

Supplementary Information

PCDD/Fs and PCBs in Soils: a Study of Case in the City of Belo Horizonte-MG

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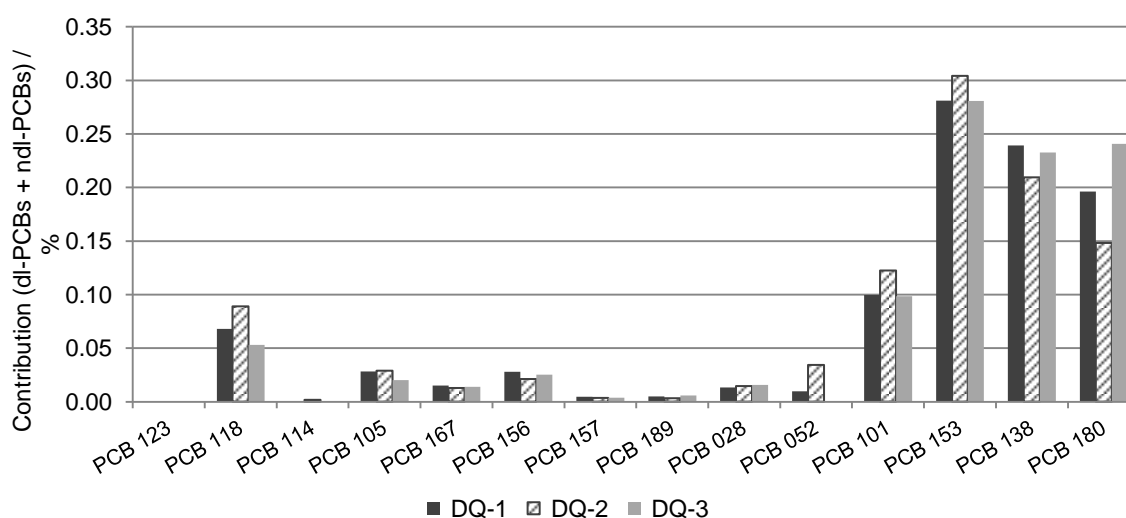


Figure S1. Contribution of MO-PCBs and ndl-PCBs in soils from the DQ area.

Table S1. Information on native and labeled PCDD/Fs and PCBs compounds

Labeled compound		Native compound	
Code	PCDD/Fs	Code	PCDD/Fs
EF-999	¹³ C-2,3,7,8-TCDF	EF-909B-5	2,3,7,8-TCDF
EF-999	¹³ C-1,2,3,7,8-PeCDF	EF-909B-5	1,2,3,7,8-PeCDF
EF-999	¹³ C-2,3,4,7,8-PeCDF	EF-909B-5	2,3,4,7,8-PeCDF
EF-999	¹³ C-1,2,3,4,7,8-HxCDF	EF-909B-5	1,2,3,4,7,8-HxCDF
EF-999	¹³ C-1,2,3,6,7,8-HxCDF	EF-909B-5	1,2,3,6,7,8-HxCDF
EF-999	¹³ C-1,2,3,7,8,9-HxCDF	EF-909B-5	2,3,4,6,7,8-HxCDF
EF-999	¹³ C-1,2,3,7,8,9-HxCDF	EF-909B-5	1,2,3,7,8,9-HxCDF
EF-999	¹³ C-1,2,3,4,6,7,8-HpCDF	EF-909B-5	1,2,3,4,6,7,8-HpCDF

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Table S1. Information on native and labeled PCDD/Fs and PCBs compounds (cont.)

