Experiment Number: S0592
Route: Gavage, IV
Species/Strain: Mouse/B6C3F1

Toxicokinetics Data Summary
Test Compound: Benzophenone
CAS Number: 119-61-9

Date Report Requested: 11/09/2016
Time Report Requested: 14:01:02
Lab: Research Triangle Institute

Male

Treatment Groups (mg/kg)

	15 [a]	15 [b]	30 [b]	60 [b]	15 IV [b]
Plasma					
Alpha (min^{-1})	0.0563 ± 0.0084				
Beta (min^{-1})	0.00903 ± 0.0084	0.0159	0.00610	0.00430	0.0259
$t_{1/2(Beta)}$ (minute)		43.6	113.0	160.0	26.7
k_{01} (min^{-1})	0.0980 ± 0.036				
k_{10} (min^{-1})	0.0442 ± 0.0052				
k_{12} (min^{-1})	0.00961 ± 0.0031				
k_{21} (min^{-1})	0.0115 ± 0.011				
Cl (mL/min/kg)					110.0
$Cl_{1(F)}$ (mL/min/kg)		418.0	317.0	231.0	
V_1 (L/kg)	2.65 ± 0.19				4.26
$V_{1(F)}$ (L/kg)		26.3	51.8	53.6	
MRT (minute)		99.3	96.1	96.2	30.9
AUC_{inf} (ug*min/mL)		28.7	74.2	205.0	140.0
F (fraction)		0.263	0.347	0.475	

Female

	Treatment Groups (mg/kg)				
	15 [c]	**15 [b]**	**30 [b]**	**60 [b]**	**15 IV [b]**
	Plasma				
Alpha (min^-1)	0.0611 ± 0.010				
Beta (min^-1)	0.00821 ± 0.0061	0.00790	0.00940	0.00640	0.0128
$t_{1/2(Beta)}$ (minute)		87.5	73.9	108.0	54.0
k_{01} (min^-1)	0.0747 ± 0.018				
k_{10} (min^-1)	0.0422 ± 0.0062				
k_{12} (min^-1)	0.0153 ± 0.0045				
k_{21} (min^-1)	0.0119 ± 0.0089				
Cl (mL/min/kg)					115.0
$Cl_{1(F)}$ (mL/min/kg)		246.0	315.0	229.0	
V_1 (L/kg)	2.96 ± 0.25				8.96
$V_{1(F)}$ (L/kg)		31.0	33.5	35.9	
MRT (minute)		91.4	89.4	112.0	42.0
AUC_{inf} (ug*min/mL)		49.2	75.9	211.0	137.0
F (fraction)		0.468	0.365	0.501	

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LEGEND

Data are displayed as mean ± SEM

MODELING METHOD & BEST FIT MODEL

[a] Compartmental modeling techniques with established models or models written to simultaneously solve iv and oral data sets (WinNonlin, Version 1 .0, Scientific Consulting Inc., 1995); Best fit is two compartmental which simultaneously solves iv and oral data sets. Analyzed using compartmental modeling techniques with established models or models written to simultaneously solve iv (Study AC) and oral data sets (Study AE) using 1/Y weighting where Y is the observed plasma BPH concentration at a given time.

[b] Models 200 and 201 of the pharmacokinetic software WinNonlin, Version 1 .0 (Scientific Consulting Inc., 1995); noncompartmental model

[c] Compartmental modeling techniques with established models or models written to simultaneously solve iv and oral data sets (WinNonlin, Version 1 .0, Scientific Consulting Inc., 1995); Best fit is two compartmental which simultaneously solves iv and oral data sets. Analyzed using compartmental modeling techniques with established models or models written to simultaneously solve iv (Study AD) and oral data sets (Study AF) using 1/Y weighting where Y is the observed plasma BPH concentration at a given time.

ANALYTE

Benzophenone

TK PARAMETERS

Alpha = Hybrid rate constant of the alpha phase

Beta = Hybrid rate constant of the beta phase

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

$V_{1(F)}$ = Apparent volume of distribution for the central compartment includes $V_{d(F)}$, $V_{(F)}$ for oral groups, and $V_{c(F)}$

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 **