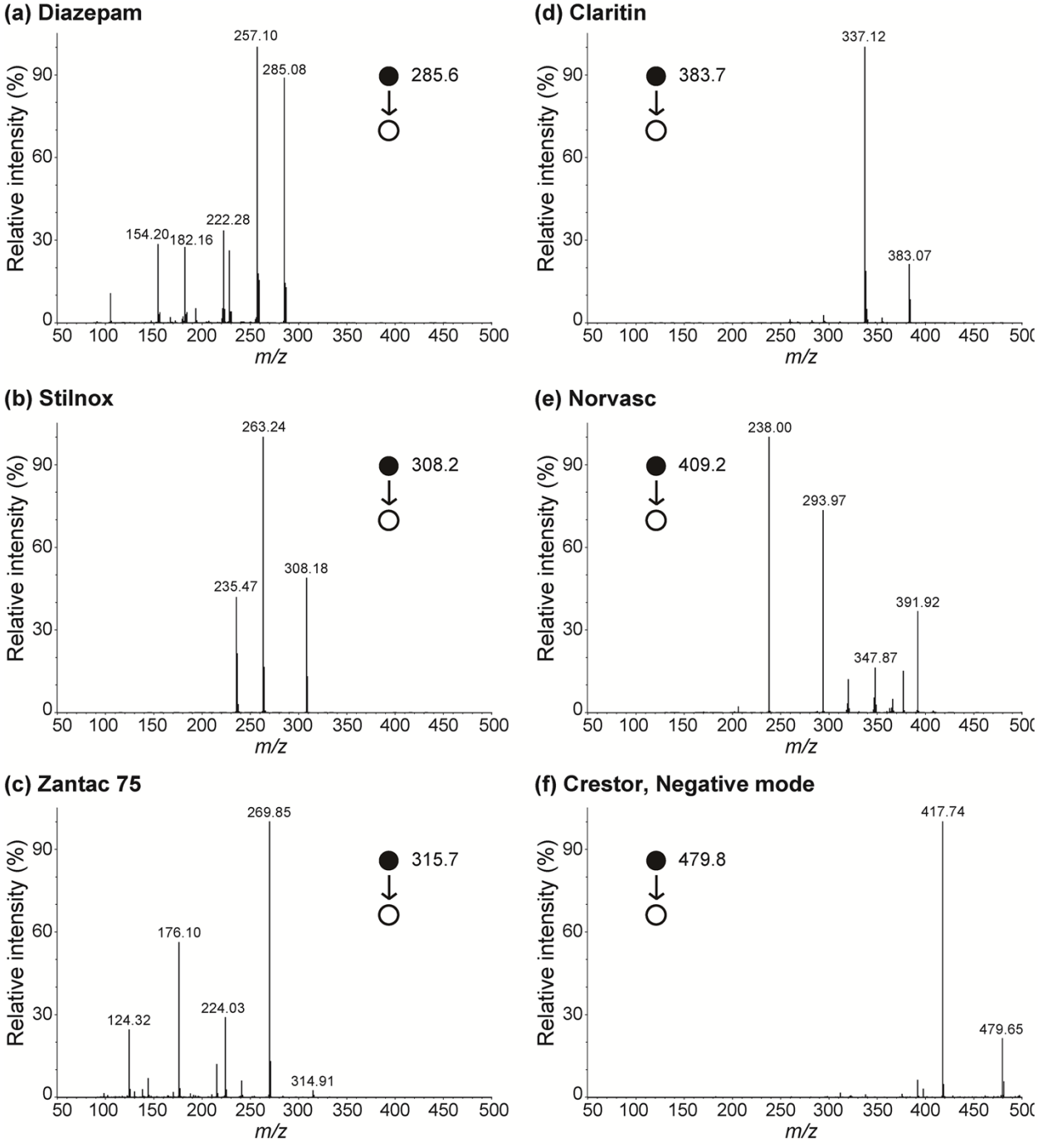
Drug	Active ingredient	Manufacturer	Amount of active ingredient per tablet	Amount of active ingredient per 1 mg of tablet powder
Diazepam	Diazepam	Myung-In Pharm.	2 mg	12.4 μg
Stilnox	Zolpidem tartrate	Sanofi-Aventis	10 mg	64 μg
Zantac 75	Ranitidine	GlaxoSmithKline	75 mg	490 μg
Claritin (Clarityne)	Loratadine	MSD	10 mg	99 μg
Norvasc	Amlodipine	Pfizer	5 mg	25 μg
Crestor	Rosuvastatin calcium	AstraZeneca	20 mg	63 μg
Zesfan gold	Dimethicone DL-carnitine	Chong Kun Dang Pharm.	50 mg (Dimethicone)	74 μg
Soksipan	Dimethicone Ursodeoxycholic acid	Green Cross	25 mg (Dimethicone)	52 μg

