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**Name:** 4-chlorobenzoyl chloride / 122-01-0

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**Legal entity owner:** National Institute of Health Sciences / Kawasaki / Japan

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# 4-chlorobenzoyl chloride

## CORE

### General information

#### Identification

**SUBSTANCE:** 4-chlorobenzoyl chloride

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**UUID:** IUC5-87ac8376-058e-4153-acc0-e69617beb555

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:25:23.000+09:00

**Remarks:**

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**Substance name**

4-chlorobenzoyl chloride

**Legal entity**

[National Institute of Health Sciences / Kawasaki / Japan](#)

#### Identification of substance

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**Reference substance**

[4-chlorobenzoyl chloride / 122-01-0 / 204-515-3](#)

**EC number**

204-515-3

**EC name**

EC Inventory

**CAS number**

122-01-0

**CAS name**

**IUPAC name**

#### Role in the supply chain

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**Manufacturer**

false

**Importer**

false

**Only representative**

false

**Downstream user**

false

# OECD

## Health Effects

Acute toxicity: oral

ENDPOINT\_STUDY\_RECORD: Acute toxicity: oral.001

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**UUID:** IUC5-a979f21c-55c9-4b3c-9783-184bbe71d749

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:17:31.000+09:00

**Remarks:**

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## Administrative data

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**Endpoint**

acute toxicity: oral

**Type of information**

experimental study

**Adequacy of study**

key study

**Robust study summary**

false

**Used for classification**

false

**Used for SDS**

false

**Reliability**

1 (reliable without restriction)

**Rationale for reliability incl. deficiencies**

other: OECD Test Guideline study under GLP condition

## Data source

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**Reference**

[Single Dose Oral Toxicity Test of 4-chlorobenzoyl chloride in Rats / MHW \(Ministry of Health and Welfare\), Japan / study report](#)

**Data access**

data published

## Materials and methods

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## Test guideline

**Qualifier**

according to

**Guideline**

OECD Guideline 423 (Acute Oral toxicity - Acute Toxic Class Method)

**Deviations**

no

**GLP compliance**

yes

**Test type**

acute toxic class method

**Limit test**

yes

## Test material

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**Test material information**

[1220-01-0](#)

## Test animals

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**Species**

rat

common species

**Strain**

Crj: CD(SD)

rat

**Sex**

female

**Details on test animals and environmental conditions**

TEST ANIMALS- Source: Charles River Japan Inc.

- Age at the time of purchase: 7 weeks old

- Weight at dosing: Females, 190 - 198 g

- Fasting period before study: Approximately 16 hrs

- Housing: One animal/cage- Diet (e.g. ad libitum): Ad libitum except fasting period for 16 hrs before administration to 3 hrs after administration

- Water (e.g. ad libitum): Ad libitum

- Acclimation period: 7 - 8 days.

**ENVIRONMENTAL CONDITIONS**

- Temperature (°C): 22.6 - 23.6

- Humidity (%): 45.6 - 62.2

- Ventilation (per hr): Approximately > 12 times

- Photoperiod (hrs light / hrs dark): 12/12

## Administration / exposure

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**Route of administration**

oral: gavage

**Vehicle**

corn oil

**Details on oral exposure**

VEHICLE

- Concentration in vehicle: 40 w/v%
  - Lot no.: V4F1900 produced by Nacalai Tesque, INC..
- MAXIMUM DOSE VOLUME APPLIED: 5 ml/kg bw

**Doses**

2000 mg/kg bw

**No. of animals per sex per dose**

First time of administration: 3 females (animal ID No. 3, 7, 10) /dose  
Second time of administration: 3 females (animal ID No. 6, 8, 9)/dose

**Control animals**

no

**Details on study design**

- Duration of observation period following administration: 14 days
- Frequency of observations: Day 1 (day of administration): within 30 minutes and 1, 2, 3, 4, 5 and 6 hrs after administration. After day 2: once a day
- Frequency of weighing: Days 1 (before administration), 7, and 14
- Necropsy of survivors performed: Yes

The LD50 value was estimated to be around 820 mg / kg from information of the test substance. Therefore, the starting administration dose was set as 2000 mg/kg bw. No clinical changes were observed in the first administration, therefore the second dose was also set as 2000 mg/kg bw

**Statistics**

No

## Results and discussion

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**Effect levels**

**Key result**  
false

**Sex**  
female

**Dose descriptor**  
LD50

**Effect level**

> 2000 mg/kg bw

**Based on**  
act. ingr.

**Mortality**

No deaths were observed in first and second times.

**Clinical signs**

No changes related to the test substance were observed in first and second times.

**Body weight**

No changes related to the test substance were observed in first and second times.

**Gross pathology**

No changes related to the test substance were observed in first and second times.

**Other findings**

- Organ weights: No data
- Histopathology: No data
- Potential target organs: Not identified
- Other observations: No data

**Applicant's summary and conclusion**

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**Conclusions**

The LD50 value was more than 2000 mg/kg bw for female rats.

## Repeated dose toxicity: oral

ENDPOINT\_STUDY\_RECORD: Repeated dose toxicity: oral.001

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**UUID:** IUC5-2c9bcc31-9c27-489b-aab9-4ae7f1fdf45c

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:26:31.000+09:00

**Remarks:**

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## Administrative data

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### Endpoint

short-term repeated dose toxicity: oral combined repeated dose and reproduction / developmental screening

### Type of information

experimental study

### Adequacy of study

key study

### Robust study summary

false

### Used for classification

false

### Used for SDS

false

### Reliability

1 (reliable without restriction)

### Rationale for reliability incl. deficiencies

other: OECD Test Guideline study under GLP condition

### Cross-reference

#### Reason / purpose

reference to same study

#### Remarks

7.8.1 Toxicity to reproduction: Toxicity to reproduction.001

7.8.2 Developmental toxicity/teratogenicity: Developmental toxicity/teratogenicity.001

## Data source

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### Reference

[A combined repeated-dose/reproductive-developmental toxicity study of 4-chlorobenzoyl chloride by or... / MHW \(Ministry of Health and Welfare\), Japan / study report](#)

### Data access

data published

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## Materials and methods

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### Test guideline

**Qualifier**

according to

**Guideline**

OECD Guideline 422 (Combined Repeated Dose Toxicity Study with the Reproduction / Developmental Toxicity Screening Test)

**Deviations**

no

**GLP compliance**

yes

**Limit test**

no

## Test material

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**Test material information**

[122-01-0 / 204-515-3](#)

## Test animals

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**Species**

rat

common rodent species

**Strain**

Crj: CD(SD)

rat

**Sex**

male/female

**Details on test animals and environmental conditions****TEST ANIMALS**

- Source: Atsugi Breeding Center, Charles River Laboratories Japan, Inc.
- Age at study initiation: 10 weeks of age
- Weight at study initiation: 395-476 g for males and 225-282 g for females
- Housing: bracket-type metallic wire-mesh cages (W 250 × D 350 × H 170 mm)- Diet (e.g. ad libitum): ad libitum
- Water (e.g. ad libitum): ad libitum
- Acclimation period: 19 days

**ENVIRONMENTAL CONDITIONS**

- Temperature (°C): 21 to 24°C
- Humidity (%): 40 to 56%
- Air changes (per hr): 10 to 15 times per hour
- Photoperiod (hrs dark / hrs light): 12-hour lighting per day

## Administration / exposure

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**Route of administration**

oral: gavage

**Vehicle**

corn oil

**Details on oral exposure**

PREPARATION OF DOSING SOLUTIONS: Test substance was dissolved in corn oil for injection.  
VEHICLE