Labeled compound		Native compound	
EF-999	¹³ C-1,2,3,4,7,8,9-HpCDF	EF-909B-5	1,2,3,4,7,8,9-HpCDF
EF-999	¹³ C-OCDF	EF-982	OCDF
ED-998	¹³ C-2,3,7,8-TCDD	ED-906B-5	2,3,7,8-TCDD
ED-998	¹³ C-1,2,3,7,8-PeCDD	ED-906B-5	1,2,3,7,8-PeCDD
ED-998	¹³ C-1,2,3,4,7,8-HxCDD	ED-906B-5	1,2,3,4,7,8-HxCDD
ED-998	¹³ C-1,2,3,6,7,8-HxCDD	ED-906B-5	1,2,3,6,7,8-HxCDD
ED-998	¹³ C-1,2,3,7,8,9-HxCDD	ED-906B-5	1,2,3,7,8,9-HxCDD
ED-998	¹³ C-1,2,3,4,6,7,8-HpCDD	ED-906B-5	1,2,3,4,6,7,8-HpCDD
ED-998	¹³ C-OCDD	ED-980	OCDD
	NO-PCBs		NO-PCBs
EC-4187	¹³ C-PCB81	EC-4986	PCB 81
EC-4187	¹³ C-PCB77	EC-4986	PCB 77
EC-4187	¹³ C-PCB126	EC-4986	PCB 126
EC-4187	¹³ C-PCB169	EC-4986	PCB 169
	MO-PCBs		MO-PCBs
EC-4188	¹³ C-PCB123	EC-4987	PCB 123
EC-4188	¹³ C-PCB118	EC-4987	PCB 118
EC-4188	¹³ C-PCB114	EC-4987	PCB 114
EC-4188	¹³ C-PCB105	EC-4987	PCB 105
EC-4188	¹³ C-PCB167	EC-4987	PCB 167
EC-4188	¹³ C-PCB156	EC-4987	PCB 156
EC-4188	¹³ C-PCB157	EC-4987	PCB 157
EC-4188	¹³ C-PCB189	EC-4987	PCB 189
	ndl-PCBs		ndl-PCBs
EC-4058	¹³ C-PCB028	EC-5179	PCB 28
EC-4058	¹³ C-PCB052	EC-5179	PCB 52
EC-4058	¹³ C-PCB101	EC-5179	PCB 101
EC-4058	¹³ C-PCB153	EC-5179	PCB 153
EC-4058	¹³ C-PCB138	EC-5179	PCB 138
EC-4058	¹³ C-PCB180	EC-5179	PCB 180
ED-911	recovery standard ¹³ C-1,2,3,4-TCDD		
EF-999	recovery standard ¹³ C-2,3,4,6,7,8-HxCDF		
ED-907	clean up standard ³⁷ Cl ₄ -2,3,7,8-TCDD		

PCDD/Fs: polychlorinated dibenzo-*p*-dioxins and polychlorinated dibenzofurans; TCDF: tetra chlorinated furan; PeCDF: penta chlorinated furan; HxCDF: hexa chlorinated furan; HpCDF: hepta chlorinated furan; OCDF: octa chlorinated furan; TCDD: tetra chlorinated dioxin; PeCDD: penta chlorinated dioxin; HpCDD: hexa chlorinated dioxin; HpCDD: hepta chlorinated dioxin; OCDD: octa chlorinated dioxin; dl-PCBs: dioxin-like PCBs; PCB: polychlorinated biphenyls; ndl-PCBs: non-dioxin-like PCBs.

Table S2. Program of automated clean up system with 24 steps described

Step	Step time / min	End step after start / min	Flow / (mL min ⁻¹)	Eluent	Wash	Elute	Tubing	Si	Al ₂ O ₃	Carbon	Collect
1	5	5	10	hexane	x						
2	1	6	10	hexane	x		x	x	x		
3	3	9	10	hexane	x						
4	2	11	10	hexane	x					x	
5	25	36	10	hexane	x			x			
6	1.2	37.2	10	toluene	x		x				
7	4	41.2	10	toluene	x					x	
8	1.2	42.4	10	etac/toluene 1:1	x		x				
9	1	43.4	10	etac/toluene 1:1	x					x	
10	1.2	44.6	10	dcm/hexane 1:1	x		x				
11	2	46.6	10	dcm/hexane 1:1	x					x	
12	1.2	47.8	10	hexane	x		x				
13	3	50.8	10	hexane						x	
14	7.4	58.2	5	aspirate sample				x	x		
15	20	78.2	10	hexane		x		x	x		
16	1.2	79.4	10	dcm/hexane 1:1	x		x				
17	12	91.4	10	dcm/hexane 1:1		x			x	x	A-fraction
18	1.2	92.6	10	etac/toluene 1:1	x		x				
19	0.4	93	10	etac/toluene 1:1		x				x	
20	1.2	94.2	10	hexane	x		x				
21	1	95.2	10	hexane		x				x	
22	1.2	96.4	10	toluene	x		x				
23	15	111.4	5	toluene		x				x	B-fraction
24	1	112.4	1	hexane	x		x				

etac: ethyl acetate; dcm: dichloromethane.

