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Supporting Information

CARCINOGENIC POTENTIAL OF SOILS CONTAMINATED WITH POLYCYCLIC AROMATIC HYDROCARBONS (PAHs) IN XIAMEN METROPOLIS, CHINA

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Additional analytical method details: For PAHs analysis, the samples were analyzed by gas chromatography (Agilent 7890A, Agilent Co., USA) equipped with a mass selective detector (Agilent 5975C, Agilent Co., USA). The DB-5 capillary column (Agilent Co.,USA) used in this study was 30 m in length with an internal diameter of 0.25 mm and a film thickness of 0.25 μm. The column temperature was programmed to initially hold at 60^0C for 1 min, to rise from 60^0C to 150^0C at a rate of 15^0C/min, and to then increase to 220^0C at 5^0C/min and finally to increase to 300^0C at 10^0C/min, thereafter 300^0C was maintained for 5 min. 1 μL sample was injected in a splitless mode. Helium was used as the carrier gas at flow rate of 1.2 ml min^{-1}. The electron-impact energy was 70 eV and the mass-to-change ration scan (m/z) was from 50 to 500 amu. The selected ion mode (SIM) was chosen and data acquisition and processing were controlled by a Agilent Chem-Station data system. Final amount of corresponding PAHs were calculated from the relative signal ratio of PAHs in samples to those in internal standard.

All analytical procedures were subjected to strict quality control. Quantification of method blanks (solvent), spiked blanks (standards spiked into solvent), and matrix spike (standards spiked into matrix) was undertaken. Surrogate standards were added to all samples (including those for QA) to monitor the procedures of sample extraction, cleanup and analysis. During the GC–MS analysis, the response factors for individual PAHs relative to the internal standard were determined by the analysis of the calibration solution containing 16 PAHs, 5 deuterated PAHs and one internal standard (fluoranthene-d10). The recovery efficiencies of naphthalene-d8 acenaphthene-d10, phenanthrene-d10, chrysene-d12 and perylene-d12 were 42.39%–55.32%%, 77.24%-92.39%, 79.09%–99.15%, 81.22%–117.68%% and 58.17%–86.05%, respectively. The recovery efficiency was also checked by analyzing soil samples spiked with known amount of PAHs standard. The spiking recovery of individual PAHs ranges from 54.5 to 116.5% with a mean value of 97.1% for the 16 PAHs. The concentrations reported in this paper were calibrated by the blank levels and not corrected by the surrogate recovery efficiencies. The limit of detection (LOD) for PAHs ranged from 0.098-1.33 ng g^{-1}. A random selection of samples (about 25% of total) was analysed in duplicate (RSD for replicates were <10%).

Table S1. PAH concentrations in soil samples from the HUA and the LUA of Xiamen.

Area	Land use	Nap			Ace			Acy			Ant			Flu			Phe		
		Mean	Median	Range	Mean	Median	Range	Mean	Median	Range	Mean	Median	Range	Mean	Median	Range	Mean	Median	Range
HUA	B(n=5)	8.9	8.1	5.9-14.6	1.5	1.6	1.0-2.1	13.6	14.2	1.0-22.0	6.2	3.6	2.1-13.7	22.1	2.7	0.4-96.8	5.3	1.4	UC-22.2
	F(n=4)	14.9	11.0	7.3-30.5	2.4	2.1	1.3-4.0	1.7	1.5	1.2-2.5	3.6	2.8	2.4-6.5	11.8	10.3	3.6-23.0	30.2	27.2	13.9-52.7
	R(n=5)	20.0	11.6	9.4-37.5	4.5	3.4	1.3-9.3	3.2	4.2	1.1-4.7	5.6	4.8	2.0-9.1	17.8	13.9	3.5-44.6	52.5	54.1	26.5-75.5
	I (n=7)	20.1	17.8	5.9-40.0	3.3	2.3	1.3-7.1	12.3	14.5	1.8-31.9	12.7	4.9	1.1-43.8	10.7	9.2	4.7-20.2	72.6	56.8	4.4-212.5
	T(n=4)	45.7	27.7	12.0-115.4	4.3	4.4	2.0-6.3	13.8	8.5	2.0-36.2	20.5	16.9	3.5-44.8	11.7	9.2	4.1-24.1	122.7	81.8	42.6-284.6
LUA	B(n=4)	21.6	15.1	4.5-51.7	2.6	2.6	0.5-4.7	2.4	2.2	0.9-4.1	2.0	1.3	0.8-4.6	14.3	11.2	3.0-31.8	25.5	17.3	7.3-60.4
	F(n=7)	24.4	21.9	6.5-50.7	6.2	7.9	2.2-8.8	2.5	2.5	1.5-3.5	2.6	2.8	1.0-3.2	16.8	13.9	3.8-30.8	25.4	26.1	12.5-33.2
	R(n=4)	25.9	27.8	9.0-39.1	5.1	4. 9	3.1-7.3	2.5	2.4	1.3-3.9	2.6	2.5	1.2-4.1	14.6	15.3	2.8-24.9	26.2	28.3	9.8-38.2
	I (n=5)	17.7	13.9	7.7-31.9	3.7	3.8	1.1-6.6	2.8	2.7	2.1-3.8	2.7	2.2	0.8-4.9	18.7	14.4	7.6-38.5	27.5	21.9	10.2-42.9
	T(n=6)	33.8	31.1	17.5-61.7	7.1	5.6	3.6-15.3	3.3	3.5	2.0-4.5	2.8	2.9	1.4-3.8	27.0	23.7	18.3-50.8	37.2	38.2	22.3-51.4

