

Male						
	Treatment Groups (mg/kg)					
	20 ^a	100 ^a	400 ^a	20 IV ^a	40 IV ^a	80 IV ^a
	Brain					
C _{max(pred)} (ug/mL)						
T _{max(pred)} (minute)						
C _{max(obs)} (ug/g) *	3.35 ± 1.29	41.7 ± 14.3	122 ± 35	32.0 ± 5.7	33.5 ± 11.5	75.2 ± 19.5
T _{max(obs)} (minute)	8	13	21	6	9	7
t _{1/2} (minute)	4.47	9.2	14.9	5.07	3.68	5.63
k ₀₁ (minute ⁻¹)						
t _{1/2(k01)} (minute)						
k ₁₀ (minute ⁻¹)						
t _{1/2(k10)} (minute)						
Cl (mL/min/kg)						
Cl _{1(F)} (mL/min/kg)						
V ₁ (mL/kg)						
V _{1(F)} (mL/kg)						
AUC _{0-t} (ug*min/g)	41.1	1070	7180	620	1280	2410
AUC _{inf} (ug*min/g)	41.2	1070	7190	620	1290	2410

Experiment Number: NA
Route: Gavage, IV
Species/Strain: Mouse/B6C3F1

Toxicokinetics Data Summary
Test Compound: 2-Methyltetrahydrofuran
CAS Number: 96-47-9

Date Report Requested: 01/09/2017
Time Report Requested: 11:24:53
Lab: Battelle Columbus

Male																					
	Treatment Groups (mg/kg)																				
	20 ^b		100 ^c		400 ^b		20 IV ^d		40 IV ^e		40 IV ^f										
	Plasma																				
C _{max(pred)} (ug/mL)	5.65	±	0.88	66.4	±	6.1	342	±	38												
T _{max(pred)} (minute)	2.95	±	0.78	9.34	±	0.65	11	±	2												
C _{max(obs)} (ug/g) *																					
T _{max(obs)} (minute)																					
t _{1/2} (minute)																					
k ₀₁ (minute^-1)	0.677	±	0.299	0.107	±	0.007	0.2	±	0.06												
t _{1/2(k01)} (minute)	1.02	±	0.45	6.48	±	0.45	3.47	±	1.04												
k ₁₀ (minute^-1)	0.138	±	0.008	0.107	±	0.007	0.0326	±	0.0019	0.19	±	0.011	0.15	±	0.004						
t _{1/2(k10)} (minute)	5.02	±	0.28	6.48	±	0.45	21.3	±	1.2	3.64	±	0.21	4.62	±	0.13						
Cl (mL/min/kg)										146	±	8	104	±	11						
Cl _{1(F)} (mL/min/kg)	325		±	32	59.3		±	5.5	26.7		±	2.8									
V ₁ (mL/kg)										768		±	57	694		±	89	976	±	219	
V _{1(F)} (mL/kg)	2360		±	300	554		±	51	820		±	120									
AUC _{0-t} (ug*min/g)	60.4				1610				13800				148				374			374	
AUC _{inf} (ug*min/g)	61.5		±	6.1	1690		±	160	15000		±	1500	137		±	7	384		±	42	374

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Male		
Treatment Groups (mg/kg)		
80 IV ^g		
Plasma		
C _{max(pred)} (ug/mL)		
T _{max(pred)} (minute)		
C _{max(obs)} (ug/g) *		
T _{max(obs)} (minute)		
t _{1/2} (minute)		
k ₀₁ (minute ⁻¹)		
t _{1/2(k01)} (minute)		
k ₁₀ (minute ⁻¹)		
t _{1/2(k10)} (minute)		
Cl (mL/min/kg)		
Cl _{1(F)} (mL/min/kg)		
V ₁ (mL/kg)	712 ± 110	
V _{1(F)} (mL/kg)		
AUC _{0-t} (ug*min/g)	1210	
AUC _{inf} (ug*min/g)	1210	

