Published in final edited form as:

J Environ Sci Health B. 2014 ; 49(11): 828–835. doi:10.1080/03601234.2014.938552.

Determination of polycyclic aromatic hydrocarbons in roasted coffee

ANGELICA JIMENEZ, AFOLABI ADISA, CARA WOODHAM, and MAHMOUD SALEH

Department of Chemistry, Texas Southern University, Houston, Texas, USA

Abstract

Polycyclic aromatic hydrocarbons (PAHs) are suspected to be carcinogenic and mutagenic. This study describes the presence of PAHs in light, medium and dark roasted coffee including instant and decaffeinated brands. Total PAHs concentration was related to the degree of roasting with light roasted coffee showing the least and dark roasted coffee showing the highest level. Both instant and decaffeinated coffee brand showed lower levels of PAHs. Naphthalene, acenaphthylene, pyrene and chrysene were the most abundant individual isomers. The concentrations ranged from 0 to 561 ng g⁻¹ for naphthalene, 0 to 512 ng g⁻¹ for acenaphthylene, 60 to 459 ng g⁻¹ for pyrene and 56 to 371 ng g⁻¹ for chrysene. Thus, roasting conditions should be controlled to avoid the formation of PAHs due to their suspected carcinogenic and mutagenic properties.

Keywords

PAH; coffee; food contaminants; carcinogens; roasting; HPLC

Introduction

Roasting is a crucial step for the manufacture of coffee, as it enables the development of color, aroma and flavor, which are essential for the characterization of the coffee quality. Roasting time and temperature conditions of the roasting step must be optimized and controlled to achieve maximum aroma and flavor development. The roasting conditions differ depending on the coffee quality expected and the type of roaster used as light, medium or dark. Chemical reactions are known to be responsible for the development of aroma and flavor during the roasting step, at the same time, toxic compounds may be formed during the roasting process.^[1–3] The presence of polycyclic aromatic hydrocarbons (PAHs) in coffee samples has been reported and may be attributed to either contamination of the initial green beans or formation of these compounds during the roasting process.^[4–8]

According to the world health organization (WHO), PAHs are toxic compounds and suspected carcinogens or procarcinogens.^[9] They have been included in the USA Environmental Protection Agency (EPA) and the European Union (EU) on their priority pollutant lists. The presence of PAHs in environmental samples such as water, sediments and

Address correspondence to Mahmoud A. Saleh, Department of Chemistry, Texas Southern University, Houston, TX 77004, USA; saleh_ma@tsu.edu.

Color versions of one or more of the figures in this article can be found online at www.tandfonline.com/lesb.

particulate air has been extensively studied, but food samples have received less attention.^[10–15] PAHs have been found as contaminants in different food categories such as dairy products, vegetables, fruits, oils, coffee, tea, cereals and smoked meat, their presence originate mainly from processing and cooking.^[16–19] The present work was undertaken to identify and determine the concentration of PAHs in different types of roasted coffee from light, medium to dark as well as instant and decaffeinated coffee.

Materials and methods

Reagents and materials

HPLC acetonitrile and water were obtained from VWR International LLC (Sugar Land, TX, USA). PAH calibration mixtures were obtained from Restek Corporation (Bellefonte, PA, USA). Thirteen commercial coffee samples of different roasting grades (light, medium and dark) as well as instant and decaffeinated were purchased from local markets. Their brand names manufacture origins are: Dark Italian-Roast[®] (instant coffee), Dark Italian-Roast[®] (instant decaffeinated), Dark Komodo Dragon Blend[®], Dark Espresso Roast[®], Blonde Willow Blend[®], Blonde Veranda Blend[®], Medium Colombia[®], Medium Pike Place Roast[®], Dark Coffee Verona[®], Dark Caffè Verona[®] (Decaffeinated), Dark French Roast[®], Dark Italian Roast[®] and Dark Sumatra[®]. Each sample was given a code number according to their roasting type as shown in Table 1.

