A novel approach to the extraction and analysis of dioxins and furans sampled onto Amberlite XAD-2 sorbent

Reinardt Cromhout[a,b], Jean-François Focant[c] and Patricia Forbes[b]

[a]Environmental Pollution Laboratory (Pty) Ltd., Pretoria, South Africa.
[b]Department of Chemistry, Faculty of Natural and Agricultural Sciences, University of Pretoria, Pretoria, South Africa.
[c]Organic and Biological Analytical Chemistry Group, MolSys Research Unit, University of Liège, Belgium.

SUPPLEMENTARY INFORMATION

Table S1: Dioxin multiple reaction monitoring (MRM) masses used for quantification of dioxins using triple quadrupole mass spectrometry.

	Quantifier ions			Qualifier ions		
Native PCDD	Parent (m/z)	Daughter (m/z)	Electron volt (eV)	Parent (m/z)	Daughter (m/z)	Electron volt (eV)
2,3,7,8-TCDD	319.90	256.90	24	321.90	258.90	24
1,2,3,7,8-PeCDD	355.90	292.90	25	353.90	290.90	25
1,2,3,4,7,8-HxCDD	389.80	326.90	25	391.80	328.80	25
1,2,3,6,7,8-HxCDD	389.80	326.90	25	391.80	328.80	25
1,2,3,7,8,9-HxCDD	389.80	326.90	25	391.80	328.80	25
1,2,3,4,6,7,8-HpCDD	423.80	360.80	25	425.80	362.80	25
1,2,3,4,6,7,8,9-OCDD	457.70	394.80	26	459.70	396.80	26

Table S2: Furan multiple reaction monitoring (MRM) masses used for the quantification of furans using triple quadrupole mass spectrometry.

	Quantifier ions			Qualifier ions		
Native PCDF	Parent (m/z)	Daughter (m/z)	Electron volt (eV)	Parent (m/z)	Daughter (m/z)	Electron volt (eV)
2,3,7,8-TCDF	303.90	240.90	33	305.60	242.90	33
1,2,3,7,8-PeCDF	339.90	276.90	35	337.90	274.90	35
2,3,4,7,8-PeCDF	339.90	276.90	35	337.90	274.90	35
1,2,3,4,7,8-HxCDF	373.80	310.90	35	375.80	312.90	35
1,2,3,6,7,8-HxCDF	373.80	310.90	35	375.80	312.90	35
1,2,3,7,8,9-HxCDF	373.80	310.90	35	375.80	312.90	35
2,3,4,6,7,8-HxCDF	373.80	310.90	35	375.80	312.90	35
1,2,3,4,6,7,8-HpCDF	407.80	344.80	36	409.80	346.80	36
1,2,3,4,7,8,9-HpCDF	407.80	344.80	36	409.80	346.80	36
1,2,3,4,6,7,8,9-OCDF	441.70	378.80	35	443.70	380.80	35

Table S3: $^{13}C_{12}$ – Labelled internal standard (IS) multiple reaction monitoring (MRM) masses used for the quantification of dioxins and furans using triple quadrupole mass spectrometry.

	Quantifier ions			Qualifier ions		
^{13}C-PCDD/F Internal standard	Parent (m/z)	Daughter (m/z)	Electron volt (eV)	Parent (m/z)	Daughter (m/z)	Electron volt (eV)
^{13}C-2,3,7,8-TCDD	331.90	267.90	24	333.90	269.90	24
^{13}C -2,3,7,8-TCDF	315.90	251.90	33	317.90	253.90	33
^{13}C -1,2,3,7,8-PeCDD	365.90	301.90	25	367.90	303.90	25
^{13}C -1,2,3,7,8-PeCDF	351.90	287.90	35	349.90	285.90	35
^{13}C -1,2,3,6,7,8-HxCDD	403.80	339.80	25	401.80	337.90	25
^{13}C -1,2,3,6,7,8-HxCDF	385.80	321.90	35	387.80	323.90	35
^{13}C -1,2,3,4,6,7,8-HpCDD	437.80	373.80	25	435.80	371.80	25
^{13}C -1,2,3,4,6,7,8-HpCDF	419.80	355.80	36	421.80	357.80	36

Table S4: Internal standard calibration of dioxins and furans using four calibration levels in DMSO analysed by GC-TQMS.

Calibration level	TeCDD/TeCDF (µg/L)	PeCDD/PeCDF-HpCDD/HpCDF (µg/L)	OCDD/OCDF (µg/L)
1	1.0	2.5	5
2	2.0	5	10
3	3.0	7.5	15
4	4.0	10	20

Table S5: PCDD/Fs calibration linearity, and lower and upper quantification limits determined in triplicate by GC-TQMS.

