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

Toxicokinetics Data Summary
Test Compound: Fluorotelomer alcohol 8+2
CAS Number: 678-39-7

Date Report Requested: 02/06/2017
Time Report Requested: 17:17:34
Lab: Battelle Columbus

	Male				
	Treatment Groups (mg/kg)				
	24 [a, #]	24 [a, ~]	24 [a, #]	24 [a, o]	24 [a, ~]
	Brain		Kidney		
$C_{max(pred)}$ (ng/mL)					
$T_{max(pred)}$ (hour)					
$C_{max(obs)}$	443 ng/mL	2440 ng/g	1470 ng/mL	455 ng/g	2080 ng/g
$T_{max(obs)}$ (hour)	3.00	0.640	3.00	12.0	0.620
$t_{1/2}$ (hour)	5.86	2.72	11.2	ND	3.74
$t_{1/2(Alpha)}$ (hour)					
$t_{1/2(Beta)}$ (hour)					
k_{01} (hour^-1)					
$t_{1/2(k01)}$ (hour)					
k_{10} (hour^-1)					
$t_{1/2(k10)}$ (hour)					
k_{12} (hour^-1)					
k_{21} (hour^-1)					
Cl_{1} (mL/hr/kg)					
$Cl_{1(F)}$ (mL/hr/kg)					
V_{1} (mL/kg)					
V_{2} (mL/kg)					
$V_{1(F)}$ (mL/kg)					
$V_{2(F)}$ (mL/kg)					
MRT (hour)					
AUC_{0-t} (ng/mL*hr)					
AUC_{inf} (ng/mL*hr)					
F (percent)					

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Male

	Treatment Groups (mg/kg)					
	24 [a, o]	**24 [a, ~]**	**24 [a, #]**	**12 [a, o]**	**12 [a, #]**	**12 [b, ~]**
	Liver			**Plasma**		
$C_{max(pred)}$ (ng/mL)						350 ± 59
$T_{max(pred)}$ (hour)						0.545 ± 0.167
$C_{max(obs)}$	1680 ng/g	9030 ng/g	2900 ng/mL	743 ng/mL	795 ng/mL	
$T_{max(obs)}$ (hour)	12.0	0.617	3.00	24.0	3.00	
$t_{1/2}$ (hour)	ND	5.35	27.0	198	56.1	
$t_{1/2(Alpha)}$ (hour)						1.32 ± 0.38
$t_{1/2(Beta)}$ (hour)						13.0 ± 11.3
k_{01} (hour^-1)						4.54 ± 2.38
$t_{1/2(k01)}$ (hour)						0.153 ± 0.080
k_{10} (hour^-1)						0.394 ± 0.102
$t_{1/2(k10)}$ (hour)						1.76 ± 0.46
k_{12} (hour^-1)						0.113 ± 0.052
k_{21} (hour^-1)						0.0708 ± 0.0626
Cl_1 (mL/hr/kg)						
$Cl_{1(F)}$ (mL/hr/kg)						10300 ± 1600
V_1 (mL/kg)						
V_2 (mL/kg)						
$V_{1(F)}$ (mL/kg)						26000 ± 6800
$V_{2(F)}$ (mL/kg)						41500 ± 38000
MRT (hour)						
AUC_{0-t} (ng/mL*hr)						1070
AUC_{inf} (ng/mL*hr)				213000	30500	1170 ± 180
F (percent)						41.2