Extraction of PAHs

One gram of each sample was extracted with 15 mL of HPLC grade hexane for 2 h using rotor mixer. Extracts were then centrifuged and supernatants were cleaned up using silica gel cartridge and passing additional 7 mL hexane through the cartridge to complete PAHs elution. The collected hexane solution was taken to dryness using Centrifan[™] PE-Personal Evaporator (Sorbent Technologies, Inc., Norcross, GA, USA) and the residue obtained was dissolved in 1 mL acetonitrile, filtered using 0.2 µ syringe filter and transferred to HPLC vials for analysis. All extractions were performed in three replicates.

High-performance liquid chromatography (HPLC) analysis

HPLC analysis was developed and performed using an Agilent 1100 (Santa Clara, CA, USA) LC system consisting of quaternary pump, autosampler, thermostatted column compartment and fluorescence detector with standard FLD flow cell using Agilent software Chemstation B.04.03. Pinnacle[®] II PAH column (RESTEK, Restek Corporation 110 Benner Circle Bellefonte, PA, USA) 150 mm × 3.0 mm ID, Particle Size: 4 µm, Pore Size: 110 Å running at 30 °C, Mobile Phase was A: water, B: acetonitrile. Separation was carried out at a flow rate of 1 mL min⁻¹, starting at 45% B and increasing to 100% B at 12 min and kept at 100% B for 5 min before it recycled and equilibrated back to the original 45% B. Column was equilibrated for 5 min between samples. Samples were detected using multiple wavelength fluorescence at excitation wave lengths of 260 nm and emission at 350, 420 and 500 nm. Peaks identification was based on the standard peak's retention time. The HPLC elution profile of the PAH compounds analyzed in this investigation are shown in Figure 1. External standard method was used to determine PAH concentration in the samples.

Quality assurance and control (QA/QC)

Linearity and precision were determined by analysis of a dilution series of the standard PAH mixtures in acetonitrile, ranging from 1 ng mL⁻¹ to 20 ng mL⁻¹ of individual PAHs in six dilution steps. Blank and low spike samples were analyzed directly, limits of detection and quantification were evaluated from the concentration of PAHs required to give at least a signal to noise ratio of 3 and are shown in Table 2. The recoveries for all three spiked samples were greater than 80%. Linear regression was applied to construct a calibration curve reporting peak area versus PAH concentration. A calibration curve was made for every sequence of analysis and were found to have an R^2 higher than 0.99 as shown in Figure 2. Chemical structures of the 18 tested PAHs, their HPLC retention times and toxicity factor equivalent are shown in Table 3.

Results and discussion

The total concentration of the 18 PAHs compounds in the tested coffee samples were found to be associated with the degree of darkens in the roasted coffee being the highest in the dark roasted coffee and lower in the light or medium roasted coffee (Fig. 3). Instant coffee and decaffeinated coffees showed much lower concentration of PAHs. The sum of the concentration of the identified PAHs isomers ranged from 197 µg kg⁻¹ in instant coffee to 3 mg kg⁻¹ in dark roasted coffee. Fluorene, Pyrene, Chrysene and Benzo(k)fluoranthene were found in all of the tested samples, other PAHs isomers were found in some samples, but not the others. Concentration of the individual 18 tested PAHs for all samples are shown in Table 4.

Benzo(a)pyrene (B[a]P) is known to be the most toxic and the most carcinogenic compound, the carcinogenic potency of each collected sample was determined in terms of its B[a]P equivalent concentration (B[a]P eq). To calculate the B[a]P eq for each individual PAH species, the use of its toxic equivalent factor (TEF) is required for the given species relative to B[a]P carcinogenic potency. In this study, the list of TEFs reported by Nisbet and LaGoy^[20] are shown in Table 3. Concentrations of carcinogenic PAHs were calculated using the equation:

$$TEQ = \sum PAH_i \times TEF_i$$

where TEQ is the toxic equivalents of reference compound; PAH_i is concentration of PAH congener i ; TEF_i is toxic equivalent factor for PAH congener i .

