Supporting Information

Nebulization Swab Assisted Photoionization Tandem Miniaturized Ion Trap Mass Spectrometry for On-site Analysis of Nonvolatile Compounds

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Molecular structure of analyzed nonvolatile compounds in this article

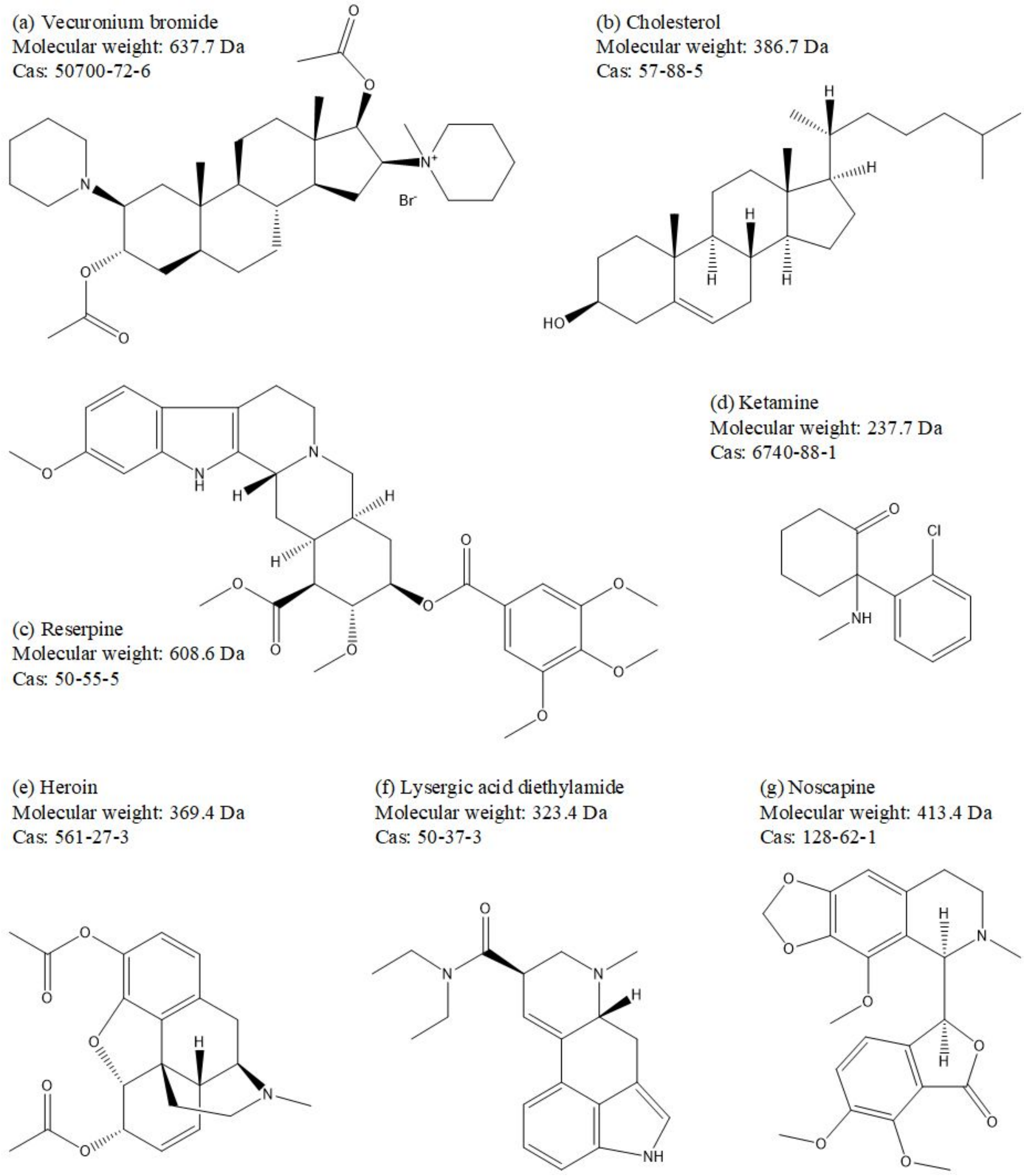

Figure S-1. The molecular structure and cas number of analyzed nonvolatile compounds in this article

Numerical Simulation

A commercial CFD software package ANSYS Fluent (No commercial using) was customized to simulate flow dynamics and ion transport in the NSAP source[1]. Turbulent flow and heat transfer were modeled using the pressure-velocity coupled solver for the Navier-Stokes equations. Menter's Shear Stress Transport (SST) k-ω turbulence model was applied for an unsteady/transient Reynolds Averaged N-S (RANS) simulation.