- Justification for use and choice of vehicle: No data
- Amount of vehicle (if gavage): 5 ml/kg bw
- Lot/batch no. (if required): V0M3906 produced by Nacalai Tesque, INC.
- Dosing volume: 5 mL/kg bw
- Stability (test solutions): At least 7 days
- Storage condition of test solution: Stored in a refrigerator

**Analytical verification of doses or concentrations**

yes

**Details on analytical verification of doses or concentrations**

Test suspensions at each concentration to be used for males in week 1 and six week of administration were analyzed by the HPLC method at Bozo Research Center Inc. Results showed that the concentration of the test article in each suspension was 98.0 to 104.0% of the nominal concentration and both values were within the acceptable range (concentration: percentage of the nominal concentration, 100 ± 10%; C.V.: 10% or below)

**Duration of treatment / exposure**

(P) Males: 42 days including 14 days pre-mating, mating, and thereafter 14 days (P)Females: 42–48 days including 14 days pre-mating, mating and gestation periods and the days until day 4 of lactation

**Frequency of treatment**

Daily: 7 times / week

**Doses / concentrations**

**Remarks**

Doses / Concentrations:  
0 (vehicle), 20, 100 and 500 mg/kg bw/day  
Basis:  
actual ingested

**No. of animals per sex per dose**

12 animals/sex/dose (main dose group)

Five out of 12 males at 0 and 500 mg/kg bw/day were used as a recovery assessment group. In addition, 10 females/dose were administered 0 and 500 mg/kg bw/day for 42 days without mating and examined after the administration period or after a 14 day recovery period.

**Control animals**

yes, concurrent vehicle

**Details on study design**

- Dose selection rationale: A preliminary study was conducted to determine the doses to be employed. Male and female rats were receiving 0, 250, 500, and 1000 mg/kg bw/day of the substance was administered for 14 days. As a result, no death, and no effects of food consumption and hematology were observed in all treated groups. Loose stool, salivation, pale stool (females), slight depression of body weights, increase in T-CHO, decrease in BUN (males) and increase in liver weight (females) were observed in both sexes receiving 1000 mg/kg. In addition, raised lesion in the forestomach in both sexes and dark red colored lesion in the glandular in males were observed in the 1000 mg/kg bw/day group. Raised focus in the forestomach in both sexes and dark red colored lesion in the glandular in males were observed in the 500 mg/kg bw/day group. Raised focus in the forestomach in females was observed in the 250 mg/kg bw/day group. Therefore, the highest dose was set at 500 mg/kg bw/day, the concentration in which the expression of apparent toxicity is expected, and the middle and low dose were set at 100 and 20 mg/kg bw/day using a common ratio of 5.

**Positive control**

no

**Examinations**

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**Observations and examinations performed and frequency**

CAGE SIDE OBSERVATIONS: Yes

- Time schedule:

Males and females: once before the start of administration, 3 times/day during the administration period, and once during the recovery period

DETAILED CLINICAL OBSERVATIONS: Yes

- Time schedule:

Males: once before the start of administration, during the administration and recovery periods

Females: once before the start of administration, days 1, 7, 14 and 20 of gestation, and day 4 of lactation

BODY WEIGHT: Yes

- Time schedule for examinations:

Males in the main groups were weighed on days 1, 4, 8, 11, 15, 18, 22, 25, 29, 32, 36, 39 and 42 of administration and on the day of necropsy, and males and females in the recovery groups were weighed on days 1, 4, 8, 11 and 14 of recovery and on the day of necropsy in addition to the measurement days for males in the main groups.

Females in the main groups were weighed on days 1, 4, 8, 11 and 15 of administration (uncopulated animals were weighed on day 18 and 22 of administration as well), days 0, 4, 7, 11, 14, 17 and 20 of gestation, days 0 and 4 of lactation and the day of necropsy.

FOOD CONSUMPTION : Yes

- Food consumption (g/day/rat) for each animal determined from the difference of the of the previous day's feeding amount: Yes

Measurement of food consumption was conducted on all animals at the following frequencies:

males in the main groups on days 1, 4, 8, 11, 15, 32, 36, 39 and 42 of administration; males and females in the recovery groups on days 1, 4, 8, 11 and 14 of recovery in addition to the measurement days for males in the main groups; and females in the main groups on days 1, 4, 8, 11 and 15 of administration, days 1, 4, 7, 11, 14, 17 and 20 of gestation and days 2 and 4 of lactation.

FOOD INTAKE: No

HAEMATOLOGY: Yes

- Time schedule for collection of blood: On the day after the final day of administration and on the final day of the recovery period

- Anaesthetic used for blood collection: Yes (identity)

- Animals fasted: Yes

- How many animals: 5 animals/sex/group

- Parameters examined red blood cell count, hemoglobin, hematocrit, mean corpuscular volume, mean corpuscular hemoglobin, mean corpuscular hemoglobin concentration, reticulocyte percentage, platelet count, white blood cell count, differential white blood cell count, absolute number of each white blood cell, prothrombin time, activated partial thromboplastin time, fibrinogen

CLINICAL CHEMISTRY: Yes

- Time schedule for collection of blood: On the day after the final day of administration and on the final day of the recovery period

- Animals fasted: Yes

- How many animals: 5 animals/sex/group

- Parameters checked: ALP, total cholesterol, triglyceride, phospholipids, total bilirubin, glucose, blood urea nitrogen, creatinine, sodium, potassium, chloride, calcium, inorganic phosphorus, total protein, albumin, A/G ratio, AST (GOT), ALT (GPT), LDH,  $\gamma$ -GTP

URINALYSIS: Yes

- Time schedule for collection of urine: final week of administration (days 39 to 40 of administration) and in the final week of recovery (days 11 to 12 of recovery)

- Metabolism cages used for collection of urine: Yes

- Animals fasted: Yes ,

A urine collector to collect four-hour urine samples under fasting but ad libitum drinking conditions, followed by collection of 20-hour urine samples under ad libitum feeding and drinking conditions.

- Parameters checked: pH, protein, ketones, glucose, occult blood, bilirubin, urobilinogen, color, sediment, urine volume (4-hour volume), osmotic pressure, urine volume (20-hour volume), water intake (24-hour volume)

**BLOOD HORMONE:** Yes

- Time schedule for collection of serum: Same as clinical chemistry

- Parameters checked: Triiodothyronine (T3), Thyroxin (T4), and thyroid stimulating hormone (TSH) of thyroid hormone

**NEUROBEHAVIOURAL EXAMINATION:** Yes

- Time schedule for examinations: Manipulative test and measurements of grip strength and motor activity were conducted on 5 animals per group with the following frequencies: males in the main groups were examined in the final week of administration (day 37 of administration), females in the main groups on day 4 of lactation (day 42 to day 44 of administration) after necropsy of F1 pups, and males and females in the recovery groups in the final week of administration (day 37 of administration) and in the final week of recovery (day 9 of recovery).

- Dose groups that were examined: All animals were examined for detailed clinical signs once before the start of administration. Thereafter, males in the main groups were examined once weekly during the administration period, whereas females were observed once weekly during the pre-mating administration period and mating period as well as on designated days during the gestation and lactation periods (days 1, 7, 14 and 20 of gestation, and day 4 of lactation). Animals in the recovery groups were examined once weekly during the administration and recovery periods.