Two brands of instant coffees were analyzed for their contents of the 18 selected PAHs isomers. Either caffeinated or decaffeinated instant coffee showed very low concentration of the total PAHs concentration or concentration of individual PAH isomers. Only fluorene, pyrene, chrysene and Benzo(k)fluoranthene were detected in the two samples with closely similar concentrations. TEQ values were 0.9 for instant coffee and 6.9 for the decaffeinated instant coffee.

One sample of espresso coffee was examined and was found to contain all of the tested 18 PAH isomers. Pyrene, chrysene, indeno(1,2,3-cd)pyrene and acenaphthylene were the most abundant isomers detected with a TEQ value of 22.3.

Three different brands of light roasted coffee were examined and total PAHs were found to be in the range of 333 to 740 $\mu\text{g kg}^{-1}$. Acenaphthylene, fluorene, pyrene, chrysene and Indeno(1,2,3-cd)pyrene were the most abundant components with a TEQ values of 4.7, 29.1 and 39.9, respectively, for the three tested light coffee blends.

Two brands of medium roasted coffee were examined and total PAHs contents were in the range of 510 to 1120 $\mu\text{g kg}^{-1}$. All isomers were detected except 2-methylnaphthalene and benzo(g,h,i)perylene. Naphthalene, 1-methylnaphthalene, acenaphthylene, fluorene, pyrene, chrysene, indeno(1,2,3-cd)pyrene and dibenz(a,h)anthracene were the most abundant PAHs isomers detected in the samples. Their TEQ values were 30.9 and 35.5.

Only one brand of dark blend decaffeinated coffee was analyzed and found to contain a total PAH of 999 $\mu\text{g kg}^{-1}$. All of the 18 isomers were detected in this sample with naphthalene, 1-methylnaphthalene, acenaphthylene, fluorene, pyrene, chrysene and indeno(1,2,3-cd)pyrene as the most abundant isomers with a TEQ value of 38.4.

Four different brands of dark roasted coffees were examined and total PAHs were found to be high in all of the examined brands with a total values reaching as high as 3 mg kg^{-1} . All isomers were detected in all of the samples with naphthalene, 1-methylnaphthalene, acenaphthylene, fluorene, pyrene, chrysene and indeno(1,2,3-cd) pyrene, Dibenz(a,h)anthracene, Benzo(k)fluoranthene as the most abundant PAH isomers. Their TEQ were 26.2, 62.0, 89.5 and 86.1, respectively.

Conclusion

Phenanthrene, fluoranthene and pyrene were the major PAHs in the coffee samples analyzed in this study, their contents increased during the roasting process under elevated temperatures. Of all PAH analyzed in this context, some of them, especially the slightly volatile ones (2 to 3 benzene rings), are not regarded as carcinogenic. Within the remaining PAHs, there are substantial differences of potency in the size of several orders of magnitude with benzo[a]pyrene and dibenz(a,h)anthracene being the most toxic/carcinogenic ones. Total PAH contents are dependent on the degree of darkens or time of roasting. Thus, roasting conditions should be controlled to avoid the formation of PAHs due to their suspected carcinogenic and mutagenic properties.

Acknowledgments

Funding

This research was performed with the financial support of the NASA CBER center at Texas Southern University.

