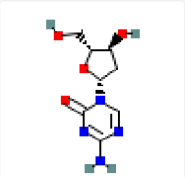
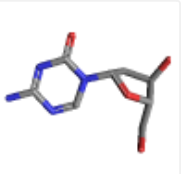
PubChem

COMPOUND SUMMARY

Decitabine

PubChem CID	451668
Structure	 2D  3D Find Similar Structures
Chemical Safety	 Irritant Health Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_8H_{12}N_4O_4$
Synonyms	Decitabine 5-Aza-2'-deoxycytidine 2353-33-5 Dacogen 2'-Deoxy-5-azacytidine More...
Molecular Weight	228.21
Dates	Modify 2022-08-06 Create 2005-08-01

Decitabine is a cytosine analogue and an intravenously administered antineoplastic agent used in the therapy of myelodysplastic syndromes. Decitabine is associated with a low rate of transient serum enzyme elevations during therapy, but has not been implicated in causing clinically apparent liver injury with jaundice.

▸ LiverTox

Decitabine is a cytidine antimetabolite analogue with potential antineoplastic activity. Decitabine incorporates into DNA and inhibits DNA methyltransferase, resulting in hypomethylation of DNA and intra-S-phase arrest of DNA replication. (NCI04)

▸ NCI Thesaurus (NCIt)

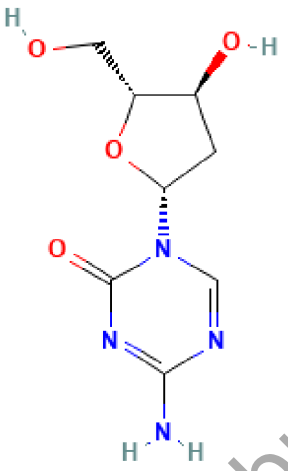
Myelodysplastic syndromes (MDS) are a heterogeneous group of hematopoietic neoplasms with variable underlying etiology and presentation, including neutropenia and thrombocytopenia. Further mutations leading to increased proliferation of cancerous cells can eventually lead to secondary acute myeloid leukemia, which has a poor prognosis. Among treatment options, nucleoside analogues such as decitabine and [azacitidine] integrate into cellular DNA and inhibit the action of DNA methyltransferases, leading to global hypomethylation and related downstream therapeutic benefits. Decitabine was developed by MGI Pharma/SuperGen Inc. and was approved by the FDA for the treatment of MDS on February 5, 2006. It was first marketed under the name Dacogen®. It is also available as an oral combination product together with the cytidine deaminase inhibitor [cedazuridine].

▸ DrugBank

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Conformer

PubChem

2 Biologic Description

IUPAC Condensed	z5Cyt-dRibf
Sequence	N
HELM	RNA1{[dR]([*n1cnc(nc1=O)N |$_R1;;;;;;;;$|])}$$$$
IUPAC	2'-deoxy-5-aza-cytidine

PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

4-amino-1-[(2*R*,4*S*,5*R*)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,3,5-triazin-2-one

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

3.1.2 InChI

InChI=1S/C8H12N4O4/c9-7-10-3-12(8(15)11-7)6-1-4(14)5(2-13)16-6/h3-6,13-14H,1-2H2,(H2,9,11,15)/t4-,5+,6+/m0/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.3 InChIKey

XAUDJQYHKZQPEU-KVQBGUIXSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.4 Canonical SMILES

C1C(C(OC1N2C=NC(=NC2=O)N)CO)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

3.1.5 Isomeric SMILES

C1[C@@H]([C@H](O[C@H]1N2C=NC(=NC2=O)N)CO)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

3.2 Molecular Formula

C8H12N4O4

CAMEO Chemicals; PubChem

3.3 Other Identifiers

3.3.1 CAS

2353-33-5

CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DrugBank; EPA DSSTox; European Chemicals Agency (ECHA); Human Metabolome Database (HMDB)

22432-95-7

European Chemicals Agency (ECHA)

3.3.2 Deprecated CAS

123795-43-7, 105597-46-4

ChemIDplus

3.3.3 European Community (EC) Number

219-089-4

European Chemicals Agency (ECHA)

815-973-4

European Chemicals Agency (ECHA)

