

**Experiment Number:** K07378  
**Route:** IV, Gavage, Dosed Water  
Gavage Challenge, Dosed Water  
**Species/Strain:** Mouse/B6C3F1

**Toxicokinetics Data Summary**  
**Compound:** Sodium Bromochloroacetic acid/ **Analyte:** Bromochloroacetic acid

**Request Date:** 7/11/2023  
**Request Time:** 10:03:16

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

Male

**Treatment Group (mg/kg)**

**100 IV Plasma<sup>a</sup>      100 Gavage Plasma<sup>b</sup>      200 Gavage Plasma<sup>b</sup>      400 Gavage Plasma<sup>b</sup>**

Cmax_pred (ug/mL)	182 ± 24	7.26 ± 1.33	23.4 ± 2.2	62.6 ± 5.6
Tmax_pred (min)		13.1 ± 2.2	21.9 ± 2.0	27.2 ± 2.0
Cmax_obs (ug/mL)		9.48 ± 7.25	28.2 ± 5.7	74.0 ± 18.6
Tmax_obs (min)		20.0	30.0	20.0
k01 (min <sup>-1</sup> )		0.0764 ± 0.013	0.0456 ± 0.0041	0.0367 ± 0.0027
k01 Half-life (min)	5.34 ± 0.68	9.07 ± 1.55	15.2 ± 1.4	18.9 ± 1.4
k10 (min <sup>-1</sup> )	0.130 ± 0.016	0.0764 ± 0.013	0.0456 ± 0.0041	0.0367 ± 0.0027
k10 Half-life (min)		9.07 ± 1.55	15.2 ± 1.4	18.9 ± 1.4
Cl (mL/min/kg)	71.3 ± 7.1			
Cl1_F (mL/min/kg)		387 ± 79	144 ± 16	86.4 ± 9
V1 (mL/kg)	550 ± 72			
V1_F (mL/kg)		5070 ± 931	3150 ± 300	2350 ± 210
MRT (min)	7.71 ± 0.97			
AUC_0-T (ug/ml*min)		248	1390	4100
AUCinf_pred (ug/mL*min)	1400 ± 140	258 ± 53	1390 ± 160	4630 ± 480

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Species/Strain: Mouse/B6C3F1

CAS Number: 5589-96-8

Lab: Battelle Columbus

Female

Treatment Group (mg/kg)

100 IV Plasma<sup>a</sup>

100 Gavage Plasma<sup>b</sup>

200 Gavage Plasma<sup>b</sup>

400 Gavage Plasma<sup>b</sup>

Cmax_pred (ug/mL)	247 ± 11	3.68 ± 0.47	16.3 ± 1.7	58.7 ± 5.6
Tmax_pred (min)		15.5 ± 1.9	17.3 ± 1.7	21.6 ± 1.8
Cmax_obs (ug/mL)		4.96 ± 1.06	15.9 ± 6.5	66.0 ± 5.7
Tmax_obs (min)		10	5.0	15.0
k01 (min <sup>-1</sup> )		0.0646 ± 0.0081	0.0579 ± 0.0056	0.0462 ± 0.0038
k01 Half-life (min)	3.73 ± 0.16	10.7 ± 1.3	12.0 ± 1.2	15.0 ± 1.2
k10 (min <sup>-1</sup> )	0.186 ± 0.008	0.0646 ± 0.0081	0.0579 ± 0.0056	0.0462 ± 0.0038
k10 Half-life (min)		10.7 ± 1.3	12.0 ± 1.2	15.0 ± 1.2
Cl (mL/min/kg)	75.3 ± 2.2			
Cl1_F (mL/min/kg)		646 ± 97	260 ± 31	116 ± 13
V1 (mL/kg)	405 ± 18			
V1_F (mL/kg)		10000 ± 1000	4500 ± 460	2510 ± 240
MRT (min)	5.38 ± 0.23			
AUC_0-T (ug/ml*min)		152	680	3090
AUCinf_pred (ug/mL*min)	1330 ± 40	155 ± 23	768 ± 92	3450 ± 390

