Supplementary Information

Exposure biomarker profiles of polycyclic aromatic hydrocarbons based on a rat model using a versatile analytical framework

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Material list:

Table S1. Daily total exposure levels of individual parent polycyclic aromatic hydrocarbons (pPAHs) for adult females in Beijing in previous studies and exposure levels of rats in this study

Compounds	Abbreviation	Estimated exposure levels for adult females (ng/kg/day)	Exposure levels for rats (ng/day)			
			Control	Low[b]	Middle[c]	High[d]
Naphthalene	NAP	100 [a]	0	4000	40000	400000
Acenaphthylene	ANY	19.7	0	788	7880	78800
Acenaphthene	ACE	23	0	920	9200	92000
Fluorene	FLU	70	0	2800	28000	280000
Phenanthrene	PHE	129	0	5160	51600	516000
Anthracene	ANT	13.9	0	556	5560	55600
Fluoranthene	FLO	34	0	1360	13600	136000
Pyrene	PYR	33.4	0	1336	13360	133600
Benz(a)anthracene	BAA	5.86	0	234.4	2344	23440
Benzo(k)fluoranthene	BkF	4.15	0	166	1660	16600
Benzo(a)pyrene	BAP	3.8	0	152	1520	15200
Dibenz(a,h)anthracene	DahA	1.11	0	44.4	444	4440
Benzo(g,h,i)perylene	BghiP	2.28	0	91.2	912	9120

[a] There were no exposure levels of NAP in the reference, so it was estimated based on phenanthrene;

[b] Calculated by (estimated exposure levels for adult females/1000)*200*200;

[c] Calculated by (estimated exposure levels for adult females/1000)*200*2000;

[d] Calculated by (estimated exposure levels for adult females/1000)*200*20000;

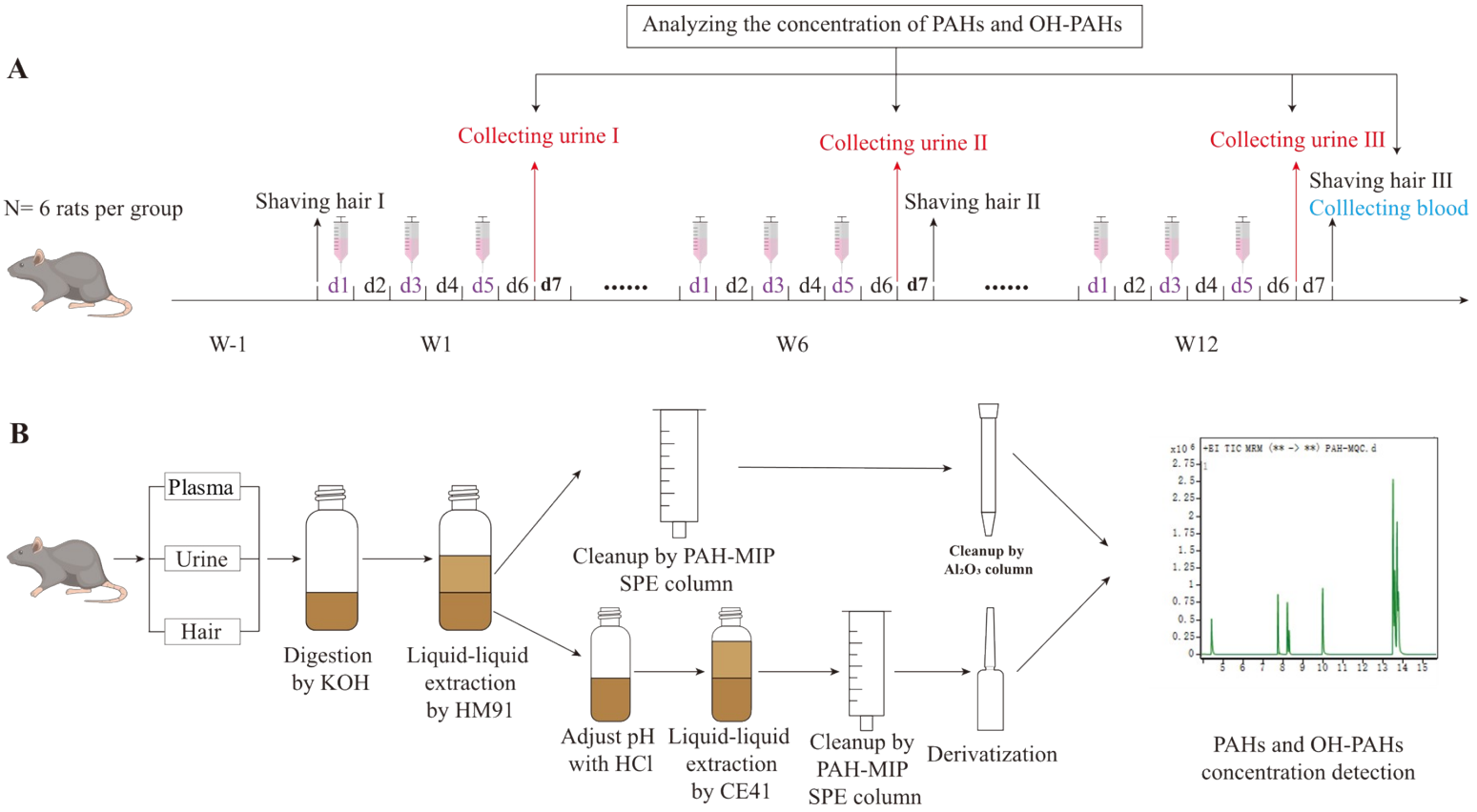

Fig. S1. Schematic diagram of the animal experiment with polycyclic aromatic hydrocarbon (PAHs) administration and flow chart of the experimental method for the detection of PAH exposure biomarkers. (A) "W" represents week; for example, "W-1" represents one week prior to the start of the experiment for adaptive feeding, while "W1", "W6", and "W12" represent the first, sixth and twelfth weeks with gavage, respectively. "d" represents day; for example, "d1" represents the first day in the week. (B) KOH (4 M) was used for plasma and urine samples, while KOH (2 M) was used for hair samples. The PAH-MIP SPE column represents PAH molecularly imprinted polymer solid-phase extraction columns (model: 500 mg). HM91 represents HEX:MTBE = 1:1 (*v*:*v*), and CE41 represents CYC:EA = 4:1 (*v*:*v*).