References

1. Lantz I, Ternité R, Wilkens J, Hoenicke K, Guenther H, van der Stegen GHD. Studies on acrylamide levels in roasting, storage and brewing of coffee. *Mol Nutr Food Res*. 2006; 50:1039–1046. [PubMed: 17054100]
2. Murkovic M, Bornik MA. Formation of 5-hydroxymethyl-2-furfural (HMF) and 5-hydroxymethyl-2-furoic acid during roasting of coffee. *Mol Nutr Food Res*. 2007; 51:390–394. [PubMed: 17357981]
3. Maier HG. Carcinogenic compound content in coffee beans. *Cafe Cacao The*. 1991; 35:133–142.
4. Kruijf N, Schouten A, Van der Stegen GHD. Occurrence of benzo[a]pyrene in roasted coffee, instant coffee and coffee brew. *Cafe Cacao The*. 1987; 31:151–154.
5. Kruijf N, Schouten T, Van der Stegen GHD. Rapid determination of benzo[a]pyrene in roasted coffee and coffee brew by high-performance liquid chromatography with fluorescence detection. *J Agric Food Chem*. 1987; 35:545–549.
6. Kayali-Sayadi MN, Rubio-Barroso S, Cuesta-Jimenez MP, Polo-Diez LM. A new method for the determination of selected PAHs in coffee brew samples by HPLC with fluorimetric detection and solid-phase extraction. *J Liq Chromatogr Relat Technol*. 1999; 22:615–627.
7. Houessou JK, Benac C, Delteil C, Camel V. Investigation of sample treatment steps for the analysis of polycyclic aromatic hydrocarbons in ground coffee. *J Agric Food Chem*. 2006; 54:7413–7421. [PubMed: 17002402]
8. Badolato ESG, Martins MS, Aued-Pimentel S, Alaburda J, Kumagai EE, Baptista GG, Rosenthal A. Systematic study of benzo[a]pyrene in coffee samples. *J Braz Chem Soc*. 2006; 17:989–993.
9. WHO – World Health Organization. Summary and Conclusions of the Sixty-Fourth Meeting of the Joint FAO/WHO Expert Committee on Food Additives. World Health Organization; Geneva, Switzerland: 2005. p. 47Rome
10. Kayali-Sayadi MN, Rubio-Barroso S, Polo-Diez LM. Rapid PAH Determination in urban particulate air samples by HPLC with fluorometric detection and programmed excitation and emission wavelength Pairs. *J Chromatogr Sci*. 1995; 33(4):181–185.
11. Kayali-Sayadi MN, Rubio-Barroso S, Polo-Diez LM. Determination of PAHs in particulate air by Micellar liquid chromatography. *J Liq Chromatogr*. 1994; 17(17):3623–3640.
12. Kayali-Sayadi MN, Rubio-Barroso S, Beceiro-Roldan C, Polo-Diez LM. Rapid determination of PAHs in drinking water samples using solid-phase extraction and HPLC with programmed fluorescence detection. *J Liq Chromatogr Relat Technol*. 1996; 19(19):3135–3146.
13. Koester CJ, Clement RE. Analysis of drinking water for trace organics. *Crit Rev Anal Chem*. 1993; 24(4):263–316.
14. Eisert R, Levsen K. Solid-phase microextraction coupled to gas chromatography: A new method for the analysis of organics in water. *J Chromatogr*. 1996; 733(1–2):143–157.
15. Camargo MCR, Toledo MCF. Polycyclic aromatic hydrocarbons in Brazilian vegetables and fruits. *Food Control*. 2003; 14(1):49–53.
16. De Vos RH, Van Dokkum W, Schouten A, Jong-Berkhout P. Polycyclic aromatic hydrocarbons in Dutch total diet samples (1984–1986). *Food Chem Toxicol*. 1990; 28(4):263–268. [PubMed: 2358252]
17. Kazerouni N, Sinha R, Hsu CH, Greenberg A, Rothman N. Analysis of 200 food items for benzo[a]pyrene and estimation of its intake in an epidemiologic study. *Food Chem Toxicol*. 2001; 39(5):423–436. [PubMed: 11313108]
18. Lin D, Tu Y, Zhu L. Concentrations and health risk of polycyclic aromatic hydrocarbons in tea. *Food Chem Toxicol*. 2005; 43(1):41–48. [PubMed: 15582194]
19. Simko P. Determination of polycyclic aromatic hydrocarbons in smoked meat products and smoke flavouring food additives. *J Chromatogr B*. 2002; 770:3–18.
20. Nisbet C, LaGoy P. Toxic equivalency factors (TEFs) for polycyclic aromatic hydrocarbons (PAHs). *Regul Toxicol Pharm*. 1992; 16:290–300.

Fig. 1. HPLC chromatograms of calibrated solution of PAH monitored at fluorescent emission at 350 nm (signal 1), 420 nm (signal 2) and 500 nm (signal 3) produced by excitation at 260 nm. Retention times (minutes) are shown in Table 3.

