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Supplementary Materials

A revised and improved toxicokinetic model to simulate serum concentrations of bioaccumulative PFAS

Christopher W Greene, Alexander R Bogdan, Helen M Goeden

Health Risk Assessment Unit, Minnesota Department of Health, St. Paul, MN 55164-0975, USA.

Correspondence to: Christopher Greene, Minnesota Department of Health, 625 Robert St. N, P.O. Box 64975, St. Paul, MN 55164-0975, USA. E-mail: christopher.greene@state.mn.us

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PLACENTAL TRANSFER FACTORS

Supplementary Table 1. Summary of placental: maternal transfer efficiencies for PFOA

Ref.	PFOA placental transfer factor		
	Mean	**Median**	**Upper %ile**
Fei *et al.*, 2007[1]	0.68		
Midasch *et al.*, 2007[2]	1.26		1.69
Monroy *et al.*, 2008[3]	0.81		
Fromme *et al.*, 2010[4]	0.7		
Kim et al., 2011a[5]	0.69		0.95
Kim *et al.*, 2011b[6]	1.02	0.79	2.39
Liu *et al.*, 2011[7]	0.91	0.89	
Needham *et al.*, 2011[8]		0.72	
Gutzkow *et al.*, 2012[9]	0.82	0.785	
Lee *et al.*, 2013[10]	0.84	0.8	1.44
Hanssen *et al.*, 2013[11]		0.84	
Ode *et al.*, 2013[12]	1.3	0.8	1.6
Porpora *et al.*, 2013[13]	0.87		
Zhang *et al.*, 2013[14]	0.58		
Kato *et al.*, 2014[15]	0.83		
Cariou *et al.*, 2015[16]	0.78		1.11
Wilhelm *et al.*, 2015[17]		0.7	
Yang *et al.*, 2016[18]	0.71	0.65	1.15
Yang *et al.*, 2016[19]	0.88	0.83	
Morello-Frosch *et al.*, 2016[20]		0.8	
Chen *et al.*, 2017[21]	0.81	0.77	
Pan *et al.*, 2017[22]	0.65	0.66	0.98
Zhao *et al.*, 2017[23]	0.59	0.57	0.88
Eryasa *et al.*, 2019[24]		0.8	
Han *et al.*, 2018[25]		0.81	
Wang *et al.*, 2019[26]		0.83	1.35
Gao *et al.*, 2019[27]	0.83		
Li *et al.*, 2020[28]		0.85	

Cai *et al.*, 2020[29]	0.8	0.73	1.6
Liu *et al.*, 2021[30]	0.85	0.83	1.25
Kaiser *et al.*, 2021[31]		0.6	
Gundacker *et al.*, 2021[32]		0.66	
Li *et al.*, 2021[33]	1.44		
Kang *et al.*, 2021[34]	0.32		
Zheng *et al.*, 2022[35]	0.8	0.74	1.7
Bao *et al.*, 2022[36]		0.56	
Count	25	24	13
Min	0.32	0.56	0.88
Max	1.44	0.89	2.39
Mean	**0.83**	**0.75**	**1.39**
Median	0.81	0.79	1.35
95th percentile	1.29	0.85	1.98

Values represent the ratio of cord to maternal serum concentration.

BREASTMILK TRANSFER FACTORS

For the breastmilk transfer factor for PFOA, we identified seven usable mean values [Supplementary Table 2]. An eighth study (Karrman *et al.*, 2007)[37] was excluded from the analysis because only one sample had a detectable level of PFOA.

Supplementary Table 2. Breastmilk transfer factors for PFOA

Source	Transfer factor (mean value)
Haug *et al.*, 2011[38]	0.038
Liu *et al.*, 2011[7]	0.11
Kim *et al.*, 2011a[5]	0.025
Kim *et al.*, 2011b[6]	0.04
Cariou *et al.*, 2015[16]	0.038
Zheng *et al.*, 2022[35]	0.05
Criswell *et al.*, 2023[39]	0.02
Mean value	**0.046**

Values represent the ratio of milk concentration to maternal serum concentration.

The 95% Upper Confidence Limit (UCL) on the mean breastmilk transfer factor was calculated using a standard equation for a one-tailed upper confidence limit (Gilbert, 1987)[40]. This approach assumes that the underlying distribution of the transfer factor is normal.

The following general equation is used to calculate a UCL on the mean at any given percentage (1 - α):

$$UCL_{1-\alpha} = \bar{x} + t_{1-\alpha,n-1}\frac{s}{\sqrt{n}} \quad \text{(S1)}$$

Where α is equal to 1 minus the percentage UCL being calculated, $\bar{x}$ is the mean, s is the standard deviation, n is the number of measurements, and t is a value in the t distribution corresponding to the desired α and the number of degrees of freedom (n - 1).

For a 95% UCL on the mean of the seven values in Supplementary Table 2, α = 0.05 (1 - 0.95), $\bar{x}$ = 0.04586, n = 7, s = 0.02998, and the value of *t* (sourced from Table A2 in Gilbert (1987)[40] for α = 0.05 and 6 degrees of freedom) is 1.943.

Using the equation above, the 95% UCL on the mean is then calculated to be 0.068.

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