

Supplementary Data

Analysis of oxy-PAHs by Liquid Chromatography-Tandem Mass Spectrometry

9-fluorenone (FLO), 9,10-phenanthrenequinone (PQ), 9,10-anthraquinone (AQ), and benz[*a*]anthracene-7,12-dione (BAQ) were analyzed by liquid chromatography-tandem mass spectrometry (LC-MS/MS). LC-MS/MS analysis was performed using a Thermo Scientific TSQ Quantum Ultra Triple Quadrupole Mass Spectrometer (Thermo Fisher Scientific, Waltham, MA) with a Thermo Scientific Atmospheric Pressure Chemical Ionization (APCI) source, a Waters Acquity UPLC system (Waters Corporation, Milford, MA), and a Waters BEH C₁₈ UPLC Column (1.7 μ m, 2.1 mm \times 50 mm). AQ and PQ standards were purchased from Sigma Aldrich (St. Louis, MO). FLO and BAQ standards were purchased from Acros Organics (Morris Plains, NJ).

The column temperature was maintained at 35°C, and the sample injection volume was 10 μ L. The mobile phase consisted of deionized water and LC-MS-grade methanol. The

mobile phase was started at a flow rate of 0.294 mL/min with 30% methanol for 2.07 min followed by a linear increase to 75% methanol over 2.72 min and was held at 75% methanol for 2.95 min. Then, at a flow rate of 0.5 mL/min, the mobile phase was linearly increased to 100% methanol over 0.45 min and held at 100% methanol for 3.81 min. Finally, at a flow rate of 0.294 mL/min, the mobile phase was linearly decreased to 30% methanol over 0.20 min and held at 30% methanol for 2.8 min.

AQ and BAQ were quantified in APCI negative ionization mode using the molecular ions $m/z=208$ and $m/z=258$, respectively. PQ and FLO were quantified in APCI positive ionization mode using the precursor to fragment ion transition $m/z=209 > 152$ and $m/z=181 > 153$, respectively. Quantification of each compound was performed according to the corresponding standard curve. The method detection limit is 6.88 μ g/L for FLO, 1.69 μ g/L for PQ, 21.2 μ g/L for AQ, and 3.87 μ g/L for BAQ.