Table S3. Exact masses and ion ratios for each PCDD/F and PCB. Determination coefficients (r^2) for the calibration curves of each PCDD/F and PCB

Compound	Quan m/z	Target m/z	Cl	^{13}C quan m/z	^{13}C Quan m/z	Quan abundance	Target abundance	Ratio	r^2
2378-TCDF	303.9016	305.8987	4	315.9419	317.9389	76	100	0.764	0.9999
12378-PeCDF	339.8597	341.8567	5	351.9000	353.8970	100	65	1.529	0.9999
23478-PeCDF	339.8597	341.8567	5	351.9000	353.8970	100	65	1.529	0.9999
123478-HxCDF	373.8208	375.8178	6	385.8610	387.8580	100	82	1.225	0.9999
123678-HxCDF	373.8208	375.8178	6	385.8610	387.8580	100	82	1.225	0.9999
234678-HxCDF	373.8208	375.8178	6	385.8610	387.8580	100	82	1.225	0.9999
123789-HxCDF	373.8208	375.8178	6	385.8610	387.8580	100	82	1.225	0.9998
1234678-HpCDF	407.7818	409.7789	7	419.8220	421.8191	100	98	1.022	0.9999
1234789-HpCDF	407.7818	409.7789	7	419.8220	421.8191	100	98	1.022	0.9993
OCDF	441.7428	443.7399	8	453.7830	455.7801	88	100	0.877	0.9999
2378-TCDD	319.8965	321.8936	4	331.9368	333.9339	76	100	0.764	0.9999
12378-PeCDD	353.8576	355.8546	5	367.8949	369.8919	61	100	0.613	0.9999
123478-HxCDD	389.8157	391.8127	6	401.8559	403.8530	100	82	1.224	0.9997
123678-HxCDD	389.8157	391.8127	6	401.8559	403.8530	100	82	1.224	0.9998
123789-HxCDD	389.8157	391.8127	6	401.8559	403.8530	100	82	1.224	0.9998
1234678-HpCDD	423.7766	425.7737	7	435.8169	437.8140	100	98	1.021	0.9998
OCDD	457.7377	459.7348	8	469.7780	471.7750	88	100	0.876	0.9988
PCB 081	289.9224	291.9154	4	301.9626	303.9597	77	100	0.767	0.9999
PCB 077	289.9224	291.9154	4	301.9626	303.9597	77	100	0.767	0.9998
PCB 126	325.8804	327.8776	5	337.9207	339.9178	100	65	1.531	0.9997
PCB 169	359.8415	361.8386	6	371.8817	373.8788	100	82	1.227	0.9999

Table S3. Exact masses and ion ratios for each PCDD/F and PCB. Determination coefficients (r^2) for the calibration curves of each PCDD/F and PCB (cont.)