Table S2. The quantification-related information of pPAHs and OH-PAHs in the present study

Compound	Abbreviation	CAS No.	Precursor (m/z)	Product (m/z)	Collision Energy (V)	RT(min)[a]	Internal Standard
PAHs							
Naphthalene	NAP	91-20-3	128.0	102.0	40	4.422	ACE-D10
Acenaphthylene	ANY	208-96-8	152.0	152.0	30	7.743	ACE-D10
Acenaphthene	ACE	83-32-9	153.0	153.0	25	8.310	ACE-D10
Fluorene	FLU	86-73-7	166.0	165.1	40	9.985	ACE-D10
Phenanthrene	PHE	85-01-8	178.0	176.0	50	13.595	ANT-D10
Anthracene	ANT	120-12-7	178.0	176.0	50	13.778	ANT-D10
Fluoranthene	FLO	206-44-0	202.1	202.1	35	18.709	ANT-D10
Pyrene	PYR	129-00-0	202.1	202.1	30	19.612	CHR-D12
Benz(a)anthracene	BAA	56-55-3	228.0	226.0	50	25.173	CHR-D12
Benzo(k)fluoranthene	BKF	207-08-9	252.0	250.0	50	29.895	CHR-D12
Benzo(a)pyrene	BAP	50-32-8	252.0	250.0	50	30.985	CHR-D12
Dibenz(a,h)anthracene	DahA	53-70-3	278.0	276.0	50	35.227	CHR-D12
Benzo(g,h,i)perylene	BghiP	191-24-2	276.0	274.0	60	35.808	CHR-D12
Acenaphthene- D10	ACE-D10	15067-26-2	164.0	162.0	35	8.216	-
Anthracene- D10	ANT-D10	1719-06-8	188.1	188.1	30	13.709	-
Chrysene-D12	CHR-D12	1719-03-5	240.0	236.0	50	25.225 c	-
OH-PAHs [b]							
1-Hydroxynaphthalene	1-OH-NAP	90-15-3	216.1	201.1	10	14.481	1-OH-NAP-D7
2-Hydroxynaphthalene	2-OH-NAP	135-19-3	216.1	201.1	15	14.979	1-OH-NAP-D7
2-Hydroxyfluorene	2-OH-FLUO	2443-58-5	254.1	239.1	15	21.204	1-OH-NAP-D7
1-Hydroxyphenanthrene	1-OH-PHE	2433-56-9	266.1	251.1	20	23.498	1-OH-NAP-D7
2-Hydroxyphenanthrene	2-OH-PHE	605-55-0	266.1	251.1	20	24.014	1-OH-NAP-D7
3-Hydroxyphenanthrene	3-OH-PHE	605-87-8	266.1	251.1	20	23.377	1-OH-NAP-D7
4-Hydroxyphenanthrene	4-OH-PHE	7651-86-7	266.1	235.0	30	22.356	1-OH-NAP-D7

9-Hydroxyphenanthrene	9-OH-PHE	484-17-3	266.2	251.1	20	22.962	1-OH-NAP-D7
1-Hydroxypyrene	1-OH-PYR	5315-79-7	290.2	275.1	20	29.392	1-OH-NAP-D7
1-Hydroxynaphthalene-D7	1-OH-NAP-D7	124251-84-9	222.2	207.1	15	14.431	-
1-Hydroxypyrene-D9	1-OH-PYR-D9	132603-37-3	299.0	284.1	20	29.346	-

[a] RT, retention time;

[b] The precursor (m/z), product (m/z), collision energy and RT of OH-PAHs referred to compounds after derivatization by BSTFA-TMCS;

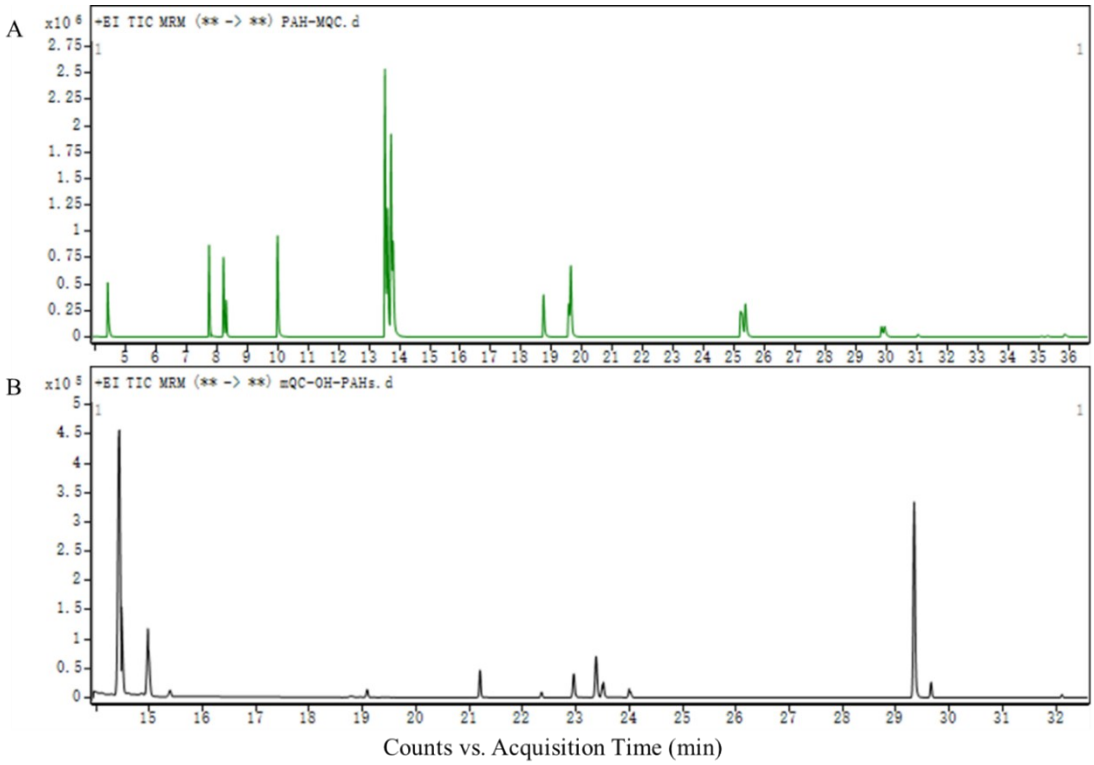

Fig. S2. Chromatographic peaks of targeted pPAHs, OH-PAHs and internal standards. (A) Chromatographic peaks of targeted pPAHs and internal standards (0.067 ppm, each). (B) Chromatographic peaks of targeted OH-PAHs and internal standards (0.007 ppm, each).

