

nite

HESS DBの概要と操作説明

HESSに付属する詳細なデータベース：
HESS DBに収載されている情報

HESS DBとは

- 化学構造情報のほか、毒性所見に基づいた検索機能を備えており、独立した毒性データベースとして使用することも可能。
- 一般化学物質に対するラットの反復経口投与毒性試験報告書が収載。（GLP準拠またはそれに類似した試験条件下で行われ、詳細なデータが公表されているものを選定）。
- 現在（2024年7月）、約830物質の試験報告書（投与経路：強制経口・混餌・飲水、投与期間：28日～17週）を収載。

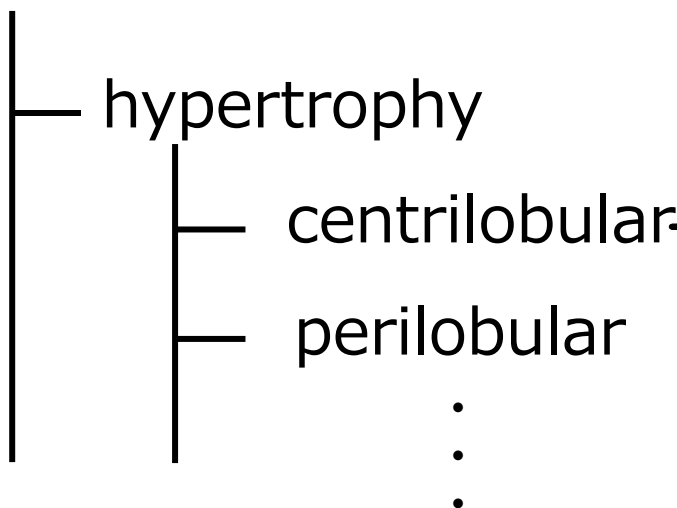
	報告書群
1	厚労省/国衛研 化審法試験
2	厚労省 安衛法長期試験（予備試験）
3	経産省/C E R I 試験（T o x - O m i c s）
4	経産省/N I T E 試験
5	米国N T P 短期試験
6	米国N T P 長期試験（予備試験）
7	医薬品データ（企業から提供）
8	J o u r n a l P a p e r

病理所見シソーラス

HESS DB

オリジナル試験報告書

Liver



hypertrophy of centrilobular hepatocyte

hypertrophy, hepatocyte, centrilobular

hypertrophy of hepatocyte, ground glass appearance in the central zone

データの検索を正確に行えるよう、データベースに入力する病理所見について、専門家が同義語を分類し関連付けることによって、用語の統一を行い、シソーラスを作成（全83臓器・11302所見）

試験報告書の用量-反応関係データ

Test Result | Flag Summary | Test Method | Measured Data

Test Item

Blood Chemistry_Male

Actual

Comment

*, significantly different from control, P<0.05

**, significantly different from control, P<0.01

		Admi...																			
DOSE	mq / kq	0					20					100					500				
No. of animals		5					5					5					5				
		mean	SD	s...	F1	F3	mean	SD	s...	F1	F3	mean	SD	s...	F1	F3	mean	SD	s...	F1	F3
BUN	mq / dL	12	1				15	2				12	1				20	2	**	△	
CRN	mq / dL	0.6	0.1				0.6	0.1				0.6	0.0				0.6	0.0			
T-CHO	mq / dL	44	3				39	6				40	7				59	11	*	△	
TG	mq / dL	51	9				37	10				44	14				33	23			
PL																					
T-BIL	mq / dL	0.11	0.03				0.14	0.02				0.12	0.02				0.16	0.06			
GLUC	mq / dL	133	16				140	21				125	16				132	24			
TP	q / dL	5.2	0.2				5.1	0.1				5.2	0.2				5.3	0.3			
BA																					
ALB	q / dL	3.3	0.1				3.1	0.1				3.1	0.1				3.1	0.2			
A/G		1.67	0.15				1.58	0.08				1.54	0.17				1.38	0.08	**		
Protein %	ALB																				

フ

フラグ

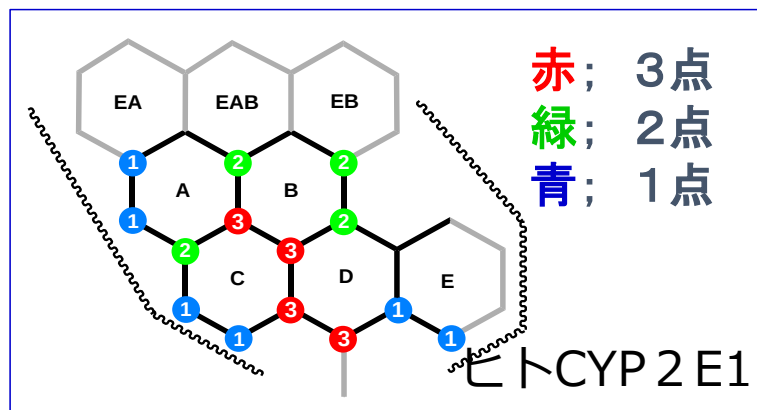
報告書に記載されている毒性所見の有意差マークのほか、**毒性・病理専門家の意見**や**既存点検時の化学物質審議会判定**に基づく、**有意差マーク(フラグ)**を付与するなどして、毒性学的な注意喚起を図っている。