Area	Land use	BaA			Chr			Flt			Pyr			BaP			BbF		
		Mean	Median	Range	Mean	Median	Range	Mean	Median	Range	Mean	Median	Range	Mean	Median	Range	Mean	Median	Range
HUA	B(n=5)	6.5	5.3	2.5-11.2	7.5	6.5	5.3-10.0	12.3	11.7	10.8-14.1	11.6	9.9	8.7-18.8	3.4	2.3	1.5-7.9	8.1	8.7	2.7-12.3
	F(n=4)	24.5	24.2	12.1-37.7	26.1	28.3	9.7-38.4	33.4	32.1	19.6-49.6	28.2	26.7	18.3-41.2	31.6	34.2	11.7-46.1	39.3	39.1	16.7-62.3
	R(n=5)	34.2	22.3	7.8-67.0	35.4	19.2	4.9-80.6	48.0	31.8	13.9-91.1	45.6	32.2	17.4-86.3	42.4	26.4	5.5-91.1	52.5	33.0	9.5-108.1
	I (n=7)	99.7	95.4	20.0-203.5	95.5	76.2	16.8-265.7	119.2	95.8	22.2-284.4	107.2	113.8	22.4-207.4	119.5	103.3	18.3-269.3	141.5	111.6	24.8-395.0
	T(n=4)	81.6	86.4	10.9-142.7	91.2	83.1	6.7-191.7	115.7	122.0	14.2-204.4	93.8	95.6	14.9-169.0	92.6	74.8	9.7-211.2	116.8	104.5	13.0-245.4
LUA	B(n=4)	6.5	7.1	2.3-9.8	3.9	4.3	0.5-6.6	10.8	10.1	5.5-17.5	11.9	12.4	5.1-17.7	4.20	3.70	0.7-8.7	8.2	9.20	1.4-12.9
	F(n=7)	13.8	13.8	6.5-21.4	11.4	10.2	3.3-23.5	18.4	19.4	8.8-29.7	18.5	20.8	7.6-28.7	13.1	11.5	2.7-25.6	21.1	20.0	6.9-36.8
	R(n=4)	9.5	10.5	3.3-13.8	5.3	5.1	2.2-8.9	11.1	11.8	5.4-15.1	12.2	12.1	6.9-17.6	5.4	4.9	1.9-10.0	9.5	9.2	4.0-15.9
	I (n=5)	12.1	12.2	4.5-24.9	10.0	9.2	4.4-17.3	17.2	19.7	8.3-27.0	25.7	23.8	17.5-33.8	10.4	10.0	4.4-20.0	18.2	18.2	8.7-30.8
	T(n=6)	19.8	20.4	4.8-40.2	19.7	8.4	1.7-79.4	24.5	28.7	7.8-38.5	23.3	24.4	10.9-36.8	17.0	9.8	1.5-58.9	29.2	21.3	5.3-88.7

