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Thermal Bursting Ionization for Ambient Mass Spectrometry

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Materials and reagents

HPLC grade methanol (CH_3OH) was purchased from Honeywell Burdick&Jackson Inc. (USA). Reserpine, formic acid, and tyrosine were obtained from Sigma-Aldrich Chemical Co. Ltd. (USA). Sucrose, angiotensin II (Ang II), and PEG 400 were obtained from Sangon Biotech (Shanghai Sangon Biological Engineering Technology & Services Co. Ltd.). All these reagents were used directly without any further purification. Distilled water (18.2 MΩ) was produced by Milli-Q system (Millipore Inc., Bedford, MA, USA). Fruit juice (The Coca-Cola Company) and skin-care products (lotion and cream of Proya brand and cream of Chando brands, affiliated to Zhejiang Proya Cosmetics Co., Ltd. (China) and Jala Co., Ltd. in Beauty and Personal Care (China) respectively) were purchased from local supermarket and cosmetics store respectively.

Experimental procedures

In this experiment, a soldering iron (AT936D, Atten Electronic Co. Ltd., Shenzhen, China) was used to ionize samples (Fig. S1). The adjustable temperature range is between 150-450 °C. When lower temperature (<150 °C) was used, an iron plate was tied to the soldering tip for reducing temperature via heat diffusion. The actual temperature was measured by a thermocouple (Tenmars Electronics Co. Ltd., Taiwan). The distance between the soldering tip (called as probe in the text) and mass spectrometer inlet capillary varied from 0.5 to 1.0 cm. For sample analysis, the probe was heated to a constant value first, and then sample was introduced by dropping on the heated probe directly with a home-made pipette tip. Since the probe was heated over the solvent boiling temperature, solvent would bump intensively accompanying with the transfer of analytes from liquid phase to gas phase for mass spectrometric detection.

Fig. S1 TBI setup for solution sample analysis

The pipette tip used to load sample is modified as follows: A 2 cm long fused silica capillary was inserted into the pipetted tip, with the end of the polyimide coating burned off to avoid melting during sample loading. For sample analysis in pure solvent, 2 μL of sample was loaded onto the metal probe directly. For viscous sample analysis, 2 μL of sample was taken in and expelled by the pipetted tip first, and then 5 μL of CH_3OH-H_2O (v/v, 1:1) was used to flush the sample remaining on the inwall of the pipette tip for mass spectrometer detection. This is because too viscous sample doesn't readily burst on the heated metal probe, and flushing of the pipette tip plays the role of dilution.

Mass spectrometry

All MS experiments were carried out using a Thermo LTQ mass spectrometer (Thermo Fisher Scientific, San Jose, CA, U.S.A.). The commercial ESI source was substituted by our home-made TBI source. The mass spectrometer conditions throughout the experiments were as follows: S lens voltage, 42% (positive mode) and 60% (negative mode); capillary temperature, 275 °C. The ion injection time was set as 100 ms and the number of microscan was set as one.

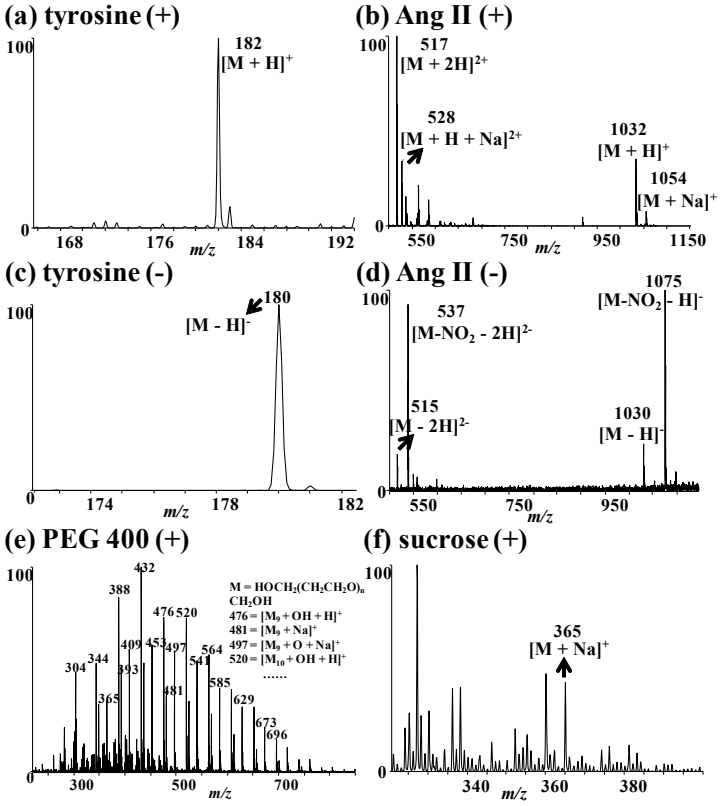

Fig. S2 Mass spectra of (a-d) tyrosine (4 μg/mL) and Ang II (2.5 μg/mL) in positive and negative mode, and (e, f) PEG 400 (5 μg/mL) and sucrose (1 μg/mL) in positive mode detected by ESI MS.

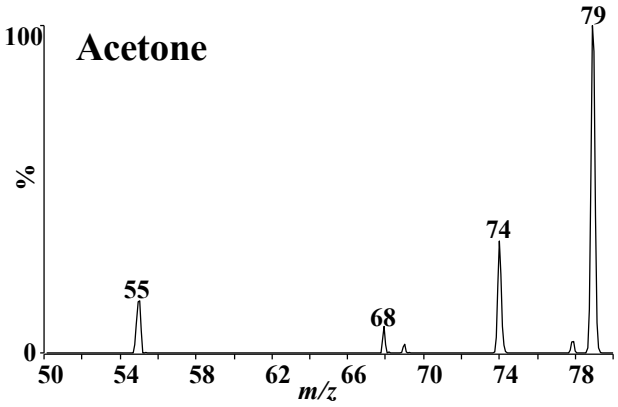

Fig. S3 Mass spectra of acetone detected by TBI MS. Conditions: $C_{acetone}$ = 5 μg/mL, solvent: CH_3OH/H_2O (v/v, 1:1), T_{probe} = 125 °C