Species transport was manipulated to simulate the mixture of air and acetone. The boundary conditions used in the simulation and the detail simulation process were summarized in Table S-1. The particle motions were modeled via DPM (discrete phase model), which is a Eulerian-Lagrangian technique in which the particulate system was considered a continuum flow of gas containing numerous discrete particle parcels with each parcel comprised of a group of dilute physical particles[2]. Then, solutions for the airflow patterns were found by calculating approximate solutions of the described Navier-Stokes and continuity equations on a grid of control volumes. The simulation model was operated under the ambient pressure and temperature conditions, where the density of the gas was 1.225 kg/m^3. The gas viscosity was 1.79×10^{-5} kg/(ms). The gas flow was simulated with second-order implicit unsteady solver with a time step of 0.0001 s. For the processing gas phase, a spatial discretization was performed that used a second-order upwind scheme for all conservation equations. Detail calculation process and equation derivation was not the point of this article, programmed files and project in this article are available for public download from github. (https://github.com/wwm0909501/fluent-nebulization)

Table. S-1 Applied boundary conditions and parameters used in the fluent simulation

Condition	Boundary condition
Dopant Inlet/diameter	Velocity inlet/2.5 mm
Mass fraction of dopant inlet	Acetone (3.7 %), Oxygen (22.3 %), N_2 (74 %)
Outlet/diameter	Pressure outlet(1atm)/ 2mm
Mass fraction of outlet	Oxygen (21 %), N_2 (79%)
ionization chamber	Wall/No slip/ (373 K)
Gas temperature	Constant temperature(300K)
Calculate type	Steady/Pressure-based
Turbulence model	SST k-omega
Species model	Species transport
Injection Type	Air-blast-atomizer
Number of Streams	300
Relative Velocity	1.3 mL/min

