

Supplementary material of “**Heart failure and PAHs, OHPAHs and trace elements levels in human serum: results from a preliminary pilot study in Greek population and the possible impact of different air pollution**”

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Table S1. Detection frequencies, median, mean and ranges of PAHs concentrations ($\mu\text{g L}^{-1}$) in cases' and controls' samples.

	NAP	ACY	ACE	FL	PHE	ANT	FLT	PYR	CHR	BaA	BFA	BaP	IPY	DBA	BPE	Σ PAHs
Cases (n=96)																
Detection Frequency (%)	100	13.5	100	100	100	91.7	100	100	35.4	78.1	93.7	25.0	4.2	67.7	0	
Median	7.85	0.02	51.8	69.1	224	3.81	54.6	22.4	0.02	2.67	2.82	0.0004	0.01	35.8	ND	506
Mean	10.5	0.03	63.0	76.7	231	4.26	61.6	23.4	1.24	3.62	2.99	0.53	0.02	38.5	ND	517
Geometric mean	8.04	0.02	54.1	67.7	209	2.34	54.4	20.3	0.11	0.83	1.80	0.003	0.01	1.68	ND	473
Geometric SD	1.41	1.34	1.28	1.25	1.22	2.16	1.25	1.27	2.83	3.48	2.27	4.23	1.35	8.35	ND	1.21
Range	0.84-32.9	0.02-0.39	11.8-183	23.3-264	72.5-588	0.01-10.9	14.3-167	5.18-83.7	0.02-8.58	0.004-12.5	0.001-7.40	0.0004-10.4	0.01-0.44	0.001-111	ND	163-1160
Controls (n=35)																
Detection Frequency (%)	100	22.9	100	100	100	77.1	100	100	28.6	71.4	77.1	14.3	8.57	65.7	0	
Median	5.73	0.02	16.9	22.8	54.7	1.80	13.8	5.86	0.03	1.09	0.99	0.0004	0.01	9.44	ND	142
Mean	6.67	0.03	19.0	26.6	56.5	1.98	15.3	7.04	0.40	1.69	1.20	0.08	0.02	9.81	ND	146
Geometric mean	5.09	0.02	17.0	23.9	52.9	0.62	13.1	6.12	0.06	0.33	0.27	0.001	0.01	0.57	ND	142
Geometric SD	1.42	1.32	1.21	1.21	1.17	2.79	1.29	1.27	2.22	3.44	3.58	2.81	1.35	6.67	ND	1.12
Range	0.74-16.4	0.02-0.24	7.83-70.8	12.4-82.8	24.8-104	0.01-5.27	3.75-36.2	2.63-16.7	0.02-3.93	0.004-7.66	0.001-3.81	0.0004-1.16	0.01-0.26	0.001-28.3	ND	87.4-230
<i>p</i> -Value	0.007	0.266	0.000	0.000	0.000	0.000	0.000	0.000	0.190	0.003	0.000	0.163	0.357	0.000	-	0.000

Table S2. Detection frequencies, median, mean and ranges of OHPAHs concentrations ($\mu\text{g L}^{-1}$) in cases' and controls' samples.

	1OHNAP	2OHNAP	1OHPHE	2OHPHE	3OHPHE	9OHPHE	1OHPYR	Σ OHPAHs
Cases (n=96)								
Detection Frequency (%)	65.6	25.0	96.9	31.2	14.6	36.5	100	
Median	0.71	0.02	1.48	0.01	0.03	0.01	1.87	5.34
Mean	1.02	1.40	2.10	0.12	0.09	0.37	3.13	8.24
Geometric mean	0.29	0.07	1.20	0.03	0.04	0.04	1.88	5.90
Geometric SD	2.45	2.56	1.73	2.03	1.50	2.41	1.58	1.41
Range	0.01-4.59	0.02-29.8	0.02-11.2	0.01-0.78	0.03-1.09	0.01-4.09	0.06-14.9	0.58-45.3
Controls (n=35)								
Detection Frequency (%)	28.6	17.1	62.9	20.0	8.57	11.4	77.1	
Median	0.01	0.015	0.18	0.01	0.03	0.01	0.99	1.76
Mean	0.12	0.13	0.40	0.06	0.03	0.04	1.87	2.67
Geometric mean	0.02	0.03	0.13	0.02	0.03	0.01	0.63	1.57
Geometric SD	1.73	1.73	2.06	1.67	1.17	1.46	2.43	1.68
Range	0.01-1.54	0.01-1.76	0.01-1.95	0.01-1.09	0.03-0.25	0.01-0.80	0.01-8.67	0.11-10.7
<i>p</i> -Value	0.000	0.216	0.000	0.114	0.289	0.003	0.014	0.000

Table S3. Detection frequencies, median, mean and ranges of trace elements' concentrations ($\mu\text{g L}^{-1}$) in cases' and controls' samples.