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**Request Date:** 7/11/2023

**Request Time:** 10:03:16

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

**Male**

**Treatment Group (mg/kg)**

**8.00 Dosed Water and  
Gavage Challenge Plasma<sup>c</sup>**

**80.0 Dosed Water and  
Gavage Challenge Plasma<sup>d</sup>**

**160 Dosed Water and  
Gavage Challenge Plasma<sup>d</sup>**

**NO DATA RECORDED**

Cmax_pred (ug/mL)		8.47 ± 1.78	55.0 ± 5.6
Tmax_pred (min)		8.37 ± 1.08	18.9 ± 1.8
Cmax_obs (ug/mL)		7.01 ± 0.48	59.0 ± 9.0
Tmax_obs (min)		5.0	10.0
k01 (min <sup>-1</sup> )		0.120 ± 0.015	0.0530 ± 0.0051
k01 Half-life (min)		5.80 ± 0.75	13.1 ± 1.2
k10 (min <sup>-1</sup> )		0.120 ± 0.015	0.0530 ± 0.0051
k10 Half-life (min)		5.80 ± 0.75	13.1 ± 1.2
Cl1_F (mL/min/kg)		415 ± 83	56.7 ± 7.1
V1_F (mL/kg)		3480 ± 730	1070 ± 110
AUC_0-T (ug/mL*min)		90.2	2540
AUCinf_pred (ug/mL*min)		193 ± 38	2820 ± 360

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**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

**Female**

**Treatment Group (mg/kg)**

**10.00 Dosed Water and  
Gavage Challenge Plasma<sup>c</sup>**

**100 Dosed Water and  
Gavage Challenge Plasma<sup>d</sup>**

**200 Dosed Water and  
Gavage Challenge Plasma<sup>h</sup>**

**NO DATA RECORDED**

Cmax_pred (ug/mL)		26.3 ± 3.1	68.0 ± 6.0
Tmax_pred (min)		19.4 ± 1.9	18.4 ± 1.5
Cmax_obs (ug/mL)		32.4 ± 0.3	77.7 ± 17.4
Tmax_obs (min)		20.0	20.0
k01 (min <sup>-1</sup> )		0.0515 ± 0.0050	0.0543 ± 0.0045
k01 Half-life (min)		13.4 ± 1.3	12.8 ± 1.0
k10 (min <sup>-1</sup> )		0.0515 ± 0.0050	0.0543 ± 0.0045
k10 Half-life (min)		13.4 ± 1.3	12.8 ± 1.0
Cl1_F (mL/min/kg)		72.0 ± 9.6	58.8 ± 6.4
V1_F (mL/kg)		1400 ± 170	1080 ± 100
AUC_0-T (ug/mL*min)		1280	3330
AUCinf_pred (ug/mL*min)		1390 ± 190	3400 ± 370

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**Toxicokinetics Data Summary**

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**Request Time:** 10:03:16

**Species/Strain:** Mouse/B6C3F1

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

**Male**

**Treatment Group (mg/kg)**

**8.0 Dosed Water Plasma<sup>e,i</sup>**

**80.0 Dosed Water Plasma<sup>f</sup>**

**160 Dosed Water Plasma<sup>f</sup>**

Cmax_obs (ug/mL)	.	0.732	1.09
Tmax_obs (hour)	.	18	15

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**Request Time:** 10:03:16

**Species/Strain:** Mouse/B6C3F1

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

**Female**

**Treatment Group (mg/kg)**

**10.0 Dosed Water Plasma<sup>e,i</sup>**

**100 Dosed Water Plasma<sup>f</sup>**

**200 Dosed Water Plasma<sup>f</sup>**

Cmax_obs (ug/mL)	.	0.99	1.37
Tmax_obs (hour)	.	15	21

**Experiment Number:** K07378  
**Route:** IV, Gavage, Dosed Water  
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**Species/Strain:** Mouse/B6C3F1

