Experiment Number: S0640	**Toxicokinetics Data Summary**	**Date Report Requested:** 11/09/2016
Route: Gavage, IV	**Test Compound:** Dibromoacetic Acid	**Time Report Requested:** 14:01:59
Species/Strain: Mouse/B6C3F1	**CAS Number:** 631-64-1	**Lab:** Battelle Columbus

Male

Treatment Groups (mg/kg)

Plasma

	70 [a]		175 [a]		350 [a]		70 IV [b]	
$C_{0min(pred)}$ (ug/mL)							94.79 ±	12.04
C_{max} (ug/mL)	6.045 ±	0.747	32.15 ±	4.00	91.06 ±	13.89		
T_{max} (hour)	0.2816 ±	0.0510	0.2510 ±	0.0830	0.3973 ±	0.1539		
k_{01} (hour^-1)	5.890 ±	2.311	10.97 ±	5.40	7.938 ±	4.407		
$t_{1/2(k01)}$ (hour)	0.1177 ±	0.0461	0.06318 ±	0.03107	0.08732 ±	0.04843		
k_{10} (hour^-1)	1.932 ±	0.311	0.8688 ±	0.0613	0.3967 ±	0.0368	6.307 ±	0.240
$t_{1/2(k10)}$ (hour)	0.3588 ±	0.0577	0.7978 ±	0.0562	1.747 ±	0.162	0.1099 ±	0.0042
Cl_1 (mL/hr/kg)							4657 ±	465
$Cl_{1(F)}$ (mL/hr/kg)	12983.0 ±	1331.0	3802.0 ±	393.0	1302.0 ±	173.0		
V_1 (mL/kg)							738.5 ±	93.9
$V_{1(F)}$ (mL/kg)	6720.0 ±	1439.0	4377.0 ±	629.0	3283.0 ±	606.0		
AUC_{0-t} (ug/mL*hr)	5.960		32.04		112.5		15.52	
AUC_{inf} (ug/mL*hr)	5.392 ±	.552	46.02 ±	4.75	268.8 ±	35.7	15.03 ±	1.50
F (percent)	12.6		28.5		43.2			

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Female

Treatment Groups (mg/kg)

Plasma

	70 [a]		175 [a]		350 [a]		70 IV [b]	
$C_{0min(pred)}$ (ug/mL)							98.61	± 17.12
C_{max} (ug/mL)	6.753	± 1.121	36.42	± 5.12	72.22	± 10.72		
T_{max} (hour)	0.2174	± 0.0590	0.2446	± 0.0831	0.2322	± 0.1610		
k_{01} (hour^-1)	8.572	± 4.375	10.52	± 5.52	17.13	± 15.73		
$t_{1/2(k01)}$ (hour)	0.08086	± 0.04123	0.06589	± 0.0346	0.04047	± 0.03713		
k_{10} (hour^-1)	2.099	± 0.327	1.033	± 0.102	0.3479	± 0.0341	8.253	± 0.462
$t_{1/2(k10)}$ (hour)	0.3302	± 0.0514	0.6710	± 0.06589	1.992	± 0.195	0.0840	± 0.0047
Cl_1 (mL/hr/kg)							5858	± 795
$Cl_{1(F)}$ (mL/hr/kg)	13788.0	± 1785.0	3855.0	± 433.0	1555.0	± 188.0		
V_1 (mL/kg)							709.8	± 123.4
$V_{1(F)}$ (mL/kg)	6568.0	± 1522.0	3732.0	± 640.0	4470.0	± 747.0		
AUC_{0-t} (ug/mL*hr)	4.236		28.83		84.33		15.82	
AUC_{inf} (ug/mL*hr)	5.077	± 0.657	45.39	± 5.09	225.1	± 27.1	11.95	± 1.62
F (percent)	10.7		26.1		43.5			

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 **