

Experiment Number: S0539
Route: Gavage
Species/Strain: Mouse/B6C3F1

Toxicokinetics Data Summary
Test Compound: 1-Chloro-2-propanol
CAS Number: 127-00-4

Date Report Requested: 01/09/2017
Time Report Requested: 12:42:16
Lab: T.S.I. Mason Laboratories

	Male	
	Treatment Groups (mg/kg)	
	22.5 ^a	45 ^b
	Plasma	
C _{0min(pred)} (ug/mL)		19.82
C _{max} (ug/mL)	7.64	
T _{max} (minute)	5.0	
Lambdaz (minute ⁻¹)	0.0991	
t _{1/2} (minute)	6.99	
Cl _{1(F)} (mL/min/kg)	264.18	
V ₁ (L/kg)		2.27
AUC _{0-t} (ug*min/mL)	86.19	449.02
AUC _{inf} (ug*min/mL)	85.17	426.66

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Female			
Treatment Groups (mg/kg)			
		22.5 ^a	45 ^c
Plasma			
C _{0min(pred)} (ug/mL)			29.75
C _{max} (ug/mL)	9.73		
T _{max} (minute)	5.0		
Lambdaz (minute ⁻¹)	0.0932		
t _{1/2} (minute)	7.43		
Cl _{1(F)} (mL/min/kg)	161.35		
V ₁ (L/kg)			1.51
AUC _{0-t} (ug*min/mL)	138.61		554.45
AUC _{inf} (ug*min/mL)	139.45		506.70

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LEGEND

Data are displayed as mean values

MODELING METHOD & BEST FIT MODEL

^a Calculations, linear regression; linear elimination profile

^b Calculations, linear regression; Michaelis-Menten due to saturation of the elimination kinetics (metabolism or excretion) as indicated by the convex profile of the elimination curve. Assuming instantaneous absorption, best fit of the data is a single capacity limited elimination process. K_m 10.32, V_m 0.94, intercept C_0^* 135.44, and C_0 is C_{max} .

^c Calculations, linear regression; Michaelis-Menten due to saturation of the elimination kinetics (metabolism or excretion) as indicated by the convex profile of the elimination curve. Assuming instantaneous absorption, best fit of the data is a single capacity limited elimination process. K_m 26.07, V_m 2.40, intercept C_0^* 93.12, and C_0 is C_{max}

ANALYTE

1-Chloro-2-propanol

TK PARAMETERS

$C_{0min(pred)}$ = Fitted plasma concentration at time zero (IV only)

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

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

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

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

$Cl_{1(F)}$ = 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

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

**** END OF REPORT ****