**Toxicokinetics Data Summary**  
**Compound:** Sodium Bromochloroacetic acid  
**Analyte:** Bromochloroacetic acid plus Isomer  
**CAS Number:** 5589-96-8

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

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**Male**

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**Treatment Group (mg/kg)**

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**100 IV Plasma<sup>g,j</sup>**

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Cmax_pred (ug/mL)	123 ± 8
k10 (min <sup>-1</sup> )	0.142 ± 0.009
k10 Half-life (min)	4.88 ± 0.32
Cl (mL/min/kg)	115 ± 6
V1 (mL/kg)	812 ± 56
MRT (min)	7.04 ± 0.46
AUCinf_pred	867 ± 45

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**Toxicokinetics Data Summary**  
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**Analyte:** Bromochloroacetic acid plus Isomer  
**CAS Number:** 5589-96-8

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

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**Female**

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**Treatment Group (mg/kg)**

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**100 IV Plasma<sup>g,i</sup>**

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Cmax_pred (ug/mL)	144 ± 8
k10 (min <sup>-1</sup> )	0.143 ± 0.007
k10 Half-life (min)	4.86 ± 0.25
Cl (mL/min/kg)	98.9 ± 4.0
V1 (mL/kg)	693 ± 38
MRT (min)	7.01 ± 0.37
AUCinf_pred	1010 ± 40



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**Compound:** Sodium Bromochloroacetic acid  
**Analyte:** Bromochloroacetic acid minus Isomer  
**CAS Number:** 5589-96-8

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

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Male

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Treatment Group (mg/kg)

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100 IV Plasma<sup>g,i</sup>

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Cmax_pred (ug/mL)	190 ± 22
k10 (min <sup>-1</sup> )	0.360 ± 0.031
k10 Half-life (min)	1.92 ± 0.16
Cl (mL/min/kg)	189 ± 13
V1 (mL/kg)	525 ± 61
MRT (min)	2.78 ± 0.24
AUCinf_pred	529 ± 36

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**Toxicokinetics Data Summary**  
**Compound:** Sodium Bromochloroacetic acid  
**Analyte:** Bromochloroacetic acid minus Isomer  
**CAS Number:** 5589-96-8

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

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**Female**

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**Treatment Group (mg/kg)**

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**100 IV Plasma<sup>g,i</sup>**

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Cmax_pred (ug/mL)	219 ± 16
k10 (min <sup>-1</sup> )	0.384 ± 0.020
k10 Half-life (min)	1.80 ± 0.09
Cl (mL/min/kg)	175 ± 7
V1 (mL/kg)	456 ± 33
MRT (min)	2.60 ± 0.14
AUCinf_pred	571 ± 23

**Experiment Number:** K07378

**Toxicokinetics Data Summary**

**Request Date:** 7/11/2023

**Route:** IV, Gavage, Dosed Water Gavage Challenge

**Compound:** Sodium Bromochloroacetic acid

**Request Time:** 10:03:16

Dosed Water

**Analyte:** Bromochloroacetic acid, Bromochloroacetic acid plus Isomer, Bromochloroacetic acid minus Isomer

**Species/Strain:** Mouse/B6C3F1

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

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LEGEND

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MODELING SOFTWARE

WinNonlin, Version 4.0, 5.0, 5.0.1

MODELING METHOD & BEST FIT MODEL

<sup>a</sup> WinNonlin, Pharsight Corp., One-compartment model with bolus input, first order output, and 1/Y<sup>hat</sup> weighting. Parameter estimates are reported to three significant figures.

<sup>b</sup> WinNonlin, Pharsight Corp., One-compartment equal first order absorption and elimination with 1/Y<sup>hat</sup> weighting. Model 5 with Ka equals to ke (a one-compartment model with equal first order absorption and elimination). Parameter estimates and SEM are reported to three significant figures. GXA and OXA plasma concentration time point data were not presented because most of GXA and OXA values were near or at BLOQ (4.209 ug/mL GXA and 4.192 ug/mL OXA).

