Experiment Number: S0640
Route: Gavage, IV
Species/Strain: Rat/F33

Toxicokinetics Data Summary
Test Compound: Dibromoacetic Acid
CAS Number: 631-64-1

Date Report Requested: 11/09/2016
Time Report Requested: 14:02:09
Lab: Battelle Columbus

Male

	Treatment Groups (mg/kg)			
	25 [a]	**50** [a]	**125** [a]	**25 IV** [b]
	Plasma			
$C_{0min(pred)}$ (ug/mL)				66.77 ± 2.99
C_{max} (ug/mL)	10.47 ± 1.29	24.20 ± 2.42	77.50 ± 5.91	
T_{max} (hour)	0.4793 ± 0.0952	0.4871 ± 0.0836	0.4142 ± 0.0624	
k_{01} (hour^-1)	4.114 ± 1.558	4.420 ± 1.306	6.169 ± 1.544	
$t_{1/2(k01)}$ (hour)	0.1685 ± 0.0638	0.1568 ± 0.0463	0.1124 ± 0.0281	
k_{10} (hour^-1)	0.8682 ± 0.1277	0.7338 ± 0.0612	0.6194 ± 0.0606	3.329 ± 0.075
$t_{1/2(k10)}$ (hour)	0.7984 ± 0.1173	0.9446 ± 0.0787	1.119 ± 0.109	0.2083 ± 0.0047
Cl_1 (mL/hr/kg)				1246 ± 37
$Cl_{1(F)}$ (mL/hr/kg)	1367.0 ± 146.0	1060.0 ± 95.0	773.0 ± 49.8	
V_1 (mL/kg)				374.5 ± 16.8
$V_{1(F)}$ (mL/kg)	1575.0 ± 319.0	1445.0 ± 205.0	1248.0 ± 142.0	
AUC_{0-t} (ug/mL*hr)	13.85	41.07	151.9	17.99
AUC_{inf} (ug/mL*hr)	18.28 ± 1.95	47.16 ± 4.21	161.7 ± 10.4	20.06 ± 0.59
F (percent)	43.2	57.3	60.8	

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Female

	Treatment Groups (mg/kg)			
	25 [a]	50 [a]	125 [a]	25 IV [b]
Plasma				
$C_{0min(pred)}$ (ug/mL)				62.70 ± 3.04
C_{max} (ug/mL)	14.78 ± 2.02	29.25 ± 2.66	94.92 ± 7.72	
T_{max} (hour)	0.2747 ± 0.0939	0.4018 ± 0.0645	0.3634 ± 0.0629	
k_{01} (hour^-1)	10.01 ± 5.24	5.328 ± 1.508	7.034 ± 1.908	
$t_{1/2(k01)}$ (hour)	0.06927 ± 0.03623	0.1301 ± 0.0368	0.09854 ± 0.0267	
k_{10} (hour^-1)	0.7970 ± 0.1009	0.8988 ± 0.0827	0.7055 ± 0.0422	3.322 ± 0.806
$t_{1/2(k10)}$ (hour)	0.8697 ± 0.1099	0.7712 ± 0.0709	0.9825 ± 0.0587	0.2087 ± 0.0051
Cl_1 (mL/hr/kg)				1324 ± 42
$Cl_{1(F)}$ (mL/hr/kg)	1083.0 ± 117.0	1071.0 ± 83.0	719.0 ± 51.3	
V_1 (mL/kg)				398.7 ± 19.3
$V_{1(F)}$ (mL/kg)	1359.0 ± 240.0	1191.0 ± 161.0	1019.0 ± 109.0	
AUC_{0-t} (ug/mL*hr)	15.47	44.66	168.7	16.93
AUC_{inf} (ug/mL*hr)	23.09 ± 2.48	46.70 ± 3.60	173.9 ± 12.4	18.88 ± 0.60
F (percent)	63.7	77.8	90.8	

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LEGEND

Data are displayed as mean ± SEM

MODELING METHOD & BEST FIT MODEL

[a] WinNONLIN (version 2.1, Scientific Consulting, Inc., Freeman SD); one-compartment model with no lag time and first-order absorption and elimination (Flip-flop model--In the flip-flop situation, the initial upward phase of the profile is a measure of the elimination phase and the terminal linear phase actually reflects the absorption phase -- the reverse situation of the typical plasma concentration time profile. A flip-flop situation often occurs with chemicals that undergo very fast elimination.)

[b] WinNONLIN (version 2.1, Scientific Consulting, Inc., Freeman SD); one-compartment model with first order elimination.

ANALYTE

Dibromoacetic acid

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

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_1 = Clearance of central compartment, Cl_{app} or apparent clearance for intravenous groups

$Cl_{1(F)}$ = 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

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

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 **