- Battery of functions tested:

1) Open field observation. Arousal, gait, posture, tremor, convulsion, rearing count, defecation (defecation count, urination), stereotypy (grooming, circling, etc.), abnormal behavior (self-biting, backward walking, etc.)

2) Manipulative Test. Auditory response, approach response, touch response, tail pinch response, pupillary reflex, aerial righting reflex, landing foot splay

3) Measurement of Grip Strength. Following manipulative test, grip strength of forelimb and hind limb was measured by CPU gauge MODEL-9502A (AIKOH Engineering Co., Ltd.).

4) Measurement of Motor Activity. Following measurement of grip strength, motor activity was measured by a motor activity sensor for experimental animals NS-AS01 (NeuroScience, Inc). The measurement was conducted for 1 hour, and measured values at 10-minute intervals and from 0 to 60 minutes were collected.

### **Sacrifice and pathology**

**GROSS PATHOLOGY AND ORGAN WEIGHTS:** Brain, pituitary, thyroids (including parathyroids), thymus, heart, liver, spleen, kidneys, adrenals, seminal, prostate, testes, epididymis, ovaries, uterus  
**HISTOPATHOLOGY:** Cerebrum, cerebellum (including pontocerebellar), sciatic nerve, spinal cord (thoracic), eye, optic nerve, Harder gland, pituitary, thyroid, parathyroid, adrenal glands, thymus, spleen, submandibular lymph nodes, mesenteric lymph nodes, heart, thoracic aorta, trachea, lung (including bronchial), tongue, larynx, esophagus, stomach, duodenum, jejunum, ileum (including Peyer's patches), cecum, colon, rectum, submandibular gland, sublingual gland, liver, pancreas, kidney, bladder, testis, ovary, epididymis, uterus, vagina, prostate, seminal vesicles (including the coagulating gland), mammary gland (groin), sternum and femur (including bone marrows), femoral skeletal muscle, skin (groin), macroscopic lesions, and parts for identification (auricles)

### **Statistics**

The data were analyzed for homogeneity of variance by the Bartlett test (level of significance: 0.01, two-tailed). If variances were homogeneous, data was analyzed by the Dunnett test, whereas heterogeneous data was analyzed by a Steel test. In the recovery test, these values of two groups were analyzed by F test and Student or Aspin-Welch t-test. Frequency data were analysed by Fisher test. Statistical significance was set at < 5% by two-sided

## **Results and discussion**

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### **Results of examinations**

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#### **Clinical signs**

effects observed, treatment-related

**Description (incidence and severity)**

No animal died in any group. Clinical signs: Salivation was observed in 1 to 7 males receiving 500 mg /kg bw/day after Day 12 during the dosing period. Salivation was observed in 1 mating female receiving 500 mg/kg bw/day after Day 12, however this sign was not observed after Day 16 of gestation. No clinical signs were observed in both sexes of recovery animals during the recovery period.

**Mortality**

mortality observed, treatment-related

**Description (incidence)**

No animal died in any group. Clinical signs: Salivation was observed in 1 to 7 males receiving 500 mg /kg bw/day after Day 12 during the dosing period. Salivation was observed in 1 mating female receiving 500 mg/kg bw/day after Day 12, however this sign was not observed after Day 16 of gestation. No clinical signs were observed in both sexes of recovery animals during the recovery period.

**Body weight and weight changes**

no effects observed

**Food consumption and compound intake (if feeding study)**

no effects observed

**Food efficiency**

not examined

**Ophthalmological findings**

no effects observed

**Haematological findings**

no effects observed

**Clinical biochemistry findings**

no effects observed

**Urinalysis findings**

no effects observed

**Description (incidence and severity)**

Significant increases in water consumption and urine volume were observed in males receiving 500 mg/kg bw/day, but it was not considered to be toxicological effects. during the dosing period.

**Behaviour (functional findings)**

no effects observed

**Organ weight findings including organ / body weight ratios**

effects observed, treatment-related

**Description (incidence and severity)**

see Details on results

**Gross pathological findings**

effects observed, treatment-related

**Description (incidence and severity)**

see Details on results

**Histopathological findings: non-neoplastic**

effects observed, treatment-related

**Description (incidence and severity)**

see Details on results

**Histopathological findings: neoplastic**

not examined

**Details on results**

**DETAILED CLINICAL OBSERVATIONS, MANIPULATIVE TEST, GRIP STRENGTH TEST AND LOCOMOTOR ACTIVITY MEASUREMENT:** There were no changes in main males and females and satellite females during the dosing and recovery periods.

**ORGAN WEIGHTS:** An Increase in relative kidney weight was observed in males receiving 500 mg/kg bw/day at the end of the administration period. Decreases in absolute and relative thymus weights were observed in mating females receiving 500 mg/kg bw/day at the end of the administration. In addition, a decrease in relative thyroid weight and increases in relative weights of the heart and testis were observed in males and decreases in relative weights of the pituitary and heart were observed in females at 500 mg/kg bw/day at end of the recovery period; however, these changes were determined to be within physiological variation range.

**GROSS PATHOLOGY:**

**Kidneys:** Irregular surface was observed in 1 male receiving 500 mg/kg bw/day.

**Stomach:** Thickening wall and focus/raised of forestomach was observed in both sexes receiving 500 mg/kg bw/day.

**HISTOPATHOLOGY**

basophilic changes in the tubular cells of kidneys from males and both mating and non-mating females, and tubular dilatation, granular casts, and fibrosis was observed in male kidneys. Atrophy of the thymus was observed in all mating females, including the control group; however, the incidence was particularly high in the 500 mg/kg bw/day group. Furthermore, histopathological changes were observed in the stomach, including intercellular edema in squamous cells and cell infiltration or hyperplasia of the forestomach mucosa, in males and mating and non-mating females. Forestomach erosion and ulceration were present in one mating female administered 500 mg/kg bw/day. These histopathological changes tended to resolve after the 14 day recovery period.

**Effect levels****Dose descriptor**

NOAEL

**Effect level**

100

mg/kg bw/day (actual dose received)

**Based on**

act. ingr.

**Sex**

male/female

**Basis for effect level**

other: Effects of lesions in the kidneys and stomach of both sexes and the thymus of females at 500 mg/kg bw/day

**Target system / organ toxicity****Key result**

false

**Critical effects observed**

not specified

**Any other information on results incl. tables**

Figures and Tables (in English) are available in the following full report of the study.

[http://dra4.nihs.go.jp/mhlw\\_data/home/pdf/PDF122-01-0d.pdf](http://dra4.nihs.go.jp/mhlw_data/home/pdf/PDF122-01-0d.pdf)

## **Applicant's summary and conclusion**

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### **Conclusions**

Based on the effects of 4-chlorobenzoyl chloride on the thymus, kidney, and stomach, the no observed adverse effect level (NOAEL) for repeated oral dosing was determined to be 100 mg/kg bw/day in male and female rats.