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Table S3. The limit of detection, limit of quantification and quantitative linear R^2 for parent polycyclic aromatic hydrocarbons (pPAHs) and hydroxyl polycyclic aromatic hydrocarbons (OH-PAHs) in three samples

Compounds	Plasma and urine (ng/mL)		Hair (ng/g)		R^2
	LOD[a]	LOQ[b]	LOD[a]	LOQ[b]	
PAHs					
ANY	0.009	0.031	0.073	0.244	0.9996
ACE	0.005	0.015	0.037	0.122	0.9999
FLU	0.037	0.122	0.293	0.977	0.9967
PHE	0.037	0.122	0.293	0.977	0.9947
ANT	0.037	0.122	0.293	0.977	0.9869
FLO	0.073	0.244	0.587	1.953	0.9884
PYR	0.073	0.244	0.587	1.953	0.9989
BAA	0.009	0.031	0.073	0.244	0.9979
BKF	0.037	0.122	0.293	0.977	0.9906
BAP	0.037	0.122	0.293	0.977	0.9811
DahA	0.018	0.061	0.147	0.488	0.9724
BghiP	0.018	0.061	0.147	0.488	0.9816
OH-PAHs					
1-OH-NAP	0.015	0.049	0.117	0.391	0.9994
2-OH-NAP	0.007	0.024	0.059	0.195	0.9992
2-OH-FLUO	0.007	0.024	0.059	0.195	0.9998
1-OH-PHE	0.007	0.024	0.059	0.195	0.9965
2-OH-PHE	0.007	0.024	0.059	0.195	0.9996
3-OH-PHE	0.002	0.006	0.015	0.049	0.9999
4-OH-PHE	0.015	0.049	0.117	0.391	0.9986
9-OH-PHE	0.007	0.024	0.059	0.195	0.9993
1-OH-PYR	0.015	0.049	0.117	0.391	0.9993

[a] LOD: limit of detection; [b] LOQ: limit of quantification;

Recoveries of the matrix-spiked method in this study were calculated as follows: (measured compound concentration in matrix spiked with respect standard – measured compound concentration in matrix without standard)/the spiked compound concentration × 100%. 10ng pPAHs and 1ng OH-PAHs standard were added to each sample. Matrix spiked recoveries in three types of samples by enzymatic hydrolysis and alkali solution hydrolysis are presented in **Fig. S3**. For OH-PAHs in plasma, the recoveries of alkaline hydrolysis were apparently higher than those of enzymatic hydrolysis, especially 1-OH-NAP (70.7% *vs*. 26.6%), 2-OH-NAP (91.1 *vs*. 59.0%), 9-OH-PHE (77.6% *vs*. 20.2%), and 1-OH-PYR (71.8% *vs*. 12.3%). For pPAHs in plasma and urine, and OH-PAHs in urine, the recoveries of the two methods were both relatively close. For hair sample, inorganic alkaline hydrolysis has been widely used previously, which can bring satisfactory recovery for OH-PAHs[1,2]. Therefore, we only illustrate the matrix spiked recovery of alkaline solution hydrolysis. The recoveries of pPAHs and OH-PAHs were stable.

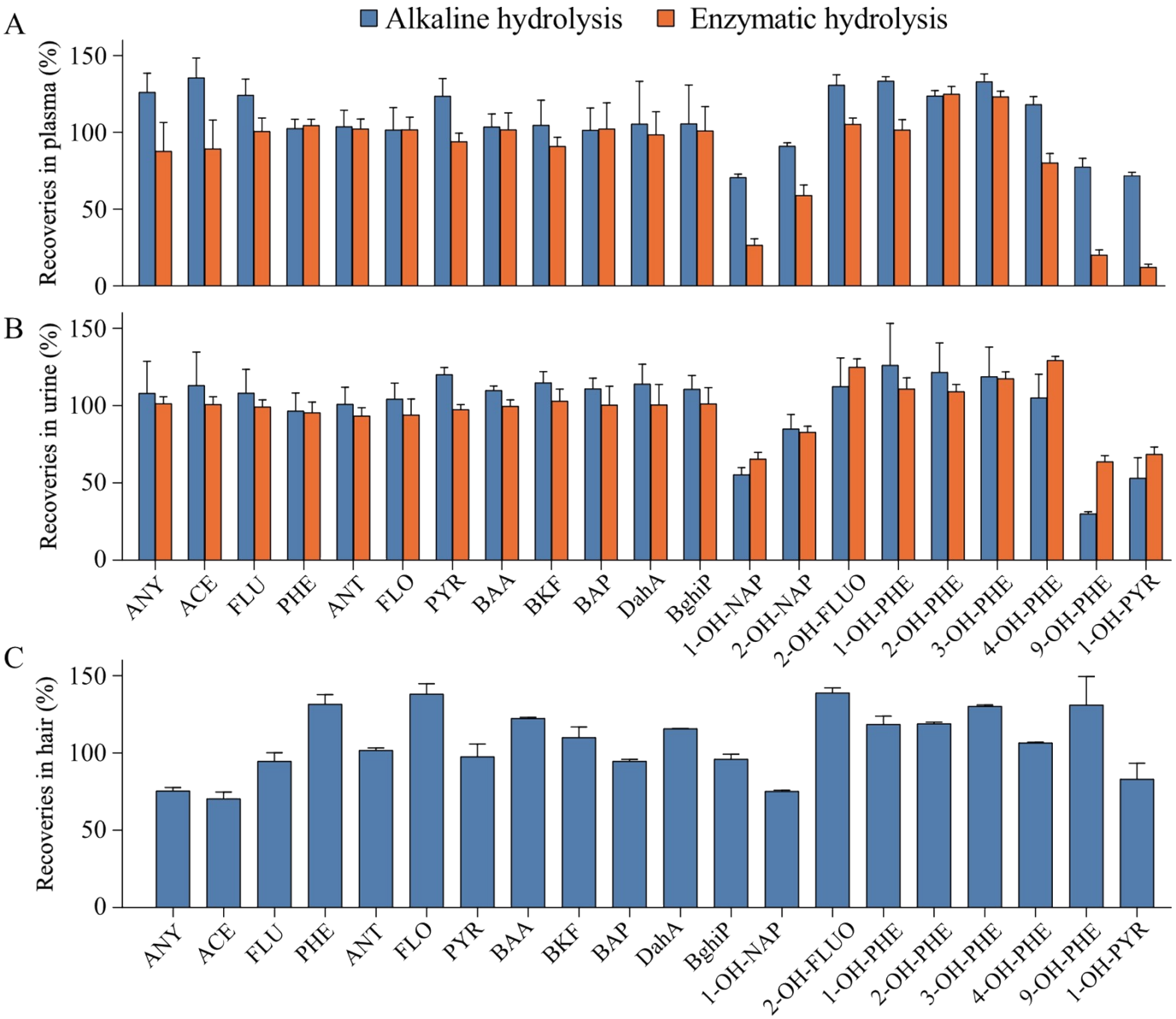

Fig. S3. Matrix spiked recoveries of the detection method in this study using the samples of plasma, urine, and hair. (A) Matrix spiked recoveries in plasma, (B) Matrix spiked recoveries in urine, and (C) Matrix spiked recoveries in hair.

