**Experiment Number:** S0592

Route: Gavage, IV

Species/Strain: Rat/F344

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

Date Report Requested: 11/09/2016 Time Report Requested: 14:01:12

Lab: Research Triangle Institute

Male								
	Treatment Groups (mg/kg)							
	2.5 a	2.5 b	5 b	10 b	2.5 IV <sup>b</sup>			
	Plasma							
Alpha (min^-1)	$0.0675 \pm 0.0074$							
Beta (min^-1)	0.00258 ± 4.4E-4	0.00280	0.00120	0.00140	0.00260			
t <sub>1/2(Beta)</sub> (minute)		245.0	594.0	506.0	268.0			
k <sub>01</sub> (min^-1)	$0.0171 \pm 0.0022$							
k <sub>10</sub> (min^-1)	$0.0198 \pm 0.0021$							
k <sub>12</sub> (min^-1)	$0.0415 \pm 0.0056$							
k <sub>21</sub> (min^-1)	$0.0881 \pm 0.0014$							
CI (mL/min/kg)					47.4			
CI <sub>1(F)</sub> (mL/min/kg)		57.5	40.2	37.4				
V <sub>1</sub> (L/kg)	$2.48 \pm 0.16$				18.3			
V <sub>1(F)</sub> (L/kg)		20.3	34.4	27.3				
MRT (minute)		349	809	737	264			
AUC <sub>inf</sub> (ug*min/mL)		32.7	95.6	208	51.9			
F (fraction)		0.824	1.18	1.27				

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Female								
	Treatment Groups (mg/kg)							
	2.5 °	2.5 b	5 b	10 b	2.5 IV b			
	Plasma							
Alpha (min^-1)	$0.196 \pm 0.030$							
Beta (min^-1)	$0.00350 \pm 0.0012$	0.00120	0.00180	0.00140	0.00280			
<sub>1/2(Beta)</sub> (minute)		567.0	395.0	499.0	247.0			
(min^-1)	$0.00385 \pm 0.0013$							
(min^-1)	$0.0505 \pm 0.010$							
(min^-1)	$0.135 \pm 0.026$							
<sub>21</sub> (min^-1)	$0.0136 \pm 0.0041$							
CI (mL/min/kg)					48.6			
il <sub>1(F)</sub> (mL/min/kg)		34.9	44.0	46.2				
′ <sub>1</sub> (L/kg)	1.11 ± 0.21				17.3			
′ <sub>1(F)</sub> (L/kg)		28.5	25.1	33.3				
MRT (minute)		816	553	662	254			
NUC <sub>inf</sub> (ug*min/mL)		53.8	86.8	166	51.6			
(fraction)		1.39	1.10	1.05				

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## **LEGEND**

Data are displayed as mean ± SEM

### MODELING METHOD & BEST FIT MODEL

<sup>a</sup> 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 U) and oral data sets (Study W) 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

 $t_{\frac{1}{2}(beta)}$  = Half-life for the beta phase

 $k_{01}$  = Absorption rate constant,  $k_a$ 

k<sub>10</sub> = Elimination rate constant from the central compartment also k<sub>e</sub> or k<sub>elim</sub>

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

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

CI = 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

AUCinf = Area under the plasma concentration versus time curve, AUC, extrapolated to time equals infinity

F = Bioavailability, absolute bioavailability

\*\* END OF REPORT \*\*

<sup>&</sup>lt;sup>b</sup> Models 200 and 201 of the pharmacokinetic software WinNonlin, Version 1.0 (Scientific Consulting Inc., 1995); noncompartmental model

<sup>&</sup>lt;sup>c</sup> 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 V) and oral data sets (Study X) using 1/Y weighting where Y is the observed plasma BPH concentration at a given time.