

Experiment Number: C99028
Route: IV
Species/Strain: Mouse/B6C3F1

Toxicokinetics Data Summary
Test Compound: Thiodiglycolic Acid
CAS Number: 123-93-3

Date Report Requested: 12/22/2016
Time Report Requested: 15:48:44
Lab: Battelle Columbus

Male

Treatment Groups (mg/kg)

| | 50 IV ^a | 50 IV ^a | 50 IV ^b | 50 IV ^a |
|---|--------------------|--------------------|--------------------|--------------------|
| | Heart | Liver | Plasma | Thymus |
| C _{max(pred)} (ug/mL) | | | 124 ± 18 | |
| C _{max(obs)} (ug/g) | 40.4 | 78.3 | | 23.9 |
| T _{max} (minute) | 3.76 | 16.3 | | 6.93 |
| t _{1/2} (minute) | 92.8 | 51.1 | | 128 |
| t _{1/2(Alpha)} (minute) | | | 3.80 ± 0.33 | |
| t _{1/2(Beta)} (minute) | | | 72.1 ± 8.1 | |
| k ₁₀ (minute ⁻¹) | | | 0.140 ± 0.013 | |
| t _{1/2(k10)} (minute) | | | 4.97 ± 0.46 | |
| k ₁₂ (minute ⁻¹) | | | 0.0399 ± 0.0045 | |
| k ₂₁ (minute ⁻¹) | | | 0.0126 ± 0.0014 | |
| Cl (mL/min/kg) | | | 56.3 ± 4.0 | |
| V ₁ (mL/kg) | | | 403 ± 58 | |
| V ₂ (mL/kg) | | | 1280 ± 230 | |
| MRT (minute) | | | 29.9 ± 3.6 | |
| AUC _{inf} (ug/mL*min) | | | 888 ± 63 | |

Experiment Number: C99028
 Route: IV
 Species/Strain: Mouse/B6C3F1

Toxicokinetics Data Summary
 Test Compound: Thiodiglycolic Acid
 CAS Number: 123-93-3

Date Report Requested: 12/22/2016
 Time Report Requested: 15:48:44
 Lab: Battelle Columbus

Female

Treatment Groups (mg/kg)

| | Treatment Groups (mg/kg) | | | |
|---|--------------------------|--------------------|--------------------|--------------------|
| | 50 IV ^a | 50 IV ^a | 50 IV ^b | 50 IV ^a |
| | Heart | Liver | Plasma | Thymus |
| C _{max(pred)} (ug/mL) | | | 111 ± 11 | |
| C _{max(obs)} (ug/g) | 37.9 | 96.6 | | 38.9 |
| T _{max} (minute) | 3.89 | 16.6 | | 3.89 |
| t _{1/2} (minute) | 73.4 | 52.0 | | 181 |
| t _{1/2(Alpha)} (minute) | | | 4.43 ± 0.32 | |
| t _{1/2(Beta)} (minute) | | | 72.2 ± 5.7 | |
| k ₁₀ (minute ⁻¹) | | | 0.111 ± 0.008 | |
| t _{1/2(k10)} (minute) | | | 6.23 ± 0.45 | |
| k ₁₂ (minute ⁻¹) | | | 0.0414 ± 0.0041 | |
| k ₂₁ (minute ⁻¹) | | | 0.0135 ± 0.0012 | |
| Cl (mL/min/kg) | | | 50.2 ± 2.3 | |
| V ₁ (mL/kg) | | | 451 ± 46 | |
| V ₂ (mL/kg) | | | 1380 ± 160 | |
| MRT (minute) | | | 36.6 ± 2.9 | |
| AUC _{inf} (ug/mL*min) | | | 997 ± 46 | |

Experiment Number: C99028

Route: IV

Species/Strain: Mouse/B6C3F1

Toxicokinetics Data Summary

Test Compound: Thiodiglycolic Acid

CAS Number: 123-93-3

Date Report Requested: 12/22/2016

Time Report Requested: 15:48:44

Lab: Battelle Columbus

LEGEND

Data are displayed as mean \pm SEM

MODELING METHOD & BEST FIT MODEL

^a WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Non-compartment model with bolus input, first order output, and uniform weighting.

^b WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; Two-compartment model with bolus input, first order output, and 1/Yhat2 weighting.

ANALYTE

Thiodiglycolic Acid

TK PARAMETERS

$C_{\max(\text{pred})}$ = Observed or Predicted Maximum plasma (or tissue) concentration

$C_{\max(\text{obs})}$ = Observed or Predicted Maximum plasma (or tissue) concentration

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

$t_{1/2}$ = λ_z half-life, $t_{1/2}$, the terminal elimination half-life based on non-compartmental analysis

$t_{1/2(\text{alpha})}$ = Half-life for the alpha phase

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

k_{10} = Elimination rate constant from the central compartment also k_e or k_{elim}

$t_{1/2(k10)}$ = Half-life for the elimination process from the central compartment

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

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_2 = Volume of distribution for the peripheral compartment

MRT = Mean residence time

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

**** END OF REPORT ****