### **Executive summary**

A combined repeated oral dose toxicity study with the reproduction/developmental toxicity screening test was performed according to the OECD TG 422. Male and female rats (12 animals/sex/dose) were administered 4-chlorobenzoyl chloride at 0, 20, 100, and 500 mg/kg bw/day. Males were dosed for 42 days, including a 14 day pre-mating period and subsequent mating period; whereas females were dosed for 42–48 days, including the 14 day pre-mating, mating, and gestation periods, and the time until day 4 of lactation. Five out of 12 males at 0 and 500 mg/kg bw/day were used as a recovery assessment group. In addition, 10 females/dose were administered 0 and 500 mg/kg bw/day for 42 days without mating and examined after the administration period or after a 14 day recovery period. At 500 mg/kg bw/day, the absolute and relative thymus weights had decreased in the mating group females. Relative kidney weight increased in males at 500 mg/kg bw/day. Histopathological examination revealed basophilic changes in the tubular cells of kidneys from males and both mating and non-mating females, and tubular dilatation, granular casts, and fibrosis was observed in male kidneys. Atrophy of the thymus was observed in all mating females, including the control group; however, the incidence was particularly high in the 500 mg/kg bw/day group. Furthermore, histopathological changes were observed in the stomach, including intercellular edema in squamous cells and cell infiltration or hyperplasia of the forestomach mucosa, in males and mating and non-mating females. Forestomach erosion and ulceration were present in one mating female administered 500 mg/kg bw/day. These histopathological changes tended to resolve after the 14 day recovery period. Based on the effects of 4-chlorobenzoyl chloride on the thymus, kidney, and stomach, the no observed adverse effect level (NOAEL) for repeated oral dosing was determined to be 100 mg/kg bw/day in male and female rats.

## Genetic toxicity in vitro

### ENDPOINT\_STUDY\_RECORD: Genetic toxicity in vitro.001

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**UUID:** IUC5-2e59c227-c537-4b93-b700-e6a72a4ec840

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:18:22.000+09:00

**Remarks:**

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## Administrative data

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### Endpoint

in vitro gene mutation study in bacteria Type of genotoxicity: gene mutation

### Type of information

experimental study

### Adequacy of study

key study

### Robust study summary

false

### Used for classification

false

### Used for SDS

false

### Reliability

1 (reliable without restriction)

### Rationale for reliability incl. deficiencies

other: OECD Test Guideline study under GLP condition

## Data source

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### Reference

[Reverse Mutation Test of 4-chlorobenzoyl chloride on Bacteria. / MHW \(Ministry of Health and Welfare\), Japan / study report](#)

### Data access

data published

## Materials and methods

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### Test guideline

#### Qualifier

according to

#### Guideline

OECD Guideline 471 (Bacterial Reverse Mutation Assay)  
in vitro gene mutation study in bacteria

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**Deviations**

no

**Qualifier**

according to

**Guideline**

OECD Guideline 472 (Genetic Toxicology: Escherichia coli, Reverse Mutation Assay)  
in vitro gene mutation study in bacteria (before 21 July 1997)

**Deviations**

no

**Qualifier**

according to

**Guideline**

JAPAN: Guidelines for Screening Mutagenicity Testing Of Chemicals

**Deviations**

no

**GLP compliance**

yes

**Type of assay**

bacterial reverse mutation assay  
in vitro gene mutation study in bacteria

**Test material**

**Test material information**

[120-01-0](#)

**Method**

**Species / strain**

**Species / strain**

S. typhimurium TA 1535, TA 1537, TA 98 and TA 100  
bacteria

**Metabolic activation**

with and without

**Metabolic activation system**

rat liver, induced by phenobarbital and 5,6-benzoflavone

**Species / strain**

E. coli WP2 uvr A  
bacteria

**Metabolic activation**

with and without

**Metabolic activation system**

rat liver, induced by phenobarbital and 5,6-benzoflavone

**Test concentrations with justification for top dose**

-S9 mix: 7.81, 15.6, 31.3, 62.5, 125, 250, 500 µg/plate (TA100, TA1535, TA98 strains)

, 15.6, 31.3, 62.5, 125, 250, 500, 1000 µg/plate (WP2uvrA strain), and 3.91, 7.81, 15.6, 31.3, 62.5, 125, 250 µg/plate (TA1537 strain)  
+S9 mix: 15.6, 31.3, 62.5, 125, 250, 500, 1000 µg/plate (all strains)

**Vehicle**

- Vehicle(s)/solvent(s) used: Acetone

**Controls**

**Negative controls**

no

**Solvent controls**

yes

**True negative controls**

no

**Positive controls**

yes

**Positive control substance**

other: other: -S9 mix: 2-(2-Furyl)-3-(5-nitro-2-furyl) acrylamide (TA 100, TA98 and WP2 uvrA), sodium azide (TA1535) and 9-aminoacridine hydrochloride (TA1537). +S9 mix: 2-aminoanthracene (all strains)

**Details on test system and conditions**

RANGE-FINDING/SCREENING STUDIES: Concentration: 9.19, 20.5, 51.2, 128, 320, 800, 2000, 5000 µg/plate

Cytotoxic conc.: No

METHOD OF APPLICATION: Preincubation

DURATION

- Preincubation period: 20 min at 37 °C

- Exposure duration: 48 hrs

NUMBER OF PLATES: 3

NUMBER OF REPLICATIONS: 1

DETERMINATION OF CYTOTOXICITY

- Method: other: growth inhibition

**Evaluation criteria**

In any strain(s) tested with or without S9 mix, when the mean number of revertant colonies per plate increased twice more than that of the negative control and when the increase was shown to be dose-related and reproducible, the chemical was judged mutagenic.

**Statistics**

No

---

## Results and discussion

**Test results**

**Key result**

false

**Species / strain**

S. typhimurium TA 1535, TA 1537, TA 98 and TA 100  
bacteria

**Metabolic activation**

with and without

**Genotoxicity**

negative

**Cytotoxicity**

no

**Vehicle controls valid**

yes

**Negative controls valid**

not examined

**Positive controls valid**

yes

**Remarks on result**

other: all strains/cell types tested Migrated from field 'Test system'.

**Key result**

false

**Species / strain**

E. coli WP2 uvr A  
bacteria

**Metabolic activation**

with and without

**Genotoxicity**

negative

**Cytotoxicity**

no

**Vehicle controls valid**

yes

**Negative controls valid**

not examined

**Positive controls valid**

yes

**Remarks on result**

other: all strains/cell types tested Migrated from field 'Test system'.

**Any other information on results incl. tables**

Figures and Tables (in English) are available in the following full report of the study.

[http://dra4.nihs.go.jp/mhlw\\_data/home/pdf/PDF122-01-0e.pdf](http://dra4.nihs.go.jp/mhlw_data/home/pdf/PDF122-01-0e.pdf)

**Applicant's summary and conclusion**

**Conclusions**

Interpretation of results (migrated information):

negative

In a bacterial reverse mutation assay using *Salmonella typhimurium* TA100, TA1535, TA98, and TA 1537, and *Escherichia coli* WP2uvrA (OECD TG 471), 4-chlorobenzoyl chloride was negative with or without metabolic activation.

