Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

High-sensitive detection of low-polar fluorene by ambient ionization mass spectrometry

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Experimental materials

The working solution for MS detection was prepared by further diluting the standard solution with methanol. Helium (purity ⩾ 99.99%) used as both the nebulization gas and discharge gas was purchased from Jinghua Industry Co. (Hangzhou, China). Glass tubes with different I.D. used as heated tubes were purchased from Tianbo Glass Instrument Co. Ltd (Tianjin, China). TSP capillary tubes with I.D. of 100 μm used for sprayer were purchased from Polymicro Technologies (Taiwan, China). Stainless steel capillary tubes (I.D. 0.51 mm) were bought from Thermo Scientific (US). All solutions were prepared on the day of use.

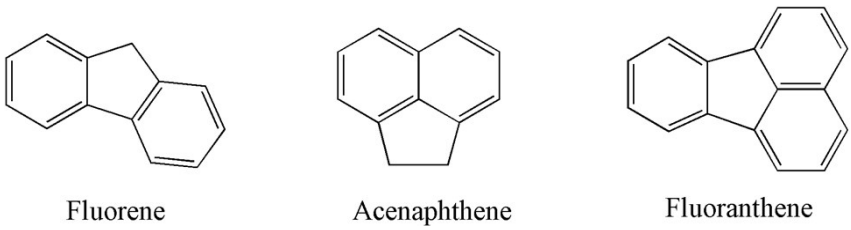

Figure S-1. Structure of fluorene, acenaphthene and fluoranthene.

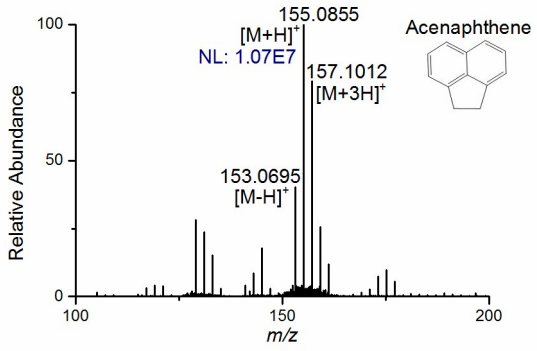

Figure S-2. Mass spectrum of acenaphthene (1.5 mg/ml) by N-DBDI method. The flow rate was 10 μL/min, the distance of two Cu electrodes was 25 mm, the i.d. of the glass tube was 1.9 mm, and the length of the glass tube was 32 cm.

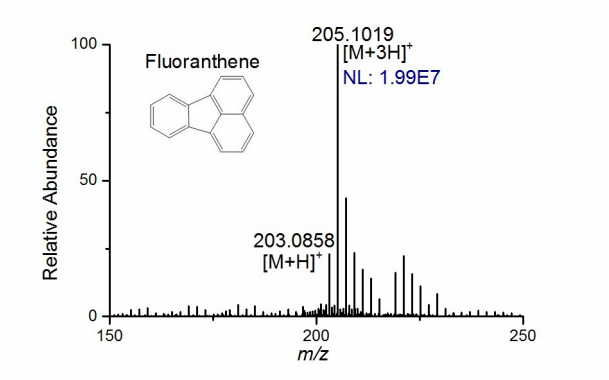

Figure S-3. Mass spectrum of fluoranthene (2 mg/mL) by N-DBDI method. The flow rate was 10 μL/min, the distance of two Cu electrodes was 25 mm, the i.d. of the glass tube was 1.9 mm, and the length of the glass tube was 32 cm.