PCDD/F	Correlation coefficient (R^2)	Response factor %RSD	Lower quantification limit (µg/L)	Upper quantification limit (µg/L)
2,3,7,8-TCDF	0.998959	2.1	0.4	30
2,3,7,8-TCDD	0.978893	16.7	0.4	30
1,2,3,7,8-PeCDF	0.991838	5.6	1.0	75
2,3,4,7,8-PeCDF	0.987223	9.8	1.0	75
1,2,3,7,8-PeCDD	0.995078	10.3	1.0	75
1,2,3,4,7,8-HxCDF	0.999808	2.3	1.5	75
1,2,3,6,7,8-HxCDF	0.992659	8.2	1.5	75
2,3,4,6,7,8-HxCDF	0.996361	3.7	1	75
1,2,3,4,7,8-HxCDD	0.950517	14.2	1.5	75
1,2,3,6,7,8-HxCDD	0.995436	4.7	1.5	75
1,2,3,7,8,9-HxCDD	0.994314	5.0	1.5	75
1,2,3,7,8,9-HxCDF	0.999657	2.8	1.5	75
1,2,3,4,6,7,8-HpCDF	0.995696	4.1	1.5	75
1,2,3,4,6,7,8-HpCDD	0.996771	5.2	1.5	75
1,2,3,4,7,8,9-HpCDF	0.986575	10.4	1.5	75
1,2,3,4,6,7,8,9-OCDD	0.994045	9.6	2	20
1,2,3,4,6,7,8,9-OCDF	0.984505	8.9	2	20

