

**Experiment Number:** S0811  
**Route:** Gavage, IV  
**Species/Strain:** Rat/Sprague-Dawley

**Toxicokinetics Data Summary**  
**Test Compound:** Hexachlorobenzene  
**CAS Number:** 118-74-1

**Date Report Requested:** 11/09/2016  
**Time Report Requested:** 14:03:22  
**Lab:** Midwest Research Institute

Female									
	Treatment Groups (ug/kg)								
	300 <sup>a</sup>	100 IV <sup>b</sup>	1000 IV <sup>b</sup>	300 <sup>a</sup>	100 IV <sup>a</sup>	1000 IV <sup>a</sup>	300 <sup>a</sup>	100 IV <sup>a</sup>	1000 IV <sup>a</sup>
	Blood			Fat (Mesenteric)			Liver		
C <sub>max</sub>	0.087 ug/mL	0.172 ug/mL	2.31 ug/mL	1.32 ug/g	0.334 ug/g	3.18 ug/g	0.202 ug/g	0.082 ug/g	0.630 ug/g
T <sub>max</sub> (hour)	3	0	0	72	336	72	3	2	2
Lambda <sub>z</sub> (hour <sup>-1</sup> )	4.0E-4								
t <sub>1/2</sub> (day)	38.0			48	68	71	75	90	85
Alpha (hour <sup>-1</sup> )		1.49	1.83						
t <sub>1/2</sub> (Alpha) (hour)		0.47	0.38						
Beta (hour <sup>-1</sup> )		0.0009	0.0008						
t <sub>1/2</sub> (Beta) (day)		34	38						
Cl (mL/hr/kg)		12.0	10.1						
Cl <sub>(F)</sub> (mL/hr/kg)	8.8								
V <sub>1</sub> (L/kg)		0.580	0.433						
V <sub>ss</sub> (L/kg)		11.2	10.1						
V <sub>1(F)</sub> (L/kg)	11.6								
MRT (day)				71	94	103	106	125	121
AUC <sub>0-t</sub> (ug*hr/mL)	34.2	8.35	99.5						
AUC <sub>inf</sub>	58.4 ug*hr/mL	12.1 ug*hr/mL	142.0 ug*hr/mL	2485 ug*hr/g	687 ug*hr/g	8179 ug*hr/g	158.6 ug*hr/g	57.9 ug*hr/g	413 ug*hr/g
F (fraction)	1.2								

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	Treatment Groups (ug/kg)		
	300 <sup>a</sup>	100 IV <sup>a</sup>	1000 IV <sup>a</sup>
	Lung		
C <sub>max</sub>	0.127 ug/g	0.101 ug/g	2.176 ug/g
T <sub>max</sub> (hour)	3	2	2
Lambda <sub>z</sub> (hour <sup>-1</sup> )			
t <sub>1/2</sub> (day)	77	55	54
Alpha (hour <sup>-1</sup> )			
t <sub>1/2</sub> (Alpha) (hour)			
Beta (hour <sup>-1</sup> )			
t <sub>1/2</sub> (Beta) (day)			
Cl (mL/hr/kg)			
Cl <sub>1(F)</sub> (mL/hr/kg)			
V <sub>1</sub> (L/kg)			
V <sub>ss</sub> (L/kg)			
V <sub>1(F)</sub> (L/kg)			
MRT (day)	108	77	78
AUC <sub>0-t</sub> (ug*hr/mL)			
AUC <sub>inf</sub>	117.1 ug*hr/g	24.4 ug*hr/g	254.4 ug*hr/g
F (fraction)			

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## LEGEND

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Data are displayed as mean  $\pm$  SEM

### MODELING METHOD & BEST FIT MODEL

<sup>a</sup> WinNonlin (Version 1, Pharsight Corporation, Cary, NC); Non-compartmental model

<sup>b</sup> WinNonlin (Version 1, Pharsight Corporation, Cary, NC); Two-compartment model with first order elimination from the central compartment best fit the data.

### ANALYTE

Hexachlorobenzene

### TK PARAMETERS

$C_{max}$  = Observed or Predicted Maximum plasma (or tissue) concentration

$T_{max}$  = Time at which  $C_{max}$  predicted or observed occurs

$\lambda_{dz}$  = Non-compartmental analysis (NCA) terminal elimination rate constant, NCA  $k_e$  or  $k_{elim}$

$t_{1/2}$  =  $\lambda_{dz}$  half-life,  $t_{1/2}$ , the terminal elimination half-life based on non-compartmental analysis

Alpha = Hybrid rate constant of the alpha phase

$t_{1/2(\alpha)}$  = Half-life for the alpha phase

Beta = Hybrid rate constant of the beta phase

$t_{1/2(\beta)}$  = Half-life for the beta phase

Cl = Clearance, includes total clearance

$Cl_{1(F)}$  = Apparent clearance of the central compartment, also  $Cl_{(F)}$  for gavage groups in non-compartmental model

$V_1$  = Volume of distribution of the central compartment, includes  $V_d$  and  $V_{volume}$  of distribution,  $V_z$  apparent volume of distribution NCA,  $V_{app}$  apparent volume of distribution for intravenous studies

$V_{ss}$  = Volume of distribution at steady state

$V_{1(F)}$  = Apparent volume of distribution for the central compartment includes  $V_{d(F)}$ ,  $V_{(F)}$  for oral groups, and  $V_{c(F)}$

MRT = Mean residence time

$AUC_{0-t}$  = Area under the plasma concentration versus time curve, AUC, from time  $t_i$  (initial) to  $t_f$  (final),  $AUC_{last}$

$AUC_{inf}$  = Area under the plasma concentration versus time curve, AUC, extrapolated to time equals infinity

F = Bioavailability, absolute bioavailability

**\*\* END OF REPORT \*\***