	As	Ba	Cd	Co	Cr	Cu	Hg	Ni	Pb	Rb
Cases (n=96)										
Detection Frequency (%)	75	100	80.2	73.9	100	100	93.7	86.5	100	100
Median	3.39	1.35	0.64	0.74	0.40	1369	3.33	0.98	19.8	166
Mean	3.25	1.53	0.76	0.69	0.47	1332	3.84	1.06	22.0	186
Geometric mean	1.87	1.26	0.49	0.46	0.32	1285	2.37	0.69	20.1	171
Geometric SD	1.74	1.35	1.60	1.60	1.52	1.12	1.96	1.67	1.20	1.19
Range	0.25-13.9	0.15-4.67	0.08-2.97	0.08-2.57	0.05-1.90	694-2308	0.01-12.4	0.05-3.37	5.18-77.0	71.6-597
Controls (n=35)										
Detection Frequency (%)	60	85.7	57.1	60	94.2	100	71.4	68.6	82.9	100
Median	0.98	1.48	0.17	0.56	0.57	1037	0.68	0.23	6.44	178
Mean	1.26	1.44	0.22	0.69	0.70	1027	0.80	0.30	5.94	195
Geometric mean	0.77	1.24	0.16	0.36	0.51	1009	0.25	0.19	2.75	188
Geometric SD	1.57	1.31	1.39	1.76	1.48	1.08	2.54	1.59	2.30	1.13
Range	0.25-4.57	0.35-2.92	0.08-1.05	0.08-2.80	0.05-2.39	654-1583	0.01-3.57	0.05-0.94	0.05-13.8	111-353
<i>p</i> -Value	0.000	0.942	0.000	0.520	0.006	0.000	0.000	0.000	0.000	0.102

Table S4. Varimax rotated PCA for PAHs, OHPAHs and trace elements for overall dataset used for logistic regression model.

Variance (%)	16.9	13.4	10.5
	1	2	3
ACE	.765	.352	.220
PHE	.748	.256	.419
FLT	.742	.304	.401
NAP	.690	.016	.278
1OHPYR	.686	.302	-.299
FL	.653	.303	.399
PYR	.643	.362	.389
ANT	.641	.206	.311
3OHPHE	.544	-.042	-.157
2OHPHE	.456	-.113	.031
9OHPHE	.456	.246	-.168
Ba	.386	.135	-.117
ACY	.294	-.051	.001
Rb	-.207	.093	-.154
Cd	.182	.710	.103
Hg	.140	.666	.182
1OHPHE	-.003	.641	-.095
Ni	.080	.604	.251
1OHNAP	.127	.577	.016
Pb	.242	.543	.317
Cu	.091	.506	.065
As	-.001	.504	.369
2OHNAP	.216	.402	-.199
Co	-.061	.399	-.147
BaP	-.014	.371	-.035
CHR	.023	-.006	.707
DBA	-.054	.085	.632
BFA	.248	.250	.601
BaA	.288	.062	.585
Cr	.035	.094	-.370
IPY	.022	.012	.215

Table S5. Hosmer and Lemeshow Test.

Hosmer and Lemeshow Test			
Step	Chi-square	df	Sig.
1	.099	8	1.000

Table S6. Varimax rotated PCA for PAHs, OHPAHs and trace elements for cases' samples classified in terms of the residence area. (Loadings > 0.600 appeared in bold).