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Male

	Treatment Groups (mg/kg)					
	24 [a, #]	**24 [a, o]**	**24 [b, ~]**	**48 [a, o]**	**48 [a, #]**	**48 [b, ~]**
			Plasma			
$C_{max(pred)}$ (ng/mL)			470 ± 94			689 ± 136
$T_{max(pred)}$ (hour)			0.853 ± 0.226			1.37 ± 0.30
$C_{max(obs)}$	1610 ng/mL	1080 ng/mL		2340 ng/mL	2370 ng/mL	
$T_{max(obs)}$ (hour)	3.00	24.0		6.00	6.00	
$t_{1/2}$ (hour)	52.5	269		353	105	
$t_{1/2(Alpha)}$ (hour)			0.702 ± 1.19			1.00 ± 2.58
$t_{1/2(Beta)}$ (hour)			5.16 ± 1.16			6.65 ± 1.20
k_{01} (hour^-1)			1.57 ± 2.79			0.901 ± 2.34
$t_{1/2(k01)}$ (hour)			0.441 ± 0.782			0.769 ± 1.99
k_{10} (hour^-1)			0.591 ± 0.910			0.415 ± 0.994
$t_{1/2(k10)}$ (hour)			1.17 ± 1.80			1.67 ± 3.99
k_{12} (hour^-1)			0.306 ± 0.723			0.208 ± 0.761
k_{21} (hour^-1)			0.224 ± 0.095			0.174 ± 0.074
Cl_1 (mL/hr/kg)						
$Cl_{1(F)}$ (mL/hr/kg)			14500 ± 2100			12800 ± 1800
V_1 (mL/kg)						
V_2 (mL/kg)						
$V_{1(F)}$ (mL/kg)			24500 ± 38400			30900 ± 75800
$V_{2(F)}$ (mL/kg)			33400 ± 21200			37000 ± 35500
MRT (hour)						
AUC_{0-t} (ng/mL*hr)			1540			3520
AUC_{inf} (ng/mL*hr)	55000	418000	1660 ± 240	1030000	118000	3740 ± 530
F (percent)			29.2			32.9

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Male

	Treatment Groups (mg/kg)		
	12 IV [c, o]	**12 IV [c, #]**	**12 IV [d, ~]**
	Plasma		
$C_{max(pred)}$ (ng/mL)			3020 ± 390
$T_{max(pred)}$ (hour)			
$C_{max(obs)}$	534 ng/mL	747 ng/mL	
$T_{max(obs)}$ (hour)	24.0	3.00	
$t_{1/2}$ (hour)	225	60.6	
$t_{1/2(Alpha)}$ (hour)			0.508 ± 0.060
$t_{1/2(Beta)}$ (hour)			6.62 ± 0.95
k_{01} (hour^-1)			
$t_{1/2(k01)}$ (hour)			
k_{10} (hour^-1)			1.06 ± 0.11
$t_{1/2(k10)}$ (hour)			0.651 ± 0.069
k_{12} (hour^-1)			0.270 ± 0.056
k_{21} (hour^-1)			0.134 ± 0.021
Cl_1 (mL/hr/kg)			4230 ± 310
$Cl_{1(F)}$ (mL/hr/kg)			
V_1 (mL/kg)			3970 ± 520
V_2 (mL/kg)			7990 ± 1570
$V_{1(F)}$ (mL/kg)			
$V_{2(F)}$ (mL/kg)			
MRT (hour)			2.83 ± 0.32
AUC_{0-t} (ng/mL*hr)			2840
AUC_{inf} (ng/mL*hr)	176000	20700	2840 ± 210
F (percent)			

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Toxicokinetics Data Summary
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CAS Number: 678-39-7

Date Report Requested: 02/06/2017
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Lab: Battelle Columbus

	Female				
	Treatment Groups (mg/kg)				
	80 [a, ~]	80 [a, #]	80 [a, ~]	80 [a, #]	80 [a, o]
	Brain		Kidney		
$C_{max(pred)}$ (ng/mL)					
$T_{max(pred)}$ (hour)					
$C_{max(obs)}$	8570 ng/g	1250 ng/mL	4480 ng/g	4900 ng/mL	2080 ng/g
$T_{max(obs)}$ (hour)	3.17	3.17	3.16	3.16	6
$t_{1/2}$ (hour)	2.26	6.44	2.58	11.9	6.24
$t_{1/2(Alpha)}$ (hour)					
$t_{1/2(Beta)}$ (hour)					
k_{01} (hour^-1)					
$t_{1/2(k01)}$ (hour)					
k_{10} (hour^-1)					
$t_{1/2(k10)}$ (hour)					
k_{12} (hour^-1)					
k_{21} (hour^-1)					
Cl_{1} (mL/hr/kg)					
$Cl_{1(F)}$ (mL/hr/kg)					
V_{1} (mL/kg)					
V_{2} (mL/kg)					
$V_{1(F)}$ (mL/kg)					
$V_{2(F)}$ (mL/kg)					
MRT (hour)					
AUC_{0-t} (ng/mL*hr)					
AUC_{inf} (ng/mL*hr)					
F (percent)					