Fig. 2.
Quantitative calibration curve for selected PAH standards.

Fig. 3.
Total PAHs concentration and standard deviations in the different brands of coffee.

Table 1

Coffee type, brand names and their code numbers.

Instant coffee			
Dark Italian-Roast®	Dark Italian-Roast® Decaffeinated		
A1	A2		
Espresso Coffee			
Dark Espresso Roast®			
B1			
Light Blend Coffee			
Dark Komodo Dragon Blend®	Blonde Willow Blend®	Blonde Veranda Blend®	
C1	C2	C3	
Medium Blend Coffee			
Medium Colombia®	Medium Pike Place Roast®		
D1	D2		
Dark Blend Coffee Decaffeinated			
Dark Caffè Verona® (Decaffeinated),			
E1			
Dark Blend Coffee			
Dark Coffee Verona®	Dark French Roast®	Dark Italian Roast®	Dark Sumatra®
F1	F2	F3	F4

Table 2

Limits of detection (LOD) and quantification (LOQ), linearity of each PAHs.

<i>PAH</i>	<i>LOD ($\mu\text{g Kg}^{-1}$)</i>	<i>LOQ ($\mu\text{g Kg}^{-1}$)</i>	<i>R²</i>	<i>Equation for calibration line</i>
Naphthalene	0.18	0.61	0.99965	Area = $0.1185 \times \text{Amount} - 0.0195$
1-Methylnaphthalene	0.14	0.47	0.99988	Area = $0.1185 \times \text{Amount} - 0.0195$
2-Methylnaphthalene	0.11	0.36	0.99195	Area = $0.1606 \times \text{Amount} + 0.0177$
Acenaphthylene	0.11	0.38	0.99876	Area = $0.1492 \times \text{Amount} + 0.0895$
Acenaphthene	0.11	0.37	0.99932	Area = $0.3332 \times \text{Amount} + 0.1612$
Fluorene	0.03	0.11	0.99546	Area = $0.0520 \times \text{Amount} + 0.9594$
Phenanthrene	0.01	0.03	0.99983	Area = $1.2824 \times \text{Amount} + 0.5322$
Anthracene	0.07	0.24	0.99970	Area = $0.1048 \times \text{Amount} + 0.0734$
Fluoranthene	0.07	0.24	0.99504	Area = $0.2085 \times \text{Amount} + 0.4726$
Pyrene	0.10	0.35	0.99410	Area = $0.0403 \times \text{Amount} + 0.4966$
Benz(a)anthracene	0.01	0.04	0.99907	Area = $0.7171 \times \text{Amount} + 0.5026$
Chrysene	0.21	0.71	0.99907	Area = $0.1565 \times \text{Amount} + 0.7083$
Benzo(b)fluoranthene	0.01	0.04	0.99971	Area = $0.3139 \times \text{Amount} + 0.1467$
Benzo(k)fluoranthene	0.01	0.04	0.99965	Area = $2.4442 \times \text{Amount} + 1.3522$
Benzo(a)pyrene	0.01	0.04	0.99968	Area = $2.0054 \times \text{Amount} + 1.2464$
Indeno(1,2,3-cd)pyrene	0.15	0.50	0.99440	Area = $0.0972 \times \text{Amount} + 0.1834$
Dibenz(a,h)anthracene	0.09	0.31	0.99697	Area = $0.2351 \times \text{Amount} + 0.3088$
Benzo(g,h,i)perylene	0.07	0.22	0.99974	Area = $0.1556 \times \text{Amount} + 0.0566$

Table 3

PAHs chemical structures, HPLC retention times and toxicity equivalent factor.

