

Experiment Number: K93026
Route: Whole Body Inhalation
Species/Strain: Mouse/B6C3F1

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

	25 Inhalation Blood^a	100 Inhalation Blood^a	400 Inhalation Blood^a
C ₀ min _{pred} (ug/g)	0.649 ± 0.087	4.50 ± 0.59	39.3 ± 6.6
Alpha (minute ⁻¹)	0.0987 ± 0.033	0.0790 ± 0.033	0.0294 ± 0.031
Alpha Half-life (minute)	7.02 ± 2.4	8.77 ± 3.7	23.6 ± 25
Beta (minute ⁻¹)	0.00632 ± 0.0017	0.00706 ± 0.0019	0.00650 ± 0.0046
Beta Half-life (minute)	110 ± 29	98.2 ± 26	107 ± 75
AUC _{inf} _{pred} (ug/mL*min)	34.0 ± 2.0	250 ± 14	3340 ± 260

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25 Inhalation Blood^a

100 Inhalation Blood^a

400 Inhalation Blood^a

C ₀ min _{pred} (ug/g)	0.582 ± 0.089	5.99 ± 1.1	42.7 ± 5.5
Alpha (minute ⁻¹)	0.0570 ± 0.019	0.120 ± 0.040	0.0267 ± 0.014
Alpha Half-life (minute)	12.2 ± 4.1	5.79 ± 1.9	26.0 ± 14
Beta (minute ⁻¹)	0.00561 ± 0.0019	0.00732 ± 0.0015	0.00527 ± 0.0033
Beta Half-life (minute)	124 ± 43	94.8 ± 20	131 ± 82
AUC _{inf} _{pred} (ug/mL*min)	31.3 ± 2.2	245 ± 16	3430 ± 250

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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), Toxicokinetic parameters were determined by fitting the equation $C(t) = A_0 e^{-\alpha t} + B_0 e^{-\beta t}$ to the data, where $C(t)$ is the blood concentration of Decalin at any postexposure time (t), α and β are the hybrid rate constants (minute^{-1}) obtained from the fit, and A_0 and B_0 are the intercepts on the ordinate (concentration) axis of the extrapolated initial and terminal phases, respectively. $C_0 = A_0 + B_0$. weighting factor of [mean Decalin blood concentration]⁻¹ for mice.

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

AUC_{inf_pred} = Area under the plasma concentration versus time curve, AUC, extrapolated to time equals infinity

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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.