Compound	Quan m/z	Target m/z	Cl	^{13}C quan m/z	^{13}C Quan m/z	Quan abundance	Target abundance	Ratio	r^2
PCB 123	325.8804	327.8776	5	337.9207	339.9178	100	65	1.531	0.9988
PCB 118	325.8804	327.8776	5	337.9207	339.9178	100	65	1.531	0.9987
PCB 114	325.8804	327.8776	5	337.9207	339.9178	100	65	1.531	0.9985
PCB 105	325.8804	327.8776	5	337.9207	339.9178	100	65	1.531	0.9985
PCB 167	359.8415	361.8386	6	371.8817	373.8788	100	82	1.227	0.9985
PCB 156	359.8415	361.8386	6	371.8817	373.8788	100	82	1.227	0.9978
PCB 157	359.8415	361.8386	6	371.8817	373.8788	100	82	1.227	0.9983
PCB 189	393.8025	395.7996	7	405.8428	407.8398	100	98	1.024	0.9976
PCB 028	255.9613	257.9585	3	268.0016	269.9986	100	98	1.020	0.9993
PCB 052	289.9224	291.9154	4	301.9626	303.9597	77	100	0.767	0.9980
PCB 101	325.8804	327.8776	5	337.9207	339.9178	100	65	1.531	0.9982
PCB 153	359.8415	361.8386	6	371.8817	373.8788	100	82	1.227	0.9989
PCB 138	359.8415	361.8386	6	371.8817	373.8788	100	82	1.227	0.9980
PCB 180	393.8025	395.7996	7	405.8428	407.8398	100	98	1.024	0.9981

TCDF: tetra chlorinated furan; PeCDF: penta chlorinated furan; HxCDF: hexa chlorinated furan; HpCDF: hepta chlorinated furan; OCDF: octa chlorinated furan; TCDD: tetra chlorinated dioxin; PeCDD: penta chlorinated dioxin; HpCDD: hexa chlorinated dioxin; HxCDD: hepta chlorinated dioxin; OCDD: octa chlorinated dioxin.

Table S4. Recoveries for the native PCDD/Fs, dl-PCBs, and ndl-PCBs in the blank (diatomaceous earth) spiked and ¹³C-labelled compounds in the soil samples, including the data for the recovery (RS-¹³C-1,2,3,4-TCDD and RS-¹³C-2,3,4,6,7,8-HxCDF) and clean up (CS-³⁷Cl₄-2,3,7,8-TCDD) standards