<i>PAHs Name</i>	<i>Retention time (min)</i>	<i>Toxicity Equivalent Factor</i>	<i>Structure</i>	<i>PAHs Name</i>	<i>Retention time (min)</i>	<i>Toxicity Equivalent Factor</i>	<i>Structure</i>
Naphthalene	5.72 min	0.001		Pyrene	10.97	0.001
1-Methylnaphthalene	7.21	0.001		Benz(a)anthracene	12.19	0.1
2-Methylnaphthalene	7.54	0.001		Chrysene	12.32	0.01
Acenaphthylene	7.82	0.001		Benzo(b)fluoranthene	13.21	0.1
Acenaphthene	8.21	0.001		Benzo(k)fluoranthene	13.65	0.1
Fluorene	9.00	0.001		Benzo(a)pyrene	13.97	1
Phenanthrene	9.66	0.001		Indeno(1,2,3-cd)pyrene	14.94	0.1
Anthracene	10.36	0.01		Dibenz(a,h)anthracene	15.28	1

<i>PAHs Name</i> <i>Retention time (min)</i> <i>Toxicity Equivalent Factor</i>	<i>Structure</i>	<i>PAHs Name</i> <i>Retention time (min)</i> <i>Toxicity Equivalent Factor</i>	<i>Structure</i>
Fluoranthene 10.76 0.001		Benzo(g,h,i)perylene 15.56 0.01

Table 4

PAHs concentration in the different types of coffee.

A.						
PAHs/Sample code #	Instant coffee		Espresso coffee		Light blend coffee	
	AI	A2	BI	CI	C2	C3
Naphthalene			22.8 ± 0.7		8.2 ± 1.0	13.4 ± 3.1
1-Methylnaphthalene			24.0 ± 4.6			
2-Methylnaphthalene			9.9 ± 5.3			28.2 ± 3.9
Acenaphthylene			34.7 ± 5.7		39.3 ± 13.8	55.5 ± 2.4
Acenaphthene			6.7 ± 0.7		6.8 ± 1.7	11.4 ± 3.8
Fluorene	11.7 ± 1.5	14.2 ± 0.9	21.2 ± 2.0	23.1 ± 1.1	24.4 ± 4.0	42.1 ± 16.4
Phenanthrene			2.3 ± 0.3		1.6 ± 0.7	4.0 ± 1.8
Anthracene			3.4 ± 1.2		1.7 ± 0.5	5.1 ± 1.5
Fluoranthene			9.5 ± 1.0		6.1 ± 0.7	10.2 ± 0.3
Pyrene	114.1 ± 18.3	125.5 ± 12.1	130.4 ± 23.0	189.5 ± 14.7	191.5 ± 12.0	274.5 ± 30.6
Benz(a) anthracene			3.7 ± 1.1	2.9 ± 0.1	2.9 ± 0.5	4.9 ± 1.6
Chrysene	69.9 ± 15.0	71.8 ± 0.6	56.5 ± 12.0	95.6 ± 3.8	126.1 ± 11.2	185.2 ± 29.3
Benzo(b)fluoranthene			1.3 ± 0.2		0.4 ± 0.2	1.2 ± 0.5
Benzo(k)fluoranthene	1.8 ± 0.6	1.4 ± 0.2	15.6 ± 2.9	18.1 ± 3.3	8.8 ± 1.6	10.8 ± 0.9
Benzo(a)pyrene		6.0 ± 0.5	3.4 ± 2.2	3.4 ± 0.1	1.4 ± 1.3	3.3 ± 1.1
Indeno(1,2,3-cd)pyrene			46.0 ± 28.4		51.2 ± 17.0	70.5 ± 3.9
Dibenz(a,h)anthracene			13.3 ± 2.5		21.4 ± 2.3	27.0 ± 9.0
Benzo(g,h,i)perylene			2.0 ± 0.8			1.8 ± 1.8
Total	197.4 ± 35.3	219.0 ± 14.1	406.6 ± 94.5	332.6 ± 22.9	491.8 ± 68.6	749.0 ± 112.0

B.						
PAHs/Sample code #	Medium blend coffee		Dark blend decaffeinated		Dark blend coffee	
	D1	D2	E1	F1	F2	F4
Naphthalene	27.9 ± 18.8	79.1 ± 18.8	101.7 ± 0.8	27.8 ± 5.2	269.2 ± 23.5	221.4 ± 37.8
1-Methylnaphthalene	28.1 ± 13.3	39.7 ± 22.7	97.6 ± 0.4	27.2 ± 5.6	177.0 ± 1.7	306.0 ± 6.6
2-Methylnaphthalene			7.2 ± 0.3	10.5 ± 1.0	55.4 ± 10.0	16.8 ± 1.9
						286.9 ± 1.5

B.