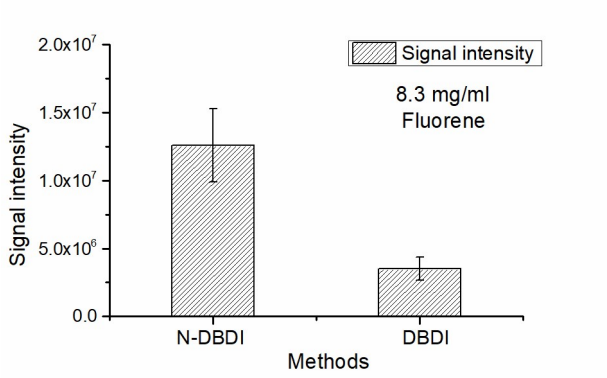

Figure S-4. Comparison of conventional DBDI and N-DBDI in analysis of fluorene, and the data represent the average of three measurements.

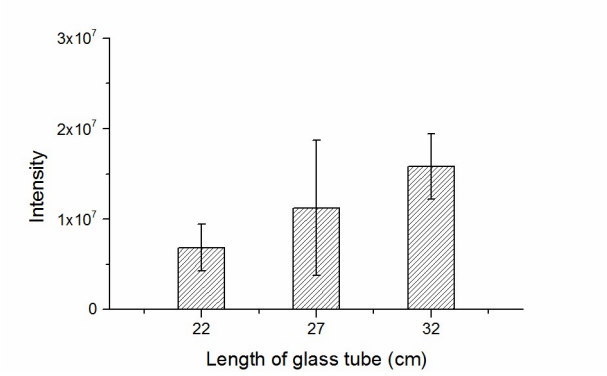

Figure S-5. The relationship between the length of glass tube and analytes signal intensity. Signal intensity acquired from fluorene (8.3 mg/mL) was used, and the data represent the

average of three measurements.

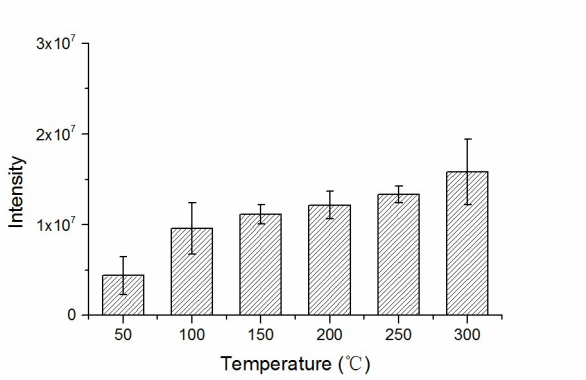

Figure S-6. The relationship between temperature and analytes signal intensity. Signal intensity acquired from fluorene (8.3 mg/mL) was used, and the data represent the average of three measurements.