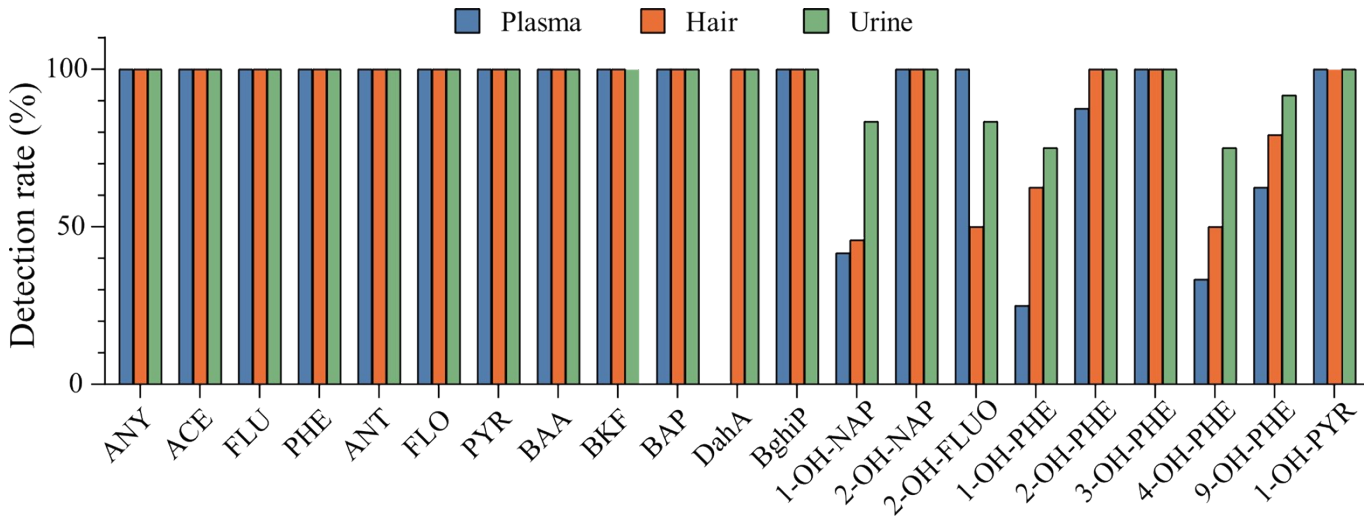

Fig. S4. Detection rates of parent polycyclic aromatic hydrocarbons (pPAHs) and hydroxylated polycyclic aromatic hydrocarbons (OH-PAHs) in plasma, hair, and urine of rats with pPAH exposure.

Table S4. Detection rates of parent polycyclic aromatic hydrocarbons (pPAHs) and hydroxyl polycyclic aromatic hydrocarbons (OH-PAHs) in rat plasma, hair and urine [a]

	Plasma				Hair				Urine			
	Control	Low	Middle	High	Control	Low	Middle	High	Control	Low	Middle	High
PAHs												
ANY	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
ACE	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
FLU	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
PHE	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
ANT	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
FLO	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
PYR	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
BAA	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
BKF	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
BAP	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
DahA	0 (0)	0 (0)	0 (0)	0 (0)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
BghiP	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
OH-PAHs												
1-OH-NAP	0 (0)	2 (33.3)	2 (33.3)	6 (100)	0 (0)	0 (0)	5 (83.3)	6 (100)	1 (33.3)	3 (100)	3 (100)	3 (100)
2-OH-NAP	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
2-OH-FLUO	6 (100)	6 (100)	6 (100)	6 (100)	4 (66.7)	0 (0)	2 (33.3)	6 (100)	2 (66.7)	2 (66.7)	3 (100)	3 (100)
4-OH-PHE	0 (0)	0 (0)	2 (33.3)	6 (100)	0 (0)	0 (0)	6 (100)	6 (100)	0 (0)	3 (100)	3 (100)	3 (100)
9-OH-PHE	1 (16.7)	2 (33.3)	6 (100)	6 (100)	3 (0.5)	4 (66.7)	6 (100)	6 (100)	2 (66.7)	3 (100)	3 (100)	3 (100)
3-OH-PHE	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
1-OH-PHE	0 (0)	0 (0)	0 (0)	6 (100)	2 (33.3)	1 (16.7)	6 (100)	6 (100)	0 (0)	3 (100)	3 (100)	3 (100)
2-OH-PHE	4 (66.7)	5 (83.3)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)
1-OH-PYR	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	6 (100)	3 (100)	3 (100)	3 (100)	3 (100)

[a] [*N(%)*];

Table S5. Linear trend test of hydroxyl polycyclic aromatic hydrocarbons (OH-PAHs) concentrations in rat urine with exposure times in the same exposure group

Compounds	Control		Low		Middle		High	
	t	P_{-trend}	*t*	P_{-trend}	*t*	P_{-trend}	*t*	P_{-trend}
1-OH-NAP	0.283	0.825	0.149	0.906	2.296	0.261	0.229	0.857
2-OH-NAP	5.208	0.121	2.086	0.285	2.378	0.253	3.928	0.159
2-OH-FLUO	0	1	0	1	330.7	0.002	2.314	0.260
1-OH-PHE	1.436	0.387	0.357	0.782	2.836	0.216	45.216	0.014
2-OH-PHE	2.464	0.245	-1.355	0.405	12.97	0.049	-0.146	0.908
3-OH-PHE	0.129	0.919	0.759	0.587	8.821	0.072	4.593	0.136
4-OH-PHE	1.436	0.387	1.868	0.313	2.146	0.278	2.041	0.290
9-OH-PHE	-0.012	0.992	-0.155	0.902	-0.002	0.986	-0.192	0.879
1-OH-PYR	-9.856	0.064	-0.107	0.932	0.203	0.873	-0.379	0.769

Table S6. Correlation between target compound concentrations measured in plasma and hair [a]