## ENDPOINT\_STUDY\_RECORD: Genetic toxicity in vitro.002

---

**UUID:** IUC5-1cc6257a-ecfb-4760-896a-031e4df5890e

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:18:26.000+09:00

**Remarks:**

---

## Administrative data

---

### Endpoint

in vitro cytogenicity / chromosome aberration study in mammalian cells Type of genotoxicity: chromosome aberration

### Type of information

experimental study

### Adequacy of study

key study

### Robust study summary

false

### Used for classification

false

### Used for SDS

false

### Reliability

1 (reliable without restriction)

### Rationale for reliability incl. deficiencies

other: OECD Test Guideline study under GLP condition

## Data source

---

### Reference

[In Vitro Chromosomal Aberration Test of 4-chlorobenzoyl chloride on Cultured Chinese Hamster Cells. / MHW \(Ministry of Health and Welfare\), Japan / study report](#)

### Data access

data published

## Materials and methods

---

### Test guideline

#### Qualifier

according to

#### Guideline

OECD Guideline 473 (In Vitro Mammalian Chromosome Aberration Test)  
in vitro cytogenicity / chromosome aberration study in mammalian cells

---

**Deviations**

no

**Qualifier**

according to

**Guideline**

JAPAN: Guidelines for Screening Mutagenicity Testing Of Chemicals

**Deviations**

no

**GLP compliance**

yes

**Type of assay**

in vitro mammalian chromosome aberration test  
chromosome aberration

**Test material**

**Test material information**

[120-01-0](#)

**Method**

**Target gene**

Chromosome

**Species / strain**

**Species / strain**

other: Chinese hamster lung(CHL/IU) cells

**Metabolic activation**

with and without

**Metabolic activation system**

rat liver, induced by phenobarbital and 5,6-benzoflavone

**Test concentrations with justification for top dose**

-S9 mix (continuous treatment): 0, 74.1, 106, 151, 216, 309, 441 ug/mL-S9 mix (short-term treatment)  
: 0, 106, 151, 216, 309, 441, 630 ug/mL+S9 mix (short-term treatment): 0, 106, 151, 216, 309, 441,  
630, 900 ug/mL

**Vehicle**

- Vehicle(s)/solvent(s) used: Acetone

**Controls**

**Negative controls**

no

**Solvent controls**

yes

**True negative controls**

no

**Positive controls**

yes

**Positive control substance**

cyclophosphamide  
mitomycin C

**Details on test system and conditions**

METHOD OF APPLICATION: Exposure duration: [continuous treatment]: 24 hrs [short-term treatment]: 6 hrs + 18 hr

SPINDLE INHIBITOR: Colcemid

STAIN: Giemsa stain for 12 min.

NUMBER OF REPLICATIONS: 2

NUMBER OF CELLS EVALUATED: 200 cells / dose

DETERMINATION OF CYTOTOXICITY

- Method: relative total growth

**Evaluation criteria**

For the evaluation of the frequencies of structural aberrations and of polyploidy induced, the following criteria, which are usually used for chromosomal aberration testing with CHL, were employed. Appearance incidence of cell with chromosomal aberrations: Negative(-): less than 5% Equivocal(±): 5% or more, less than 10% Positive(+): 10% or more

**Statistics**

Fisher and Cochran-Armitage trend tests (one-sided test, P = 2.5%)

## Results and discussion

**Test results**

**Key result**

false

**Species / strain**

other: Chinese hamster lung (CHL/IU) cells

**Metabolic activation**

with and without

**Genotoxicity**

negative

**Cytotoxicity**

no

**Vehicle controls valid**

yes

**Negative controls valid**

not examined

**Positive controls valid**

yes

**Remarks on result**

other: all strains/cell types tested Migrated from field 'Test system'.

## Any other information on results incl. tables

Figures and Tables (in English) are available in the following full report of the study.

[http://dra4.nihs.go.jp/mhlw\\_data/home/pdf/PDF122-01-0f.pdf](http://dra4.nihs.go.jp/mhlw_data/home/pdf/PDF122-01-0f.pdf)

## **Applicant's summary and conclusion**

---

### **Conclusions**

Interpretation of results (migrated information):  
negative

4-Chlorobenzoyl chloride did not induce chromosomal aberrations in cultured cells.

### **Executive summary**

An in vitro chromosomal aberration test using CHL/IU cells (OECD TG 473) was negative with or without metabolic activation.



## Toxicity to reproduction

### ENDPOINT\_STUDY\_RECORD: Toxicity to reproduction.001

---

**UUID:** IUC5-425c2820-7a3b-4906-ba61-2f2048c78a20

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:18:44.000+09:00

**Remarks:**

---

## Administrative data

---

### Endpoint

screening for reproductive / developmental toxicity based on test type (migrated information)

### Type of information

experimental study

### Adequacy of study

key study

### Robust study summary

false

### Used for classification

false

### Used for SDS

false

### Reliability

1 (reliable without restriction)

### Rationale for reliability incl. deficiencies

other: OECD Test Guideline study under GLP condition

### Cross-reference

#### Reason / purpose

reference to same study

#### Remarks

7.5.Repeated dose toxicity: oral: Repeated dose toxicity: oral.001

## Data source

---

### Reference

[A combined repeated-dose/reproductive-developmental toxicity study of 4-chlorobenzoyl chloride by or... / MHW \(Ministry of Health and Welfare\), Japan / study report](#)

### Data access

data published

## Materials and methods

---

## Test guideline

**Qualifier**

according to

**Guideline**

OECD Guideline 422 (Combined Repeated Dose Toxicity Study with the Reproduction / Developmental Toxicity Screening Test)

**Deviations**

no

**GLP compliance**

yes

**Limit test**

no

## Test material

---

**Test material information**

120-01-0

## Test animals

---

**Species**

rat

**Strain**

Crj: CD(SD)

rat

**Sex**

male/female

**Details on test animals and environmental conditions****TEST ANIMALS**

- Source: Atsugi Breeding Center, Charles River Laboratories Japan, Inc.
- Age at study initiation: 10 weeks of age
- Weight at study initiation: 395-476 g for males and 225-282 g for females
- Housing: bracket-type metallic wire-mesh cages (W 250 × D 350 × H 170 mm)- Diet (e.g. ad libitum): ad libitum
- Water (e.g. ad libitum): ad libitum
- Acclimation period: 19 days

**ENVIRONMENTAL CONDITIONS**

- Temperature (°C): 21 to 24°C
- Humidity (%): 40 to 56%
- Air changes (per hr): 10 to 15 times per hour
- Photoperiod (hrs dark / hrs light): 12-hour lighting per day

## Administration / exposure

---

**Route of administration**

oral: gavage

**Vehicle**

corn oil

**Details on exposure**

PREPARATION OF DOSING SOLUTIONS: Test substance was dissolved in corn oil for injection.

#### VEHICLE

- Justification for use and choice of vehicle: No data
- Amount of vehicle (if gavage): 5 ml/kg bw
- Lot/batch no. (if required): V0M3906 produced by Nacalai Tesque, INC.
- Dosing volume: 5 mL/kg bw
- Stability (test solutions): At least 7 days
- Storage condition of test solution: Stored in a refrigerator

#### Details on mating procedure

- M/F ratio per cage: 1:1
- Length of cohabitation: up to 14 days
- Proof of pregnancy: [vaginal plug / sperm in vaginal smear] referred to as [day 0] of pregnancy
- After ... days of unsuccessful pairing replacement of first male by another male with proven fertility.
- Further matings after two unsuccessful attempts: [no]

#### Analytical verification of doses or concentrations

yes

#### Details on analytical verification of doses or concentrations

Test suspensions at each concentration to be used for males in week 1 and six week of administration were analyzed by the HPLC method at Bozo Research Center Inc. Results showed that the concentration of the test article in each suspension was 98.0 to 104.0% of the nominal concentration and both values were within the acceptable range (concentration: percentage of the nominal concentration, 100 ± 10%; C.V.: 10% or below)

#### Duration of treatment / exposure

(P) Males: 42 days including 14 days pre-mating, mating, and thereafter 14 days

(P) Females: 42-48 days including 14 days pre-mating, mating and gestation periods and the days until day 4 of lactation

#### Frequency of treatment

Daily: 7 times / week

#### Doses / concentrations

##### Remarks

Doses / Concentrations:

0 (vehicle), 20, 100 and 500 mg/kg bw/day

Basis:

actual ingested

#### No. of animals per sex per dose

12 animals/sex/dose

Five out of 12 males at 0 and 500 mg/kg bw/day were used as a recovery assessment group. In addition, 10 females/dose were administered 0 and 500 mg/kg bw/day for 42 days without mating and examined after the administration period or after a 14 day recovery period.

