Supporting Information

A Tapered Capillary-based Contactless Atmospheric Pressure Ionization Mass spectrometry for On-line Preconcentration and Separation of Small Organics

Yen-Chun Chen,[1,2†] Arun Krishnamurthy,[1,2†] Szu-Hua Chen,[1,2] Yu-Chie Chen[1,2*]

[1]Department of Applied Chemistry, National Yang Ming Chiao Tung University
Hsinchu 300, Taiwan
[2]Department of Applied Chemistry, National Chiao Tung University
Hsinchu 300, Taiwan

[*]E-mail: yuchie@nctu.edu.tw
[†]These authors contributed equally to this work.

Additional Experimental Details

Chemicals and reagents

Fused silica capillaries (inner diameter (ID): ~50 μm, outer diameter (OD): ~360 μm) were purchased from Polymicro Technologies (Phoenix, AZ, USA). Adenosine, arginine, L-lysine, and L-histidine were purchased from Sigma (St. Louis, MO, USA). Trichloro(octadecyl)silane (C18) was purchased from Aldrich (Allentown, PA). Atrazine, ametryn, prometryn, and ammonium acetate were purchased from Riedel-de Haën (St. Louis, MO, USA). Ammonium bicarbonate was obtained from J. T. Baker (Center Valley, PA, USA). Isopropyl alcohol and ethanol were obtained from Macron fine chemicals (Center valley, PA, USA), whereas acetonitrile and hydrofluoric acid (HF) were obtained from Merck (Darmstadt, Germany). Ultrapure water (18.2 21Ω) was obtained from Merck Millipore water purifier (Billerica, MA, USA).

Instrumentation

Mass spectra were obtained using either an Amazon SL ion trap mass spectrometer (Bruker Daltonics, Bremen, Germany) or a micrOTOF-Q II mass spectrometer (Bruker Daltonics, Bremen, Germany). The optimized voltage set at the orifice of the mass spectrometer was -4.5 kV when operating the mass spectrometer in the positive ion mode. The temperature of the capillary used for ion transfer was set at 200 ^{o}C. A metal tube (ID: ~0.8 mm; OD: ~1 mm) with a length of 5 cm was connected to the orifice of the mass spectrometer.

Preparation of C18 coated capillaries

The coating procedure for the wall of the capillary was similar to that reported by Tsuda et al. (*Chromatogr*. 1978, 158, 227) with slight modifications. The capillary was flushed by a water aspirator pump (10.3 psi). A fused silica capillary (length: 15 cm; ID: 50 μm, OD: 365 μm) was initially conditioned by flushing with aqueous NaOH (1 N) for 2 h followed by flushing with water for 1 h using a water aspirator vacuum pump. The capillary was dried in an oven at 150 ^{o}C for 4 h. C18 (20%, v/v) was prepared in toluene and sucked

into the conditioned capillary using a water aspirator pump (10.3 psi). The two ends of the capillary were sealed using polymer glue. The capillary was heated at 90 ºC for 12 h. After cooling, the two ends of the capillary were cut, and the capillary was flushed with nitrogen gas (30 psi) to remove remaining residues. Subsequently, the capillary was flushed with toluene for 30 min using a water aspiratory pump to remove unreacted reagents followed by flushing with the solvent of deionized water and acetonitrile (1:1, v/v) for another 30 min.

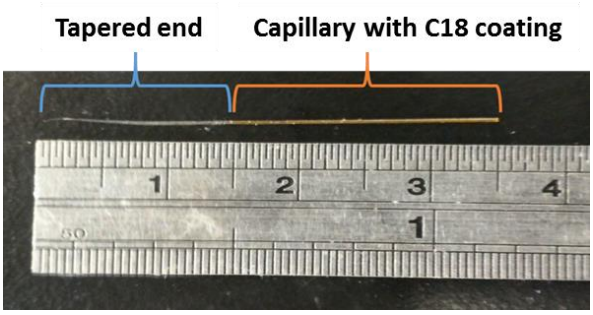

Figure S1. Photograph of the as-prepared capillary with a tapered end.