**Experiment Number:** C06100
**Route:** Gavage, IV
**Species/Strain:** Rat/Harlan Sprague-Dawley

**Toxicokinetics Data Summary**
**Test Compound:** Perfluorohexane-1-Sulphonic Acid - Potassium Salt
**CAS Number:** 3871-99-6

**Date Report Requested:** 01/09/2017
**Time Report Requested:** 11:25:37
**Lab:** Battelle Columbus

**Male**

| | Treatment Groups (mg/kg) | | | |
|---|---|---|---|---|
| | **16 [a]** | **16 [a]** | **16 [a]** | **4 [b]** |
| | **Brain** | **Kidney** | **Liver** | **Plasma** |
| $C_{max(pred)}$ (ng/mL) | | | | 32200 ± 2900 |
| $T_{max(pred)}$ (hour) | | | | 6.90 ± 1.26 |
| $C_{max(obs)}$ (ng/g) | 1800 | 38,100 | 76,700 | |
| $T_{max(obs)}$ (hour) | 12.0 | 12.0 | 6.00 | |
| $t_{1/2}$ (hour) | 184 | 508 | 639 | |
| $t_{1/2(Alpha)}$ (hour) | | | | |
| $t_{1/2(Beta)}$ (hour) | | | | |
| $k_{01}$ (hour^-1) | | | | 0.919 ± 0.204 |
| $t_{1/2(k01)}$ (hour) | | | | 0.755 ± 0.168 |
| $k_{10}$ (hour^-1) | | | | 0.00164 ± 1.6E-4 |
| $t_{1/2(k10)}$ (hour) | | | | 423 ± 42 |
| $k_{12}$ (hour^-1) | | | | |
| $k_{21}$ (hour^-1) | | | | |
| $Cl_1$ (mL/hr/kg) | | | | |
| $Cl_{1(F)}$ (mL/hr/kg) | | | | 0.201 ± 0.016 |
| $V_1$ (mL/kg) | | | | |
| $V_2$ (mL/kg) | | | | |
| $V_{1(F)}$ (mL/kg) | | | | 123 ± 11 |
| MRT (hour) | | | | |
| $AUC_{0-t}$ (ng/mL*hr) | | | | 14400000 |
| $AUC_{inf}$ (ng/mL*hr) | | | | 19900000 ± 1600000 |
| F (percent) | | | | 98.0 |

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| | Treatment Groups (mg/kg) | | |
|---|---|---|---|
| | **16 [b]** | **32 [b]** | **4 IV [c]** |
| | **Plasma** | | |
| $C_{max(pred)}$ (ng/mL) | 116000 ± 8000 | 165000 ± 14000 | 45300 ± 2600 |
| $T_{max(pred)}$ (hour) | 5.89 ± 0.82 | 5.28 ± 0.99 | |
| $C_{max(obs)}$ (ng/g) | | | |
| $T_{max(obs)}$ (hour) | | | |
| $t_{1/2}$ (hour) | | | |
| $t_{1/2(Alpha)}$ (hour) | | | 13.0 ± 3.8 |
| $t_{1/2(Beta)}$ (hour) | | | 811 ± 154 |
| $k_{01}$ (hour^-1) | 1.09 ± 0.19 | 1.22 ± 0.28 | |
| $t_{1/2(k01)}$ (hour) | 0.632 ± 0.107 | 0.567 ± 0.129 | |
| $k_{10}$ (hour^-1) | 0.00175 ± 1.2E-4 | 0.00196 ± 1.5E-4 | 0.00223 ± 2.6E-4 |
| $t_{1/2(k10)}$ (hour) | 397 ± 27 | 354 ± 28 | 311 ± 36 |
| $k_{12}$ (hour^-1) | | | 0.0314 ± 0.0095 |
| $k_{21}$ (hour^-1) | | | 0.0204 ± 0.0070 |
| $Cl_1$ (mL/hr/kg) | | | 0.197 ± 0.019 |
| $Cl_{1(F)}$ (mL/hr/kg) | 0.239 ± 0.014 | 0.376 ± 0.027 | |
| $V_1$ (mL/kg) | | | 88.4 ± 5.1 |
| $V_2$ (mL/kg) | | | 136 ± 27 |
| $V_{1(F)}$ (mL/kg) | 137 ± 9 | 192 ± 17 | |
| MRT (hour) | | | 1140 ± 210 |
| $AUC_{0-t}$ (ng/mL*hr) | 54000000 | 72900000 | 14200000 |
| $AUC_{inf}$ (ng/mL*hr) | 66800000 ± 3800000 | 85100000 ± 6000000 | 20300000 ± 1990000 |
| F (percent) | 82.3 | 52.4 | |