ADME情報

毒性試験が行われた化合物を対象にADME情報を収集し、DB化。

吸収	吸収率、Cmax、Tmax トランスポータの関与
分布	見かけの分布容積、反復に伴う経時変化 脳→中枢作用、脂肪組織→蓄積 肝臓→酸化抱合代謝、腎臓→尿中排泄 腎臓→タンパク結合 血液よりも高い濃度を示す臓器/器官 トランスポータの関与

代謝	関連酵素と分子情報 細胞内画分、代謝物 種差・系統差
排泄	排泄率 トランスポータの関与 種差・系統差
相互作用、酵素阻害、酵素誘導試験の結果	
毒性との関連性	



リガンド構造に基づいた薬物代謝酵素
P450代謝予測モデルによる代謝予測
データも収載

毒性作用機序DBのデータ項目

変性・壊死など重篤な毒性に対する毒性メカニズム情報を収集しDB化

対象毒性：血液、肝臓、腎臓、精巣、神経、膀胱、甲状腺

収載情報の分類	データ項目
A：物質情報	CAS. No., 物質名, 構造式
B：文献情報	毒性メカニズム情報等が収載されている文献の情報
C:試験方法情報	細胞株/動物種、実験デザイン、in vitro/ in vivo/ex vivo、濃度/投与量
D:作用機序関連情報	キーワード, 要約, 化学反応/代謝, トキシカント, 生体分子との相互作用, エフェクト, 標的細胞/組織/臓器, 有効濃度/投与量
E：その他	関連物質, 追加情報, 著者の機序的考察, 備考, 関連文献

HESS DBの操作説明

HESSとHESS DBのリンク

The screenshot displays the Hazard Evaluation Support System (HESS) interface, which is used for chemical hazard evaluation. The main window shows the chemical name **3,4-dimethylaniline; 3,4-xylidine** with CAS No. **95-64-7** and SMILES **c1(C)c(C)cc(N)cc1**. The chemical structure is shown as a benzene ring with methyl groups at positions 3 and 4, and an amino group at position 1.

On the left, the **Input** section includes **Profiling**, **RDT Data**, **Categories**, **Gap Filling**, **Report**, and **Metabolism**. The **Metabolism** section is expanded, showing various metabolic pathways and chemical classes.

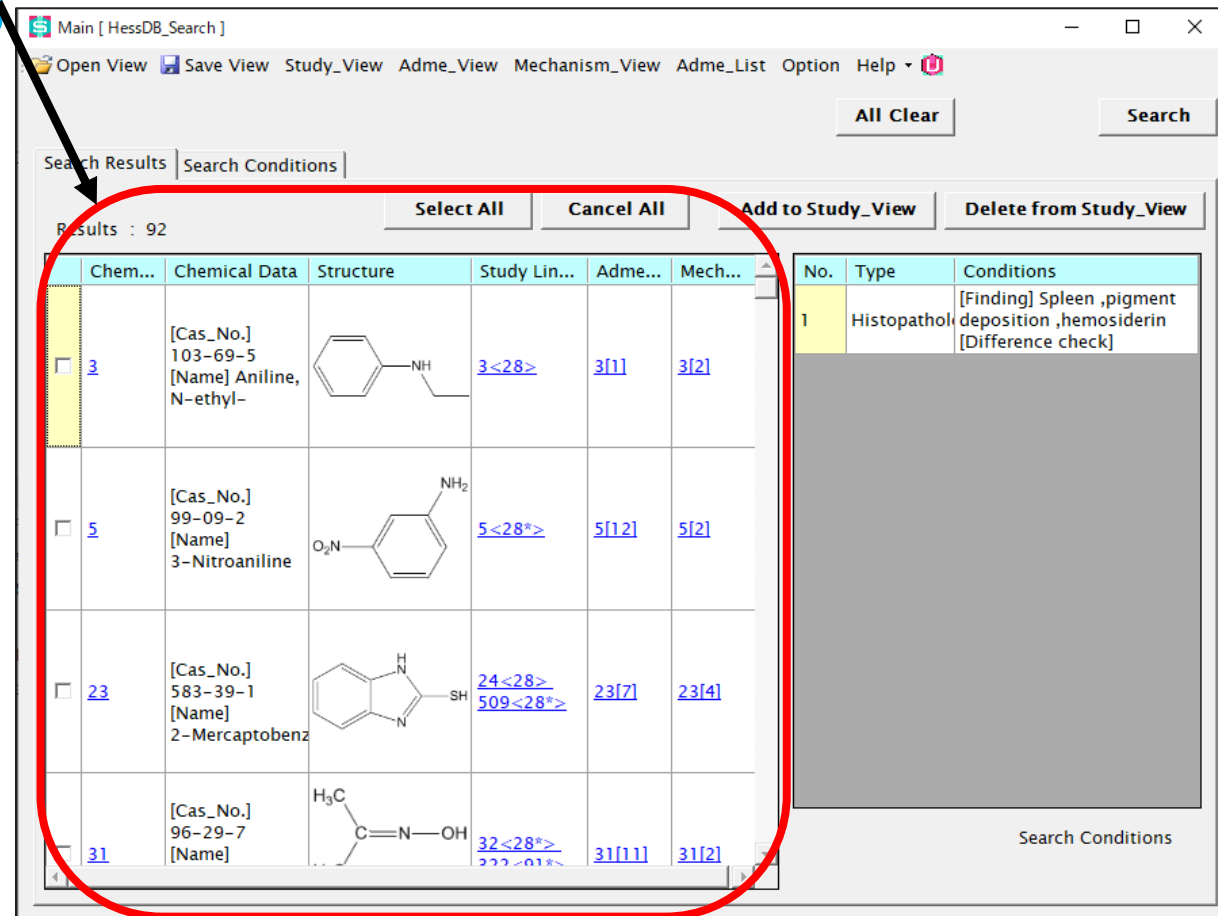
The **Study** section shows a list of studies. The first study is highlighted, showing its **Chemical No.** (Link to HESS DB) as **1**. This number is linked to the **Study Link ID** in the **Study (HESSDB_Search)** window.

