

1 **Supplementary Material: tobacco-specific and combustion pollutants in settled**
2 **house dust in Malta**

3
4 **Details of the extraction, cleaning and concentration of PAHs, Nicotine, Nicotelline**
5 **and TSNA from settled house dust (SHD).**

6
7 **Extraction of PAHs**

8 Approximately 200 mg of sieved SHD were weighed and placed in a 16 × 125 culture
9 tube. 50 µL of Nicotine-d₄ internal standard and 50 µL of Nicotelline + TSNA internal
10 standard mix were prepared in advance in 0.5 mL 1M H₂SO₄ per sample. Similarly, 50
11 µL of PAH internal standard mix was prepared in 0.5 mL DCM/Pentane (50:50) per
12 sample. Each dust sample was spiked with the abovementioned internal standard mixes
13 and 1.5 mL of water and 5 mL of DCM/Pentane(50:50) were added. The mix was
14 vortexed for 30 s and sonicated for 30 min at 25 °C. After vortexing for 30 s, the tubes
15 were centrifuged at 3700 rpm for 4 min and then frozen in an acetone-dry ice bath.

16
17 The organic phase (this is Fraction 1) was transferred in a 13 × 100 tube and kept for
18 PAHs analysis.

19
20 **Fraction 1: PAHs**

21 This fraction was blown to dryness at 25 °C under a gentle stream of nitrogen and
22 reconstituted with 500 µL of hexane. 300 mg of anhydrous sodium sulfate as a drying
23 agent were added to an Agilent Bond Elut 10 mL, 1 mg silica column. The silica
24 column was prewashed with 3 mL MeOH followed by 3 mL acetone, conditioned with
25 3mL hexane/DCM (50:50) followed by 6 mL hexane, loaded with 500 µL of
26 reconstituted extract in hexane and eluted with 6 mL of hexane/DCM (70:30) in a 13 ×
27 100 tube. 200 µL of m-xylene were spiked in the collected eluent and blown down
28 under a gentle stream of nitrogen to a final extract volume of 200 µL which was



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29 transferred with a glass Pasteur pipette in a GC vial with a 250 μ L insert. 2 μ L were
30 injected in a GC-MS.

31

32 **Extraction of Nicotelline + TSNAs**

33 After Fraction 1 was removed, 1 mL of 45% potassium carbonate + 5% Na₄EDTA were
34 added to the remaining aqueous phase followed by 8 mL of DCM/Pentane/EtOAc/IPA
35 (40:40:15:5). After vortexing for 1 min and centrifuging at 3700 rpm for 4 min, the two
36 phases were placed in an acetone-dry ice bath.

37

38 At this stage the organic phase was split as follows:

39 Fraction 2: In a 13 \times 100 tube containing 0.5 mL of 1M H₂SO₄, 3 mL of the organic
40 phase were poured, for **Nicotine** to be extracted from it.

41

42 Fraction 3: In another 13 \times 100 tube containing 0.5 mL of 1M H₂SO₄, the remaining 5
43 mL of the organic phase were poured, for **Nicotelline + TSNAs** to be extracted from it.

44

45 Both Fractions 2 & 3 were vortexed for 1 min, centrifuged at 3700 rpm for 4 min and
46 frozen in an acetone-dry ice bath after which the organic phase was discarded.

47

48 Fraction 2: Nicotine

49 The remaining aqueous phase was neutralized with 0.5 mL 50% K₂CO₃/2N NH₄OH
50 and 0.5 mL 90:10 Toluene/Butanol were added. The two phases were vortexed for 1
51 min, centrifuged at 3700 rpm for 3 min and frozen in an acetone-dry ice bath. The 0.5
52 mL organic phase was poured in an EDTA deactivated GC vial and injected 2 μ L in
53 GC-MS.