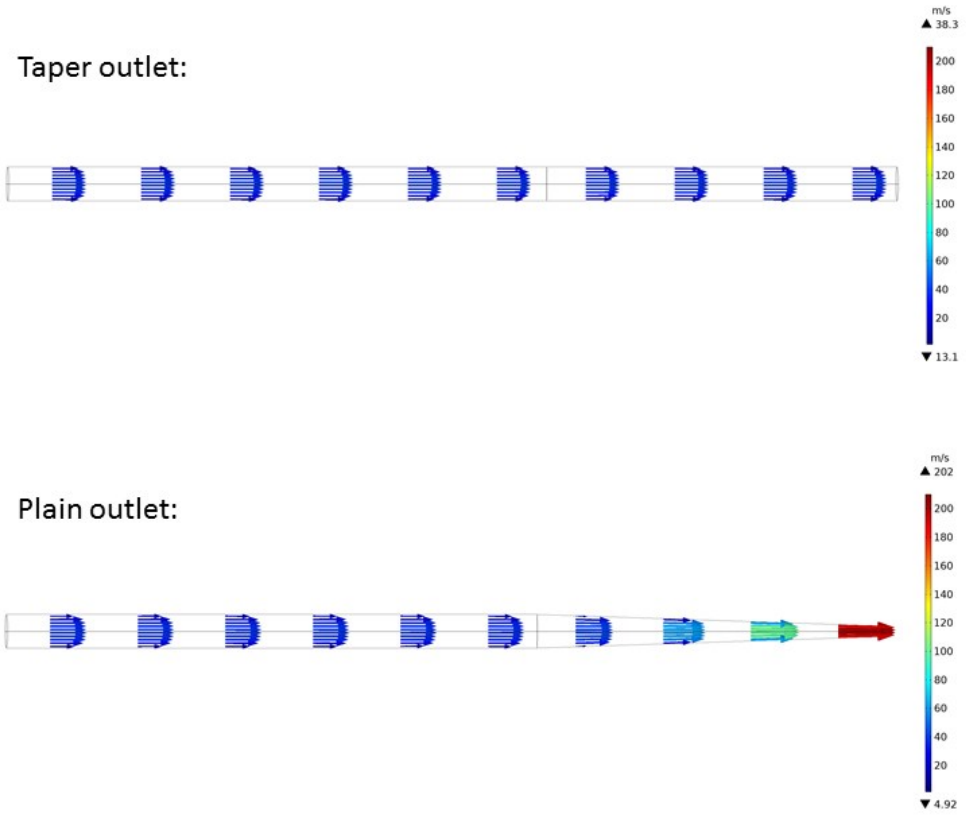

Figure S-7. Comparison of gas flow rate with taper and plain outlet. The images were obtained by COMSOL Multiphyscis 5.5.

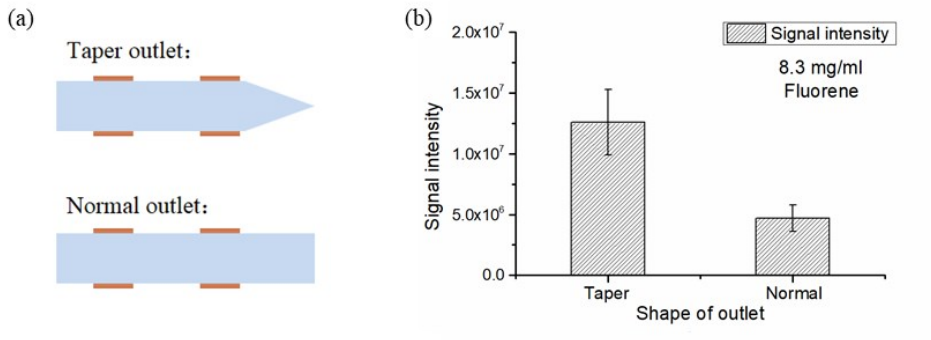

Figure S-8. Comparison of taper and plain outlet: (a) schematic; (b) signal intensities. Signal intensity acquired from fluorene (8.3 mg/mL) was used, and the data represent the average of three measurements.