Sample product	Blank spiked	DQ-1 soil	DQ-2 soil	DQ-3 soil	CS-1 soil	CS-2 soil	CS-3 soil	PC-1 soil	PC-2 soil	PC-3 soil	PR-1 soil	PR-2 soil	PR-3 soil	BV-1 soil	BV-2 soil	BV-3 soil	AL-1 soil	AL-2 soil	AL-3 soil
PCDD/Fs																			
¹³ C-2,3,7,8-	80	81	90	80	85	89	98	82	81	80	91	90	95	97	96	95	99	96	87
¹³ C-1,2,3,7,8-	88	89	87	90	112	87	81	93	90	92	96	105	88	89	93	99	97	96	99
¹³ C-2,3,4,7,8-	93	91	92	94	114	95	96	92	96	98	89	104	90	93	96	104	101	102	100
¹³ C-1,2,3,4,7,8-	86	91	87	86	98	86	91	89	89	90	90	86	87	90	90	90	93	89	85
¹³ C-1,2,3,6,7,8-	84	89	85	84	96	85	83	88	87	88	89	84	85	88	89	88	91	87	83
¹³ C-1,2,3,7,8,9-	96	103	97	91	84	94	101	97	99	92	99	92	94	99	96	98	99	100	92
¹³ C-	83	89	87	83	80	90	94	90	89	84	95	84	83	87	86	84	86	84	84
¹³ C-	87	93	82	83	87	82	80	82	85	81	88	89	90	82	92	91	94	89	80
¹³ C-OCDF	89	94	96	93	82	83	92	92	80	85	81	80	83	80	83	85	88	82	86
¹³ C-2,3,7,8-	87	93	90	89	93	92	88	96	95	93	93	98	89	96	91	91	94	90	92
¹³ C-1,2,3,7,8-	88	89	90	92	113	91	83	93	92	93	92	105	89	90	93	98	97	97	98
¹³ C-1,2,3,4,7,8-	88	96	88	92	80	90	84	93	94	95	93	93	89	93	94	96	98	92	87
¹³ C-1,2,3,6,7,8-	86	95	87	91	89	91	89	91	90	94	93	91	89	92	93	94	97	92	85
¹³ C-1,2,3,7,8,9-	93	88	94	88	98	90	92	88	90	88	99	83	83	95	99	98	102	98	84
¹³ C-	81	86	86	87	83	85	89	87	93	88	91	91	82	90	87	91	94	89	86
¹³ C-OCDD	85	93	89	85	92	84	87	88	80	83	81	80	89	82	85	86	87	84	90
dl-PCBs																			
¹³ C-PCB81	94	95	89	85	102	88	88	82	90	84	83	80	96	87	84	93	81	89	92
¹³ C-PCB77	83	87	89	92	88	88	81	81	82	84	81	93	89	89	83	83	87	87	84
¹³ C-PCB126	88	82	90	83	99	81	80	82	82	95	89	82	88	98	88	81	85	89	84
¹³ C-PCB169	92	91	90	94	111	90	81	91	88	94	88	100	90	87	91	102	93	98	96
¹³ C-PCB123	84	85	82	83	85	88	100	83	84	84	86	87	82	84	85	84	82	98	81
¹³ C-PCB118	89	84	98	82	83	83	92	83	81	85	85	94	83	87	81	84	82	91	85
¹³ C-PCB114	97	91	83	89	82	82	83	81	84	82	84	82	82	84	86	84	86	84	90
¹³ C-PCB105	89	84	82	85	82	87	82	91	98	83	94	93	85	98	82	83	83	88	95
¹³ C-PCB167	85	86	81	88	88	83	88	92	99	82	84	90	82	91	86	85	88	83	82
¹³ C-PCB156	86	90	88	90	92	84	95	90	87	99	92	95	86	95	81	83	82	83	82
¹³ C-PCB157	88	81	82	83	87	93	83	86	86	87	86	96	89	89	85	88	84	82	82
¹³ C-PCB189	84	87	83	88	85	92	89	83	85	88	85	87	90	101	89	87	83	83	94
ndl-PCBs																			
¹³ C-PCB028	83	106	103	107	101	90	87	106	105	104	98	105	99	97	101	99	103	99	101
¹³ C-PCB052	98	112	114	115	108	82	101	100	109	104	111	112	115	111	98	98	106	115	111
¹³ C-PCB101	84	84	85	97	89	88	89	104	98	101	88	105	102	87	89	101	97	99	96
¹³ C-PCB153	85	86	86	84	83	90	83	89	90	84	88	89	93	89	82	87	89	82	88
¹³ C-PCB138	93	99	99	95	99	88	86	91	92	93	98	94	101	102	95	92	95	92	97
¹³ C-PCB180	96	108	107	109	104	99	103	92	92	90	107	92	99	103	83	92	94	92	98

Table S4. Recoveries for the native PCDD/Fs, dl-PCBs, and ndl-PCBs in the blank (diatomaceous earth) spiked and ¹³C-labelled compounds in the soil samples, including the data for the recovery (RS-¹³C-1,2,3,4-TCDD and RS-¹³C-2,3,4,6,7,8-HxCDF) and clean up (CS-³⁷Cl₄-2,3,7,8-TCDD) standards (cont.)

Sample product	Blank	DQ-1	DQ-2	DQ-3	CS-1	CS-2	CS-3	PC-1	PC-2	PC-3	PR-1	PR-2	PR-3	BV-1	BV-2	BV-3	AL-1	AL-2	AL-3
	spiked	soil	soil	soil	soil	soil	soil	soil	soil	soil	soil	soil	soil	soil	soil	soil	soil	soil	soil
RS- ¹³ C-1,2,3,4-	100	101	98	101	103	104	102	107	103	104	100	95	106	106	98	87	84	98	114
RS- ¹³ C-	99	104	99	105	104	101	100	104	108	109	94	103	96	103	97	90	81	97	105
CS- ³⁷ Cl ₄ -	90	94	92	97	97	84	88	94	94	93	93	91	89	94	88	96	94	90	98

PCDD/Fs: polychlorinated dibenzo-*p*-dioxins and polychlorinated dibenzofurans; TCDF: tetra chlorinated furan; PeCDF: penta chlorinated furan; HxCDF: hexa chlorinated furan; HpCDF: hepta chlorinated furan; OCDF: octa chlorinated furan; TCDD: tetra chlorinated dioxin; PeCDD: penta chlorinated dioxin; HpCDD: hexa chlorinated dioxin; HpCDD: hepta chlorinated dioxin; OCDD: octa chlorinated dioxin; dl-PCBs: dioxin-like PCBs; PCB: polychlorinated biphenyls; ndl-PCBs: non-dioxin-like PCBs.