54

55 Fraction 3: Nicotelline + TSNAs

56 The remaining aqueous phase was neutralized with 0.5 mL 45% K₂CO₃/5% Na₄EDTA
57 and 5 mL 40:40:15:5 DCM/Pent/EtAc/IPA were added. The mixture was vortexed for 1
58 min, centrifuged at 3700 rpm for 3 min and frozen in an acetone-dry ice bath. The
59 organic phase was poured in a 13 \times 100 tube and spiked with 100 μ L of 1% HCl in
60 MeOH and dried at 60 °C under a gentle nitrogen flow. Reconstitution of analytes was
61 done with 200 μ L 0.1 M ammonium formate in 20% MeOH. 30 μ L were injected in

62 LC-MS/MS.

63

64 **Supplementary Table 1. Characteristics and statistics of districts in Malta**

District	Name	Population	Area ^a (%)	Type
1	Northern Harbour	131,056	7.6	Urban
2	Northern	69,467	23.3	Urban background/Rural
3	Southern Harbour	80,170	8.3	Urban/Harbour
4	Western	59,817	22.9	Urban background/Rural
5	South Eastern	68,044	17.2	Quarries/industrial/ Trans-shipment hub

65 ^aPercentage area occupied by district in relation to the surface area of Malta.

66

67 **Supplementary Table 2. Precision and accuracy for determination of nicotine,**
68 **nicotelline, TSNAs and PAHs in analyte spiked clay soil^a used as QC samples**

Pollutant	LOQ (ng/g)	Actual (ng/g)	Measured (ng/g)	SD (ng/g)	% RSD	% Accuracy	% Recovery
Nicotine	1.4	1000.0	976.9	20.7	2.1	-2.3	97.7
		333.3	351.3	0.5	0.1	5.4	105.4
		111.1	115.2	0.5	0.4	3.7	103.7
		37.0	38.0	0.3	0.7	2.7	102.7
		12.3	12.4	0.0	0.3	0.3	100.3
		4.1	4.3	0.1	1.5	4.8	104.8
		1.4	1.2	0.0	1.6	-14.5	85.5
Nicotelline	0.36	100.0	91.4	7.6	8.3	-8.6	91.4
		33.3	32.1	2.6	8.3	-3.7	96.3
		11.1	11.8	1.2	9.9	5.8	105.8

		3.7	4.0	0.2	5.5	8.8	108.8
		1.2	1.3	0.1	6.3	6.4	106.4
		0.4	0.4	0.0	6.2	-4.9	95.1
NNK	0.14	100.0	100.3	0.4	0.4	0.3	100.3
		33.3	30.4	3.7	12.3	-8.7	91.3
		11.1	10.9	0.4	3.5	-2.2	97.8
		3.7	3.7	0.2	6.3	-0.2	99.8
		1.2	1.2	0.1	9.4	0.7	100.7
		0.4	0.4	0.0	5.8	3.5	103.5
		0.1	0.1	0.0	9.5	4.2	104.2
NNN	0.02	100.0	79.5	18.0	22.6	-20.5	79.5
		33.3	26.9	0.6	2.2	-19.3	80.7
		11.1	10.5	0.8	7.7	-5.4	94.6
		3.7	3.8	0.2	4.8	2.5	102.5
		1.2	1.3	0.0	3.6	3.2	103.2
		0.4	0.4	0.0	7.1	-5.2	94.8
NAB	1.23	100.0	92.9	4.9	5.2	-7.1	92.9
		33.3	34.1	0.9	2.6	2.3	102.3
		11.1	11.4	0.7	6.2	2.8	102.8
		3.7	3.9	0.1	2.8	4.9	104.9
		1.2	1.2	0.1	7.1	1.0	101.0
NAT	0.02	100.0	100.2	4.2	4.2	0.2	100.2
		33.3	33.3	0.1	0.3	-0.2	99.8
		11.1	11.0	0.3	3.1	-1.2	98.8
		3.7	3.7	0.0	1.0	1.2	101.2
		1.2	1.2	0.0	1.0	0.8	100.8
		0.4	0.4	0.0	2.1	1.9	101.9
		0.1	0.1	0.0	1.2	-2.0	98.0

