## 26th Australian Total Diet Study



Appendix 2: Compounds analysed, WHO derived toxic equivalency factors (TEFs), and analytical methodology

Appendix 2.1: WHO derived toxic equivalency factors (TEFs) for human risk assessment for dioxins and dioxin-like compounds

Dioxins and furans (PCDD/Fs)	WHO 1998 TEF*	WHO 2005 TEF*	Dioxin-like PCBs (DL-PCBs)	WHO 1998 TEF*	WHO 2005 TEF*
Chlorinated dibenzo-p-dioxins (PCDDs)			Non- <i>ortho</i> substituted PCBs		
2,3,7,8-TCDD	1	1	PCB 77	0.0001	0.0001
1,2,3,7,8-PeCDD	1	1	PCB 81	0.0001	0.0003
1,2,3,4,7,8-HxCDD	0.1	0.1	PCB 126	0.1	0.1
1,2,3,6,7,8-HxCDD	0.1	0.1	PCB 169	0.01	0.03
1,2,3,7,8,9-HxCDD	0.1	0.1			
1,2,3,4,6,7,8-HpCDD OCDD	0.01 0.0001	0.01 <b>0.0003</b>			
Chlorinated dibenzofurans (PCDFs)			Mono- <i>ortho</i> substituted PCBs		
2,3,7,8-TCDF	0.1	0.1	PCB 105	0.0001	0.00003
1,2,3,7,8-PeCDF	0.05	0.03	PCB 114	0.0005	0.00003
2,3,4,7,8-PeCDF	0.5	0.3	PCB 118	0.0001	0.00003
1,2,3,4,7,8-HxCDF	0.1	0.1	PCB 123	0.0001	0.00003
1,2,3,6,7,8-HxCDF	0.1	0.1	PCB 156	0.0005	0.00003
1,2,3,7,8,9-HxCDF	0.1	0.1	PCB 157	0.0005	0.00003
2,3,4,6,7,8-HxCDF	0.1	0.1	PCB 167	0.00001	0.00003
1,2,3,4,6,7,8-HpCDF	0.01	0.01	PCB 189	0.0001	0.00003
1,2,3,4,7,8,9-HpCDF	0.01	0.01			
OCDF	0.0001	0.0003			

<sup>\*</sup>Van den Berg, 2006

Changes in WHO toxicity equivalency factors between 1998 and 2005 assessments (TEFwH098 and TEFwH005) are in bold.

Appendix 2.2: Analytical limits for dioxins and dioxin-like compounds

Dioxins and dioxin-like congener	CAS Registry Number	LOD* (pg/g)	LOQ** (pg/g)	LOR*** (pg/g)	
Chlorinated dibenzo-p- dioxins (PCDDs)					
2,3,7,8-TCDD	1746-01-6	0.0003 - 0.09	0.0003 - 0.09	0.0003 - 0.09	
1,2,3,7,8-PeCDD	40321-76-4	0.0002 - 0.08	0.0002 - 0.08	0.0002 - 0.08	
1,2,3,4,7,8-HxCDD	39227-28-6	0.0002 - 0.06	0.0002 - 0.06	0.0002 - 0.06	
1,2,3,6,7,8-HxCDD	57653-85-7	0.0002 - 0.06	0.0002 - 0.06	0.0002 - 0.06	
1,2,3,7,8,9-HxCDD	19408-74-3	0.0002 - 0.06	0.0002 - 0.06	0.0002 - 0.06	
1,2,3,4,6,7,8-HpCDD	35822-46-9	0.0003 - 0.2	0.0003 - 0.2	0.0003 - 0.2	
OCDD	3268-87-9	0.0004 - 1	0.0004 - 1	0.0004 - 1	
Chlorinated dibenzofurans (PCDFs)					
2,3,7,8-TCDF	51207-31-9	0.0003 - 0.05	0.0003 - 0.05	0.0003 - 0.05	
1,2,3,7,8-PeCDF	57117-41-6	0.0003 - 0.05	0.0003 - 0.05	0.0003 - 0.05	
2,3,4,7,8-PeCDF	57117-31-4	0.0002 - 0.04	0.0002 - 0.04	0.0002 - 0.04	
1,2,3,4,7,8-HxCDF	70648-26-9	0.0002 - 0.04	0.0002 - 0.04	0.0002 - 0.04	
1,2,3,6,7,8-HxCDF	57117-44-9	0.0002 - 0.04	0.0002 - 0.04	0.0002 - 0.04	
1,2,3,7,8,9-HxCDF	72918-21-9	0.0002 - 0.05	0.0002 - 0.05	0.0002 - 0.05	
2,3,4,6,7,8-HxCDF	60851-34-5	0.0002 - 0.05	0.0002 - 0.05	0.0002 - 0.05	
1,2,3,4,6,7,8-HpCDF	38998-75-3	0.0002 - 0.2	0.0002 - 0.2	0.0002 - 0.2	
1,2,3,4,7,8,9-HpCDF	55673-89-7	0.0002 - 0.2	0.0002 - 0.2	0.0002 - 0.2	
OCDF	39001-02-0	0.0002 - 0.1	0.0002 - 0.1	0.0002 - 0.1	
Non- <i>ortho</i> substituted PCBs					
PCB 77	32598-13-3	0.0008 - 4	0.0008 - 4	0.0008 - 4	
PCB 81	70362-50-4	0.0003 - 0.2	0.0003 - 0.2	0.0003 - 0.2	
PCB 126	57465-28-8	0.0006 - 1	0.0006 - 1	0.0006 - 1	
PCB 169	32774-16-6	0.0004 - 0.2	0.0004 - 0.2	0.0004 - 0.2	
Mono- <i>ortho</i> substituted PCBs					
PCB 105	32598-14-4	0.007 - 10	0.007 - 10	0.007 - 10	
PCB 114	74472-37-0	0.0009 - 5	0.0009 - 5	0.0009 - 5	
PCB 118	31508-00-6	0.01 - 30	0.01 - 30	0.01 - 30	
PCB 123	65510-44-3	0.002 - 6	0.002 - 6	0.002 - 6	
PCB 156	38380-08-4	0.001 - 20	0.001 - 20	0.001 - 20	
PCB 157	69782-90-7	0.0006 - 7	0.0006 - 7	0.0006 - 7	
PCB 167	52663-72-6	0.0007 - 10	0.0007 - 10	0.0007 - 10	
PCB 189	39635-31-9	0.0004 - 2	0.0004 - 2	0.0004 - 2	
OD: Limit of Detection: **LOO: Limit of Quantification: ***LOR: Limit of Reporting					

