Supporting Information

Analysis of human breath samples of lung cancer patients and healthy controls with solid-phase microextraction (SPME) and flow-modulated comprehensive two-dimensional gas chromatography (GC × GC)

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Table S1. GC×GC Chromatographic Conditions

GC×GC: Agilent 7890A FID

Carrier: Hydrogen, constant flow

Inlet: Pulsed splitless; 250 ℃

Inlet liner: Deactivated dual taper direct connect

Column 1: J&W 122-5532 : 60 m ×250 μm ×0.25 μm DB-5ms, 0.8 mL/min

Column 2: Agilent 19091N-030: 5 m ×250 μm ×0.15 μm HP-INNOWax，21 mL/min

Oven: 50 ℃ (1 min) to 150 ℃ (15 ℃/min), hold 15 min,150 ℃ to 220 ℃ (10 ℃/min), hold 5 min

Modulator period: modulator period 1.5 seconds,1.4 seconds collect (sampling time), 0.10 s injection time. ,

Detection: FID at 200 Hz, 250 ℃, H_2 20 mL/min, Air 400 mL/min, N_2 25 mL/min.

Processing software: GC-image software, Version 2.1, Zoex Corporation, Pasadena, TX ,USA,

Table S2: Retention time, linear ranges (LR), limit of detection(LOD), regression equation (Y, Peak volume; X, concentration), correlation coefficient and relative standard deviation (RSD) for the studied compounds.

No.	Targets	Retention Time (T_a, T_b)(min)	LR (μg/L)	LOD (μg/L)	Regression equation	Correlation coefficient	RSD [a] (%)
1	Methanol	（17.4, 0.9）	0.05-2.5	0.01	y = 11.7x + 87.4	0.9447	5
2	Pentane	（18.8, 0.9）	0.05-2.5	0.01	y = 23.8x + 15.4	0.9247	6
3	Acetone	（19.3, 0.8）	0.1-5	0.1	y = 37.7x + 122.1	0.9496	3
4	Isoprene	（19.6, 0.9）	0.1-5	0.1	y = 257.2x + 501.5	0.9748	4
5	Propanol	（21.2, 0.9）	0.1-20	0.1	y = 1495.9x + 2723.5	0.9533	5

a) The RSD experiments were carried out five times using GC×GC under the same conditions.

Table S3. Pearson correlation between BMW and Methanol, Pentane, Acetone, Isoprene, Propanol.BMW

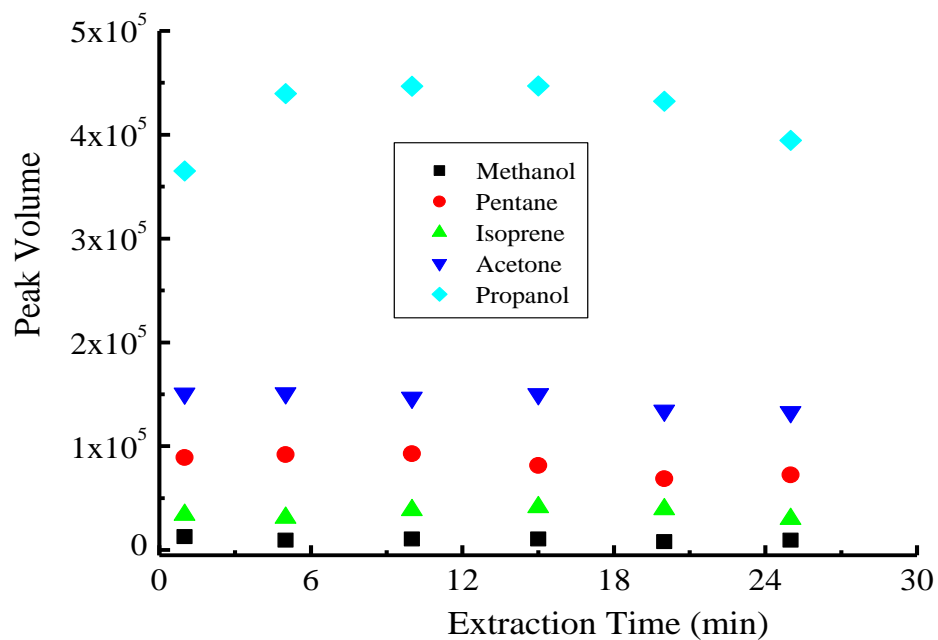|	Methanol	Pentane	Acetone	Isoprene	Propanol
Correlation coefficient	0.339	0.287	-0.086	0.134	0.272
P-Value	0.097	0.164	0.681	0.522	0.189