		0.05	0.0	0.0	0.9	-2.1	97.9
		0.02	0.0	0.0	1.8	-0.2	99.8
Ph	0.82	200.0	172.2	23.2	13.5	-13.9	86.1
		66.7	66.1	1.4	2.1	-0.9	99.1
		22.2	22.6	0.9	4.0	1.7	101.7
		7.4	6.8	0.1	0.7	-8.2	91.8
		2.5	2.5	0.2	8.6	0.6	100.6
		0.8	0.9	0.0	4.3	3.7	103.7
An	0.09	200.0	179.6	18.1	10.1	-10.2	89.8
		66.7	66.0	1.5	2.3	-0.9	99.1
		22.2	23.5	0.9	4.0	5.7	105.7
		7.4	6.8	0.3	4.6	-7.6	92.4
		2.5	2.4	0.1	5.3	-3.5	96.5
		0.8	0.9	0.0	2.4	8.0	108.0
Fluo	2.47	200.0	182.1	13.8	7.6	-8.9	91.1
		66.7	65.6	0.4	0.6	-1.6	98.4
		22.2	23.6	0.2	1.0	6.4	106.4
		7.4	7.1	0.2	2.2	-3.6	96.4
		2.5	2.4	0.1	2.7	-1.2	98.8
Pyr	7.41	200.0	186.8	16.8	9.0	-6.6	93.4
		66.7	66.5	4.1	6.2	-0.3	99.7
		22.2	23.9	1.2	4.9	7.5	107.5
		7.4	6.9	0.3	4.6	-6.8	93.2
		2.5	2.5	0.1	2.3	1.7	101.7
B(a)A	0.09	200.0	184.5	11.4	6.2	-7.7	92.3
		66.7	64.9	2.0	3.2	-2.7	97.3
		22.2	23.9	0.4	1.7	7.4	107.4
		7.4	6.8	0.2	3.6	-7.7	92.3
		2.5	2.3	0.1	4.3	-4.9	95.1

		0.3	0.3	0.0	1.1	10.7	110.7
		0.1	0.1	0.0	12.3	2.8	102.8
Chry	2.47	200.00	181.73	18.01	9.91	-9.14	90.86
		66.67	64.11	4.64	7.23	-3.84	96.16
		22.22	24.40	1.79	7.34	9.82	109.82
		7.41	7.01	0.27	3.85	-5.39	94.61
		2.47	2.52	0.13	5.01	2.10	102.10
B(b)F	2.47	200.0	181.5	14.6	8.0	-9.2	90.8
		66.7	62.6	4.0	6.4	-6.1	93.9
		22.2	23.7	1.0	4.4	6.7	106.7
		7.4	6.9	0.2	3.4	-7.2	92.8
		2.5	2.5	0.1	5.4	1.6	101.6
B(a)P	0.09	200.0	185.8	12.0	6.4	-7.1	92.9
		66.7	64.5	3.1	4.8	-3.2	96.8
		22.2	24.2	1.6	6.6	8.9	108.9
		7.4	6.8	0.3	3.9	-7.6	92.4
		2.5	2.4	0.2	9.4	-1.3	98.7
IndP	2.47	200.0	187.1	9.9	5.3	-6.5	93.5
		66.7	66.0	1.4	2.2	-1.0	99.0
		22.2	26.4	2.5	9.4	18.9	118.9
		7.4	7.0	0.2	3.4	-5.8	94.2
		2.5	2.5	0.1	3.6	-0.4	99.6
		0.8	1.0	0.1	13.1	15.5	115.5
D(ah)A	0.09	200.0	195.2	4.8	2.5	-2.4	97.6
		66.7	66.0	1.6	2.4	-1.0	99.0
		7.4	7.2	0.3	4.4	-2.5	97.5
		2.5	2.6	0.1	3.7	5.7	105.7
		0.3	0.3	0.0	3.3	-5.1	94.9

		0.1	0.1	0.0	5.4	4.0	104.0
B(ghi)P	0.27	200.0	201.0	6.7	3.3	0.5	100.5
		66.7	68.4	2.2	3.2	2.6	102.6
		7.4	7.0	0.3	4.6	-5.2	94.8
		2.5	2.4	0.1	4.7	-2.0	98.0
		0.8	0.9	0.0	2.9	10.4	110.4

69 ^aAn aqueous solution of nicotelline, nicotine, TSNAs and PAHs containing the
70 specified amounts was added to 200 mg powdered, dried clay soil. Samples were
71 extracted and analyzed as described for the SHD in the experimental section. For all
72 compounds, results are based on the mean of four replicates. LOQ: Limit of
73 quantitation (ng/g); SD: standard deviation; RSD: relative standard deviation.

