

ELECTRONIC SUPPLEMENTARY INFORMATION

Comparative Assessment of the Chromatographic Separation of 2,3,7,8-Substituted Polychlorinated  
Dibenzo-*p*-Dioxins and Polychlorinated Dibenzofurans Using Supercritical Fluid Chromatography and  
High Resolution Gas Chromatography

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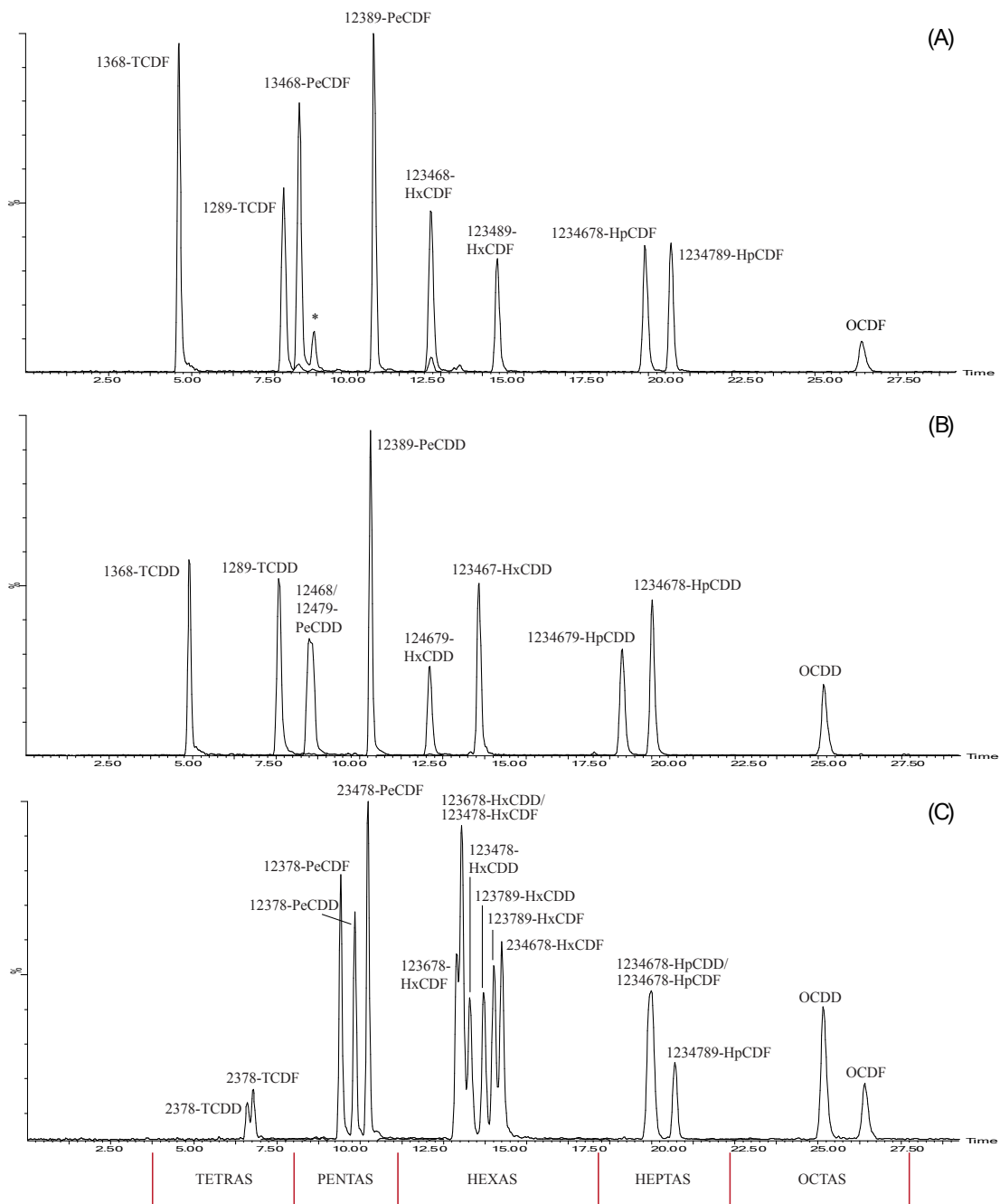


Figure S1: Chromatograms illustrating the separation of the (A) PCDF HRGC window definers (\* indicates a PCDF impurity in the mixture), (B) PCDD HRGC window definers, and (C) a mixture of 2,3,7,8-substituted PCDD and PCDF congeners using the developed pSFC-MS/MS method.

Table S1: Components and Concentrations of EPA-1613STOCK

<b>Component</b>	<b>Concentration (ng/ml)</b>
2,3,7,8-Tetrachlorodibenzo-p-dioxin	400
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	2000
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	2000
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	2000
1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	2000
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	2000
Octachlorodibenzo-p-dioxin	4000
2,3,7,8-Tetrachlorodibenzofuran	400
1,2,3,7,8-Pentachlorodibenzofuran	2000
2,3,4,7,8-Pentachlorodibenzofuran	2000
1,2,3,4,7,8-Hexachlorodibenzofuran	2000
1,2,3,6,7,8-Hexachlorodibenzofuran	2000
1,2,3,7,8,9-Hexachlorodibenzofuran	2000
2,3,4,6,7,8-Hexachlorodibenzofuran	2000
1,2,3,4,6,7,8-Heptachlorodibenzofuran	2000
1,2,3,4,7,8,9-Heptachlorodibenzofuran	2000
Octachlorodibenzofuran	4000