The **Study (HESSDB_Search)** window displays search results for the chemical. The first result is highlighted, showing the **Study Link ID** as **1** and the **Chemical No.** as **1**. This link is used to access the detailed test data in the **Study (HESSDB_Search)** window.

The **Study (HESSDB_Search)** window shows detailed test data for the chemical, including **Test Result**, **Flag Summary**, **Test Method**, and **Measured Data**. The data is organized into tables for **Hematology**, **Blood Chemistry**, **Relative organ weight**, **Necropsy (Survival)**, **Necropsy (Dead)**, **Histopathology (Survival)**, and **Histopathology (Dead)**. The data is presented for both **Male** and **Female** subjects.

The **Study (HESSDB_Search)** window also includes a **Descriptive Data** section, which provides information on **Clinical sign**, **FOB**, **Urinalysis**, **Body weight**, **Food consumption**, **Water consumption**, and **Toxicological index**. The **Toxicological index** table shows the **NOEL**, **NOEL**, **LOEL**, and **LOEL** values for the chemical.

HESSからHESS DBへ直接リンクさせることができ、試験データの詳細情報を閲覧できる。



検索条件の入力(Measured Data)

Main [HessDB_Search]

Open View Save View Study_View Adme_View Mechanism_View Adme_List Option Help

All Clear Search

Search Results Search Conditions

Please set the search conditions.

Chemical Histopathology **Measured Data**

Test Item **2** Hematology

Group ☒ All ☐ Administration ☐ Recovery

Sex ☒ All ☐ Male ☐ Female

Search Keyword RBC ≤ 30

Difference ☐ Signif ☐ F

3 Add

No.	Type	Conditions
1	Test Item	[Test Item] Hematology [Group]All [Sex]All [Search Keyword]RBC ≤ 30 [Difference]

Clear 1 Delete

Main [HessDB_Search]