<sup>c</sup> WinNonlin, version 4.0, 5.0, or 5.0.1, Pharsight Corporation, Mountain View, CA, For mice, data sets for the low dosage gavage challenge group did not allow for reliable TK parameters to be generated which was attributed to an undefined terminal linear phase as a result of little decay in plasma BCA concentrations at the later time points and proximity to the LOQ>

<sup>d</sup> WinNonlin, version 4.0, 5.0, or 5.0.1, Pharsight Corporation, Mountain View, CA, One-compartment model with equal first order absorption and elimination. Parameter estimates and SEM are reported to three significant figures.

<sup>e</sup> WinNonlin, version 4.0, 5.0, or 5.0.1, Pharsight Corporation, Mountain View, CA, No kinetic modeling was possible for the non-challenge group animals. BCA, GXA, and OXA plasma concentrations were BLOQ (0.0750 ug/mL for BCA, 4.349 ug/mL for GXA, and 4.169 ug/mL for OXA) for the low dosage groups.

<sup>f</sup> WinNonlin, version 4.0, 5.0, or 5.0.1, Pharsight Corporation, Mountain View, CA, No extensive TK analysis was performed for the non-challenge group data, however, non-compartmental analysis was used to determine C<sub>max</sub> and AUC values for the mid and high dose BCA groups for the purpose of examining dose proportionality. No kinetic modeling was possible for the non-challenge group animals for GXA and OXA. The plasma concentrations of GXA and OXA were either BLOQ (4.349 and 4.169 µg/mL, respectively), or not detected, for all dosage groups.

<sup>g</sup> WinNonlin Pharsight Corp., One-compartment model with bolus input, first order output, and 1/Y weighting. The BCA minus isomer was eliminated much faster than BCA plus isomer for rats and mice.

<sup>h</sup> One-compartment model with equal first order absorption and elimination. Parameter estimates and SEM are reported to three significant figures. The BCA minus isomer was eliminated much faster than BCA plus isomer for rats and mice.

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**Experiment Number:** K07378

**Toxicokinetics Data Summary**

**Request Date:** 7/11/2023

**Route:** IV, Gavage, Dosed Water Gavage Challenge

**Compound:** Sodium Bromochloroacetic acid

**Request Time:** 10:03:16

Dosed Water

**Analyte:** Bromochloroacetic acid, Bromochloroacetic acid plus Isomer, Bromochloroacetic acid minus Isomer

**Species/Strain:** Mouse/B6C3F1

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

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EXCEPTIONS

<sup>l</sup>C<sub>max</sub> observed is below the LOQ of 0.0750 ug/mL plasma. T<sub>max</sub> is not applicable

<sup>i</sup>V<sub>1</sub> represents V<sub>d</sub>

ANALYTE

Bromochloroacetic acid

Bromochloroacetic acid minus Isomer

Bromochloroacetic acid plus Isomer

TK PARAMETERS

C<sub>max\_pred</sub> = Observed or Predicted Maximum plasma (or tissue) concentration

T<sub>max\_pred</sub> = Time at which C<sub>max</sub> predicted or observed occurs

C<sub>max\_obs</sub> = Observed or Predicted Maximum plasma (or tissue) concentration

T<sub>max\_obs</sub> = Time at which C<sub>max</sub> predicted or observed occurs

k<sub>01</sub> = Absorption rate constant, k<sub>a</sub>

k<sub>01</sub> Half-life = Half-life of the absorption process to the central compartment

k<sub>10</sub> = Elimination rate constant from the central compartment also k<sub>e</sub> or k<sub>elim</sub>

k<sub>10</sub> Half-life = Half-life of the absorption process to the central compartment

Cl = Clearance, includes total clearance

Cl<sub>1\_F</sub> = Apparent clearance of the central compartment, also Cl<sub>1\_F</sub> for gavage groups in non-compartmental model

V<sub>1</sub> = Volume of distribution of the central compartment, includes V<sub>d</sub> and V volume of distribution, V<sub>z</sub> apparent volume of distribution NCA,