#### Control animals

yes, concurrent vehicle

## Examinations

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#### Parental animals: Observations and examinations

CAGE SIDE OBSERVATIONS: Yes

- Time schedule:

Males and females: once before the start of administration, 3 times/day during the administration period, and once during the recovery period

DETAILED CLINICAL OBSERVATIONS: Yes

- Time schedule:

Males: once before the start of administration, during the administration and recovery periods  
Females: once before the start of administration, days 1, 7, 14 and 20 of gestation, and day 4 of lactation

BODY WEIGHT: Yes

- Time schedule for examinations:

Males in the main groups were weighed on days 1, 4, 8, 11, 15, 18, 22, 25, 29, 32, 36, 39 and 42 of administration and on the day of necropsy, and males and females in the recovery groups were weighed on days 1, 4, 8, 11 and 14 of recovery and on the day of necropsy in addition to the measurement days for males in the main groups.

Females in the main groups were weighed on days 1, 4, 8, 11 and 15 of administration (uncopulated animals were weighed on day 18 and 22 of administration as well), days 0, 4, 7, 11, 14, 17 and 20 of gestation, days 0 and 4 of lactation and the day of necropsy.

FOOD CONSUMPTION : Yes

- Food consumption (g/day/rat) for each animal determined from the difference of the of the previous day's feeding amount: Yes

Measurement of food consumption was conducted on all animals at the following frequencies:

males in the main groups on days 1, 4, 8, 11, 15, 32, 36, 39 and 42 of administration; males and females in the recovery groups on days 1, 4, 8, 11 and 14 of recovery in addition to the measurement days for males in the main groups; and females in the main groups on days 1, 4, 8, 11 and 15 of administration, days 1, 4, 7, 11, 14, 17 and 20 of gestation and days 2 and 4 of lactation.

COMPOUND INTAKE: No

FOOD EFFICIENCY: No

WATER CONSUMPTION: No

#### **Estrous cyclicity (parental animals)**

Vaginal smears were collected from all females in the main groups and microscopically examined every day from the day after the start of administration until the day copulation was confirmed.

During the pre-mating administration period, vaginal smear pictures were classified as proestrus, estrus, metestrus or diestrus and examined for the frequency of estrus and interval between estruses (estrous cycle). During the mating period, vaginal smears were examined for the presence of sperm.

#### **Sperm parameters (parental animals)**

Parameters examined in P male parental generations: testes weight, epididymides weight

#### **Litter observations**

PARAMETERS EXAMINED: The following parameters were examined in F1 offspring: Number and sex of pups, stillbirths, live births, postnatal mortality, presence of gross anomalies, and weight gain.

GROSS EXAMINATION OF DEAD PUPS: Yes, for external and internal abnormalities.

#### **Postmortem examinations (parental animals)**

SACRIFICE: Male animals: Rats were euthanized by exsanguination under ether anesthesia on the day after the last administration. Maternal animals: Rats were euthanized by exsanguination under ether anesthesia on day 4 of lactation.

GROSS PATHOLOGY AND ORGAN WEIGHTS : Yes Brain, pituitary, thyroids(including parathyroids), thymus, heart, liver, spleen, kidneys, adrenals, seminal, prostate, testes, epididymis, ovaries, uterus

HISTOPATHOLOGY: Yes Cerebrum, cerebellum (including pontocerebellar), sciatic nerve, spinal cord (thoracic), eye, optic nerve, Harder gland, pituitary, thyroid, parathyroid, adrenal glands, thymus, spleen, submandibular lymph nodes, mesenteric lymph nodes, heart, thoracic aorta, trachea, lung (including bronchial), tongue, larynx, esophagus, stomach, duodenum, jejunum, ileum (including Peyer's patches), cecum, colon, rectum, submandibular gland, sublingual gland, liver, pancreas, kidney, bladder, testis, ovary, epididymis, uterus, vagina, prostate, seminal vesicles (including the coagulating gland), mammary gland (groin), sternum and femur (including bone marrows), femoral skeletal muscle, skin (groin), macroscopic lesions, and parts for identification (auricles)

#### **Postmortem examinations (offspring)**

SACRIFICE: The F1 pups were euthanized on PND 4 by exsanguination under ether anesthesia.

GROSS NECROPSY: Yes

### Statistics

The data were analyzed for homogeneity of variance by the Bartlett test (level of significance: 0.01, two-tailed). If variances were homogeneous, data was analyzed by the Dunnett test, whereas heterogeneous data was analyzed by a Steel test. In the recovery test, these values of two groups were analyzed by F test and Student or Aspin-Welch t-test. Frequency data were analysed by Fisher test. Statistical significance was set at < 5% by two-sided

### Reproductive indices

) Each parameter was determined by the following equations:

Copulation index (%) = (No. of copulated animals/No. of co-housed animals) × 100

Fertility index (%) = (No. of pregnant females/No. of copulated females) × 100

Insemination index (%) = (No. of pregnant females/No. of copulated males) × 100

Duration of gestation (days) = day 0 of lactation – day 0 of gestation

Delivery index (%) = (No. of females delivered liveborn pups/No. of pregnant females) × 100

Implantation index (%) = (No. of implantation sites/No. of corpora lutea) × 100

Stillborn index (%) = (No. of stillborn pups/Total No. of pups born) × 100

Liveborn index (%) = (No. of liveborn pups/Total No. of pups born) × 100

External abnormalities (%) = (No. of pups with external abnormalities/No. of liveborn pups) × 100

Sex ratio = No. of males/(No. of males + No. of females)

Viability index (%) = (No. of surviving pup on day 4 after birth/No. of liveborn pups on day 0 after birth) × 100

### Offspring viability indices

Number of live pups on day 0 of lactation  
Birth index (%) = (Number of live pups on day 0/Number of implantation sites) × 100

Live birth index (%) = (Number of live pups on day 0/Number of pups born) × 100

Pups weight on day 0 of lactation  
Sex ratio on day 0 of lactation

Number of live pups on day 4 of lactation

Pups weight on day 4 of lactation

Sex ratio on day 4 of lactation

Viability index = (Number of live pups on day 4 after birth/Number of live pups born) × 100

## Results and discussion

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### Results: P0 (first parental animals)

---

#### General toxicity (P0)

---

##### Clinical signs

effects observed, treatment-related

##### Description (incidence and severity)

see Details on results

##### Body weight and weight changes

no effects observed

##### Food consumption and compound intake (if feeding study)

no effects observed

##### Organ weight findings including organ / body weight ratios

no effects observed

##### Gross pathological findings

no effects observed

##### Description (incidence and severity)

on reproductive organs

**Histopathological findings: non-neoplastic**  
no effects observed

**Description (incidence and severity)**  
on reproductive organs

**Other effects**  
no effects observed

## Reproductive function / performance (P0)

---

**Reproductive function: estrous cycle**  
no effects observed

**Reproductive function: sperm measures**  
not examined

**Reproductive performance**  
no effects observed

## Details on results (P0)

---

CLINICAL SIGNS AND MORTALITY: Mortality: No animal died in any group. Clinical signs: Salivation was observed in 1 to 7 males receiving 500 mg/kg bw/day after Day 12 during the dosing period. Salivation was observed in 1 mating female receiving 500 mg/kg bw/day after Day 12, however this sign was not observed after Day 16 of gestation. No clinical signs were observed in both sexes of recovery animals during the recovery period.

