

**Table S2. Physiological and Biochemical Parameters of the Human DLC Mixture PBPK Model**

Parameter	Symbol	Value or Equation	Unit
Body weight	<i>BW</i>	<b>Male:</b> $0.00058 \cdot \text{ageInYears}^3 - 0.0948 \cdot \text{ageInYears}^2 + 4.8434 \cdot \text{ageInYears} + 2.2785$ <b>Female:</b> $0.0006 \cdot \text{ageInYears}^3 - 0.0912 \cdot \text{ageInYears}^2 + 4.3200 \cdot \text{ageInYears} + 3.6520$	kg
Tissue volume fraction of <i>BW</i>			
Liver	<i>VLC</i>	$3.59\text{E-}2 - 4.76\text{E-}7 \cdot BW^{1\text{E}3}$ $+ 8.50\text{E-}12 \cdot (BW^{1\text{E}3})^2 - 5.45\text{E-}17 \cdot (BW^{1\text{E}3})^3$	-
Fat	<i>VFC</i>	<b>Male:</b> $- 5.26\text{E-}20 \cdot (BW^{1000})^4 + 1.09\text{E-}14 \cdot (BW^{1000})^3$ $- 6.99\text{E-}10 \cdot (BW^{1000})^2 + 1.59\text{E-}5 \cdot BW^{1000}$ $+ 3.95\text{E-}2$ <b>Female:</b> $- 6.36\text{E-}20 \cdot (BW^{1000})^4 + 1.12\text{E-}14 \cdot (BW^{1000})^3$ $- 5.8\text{E-}10 \cdot (BW^{1000})^2 + 1.2\text{E-}5 \cdot BW^{1000}$ $+ 5.91\text{E-}2$	-
Rest of Body (RB)	<i>VRBC</i>	$(0.91 - VLBC \cdot VLC - VFBC \cdot VFC - VLC - VFC) /$ $(1 + VRBBC)$	-
Tissue blood volume fraction			
Liver	<i>VLBC</i>	0.266	-
Fat	<i>VFBC</i>	0.05	-
RB	<i>VRBBC</i>	0.03	-
Cardiac Output	<i>QCC</i>	15.36	L/kg/h
Tissue fractional blood flow of <i>QCC</i>			
Liver	<i>QLC</i>	0.266	-
Fat	<i>QFC</i>	0.05	-
RB	<i>QRBC</i>	0.03	-
AHR total	<i>AHR<sub>tot</sub></i>	0.35	nM
Basal concentration of CYP1A2	<i>CYP1A2_1BASAL</i>	1600	nM
Affinity constant of AHR-mediated CYP1A2 induction	<i>CYP1A2_1EC50</i>	130	nM
Maximal fold of CYP1A2 induction	<i>CYP1A2_1EMAX</i>	9300	-
Rate constant of CYP1A2 mRNA transcription	<i>k<sub>transcription_1A2</sub></i>	16	nM/h

Rate constant of CYP1A2 mRNA degradation	$kdeg_{CYP1A2\_mRNA}$	0.1	1/h
Rate constant of CYP1A2 translation	$ktranslation\_1A2$	1.25	1/h
Rate constant of CYP1A2 degradation	$kdeg_{CYP1A2}$	0.125	1/h

**Note:** All parameter values or equations are from Emond et al. 2018, except for  $ktranslation\_1A2$ ,  $kdeg_{CYP1A2}$ ,  $ktranscription\_1A2$ , and  $kdeg_{CYP1A2\_mRNA}$ , which were adjusted such that the basal and maximally induced steady-state levels of CYP1A2 remain the same as in the Emond model and the steady-state mRNA level was kept to be 10% of the protein level.