Variance (%)	Urban			Industrial			Rural		
	17.0	11.9	9.8	19.3	13.5	10.4	17.1	15.6	13.4
	1	2	3	1	2	3	1	2	3
NAP	.587	.337	-.241	.759	-.031	.149	.041	-.408	.079
ACY	.156	.537	.063	.439	-.129	-.162	-.128	.032	.587
ACE	.434	.783	-.063	.696	.388	.300	.412	.079	.808
FL	.374	.169	-.046	.845	.202	.116	.933	-.224	.058
PHE	.804	.285	-.151	.857	.081	-.229	.401	-.619	.164
ANT	.387	.312	-.003	.792	.147	.110	.554	.062	.273
FLT	.709	.388	-.075	.880	.132	-.154	.849	-.370	.110
PYR	.820	.218	.161	.675	.085	.306	.233	-.005	.243
CHR	.006	.000	.261	.399	-.605	.304	.023	-.225	.805
BaA	.272	.052	.603	.539	-.488	.206	.201	-.320	.537
BFA	.212	-.019	.336	.664	-.214	.101	-.069	-.009	.627
BaP	.305	-.075	.050	-.051	-.120	.412	.678	.337	-.179
IPY	-.068	-.016	.369	.033	-.178	.587	.085	.128	.558
DBA	-.453	-.135	-.121	.134	-.669	.466	.093	-.515	.340
OHNAP1	.274	-.251	.227	-.132	.366	.550	.366	.809	.126
OHNAP2	-.196	.785	-.013	.038	.454	.183	.876	.178	-.057
OHPHE1	-.163	.611	.109	-.130	.432	-.095	.028	.631	-.122
OHPHE2	.719	-.106	-.093	.157	.228	.269	-.038	-.518	-.041
OHPHE3	.419	.058	-.091	.271	.324	-.134	.186	-.155	.295
OHPHE9	.598	-.022	.021	.107	.550	.061	.006	.211	.631
OHPYR1	.689	.177	.096	.356	.819	.044	.507	.380	-.031
As	-.218	.085	.600	.215	-.099	-.219	.244	.566	.096
Ba	.269	.528	-.162	.183	.562	.195	.359	-.184	-.328
Cd	.331	.409	.514	.090	.216	.499	.631	.496	-.203
Co	-.195	.242	.663	-.190	.520	.073	.470	.296	.300
Cr	.154	.496	.045	-.035	.350	.494	.265	.582	.182
Cu	.047	.355	.323	-.187	.167	-.610	.103	.598	-.004
Hg	-.069	.000	.560	-.119	.480	.620	.504	.159	.079
Ni	.143	-.123	.746	.119	.334	.134	.363	.323	.185
Pb	.330	.488	.176	.147	-.007	-.168	.039	.668	.021
Rb	-.315	.049	-.143	-.206	-.029	-.426	.014	.135	-.588

Table S7: Analytical method recovery rates, LoD and LoQ for the determination of PAHs and OH-PAHs in human serum

NAME	Recovery rate				LOD ng mL ⁻¹	LOQ ng mL ⁻¹
	25ng mL ⁻¹	RSD%	50ng mL ⁻¹	RSD%		
NaP	110	10.2	82.6	30.3	0.11	0.32
ACY	136	17.7	132	8.09	0.03	0.09
ACE	96.5	5.94	128	9.42	0.03	0.01
FL	99.1	10.8	124	6.38	0.02	0.07
PHE	89.4	60.1	104	10.1	0.03	0.10
ANT	138	19.9	131	7.72	0.01	0.034
FLT	106	14.3	96	1.41	0.09	0.27
PYR	98.3	2.43	107	7.54	0.09	0.27
CHR	122	13.1	131	0.33	0.04	0.12
BaA	77.8	8.10	80.8	1.07	0.01	0.026
BFA	70.2	11.1	84.9	6.83	0.003	0.009
BaP	112	8.61	114	15.5	0.001	0.003
IPY	89.4	10.2	81.3	9.24	0.02	0.07
DBA	79.0	10.0	72.5	14.2	0.003	0.009
BPE	78.7	9.35	70.9	4.23	0.002	0.006
1OHNAP	72.5	10.9	77.7	16.7	0.03	0.09
2OHNAP	77.3	12.3	79.1	14.2	0.03	0.09
1OHPHE	82.1	9.9	83.2	12.2	0.03	0.09
2OHPHE	86.7	8.8	85.6	14.3	0.02	0.06
3OHPHE	88.0	10.4	89.4	12.2	0.05	0.15
9OHPHE	93.1	8.6	92.1	9.7	0.02	0.06
1OHPYR	91.8	10.3	94.4	10.9	0.03	0.09