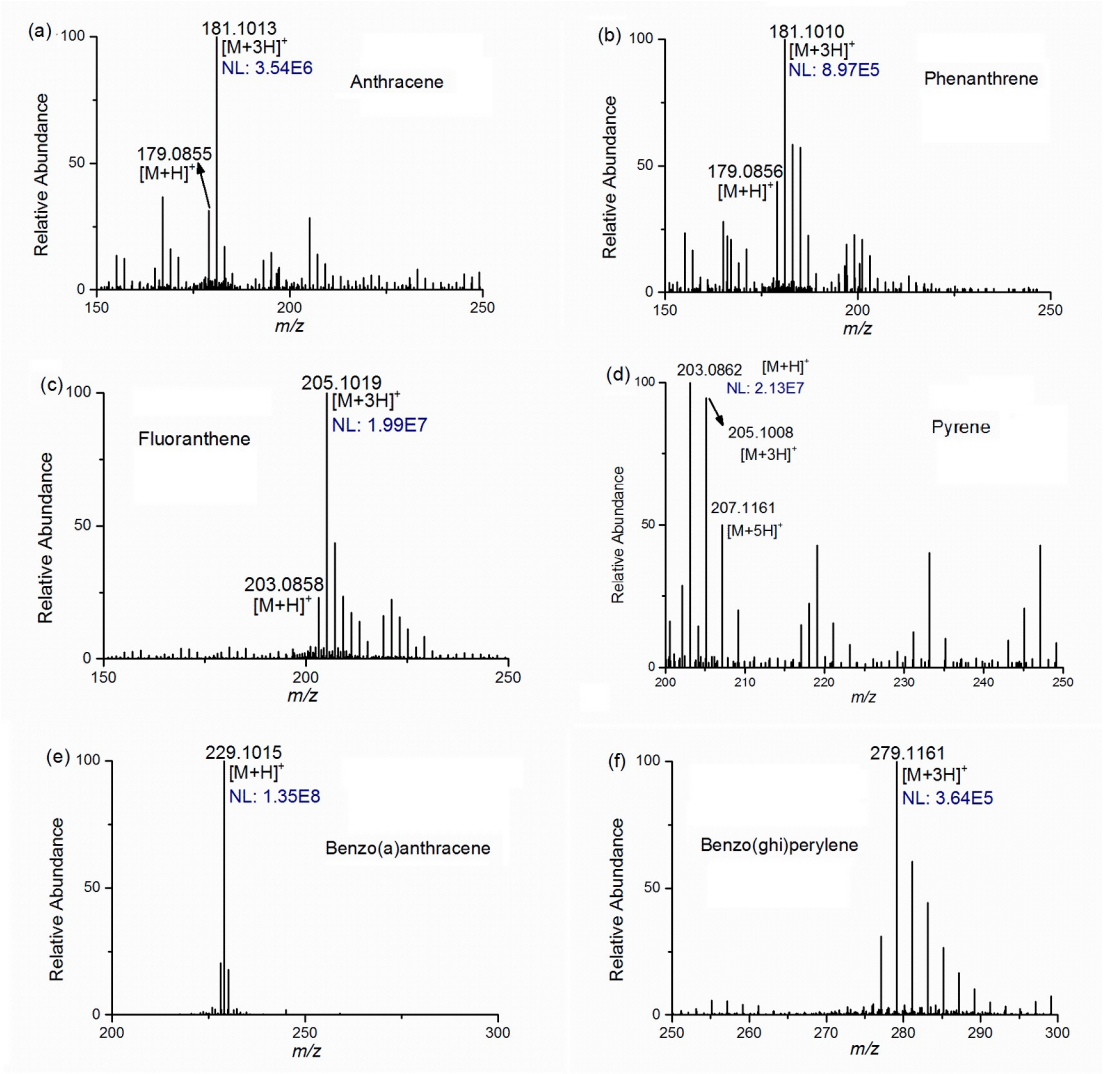

Figure S-9. Mass spectra of other PAHs by N-DBDI method: (a) anthracene, (b) phenanthrene, (c) fluoranthene, (d) pyrene, (e) benzo(a)anthracene, (f) benzo(ghi)perylene.