	ANY	ACE	FLU	PHE	ANT	FLO	PYR	BAA	BKF	BAP	BghiP	1-OH-NAP	2-OH-NAP	2-OH-FLUO	1-OH-PHE	2-OH-PHE	3-OH-PHE	4-OH-PHE	9-OH-PHE	1-OH-PYR
r [b]																				
ANY	0.24	0.20	0.07	0.11	0.23	0.14	-0.24	0.14	-0.07	0.06	-0.01	0.14	-0.23	0.14	0.22	0.20	0.22	0.22	0.20	0.28
ACE	0.31	0.23	0.05	0.10	0.17	0.06	-0.17	0.10	-0.13	-0.05	-0.08	-0.06	-0.26	-0.07	-0.05	-0.04	-0.01	-0.02	-0.07	0.06
FLU	0.30	0.16	<0.01	0.06	0.01	0.03	-0.11	0.09	<0.01	0.06	0.12	-0.08	-0.16	-0.10	-0.05	-0.06	-0.01	-0.02	-0.08	0.12
PHE	0.34	0.27	0.13	0.25	0.27	0.23	-0.04	0.35	0.14	0.20	0.09	0.26	-0.09	0.26	0.29	0.28	0.35	0.34	0.25	0.36
ANT	0.31	0.24	0.01	0.03	0.15	0.04	-0.20	0.06	-0.18	-0.06	-0.06	-0.11	-0.20	-0.12	-0.06	-0.07	<0.01	-0.03	-0.08	0.03
FLO	0.25	0.20	0.12	0.16	0.17	0.10	-0.16	0.06	-0.09	0.01	-0.01	-0.14	-0.19	-0.15	-0.06	-0.10	-0.07	-0.08	-0.09	0.12
PYR	0.44	0.31	0.08	0.25	0.42	0.26	-0.12	0.21	-0.01	0.09	0.14	<0.01	-0.20	0.01	0.09	0.04	0.13	0.10	0.05	0.15
BAA	0.27	0.21	0.07	0.11	0.20	0.09	-0.18	0.06	-0.13	-0.04	-0.06	-0.12	-0.20	-0.13	-0.03	-0.07	-0.04	-0.05	-0.07	0.13
BKF	0.28	0.21	0.08	0.15	0.23	0.12	-0.15	0.07	-0.11	-0.03	-0.06	-0.11	-0.20	-0.11	-0.02	-0.07	-0.04	-0.05	-0.06	0.15
BAP	0.26	0.20	0.06	0.12	0.21	0.11	-0.15	0.08	-0.10	-0.02	-0.07	-0.09	-0.19	-0.09	<0.01	-0.04	-0.02	-0.02	-0.04	0.16
BghiP	0.28	0.22	0.08	0.14	0.22	0.12	-0.15	0.08	-0.11	-0.03	-0.07	-0.11	-0.20	-0.10	-0.02	-0.06	-0.04	-0.04	-0.06	0.14
1-OH-NAP	0.14	0.08	0.13	0.30	0.13	0.32	<0.01	0.29	0.40	0.62	0.54	0.62	0.30	0.60	0.58	0.56	0.65	0.65	0.64	0.41
2-OH-NAP	0.04	0.02	-0.20	-0.22	-0.08	-0.16	-0.09	-0.16	-0.02	-0.03	-0.06	-0.14	0.20	-0.15	-0.17	-0.14	-0.16	-0.16	-0.15	-0.16
2-OH-FLUO	-0.01	0.02	0.12	0.32	0.21	0.52	0.20	0.66	0.57	0.57	0.41	0.67	0.63	0.69	0.74	0.64	0.68	0.70	0.68	0.53
1-OH-PHE	0.04	0.05	0.05	0.17	0.09	0.33	0.05	0.43	0.46	0. 60	0.42	0.84	0.19	0.84	0.92	0.87	0.95	0.94	0.88	0.73
2-OH-PHE	-0.01	0.04	0.10	0.22	0.13	0.39	0.11	0.43	0.47	0.53	0.33	0.73	0.11	0.73	0.89	0.78	0.87	0.87	0.79	0.86
3-OH-	0.06	0.02	-0.04	0.06	0.07	0.25	-0.07	0.32	0.36	0.47	0.29	0.56	0.19	0.55	0.71	0.62	0.69	0.68	0.63	0.66

PHE																			
4-OH-PHE	0.03	0.07	0.11	0.21	0.11	0.37	0.11	0.45	0.50	0.58	0.38	0.80	0.21	0.81	0.92	0.83	0.93	0.92	0.85	0.79
9-OH-PHE	0.01	<0.01	0.07	0.21	0.12	0.40	0.13	0.56	0.50	0.59	0.42	0.89	0.28	0.90	0.93	0.90	0.95	0.95	0.90	0.63
1-OH-PYR	-0.10	-0.08	0.12	0.07	-0.16	-0.17	0.25	-0.21	-0.12	-0.24	-0.18	-0.11	-0.04	-0.08	-0.18	-0.13	-0.22	-0.20	-0.14	-0.10
P [c]																				
ANY	0.27	0.35	0.76	0.61	0.28	0.53	0.27	0.52	0.74	0.79	0.95	0.51	0.27	0.53	0.30	0.35	0.31	0.31	0.36	0.19
ACE	0.18	0.28	0.82	0.66	0.42	0.79	0.44	0.63	0.54	0.81	0.72	0.77	0.21	0.75	0.80	0.87	0.98	0.93	0.76	0.80
FLU	0.15	0.45	0.98	0.77	0.96	0.88	0.62	0.66	0.98	0.79	0.56	0.71	0.46	0.64	0.82	0.80	0.98	0.92	0.73	0.58
PHE	0.11	0.20	0.54	0.24	0.21	0.28	0.85	0.10	0.51	0.36	0.69	0.22	0.66	0.22	0.17	0.19	0.10	0.11	0.25	0.09
ANT	0.14	0.26	0.97	0.90	0.47	0.87	0.36	0.77	0.39	0.80	0.80	0.62	0.34	0.58	0.78	0.74	0.97	0.90	0.71	0.89
FLO	0.25	0.35	0.56	0.53	0.43	0.64	0.46	0.79	0.69	0.96	0.96	0.50	0.36	0.48	0.78	0.65	0.74	0.72	0.68	0.58
PYR	0.03	0.15	0.70	0.24	0.04	0.22	0.59	0.34	0.96	0.69	0.50	0.98	0.35	0.95	0.69	0.85	0.55	0.66	0.83	0.49
BAA	0.21	0.33	0.77	0.60	0.36	0.66	0.41	0.80	0.54	0.87	0.78	0.56	0.35	0.56	0.88	0.73	0.86	0.82	0.75	0.53
BKF	0.19	0.32	0.701	0.49	0.28	0.58	0.49	0.75	0.60	0.89	0.78	0.60	0.36	0.60	0.91	0.75	0.85	0.82	0.78	0.48
BAP	0.22	0.36	0.80	0.59	0.33	0.60	0.48	0.703	0.64	0.92	0.74	0.68	0.38	0.69	>0.99	0.85	0.94	0.92	0.87	0.44
BghiP	0.19	0.31	0.73	0.52	0.29	0.57	0.50	0.71	0.61	0.89	0.74	0.62	0.36	0.63	0.92	0.78	0.86	0.84	0.80	0.51
1-OH-NAP	0.53	0.71	0.53	0.16	0.55	0.13	0.99	0.16	0.06	<0.01	<0.01	<0.01	0.15	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.05
2-OH-NAP	0.84	0.94	0.34	0.29	0.71	0.45	0.68	0.45	0.94	0.90	0.78	0.52	0.34	0.48	0.44	0.51	0.47	0.46	0.48	0.46
2-OH-FLUO	0.96	0.94	0.59	0.13	0.33	<0.01	0.36	<0.01	<0.01	<0.01	0.05	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
1-OH-PHE	0.86	0.82	0.81	0.42	0.68	0.12	0.83	0.04	0.02	<0.01	0.04	<0.01	0.38	<0.01	<0.01	<0.01	<0.01	<0.0	<0.01	<0.01

