

**Table S1. ODEs of the Human DLC Mixture PBPK Model**

1	Amount in GI track	$\frac{dMST}{dt} = - (KST + KABS) \odot MST + ORAL\_DOSE\_RATE$
2	Amount absorbed into lymph circulation	$\frac{dLYMLUM}{dt} = KABS \odot MST \odot a$
3	Amount absorbed into portal circulation	$\frac{dLIMLUM}{dt} = KABS \odot MST \odot b$
4	Amount of urinary excretion	$\frac{dAURI}{dt} = CLURI \odot CB$
5	Amount in fat blood	$\frac{dAFB}{dt} = QF * (CA - \frac{AFB}{VFB}) - PAF \odot (\frac{AFB}{VFB} - (\frac{AF}{VF}) \odot \frac{1}{PF})$
6	Amount in fat tissue	$\frac{dAF}{dt} = PAF \odot (\frac{AFB}{VFB} - (\frac{AF}{VF}) \odot \frac{1}{PF})$
7	Amount in RB blood	$\frac{dARBB}{dt} = QRB * (CA - \frac{ARBB}{VRBB}) - PARB \odot (\frac{ARBB}{VRBB} - \frac{ARB}{VRB} \odot \frac{1}{PRB})$
8	Amount in RB tissue	$\frac{dARB}{dt} = PARB \odot (\frac{ARBB}{VRBB} - \frac{ARB}{VRB} \odot \frac{1}{PRB})$
9	Amount in liver blood	$\frac{dALB}{dt} = QL * (CA - \frac{ALB}{VLB}) - PAL \odot (\frac{ALB}{VLB} - (\frac{AL}{VL}) \odot \frac{1}{PL}) + KABS \odot MST \odot b$
10	Amount of free and nonspecific bound in liver tissue	$\begin{aligned} \frac{dAL}{dt} = & PAL \odot (\frac{ALB}{VLB} - (\frac{AL}{VL}) \odot \frac{1}{PL}) + (-kelim \odot (\frac{AL}{VL}) \odot \frac{1}{PL} * \frac{CYP1A2 + \Sigma(\frac{A\_Dioxin\_CYP1A2}{VL}) - CYP1A2\_1BASAL}{CYP1A2\_1BASAL} - kfAHR \odot \\ & (\frac{AL}{VL}) \odot \frac{1}{PL} * (AHR_{tot} - \Sigma(\frac{A\_Dioxin\_AHR}{VL}))) + kbAHR \odot \frac{A\_Dioxin\_AHR}{VL} - kf1A2 \odot (\frac{AL}{VL}) \odot \frac{1}{PL} * CYP1A2 + kb1A2 \odot \\ & \frac{A\_Dioxin\_CYP1A2}{VL}) * VL \end{aligned}$
11	Amount of Dioxin-AHR complex	$\frac{dA\_Dioxin\_AHR}{dt} = (kfAHR \odot (\frac{AL}{VL}) \odot \frac{1}{PL} * (AHR_{tot} - \Sigma(\frac{A\_Dioxin\_AHR}{VL}))) - kbAHR \odot \frac{A\_Dioxin\_AHR}{VL} * VL$

12	Amount of Dioxin-CYP1A2 complex	$\frac{dA\_Dioxin\_CYP1A2}{dt} = (kf1A2 \odot (\frac{AL}{VL}) \odot \frac{1}{PL} * CYP1A2 - kb1A2 \odot \frac{A\_Dioxin\_CYP1A2}{VL}) * VL$
13	Concentration of CYP1A2 mRNA	$\frac{dCYP1A2\_mRNA}{dt} = ktranscription\_1A2 * (1 + \frac{CYP1A2\_1EMAX * (\Sigma \frac{A\_Dioxin\_AHR}{VL})^{0.6}}{CYP1A2\_1EC50^{0.6} + (\Sigma \frac{A\_Dioxin\_AHR}{VL})^{0.6}}) - kdegCYP1A2\_mRNA * CYP1A2\_mRNA$
14	Concentration of free CYP1A2	$\frac{dCYP1A2}{dt} = ktranslation\_1A2 * CYP1A2\_mRNA - kdegCYP1A2 * CYP1A2 - \Sigma(kf1A2 \odot (\frac{AL}{VL}) \odot \frac{1}{PL} * CYP1A2) + \Sigma(kb1A2 \odot \frac{A\_Dioxin\_CYP1A2}{VL})$