Supplemental Table 1. Kinetic parameter estimates of model C.

Parameter	Notes	Final Value	Clearance, L/hr	Half-life, hr
k_{1fT}	TCE→TCA formation	0.0271	-	-
k_{Te}	TCA elimination	0.0563	0.00336	12.3
V_{mT}	Volume of distribution for TCA	0.0598	-	-
k_{TfD}	TCA→ DCA formation	1.53×10^{-6}	-	-
K_{1fD}	TCE→DCA formation	7.96×10^{-8}	-	-
k_{De}	DCA elimination	8.65	0.00050	0.080
V_{MD}	Volume of distribution for DCA	5.79×10^{-5}	-	-
k_{1fG}	TCE→DCVG formation	4.39×10^{-6}	-	-
k_{GfC}	DCVG→DCVC formation	0.492	0.0178	1.41
V_{mG}	Volume of distribution for DCVG	0.0361	-	-
k_{Ce}	DCVC elimination	0.603	0.187	1.15
V_{mC}	Volume of distribution for. DCVC	0.309	-	-
k_{1fT}	TCE→TCA formation	0.0271	-	-

Clearance is the product between elimination constant and volume of distribution of each metabolite, reflecting systemic clearance. Units of the reaction constants and volume of distributions are hr^{-1} and liter, respectively. Parameter estimates of parent compound can be found in Table 4.