Open View Save View Study_View Adme_View Mechanism_View Adme_List Option Help

All Clear Search

Search Results Search Conditions

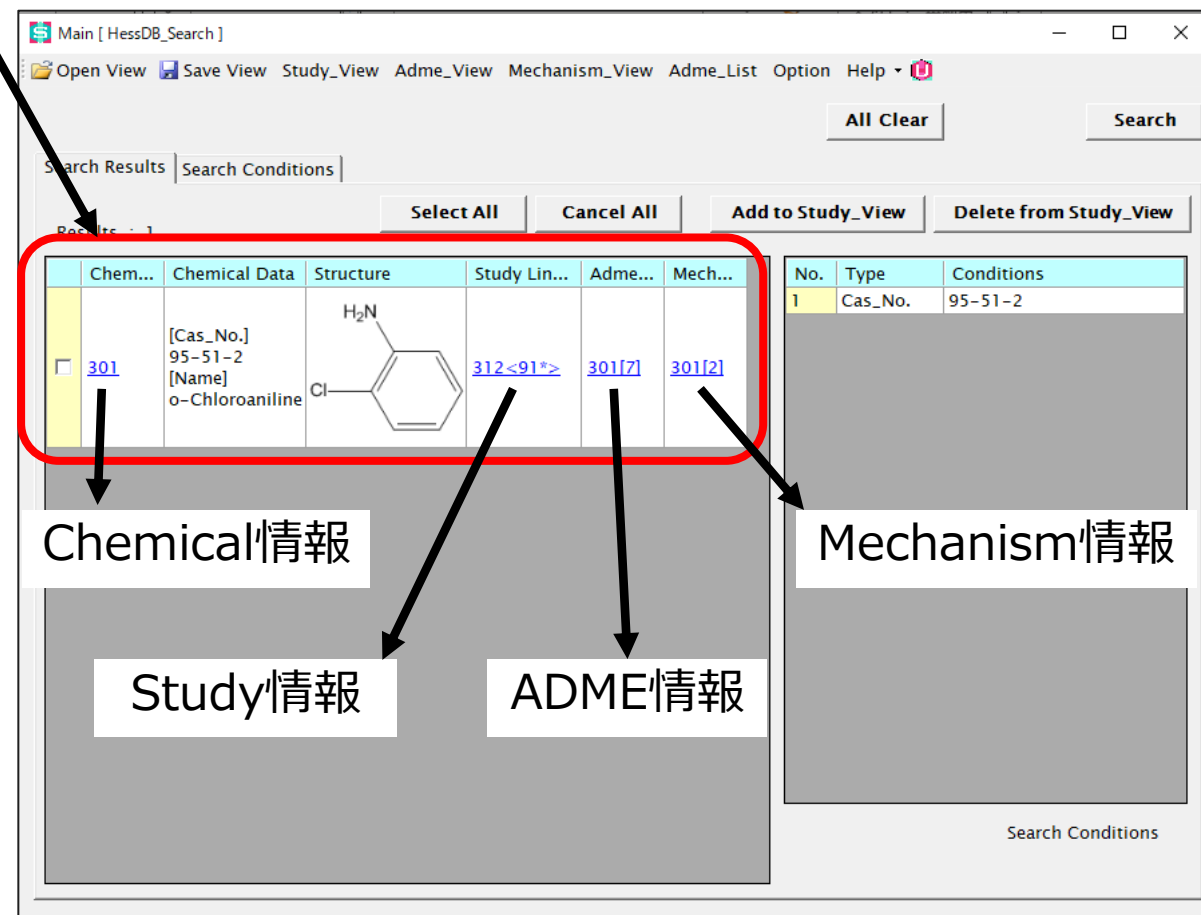
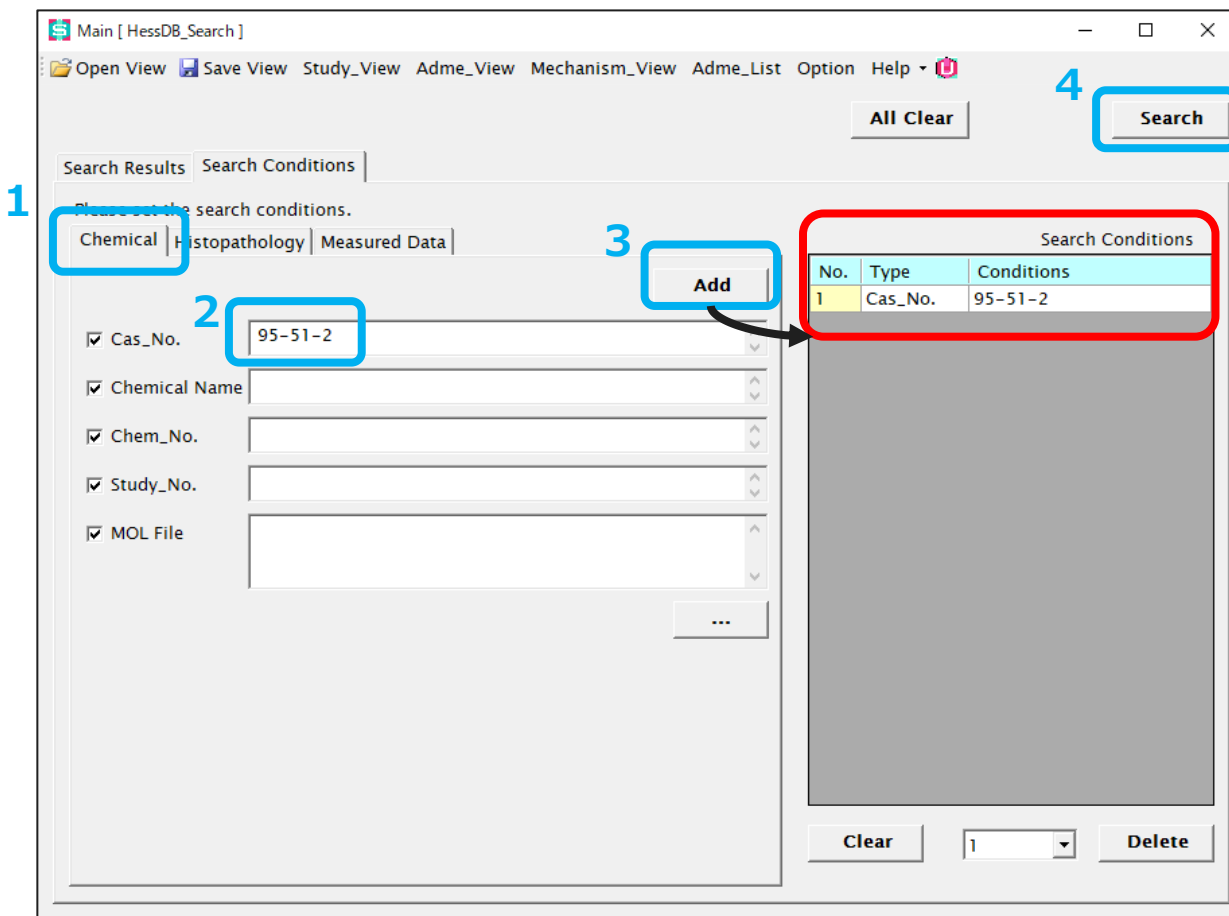
Results : 298