2-OH-PHE	0.95	0.87	0.65	0.30	0.56	0.06	0.61	0.03	0.02	<0.01	0.12	<0.01	0.60	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
3-OH-PHE	0.77	0.94	0.84	0.79	0.73	0.23	0.74	0.13	0.08	0.02	0.17	<0.01	0.37	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
4-OH-PHE	0.88	0.74	0.62	0.32	0.61	0.08	0.62	0.03	0.01	<0.01	0.06	<0.01	0.31	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
9-OH-PHE	0.96	>0.99	0.75	0.32	0.59	0.06	0.56	<0.01	0.01	<0.01	0.04	<0.01	0.18	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
1-OH-PYR	0.65	0.70	0.57	0.75	0.53	0.43	0.25	0.34	0.58	0.27	0.40	0.61	0.84	0.72	0.41	0.53	0.31	0.35	0.51	0.64

Rows in the table represent compounds in plasma, while columns represent compounds in hair;

[a] The results were calculated by Pearson correlation test; [b] Correlation coefficients; [c] *P* values for Pearson correlation test;

Table S7. Correlation between target compound concentrations measured in plasma and urine [a]

	ANY	ACE	FLU	PHE	ANT	FLO	PYR	BAA	BKF	BAP	DahA	BghiP	1-OH-NAP	2-OH-NAP	2-OH-FLUO	1-OH-PHE	2-OH-PHE	3-OH-PHE	4-OH-PHE	9-OH-PHE	1-OH-PYR
r [b]																					
ANY	0.61	0.44	0.25	0.19	0.55	0.20	-0.60	-0.60	-0.29	0.68	0.68	-0.47	0.75	0.77	0.80	0.76	0.78	0.79	0.79	0.78	0.74
ACE	0.89	0.16	-0.56	-0.74	-0.37	-0.39	-0.54	-0.54	0.02	0.98	0.98	-0.29	-0.15	-0.14	-0.10	-0.15	-0.12	-0.11	-0.12	-0.12	-0.19
FLU	0.87	0.41	-0.43	-0.86	-0.74	-0.11	0.04	0.04	0.58	0.80	0.76	0.40	-0.52	-0.49	-0.42	-0.52	-0.47	-0.45	-0.46	-0.49	-0.49
PHE	0.67	0.55	0.30	0.16	0.50	0.28	-0.51	-0.51	-0.17	0.68	0.70	-0.36	0.72	0.74	0.78	0.72	0.75	0.76	0.76	0.74	0.72
ANT	0.95	0.32	-0.42	-0.67	-0.32	-0.24	-0.47	-0.47	0.12	>0.99	0.99	-0.12	-0.08	-0.05	-0.01	-0.07	-0.04	-0.02	-0.03	-0.04	-0.10
FLO	0.66	-0.20	-0.82	-0.82	-0.45	-0.70	-0.64	-0.64	-0.16	0.83	0.85	-0.33	-0.32	-0.32	-0.31	-0.32	-0.32	-0.32	-0.32	-0.30	-0.40
PYR	0.68	0.27	-0.04	-0.05	0.39	-0.07	-0.75	-0.75	-0.37	0.79	0.83	-0.57	0.59	0.60	0.62	0.59	0.60	0.61	0.61	0.61	0.54
BAA	0.72	-0.12	-0.72	-0.72	-0.30	-0.62	-0.72	-0.72	-0.22	0.89	0.91	-0.42	-0.15	-0.15	-0.13	-0.17	-0.14	-0.14	-0.14	-0.13	-0.23
BKF	0.78	-0.03	-0.67	-0.73	-0.32	-0.55	-0.67	-0.67	-0.15	0.92	0.94	-0.35	-0.15	-0.14	-0.12	-0.17	-0.14	-0.13	-0.13	-0.13	-0.22
BAP	0.80	0.02	-0.61	-0.66	-0.24	-0.50	-0.70	-0.70	-0.17	0.94	0.96	-0.38	-0.06	-0.05	-0.03	-0.06	-0.04	-0.04	-0.04	-0.03	-0.12
BghiP	0.76	-0.06	-0.68	-0.71	-0.30	-0.57	-0.70	-0.70	-0.19	0.91	0.93	-0.39	-0.13	-0.13	-0.11	-0.13	-0.12	-0.11	-0.12	-0.11	-0.20