3.3.4 UNII

776B62CQ27

FDA/SPL Indexing Data

3.3.5 DSSTox Substance ID

DTXSID7030432

EPA DSSTox

3.3.6 Wikidata

Q1181878

Wikidata

3.3.7 NCI Thesaurus Code

C981

NCI Thesaurus (NCIt)

3.3.8 RXCUI

15657

NLM RxNorm Terminology

3.4 Synonyms

3.4.1 MeSH Entry Terms

2' Deoxy 5 azacytidine	decitabine
2'-deoxy-5-azacytidine	decitabine mesylate
5 Aza 2' deoxycytidine	Mesylate, Decitabine

5 Azadeoxycytidine	NSC 127716
5 Deoxyazacytidine	NSC-127716
5-aza-2'-deoxycytidine	NSC127716
5-AzadC	
5-azadeoxycytidine	
5-deoxyazacytidine	
5AzadC	
AzadC compound	
Compound, AzadC	
Dacogen	

Medical Subject Headings (MeSH)

3.4.2 Depositor-Supplied Synonyms

Decitabine	Alpha-Decitibine	MFCD00043011
5-Aza-2'-deoxycytidine	4-amino-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-1,3,5-triazin-2(1H)-one	776B62CQ27
2353-33-5	4-amino-1-[(2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,3,5-triazin-2-one	SMR000857076
Dacogen	UNII-776B62CQ27	4-Amino-1-(2-deoxy-beta-D
2'-Deoxy-5-azacytidine	5A2dc	4-amino-1-[(2S,4S,5R)-4-hyc
5-Azadeoxycytidine	5-aza-2-deoxycytidine	DSSTox_CID_10432
AzadC	NSC-127716	DSSTox_RID_78849
5-aza-CdR	4-Amino-1-(2-deoxy-beta-D-erythro-pentofuranosyl)-s-triazin-2(1H)-one	DSSTox_GSID_30432
5-aza-dC	4-Amino-1-(2-deoxy-beta-D-erythro-pentofuranosyl)-1,3,5-triazin-2(1H)-one	4-amino-1-[(2R,4S,5R)-4-hyc
Dezocitidine	MLS001332587	5-AZAdC
NSC 127716	C8H12N4O4	NSC127716
Dac	CHEBI:50131	2-deoxyazacytidine

PubChem

4 Chemical and Physical Properties

4.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	228.21	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	-1.2	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	228.08585488	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	228.08585488	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	121 Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	16	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	356	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	3	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

PubChem

4.2 Experimental Properties

4.2.1 Physical Description

5-aza-2'-deoxycytidine is a fine white crystalline powder. Used as a drug.

CAMEO Chemicals

Solid

Human Metabolome Database (HMDB)

4.2.2 Melting Point

193-196

SignalChem Product Sheet

DrugBank

4.2.3 Solubility

11 mg/mL

SignalChem Product Sheet

DrugBank

5.50e+00 g/L

Human Metabolome Database (HMDB)

4.2.4 LogP

-1.89 (LogP)

DAYLIGHT (1999)

EPA DSSTox

5 Spectral Information

5.1 IR Spectra

5.1.1 ATR-IR Spectra

Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Forensic Spectral Research
Source of Sample	Sigma-Aldrich Company Llc
Catalog Number	A3656
Lot Number	082K1003
Copyright	Copyright © 2014-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5.2 Raman Spectra

Technique	FT-Raman
Source of Spectrum	Forensic Spectral Research
Source of Sample	Sigma-Aldrich Company Llc.
Catalog Number	A-3656
Lot Number	082K1003
Copyright	Copyright © 2015-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

6 Related Records

6.1 Related Compounds with Annotation

PubChem

6.2 Related Compounds

Same Connectivity	31 Records
Same Stereo	8 Records
Same Isotope	20 Records
Same Parent, Connectivity	54 Records
Same Parent, Stereo	27 Records
Same Parent, Isotope	43 Records
Same Parent, Exact	20 Records
Mixtures, Components, and Neutralized Forms	95 Records
Similar Compounds	278 Records
Similar Conformers	4,983 Records