Experiment Number: NA
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Toxicokinetics Data Summary
Test Compound: Fluorotelomer alcohol 8+2
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Date Report Requested: 02/06/2017
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	Female					
	Treatment Groups (mg/kg)					
	80 [a, ~]	80 [a, #]	80 [a, o]	40 [a, o]	40 [a, #]	40 [b, ~]
	Liver			Plasma		
$C_{max(pred)}$ (ng/mL)						580 ± 153
$T_{max(pred)}$ (hour)						0.921 ± 0.303
$C_{max(obs)}$	10500 ng/g	10100 ng/mL	2000 ng/g	1180 ng/mL	3250 ng/mL	
$T_{max(obs)}$ (hour)	0.607	3.00	3.00	6.00	3.00	
$t_{1/2}$ (hour)	3.32	21.8	4.72	6.35	40.0	
$t_{1/2(Alpha)}$ (hour)						0.617 ± 4.15
$t_{1/2(Beta)}$ (hour)						7.52 ± 2.50
k_{01} (hour^-1)						1.35 ± 8.98
$t_{1/2(k01)}$ (hour)						0.513 ± 3.40
k_{10} (hour^-1)						0.413 ± 2.63
$t_{1/2(k10)}$ (hour)						1.68 ± 10.6
k_{12} (hour^-1)						0.552 ± 4.82
k_{21} (hour^-1)						0.250 ± 0.193
Cl_1 (mL/hr/kg)						
$Cl_{1(F)}$ (mL/hr/kg)						12600 ± 1800
V_1 (mL/kg)						
V_2 (mL/kg)						
$V_{1(F)}$ (mL/kg)						30500 ± 193000
$V_{2(F)}$ (mL/kg)						67200 ± 126000
MRT (hour)						
AUC_{0-t} (ng/mL*hr)						2610
AUC_{inf} (ng/mL*hr)				18300	66200	3180 ± 460
F (percent)						22.2

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Female

	Treatment Groups (mg/kg)					
	80 [a, o]	**80 [a, #]**	**80 [b, ~]**	**160 [a, o]**	**160 [a, #]**	**160 [b, ~]**
	Plasma					
$C_{max(pred)}$ (ng/mL)			946 ± 203			2040 ± 420
$T_{max(pred)}$ (hour)			2.40 ± 0.51			2.76 ± 0.41
$C_{max(obs)}$	2770 ng/mL	7760 ng/mL		4890 ng/mL	8590 ng/mL	
$T_{max(obs)}$ (hour)	3.00	3.00		3.00	6.00	
$t_{1/2}$ (hour)	12.0	99.0		6.97	33.0	
$t_{1/2(Alpha)}$ (hour)			2.08 ± 2.62			1.59 ± 16.9
$t_{1/2(Beta)}$ (hour)			9.48 ± 5.05			5.4 ± 0.76
k_{01} (hour^-1)			0.532 ± 0.729			0.507 ± 4.39
$t_{1/2(k01)}$ (hour)			1.30 ± 1.79			1.37 ± 11.8
k_{10} (hour^-1)			0.297 ± 0.345			0.205 ± 1.75
$t_{1/2(k10)}$ (hour)			2.33 ± 2.70			3.37 ± 28.7
k_{12} (hour^-1)			0.0268 ± 0.0652			0.0863 ± 2.27
k_{21} (hour^-1)			0.0818 ± 0.0534			0.272 ± 0.631
Cl_1 (mL/hr/kg)						
$Cl_{1(F)}$ (mL/hr/kg)			11600 ± 2000			7860 ± 900
V_1 (mL/kg)						
V_2 (mL/kg)						
$V_{1(F)}$ (mL/kg)			39200 ± 49000			38200 ± 327000
$V_{2(F)}$ (mL/kg)			12800 ± 10100			12100 ± 190000
MRT (hour)						
AUC_{0-t} (ng/mL*hr)			6080			22200
AUC_{inf} (ng/mL*hr)	28900	27200	6870 ± 1210	93600	31900	20400 ± 2400
F (percent)			24.0			35.7