1-OH-NAP	0.04	0.35	0.67	0.76	0.93	0.47	-0.35	-0.35	-0.41	0.05	0.08	-0.46	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99
2-OH-FLUO	0.28	0.36	0.49	0.55	0.82	0.33	-0.52	-0.52	-0.43	0.32	0.36	-0.54	0.95	0.95	0.96	0.95	0.96	0.96	0.96	0.93
1-OH-PHE	0.08	0.39	0.68	0.74	0.91	0.49	-0.33	-0.33	-0.38	0.08	0.11	-0.43	0.99	>0.99	>0.99	0.99	>0.99	>0.99	>0.99	>0.99
2-OH-PHE	0.06	0.30	0.60	0.72	0.93	0.40	-0.43	-0.43	-0.47	0.10	0.14	-0.53	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	0.99
3-OH-PHE	0.05	0.43	0.74	0.78	0.91	0.56	-0.25	-0.25	-0.32	0.02	0.05	-0.36	0.98	0.99	>0.99	0.98	>0.99	>0.99	0.99	>0.99
4-OH-PHE	0.05	0.35	0.67	0.76	0.93	0.47	-0.35	-0.35	-0.42	0.06	0.09	-0.46	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99
9-OH-PHE	0.08	0.34	0.63	0.72	0.92	0.43	-0.40	-0.40	-0.44	0.10	0.14	-0.49	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	0.99
1-OH-PYR	-0.20	-0.76	-0.89	-0.67	-0.67	-0.84	-0.12	-0.12	-0.12	-0.06	-0.05	-0.06	-0.80	-0.83	-0.87	-0.80	-0.84	-0.85	-0.85	-0.82	-0.88
P [c]																				
ANY	0.39	0.56	0.73	0.81	0.45	0.80	0.40	0.40	0.71	0.34	0.32	0.53	0.25	0.23	0.20	0.24	0.22	0.21	0.21	0.22	0.26
ACE	0.12	0.84	0.44	0.27	0.63	0.61	0.46	0.46	0.98	0.03	0.02	0.80	0.85	0.86	0.90	0.85	0.88	0.89	0.88	0.88	0.81
FLU	0.13	0.59	0.57	0.14	0.26	0.89	0.97	0.97	0.42	0.20	0.24	0.60	0.48	0.51	0.58	0.48	0.53	0.55	0.54	0.51	0.51
PHE	0.33	0.45	0.70	0.84	0.51	0.72	0.49	0.49	0.83	0.32	0.30	0.64	0.28	0.26	0.22	0.28	0.25	0.24	0.24	0.26	0.28
ANT	0.05	0.68	0.58	0.33	0.68	0.77	0.53	0.53	0.88	<0.01	<0.01	0.88	0.92	0.95	>0.99	0.93	0.96	0.98	0.97	0.96	0.90
FLO	0.34	0.80	0.18	0.18	0.55	0.30	0.37	0.37	0.84	0.17	0.16	0.67	0.68	0.68	0.69	0.68	0.68	0.69	0.69	0.70	0.60
PYR	0.32	0.73	0.96	0.95	0.61	0.93	0.25	0.25	0.63	0.21	0.17	0.43	0.41	0.40	0.38	0.41	0.40	0.39	0.39	0.39	0.46
BAA	0.28	0.88	0.28	0.28	0.70	0.38	0.28	0.28	0.78	0.11	0.09	0.58	0.85	0.85	0.87	0.85	0.86	0.86	0.86	0.87	0.77
BKF	0.22	0.97	0.33	0.27	0.68	0.45	0.33	0.33	0.85	0.08	0.06	0.65	0.85	0.86	0.88	0.85	0.86	0.87	0.87	0.87	0.78
BAP	0.20	0.98	0.39	0.34	0.76	0.50	0.30	0.30	0.83	0.06	0.04	0.62	0.94	0.95	0.97	0.95	0.96	0.96	0.96	0.97	0.88

BghiP	0.24	0.94	0.32	0.29	0.70	0.43	0.30	0.30	0.82	0.09	0.07	0.61	0.87	0.87	0.89	0.87	0.88	0.89	0.89	0.89	0.80
1-OH-NAP	0.97	0.66	0.33	0.24	0.07	0.53	0.65	0.65	0.59	0.96	0.92	0.54	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
2-OH-FLUO	0.72	0.64	0.51	0.45	0.18	0.67	0.48	0.48	0.57	0.68	0.64	0.46	0.05	<0.05	0.04	>0.05	0.04	0.04	0.04	0.04	0.07
1-OH-PHE	0.92	0.61	0.32	0.26	0.09	0.51	0.67	0.67	0.62	0.92	0.89	0.57	0.01	<0.01	<0.01	0.01	<0.01	<0.01	<0.01	<0.01	<0.01
2-OH-PHE	0.94	0.70	0.40	0.28	0.07	0.60	0.57	0.57	0.53	0.90	0.86	0.47	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	0.02
3-OH-PHE	0.96	0.57	0.26	0.22	0.10	0.44	0.75	0.75	0.68	0.98	0.95	0.64	0.02	0.01	<0.01	0.02	<0.01	<0.01	<0.01	0.01	<0.01
4-OH-PHE	0.96	0.65	0.33	0.25	0.08	0.53	0.65	0.65	0.59	0.94	0.91	0.54	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
9-OH-PHE	0.92	0.66	0.37	0.28	0.08	0.57	0.60	0.60	0.56	0.90	0.86	0.51	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	0.01
1-OH-PYR	0.80	0.24	0.11	0.33	0.33	0.16	0.88	0.88	0.88	0.95	0.95	0.94	0.20	0.17	0.13	0.20	0.16	0.15	0.15	0.18	0.12

Rows in the table represent compounds in plasma, while columns represent compounds in urine;

[a] The results were calculated by Pearson correlation test; [b] Correlation coefficients; [c] *P* values for Pearson correlation test;

Table S8. Correlation between target compound concentrations measured in hair and urine [a]

	ANY	ACE	FLU	PHE	ANT	FLO	PYR	BAA	BKF	BAP	DahA	BghiP	1-OH-NAP	2-OH-NAP	2-OH-FLUO	1-OH-PHE	2-OH-PHE	3-OH-PHE	4-OH-PHE	9-OH-PHE	1-OH-PYR
r [b]																					
ANY	0.49	0.90	0.48	-0.13	-0.35	0.76	0.72	0.72	0.94	0.20	0.13	0.87	-0.17	-0.12	-0.04	-0.17	-0.10	-0.08	-0.08	-0.14	-0.04
ACE	0.99	0.61	-0.18	-0.63	-0.42	0.09	-0.12	-0.12	0.47	0.92	0.89	0.24	-0.15	-0.11	-0.03	-0.14	-0.09	-0.07	-0.07	-0.10	-0.11
FLU	-0.35	-0.71	-0.29	0.28	0.59	-0.59	-0.83	-0.83	-0.99	-0.07	0.01	-0.97	0.46	0.42	0.35	0.46	0.40	0.38	0.38	0.44	0.33
PHE	0.10	-0.32	-0.17	0.21	0.64	-0.40	-0.95	-0.95	-0.87	0.35	0.42	-0.96	0.66	0.63	0.60	0.66	0.62	0.62	0.62	0.65	0.55
ANT	0.88	0.40	-0.14	-0.31	0.10	-0.06	-0.61	-0.61	-0.10	0.94	0.95	-0.33	0.34	0.37	0.41	0.35	0.38	0.39	0.39	0.38	0.32
FLO	0.17	0.06	0.25	0.48	0.83	0.04	-0.74	-0.74	-0.68	0.31	0.36	-0.78	0.90	0.90	0.88	0.91	0.89	0.89	0.89	0.91	0.85
PYR	-0.65	-0.81	-0.20	0.42	0.57	-0.53	-0.60	-0.60	-0.94	-0.40	-0.33	-0.84	0.37	0.32	0.23	0.37	0.29	0.27	0.27	0.33	0.25
BAA	-0.02	0.22	0.59	0.76	0.96	0.36	-0.45	-0.45	-0.53	0.03	0.07	-0.57	>0.99	>0.99	0.99	>0.99	>0.99	>0.99	>0.99	>0.99	0.98
BKF	0.04	0.63	0.91	0.79	0.78	0.80	0.07	0.07	-0.02	-0.08	-0.07	-0.04	0.87	0.89	0.91	0.87	0.90	0.90	0.90	0.88	0.93
BAP	0.27	0.71	0.81	0.64	0.71	0.75	-0.05	-0.05	<0.01	0.17	0.17	-0.08	0.86	0.89	0.92	0.86	0.90	0.91	0.91	0.88	0.92
DahA	0.22	0.74	0.87	0.67	0.69	0.81	0.06	0.06	0.08	0.09	0.09	0.01	0.83	0.85	0.89	0.83	0.87	0.87	0.87	0.84	0.90
BghiP	0.04	0.77	0.98	0.72	0.57	0.95	0.38	0.38	0.28	-0.16	-0.19	0.28	0.67	0.70	0.73	0.66	0.71	0.72	0.71	0.68	0.77
1-OH-NAP	0.06	0.37	0.67	0.75	0.92	0.48	-0.34	-0.34	-0.40	0.07	0.10	-0.48	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99