PubChem

6.3 Substances

6.3.1 Related Substances

All	342 Records
Same	212 Records
Mixture	130 Records

PubChem

6.3.2 Substances by Category

PubChem

6.4 Entrez Crosslinks

PubMed	3,050 Records
Taxonomy	7 Records
OMIM	48 Records
Gene	2,297 Records

PubChem

6.5 NCBI LinkOut

NCBI

7 Chemical Vendors

PubChem

8 Drug and Medication Information

8.1 Drug Indication

Showing 3 of 4 View More

Decitabine is indicated for the treatment of patients with myelodysplastic syndromes (MDS) including all French-American-British subtypes (refractory anemia, refractory anemia with ringed sideroblasts, refractory anemia with excess blasts, refractory anemia with excess blasts in transformation, and chronic myelomonocytic leukemia), as well as for MDS scored as belonging to the intermediate-1, intermediate-2, or high-risk group in the International Prognostic Scoring System.

- DrugBank

FDA Label

- DrugBank

Treatment of adult patients with newly diagnosed de novo or secondary acute myeloid leukaemia (AML), according to the World Health Organization (WHO) classification, who are not candidates for standard induction chemotherapy.

- European Medicines Agency (EMA)

8.2 LiverTox Summary

Decitabine is a cytosine analogue and an intravenously administered antineoplastic agent used in the therapy of myelodysplastic syndromes. Decitabine is associated with a low rate of transient serum enzyme elevations during therapy, but has not been implicated in causing clinically apparent liver injury with jaundice.

- LiverTox

8.3 Drug Classes

Antineoplastic Agents

- LiverTox

8.4 FDA Orange Book

- FDA Orange Book

8.5 FDA National Drug Code Directory

▸ National Drug Code (NDC) Directory

DECITABINE is an active ingredient in 3 products including: DACOGEN, DECITABINE, and INQOVI.

▸ National Drug Code (NDC) Directory

8.6 Drug Labels for Ingredients

Label Information	Total 30 labels
Drug Ingredient	DECITABINE
NDC Code(s)	0781-3296-80, 16714-749-01, 16714-928-01, 16729-224-05, 25021-231-20, 43598-348-37, 43598-427-37, 47335-361-41, 47335-362-40, 50742-430-01 ... total 33
Packagers	Accord Healthcare Inc.; Amneal Pharmaceuticals LLC; Athenex Pharmaceutical Division, LLC.; AuroMedics Pharma LLC; BluePoint Laboratories; Cipla USA Inc.; Dr. Reddy's Laboratories Inc.; Dr.Reddy's Laboratories Limited; Fresenius Kabi USA, LLC; Gland Pharma Limited; Ingenus Pharmaceuticals, LLC; Lupin Pharmaceuticals, Inc.; MSN LABORATORIES PRIVATE LIMITED; Meitheal Pharmaceuticals Inc.; Mylan Institutional LLC; Nivagen Pharmaceuticals, Inc.; NorthStar RxLLC; Northstar Rx LLC; Novadoz Pharmaceuticals LLC; Otsuka America Pharmaceutical, Inc.; Qilu Pharmaceutical Co., Ltd.; Sagent Pharmaceuticals; Sandoz Inc; Sun Pharmaceutical Industries, Inc.; Taiho Pharmaceutical Co., Ltd.; Wockhardt USA LLC.

▸ DailyMed

Label Title	INQOVI- cedazuridine and decitabine tablet, film coated
Drug Ingredient	CEDAZURIDINE; DECITABINE
Label Image	

Label Download	PDF Label
NDC Code(s)	64842-0727-9
Packager	Taiho Pharmaceutical Co., Ltd.

DailyMed

8.7 Clinical Trials

8.7.1 ClinicalTrials.gov

ClinicalTrials.gov

8.7.2 EU Clinical Trials Register

EU Clinical Trials Register

8.7.3 NIPH Clinical Trials Search of Japan

NIPH Clinical Trials Search of Japan

8.8 EMA Drug Information

Medicine	Dacogen
Therapeutic area	Leukemia, Myeloid
Active Substance	Decitabine
INN/Common name	decitabine
Pharmacotherapeutic Classes	Antineoplastic agents
Status	This medicine is authorized for use in the European Union
Company	Janssen-Cilag International N.V.
Market Date	2012-09-20

European Medicines Agency (EMA)

9 Pharmacology and Biochemistry

9.1 Pharmacodynamics

Decitabine is a prodrug analogue of the natural nucleotide 2'-deoxycytidine, which, upon being phosphorylated intracellularly, is incorporated into DNA and exerts numerous effects on gene expression. The use of decitabine is associated with neutropenia and thrombocytopenia. In addition, decitabine can cause fetal harm in pregnant women; effective contraception and avoidance of pregnancy are recommended during treatment with decitabine.