Table S5. Summary of PCDD/Fs and dl-PCBs concentrations in soil from EU Member States. Concentrations in ng TEQ kg⁻¹ d.m.

Country	Type soil	PCDD/Fs-TEQ / (ng TEQ kg ⁻¹ d.m)	dl-PCBs-TEQ / (ng TEQ kg ⁻¹ d.m)	TOTAL-TEQ / (ng TEQ kg ⁻¹ d.m)
Austria ¹	forest	0.01-64 ^a		
Belgium ²	pasture	1.6-14 ^a		
	any type	2.7-8.9 ^a		
Finland ³	rural	2.1-2.7 ^a		
	any type	9.1-90.000 ^a		
Germany ⁴	any type	0.1-42 ^a		
	forest	10-30 ^a		
	pasture	0.004-30 ^a		
	arable	0.03-25 ^a		
Greece ⁵	rural	1.0 ^a		
	any type	2-45 ^a		
Ireland	any type	0.15-8.6 ^a		
	forest	4.8 ^a		
Italy ⁶	pasture	0.8-13 ^a		
	any type	0.057-0.12 ^a		
	pasture	0.1-43 ^a		
Luxembourg ⁷	arable	1.9-3.1 ^a		
	any type	1.8-20 ^a		
	forest	6.0 ^a		
The Netherlands ⁸	rural	1.4 ^a		
	any type	2-55 ^a		
Russia ⁹	rural	2.2-17 ^a		
	inhabited industrial			0.022-0.1 ^a > 40 ^a
Slovakia ¹⁰	industrial area	0.28-5.9 ^b	0.069-6.5 ^b	
Spain ¹¹	urban	0.63-24.2 ^a		
	rural	0.08-8.40 ^a		
Sweden ¹²	rural	0.11-11.446 ^a		
United Kingdom ¹³	any type	0.78-87 ^a		
	rural	0.78-20 ^a		
Brazil ¹⁴	urban	0.03-900 ^a		
Chile ¹⁵	urban	0.22-2.2 ^a		
USA ¹⁶	urban	0.13-19 ^a		
	open	0.04-4.6 ^a		
	forest	0.033-5.2 ^a		
Canada ¹⁷	urban	0-99 ^a		
	rural	0-57 ^a		
China ¹⁸	any type			0.017-5.04 ^c
Japan ¹⁹	any type	7.9-424 ^a		
South Africa ²⁰	industrial and urban	0.08-11.1 ^c	0.04-4.4 ^c	
Korea ²¹	industrial and urban			4.0-8.0 ^a
Australia ²²	industrial	0.12-11 ^b	0.015-1.8 ^b	
	urban	0.11-42 ^b	0.0058-1.6 ^b	
	agricultural	0.027-4.2 ^b	0.003-0.089 ^b	
	remote	0.037-5.1 ^b	0.0012-0.079 ^b	
New Zealand ²³	forest and grassland	0.17-1.99 ^a		
	agricultural	0.17-0.90 ^a	0.065-1.33 ^a	
	urban	0.26-6.67 ^a		

^aI-TEQ; ^bTEF-WHO₁₉₉₈; ^cTEF-WHO₂₀₀₅.

Table S6. Levels of PCDD/Fs in soil from Brazilian cities

City-State	Deposition / (ng I-TEQ kg ⁻¹)
Cubatão-SP	11-341
Araraquara-SP	0.1-1.2
Cantagalo-RJ	0.6-2.5
Formiga-MG	1.4-654
Duque de Caxias-RJ	13-900
Industrial area-RJ	1.1-654
Recreation area-RJ	0.03-1.8
Manaus-AM	0.05-0.4

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