Select All Cancel All Add to Study_View Delete from Study_View

	Chem...	Chemical Data	Structure	Study Lin...	Adme...	Mech...
☐	1	[Cas_No.] 95-64-7 [Name] 3,4-Xylidine	<chem>Nc1ccc(C)c(C)c1</chem>	1<28>	1[7]	1[3]
☐	2	[Cas_No.] 100-61-8 [Name] N-methylaniline	<chem>CNc1ccccc1</chem>	2<28>	2[54]	2[3]
☐	6	[Cas_No.] 147-14-8 [Name] Copper, phthalocyaninat	<chem>Cu(C12C=CC3=C1N(C2)C4=CC=CC=C4N3)C5=CC=CC=C5</chem>	6<28*>		
☐	8	[Cas_No.] 88-53-9	<chem>Nc1ccc(S(=O)(=O)C)cc1</chem>	8<28>	8[1]	

Search Conditions

検索条件の入力(Cheical)



ChemicalとStudy情報

Chemical情報

Chemical [HessDB_Search]

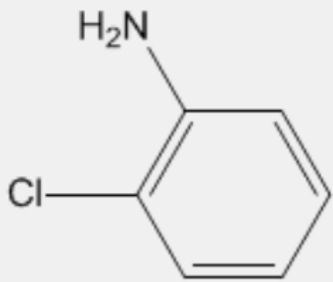
General Information

Chem_No.	301
CAS_No.	95-51-2
Name (CHRIP)	o-Chloroaniline
Name (EINECS)	2-chloroaniline
Name (TSCA)	Benzenamine, 2-chloro-
Name (OECD HPV)	Aniline, 2-chloro-
Synonym 1	2-Chlorobenzeneamine
Synonym 2	1-Amino-2-chlorobenzene
Usage	Intermediate raw materials for medicine and pesticide, resin
CSCL class	Priority assessment/ Existing/Type III Monitoring (before

Physical Chemical Properties

Molecular weight	127.57
Formula	C6H6ClN
Melting point (°C)	-1.94
Boiling point (°C)	208.84(decomposition)
Water solubility	8.76g/L (25°C)
Vapor pressure	0.034kPa (25°C)
Specific gravit/density	1.2114 (22/4°C)
logKow(est)	-
logKow(exp)	1.9

Structure



Study (Test result) 情報

Study [HessDB_Search]

Chem_No. 301 Chemical Data [Cas_No.] 95-51-2 [Name] o-Chloroaniline

Study Link ID 312<91*>

Test Result | Fig Summary | Test Method | Measured Data

	Male	Female
Hematology	Met-Hgb1: ≥10 HCT1: ≥80 HGB1: ≥40 RET1: ≥40 WBC1: ≥40 LYMPH1: ≥40 RBC1: ≥80 Plt1: ≥80 Nucleated erythrocyte1: 160 NEUT1: ≥80 Heinz1: 160	Met-Hgb1: ≥10 HCT1: ≥80 HGB1: ≥20 RET1: ≥20 WBC1: ≥20 LYMPH1: ≥20 RBC1: ≥20 Plt1: ≥20 Nucleated erythrocyte1: ≥80 NEUT1: ≥80 Heinz1: 160
Blood Chemistry	Bile acid1: ≥40	Bile acid1: 160
Absolute organ weight	Spleen1: ≥40	Spleen1: ≥40
Relative organ weight	Heart1: ≥20 Right kidney1: ≥80 Liver1: ≥80 Spleen1: ≥40	Heart1: 160 Liver1: 160 Spleen1: ≥40
Necropsy (Survival)	N/A	N/A
Necropsy (Dead)	-	-
Histopathology (Survival)	Liver-Kupffer cell, Hemosiderin: 160 Bone marrow-Erythroid cell, hyperplasia: ≥40 Spleen-Hematopoietic cell, proliferation: ≥80 Spleen-Capsule, fibrosis: ≥80 Spleen-Pigmentation, hemosiderin: 160	Liver-Kupffer cell, Hemosiderin: 160 Bone marrow-Erythroid cell, hyperplasia: ≥80 Spleen-Hematopoietic cell, proliferation: ≥80 Spleen-Capsule, fibrosis: ≥80 Spleen-Pigmentation, hemosiderin: ≥80

Descriptive Data

Clinical sign	FOB
Male:Tremors: ≥80 Female:Tremors: ≥80 Wasting: 160 Bluish discoloration of genital and footpad regions: ≥80	Male:- Female:-
Urinalysis	Body weight
Male:- Female:-	Male:1: 160 Female:N/A
Food consumption	Water consumption
Male:- Female:-	Male:- Female:-

Toxicological index

	NOEL	NOAEL	LOEL	LOAEL
Male	<10 mg/kg/day		10 mg/kg/day	
Female	<10 mg/kg/day		10 mg/kg/day	

Comment

Evaluated by toxicology experts in the NEDO project

Study情報

Study [HessDB_Search]

