Experiment Number: S0546
Route: Gavage, IV
Species/Strain: Rat/Sprague-Dawley

Toxicokinetics Data Summary
Test Compound: 2,4-Dichlorophenoxyacetic Acid
CAS Number: 94-75-7

Date Report Requested: 11/09/2016
Time Report Requested: 13:59:47
Lab: Research Triangle Institute

Male

	Treatment Groups (mg/kg)				
	1.5 [a]	**1.5 [b]**	**3.56 [b]**	**7 [b]**	**2 IV [b]**
	Plasma				
$C_{0min(pred)}$ (ug/mL)					33.4
C_{max} (ug/mL)		3.73	11.0	12.0	
T_{max} (minute)		30	30	10	
Alpha (min^-1)	0.223 ± 0.0082				
Beta (min^-1)	0.0200 ± 0.0021				
$t_{1/2(Beta)}$ (minute)		134	1066	176	61.9
k_{01} (min^-1)	0.0330 ± 0.0058				
k_{10} (min^-1)	0.0461 ± 0.0074				
k_{12} (min^-1)	0.0998 ± 0.049				
k_{21} (min^-1)	0.0968 ± 0.031				
Cl (mL/min/kg)					2.02
$Cl_{1(F)}$ (mL/min/kg)		2.92			
V_1 (L/kg)	0.0559 ± 0.0091				
MRT (minute)		180.0	1417.0	290.0	61.7
AUC_{inf} (ug/mL*min)		513.0	4821.0	2959.0	992
F (fraction)		0.69			

LEGEND

Data are displayed as mean ± SEM

MODELING METHOD & BEST FIT MODEL

[a] Analyzed using compartmental modeling techniques with established models or models written to simultaneously solve iv and oral data sets (PCNONLIN software, SCI Software, Lexington, KY); The rat data were best fit using a 2-compartment model with simultaneous solution of the iv (Study X) and low oral (Study Y) data.

[b] Models 200 and 201, PCNONLIN software, SCI Software, Lexington, KY; noncompartmental model (not best fit)

ANALYTE

2,4-Dichlorophenoxyacetic 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

Alpha = Hybrid rate constant of the alpha phase

Beta = Hybrid rate constant of the beta phase

$t_{½(beta)}$ = Half-life for the beta phase

k_{01} = Absorption rate constant, k_a

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

k_{12} = Distribution rate constant from first to second compartment etc.

k_{21} = Distribution rate constant from second to first compartment etc.

Cl = Clearance, includes total clearance

$Cl_{1(F)}$ = 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

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 **