Experiment Number: K93026
Route: Whole Body Inhalation
Species/Strain: Rats/F344/N

Toxicokinetics Data Summary
Compound: Decalin/ **Analyte:** Decalin
CAS Number: 91-17-8

Request Date: 7/11/2023
Request Time: 10:03:16
Lab: Battelle Northwest

Male

	Treatment Group (ppm)		
	25 Inhalation Blood[a]	**100 Inhalation Blood[a]**	**400 Inhalation Blood[a]**
C_0min_pred (ug/g)	0.501 ± 0.083	3.75 ± 0.64	20.2 ± 3.5
Alpha (minute^{-1})	0.0276 ± 0.0062	0.0301 ± 0.0067	0.0260 ± 0.0057
Alpha Half-life (minute)	25.1 ± 5.6	23.0 ± 5.1	26.6 ± 5.8
Beta (minute^{-1})	0.00150 ± 0.00027	0.00166 ± 0.00026	0.00136 ± 0.00027
Beta Half-life (minute)	463 ± 84	418 ± 64	511 ± 100
AUCinf_pred (ug/mL*min)	54.5 ± 2.1	370 ± 14	2110 ± 90

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Female

	Treatment Group (ppm)		
	25 Inhalation Blood[a]	**100 Inhalation Blood[a]**	**400 Inhalation Blood[a]**
C_0min_pred (ug/g)	0.639 ± 0.13	3.89 ± 0.61	19.5 ± 4.1
Alpha (minute^{-1})	0.0277 ± 0.0084	0.0199 ± 0.0044	0.0180 ± 0.0054
Alpha Half-life (minute)	25.1 ± 7.6	34.9 ± 7.8	38.4 ± 11
Beta (minute^{-1})	0.00163 ± 0.00032	0.00135 ± 0.00028	0.00127 ± 0.00039
Beta Half-life (minute)	426 ± 84	512 ± 100	546 ± 170
AUCinf_pred (ug/mL*min)	80.3 ± 5.7	507 ± 25	2680 ± 170

LEGEND

MODELING SOFTWARE

SAS PROC NLIN

MODELING METHOD & BEST FIT MODEL

[a] nonlinear least-squares fitting program (SAS PROC NLIN, SAS Institute, Inc., Cary, NC), Toxicolkinetic parameters were determined by fitting the equation C(t) equals Ao*e^alpha t plus Bo*e^beta t to the data, where C(t) is the blood concentration of Decalin at any postexposure time (t), alpha and beta are the hybrid rate constants ($minute^{-1}$) obtained from the fit, and Ao and Bo are the intercepts on the ordinate (concentration) axis of the extrapolated initial and terminal phases, respectively. Co = Ao + Bo . weighting factor of [mean Decalin blood concentration]$^{-2}$ for rats.

ANALYTE

Decalin

TK PARAMETERS – (NOTE: All parameters use Confidence Interval instead of SD or SEM)

C_0min_pred = Fitted plasma concentration at time zero (IV only)
Alpha = Hybrid rate constant of the alpha phase
Alpha Half-Life = Half-life for the alpha phase
Beta = Hybrid rate constant of the beta phase
Beta Half-Life = Half-life for the beta phase
AUCinf_pred = Area under the plasma concentration versus time curve, AUC, extrapolated to time equals infinity

TK PARAMETERS PROTOCOL

ANALYSIS METHOD

Analysis of Decalin in blood samples was conducted using a validated GC/MS method incorporating selected ion monitoring. The limit of detection (LOD), limit of quantitation (LOQ), and experimental limit of quantitation (ELOQ) were 0.0011, 0.0036, and 0.012 ug/g blood for (cis plus trans)-Decalin, respectively. The sum of cis- and trans-Decalin was used to calculate the total Decalin concentration of the exposure chamber. Separate parameter estimations were made for cis-, trans-, and total (cis + trans)-Decalin, allowing comparison of separate cis- and trans-Decalin kinetic parameter estimates. Rate constants (and half-lives) for both the initial and terminal elimination phases were not statistically different for the two isomers. Therefore, kinetic parameters are reported only for total (cis plus trans)-Decalin.

TK_WHOLE BODY INHALATION BLOOD

25 ppm, 100 ppm, 400 ppm Male and Female

Rats and mice received a single 6-hour whole-body inhalation exposure to target concentrations of 25, 100, or 400 ppm Decalin. Heparinized blood was collected at 8 time points postdosing in mice. Each animal was bled twice. Concentrations were ug/g whole blood.