Experiment Number: C07040
Route: Gavage, IV
Species/Strain: Rat/Harlan Sprague-Dawley

Toxicokinetics Data Summary
Test Compound: Potassium Perfluorobutane Sulfonate
CAS Number: 29420-49-3

Date Report Requested: 12/29/2016
Time Report Requested: 14:35:06
Lab: Battelle Columbus

Male

Treatment Groups (mg/kg)

	20 [a]	20 [b]	20 [b]	4 [c]		
	Brain	**Kidney**	**Liver**	**Plasma**		
$C_{max(pred)}$ (ng/mL)				16000	±	2500
$T_{max(pred)}$ (hour)				2.37	±	0.56
$C_{max(obs)}$ (ng/g)	1120	22500	95200			
$T_{max(obs)}$ (hour)	1.13	3.00	1.11			
$t_{1/2}$ (hour)	ND	3.13	2.83			
$t_{1/2(Alpha)}$ (hour)				1.37	±	31.5
$t_{1/2(Beta)}$ (hour)				4.89	±	1.67
k_{01} (hour^-1)				0.839	±	3.57
$t_{1/2(k01)}$ (hour)				0.826	±	3.51
k_{10} (hour^-1)				0.159	±	0.657
$t_{1/2(k10)}$ (hour)				4.37	±	18.1
k_{12} (hour^-1)				0.0366	±	2.34
k_{21} (hour^-1)				0.451	±	8.69
Cl_1 (mL/hr/kg)						
$Cl_{1(F)}$ (mL/hr/kg)				26.0	±	2.5
V_1 (mL/kg)						
V_2 (mL/kg)						
$V_{1(F)}$ (mL/kg)				164	±	677
$V_{2(F)}$ (mL/kg)				13.3	±	544
MRT (hour)						
AUC_{0-t} (ng/mL*hr)				151000		
AUC_{inf} (ng/mL*hr)				154000	±	15000
F (percent)				133		

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	Male					
	Treatment Groups (mg/kg)					
	20 [c]		**100** [c]		**4 IV** [d]	
	Plasma					
$C_{max(pred)}$ (ng/mL)	75100	± 7700	225000	± 21000	35500	± 5100
$T_{max(pred)}$ (hour)	2.18	± 0.24	1.42	± 0.18		
$C_{max(obs)}$ (ng/g)						
$T_{max(obs)}$ (hour)						
$t_{1/2}$ (hour)						
$t_{1/2(Alpha)}$ (hour)	2.37	± 1.07	2.60	± 0.61	0.532	± 0.251
$t_{1/2(Beta)}$ (hour)	5.36	± 1.24	5.25	± 1.19	4.22	± 0.28
k_{01} (hour^-1)	0.722	± 0.306	1.52	± 0.40		
$t_{1/2(k01)}$ (hour)	0.960	± 0.406	0.455	± 0.120		
k_{10} (hour^-1)	0.254	± 0.078	0.243	± 0.033	0.307	± 0.044
$t_{1/2(k10)}$ (hour)	2.73	± 0.84	2.86	± 0.39	2.26	± 0.33
k_{12} (hour^-1)	0.0192	± 0.0304	0.0112	± 0.0141	0.463	± 0.308
k_{21} (hour^-1)	0.149	± 0.058	0.145	± 0.050	0.697	± 0.311
Cl_1 (mL/hr/kg)					34.5	± 2.0
$Cl_{1(F)}$ (mL/hr/kg)	37.6	± 3.1	75.5	± 5.8		
V_1 (mL/kg)					113	± 16
V_2 (mL/kg)					74.8	± 18.8
$V_{1(F)}$ (mL/kg)	148	± 52	311	± 55		
$V_{2(F)}$ (mL/kg)	19.0	± 17.7	23.9	± 19.5		
MRT (hour)					5.43	± 0.25
AUC_{0-t} (ng/mL*hr)	499000		1280000		112000	
AUC_{inf} (ng/mL*hr)	533000	± 45000	1320000	± 100000	116000	± 7000
F (percent)	91.9		45.5			