Area	Land use	BkF			DbA			BghiP			InP			Σ 16PAHs		
		Mean	Median	Range	Mean	Median	Range	Mean	Median	Range	Mean	Median	Range	Mean	Median	Range
HUA	B(n=5)	5.5	5.9	2.2-8.8	8.1	6.9	1.9-16.0	8.7	9.3	4.3-13.3	9.6	9.5	3.2-16.7	138.9	140.7	84.6-217.8
	F(n=4)	25.4	25.7	11.2-38.8	6.9	7.2	3.0-10.2	29.3	28.3	17.2-43.6	39.9	41.7	12.6-63.4	349.2	324.8	196.4-550.6
	R(n=5)	33.2	18.4	4.8-73.2	8.5	4.8	1.2-18.5	40.7	26.5	7.0-78.3	53.2	31.2	7.7-113.1	497.5	366.3	129.3-954.9
	I (n=7)	99.2	107.0	16.0-234.7	47.0	23.3	4.6-159.4	112.9	94.3	20.3-262.2	163.7	128.2	25.9-419.5	1237.0	1229.6	263.4-2947.4
	T(n=4)	75.1	62.8	8.1-166.6	20.8	19.0	2.4-42.9	79.4	70.9	10.7-165.1	113.0	98.0	9.7-246.3	1098.6	1121.8	173.2-1977.6
LUA	B(n=4)	3.9	4.0	0.6-7.1	1.0	1.0	UC-1.8	5.5	4.7	1.9-10.5	5.7	4.1	0.5-13.9	129.9	121.7	45.9-230.4
	F(n=7)	13.1	12.4	3.1-21.7	2.9	2.5	0.7-5.1	14.2	14.8	4.7-24.0	18.2	15.1	3.8-36.7	222.5	224.1	108.7-309.5
	R(n=4)	5.3	5.3	2.2-8.3	1.0	0.9	UC-2.1	6.3	6.5	2.7-9.6	7.0	7.1	UC-13.4	149.5	151.9	75.2-219.2
	I (n=5)	8.9	8.8	4.8-17.2	2.2	1.9	0.9-4.6	13.7	12.1	7.6-23.9	13.2	12.0	6.5-24.6	204.6	178.8	140.5-346.6
	T(n=6)	16.5	9.9	1.1-59.0	4.1	2.6	UC-13.5	22.0	13.6	3.1-68.6	29.4	19.8	0.4-105.5	316.6	313.1	103.7-680.8

B-Background area; F-Farmland; R-Residential district; I-Industrial district; T-Traffic belt; UC-Unquantified concentration

Table S2. Toxicity equivalency factor (TEF) schemes. Weightings are relative to BaP (weighted 1.0)

PAH	TEF set reference and number See list of references at the end of the table																					
	[1]	[2]	[3]	[4]	[5]	[6]	[7]**	[8]***	[9]	[10]	[11]	[12]	[13]	[14]	[15]	[16]	[17]	[18]	[19]	[20]	[21]	[22]
Acenaphthene				0.001					0.001													
Acenaphthylene				0.001					0.01													
Anthracene				0.01									0.0005									
B[a]P	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Benz[a]anthracene	0.1	0.013	0.145	0.1	0.1	0.1	0.1	0.04	0.1		0.1	0.014	0.005	0.1	0.1	0.08	0.09	0.1	0.14	0.11	0.08	0.7
Benzo[b]fluoranthene	0.1	0.08	0.14	0.1	0.1	0.1	0.1		0.1	0.06	0.11	0.11	0.1	0.1	0.1	7.8	1.3					
Benzo[ghi]perylene	0.01		0.022					0.03				0.012	0.02	0.01				0.0044				0.002
Benzo[j]fluoranthene	(b+j)		0.061			0.1	0.1		0.1	0.05		0.045	0.05	0.1	0.1							
Benzo[k]fluoranthene	0.1	0.04		0.1	0.1	0.1	0.1	0.09	0.1	0.04	0.03	0.037	0.05	0.1	0.1	15	1	9.6	3.4	6.1	18.2	3.8
Chrysene	0.01	0.001		0.01	0.001	0.1	0.01	0.89	0.01		0.03	0.026	0.03	0.01	0.0044	0.6		0.26	0.16	0.59	1.1	2.7
Dibenzo[a,h]anthracene	1	0.69	1.11	5	1	1			1		1.91	0.89		1	1.1	6.3	0.26					
Dibenzo[a,h]pyrene				1			10															
Dibenzo[a,i]pyrene							10											1	1	1	1	1
Dibenzo[a,l]pyrene				1			10															
Fluoranthene				0.001				0.06	0.01				0.05					0.0004			0.0003	0.00003
Fluorene				0.001																		
Indeno[1,2,3-cd]pyrene	0.1	0.017	0.232	0.1	0.1	0.1	0.1	0.08	0.1	0.12	0.08	0.067	0.1	0.1	0.2	3	0.29	2.7	0.9		3.3	0.3
2-methylnaphthalene				0.001																		
Naphthalene				0.001																		
Phenanthrene				0.001				0.01				0.00064	0.0005									
Pyrene			0.081	0.001					0.001				0.001									