Designed NSAP source and infusion ESI source

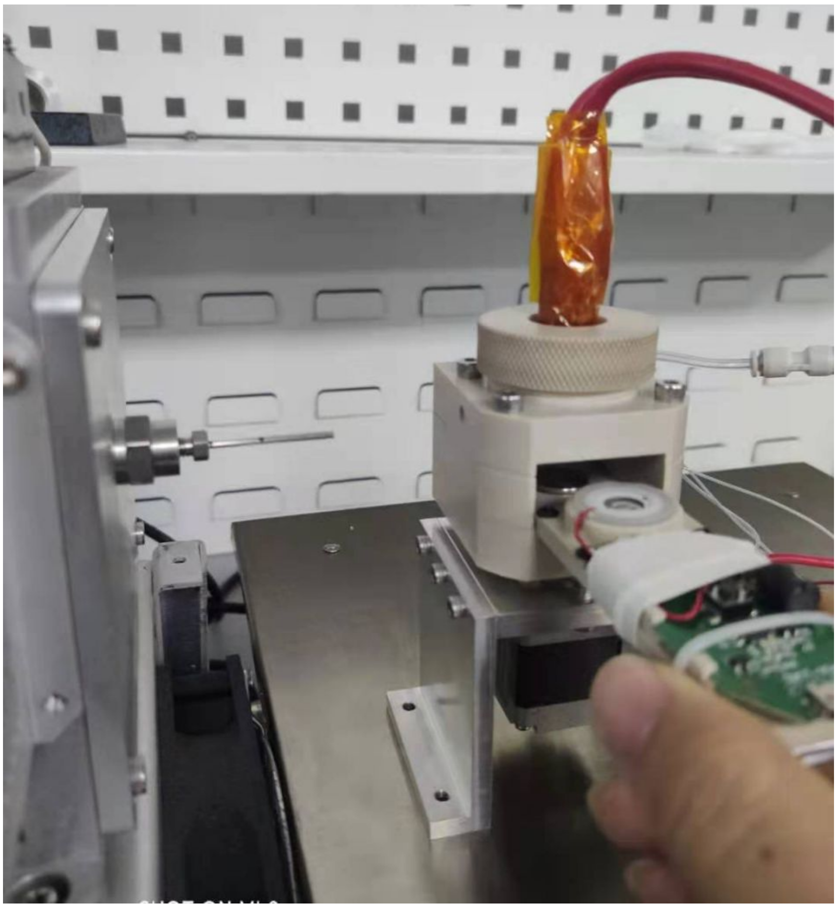

Figure S-2. Photograph of designed NSAP source

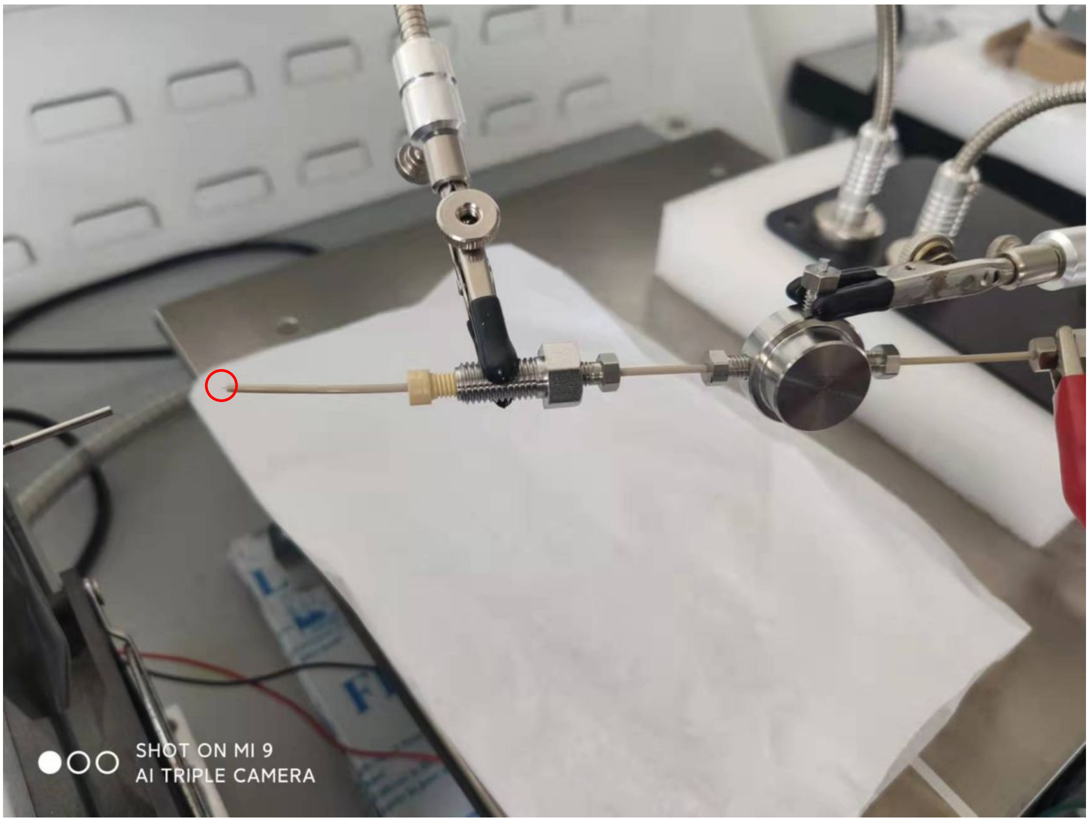

Figure S-3. Photograph of infusion ESI (10 μL/min)

