

SUPPORTING MATERIALS

Table S1. Biomarkers in this study

Biomarker	Abbreviation
<i>N'</i> -nitrosonornicotine	NNN
<i>N</i> -nitrosoanabasine	NAB
<i>N</i> -nitrosoanatabine	NAT
4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol	NNAL
S-phenylmercapturic acid	SPMA
monohydroxybutenyl mercapturic acid	MHBMA
dihydroxybutyl mercapturic acid	DHBMA
3-hydroxypropylmercapturic acid	3HPMA
3-hydroxy-1-methylpropylmercapturic acid	3HMPMA

Table S2. The information of the 224 eligible subjects

<i>Number of subjects in different cities</i>			
Shanghai	60	Suzhou	58
Hefei	56	Guiyang	50
<i>Number of male and female</i>			
Male	179	Female	45
<i>Number of subjects in different age groups</i>			
20-29	37	30-39	61
40-49	53	50-59	42
60-65	31		

Table S3. Retention time (RT) and MRM condition of biomarkers for LC-MS/MS analysis.

Analyte	tR(min)	Q1	Q3	DP	CE	CXP
NNN_1*	1.83	178.1	148.1	30	15	9
NNN_2	1.83	178.1	119.1	30	15	9
NAB*	2.54	192.1	162.1	26	18	11
NAT*	2.52	190.1	160.1	28	16	10
NNAL_1*	1.76	210	105.7	34	19	3
NNAL_2	1.76	210	131	34	19	3
NNAL_3	1.76	210	148.7	34	9	3
NNN-d4_1*	1.83	182.1	152.1	30	16	9
NNN-d4_2	1.83	182.1	124.1	30	16	9

SPMA*	2.79	237.9	108.9	-43	-15	-10
MHBMA_1*	2.15	232	102.9	-40	-15	-10
MHBMA_2	2.15	232	199	-45	-20	-10
DHBMA_1*	1.21	249.9	120.9	-35	-16	-10
DHBMA_2	1.21	249.9	127.9	-35	-16	-10
3-HPMA_1*	1.49	219.9	90.9	-45	-16	-10
3-HPMA_2	1.49	219.9	84	-45	-17	-10
3-HMPMA_1*	2.34	234	105	-30	-21	-10
3-HMPMA_2	2.34	234	102.9	-20	-39	-10
3-HPMA-d3*	1.49	222.8	90.9	-45	-16	-10

* The ion transitions is for quantitation.

Table S4. The MS source conditions

Ion source	ESI
Curtain Gas	20 arb
Collision Gas	9 arb
IonSpray voltage	4200V
Temperature	450 °C
IonSource Gas1	35 arb
IonSource Gas2	35 arb