

Experiment Number: S0539
Route: Gavage
Species/Strain: Rats/F344/N

Toxicokinetics Data Summary
Compound: 1-Chloro-2-propanol/ **Analyte:** 1-Chloro-2-propanol
CAS Number: 127-00-4

Request Date: 7/11/2023
Request Time: 10:03:16
Lab: T.S.I Mason

Male

Treatment Group (mg/kg)

1.5 Gavage Plasma^a

7.5 Gavage Plasma^b

15.0 Gavage Plasma^c

No parameters calculated

Cmax_obs (ug/mL)		1.63	5.97
Tmax_obs (minute)		5.0	10.0
Lambda_z (minute ⁻¹)		0.0292	0.0325
Half-life (minute)		23.77	21.30
Cl _{1_F} (mL/min/kg)		114.54	59.26
AUC _{0-T} (ug*min/mL)		63.18	250.89
AUC _{inf_pred} (ug*min/mL)		65.48	253.13

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Female

Treatment Group (mg/kg)

1.5 Gavage Plasma^a

7.5 Gavage Plasma^b

15.0 Gavage Plasma^c

No parameters calculated

Cmax_obs (ug/mL)		1.82	4.97
Tmax_obs (minute)		5.0	5.0
Lambda_z (minute ⁻¹)		0.0388	0.0331
Half-life (minute)		17.87	20.95
Cl _{1_F} (mL/min/kg)		148.02	83.73
AUC _{0-T} (ug*min/mL)		49.35	177.50
AUC _{inf_pred} (ug*min/mL)		50.67	179.14

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LEGEND

MODELING METHOD & BEST FIT MODEL

^a calculations, linear regression - The plasma concentration vs time data for the 1.5 mg/kg rats could not be determined due to values which were below quantifiable limits.

^b calculations, linear regression – linear kinetics

^c calculations, linear regression - linear kinetics-Kinetic analysis did not reveal any difference in kinetic disposition when the data was processed as a linear or non-linear model, so assumed linear.

ANALYTE

1-Chloro-2-propanol

TK PARAMETERS

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

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

Lambda_z = Non-compartmental analysis (NCA) terminal elimination rate constant, NCA ke or kelim

Half-Life = Lambda z 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

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

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TK PARAMETERS PROTOCOL

ANALYSIS METHOD

Plasma was analyzed with a validated method using a gas chromatograph-mass spectrometer (GC/MS) in the selected ion mode to measure levels of 1-chloro-2-propanol. Two standard curve ranges encompassed the range of 0.050 to 8.0 ug/mL and dilutions with control plasma were used to extend the upper limit of quantitation to 80 ug/ml. For the lower standard curve, the limit of detection (LOD) was 0.016 ug/mL and the experimental limit of quantitation (ELOQ) was 0.05 ug/mL. For the higher standard curve, LOD was 0.120 ug/mL and ELOQ was 0.6 ug/mL.

TK_GAVAGE PLASMA

1.5 mg/kg, 7.5 mg/kg, 15.0 mg/kg Male and Female

Mice and F344/N rats were administered a single gavage dose. Blood was collected post-dosing from 3 animals/species/route/dose/timepoint for 8 timepoints in the low and mid dose and 10 timepoints for the higher dose. The average plasma levels of 1-chloro-2-propanol were calculated and the logarithm of these values were plotted as a function of time. The terminal rate constant was determined from the slope of the terminal phase of the log plasma concentration-time profile. The slope was obtained by linear regression of the terminal data points. The half life was calculated as 0.693 divided by lambda. AUC was determined using the trapezoid rule. (last timepoint 120 minutes).