V<sub>app</sub> apparent volume of distribution for intravenous studies

V<sub>1\_F</sub> = Apparent volume of distribution for the central compartment includes V<sub>d\_F</sub>, V<sub>F</sub> for oral groups, and V<sub>c\_F</sub>

MRT = Mean residence time

AUC<sub>0-T</sub> = Area under the plasma concentration versus time curve, AUC, from time t<sub>i</sub> (initial) to t<sub>f</sub> (final), AUC<sub>last</sub>

AUC<sub>inf\_pred</sub> = Area under the plasma concentration versus time curve, AUC, from time t<sub>i</sub> (initial) to t<sub>f</sub> (final), AUC<sub>last</sub>

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**Experiment Number:** K07378

**Toxicokinetics Data Summary**

**Request Date:** 7/11/2023

**Route:** IV, Gavage, Dosed Water Gavage Challenge

**Compound:** Sodium Bromochloroacetic acid

**Request Time:** 10:03:16

Dosed Water

**Analyte:** Bromochloroacetic acid, Bromochloroacetic acid plus Isomer, Bromochloroacetic acid minus Isomer

**Species/Strain:** Mouse/B6C3F1

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

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TK PARAMETERS PROTOCOL

ANALYSIS METHOD

Mouse blood samples were collected using the cardiac puncture method. Animals were anesthetized with CO<sub>2</sub>/O<sub>2</sub> prior to bleeding. Three animals/sex/species were bled at each time point. Blood collection times are 0, 2, 5, 10, 20, 30, 40, 50, and 60 minutes. The plasma samples were analyzed by gas chromatography-flame ionization detection (GC-FID) system. The level of detection for Bromochloroacetic acid in plasma from the IV groups was 0.07445 ug/mL. Plasma and urine concentration time point values were reported to at least three significant figures.

TK\_INTRAVENTOUS PLASMA

100 mg/kg Male and Female (Analyte: Bromochloroacetic acid)

Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were administered a single IV dose through an implanted jugular catheter.

ANALYSIS METHOD

Mouse blood samples were collected using the cardiac puncture method. Animals were anesthetized with CO<sub>2</sub>/O<sub>2</sub> prior to bleeding. Three animals/sex/species were bled at each time point. Blood collection times are 0, 2, 5, 10, 15, 20, 30, 40, 60, and 90 minutes. The plasma samples were analyzed by high performance liquid chromatography- ultraviolet detection, HPLC-UVD. The LOQ for BCA in plasma for the mouse gavage group samples was 0.07757 ug/mL. Plasma and urine concentration time point values were reported to at least three significant figures.

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**Route:** IV, Gavage, Dosed Water Gavage Challenge

**Compound:** Sodium Bromochloroacetic acid

**Request Time:** 10:03:16

Dosed Water

**Analyte:** Bromochloroacetic acid, Bromochloroacetic acid plus Isomer, Bromochloroacetic acid minus Isomer

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TK PARAMETERS PROTOCOL (cont'd)

TK\_GAVAGE PLASMA

100 mg/kg Male and Female (Analyte: Bromochloroacetic acid)

Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were administered a single gavage dose.

ANALYSIS METHOD

Mouse blood samples were collected using the cardiac puncture method. Animals were anesthetized with CO<sub>2</sub>/O<sub>2</sub> prior to bleeding. Three animals/sex/species were bled at each time point. Blood collection times are 0, 2, 5, 10, 15, 20, 30, 40, 60, 90, 120, and 150 minutes. The plasma samples were analyzed by high performance liquid chromatography- ultraviolet detection, HPLC-UVD. The LOQ for BCA in plasma for the mouse gavage group samples was 0.07757 ug/mL. Plasma and urine concentration time point values were reported to at least three significant figures.

TK\_GAVAGE PLASMA

200 mg/kg Male and Female (Analyte: Bromochloroacetic acid)

Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were administered a single gavage dose. There was no TK analysis for the urine mid-level dose gavage groups because no plasma samples were taken from the separate group of animals from which urine samples were collected.