PAHs/Sample code #	Medium blend coffee		Dark blend decaffeinated		Dark blend coffee			
	D1	D2	E1	F1	F2	F3	F4	
Acenaphthylene	56.5 ± 26.3	155. ± 16.9	188.2 ± 0.4	44.6 ± 6.6	327.9 ± 16.2	398.7 ± 43.4	512.4 ± 10.9	
Acenaphthene	6.1 ± 4.3	17.3 ± 0.6	20.8 ± 0.1	7.4 ± 1.0	31.8 ± 2.2	29.4 ± 4.7	37.4 ± 0.4	
Fluorene	29.0 ± 10.6	75.5 ± 14.3	74.2 ± 1.1	25.3 ± 4.8	84.9 ± 5.4	85.9 ± 4.6	184.2 ± 24.3	
Phenanthrene	3.3 ± 1.1	5.6 ± 0.4	6.5 ± 1.1	2.6 ± 0.4	14.0 ± 1.6	13.8 ± 1.4	7.3 ± 0.7	
Anthracene	5.5 ± 1.5	9.0 ± 0.9	12.7 ± 2.1	2.8 ± 1.1	24.5 ± 2.3	28.3 ± 4.6	44.1 ± 5.5	
Fluoranthene	12.2 ± 3.8	21.7 ± 1.2	29.8 ± 0.4	9.2 ± 1.3	52.5 ± 3.9	58.9 ± 5.8	85.3 ± 6.3	
Pyrene	141.6 ± 28.7	352.8 ± 47.5	59.8 ± 5.3	156.1 ± 16.2	448.6 ± 42.5	388.7 ± 12.1	458.8 ± 27.6	
Benz(a) anthracene	5.2 ± 3.4	5.9 ± 0.8	5.3 ± 1.5	3.0 ± 0.6	9.1 ± 0.5	19.1 ± 0.5	12.0 ± 0.1	
Chrysene	84.0 ± 19.8	242. ± 64.0	258.6 ± 2.6	65.1 ± 6.5	309.4 ± 49.9	292.3 ± 35.8	371.2 ± 40.6	
Benzo(b)fluoranthene	1.0 ± 0.8	1.1 ± 0.4	1.8 ± 0.6	0.3 ± 0.1	2.6 ± 0.7	5.4 ± 1.1	10.5 ± 1.4	
Benzo(k)fluoranthene	15.6 ± 1.0	31.6 ± 7.0	7.1 ± 1.7	14.0 ± 2.9	42.5 ± 1.2	53.9 ± 10.4	36.1 ± 5.2	
Benzo(a)pyrene	4.9 ± 3.0	2.4 ± 3.6	13.7 ± 0.6	3.5 ± 0.0	11.0 ± 0.3	18.5 ± 5.5	9.5 ± 1.9	
Indeno (1,2,3-cd)pyrene	71.4 ± 32.3	57.1 ± 10.9	101.6 ± 2.5	26.4 ± 5.1	88.4 ± 10.1	212.0 ± 0.9	107.6 ± 7.3	
Dibenz(a,h)anthracene	17.0 ± 5.3	23.2 ± 2.6	10.4 ± 1.3	12.7 ± 2.1	36.0 ± 8.5	42.5 ± 22.6	57.4 ± 6.8	
Benzo(g,h,i)perylene			1.7 ± 0.0	2.8 ± 0.9	0.5 ± 0.8	5.3 ± 2.9	16.8 ± 2.1	
Total	509.5 ± 174.0	1120.0 ± 212.6	998.6 ± 22.8	441.3 ± 61.3	1985.3 ± 181.2	2197.1 ± 202.9	3091.1 ± 265.5	