III. Supplementary Figures

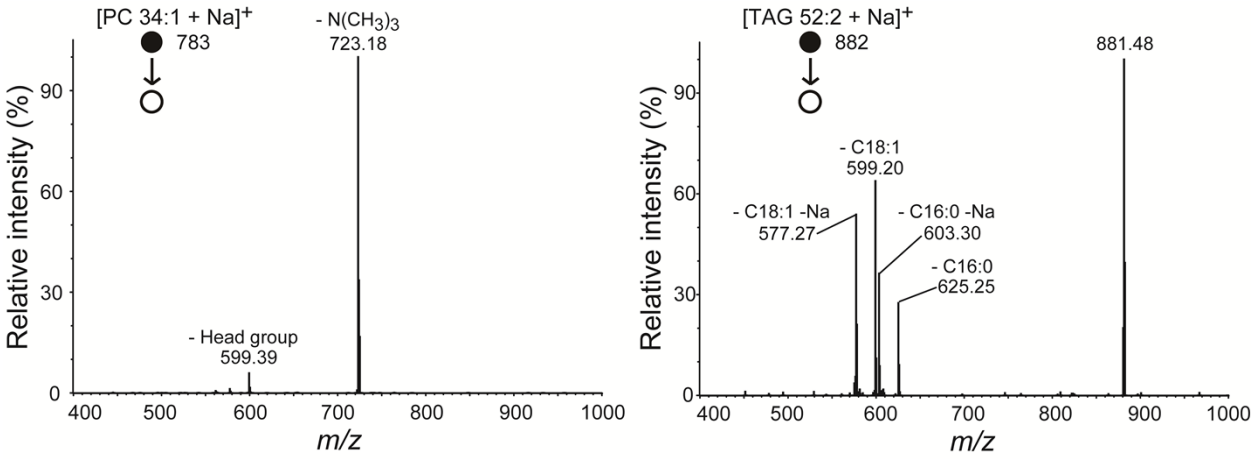
Supplementary Figure S1. The extracted ion chronograms for $[PC\ 34:1 + K]^+$ ion at *m/z* 798.8 detected from a 5.0 mg ground beef sample by PCSI MS with (a) a weighing paper cone tip and (b) a filter paper cone tip. The spraying solvent was 50 μL ethanol. As shown in the figure, more stable and higher analyte signals were observed for a longer period of time with the weighing paper cone tip. As a result, total ion counts (area of chronogram) of $[PC\ 34:1 + K]^+$ was more than 10 fold higher with the weighing paper cone tip than with the filter paper one.



Supplementary Figure S2. Tandem mass spectra of the major active components detected from various powdered tablets (Fig. 2). See supplementary references 1-6 for the reference tandem mass spectra.



Supplementary Figure S3. Tandem mass spectra for the ions [PC 34:1 + Na]$^+$ at *m/z* 783 and [TAG 52:2 + Na]$^+$ at *m/z* 882 detected from a ground beef sample [Fig. 5(c)].



IV. Supplementary References

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