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**Toxicokinetics Data Summary**

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**Route:** IV, Gavage, Dosed Water Gavage Challenge

**Compound:** Sodium Bromochloroacetic acid

**Request Time:** 10:03:16

Dosed Water

**Analyte:** Bromochloroacetic acid, Bromochloroacetic acid plus Isomer, Bromochloroacetic acid minus Isomer

**Species/Strain:** Mouse/B6C3F1

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

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TK PARAMETERS PROTOCOL (cont'd)

ANALYSIS METHOD

Mouse blood samples were collected using the cardiac puncture method. Animals were anesthetized with CO<sub>2</sub>/O<sub>2</sub> prior to bleeding. Three animals/sex/species were bled at each time point. Blood collection times are 0, 2, 5, 10, 15, 20, 40, 60, 90, 120, 150, and 180 minutes. The plasma samples were analyzed by high performance liquid chromatography- ultraviolet detection, HPLC-UVD. The LOQ for BCA in plasma for the mouse gavage group samples was 0.07757 ug/mL. Plasma and urine concentration time point values were reported to at least three significant figures.

TK\_GAVAGE PLASMA

400mg/kg Male and Female (Analyte: Bromochloroacetic acid)

Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were administered a single gavage dose. There was no TK analysis for the urine high-level dose gavage groups because no plasma samples were taken from the separate group of animals from which urine samples were collected

ANALYSIS METHOD

For the challenge Drinking Water Study groups, exposure continued up through the fourteenth day of exposure and, on the 14th day of exposure (Study Day 14), the BCA treated drinking water was replaced by untreated water (control tap water), which the animals were exposed to overnight prior to being given a single gavage administration on Day 15. Three animals/sex/species were bled at each time point. Blood collection times are 2, 5, 10, 15, 20, 30, 45, and 60 minutes. Samples were analyzed using a validated capillary gas chromatography (GC) method with electron capture detection (ECD) for BCA. LOQ for BCA in plasma and urine was 0.0750 µg/mL.

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Dosed Water

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TK PARAMETERS PROTOCOL (cont'd)

TK\_DOSED WATER AND GAVAGE CHALLENGE PLASMA

8.00 mg/kg Male, 10.0 mg/kg Female (ANALYTE: Bromochloroacetic acid)

Listed date of first exposure is Day 15 gavage dose date. Day 1 Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were dosed for two weeks from dosed drinking water available ad libitum. These animals were also challenged with a gavage dose on study day 15.

ANALYSIS METHOD

For the challenge Drinking Water Study groups, exposure continued up through the fourteenth day of exposure and, on the 14th day of exposure (Study Day 14), the BCA treated drinking water was replaced by untreated water (control tap water), which the animals were exposed to overnight prior to being given a single gavage administration on Day 15. Three animals/sex/species were bled at each time point. Blood collection times are 2, 5, 10, 20, 40, 60, 90, and 120 minutes. Samples were analyzed using a validated capillary gas chromatography (GC) method with electron capture detection (ECD) for BCA. LOQ for BCA in plasma and urine was 0.0750 µg/mL.

TK\_DOSED WATER AND GAVAGE CHALLENGE PLASMA

80.0 mg/kg Male, 100 mg/kg Female (ANALYTE: Bromochloroacetic acid)

Listed date of first exposure is Day 15 gavage dose date. Day 1 Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were dosed for two weeks from dosed drinking water available ad libitum. These animals were also challenged with a gavage dose on study day 15.



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Dosed Water

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TK PARAMETERS PROTOCOL (cont'd)

ANALYSIS METHOD

For the challenge Drinking Water Study groups, exposure continued up through the fourteenth day of exposure and, on the 14th day of exposure (Study Day 14), the BCA treated drinking water was replaced by untreated water (control tap water), which the animals were exposed to overnight prior to being given a single gavage administration on Day 15. Three animals/sex/species were bled at each time point. Blood collection times are 2, 5, 10, 20, 40, 60, 120, and 180 minutes. Samples were analyzed using a validated capillary gas chromatography (GC) method with electron capture detection (ECD) for BCA. LOQ for BCA in plasma and urine was 0.0750 µg/mL.

