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

Toxicokinetics Data Summary
Test Compound: Perfluorodecanoic acid
CAS Number: 335-76-2

Date Report Requested: 01/09/2017
Time Report Requested: 11:25:25
Lab: Battelle Columbus

Male

	Treatment Groups (mg/kg)			
	10 [a]	**10 [a]**	**10 [a]**	**2 [b]**
	Brain	**Kidney**	**Liver**	**Plasma**
$C_{max(pred)}$ (ng/mL)				7520 ± 360
$T_{max(pred)}$ (hour)				8.27 ± 0.63
$C_{max(obs)}$ (ng/g)	2590	27800	112000	
$T_{max(obs)}$ (hour)	24.0	24.0	24.0	
$t_{1/2}$ (hour)	865	832	983	
$t_{1/2(Alpha)}$ (hour)				175 ± 31
$t_{1/2(Beta)}$ (hour)				1620 ± 220
k_{01} (hour^-1)				0.656 ± 0.066
$t_{1/2(k01)}$ (hour)				1.06 ± 0.11
k_{10} (hour^-1)				0.00120 ± 8.0E-5
$t_{1/2(k10)}$ (hour)				579 ± 40
k_{12} (hour^-1)				0.00178 ± 3.9E-4
k_{21} (hour^-1)				0.00141 ± 3.4E-4
Cl_1 (mL/hr/kg)				
$Cl_{1(F)}$ (mL/hr/kg)				0.310 ± 0.014
V_1 (mL/kg)				
V_2 (mL/kg)				
$V_{1(F)}$ (mL/kg)				259 ± 13
$V_{2(F)}$ (mL/kg)				327 ± 44
MRT (hour)				
AUC_{0-t} (ng/mL*hr)				5410000
AUC_{inf} (ng/mL*hr)				6440000 ± 290000
F (percent)				172

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	Treatment Groups (mg/kg)		
	10 [b]	**20** [b]	**2 IV** [c]
	Plasma		
$C_{max(pred)}$ (ng/mL)	42400 ± 2700	81300 ± 3600	7300 ± 740
$T_{max(pred)}$ (hour)	9.06 ± 0.85	10.0 ± 0.6	
$C_{max(obs)}$ (ng/g)			
$T_{max(obs)}$ (hour)			
$t_{1/2}$ (hour)			
$t_{1/2(Alpha)}$ (hour)	123 ± 40	111 ± 24	27.0 ± 17.0
$t_{1/2(Beta)}$ (hour)	995 ± 80	1070 ± 60	854 ± 61
k_{01} (hour^-1)	0.562 ± 0.072	0.482 ± 0.042	
$t_{1/2(k01)}$ (hour)	1.23 ± 0.16	1.44 ± 0.13	
k_{10} (hour^-1)	0.00145 ± 1.1E-4	0.00143 ± 8.0E-5	0.00195 ± 2.4E-4
$t_{1/2(k10)}$ (hour)	478 ± 38	485 ± 27	356 ± 44
k_{12} (hour^-1)	0.00217 ± 9.3E-4	0.00264 ± 7.3E-4	0.0138 ± 0.0100
k_{21} (hour^-1)	0.00271 ± 9.1E-4	0.00283 ± 6.2E-4	0.0107 ± 0.0062
Cl_1 (mL/hr/kg)			0.534 ± 0.031
$Cl_{1(F)}$ (mL/hr/kg)	0.331 ± 0.013	0.338 ± 0.009	
V_1 (mL/kg)			274 ± 28
V_2 (mL/kg)			355 ± 69
$V_{1(F)}$ (mL/kg)	228 ± 16	236 ± 12	
$V_{2(F)}$ (mL/kg)	183 ± 30	220 ± 23	
MRT (hour)			1180 ± 80
AUC_{0-t} (ng/mL*hr)	28500000	55000000	3500000
AUC_{inf} (ng/mL*hr)	30200000 ± 1200000	59200000 ± 1600000	3750000 ± 220000
F (percent)	161	158	