Chem.No. 301 Chemical Data [Cas.No.] 95-51-2 [Name] o-Chloroaniline

Test Result | **Flag Summary** | Test Method | Measured Data

Study Link ID 312<91*>

Hematology

Blood Chemistry

Absolute organ weight

Relative organ weight

Necropsy (Survive)

Necropsy (Dead)

Histopathology (S)

Histopathology (D)

Male

Female

[RBC]:A80 ▽ A160 ▽ [HCT(PCV)]:A80 ▽ A160 ▽ [HGB]:A40 ▽ A80 ▽ A160 ▽ [Met-Hgb]:A10 ▽ A20 ▽ A40 ▽ A80 ▽ A160 ▽ [Heinz]:A160 ▽ [WBC]:A40 ▽ A80 ▽ A160 ▽ [LEUCO%] SEG:A80 ▽ A160 ▽ [LEUCO%]LYMPH:A40 ▽ A80 ▽ A160 ▽ [RET]:A40 ▽ A80 ▽ A160 ▽ [Plt]:A80 ▽ A160 ▽ [Nucleated erythrocytes]:A160 ▽

[RBC]:A20 ▽ A40 ▽ A80 ▽ A160 ▽ [HCT(PCV)]:A80 ▽ A160 ▽ [HGB]:A20 ▽ A40 ▽ A80 ▽ A160 ▽ [Met-Hgb]:A10 ▽ A20 ▽ A40 ▽ A80 ▽ A160 ▽ [Heinz]:A160 ▽ [WBC]:A20 ▽ A40 ▽ A80 ▽ A160 ▽ [LEUCO%] SEG:A80 ▽ A160 ▽ [LEUCO%]LYMPH:A20 ▽ A40 ▽ A80 ▽ A160 ▽ [RET]:A20 ▽ A40 ▽ A80 ▽ A160 ▽ [Plt]:A20 ▽ A40 ▽ A80 ▽ A160 ▽ [Nucleated erythrocytes]:A80 ▽ A160 ▽

[Bile salts]:A40 ▽ A80 ▽ A160 ▽

[Bile salts]:A160 ▽

[Body Weight]:A160 ▽ [Spleen]:A40 ▽ A80 ▽ A160 ▽

[Spleen]:A40 ▽ A80 ▽ A160 ▽

[Liver]:A80 ▽ A160 ▽ [Kidneys]right:A80 ▽ A160 ▽ [Spleen]:A40 ▽ A80 ▽ A160 ▽

[Heart]:A160 ▽ [Liver]:A160 ▽ [Spleen]:A40 ▽ A80 ▽ A160 ▽

Study [HessDB_Search]

Chem.No. 301 Chemical Data [Cas.No.] 95-51-2 [Name] o-Chloroaniline

Test Result | **Test Method** | Measured Data

Study Link ID 312<91*>

Basic Information of study

Test Substance Information

Information of administration

Stability and homogeneity

Dose selection

Note

Others

Study No. 312 Study type Repeated dose oral toxicity test

GLP 21 CFR 58/FDA Test guideline No description

Administration period 93 Recovery period 0 Year reported 1998

Start (year) 1992 End (year) 1992 Test facility Battelle Columbus Laboratories

Test substance o-Chloroaniline

Manufacturer Aldrich Chemical Company (Milwaukee, WI) Color Colorless

Lot No. 04921TX Purity (%) ≥99 (by GC) External appearance Liquid

Impurities No description

Stability Stable for 13 weeks when stored in amber glass bottles sealed with Teflon-lined lids at room temperature. No decomposition of test substance under the conditioned employed.

Route (method) Oral (Gavage) Dose levels 0, 10, 20, 40, 80, 160 mg/kg

Frequency/Week 5 Dose volume(ml/kg) - Vehicle Dilute

Stability and homogeneity Stable for 35 days in 1 mg/ml solution when stored sealed in the dark at room temperature or at 5 °C. Stable for 3hours under simulated dosing condition.

Dose selection <Preliminary test> Selected based on literature values.

Note -

Statistical analysis

Williams test, Dunnett test, Shirley test, Dunn test, Jonckheere's test, Fisher exact test.

Note Comparative Toxicity Studies of o-, m-, and p-Chloroanilines (CAS

Study [HessDB_Search]

Chem.No. 301 Chemical Data [Cas.No.] 95-51-2 [Name] o-Chloroaniline

Test Result | Flag Summary | Test Method | **Measured Data**

Study Link ID 312<91*>

Test Item Hematology_Male Actual Comment

Significantly different from control group; *: P<0.05 **: P<0.01 In this study, SD indicates the standard error, but not the