Fig. S1. Effect of the extraction time on the signal intensity of target compounds. Conditions: concentration, 500 ng L^{-1}; extraction temperature, 25 ℃; injection temperature, 250 ℃; desorption time, 3min.
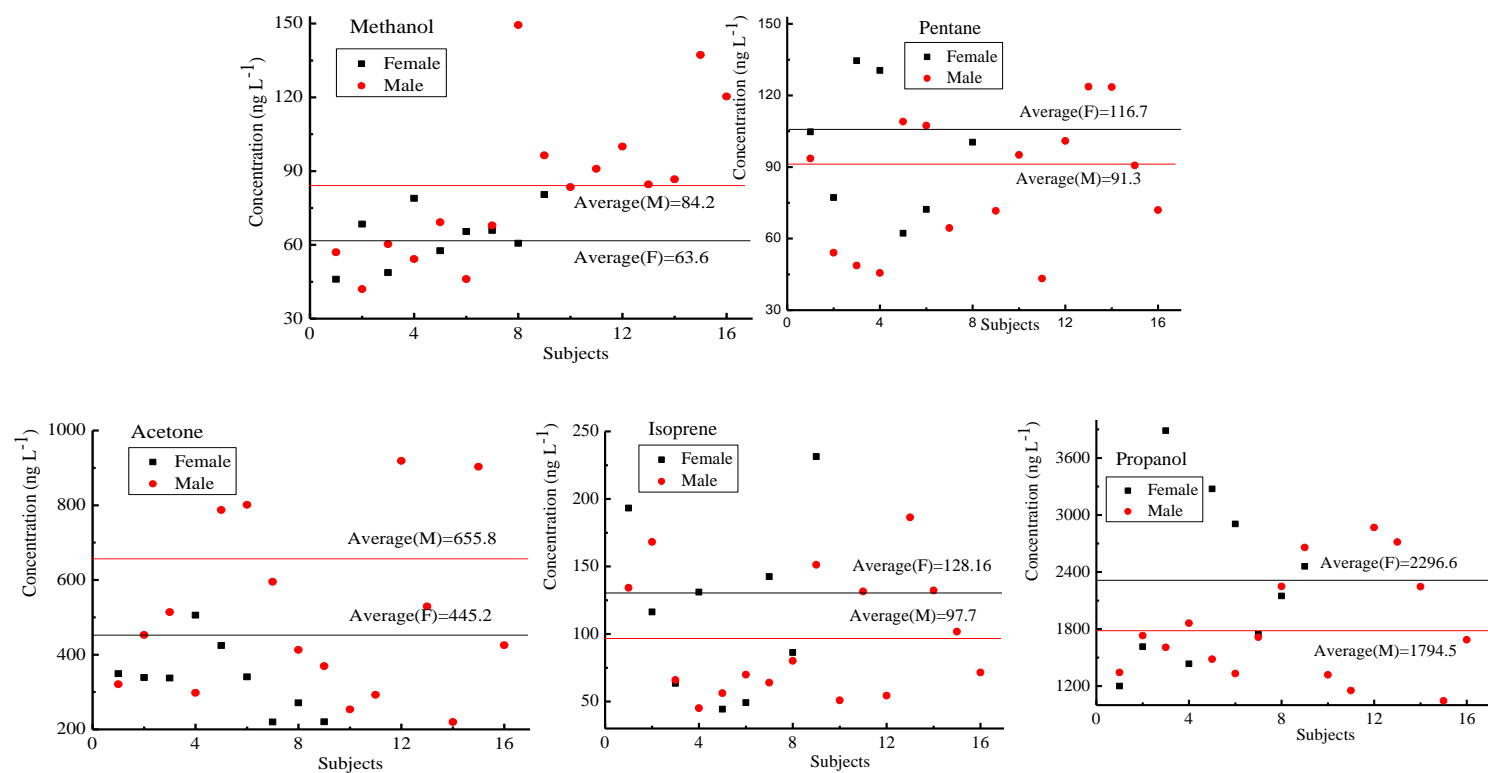
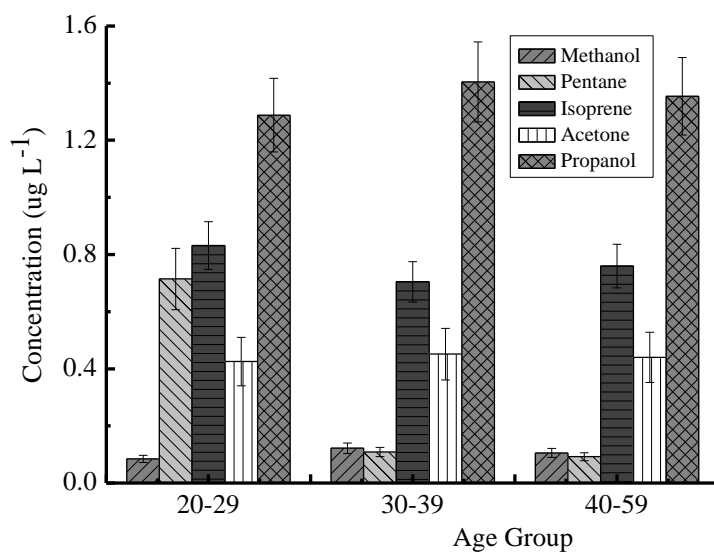**Fig. S2.** A plot of the mean breath VOCs concentration against the gender of health controls.