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Female

	Treatment Groups (mg/kg)			
	10 [a]	**10 [a]**	**10 [a]**	**2 [b]**
	Brain	**Kidney**	**Liver**	**Plasma**
$C_{max(pred)}$ (ng/mL)				10400 ± 600
$T_{max(pred)}$ (hour)				9.01 ± 0.8
$C_{max(obs)}$ (ng/g)	2380	57300	126000	
$T_{max(obs)}$ (hour)	24.0	24.0	24.0	
$t_{1/2}$ (hour)	987	918	900	
$t_{1/2(Alpha)}$ (hour)				295 ± 110
$t_{1/2(Beta)}$ (hour)				1240 ± 290
k_{01} (hour^-1)				0.672 ± 0.078
$t_{1/2(k01)}$ (hour)				1.03 ± 0.12
k_{10} (hour^-1)				0.00101 ± 7.0E-5
$t_{1/2(k10)}$ (hour)				685 ± 50
k_{12} (hour^-1)				5.99E-4 ± 2.74E-4
k_{21} (hour^-1)				0.00129 ± 6.9E-4
Cl_1 (mL/hr/kg)				
$Cl_{1(F)}$ (mL/hr/kg)				0.192 ± 0.009
V_1 (mL/kg)				
V_2 (mL/kg)				
$V_{1(F)}$ (mL/kg)				189 ± 11
$V_{2(F)}$ (mL/kg)				87.9 ± 23.9
MRT (hour)				
AUC_{0-t} (ng/mL*hr)				9740000
AUC_{inf} (ng/mL*hr)				10400000 ± 500000
F (percent)				170

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	Treatment Groups (mg/kg)		
	10 [b]	**20** [b]	**2 IV** [c]
	Plasma		
$C_{max(pred)}$ (ng/mL)	55200 ± 3200	124000 ± 10000	8400 ± 1240
$T_{max(pred)}$ (hour)	9.29 ± 0.88	10.8 ± 1.2	
$C_{max(obs)}$ (ng/g)			
$T_{max(obs)}$ (hour)			
$t_{1/2}$ (hour)			
$t_{1/2(Alpha)}$ (hour)	298 ± 116	226 ± 81	5.92 ± 4.64
$t_{1/2(Beta)}$ (hour)	1260 ± 330	1240 ± 270	904 ± 83
k_{01} (hour^-1)	0.646 ± 0.080	0.508 ± 0.078	
$t_{1/2(k01)}$ (hour)	1.07 ± 0.13	1.37 ± 0.21	
k_{10} (hour^-1)	0.00102 ± 8.0E-5	0.00122 ± 1.2E-4	0.00137 ± 2.2E-4
$t_{1/2(k10)}$ (hour)	681 ± 55	569 ± 55	506 ± 81
k_{12} (hour^-1)	6.03E-4 ± 2.86E-4	0.00100 ± 4.7E-4	0.0510 ± 0.0432
k_{21} (hour^-1)	0.00125 ± 7.1E-4	0.00141 ± 6.8E-4	0.0655 ± 0.0515
Cl_1 (mL/hr/kg)			0.327 ± 0.024
$Cl_{1(F)}$ (mL/hr/kg)	0.182 ± 0.010	0.192 ± 0.011	
V_1 (mL/kg)			238 ± 35
V_2 (mL/kg)			186 ± 57
$V_{1(F)}$ (mL/kg)	178 ± 11	158 ± 13	
$V_{2(F)}$ (mL/kg)	85.8 ± 25.3	112 ± 27	
MRT (hour)			1300 ± 120
AUC_{0-t} (ng/mL*hr)	50800000	100000000	5760000
AUC_{inf} (ng/mL*hr)	55000000 ± 2900000	104000000 ± 6000000	6130000 ± 450000
F (percent)	179	170	

LEGEND

Data are displayed as mean ± SEM

MODELING METHOD & BEST FIT MODEL

[a] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Non-compartmental (NCA) model with first order input, first order output, and uniform weighting.

[b] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Two-compartment model with first order input and first order output 1/Yhat2 weighting.

[c] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Two-compartment model with bolus input, first order output, and 1/Yhat2 weighting.

ANALYTE

Perfluorodecanoic 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

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 **