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Female

	Treatment Groups (mg/kg)			
	40 IV [c, o]	**40 IV [c, #]**	**40 IV [d, ~]**	
	Plasma			
$C_{max(pred)}$ (ng/mL)			17600	± 2700
$T_{max(pred)}$ (hour)				
$C_{max(obs)}$	2390 ng/mL	2630 ng/mL		
$T_{max(obs)}$ (hour)	1.00	3.00		
$t_{1/2}$ (hour)	4.47	71.2		
$t_{1/2(Alpha)}$ (hour)			0.475 ±	0.055
$t_{1/2(Beta)}$ (hour)			7.33 ±	1.38
k_{01} (hour^-1)				
$t_{1/2(k01)}$ (hour)				
k_{10} (hour^-1)			1.23 ±	0.14
$t_{1/2(k10)}$ (hour)			0.563 ±	0.062
k_{12} (hour^-1)			0.211 ±	0.045
k_{21} (hour^-1)			0.112 ±	0.022
Cl_1 (mL/hr/kg)			2800	± 250
$Cl_{1(F)}$ (mL/hr/kg)				
V_1 (mL/kg)			2270	± 340
V_2 (mL/kg)			4270	± 1110
$V_{1(F)}$ (mL/kg)				
$V_{2(F)}$ (mL/kg)				
MRT (hour)			2.34 ±	0.36
AUC_{0-t} (ng/mL*hr)			15100	
AUC_{inf} (ng/mL*hr)	19700	69600	14300	± 1300
F (percent)				

LEGEND

Data are displayed as mean ± SEM

*Data are displayed as mean ± SD

ND = not determined

MODELING METHOD & BEST FIT MODEL

[a] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Noncompartmental analysis (NCA) model with first order input, first order output, and uniform weighting. Parameter estimates are reported to three significant figures. NCA does not calculate a standard error.

[b] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Two-compartment model with first order input, first order output, and 1/Yhat2 weighting. Parameter estimates are reported to three significant figures. Observed values do not have a reported SEM.

[c] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Noncompartmental analysis (NCA) model with bolus input, first order output, and uniform weighting. Parameter estimates are reported to three significant figures. NCA does not calculate a standard error.

[d] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Two-compartment model with bolus input, first order output, and l/Yhat2 weighting. Parameter estimates are reported to three significant figures. AUC_0-T is an observed values that does not have a reported SEM. Cmax (predicted) based on the model prediction at 0 minutes.

ANALYTE

[#] Fluorotelomer acid 7+3

[~] Fluorotelomer alcohol 8+2

[o] Perfluorooctanoic acid

TK PARAMETERS

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

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

$t_{½}$ = $Lambda_z$ half-life, $t_{1/2}$, the terminal elimination half-life based on non-compartmental analysis

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

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

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

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

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

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

LEGEND

TK PARAMETERS

V_2 = Volume of distribution for the peripheral compartment
$V_{1(F)}$ = Apparent volume of distribution for the central compartment includes $V_{d(F)}$, $V_{(F)}$ for oral groups, and $V_{c(F)}$
$V_{2(F)}$ = Apparent volume of distribution for the peripheral compartment
MRT = Mean residence time
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 **