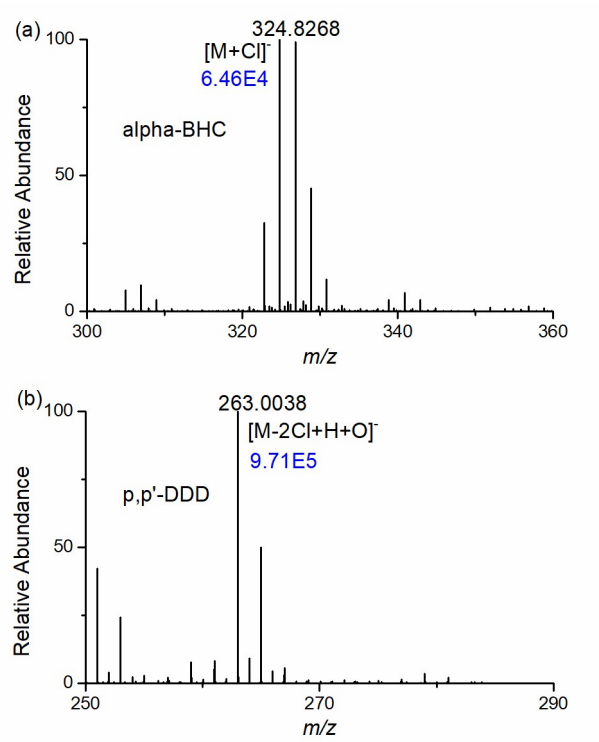

Figure S-10. Mass spectra of OCPs by N-DBDI method: (a) alpha-BHC and (b) p,p'-DDD.

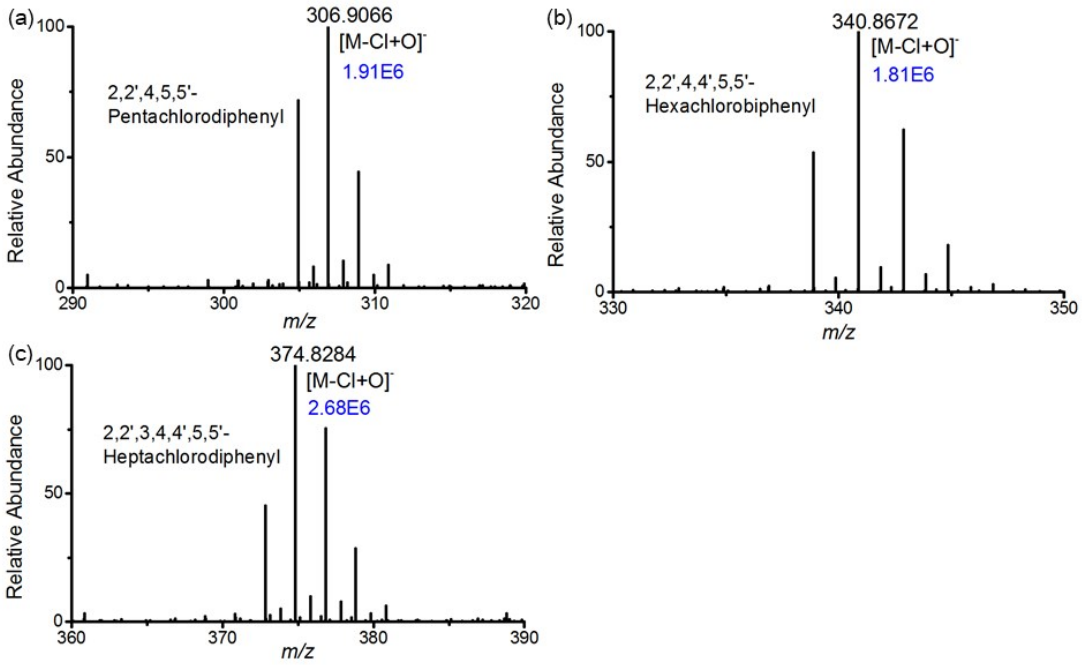

Figure S-11. Mass spectra of PCBs by N-DBDI method: (a) 2,2',4,5,5'-pentachlorobiphenyl, (b) 2,2',4,4',5,5'- hexachlorobiphenyl, (c) 2,2',3,4,4',5,5'-heptachlorobiphenyl.