<sup>\*</sup>LOD: Limit of Detection; \*\*LOQ: Limit of Quantification; \*\*\*LOR: Limit of Reporting Values for LOD, LOQ and LOR are the same and specific for each congener for each analysis The LOD, LOQ and LOR ranges represented all matrices analysed for that congener

Appendix 2.3: Analytical limits for non-dioxin like PCBs

Non-dioxin-like PCBs congener	CAS Registry Number	LOD* (μg/kg)	LOQ** (µg/kg)	LOR*** (μg/kg)
PCB 18	37680-65-2	0.01	0.04	0.05
PCB 28 (i)	7012-37-5	0.01	0.04	0.05
PCB 44	41464-39-5	0.01	0.04	0.05
PCB 52 (i)	35693-99-3	0.01	0.04	0.05
PCB 66	32598-10-0	0.01	0.04	0.05
PCB 101 (i)	37680-73-2	0.01	0.04	0.05
PCB 128	11096-82-5	0.01	0.04	0.05
PCB 138 (i)	35065-28-2	0.01	0.04	0.05
PCB 153 (i)	35065-27-1	0.01	0.04	0.05
PCB 170	35065-30-6	0.01	0.04	0.05
PCB 180 (i)	35065-29-3	0.01	0.04	0.05
PCB 187	52663-68-0	0.01	0.04	0.05
PCB 8	34883-43-7	0.2	0.7	1
PCB 195	52663-78-2	0.2	0.7	1
PCB 206	40186-72-9	0.2	0.7	1
PCB 209	2051-24-3	0.2	0.7	1

(i): indicator PCBs \*LOD: Limit of Detection; \*\*LOQ: Limit of Quantification; \*\*\*LOR: Limit of Reporting

## Appendix 2.4: Analytical methodology

The analytical methods for the determination of PCDDs, PCDFs and DL-PCBs in food for the 26th ATDS are based on the United States Environmental Protection Agency (US EPA) *Method 1613 Revision B* and *Method 1668 Revision A*, respectively, with some in-house modifications. Both methods use High Resolution Gas Chromatography (HRGC) and High Resolution Mass Spectrometry (HRMS). The methods are under accreditation by the National Association of Testing Authorities (NATA). Both methods use the technique of isotope dilution with high-resolution mass spectrometry for determination of 10 PCDDs, 12 PCDFs and 12 DL-PCBs. These methods are performance-based and the detection limits and quantitation levels are usually dependent on the level of interferences and laboratory background levels rather than instrumental limitations. The limit of reporting (LOR) for individual congener varies for different matrices and is calculated individually for each analysis. The results for PCDDs, PCDFs and DL-PCBs were reported on a fresh weight (fw) basis, where applicable, results were also reported on a lipid weight (lw) basis for samples with typically high lipid content. Analytical concentration data for PCDDs, PCDFs and DL-PCBs were reported to two significant figures.

The analytical methodology used for the 26<sup>th</sup> ATDS for PCBs was developed in-house by the National Measurement Institute (NMI) and under accreditation by NATA. The method used Gas Chromatography with Tandem Mass Spectroscopy (GC/MSMS). Each composite sample was analysed for 21 PCBs including 16 NDL-PCBs. The LORs for different NDL-PCBs congeners varied, typically at a greater sensitivity level of 0.05 µg/kg for all congeners, except for PCB8, PCB195, PCB206 and PCB209, at 1 µg/kg. Analytical results for these 16 NDL-PCBs congeners were reported on a fresh weight basis. This method also reported results for five DL-PCBs (PCB77, PCB105, PCB118, PCB126 and PCB169). However, given these five DL-PCBs congeners were already included in the analysis for dioxins and dioxin-like compounds, analytical results for these were not taken from this method, since the other offered better sensitivity.