*: Nisbet and Lagoy, 1992 also indicate: a ETF of 0.001 for acenaphthene, acephthylene, fluoranthene, 2-methylnaphtalene, naphthalene, phenanthrene, and pyrene; and a TEF of 0.1 for anthracene
*: OEHHA (1992) also indicate a ETF of 0.1 for dibenz(a,j)acridine, dibenz(a,h)acridine; a ETF of 1 for 5-methylchrysene
***: used the upper extremes

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Table S3. TEQ calculated using 22 different TEF schemes for the HUA (see Table S2 for weightings)

Land use	Samp. No.	TEF set reference 1	2	3	4*	5	6	7**	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
Bck	x107	198	16	24	32	20	21	17	23	20	15	22	18	17	20	22	344	48	145	60	72	238	80
	x148-1	238	6.3	9.0	17	7.6	8.1	5.4	11	8	5	9.6	7.1	6.0	7.7	8.1	59	8.3	31	14	19	52	28
	x151	55	17	24	50	21	22	14	24	21	13	27	19	14	21	22	189	24	95	42	54	159	70
	x47	14	7.0	11	15	8.9	9.5	7.5	12	9.1	6.4	10.0	8.0	7.4	9.0	9.7	156	21	66	27	36	111	43
	x158	33	12	18	24	15	15	12	16	15	11	16	13	12	15	16	233	33	102	42	49	164	55
Farm.	x48	526	39	56	72	48	50	42	62	48	37	52	44	41	48	52	827	115	361	149	190	605	216
	x74	368	16	24	32	20	21	17	24	20	15	22	18	17	20	22	374	50	157	65	87	269	92
	x59	154	61	91	118	77	80	67	95	77	59	84	70	65	77	84	1395	190	604	247	310	1007	343
	x86	94	50	71	95	61	64	53	76	62	48	67	56	52	62	67	1002	139	446	185	231	741	259
Res.	x66	136	30	47	58	38	40	34	48	39	29	42	35	33	39	42	692	96	291	120	149	483	170
	x40	129	33	46	57	39	41	35	47	40	32	42	36	35	40	42	595	88	253	108	137	419	150
	x71	78	7.6	13	15	9.7	10	8.6	13	10	7.2	11	8.7	8.6	9.9	11	187	26	75	31	39	125	45
	x119	160	87	129	163	108	114	95	139	109	84	117	99	94	109	119	1920	264	844	346	432	1404	489
	x136	155	118	171	221	146	154	128	190	148	114	159	134	126	147	159	2542	349	1127	464	593	1891	668
Traf.	x70	399	121	188	242	154	165	134	220	158	113	171	138	132	156	168	2811	388	1157	480	620	1955	780
	x78	85	13	19	26	16	17	14	19	16	12	18	15	14	16	17	282	39	117	49	64	198	69
	x93	341	273	388	508	334	353	293	440	338	262	365	308	289	338	364	5759	792	2540	1050	1356	4278	1536
	x102	97	83	122	171	104	110	88	133	105	77	116	94	86	105	114	1793	242	789	324	412	1323	476
Ind.	x15	47	37	56	69	46	49	41	58	47	36	50	42	40	47	51	825	117	339	141	175	563	200
	x17	130	113	168	219	141	148	122	173	142	110	155	130	120	142	156	2449	341	1057	433	515	1730	592
	x42	112	25	38	50	32	33	27	40	32	24	35	28	26	32	35	570	77	249	102	128	416	146
	x51	409	139	206	269	175	183	152	209	178	132	190	158	150	177	190	3491	462	1502	606	811	2559	820
	x85	496	376	564	802	476	502	397	596	481	353	536	434	391	481	526	8814	1178	3746	1516	1880	6234	2147
	x26	738	320	460	1045	407	417	248	328	409	229	543	368	239	409	443	3981	484	1908	813	984	3116	1071
	x73	1106	189	294	388	243	254	208	290	246	179	267	217	200	245	267	4817	640	2045	824	1051	3433	1139

*: Nisbet and Lagoy, 1992 also indicate: a ETF of 0.001 for acenaphthene, acephthylene, fluoranthene, 2-methylnaphtalene, naphthalene, phenanthrene, and pyrene; and a TEF of 0.1 for anthracene

*: OEHHA (1992) also indicate a ETF of 0.1 for dibenz(a,j)acridine, dibenz(a,h)acridine; a ETF of 1 for 5-methylchrysene

***: used the upper extremes

+: outlier not used

Table S4. TEQ calculated using 22 different TEF schemes for the LUA (see Table S2 for weightings).