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Treatment Groups (mg/kg)						
	20 ^a	100 ^a	400 ^a	10 IV ^a	20 IV ^a	40 IV ^a
Brain						
C _{max(pred)} (ug/mL)						
T _{max(pred)} (minute)						
C _{max(obs)} (ug/g) *	4.16 ± 1.41	42.4 ± 16.6	110 ± 38	13.8 ± 2.0	12.8 ± 0.8	22.0 ± 2.5
T _{max(obs)} (minute)	8	23	13	6	6	9
t _{1/2} (minute)	4.43	7.19	11.7	4.62	5.81	4.27
k ₀₁ (minute ⁻¹)						
t _{1/2(k01)} (minute)						
k ₁₀ (minute ⁻¹)						
t _{1/2(k10)} (minute)						
Cl (mL/min/kg)						
Cl _{1(F)} (mL/min/kg)						
V ₁ (mL/kg)						
V _{1(F)} (mL/kg)						
AUC _{0-t} (ug*min/g)	37.2	1260	7170	344	364	548
AUC _{inf} (ug*min/g)	37.2	1260	7180	345	364	554

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	Female																	
	Treatment Groups (mg/kg)																	
	20 ^b			100 ^c			400 ^h		10 IV ^d		20 IV ^d		40 IV ^e					
	Plasma																	
C _{max(pred)} (ug/mL)	4.25	±	0.61	57.8	±	5.1	177	±	17									
T _{max(pred)} (minute)	3.55	±	0.59	9.25	±	0.63												
C _{max(obs)} (ug/g) *																		
T _{max(obs)} (minute)																		
t _{1/2} (minute)																		
k ₀₁ (minute^-1)	0.461	±	0.144	0.108	±	0.007	0.664	±	0.267									
t _{1/2(k01)} (minute)	1.5	±	0.47	6.41	±	0.44	1.04	±	0.42									
k ₁₀ (minute^-1)	0.157	±	0.009	0.108	±	0.007				0.28	±	0.018	0.202	±	0.008	0.193	±	0.007
t _{1/2(k10)} (minute)	4.42	±	0.26	6.41	±	0.44				2.47	±	0.16	3.42	±	0.13	3.58	±	0.13
Cl (mL/min/kg)										159	±	9	144	±	5	77.2	±	10.3
Cl _{1(F)} (mL/min/kg)	424	±	42	68.8	±	6.4												
V ₁ (mL/kg)										569	±	49	710	±	35	399	±	64
V _{1(F)} (mL/kg)	2700	±	350	637	±	57	2080	±	230									
AUC _{0-t} (ug*min/g)	48.3			1390			10900			67.4			151			374		
AUC _{inf} (ug*min/g)	47.2	±	4.7	1450	±	130				62.7	±	3.4	139	±	5	518	±	69

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Female		
Treatment Groups (mg/kg)		
40 IV ^f		
Plasma		
C _{max(pred)} (ug/mL)		
T _{max(pred)} (minute)		
C _{max(obs)} (ug/g) *		
T _{max(obs)} (minute)		
t _{1/2} (minute)		
k ₀₁ (minute ⁻¹)		
t _{1/2(k01)} (minute)		
k ₁₀ (minute ⁻¹)		
t _{1/2(k10)} (minute)		
Cl (mL/min/kg)		
Cl _{1(F)} (mL/min/kg)		
V ₁ (mL/kg)	908 ± 126	
V _{1(F)} (mL/kg)		
AUC _{0-t} (ug*min/g)	374	
AUC _{inf} (ug*min/g)	374	

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LEGEND

Data are displayed as mean \pm SEM

*Data are displayed as mean \pm SD

MODELING METHOD & BEST FIT MODEL

^a WinNonlin; Noncompartmental analysis.

^b WinNonlin; Calculated using one-compartment model with first order absorption and elimination.

^c WinNonlin; Calculated using one-compartment model with the same rate constants for first order input and output.

^d WinNonlin; One-compartment model with first order elimination.

^e WinNonlin; Calculated using one-compartment model with bolus input and first-order elimination. 1/Yhat2 weighting was used.

^f WinNonlin Michaelis-Menten model; Calculated using a Michaelis-Menten one-compartment model (1/Yhat2 weighting). Trapezoidal method was used to calculate AUCs.

^g WinNonlin Michaelis-Menten model; One-compartment with Michaelis-Menten elimination. Trapezoidal method was used to calculate AUCs.

^h WinNonlin Michaelis-Menten model; Calculated using a Michaelis-Menten one-compartment model.

ANALYTE

2-Methyltetrahydrofuran

TK PARAMETERS

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

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

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

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 = 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

$V_{1(F)}$ = 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

**** END OF REPORT ****