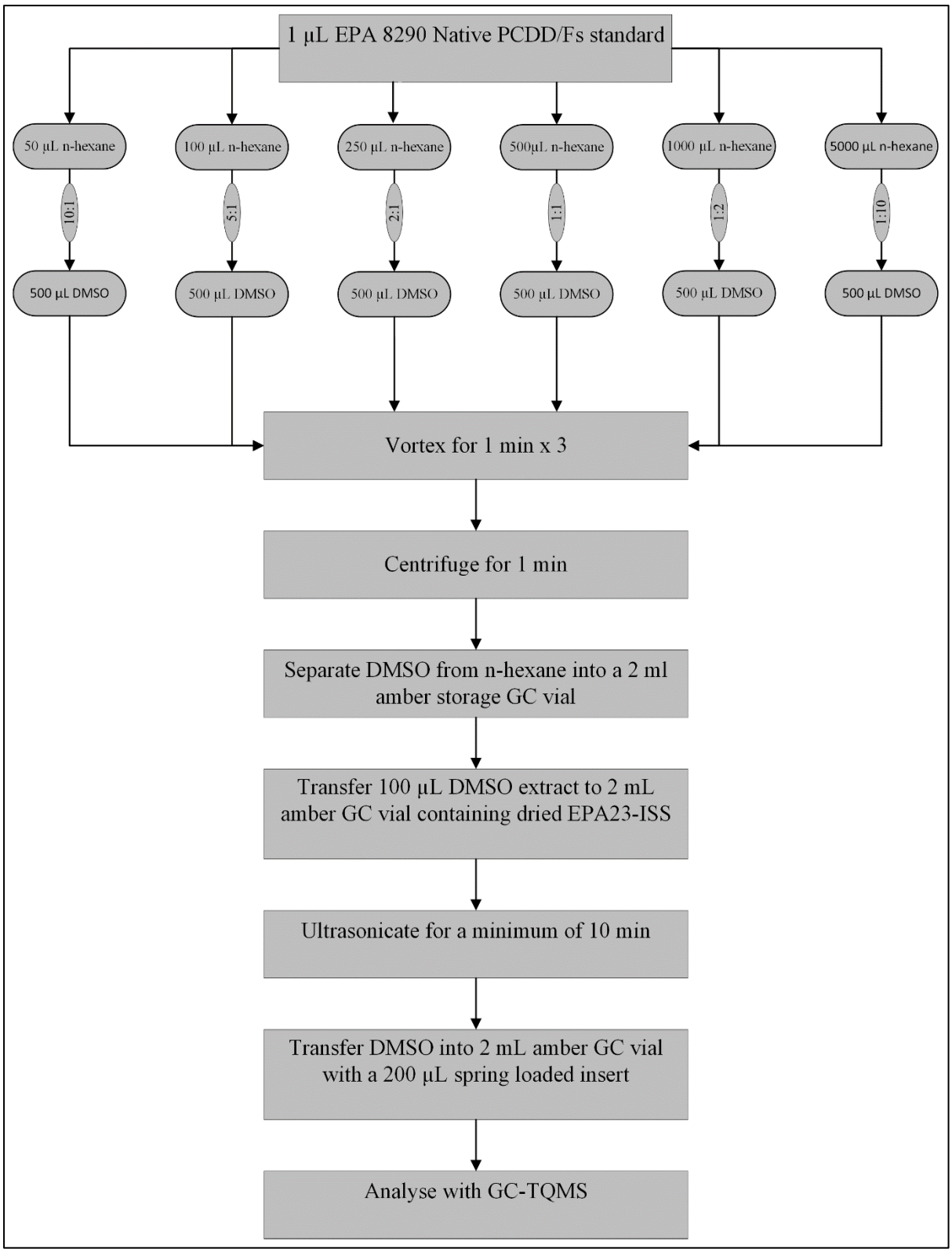

Fig. S1: Flow diagram of the investigation into dioxin and furan partitioning into a fixed DMSO volume using variable volumes of n-hexane (ratio of DMSO to n-hexane).

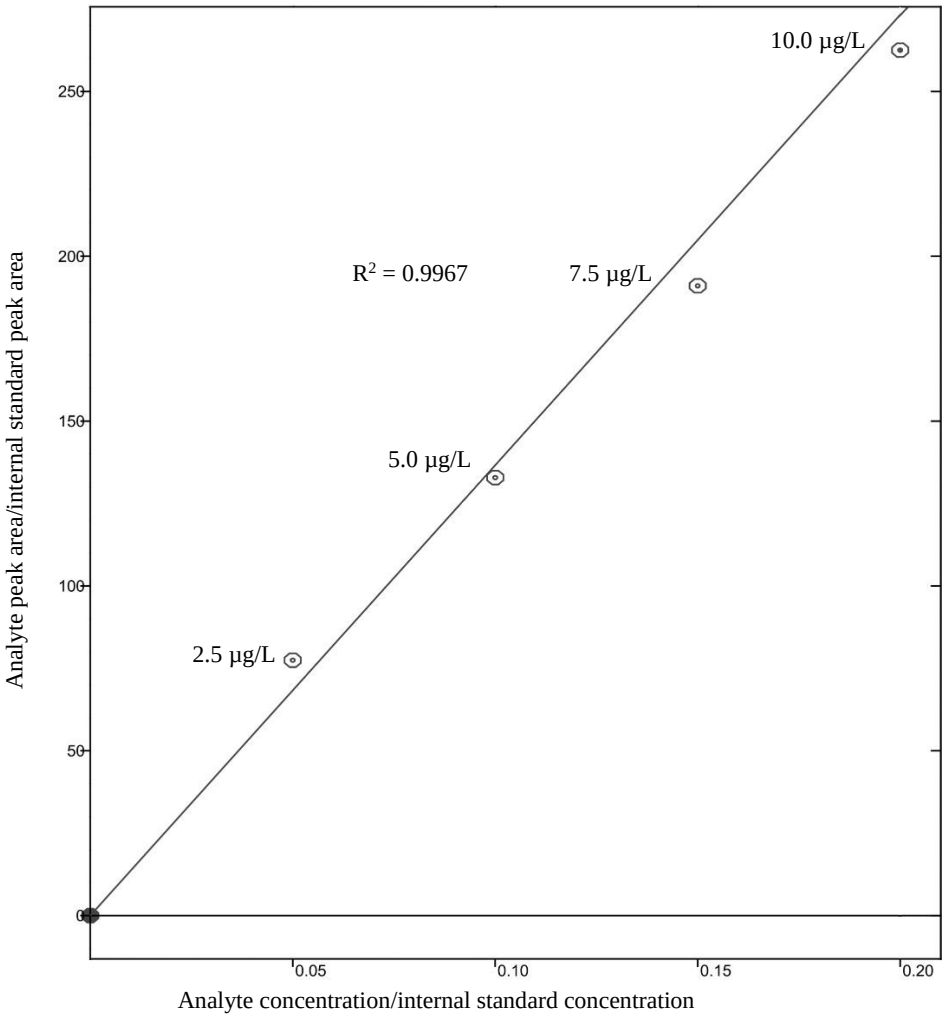

Fig. S2: Typical calibration curve for 1,2,3,7,8-PeCDD in DMSO, analysed by direct 2 µL splitless injection into the GC-TQMS. The calibration curve was prepared from dilutions of the PCDD/F native calibration standard (EPA 8290 STN) and labelled internal standard (EPA-23ISS). The final labelled internal standard concentration was 50.0 µg/L and a four level 1,2,3,7,8-PeCDD calibration curve was generated with analyte concentrations of 2.5, 5.0,7.5 and 10.0 µg/L.