Mass spectra comparison between the infusion ESI and NSAP source

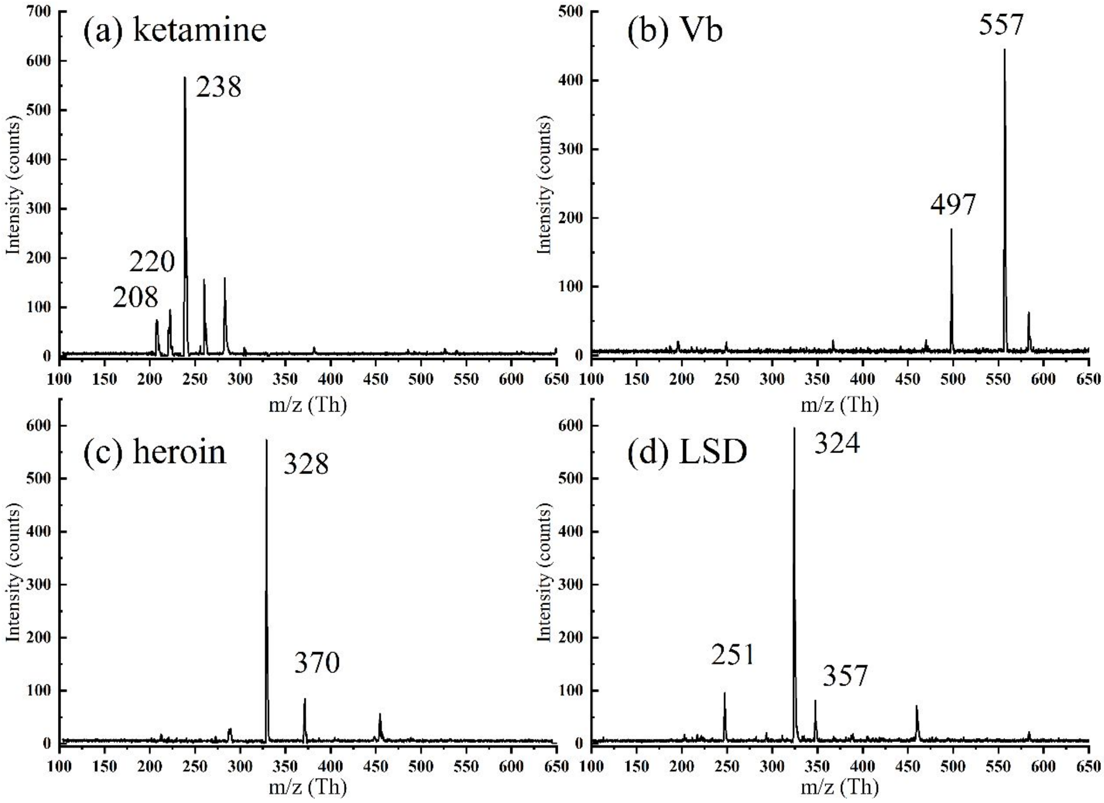

Figure S-4. Mass spectrums of four drugs (a) ketamine (b) Vb (c) heroin (d) LSD with infusion ESI system

Table. S-2 The LODs for measured compounds obtained by using infusion ESI system

Target compounds	Characteristic ion (m/z, Th)	LOD	
		Absolute amount* (pg)	Concentration (ppm)/(RSD %)
Ketamine	238.4 $[M+H]^+$	3.33	0.02 (1.20 %)
LSD	324.6 $[M+H]^+$	16.65	0.1 (3.50 %)
Heroin	328.4 $[M+H]^+$	33.30	0.2 (4.26 %)
Fentanyl	337.5 $[M+H]^+$	83.30	0.5 (4.77 %)
Cocaine	304.2 $[M+H]^+$	16.65	0.1 (2.19 %)
Reserpine	609.7 $[M+H]^+$	166.70	1 (5.67 %)
Noscapine	414.4 $[M+H]^+$	83.30	0.5 (4.38 %)
Cholesterol	369.6 $[M-H_2O+H]^+$	83.30	0.5 (3.39 %)
Norfloxacin	320.3 $[M+H]^+$	33.30	0.2 (4.61 %)
Chlorotetracycline	479.8 $[M-Cl]^+$	83.30	0.5 (5.67 %)
Tetracycline	445.5 $[M+H]^+$	16.65	0.1 (1.22 %)
Oxytetracycline	461.8 $[M+H]^+$	33.30	0.2 (3.50 %)
Dinonyl phthalate, DOP	419.6 $[M+H]^+$	833	5 (6.85 %)