2-OH-NAP	0.79	0.97	0.46	-0.08	-0.05	0.68	0.23	0.23	0.62	0.58	0.54	0.45	0.22	0.27	0.36	0.22	0.30	0.32	0.32	0.26	0.32
2-OH-FLUO	0.10	0.37	0.64	0.71	0.91	0.45	-0.38	-0.38	-0.41	0.12	0.15	-0.47	0.99	>0.99	>0.99	0.99	>0.99	>0.99	>0.99	>0.99	0.99
1-OH-PHE	<0.01	0.29	0.64	0.77	0.94	0.42	-0.39	-0.39	-0.47	0.03	0.07	-0.51	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99
2-OH-PHE	-0.01	0.28	0.65	0.78	0.95	0.43	-0.38	-0.38	-0.47	0.01	0.05	-0.51	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99
3-OH-PHE	-0.01	0.28	0.65	0.78	0.95	0.43	-0.38	-0.38	-0.47	0.02	0.05	-0.51	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99
4-OH-PHE	<0.01	0.29	0.65	0.77	0.94	0.43	-0.38	-0.38	-0.46	0.03	0.07	-0.50	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99
9-OH-PHE	<0.01	0.30	0.65	0.77	0.94	0.44	-0.37	-0.37	-0.46	0.03	0.06	-0.50	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99	>0.99
1-OH-PYR	0.10	0.19	0.46	0.64	0.91	0.24	-0.57	-0.57	-0.58	0.18	0.23	-0.65	0.98	0.97	0.96	0.98	0.97	0.97	0.97	0.98	0.94
P [c]																					
ANY	0.51	0.10	0.52	0.87	0.65	0.24	0.28	0.28	0.06	0.80	0.88	0.13	0.83	0.88	0.96	0.83	0.90	0.92	0.92	0.86	0.97
ACE	<0.01	0.39	0.82	0.37	0.58	0.91	0.89	0.89	0.53	0.08	0.11	0.76	0.85	0.89	0.97	0.86	0.92	0.93	0.93	0.90	0.89
FLU	0.65	0.29	0.71	0.72	0.41	0.41	0.17	0.17	<0.01	0.93	0.99	0.03	0.54	0.58	0.66	0.54	0.60	0.62	0.62	0.57	0.67
PHE	0.90	0.68	0.83	0.79	0.36	0.60	>0.05	0.05	0.13	0.65	0.58	0.04	0.34	0.37	0.40	0.34	0.38	0.38	0.38	0.35	0.45
ANT	0.12	0.60	0.86	0.70	0.90	0.95	0.39	0.39	0.90	0.06	<0.50	0.67	0.66	0.63	0.59	0.65	0.62	0.61	0.61	0.62	0.68
FLO	0.83	0.94	0.75	0.52	0.17	0.96	0.26	0.26	0.32	0.69	0.64	0.23	0.10	0.10	0.12	0.10	0.11	0.11	0.11	0.09	0.15
PYR	0.35	0.19	0.81	0.58	0.43	0.47	0.40	0.40	0.06	0.60	0.67	0.17	0.64	0.69	0.77	0.64	0.71	0.73	0.73	0.67	0.75
BAA	0.98	0.78	0.41	0.24	0.04	0.65	0.56	0.56	0.47	0.97	0.93	0.43	<0.01	<0.01	0.02	<0.01	<0.01	<0.01	<0.01	<0.01	0.02
BKF	0.96	0.37	0.09	0.21	0.22	0.20	0.93	0.93	0.98	0.92	0.93	0.96	0.13	0.11	0.09	0.13	0.10	0.10	0.10	0.12	0.07
BAP	0.73	0.29	0.19	0.36	0.29	0.26	0.95	0.95	>0.99	0.83	0.83	0.92	0.14	0.11	0.08	0.14	0.10	0.09	0.10	0.12	0.08

DahA	0.78	0.26	0.13	0.33	0.31	0.19	0.94	0.94	0.92	0.91	0.92	0.99	0.17	0.15	0.11	0.17	0.14	0.13	0.13	0.16	0.10
BghiP	0.96	0.23	0.02	0.28	0.43	<0.05	0.62	0.62	0.72	0.84	0.82	0.72	0.34	0.31	0.27	0.34	0.29	0.29	0.29	0.32	0.23
1-OH-NAP	0.94	0.63	0.33	0.25	0.08	0.52	0.66	0.66	0.60	0.93	0.90	0.55	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
2-OH-NAP	0.22	0.04	0.54	0.92	0.95	0.32	0.77	0.77	0.38	0.42	0.46	0.55	0.78	0.73	0.64	0.78	0.70	0.68	0.69	0.74	0.68
2-OH-FLUO	0.90	0.63	0.36	0.29	0.10	0.55	0.62	0.62	0.59	0.88	0.85	0.53	0.01	<0.01	<0.01	0.01	<0.01	<0.01	<0.01	<0.01	0.01
1-OH-PHE	>0.99	0.71	0.36	0.23	0.06	0.58	0.61	0.61	0.53	0.97	0.93	0.49	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
2-OH-PHE	0.99	0.72	0.35	0.22	>0.05	0.57	0.62	0.62	0.53	0.99	0.95	0.50	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
3-OH-PHE	0.99	0.72	0.35	0.22	>0.05	0.57	0.62	0.62	0.53	0.99	0.95	0.50	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
4-OH-PHE	>0.99	0.71	0.35	0.23	0.06	0.57	0.62	0.62	0.54	0.97	0.94	0.50	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
9-OH-PHE	>0.99	0.70	0.35	0.23	0.06	0.56	0.63	0.63	0.54	0.98	0.94	0.50	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
1-OH-PYR	0.91	0.81	0.54	0.36	0.09	0.76	0.43	0.43	0.42	0.82	0.78	0.35	0.02	0.03	0.04	0.02	0.03	0.03	0.03	0.02	0.06

Rows in the table represent compounds in hair, while columns represent compounds in urine;

[a] The results were calculated by Pearson correlation test; [b] Correlation coefficients; [c] *P* values for Pearson correlation test.

References

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