74

75 **Supplementary Table 3. Equations for typical standard curves**

Pollutant	Concentration range (ng/g)	Slope^a	Intercept	Correlation coefficient (r²)
Nicotine	0-200,000	0.191056	0.00698	0.9986
Nicotelline	0-200	0.35566	0.00184	0.9982
NNK	0-200	0.206839	-0.00759	0.9992
NNN		0.144304	-0.00012	1.0000
NAT		0.133022	1.99774	0.9993
NAB		0.786727	0.145523	0.9976
Ph	0-10,000	0.227839	0.062935	0.9975
An		0.016556	0.004256	0.9903
Fluo		0.037721	0.054607	0.9979
Pyr		0.035267	0.038995	0.9991
BaA		0.035974	0.013190	0.9939
Chry		0.032483	0.005760	0.9940
BbF		0.034311	0.003298	0.9938
BaP		0.025556	0.012023	0.9998

IndP		0.030388	0.012978	0.9998
DahA		0.047156	-0.006188	0.9992
BghiP		0.037242	0.013107	0.9993

76 ^aEquations were determined by linear regression: response ratio = a × (amount ratio) +
77 intercept.

78

79 **Supplementary Table 4. Descriptive statistics for all pollutants (in ng/g) of outdoor deposited house dust collected in Malta**

Pollutant	Valid <i>n</i>	Detection frequency (%)	Mean	SD	Min	Max (ng/g)	Q1	Q2	Q3
Nicotine	16	80	3692	11428	75	46,364	213	580	1414
Nicotelline	20	100	2	4	0	17	0	1	2
NNK	20	100	0.5	0.9	0.0	2.9	0.1	0.2	0.3
NNN	20	100	0.4	1.0	0.0	4.3	0.0	0.1	0.2
NAT	20	100	0.2	0.4	0.0	2.1	0.0	0.0	0.1
NAB	20	100	0.2	0.2	0.0	0.7	0.1	0.1	0.3
Σ TSNA	20	100	1.3	2.3	0.1	9.9	0.2	0.5	0.9
Ph	20	100	135	81	24	326	82	110	180
An	20	100	13	10	1	37	6	10	21
Fluo	20	100	178	124	32	506	83	152	246
Pyr	18	90	171	110	33	463	104	135	207



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BaA	20	100	57	37	5	146	31	54	84
Chry	20	100	110	73	15	308	56	97	156
BbF	20	100	87	62	16	276	43	85	114
BaP	20	100	78	50	11	202	44	77	101
IndP	20	100	74	49	13	196	32	70	100
DahA	20	100	18	14	2	44	7	17	27
BghiP	20	100	92	61	14	257	40	90	106
Σ PAH	20	100	1074	717	133	3034	599	1009	1265

80 Q1, Q2, Q3 are the 25th, 50th and 75th percentiles respectively.

81

82 **Supplementary Table 5. Mann Whitney U test for all pollutants in SHD to check statistical difference across smoking and non-smoking**
 83 **houses**

Test statistics^{a,b}																			
	Nico tine	Nicot elline	NN K	NN N	NA B	NA T	ΣTS NA	Ph	An	Fluo	Pyr	BaA	Chr y	BbF	BaP	Ind P	Dah A	Bgh iP	ΣP AH
Mann-W hitney <i>U</i>	8.00 0	128.0 00	132. 000	88.0 00	131. 500	99.5 00	112. 000	121. 000	157. 000	51.0 00	46.0 00	65.0 00	45.0 00	48.0 00	92.0 00	54. 000	81.0 00	101. 000	74.0 00
Wilcoxo	74.0	869.0	873.	829.	872.	840.	853.	226.	262.	106.	101.	143.	111.	103.	158.	90.	172.	192.	179.