DOSE	mg/kg	Admi...	mean	SD	s...	F1	F3	mean	SD	s...	F1	F3	mean	SD	s...
No. of animals	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10
RBC	10 ⁶ /μL	8.55	0.07	8.63	0.06	8.71	0.07	8.48	0.10						
HCT(PCV)	%	45.4	0.4	45.7	0.3	45.7	0.3	44.6	0.4						
HGB	g/dL	16.1	0.1	16.2	0.1	16.1	0.2	15.6	0.1	*					
MCV	fL	53.1	0.2	53.0	0.2	52.4	0.2	52.6	0.3						
MCH	pg	18.9	0.1	18.8	0.1	18.5	0.1	18.4	0.2						
MCHC	g/dL	35.5	0.2	35.6	0.2	35.2	0.2	34.9	0.3						
Met-Hgb	g/dL	0.30	0.02	0.40	0.02	0.59	0.04	0.84	0.04	**					
Heinz		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0						
WBC	10 ³ /μL	5.50	0.26	6.04	0.19	5.94	0.18	6.57	0.22	**					
LEUCO% NEUT															
LEUCO% STAB															
LEUCO% SEG	10 ³ /μL	1.09	0.10	1.34	0.12	1.32	0.09	1.26	0.12						
LEUCO% LYMPH	10 ³ /μL	4.25	0.19	4.60	0.17	4.49	0.23	5.19	0.23	**					
LEUCO% MONO	10 ³ /μL	0.06	0.01	0.06	0.02	0.05	0.01	0.07	0.02						
LEUCO% EOSN	10 ³ /μL	0.10	0.03	0.03	0.01	0.08	0.02	0.05	0.01						
LEUCO% BASO															
LEUCO% LUC															
LEUCO% OTHERS															
E-Blast															
RET	10 ⁶ /μL	0.16	0.01	0.15	0.02	0.19	0.01	0.21	0.02	*					
Plt	10 ³ /μL	738.5	7.2	745.6	11.5	718.7	13.5	778.6	12.2						
CT															
PT															

Penicillin (Eli Lilly)

Brothers, Inc.,

Gardners, PA)

Diet

Feeding ad libitum

Watering ad libitum

Link to Original

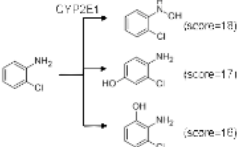
ADME情報

Adme_List [HessDB_Search]

Adme List | Adme Conditions **1**

Results : 7

Select All **Cancel All** **2 Add to Adme_View**

	Experiment ID	Chem_No.	Cas_No.	Substance	Keyword	Referenced figures and tables	Adme Link ID
☒	301-00-00-01	301	95-51-2	o-chloroaniline	in silico prediction, Human		301
☒	301-06-04-01	301	95-51-2	o-Chloroaniline (o-CA)	in vivo, Rat		301
☒	301-06-04-02	301	95-51-2	o-Chloroaniline (o-CA)	in vivo, Mouse		301
☒	301-06-04-03	301	95-51-2	m-chloroaniline (m-CA)	in vivo, Rat		301

Adme_View [HessDB_Search]

Delete selected columns

Format Set

Adme Link ID			301	301
Chem_No.			301	301
keyword			in silico prediction, Human	in vivo, Rat
Reference	ID		301-00-00	301-06-04
Reference	Author		Y.Yamazoe, K. Ito, K. Yoshinari	M. R. Hejtmancik, B. A. Tre- Ryan, J. T. Yarrington, R. S.
Reference	Journal		Drug Metabolism Reviews	Toxicological Sciences
Reference	Volume		43	69
Reference	Number		4	
Reference	Pages		409-439	234-243
Reference	Publication year		2011	2002
Reference	Title		Construction of a CYP2E1-template system for prediction of the metabolism on both site and preference order	Comparative Gavage Subcl o-Chloroaniline and m-Cl B6C3F1 Mice
Reference	Language		English	English
Reference	PubMed_Author			
Reference	PubMed_Journal			
Reference	PubMed_Volume			
Reference	PubMed_Number			
Reference	PubMed_Page			
Reference	PubMed_Public year			
Reference	PubMed_Title			
Reference	PubMed_ID		22017508	12215679
Reference	PubMed_Doi		10.3109/03602532.2011.624103	
Reference	PubMed_Pii			
Experiment	Experiment ID		301-00-00-01	301-06-04-01

Mechanism情報

Mechanism_List [HessDB_Search]

Chem_No. 301

Chemical Data [Cas_No.] 95-51-2 [Name] o-Chloroaniline

Summary of Mechanistic Information

Mechanism_List

Link Data : 2

	viewID	Reference	Key Words	Summary
☐	301-1	Nomura A. Studies on sulfhemoglobin formation by various drugs (1). Folia Pharmacol Jap. 1975; May;71(4): 351-365. PMID: 1237450	Erythrocyte; Met-Hb formation; in vivo	Met-Hb and sulfhemoglobin formations were induced by administration of 2-chloroaniline to mice. Maximum plasma concentration time of Met-Hb was 30 min, and Met-Hb was almost completely eliminated at 1 h after a
☐	301-2	Sabbioni G. Hemoglobin binding of monocyclic aromatic amines: Molecular dosimetry and quantitative structure activity relationships for the N-oxidation. Chem Biol	Erythrocyte; Covalent binding to hemoglobin; in vivo	Hemoglobin adducts were observed after administration of 2-chloroaniline to rats. The hemoglobin binding index was 0.5 ± 0.1 .