Land use	Samp. No.	TEF set reference																					
		1	**2**	**3**	**4***	**5**	**6**	**7****	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**
Bck.	x219	13	12	19	22	15	15	13	18	15	11	16	13	13	15	16	273	38	117	47	57	191	63
	x262	6.5	5.2	8.1	10.9	6.7	7.1	5.8	8.3	6.8	4.6	7.5	5.9	5.5	6.8	7.2	141	19	52	22	30	91	34
	x293	35	5.8	10.1	12	7.8	8.3	6.8	11	8.1	5.2	8.6	6.7	6.8	7.9	8.4	174	24	58	24	33	100	41
	x297	15	0.9	2.4	1.6	1.2	1.3	1.1	1.8	1.3	0.8	1.3	1.0	1.2	1.3	1.3	23	3.4	8.3	3.6	5.1	14	6.1
Farm.	x234	13	9	14	17	12	12	10	13	12	9	12	10	10	12	13	268	34	122	48	61	206	60
	x239	51	30	46	59	38	40	33	45	39	29	42	35	32	39	43	789	105	336	134	166	559	175
	x246	47	16	25	35	21	22	18	27	21	15	24	19	17	21	23	424	56	171	70	96	295	104
	x260	97	15	24	29	19	20	17	25	20	15	21	18	17	20	21	381	52	154	63	81	260	91
	x279	63	17	26	32	22	23	19	26	22	16	23	19	19	22	24	473	62	202	81	109	346	109
	x282	43	4.0	7.4	8.6	5.5	5.8	4.8	7.6	5.7	3.7	6.0	4.7	4.8	5.6	6.0	122	17	45	18	24	77	29
	x314	85	33	48	60	41	43	36	54	41	32	44	37	36	41	44	724	100	314	130	169	530	192
Res.	x251	78	3.7	7.9	9.8	5.7	6.1	4.8	7.5	5.9	3.3	6.4	4.6	4.3	5.8	6.4	160	20	62	24	32	106	37
	x277	56	12	18	18	14	15	14	21	15	12	15	13	13	15	15	217	33	96	42	54	162	68
	x288	30	11	18	23	15	15	13	17	15	10	16	13	12	15	16	314	42	126	51	63	211	70
	x290	25	2.9	4.3	4.6	3.5	3.7	3.3	5.1	3.6	2.7	3.7	3.2	3.2	3.6	3.6	70	10	25	11	17	46	19
Traf.	x287	36	4.6	8.2	10	6.2	6.5	5.3	8.0	6.4	4.2	7.0	5.4	5.1	6.3	6.8	117	17	42	18	22	70	28
	x256	51	18	29	33	23	24	21	26	23	18	24	21	20	23	26	430	60	184	75	87	298	94
	x267	104	80	121	157	102	110	89	150	103	79	111	93	87	103	114	2088	271	935	373	470	1572	557
	x208	58	11	22	28	16	17	13	20	17	10	18	13	13	16	18	385	51	142	57	68	236	86
	x305	212	2.2	4.4	4.1	2.9	3.1	2.7	4.1	3.1	1.9	3.2	2.6	2.7	3.0	3.0	63	10	14	6.4	9.5	24	14
	x310	37	26	41	52	33	35	29	42	34	25	37	30	28	34	37	630	88	253	104	131	422	153
Ind.	x285	23	14	22	27	18	18	15	22	18	13	19	16	15	18	19	346	48	135	55	71	227	81
	x296	51	27	42	53	34	36	30	43	35	25	38	31	29	35	37	634	88	259	107	138	435	157
	x306	44	7.8	12	15	9.7	10	8.6	12	9.9	7.4	11	8.8	8.5	9.8	10	176	25	72	30	39	121	43
	power plant	73	7.7	15	18	10	11	8.2	14	10	6.9	12	9.4	8.4	10	11	271	38	79	31	39	133	50
	x307	34	14	22	21	17	19	17	26	18	14	18	16	17	18	19	303	44	133	56	74	225	88

*: Nisbet and Lagoy, 1992 also indicate: a ETF of 0.001 for acenaphthene, acephthylene, fluoranthene, 2-methylnaphtalene, naphthalene, phenanthrene, and pyrene; and a TEF of 0.1 for anthracene

*: OEHHA (1992) also indicate a ETF of 0.1 for dibenz(a,j)acridine, dibenz(a,h)acridine; a ETF of 1 for 5-methylchrysene

***: used the upper extremes

+: outlier not used

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