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**Female**

| | Treatment Groups (mg/kg) | | | |
|---|---|---|---|---|
| | **16 [a]** | **16 [a]** | **16 [a]** | **4 [b]** |
| | **Brain** | **Kidney** | **Liver** | **Plasma** |
| $C_{max(pred)}$ (ng/mL) | | | | 24900 ± 1300 |
| $T_{max(pred)}$ (hour) | | | | 2.81 ± 0.38 |
| $C_{max(obs)}$ (ng/g) | 1360 | 37,500 | 53,700 | |
| $T_{max(obs)}$ (hour) | 3.00 | 6.00 | 3.00 | |
| $t_{1/2}$ (hour) | 32.9 | 55.5 | 45.2 | |
| $t_{1/2(Alpha)}$ (hour) | | | | |
| $t_{1/2(Beta)}$ (hour) | | | | |
| $k_{01}$ (hour^-1) | | | | 1.78 ± 0.30 |
| $t_{1/2(k01)}$ (hour) | | | | 0.389 ± 0.066 |
| $k_{10}$ (hour^-1) | | | | 0.0124 ± 3.0E-4 |
| $t_{1/2(k10)}$ (hour) | | | | 55.9 ± 1.6 |
| $k_{12}$ (hour^-1) | | | | |
| $k_{21}$ (hour^-1) | | | | |
| $Cl_{1}$ (mL/hr/kg) | | | | |
| $Cl_{1(F)}$ (mL/hr/kg) | | | | 1.92 ± 0.09 |
| $V_{1}$ (mL/kg) | | | | |
| $V_{2}$ (mL/kg) | | | | |
| $V_{1(F)}$ (mL/kg) | | | | 155 ± 9 |
| MRT (hour) | | | | |
| $AUC_{0-t}$ (ng/mL*hr) | | | | 2160000 |
| $AUC_{inf}$ (ng/mL*hr) | | | | 2080000 ± 90000 |
| F (percent) | | | | 142 |

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**Female**

| | Treatment Groups (mg/kg) | | |
|---|---|---|---|
| | **16** [b] | **32** [b] | **4 IV** [c] |
| | **Plasma** | | |
| $C_{max(pred)}$ (ng/mL) | 83400 ± 6000 | 118000 ± 8000 | 60300 ± 7000 |
| $T_{max(pred)}$ (hour) | 2.24 ± 0.48 | 1.87 ± 0.43 | |
| $C_{max(obs)}$ (ng/g) | | | |
| $T_{max(obs)}$ (hour) | | | |
| $t_{1/2}$ (hour) | | | |
| $t_{1/2(Alpha)}$ (hour) | | | 0.699 ± 0.311 |
| $t_{1/2(Beta)}$ (hour) | | | 37.4 ± 1.0 |
| $k_{01}$ (hour^-1) | 2.32 ± 0.62 | 2.84 ± 0.81 | |
| $t_{1/2(k01)}$ (hour) | 0.299 ± 0.079 | 0.244 ± 0.070 | |
| $k_{10}$ (hour^-1) | 0.0132 ± 4.0E-4 | 0.0145 ± 4.0E-4 | 0.0412 ± 0.0050 |
| $t_{1/2(k10)}$ (hour) | 52.6 ± 1.4 | 47.6 ± 1.2 | 16.8 ± 2.0 |
| $k_{12}$ (hour^-1) | | | 0.522 ± 0.272 |
| $k_{21}$ (hour^-1) | | | 0.446 ± 0.177 |
| $Cl_1$ (mL/hr/kg) | | | 2.73 ± 0.13 |
| $Cl_{1(F)}$ (mL/hr/kg) | 2.46 ± 0.15 | 3.84 ± 0.24 | |
| $V_1$ (mL/kg) | | | 66.3 ± 7.6 |
| $V_2$ (mL/kg) | | | 77.6 ± 10.8 |
| $V_{1(F)}$ (mL/kg) | 186 ± 14 | 264 ± 20 | |
| MRT (hour) | | | 52.7 ± 1.3 |
| $AUC_{0-t}$ (ng/mL*hr) | 6510000 | 8260000 | 1500000 |
| $AUC_{inf}$ (ng/mL*hr) | 6520000 ± 410000 | 8340000 ± 520000 | 1460000 ± 70000 |
| F (percent) | 112 | 71.4 | |

LEGEND

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Data are displayed as mean ± SEM

MODELING METHOD & BEST FIT MODEL

[a] WinNonlin, Version 5.0.1, Pharsight Corporation, Mountain View, CA; NCA model with first order input, first order output, and uniform weighting.

[b] WinNonlin, Pharsight Corporation, Mountain View, CA; One-compartment model with first order input, first order output, and 1/Yhat2 weighting.

[c] WinNonlin, Pharsight Corporation, Mountain View, CA; Two-compartment model with bolus input, first order output, and 1/Yhat2 weighting.

ANALYTE

Perfluorohexane-1-Sulphonic Acid – Potassium Salt

TK PARAMETERS

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

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

$t_{½}$ = Lambda$_z$ half-life, $t_{1/2}$, the terminal elimination half-life based on non-compartmental analysis

$t_{½(alpha)}$ = Half-life for the alpha phase

$t_{½(beta)}$ = Half-life for the beta phase

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

$t_{1/2(k01)}$ = Half-life of the absorption process to the central compartment

$k_{10}$ = 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.

$Cl_1$ = Clearance of central compartment, $Cl_{app}$ or apparent clearance for intravenous groups

$Cl_{1(F)}$ = 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

$V_2$ = Volume of distribution for the peripheral compartment

$V_{1(F)}$ = 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

$AUC_{0-t}$ = Area under the plasma concentration versus time curve, AUC, from time $t_i$ (initial) to $t_f$ (final), $AUC_{last}$

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

F = Bioavailability, absolute bioavailability

** END OF REPORT **