### 1) Estrous Cycle

There were no animals showing abnormal estrous cycles, and there were no significant differences in the average length of the estrous cycle between the control group and any treatment groups.

### 2) Results of Mating

There were no significant differences in the number of elapsed days until copulation, copulation index, insemination index or fertility index between the control group and any treatment groups.

### 3) Delivery Data and Delivery

With regard to delivery status, all pregnant animals delivered normally between day 21 and day 23 of gestation excluding one dam of 100 mg/kg bw/day group. There were no significant differences in the delivery index, duration of gestation, number of corpora lutea, number of implantation sites, implantation index, stillborn index, number of liveborn pups or liveborn index between the control group and any treatment groups. Significantly increase of delivery index was observed in dam receiving 500 mg/kg bw/day, which showed high value, however this change was determined the incidental effect.

## Effect levels (P0)

---

**Dose descriptor**  
NOAEL reproduction

**Effect level**

500

mg/kg bw/day (actual dose received)

**Sex**  
male/female

**Basis for effect level**  
other: no effects on reproduction

## Results: F1 generation

---

## General toxicity (F1)

---

**Clinical signs**

no effects observed

**Mortality / viability**

no mortality observed

**Body weight and weight changes**

effects observed, treatment-related

**Description (incidence and severity)**

The body weights of pups on postnatal day (PND) 0 and PND 4 were decreased in pups of both sexes following 500 mg/kg bw/day dosing

**Sexual maturation**

not examined

**Organ weight findings including organ / body weight ratios**

not examined

**Gross pathological findings**

no effects observed

**Histopathological findings**

not examined

## Effect levels (F1)

---

**Dose descriptor**

NOAEL development

**Generation**

F1

**Effect level**

100

mg/kg bw/day (actual dose received)

**Sex**

male/female

**Basis for effect level**

other: The body weights of pups on postnatal day (PND) 0 and PND 4 were decreased in pups of both sexes following 500 mg/kg bw/day dosing

## Overall reproductive toxicity

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**Key result**

false

**Reproductive effects observed**

not specified

## Applicant's summary and conclusion

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**Conclusions**

The NOAELs for rat reproductive toxicity and developmental toxicity were determined to be 500 mg/kg bw/day and 100 mg/kg bw/day, respectively.

**Executive summary**

In the combined repeated oral dose toxicity study with the reproduction/developmental toxicity screening test (OECD TG 422), reproductive parameters were not affected up to 500 mg/kg bw/day. The body weights of pups on postnatal day (PND) 0 and PND 4 were decreased in pups of both sexes following 500 mg/kg bw/day dosing. The NOAELs for rat reproductive toxicity and developmental toxicity were determined to be 500 mg/kg bw/day and 100 mg/kg bw/day, respectively.



---

# References

## TEST\_MATERIAL\_INFORMATION: 120-01-0

---

**UUID:** 50c7e013-2743-3358-848b-8b44357c2cb7

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:18:22.000+09:00

**Remarks:**

---

**Name**

120-01-0

## Composition

---

**Type**

Constituent

**Reference substance**

120-01-0 / 120-01-0

**EC number**

**EC name**

**CAS number**

**CAS name**

**IUPAC name**

120-01-0

## Other characteristics

---

### Details on test material

- Name of test material (as cited in study report): 4-chlorobenzoyl chloride- Molecular weight: 175.01
- Physical state: Colorless liquid
- Analytical purity: 99.79%
- Melting point/ boiling point: 12—14°C/222°C
- Solubility: Very soluble in acetone (656 mg/mL), methanol, ethanol, ether, ketone, and toluene, and insoluble in water
- Vapor pressure: 110°C /20 mmHg
- Specific gravity: 1.377/20°C
- Odor: Very irritating odor
- Supplier: Iharanikkei Chemical Industry Co., Ltd
- Lot/batch No.: I5001
- Storage condition of test material: Room temperature

---

# TEST\_MATERIAL\_INFORMATION: 120-01-0

---

**UUID:** 53052755-25fd-308c-8792-dfa3751fafa4

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:18:26.000+09:00

**Remarks:**

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**Name**

120-01-0

## Composition

---

**Type**

Constituent

**Reference substance**

120-01-0 / 120-01-0

**EC number**

**EC name**

**CAS number**

**CAS name**

**IUPAC name**

120-01-0

## Other characteristics

---

### Details on test material

- Name of test material (as cited in study report): 4-chlorobenzoyl chloride
- Molecular weight: 175.01
- Physical state: Colorless liquid
- Analytical purity: 99.79%
- Melting point/ boiling point: 12—14°C/222°C
- Solubility: Very soluble in acetone (656 mg/mL), methanol, ethanol, ether, ketone, and toluene, and insoluble in water
- Vapor pressure: 110°C /20 mmHg
- Specific gravity: 1.377/20°C
- Odor: Very irritating odor
- Supplier: Iharanikkei Chemical Industry Co., Ltd
- Lot/batch No.: I5001
- Storage condition of test material: Room temperature

---

# TEST\_MATERIAL\_INFORMATION: 120-01-0

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**UUID:** c627e21d-6b77-3b99-a596-d268f2494fbe

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:18:44.000+09:00

**Remarks:**

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**Name**

120-01-0

## Composition

---

**Type**

Constituent

**Reference substance**

120-01-0 / 120-01-0

**EC number**

**EC name**

**CAS number**

**CAS name**

**IUPAC name**

120-01-0

## Other characteristics

---

### Details on test material

- Name of test material (as cited in study report): 4-chlorobenzoyl chloride
- Molecular weight: 175.01
- Physical state: Colorless liquid to white crystal mass
- Analytical purity: 99.6%
- Melting point/ boiling point: 12°C (solid point)/220-222°C
- Flash point: 118°C
- Solubility: Very soluble in acetone (656 mg/mL), methanol, ethanol, ether, ketone, and toluene, and insoluble in water
- Vapor pressure: 110°C /20 mmHg
- Specific gravity: 1.377/20°C
- Odor: Very irritating odor
- Supplier: Iharanikkei Chemical Industry Co., Ltd
- Lot/batch No.: KSSFK
- Storage condition of test material: Room temperature

---

# TEST\_MATERIAL\_INFORMATION: 122-01-0 / 204-515-3

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**UUID:** 208c4aae-3a09-3923-bcf9-9345059a08a2

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:26:31.000+09:00

**Remarks:**

---

## Name

122-01-0 / 204-515-3

## Composition

---

### Type

Constituent

### Reference substance

4-chlorobenzoyl chloride / 122-01-0 / 204-515-3

### EC number

204-515-3

### EC name

EC Inventory

### CAS number

122-01-0

### CAS name

### IUPAC name

## Other characteristics

---

### Details on test material

- Name of test material (as cited in study report): 4-chlorobenzoyl chloride
- Molecular weight: 175.01
- Physical state: Colorless liquid to white crystal mass
- Analytical purity: 99.6%
- Melting point/ boiling point: 12°C (solid point)/220-222°C
- Flash point: 118°C
- Solubility: Very soluble in acetone (656 mg/mL), methanol, ethanol, ether, ketone, and toluene, and insoluble in water
- Vapor pressure: 110°C /20 mmHg
- Specific gravity: 1.377/20°C
- Odor: Very irritating odor
- Supplier: Iharanikkei Chemical Industry Co., Ltd
- Lot/batch No.: KSSFK
- Storage condition of test material: Room temperature