TK\_DOSED WATER AND GAVAGE CHALLENGE PLASMA

160 mg/kg Male, 200 mg/kg Female (ANALYTE: Bromochloroacetic acid)

Listed date of first exposure is Day 15 gavage dose date. Day 1 Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were dosed for two weeks from dosed drinking water available ad libitum. These animals were also challenged with a gavage dose on study day 15.

ANALYSIS METHOD

For the non-challenge Drinking Water Study groups, Bromochloroacetic acid (BCA) exposure continued through the fourteenth day of exposure and into the fifteenth day of exposure, so that beginning on the fourteenth day of exposure (Study Day 14), this group of rats and mice had blood samples collected over a 21-hour period beginning at 9:00 am on Day 14. Plasma was collected at 8 time points every 3 hours (180 minutes) Collection times were 9 AM (Day 14), 12 PM, 3 PM, 6 PM, 9 PM, 12 AM (Day 15), 3 AM, 6 AM. For the rats the glyoxylic acid (GXA) and oxalic acid (OXA) plasma concentrations were either below the level of quantitation (BLOQ) or not detected at all dosing concentrations.

**Experiment Number:** K07378

**Toxicokinetics Data Summary**

**Request Date:** 7/11/2023

**Route:** IV, Gavage, Dosed Water Gavage Challenge

**Compound:** Sodium Bromochloroacetic acid

**Request Time:** 10:03:16

Dosed Water

**Analyte:** Bromochloroacetic acid, Bromochloroacetic acid plus Isomer, Bromochloroacetic acid minus Isomer

**Species/Strain:** Mouse/B6C3F1

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

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TK PARAMETERS PROTOCOL (cont'd)

TK\_DOSED WATER

8.00 mg/kg, 80.0 mg/kg, 160 mg/kg Male and 10.0 mg/kg, 100 mg/kg, 200 mg/kg Female (ANALYTE: Bromochloroacetic acid)

Day 1 Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were dosed for two weeks from dosed drinking water available ad libitum.

ANALYSIS METHOD

Mouse blood samples were collected using the cardiac puncture method. Animals were anesthetized with CO<sub>2</sub>/O<sub>2</sub> prior to bleeding. Three animals/sex/species were bled at each time point. Blood collection times are 0, 2, 5, 10, 20, 30, 40, 50, and 60 minutes. The plasma samples were analyzed by gas chromatography-electron capture detection (GC-ECD) system. The target LOQ for plus and minus bromochloroacetic acid isomers in rat and mouse plasma samples was 0.03750 ug/mL. The actual LOQ ranged from 0.03620 to 0.03924 ug/mL. Plasma and urine concentration time point values were reported to at least three significant figures.

TK\_INTRAVENTOUS PLASMA

100 mg/kg Male and Female (ANALYTE: Bromochloroacetic acid\_minus\_isomer)

Day 1 Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were given a single bolus intravenous injection through an indwelling jugular catheter.

**Experiment Number:** K07378

**Toxicokinetics Data Summary**

**Request Date:** 7/11/2023

**Route:** IV, Gavage, Dosed Water Gavage Challenge

**Compound:** Sodium Bromochloroacetic acid

**Request Time:** 10:03:16

Dosed Water

**Analyte:** Bromochloroacetic acid, Bromochloroacetic acid plus Isomer, Bromochloroacetic acid minus Isomer

**Species/Strain:** Mouse/B6C3F1

**CAS Number:** 5589-96-8

**Lab:** Battelle Columbus

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TK PARAMETERS PROTOCOL (cont'd)

TK\_INTRAVENTOUS PLASMA

100 mg/kg Male and Female (ANALYTE: Bromochloroacetic acid plus\_isomer)

Day 1 Mean weights are based on animals available for use prior to dosing and does not take into account substituted animals. Animals were given a single bolus intravenous injection through an indwelling jugular catheter.