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	Female			
	Treatment Groups (mg/kg)			
	20 [a]	20 [b]	20 [b]	4 [c]
	Brain	Kidney	Liver	Plasma
$C_{max(pred)}$ (ng/mL)				8830 ± 860
$T_{max(pred)}$ (hour)				0.994 ± 0.132
$C_{max(obs)}$ (ng/g)	522	26700	42900	
$T_{max(obs)}$ (hour)	0.583	0.567	0.556	
$t_{1/2}$ (hour)	ND	1.42	1.16	
$t_{1/2(Alpha)}$ (hour)				1.04 ± 0.28
$t_{1/2(Beta)}$ (hour)				7.84 ± 3.66
k_{01} (hour^-1)				1.47 ± 0.59
$t_{1/2(k01)}$ (hour)				0.471 ± 0.188
k_{10} (hour^-1)				0.589 ± 0.147
$t_{1/2(k10)}$ (hour)				1.18 ± 0.29
k_{12} (hour^-1)				0.0675 ± 0.0326
k_{21} (hour^-1)				0.100 ± 0.049
Cl_1 (mL/hr/kg)				
$Cl_{1(F)}$ (mL/hr/kg)				139 ± 14
V_1 (mL/kg)				
V_2 (mL/kg)				
$V_{1(F)}$ (mL/kg)				237 ± 71
$V_{2(F)}$ (mL/kg)				159 ± 77
MRT (hour)				
AUC_{0-t} (ng/mL*hr)				26900
AUC_{inf} (ng/mL*hr)				28700 ± 2800
F (percent)				171

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Female

	Treatment Groups (mg/kg)					
	20 [c]		**100** [c]		**4 IV** [d]	
	Plasma					
$C_{max(pred)}$ (ng/mL)	37100	± 5300	225000	± 36000	32600	± 3200
$T_{max(pred)}$ (hour)	0.712	± 0.159	1.42	± 0.27		
$C_{max(obs)}$						
$T_{max(obs)}$ (hour)						
$t_{1/2}$ (hour)						
$t_{1/2(Alpha)}$ (hour)	3.29	± 0.82	1.01	± 0.78	0.282	± 0.031
$t_{1/2(Beta)}$ (hour)	1.04	± 0.50	0.454	± 3.51	0.950	± 0.104
k_{01} (hour^-1)	2.74	± 1.42	0.946	± 3.16		
$t_{1/2(k01)}$ (hour)	0.253	± 0.131	0.732	± 2.44		
k_{10} (hour^-1)	0.519	± 0.164	0.517	± 1.67	1.95	± 0.14
$t_{1/2(k10)}$ (hour)	1.34	± 0.42	1.34	± 4.33	0.356	± 0.025
k_{12} (hour^-1)	0.0893	± 0.109	-0.336	± 1.20	0.318	± 0.097
k_{21} (hour^-1)	0.272	± 0.117	2.03	± 11.1	0.920	± 0.150
Cl_1 (mL/hr/kg)					238	± 11
$Cl_{1(F)}$ (mL/hr/kg)	183	± 22	123	± 17		
V_1 (mL/kg)					123	± 12
V_2 (mL/kg)					42.4	± 6.6
$V_{1(F)}$ (mL/kg)	352	± 118	238	± 761		
$V_{2(F)}$ (mL/kg)	116	± 76	-39	± 341		
MRT (hour)					0.692	± 0.031
AUC_{0-t} (ng/mL*hr)	104000		584000		16600	
AUC_{inf} (ng/mL*hr)	109000	± 13000	812000	± 122000	16800	± 800
F (percent)	130		193			

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LEGEND

Data are displayed as mean ± SEM

ND = not detected

MODELING METHOD & BEST FIT MODEL

[a] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Unable to determine lambda z for brain elimination half-life parameter because did not have enough measurable concentrations. Non-compartment model with first order input, first order output, and uniform weighting.

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

[c] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Two-compartment model with first order input, first order output, and l/Yhat^2 weighting.

[d] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Two-compartment model with bolus input, first order output, and l/Yhat^2 weighting.

ANALYTE

Potassium Perfluorobutane Sulfonate

TK PARAMETERS

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

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

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

$t_{1/2(alpha)}$ = Half-life for the alpha phase

$t_{1/2(beta)}$ = 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 **