Electronic supplementary information

Self-aspiration sampling design for rapid analysis of volatile organic compounds based on atmospheric pressure chemical ionization/photoionization combined ionization source mass spectrometry

Yuxin Wang^{a,b}, Hengyi Xu^c, Bo Sui^{a,b}, Hui Xi^b, Yingjie Fu^b, Wuduo Zhao^{a,d}, Peng Li^b, Shihao Sun^{a,b*}, Dingzhong Wang^{a,b*}

^aFlavor Science Research Center, College of Chemistry, Zhengzhou University, Zhengzhou, 450001, China.

^bKey Laboratory of Tobacco Flavor Basic Research of CNTC, Zhengzhou Tobacco Research Institute, Zhengzhou, 450001, China.

^cTechnology Center, China Tobacco Shenzhen Tobacco Industrial Co., Ltd., Guangdong, 518110, China.

^dCenter of Advanced Analysis and Gene Sequencing, Zhengzhou University, Zhengzhou, 450001, China.

*Corresponding author. E-mail address: sunsh@ztri.com.cn (Shihao Sun); wdz426@163.com (Dingzhong Wang)



Fig. S1 Photograpg of connection between injection vial and capillary inlet.



Fig. S2 Mass spectrum of 3-pentanone and cyclohexanone solution when use different types dopants. a) without dopant in methanol b) acetone as dopant in methanol c) anisole as dopant in methanol d) acetone as dopant.



Fig. S3 Photograph of electric spark between metal needle probe and cone.



Fig. S4 Mass spectrum of standard solution of acetone and cyclohexanone (1mg·mL⁻¹, acetone solution) in APCI/VUV and APCI mode.

	•		•	-	-
Compounds	Concentration	LODs	LOQs	R ²	Standard curve
	range (µg·m⁻³)	(ng∙m ⁻³)	(ng∙m⁻³)		
Toluene	0.5~50	7.5	25	0.9971	y=12.976x+671.86
Cyclohexanone	0.5~50	1.5	5	0.9936	y=48.462x+1080
Styrene	0.5~50	7.5	25	0.9900	y=14.157x+1136.4
Ethylbenzene	0.5~50	15	50	0.9985	y=34.581x+1340.6

Table S1 Detailed quantification results of four compounds by APCI/VUV-MS

Component	Standard curve R ²		Concentration (µg·mL⁻	
			¹)	
Toluene	y=12.976x+671.86	0.9971	85.17	
Ethylbenzen	y=34.581x+1340.6	0.9985	9.45	
е				

Table S2 Quantitative results of benzene series compounds in a spray paint