Didecyl phthalate, DIDP	447.6 $[M+H]^+$	833	5 (7.90 %)
Bis(2-ethylhexyl) phthalate, DEHP	391.6 $[M+H]^+$	83.30	0.5 (4.11 %)
Vecuronium bromide	557.7 $[M-Br]^+$	83.30	0.5 (4.50 %)
Rocuronium bromide	529.7 $[M-Br]^+$	83.30	0.5 (5.90 %)

* The absolute amout is calculated from the concentration in 1 seconds.

Mean particle diameter calculation

Typically, the mean droplet size produced by an ultrasonic nebulizer is expressed by Lang's equation[3, 4]:

$$D = A(\frac{8\pi\sigma}{\rho f^2})^{1/3} \quad (1)$$

The value of A, an experimentally obtained coefficient, was reported to range between 0.34 and 0.45. ρ is the density of the droplet fluid where 0.787 g/mL was used. In this experiment, f is the frequency of the generated SAWN which is 2.5 MHz. σ is the surface tension of the bulk solution, and was calculated with equation (2):

$$\sigma = y_a\sigma_a + y_b\sigma_b \quad (2)$$

where y_a and y_b are the fractions of components a and b, respectively, and σ_a and σ_b are the surface tensions of the pure component solvents respectively, which were obtained by consulting the Lange's handbook of Chemistry. It is known that the surface tensions of pure water and pure methanol are 72.75 mN/m and 22.6 mN/m, respectively, at 20 °C. Therefore, σ can be calculated to be 47.98 mN/m. Bring the parameters A, σ, f and ρ into equation (1), the mean droplet size D could be calculated to be 2.12 μm.

Signal variation and duration of the ion signal

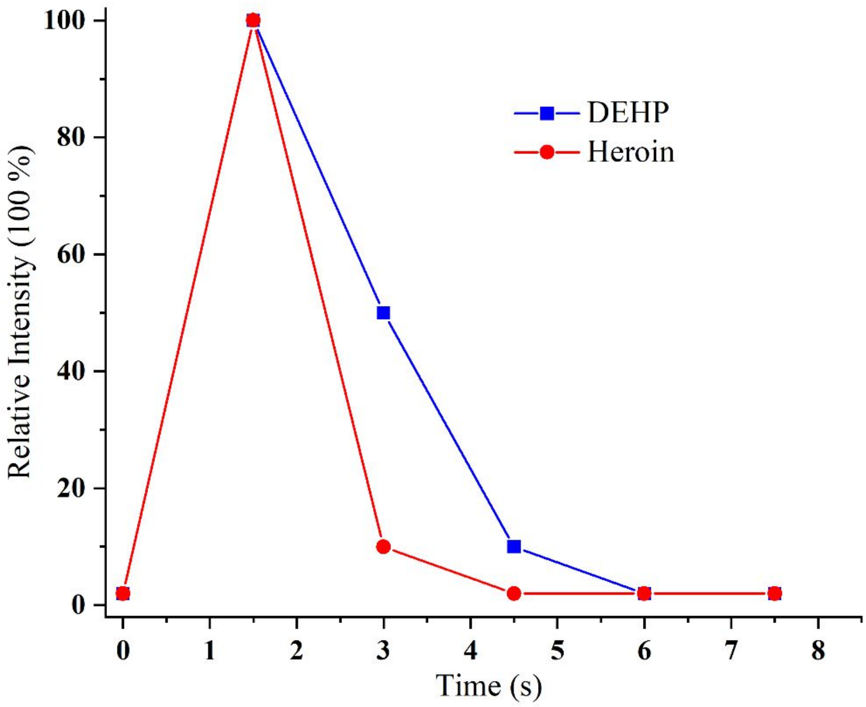

Figure S-5 The TIC of 1 μg/mL DEHP and 1 μg/mL heroin standards

References

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