Table S2: Components and Concentrations of EPA-8280CVS

Component	Concentration (ng/μl)				
	CS1	CS2	CS3	CS4	CS5
2,3,7,8-Tetrachlorodibenzofuran	0.1	0.25	0.5	1.0	2.0
1,2,3,7,8-Pentachlorodibenzofuran	0.1	0.25	0.5	1.0	2.0
2,3,4,7,8-Pentachlorodibenzofuran	-	-	0.5	-	-
1,2,3,4,7,8-Hexachlorodibenzofuran	-	-	1.25	-	-
1,2,3,6,7,8-Hexachlorodibenzofuran	0.25	0.625	1.25	2.5	5.0
2,3,4,6,7,8-Hexachlorodibenzofuran	-	-	1.25	-	-
1,2,3,7,8,9-Hexachlorodibenzofuran	-	-	1.25	-	-
1,2,3,4,6,7,8-Heptachlorodibenzofuran	0.25	0.625	1.25	2.5	5.0
1,2,3,4,7,8,9-Heptachlorodibenzofuran	-	-	1.25	-	-
Octachlorodibenzofuran	0.5	1.25	2.5	5.0	10.0
2,3,7,8-Tetrachlorodibenzo-p-dioxin	0.1	0.25	0.5	1.0	2.0
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	0.1	0.25	0.5	1.0	2.0
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	-	-	1.25	-	-
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	0.25	0.625	1.25	2.5	5.0
1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	-	-	1.25	-	-
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	0.25	0.625	1.25	2.5	5.0
Octachlorodibenzo-p-dioxin	0.5	1.25	2.5	5.0	10.0
2,3,7,8-Tetrachloro[ <sup>13</sup> C <sub>12</sub> ]dibenzofuran	0.5	0.5	0.5	0.5	0.5
1,2,3,4,6,7,8-Heptachloro[ <sup>13</sup> C <sub>12</sub> ]dibenzofuran	1.0	1.0	1.0	1.0	1.0
2,3,7,8-Tetrachloro[ <sup>13</sup> C <sub>12</sub> ]dibenzo-p-dioxin	0.5	0.5	0.5	0.5	0.5
1,2,3,6,7,8-Hexachloro[ <sup>13</sup> C <sub>12</sub> ]dibenzo-p-dioxin	0.5	0.5	0.5	0.5	0.5
Octachloro[ <sup>13</sup> C <sub>12</sub> ]dibenzo-p-dioxin	1.0	1.0	1.0	1.0	1.0
1,2,3,4-Tetrachloro[ <sup>13</sup> C <sub>12</sub> ]dibenzo-p-dioxin	0.5	0.5	0.5	0.5	0.5
1,2,3,7,8,9-Hexachloro[ <sup>13</sup> C <sub>12</sub> ]dibenzo-p-dioxin	0.5	0.5	0.5	0.5	0.5

Table S3: Components and Concentrations of 5TCDD

PCDD Congener	Concentration (μg/ml)
1,2,3,4-TCDD	0.5
1,2,3,7- and 1,2,3,8-TCDD	0.5 (total)
2,3,7,8-TCDD	1.0
1,2,3,9-TCDD	1.0
<sup>13</sup> C <sub>12</sub> -1,2,3,4-TCDD	0.5
<sup>13</sup> C <sub>12</sub> -2,3,7,8-TCDD	0.5

Table S4: Components and Concentrations of WP-STK

IUPAC #	PCB Congener	Concentration (ng/ml)
77	3,3',4,4'-Tetrachlorobiphenyl	2000
81	3,4,4',5-Tetrachlorobiphenyl	2000
105	2,3,3',4,4'-Pentachlorobiphenyl	2000
114	2,3,4,4',5-Pentachlorobiphenyl	2000
118	2,3',4,4',5-Pentachlorobiphenyl	2000
123	2',3,4,4',5-Pentachlorobiphenyl	2000
126	3,3',4,4',5-Pentachlorobiphenyl	2000
156	2,3,3',4,4',5-Hexachlorobiphenyl	2000
157	2,3,3',4,4',5'-Hexachlorobiphenyl	2000
167	2,3',4,4',5,5'-Hexachlorobiphenyl	2000
169	3,3',4,4',5,5'-Hexachlorobiphenyl	2000
189	2,3,3',4,4',5,5'-Heptachlorobiphenyl	2000

Table S5: Summary of HRGC/HRMS and pSFC-MS/MS quantification results for PE1102-2ML – a proficiency testing material for polychlorinated dioxins and furans in water by U.S. EPA Method 8280B.

Compound	IS % recovery	HRGC/HRMS ng/L	actual ng/L	% Difference	pSFC-MS/MS ng/L	actual ng/L	% Difference
2378-TCDF	92	119	124	4.0	97	124	22.0
12378-PeCDF	84	--	0	--	--	0	--
23478-PeCDF	83	--	0	--	--	0	--
123478-HxCDF	87	--	0	--	--	0	--
123678-HxCDF	86	--	0	--	--	0	--
234678-HxCDF	86	--	0	--	--	0	--
123789-HxCDF	85	--	0	--	--	0	--
1234678-HpCDF	83	--	0.34	--	--	0.34	--
1234789-HpCDF	84	--	0.09	--	--	0.09	--
OCDF	--	69	65	6.2	53	65	18.3
2378-TCDD	86	114	96	18.8	72	96	25.0
12378-PeCDD	91	51.3	46.3	10.8	41	46.3	11.1
123478-HxCDD	89	132	108	22.2	84	108	21.9
123678-HxCDD	94	81	76.8	5.5	55	76.8	27.8
123789-HxCDD	--	45.6	40.9	11.5	38	40.9	6.1
1234678-HpCDD	90	96.4	90.9	6.1	58	90.9	35.7
OCDD	78	18.7	18	3.9	14	18	21.2