Fig. S3. Concentration of breath target compounds classified by the different age group of the controls. The controls are divided into three age groups(20-29,30-39,40-59).
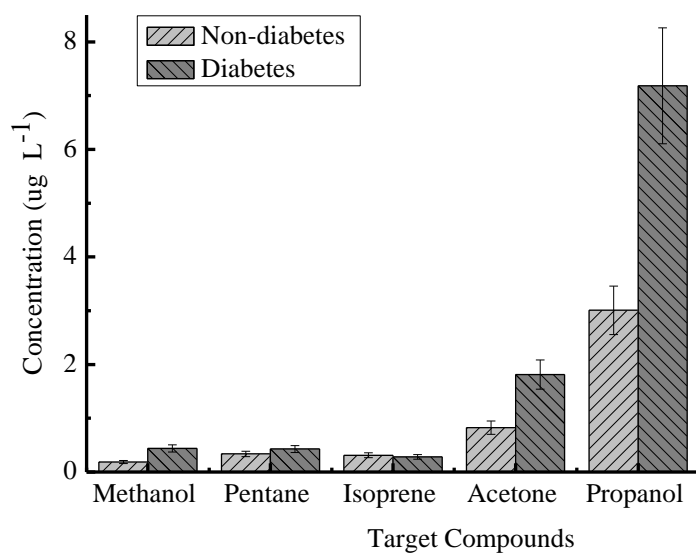
Fig. S4. Comparison of target compounds concentrations between diabetes and non-diabetes
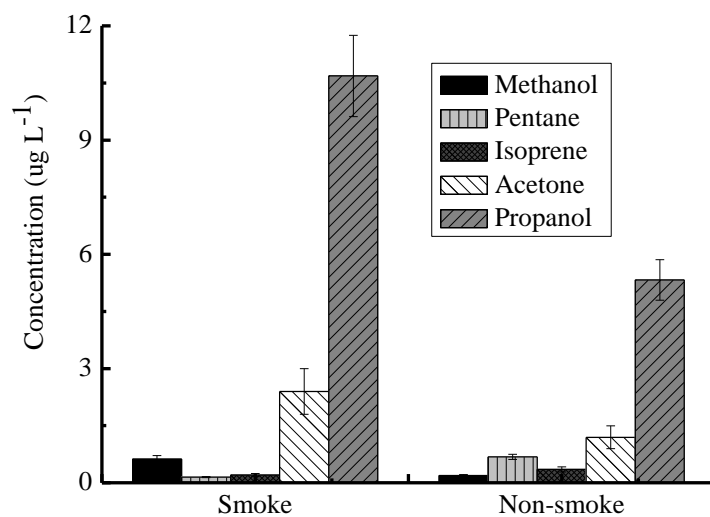
Fig. S5. Influence of the smoke on the extraction of methanol, pentane, isoprene, acetone, propanol.