Select All Cancel All Add to Mechanism_View

Chemical structure of o-chloroaniline: Nc1ccccc1Cl

Summary of Mechanistic Information [HessDB_Search]

1 / 3 Aniline-induced hemolytic effects

Summary

Repeated administration of aniline and its derivatives including some alkyl-, chloro-, alkoxy- and N-alkyl-anilines causes hemolysis as a critical effect in most of cases. These are bioactivated to the corresponding N-hydroxylated metabolites. The reactive metabolites oxidize hemoglobin in red blood cells, resulting in formation of methemoglobin (Met-Hb) accompanied by generation of reactive oxygen species (ROS). ROS appear to be responsible for damaging red blood cells. However, effects of size, number and location of the substituted groups of aniline derivatives on bioactivation seem to be complicated by the presence of multiple enzymes for metabolic activation. Hence *in vivo* indicators such as formation of Met-Hb and hemoglobin adducts may be of assistance to screen candidate aniline derivatives that might cause hemolysis via the pathway. Moreover, chemicals that form hemolytic anilines through endogenous metabolism cause hemolytic effects.

Hemolytic pathway induced by aniline

In rats, aniline is metabolized through N-hydroxylation in the liver to produce phenylhydroxylamine (PHA), one of the aniline metabolites (Blaauboer and Van Holstein, 1983; Harrison and Jollow, 1987). PHA, which is interconvertible with o-chloroaniline, is metabolized to o-chlorophenylhydroxylamine (OCPHA) and o-chlorophenylhydroxylamine (OCPHA) is metabolized to o-chlorophenylhydroxylamine (OCPHA).

Mechanism_View [HessDB_Search]

Delete selected columns Format Set

	Chem_No.	301	301
ViewID	301-1	301-2	
CAS_No.	95-51-2	95-51-2	
Chemical Name	o-Chloroaniline; 2-Chloroaniline	o-Chloroaniline; 2-Chloroaniline	
Structure	<chem>Nc1ccccc1Cl</chem>	<chem>Nc1ccccc1Cl</chem>	
Reference	Nomura A. Studies on sulfhemoglobin formation by various drugs (1). Folia Pharmacol Jap. 1975; May;71(4): 351-365. PMID: 1237450	Sabbioni G. Hemoglobin binding of monocyclic aromatic amines: Molecular dosimetry and quantitative structure activity relationships for the N-oxidation. Chem Biol Interact. 1992; Jan;81 (1-2): 91-118. PMID: 1730150	
Key Words	Erythrocyte; Met-Hb formation; in vivo	Erythrocyte; Covalent binding to hemoglobin; in vivo	
Summary	Met-Hb and sulfhemoglobin formations were induced by administration of 2-chloroaniline to mice. Maximum plasma concentration time of Met-Hb was 30 min, and Met-Hb was almost completely eliminated at 1 h after a single administration. Sulfhemoglobin was detected after consecutive administration for 3 days but not after a single administration.	Hemoglobin adducts were observed after administration of 2-chloroaniline to rats. The hemoglobin binding index was 0.5 ± 0.1 .	
Possible Chemical Reaction/ Metabolism			
Possible Toxicant			
Possible Interaction with Bio-molecule		Covalent binding to hemoglobin	
Effects	Met-Hb formation; Sulfhemoglobin formation		
Target Cell/ Tissue/ Organ etc.	Erythrocytes	Erythrocytes	
Cell line/ Species	Male ddY mice (25-30 g, 6-7 weeks old)	Female Wistar rats (200-225 g)	
Experimental Design	Levels of Met-Hb and sulfhemoglobin were examined in mice given 2-chloroaniline intraperitoneally for 1 or 3 days.	Rats were given 2-chloroaniline by gavage. Twenty-four hours after dosing, blood was collected and the released arylamines were measured after hydrolysis of hemoglobin adduct to calculate hemoglobin binding index.	
in vitro/ in vivo/ ex vivo	In vivo	In vivo	

HESS DBの入手方法と使い方マニュアル

The screenshot shows the NITE website's interface for HESS DB user registration. The top navigation bar includes links for 'Home', 'About NITE', 'Services', 'Contact', and 'English'. The main content area is titled '有害性評価支援システム統合プラットフォーム (HESS) 及び HESS DBのユーザー登録' (User Registration for HESS and HESS DB). Below the title, there is a section for 'HESSの使用許諾契約書' (Terms of Use for HESS) with a list of 9 points. The sidebar on the right contains links to '動物実験代替法 (QSAR, Read-across, IATA)', '有害性評価支援システム統合プラットフォーム (HESS)', 'OECD QSAR Toolbox', '事業者支援', '動物実験代替法についての国際動向 (OECD等)', '動画講習/学習教材サイト', 'QSAR, Read-across, IATAに関する用語集・リンク集', '外部発表', '過去の活動', and '分野サイトマップ'.

NITEのHPからユーザー登録

http://www.nite.go.jp/chem/qsar/hess_01.html
(検索キーワード“NITE”, “HESS”)



登録メールアドレスにHESS及びHESS DBダウンロードURLページが記載されたメールが送付される。



HESS及びHESS DBのインストールファイル一式を無料でダウンロード！

詳細な使い方マニュアルは、ダウンロードファイル内の以下の資料をご確認下さい。
HessDB instructions (日本語版) Feb 2020.pdf