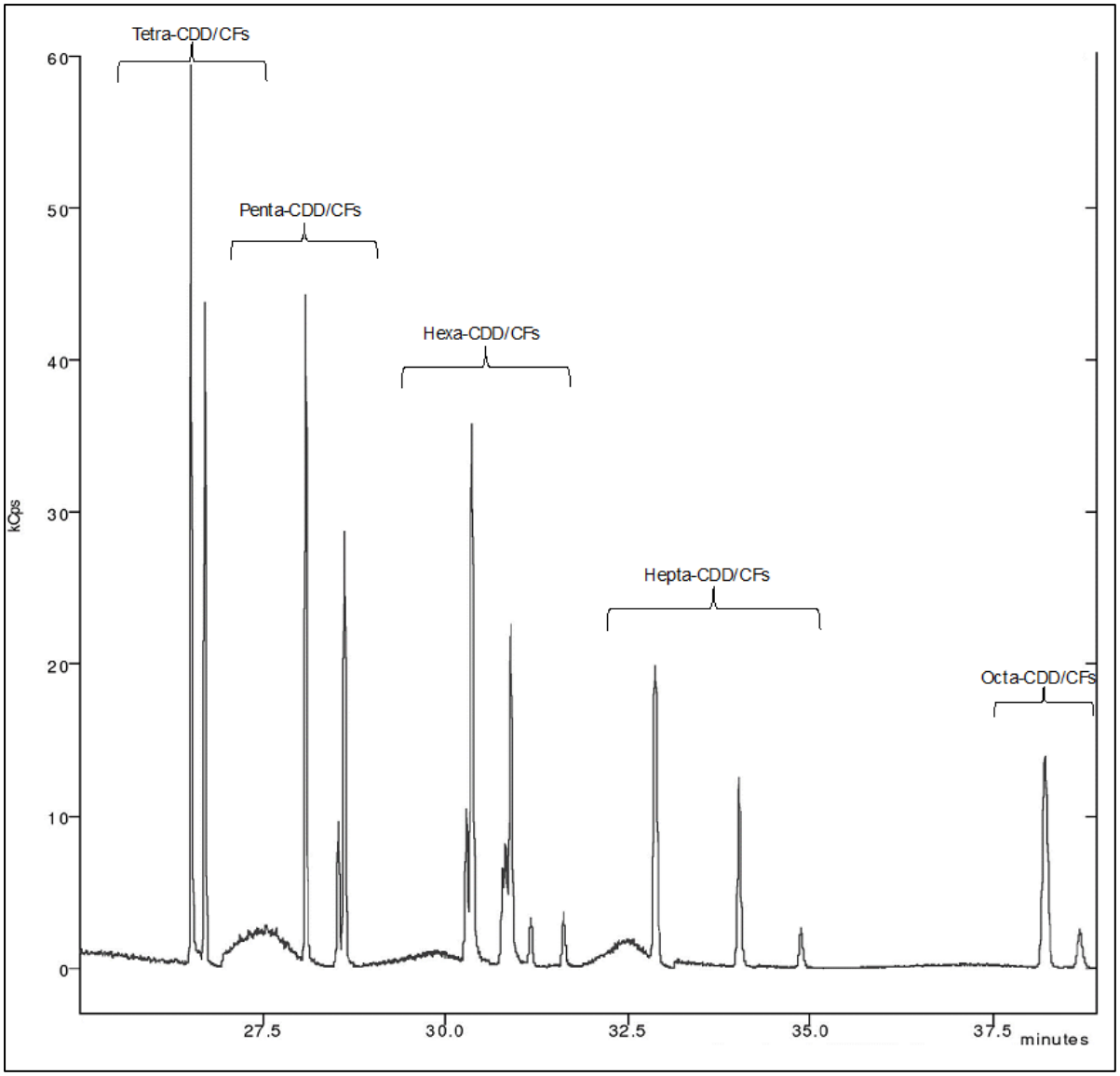

Fig. S3: Reconstructed ion chromatogram (RIC) of the 17 measured native PCDD/Fs (4.0 µg/L - tetra-CDD/Fs; 10.0 µg/L - penta to hepta-CDD/Fs; 20.0 µg/L- octa-CDD/Fs) and labelled internal standards (50.0 µg/L tetra-$^{13}C_{12}$DD/Fs- hepta-$^{13}C_{12}$DD/Fs and 100.0 µg/L octa-$^{3}C_{12}$DD) in DMSO analysed by direct 2 µL splitless injection into the GC-TQMS.