n W	00	00	000	000	500	500	000	000	000	000	000	000	000	000	000	000	000	000	000
Z	-3.3	-3.334	-3.2	-4.1	-3.2	-3.9	-3.6	-2.2	-1.3	-3.0	-3.1	-3.2	-3.5	-3.1	-2.0	-2.2	-3.0	-2.5	-3.5
	10		59	36	68	16	37	43	35	23	84	02	31	20	45	87	15	85	06
Asymp.	<	<	0.00	<	0.00	<	<	0.02	0.18	0.00	0.00	0.00	<	0.00	0.04	0.0	0.00	0.01	<
Sig.	0.00	0.001	1	0.00	1	0.00	0.00	5	2	2	1	1	0.00	2	1	22	3	0	0.00
(2-tailed)	1			1		1	1						1						1
Exact	<									0.00	<	<	<	0.00	0.04	0.0	0.00		
Sig.	0.00									2 ^b	0.00	0.00	0.00	1 ^b	1 ^b	21 ^b	2 ^b		
[2*(1-tailed Sig.)]	1 ^b										1 ^b	1 ^b	1 ^b						

84 ^aGrouping variable: smoker; ^bnot corrected for ties.

85

86 **Supplementary Table 6. Kruskal-Wallis H test for all pollutants in SHD to check statistical difference across the different districts in**

87 **Malta**

Test statistics ^{a,b}																			
	Nicoti	Nicotell	NN	NN	NA	NA	∑TS	Ph	An	Flu	Pyr	Ba	Chr	Bb	BaP	Ind	Dah	Bgh	∑PA

	ne	ine	K	N	T	B	NA			o		A	y	F		P	A	iP	H
Kruskal-Wallis H	3.941	4.262	5.995	4.010	.933	.992	5.579	4.150	1.790	5.411	3.922	3.163	3.825	4.816	4.596	3.565	3.392	4.558	4.068
df	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
Asymp. Sig.	0.414	0.372	0.200	0.405	0.920	0.911	0.233	0.386	0.774	0.248	0.417	0.531	0.430	0.307	0.331	0.468	0.495	0.336	0.397

88 ^aKruskal Wallis test; ^bGrouping variable: district.

89

90 **Supplementary Table 7. Spearman rho correlation plot for nicotine, nicotelline, TSNA and PAHs**

