Experiment Number: S0545

Route: Gavage, IV

Species/Strain: Rat/Sprague-Dawley

Toxicokinetics Data Summary

Test Compound: DI-n-butyl phthalate

CAS Number: 84-74-2

Date Report Requested: 12/27/2016 Time Report Requested: 11:23:14

Lab: Research Triangle Institute

		-	
M	а	ΙД	

	Treatment Groups (mg/kg)						
	50 ^a	100 b	200 b	20 IV ^b	20 IV °		
	Plasma						
C _{max} (ug/mL)	21.0	42.0	123	44.8			
T _{max} (minute)	20	30	60				
Alpha (minute^-1)					0.0593 ± 0.012		
Beta (minute^-1)					0.000710 ± 0.0011		
t _{1/2(Beta)} (minute)	379	290	279	163			
k ₀₁ (minute^-1)					0.0289 ± 0.0057		
k ₁₀ (minute^-1)					0.0246 ± 0.018		
k ₁₂ (minute^-1)					0.0337 ± 0.017		
k ₂₁ (minute^-1)					0.00171 ± 0.0017		
CI (mL*min/kg)	17.9	12.3	6.25	11.0			
V ₁ (L/kg)					0.407 ± 0.082		
MRT (minute)	345	317	254	122			
AUC _{inf} (ug/mL*min)	2230	6493	25583	1450			
F (fraction)	0.62	0.90	1.76				

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LEGEND

Data are displayed as mean ± SEM

MODELING METHOD & BEST FIT MODEL

^a Models 200 and 201, PCNONLIN software, SCI Software, Lexington, KY; Noncompartmental analysis.

ANALYTE

Mono-n-butyl phthalate

TK PARAMETERS

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

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

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_{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.

CI = Clearance, includes total clearance

 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

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 **

^b Models 200 and 201, PCNONLIN software, SCI Software, Lexington, KY; Noncompartmental analysis. Secondary rise is plasma concentration indicate that additional factors such as enterohepatic recirculation should be considered in the analysis of the data.

^c Compartmental modeling techniques with established models or models written to simultaneously solve IV and oral data sets (PCNONLIN); 2-compartmental model using equations derived from simultaneous fitting the IV and low oral dose data (Studies AB and AC).