

Experiment Number: S0328
Route: Dosed Feed, Gavage, IV
Species/Strain: Rat/F344

Toxicokinetics Data Summary
Test Compound: Pentachlorophenol, purified
CAS Number: 87-86-5

Date Report Requested: 01/23/2017
Time Report Requested: 15:41:04
Lab: NIEHS_Midwest Research Institute

		Male					
		Treatment Groups (mg/kg)					
		9.5 ^a	18.75 ^b	38 ^a	75 ^b	312 ^c	1250 ^c
		Plasma					
Beta (hour ⁻¹)							
k ₀₁ (hour ⁻¹)		0.87 ± 0.15		0.49 ± 0.08			
t _{1/2(k01)} (hour)			3.6		2.1		
k ₁₀ (hour ⁻¹)		0.081 ± 0.006		0.110 ± 0.008			
t _{1/2(k10)} (hour)			3.8		5.7		
Cl			21.4 mL/hr/kg		22.0 mL/hr/kg		
Cl ₁ (L/hr/kg)		0.015 ± 4.0E-4		0.016 ± 5.0E-4			
V ₁ (mL/kg)							
V _{ss}		0.19 ± 0.014 L/kg	181 mL/kg	0.17 ± 0.014 L/kg	139 mL/kg		
MRT (hour)			15.4		11.9		
AUC _{inf}		613 ± 31 ug*hr/mL	878 ug/mL*hr	2049 ± 94 ug*hr/mL	3402 ug/mL*hr		
F		100 ± 4 percent	0.55 fraction	86 ± 4 percent	0.53 fraction	52 percent	30 percent

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Male

	Treatment Groups (mg/kg)	
	5 IV ^d	5 IV ^b
	Plasma	
Beta (hour ⁻¹)	0.123 ± 0.008	
k ₀₁ (hour ⁻¹)		
t _{1/2(k01)} (hour)		
k ₁₀ (hour ⁻¹)		
t _{1/2(k10)} (hour)		2.6
Cl	0.016 ± 0.0007 L/hr/kg	11.7 mL/hr/kg
Cl ₁ (L/hr/kg)		
V ₁ (mL/kg)		46
V _{ss}	0.13 ± 0.006 L/kg	85 mL/kg
MRT (hour)		7.3
AUC _{inf}	314 ± 14 ug*hr/mL	428 ug/mL*hr
F		

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Female				
Treatment Groups (mg/kg)				
	18.75 ^b	75 ^b	5 IV ^d	5 IV ^b
Plasma				
Beta (hour ⁻¹)			0.073 ± 0.032	
t _{1/2(k01)} (hour)	3.8	1.9		
t _{1/2(k10)} (hour)	3.1	6.0		5.8
Cl	22.0 mL/hr/kg	28.8 mL/hr/kg	0.017 ± 0.002 L/hr/kg	13.9 mL/hr/kg
V ₁ (mL/kg)				125
V _{ss}	164 mL/kg	149 mL/kg	0.20 ± 0.04 L/kg	113 mL/kg
MRT (hour)	11.8	10.8		8.1
AUC _{inf}	852 ug/mL*hr	2613 ug/mL*hr	295 ± 34 ug*hr/mL	359 ug/mL*hr
F (fraction)	0.63	0.48		

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LEGEND

Data are displayed as mean \pm SD

MODELING METHOD & BEST FIT MODEL

^a Nonlin84 (Metzler et al. 1974); one-compartment model with first-order absorption and elimination kinetics.

^b No details given; One-compartment open model.

^c Plasma concentrations of PCP in the dosed feed study were analysed using a computer model based on linear theory; Yuan JH 1993 dosed feed model in Applied Pharmacology.

^d Nonlin84 (Metzler et al. 1974); Two-compartment model.

ANALYTE

Pentachlorophenol, purified

TK PARAMETERS

Beta = Hybrid rate constant of the beta phase

k_{01} = Absorption rate constant, k_a

$t_{1/2(k01)}$ = Half-life of the absorption process to the central compartment

k_{10} = Elimination rate constant from the central compartment also k_e or k_{elim}

$t_{1/2(k10)}$ = Half-life for the elimination process from the central compartment

Cl = Clearance, includes total clearance

Cl_1 = Clearance of central compartment, Cl_{app} or apparent clearance for intravenous groups

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

MRT = Mean residence time

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

F = Bioavailability, absolute bioavailability

**** END OF REPORT ****