---

# TEST\_MATERIAL\_INFORMATION: 1220-01-0

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**UUID:** 3fa0a575-f847-3842-95a4-2f3f26e9dc93

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:17:31.000+09:00

**Remarks:**

---

**Name**

1220-01-0

## Composition

---

**Type**

Constituent

**Reference substance**

1220-01-0 / 1220-01-0

**EC number**

**EC name**

**CAS number**

**CAS name**

**IUPAC name**

1220-01-0

## Other characteristics

---

### Details on test material

- Name of test material (as cited in study report): 4-chlorobenzoyl chloride
- Molecular weight: 175.01
- Physical state: Colorless liquid
- Analytical purity: 99.79%
- Melting point/ boiling point: 12—14°C/222°C
- Solubility: Very soluble in acetone (656 mg/mL), methanol, ethanol, ether, ketone, and toluene, and insoluble in water
- Vapor pressure: 110°C /20 mmHg
- Specific gravity: 1.377/20°C
- Odor: Very irritating odor
- Supplier: Iharanikkei Chemical Industry Co., Ltd
- Lot/batch No.: I5001
- Storage condition of test material: Room temperature

# REFERENCE\_SUBSTANCE: 4-chlorobenzoyl chloride

---

**UUID:** IUC5-a2a9360b-d978-4902-b119-ef75ccfb7959

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:23:46.000+09:00

**Remarks:**

---

## General information

---

**Reference substance name**

4-chlorobenzoyl chloride

## Inventory

---

**Inventory name**

4-chlorobenzoyl chloride

**Inventory**

EC

**Inventory number**

204-515-3

**CAS number**

122-01-0

**Molecular formula**

C<sub>7</sub>H<sub>4</sub>Cl<sub>2</sub>O

**Description**

## Reference substance information

---

### CAS information

---

**CAS number**

122-01-0

## Molecular and structural information

---

**Molecular formula**

C<sub>7</sub>H<sub>4</sub>Cl<sub>2</sub>O

# LITERATURE: A combined repeated-dose/ reproductive-developmental toxicity study of 4-chlorobenzoyl chloride by oral adm inistration in rats.

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**UUID:** aee93755-ee7f-3660-ba5c-00501643acc9

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:26:31.000+09:00

**Remarks:**

---

## General information

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**Reference Type**

study report

**Title**

A combined repeated-dose/reproductive-developmental toxicity study of 4-chlorobenzoyl chloride by oral administration in rats.

**Author**

MHW (Ministry of Health and Welfare), Japan

**Year**

2011

**Bibliographic source**

Japan Existing Chemical Data Base (JECDB)

**Testing facility**

BoZo Research Center Inc.

# LITERATURE: A combined repeated-dose/ reproductive-developmental toxicity study of 4-chlorobenzoyl chloride by oral adm inistration in rats.

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**UUID:** 9447876a-ad3b-3485-a963-3bae6a1ea3db

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:18:44.000+09:00

**Remarks:**

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## General information

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**Reference Type**

study report

**Title**

A combined repeated-dose/reproductive-developmental toxicity study of 4-chlorobenzoyl chloride by oral administration in rats.

**Author**

MHW (Ministry of Health and Welfare), Japan

**Year**

2011

**Bibliographic source**

Japan Existing Chemical Data Base (JECDB)

**Testing facility**

BoZo Research Center Inc.



# LITERATURE: In Vitro Chromosomal Aberration Test of 4-chlorobenzoyl chloride on Cultured Chinese Hamster Cells.

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**UUID:** 93929503-6ac9-3c0b-b65a-e1c5433986f4

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:18:26.000+09:00

**Remarks:**

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## General information

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**Reference Type**

study report

**Title**

In Vitro Chromosomal Aberration Test of 4-chlorobenzoyl chloride on Cultured Chinese Hamster Cells.

**Author**

MHW (Ministry of Health and Welfare), Japan

**Year**

2006

**Bibliographic source**

Japan Existing Chemical Data Base (JECDB)

**Testing facility**

Biosafety Research Center, Foods, Drugs and Pesticides (Anpyo Center)

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# LEGAL\_ENTITY: National Institute of Health Sciences

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**UUID:** IUC4-b036ff75-0f3c-323b-b200-ed5f46cf5101

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2019-09-03T10:05:28.255+09:00

**Remarks:** Disclaimer: The contents in this document were created based on the MHLW (Ministry of Health, Labour and Welfare) peer reviewed study reports (in Japanese) in JECDB (Japan Existing Chemical Database) at [http://dra4.nihs.go.jp/mhlw\\_data/jsp/SearchPageENG.jsp](http://dra4.nihs.go.jp/mhlw_data/jsp/SearchPageENG.jsp). Authorship is in the Division of Risk Assessment, the National Institute of Health Sciences, and the contents do not reflect any official MHLW opinions or any other regulatory policies.

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## General information

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### Legal entity name

National Institute of Health Sciences

### Remarks

Disclaimer: The contents in this document were created based on the MHLW (Ministry of Health, Labour and Welfare) peer reviewed study reports (in Japanese) in JECDB (Japan Existing Chemical Database) at [http://dra4.nihs.go.jp/mhlw\\_data/jsp/SearchPageENG.jsp](http://dra4.nihs.go.jp/mhlw_data/jsp/SearchPageENG.jsp). Authorship is in the Division of Risk Assessment, the National Institute of Health Sciences, and the contents do not reflect any official MHLW opinions or any other regulatory policies.

## Identifiers

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### Other IT system identifiers

<b>IT system</b> LEO
<b>ID</b> 10767
<b>IT system</b> IUCLID4
<b>ID</b> 16558402024DIV750

## Contact information

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### Contact address

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**Region / State**

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**Country**

Japan

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**Person**

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**Last name**

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**First name**

Akihiko

**Organisation**

National Institute of Health Sciences, Japan

**Department**

Division of Risk Assessment

**Title**

Dr

**Country**

Japan

# LITERATURE: Reverse Mutation Test of 4-chlorobenzoyl chloride on Bacteria.

---

**UUID:** 3291c047-b7ef-339b-be14-a659befe31ba

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:18:22.000+09:00

**Remarks:**

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## General information

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**Reference Type**

study report

**Title**

Reverse Mutation Test of 4-chlorobenzoyl chloride on Bacteria.

**Author**

MHW (Ministry of Health and Welfare), Japan

**Year**

2006

**Bibliographic source**

Japan Existing Chemical Data Base (JECDB)

**Testing facility**

Biosafety Research Center, Foods, Drugs and Pesticides (Anpyo Center)

# LITERATURE: Single Dose Oral Toxicity Test of 4-chlorobenzoyl chloride in Rats

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**UUID:** 9bba3071-8e05-38a8-8af7-4bef22a4ff1a

**Dossier UUID:**

**Author:** SuperUser

**Date:** 2017-01-04T16:17:31.000+09:00

**Remarks:**

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## General information

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**Reference Type**

study report

**Title**

Single Dose Oral Toxicity Test of 4-chlorobenzoyl chloride in Rats

**Author**

MHW (Ministry of Health and Welfare), Japan

**Year**

2007

**Bibliographic source**

Japan Existing Chemical Data Base (JECDB)

**Testing facility**

Biosafety Research Center, Foods, Drugs and Pesticides (An-Pyo Center)