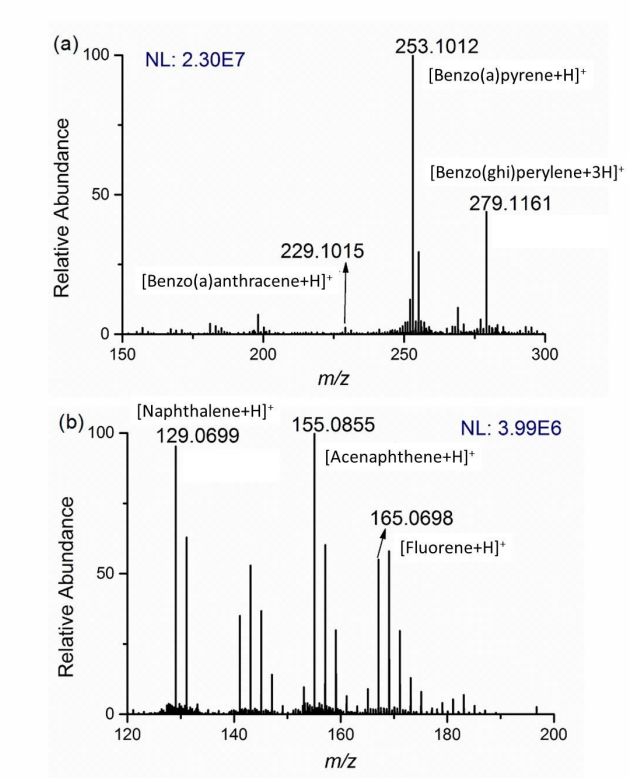

Figure S-12. Mass spectra of PAHs mixture by N-DBDI method: (a) the mixture of benzo(ghi)perylene, benzo(a)pyrene, and benzo(a)anthracene; (b) the mixture of naphthalene, acenaphthene, and fluorene.

Table S-1. POPs analyzed in the present work.

Name	Molecular formula	Molecular mass	Purity	Purchase
Acenaphthene	$C_{12}H_{10}$	154.21	> 98%	Sigma-Aldrich (Darmstadt, Germany)
Anthracene	$C_{14}H_{10}$	178.23	> 98%	J&K Scientific Co. (Beijing, China)
Phenanthrene	$C_{14}H_{10}$	178.23	> 98%	J&K Scientific Co. (Beijing, China)
Fluoranthene	$C_{16}H_{10}$	202.25	> 98%	J&K Scientific Co. (Beijing, China)
Pyrene	$C_{16}H_{10}$	202.25	> 98%	J&K Scientific Co. (Beijing, China)
Benzo(ghi)perylene	$C_{22}H_{12}$	276.33	> 98%	J&K Scientific Co. (Beijing, China)
Benzo(a)pyrene	$C_{20}H_{12}$	252.31	> 98%	J&K Scientific Co. (Beijing, China)
Benzo(a)anthracene	$C_{18}H_{12}$	228.29	> 98%	J&K Scientific Co. (Beijing, China)
2,4,4'-Trichlorobiphenyl	$C_{12}H_7Cl_3$	257.54	> 98%	J&K Scientific Co. (Beijing, China)
2,2',5,5'-Tetrachlorobiphenyl	$C_{12}H_6Cl_4$	291.99	> 98%	J&K Scientific Co. (Beijing, China)
2,2',4,5,5'-Pentachlorobiphenyl	$C_{12}H_5Cl_5$	326.43	> 98%	J&K Scientific Co. (Beijing, China)
2,2',4,4',5,5'-Hexachlorobiphenyl	$C_{12}H_4Cl_6$	360.88	> 98%	J&K Scientific Co. (Beijing, China)
2,2',3,4,4',5,5'-Heptachlorobipheny l	$C_{12}H_3Cl_7$	395.32	> 98%	J&K Scientific Co. (Beijing, China)
Gama-HCH	$C_6H_6Cl_6$	290.81	> 98%	J&K Scientific Co. (Beijing, China)
Alpha-BHC	$C_6H_6Cl_6$	290.81	> 98%	J&K Scientific Co. (Beijing, China)
p,p'-DDD	$C_{14}H_{10}Cl_4$	320.04	> 98%	J&K Scientific Co. (Beijing, China)

Table S-2. Accuracy and precision of N-DBDI (n=6).

Spiked (ng/L)	Found (ng/L)	Recovery (%)	RSD (%)
2.5	2.67±0.19	106.71	6.40
25	22.84±1.80	91.37	7.86
45	44.53±3.19	98.97	7.17