		Correlations																		
Spearman's rho	Nicotine	Nicotine	NK	NN	NAT	NAB	TOTALSNA	PH	AN	Fluo	Fyr	BAA	Chr7	BBF	BAP	INDP	DANA	BgnIP	TOTALPAH	
	Correlation Coefficient	1.000																		
	Sig. (2-tailed)																			
N	54																			
	Correlation Coefficient	.697	1.000																	
	Sig. (2-tailed)	0.000																		
N	21	21																		
	Correlation Coefficient	.905	.709	1.000																
	Sig. (2-tailed)	0.000	0.000																	
N	54	21	54																	
	Correlation Coefficient	.819	.760	.847	1.000															
	Sig. (2-tailed)	0.000	0.000	0.000																
N	54	21	54	54																
	Correlation Coefficient	.605	.760	.816	.790	1.000														
	Sig. (2-tailed)	0.000	0.000	0.000	0.000															
N	54	21	54	54	54															
	Correlation Coefficient	.459	.612	.609	.572	.530	1.000													
	Sig. (2-tailed)	0.000	0.003	0.000	0.000	0.000														
N	54	21	54	54	54	54														
	Correlation Coefficient	.883	.765	.972	.903	.717	.708	1.000												
	Sig. (2-tailed)	0.000	0.000	0.000	0.000	0.000	0.000													
N	54	21	54	54	54	54	54													
	Correlation Coefficient	-0.073	-0.187	0.026	-0.076	0.210	-0.038	-0.038	1.000											
	Sig. (2-tailed)	0.637	0.458	0.867	0.822	0.171	0.788	0.802												
N	44	18	44	44	44	44	44	44	44											
	Correlation Coefficient	0.117	-0.362	0.099	-0.019	-0.127	0.058	0.071	.625	1.000										
	Sig. (2-tailed)	0.451	0.140	0.523	0.802	0.412	0.708	0.647	0.000											
N	44	18	44	44	44	44	44	44	44	44										
	Correlation Coefficient	-0.143	-.532	-0.112	-0.283	-0.271	-0.231	-0.160	.845	.589	1.000									
	Sig. (2-tailed)	0.385	0.034	0.496	0.121	0.095	0.157	0.332	0.000	0.000										
N	39	16	39	39	39	39	39	39	39	39	39									
	Correlation Coefficient	-0.070	-0.331	-0.028	-0.241	-0.283	-0.173	-0.095	.806	.702	.936	1.000								
	Sig. (2-tailed)	0.672	0.185	0.867	0.140	0.121	0.293	0.565	0.000	0.000	0.000									
N	39	17	39	39	39	39	39	39	39	39	39	39								
	Correlation Coefficient	-0.086	-.568	-0.131	-.307	-0.174	-0.174	.769	.737	.922	.928	1.000								
	Sig. (2-tailed)	0.544	0.016	0.408	0.046	0.048	0.289	0.271	0.000	0.000	0.000	0.000								
N	42	18	42	42	42	42	42	42	42	42	42	42	42							
	Correlation Coefficient	-0.085	-.496	-0.063	-0.287	-.328	-0.176	-0.132	.777	.672	.922	.973	.949	1.000						
	Sig. (2-tailed)	0.596	0.036	0.697	0.068	0.036	0.271	0.413	0.000	0.000	0.000	0.000	0.000							
N	41	18	41	41	41	41	41	41	41	41	41	41	41	41						
	Correlation Coefficient	-0.135	-.521	-0.146	-0.299	-.325	-0.236	-0.195	.745	.616	.926	.953	.942	.956	1.000					
	Sig. (2-tailed)	0.413	0.039	0.374	0.005	0.044	0.149	0.233	0.000	0.000	0.000	0.000	0.000	0.000						
N	39	16	39	39	39	39	39	39	39	39	39	39	39	39	39					
	Correlation Coefficient	-0.102	-0.224	-0.127	-0.205	-0.204	-0.180	-0.156	.702	.773	.776	.852	.871	.813	.833	1.000				
	Sig. (2-tailed)	0.530	0.405	0.434	0.204	0.206	0.265	0.336	0.000	0.000	0.000	0.000	0.000	0.000	0.000					
N	40	16	40	40	40	40	40	40	40	40	40	40	40	40	40	40				
	Correlation Coefficient	-0.069	-0.339	-0.093	-0.199	-0.199	-0.091	-0.116	.752	.651	.926	.889	.940	.910	.969	.846	1.000			
	Sig. (2-tailed)	0.684	0.216	0.688	0.240	0.262	0.592	0.484	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000				
N	37	15	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37			
	Correlation Coefficient	-0.170	-.527	-0.180	-.304	-.322	-0.134	-0.208	.667	.676	.873	.863	.904	.889	.913	.906	.951	1.000		
	Sig. (2-tailed)	0.277	0.025	0.249	0.048	0.035	0.393	0.186	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			
N	43	18	43	43	43	43	43	43	43	43	43	43	43	43	43	43	43	43		
	Correlation Coefficient	-0.080	-0.360	-0.102	-0.212	-0.239	-0.095	-0.115	.701	.640	.894	.903	.893	.913	.936	.903	.965	.957	1.000	
	Sig. (2-tailed)	0.607	0.142	0.509	0.166	0.119	0.721	0.458	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
N	44	18	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	
	Correlation Coefficient	-0.116	-0.389	-0.095	-0.249	-.300	-0.086	-0.134	.851	.650	.935	.973	.950	.971	.946	.886	.919	.873	.905	1.000
	Sig. (2-tailed)	0.482	0.111	0.579	0.101	0.045	0.579	0.382	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	
N	45	18	45	45	45	45	45	45	45	45	45	45	45	45	45	45	45	45	45	45

***. Correlation is significant at the 0.01 level (2-tailed).
 **. Correlation is significant at the 0.05 level (2-tailed).

92

93 **Supplementary Table 8. Nicotine, Σ TSNA and Σ PAH concentrations (in ng/g) and % load of pollutant in indoor/outdoor and**
 94 **smoker/non-smokers' SHD**

Place	N	Nicotine (%)	Σ TSNA (%)	Σ PAH (%)
Indoor	54	18246 85.1	26 0.1	3169 14.8
Outdoor	20	3692 77.4	1.3 0.1	1074 22.5
Indoor-smokers	16	37366 97.9	40 0.1	762 2.0
Indoor-non-smokers	30	864 16.8	20 0.4	4256 82.8

95 All concentrations are mean values (in ng/g).