▸ DrugBank

9.2 MeSH Pharmacological Classification

Enzyme Inhibitors

Compounds or agents that combine with an enzyme in such a manner as to prevent the normal substrate-enzyme combination and the catalytic reaction. (See all compounds classified as Enzyme Inhibitors.)

▸ Medical Subject Headings (MeSH)

Antimetabolites, Antineoplastic

Antimetabolites that are useful in cancer chemotherapy. (See all compounds classified as Antimetabolites, Antineoplastic.)

▸ Medical Subject Headings (MeSH)

9.3 FDA Pharmacological Classification

FDA UNII	776B62CQ27
Active Moiety	DECITABINE
Pharmacological Classes	Mechanisms of Action [MoA] - Nucleic Acid Synthesis Inhibitors
Pharmacological Classes	Established Pharmacologic Class [EPC] - Nucleoside Metabolic Inhibitor
FDA Pharmacology Summary	Decitabine is a Nucleoside Metabolic Inhibitor. The mechanism of action of decitabine is as a Nucleic Acid Synthesis Inhibitor.

▸ FDA Pharm Classes

Non-Proprietary Name	DECITABINE
Pharmacological Classes	Nucleoside Metabolic Inhibitor [EPC]; Nucleic Acid Synthesis Inhibitors [MoA]

▸ National Drug Code (NDC) Directory

9.4 ATC Code

L01BC08

▸ European Medicines Agency (EMA); NORMAN Suspect List Exchange

L - Antineoplastic and immunomodulating agents

L01 - Antineoplastic agents

L01B - Antimetabolites

L01BC - Pyrimidine analogues

L01BC08 - Decitabine

▸ WHO Anatomical Therapeutic Chemical (ATC) Classification

9.5 Absorption, Distribution and Excretion

Absorption

Decitabine administered intravenously at 15 mg/m^2 for three hours every eight hours over three days resulted in a C_{max} of 73.8 ng/mL (66% coefficient of variation, CV), an $AUC_{0-\infty}$ of 163 ng*h/mL (62% CV), and a cumulative AUC of 1332 ng*h/mL (95% CI of 1010-1730). Similarly, decitabine at 20 mg/m^2 for one hour once daily over five days resulted in a C_{max} of 147 ng/mL (49% CV), an $AUC_{0-\infty}$ of 115 ng*h/mL (43% CV), and a cumulative AUC of 570 ng*h/mL (95% CI of 470-700).

- DrugBank

Route of Elimination

Less than 1% of administered decitabine is excreted in the urine.

- DrugBank

Volume of Distribution

Decitabine as an apparent volume of distribution of 4.59 ± 1.42 L/kg.

- DrugBank

Clearance

Decitabine has a clearance of 125 L/hr/m^2 (53% CV) when administered intravenously at 15 mg/m^2 for three hours every eight hours over three days, and a clearance of 210 L/hr/m^2 (47% CV) at 20 mg/m^2 for one hour once daily over five days.

- DrugBank

9.6 Metabolism/Metabolites

Decitabine is phosphorylated inside cells by the sequential action of **deoxycytidine** kinase, nucleotide monophosphate kinase, and nucleotide diphosphate kinase, prior to being incorporated into newly synthesized DNA by DNA polymerase. Decitabine not incorporated into cellular DNA undergoes deamination by **cytidine** deaminase followed by additional degradation prior to excretion.

- DrugBank

9.7 Biological Half-Life

Decitabine has a half-life of 0.62 hours (49% CV) when administered intravenously at 15 mg/m^2 for three hours every eight hours over three days, and a half-life of 0.54 hours (43% CV) at 20 mg/m^2 for one hour once daily over five days.

- DrugBank

9.8 Mechanism of Action

Myelodysplastic syndromes (MDS) are a group of hematopoietic neoplasms that manifest in peripheral cytopenias and may eventually progress to secondary acute myeloid leukemia (sAML). Included in the over 45 genes commonly mutated in MDS patients are those involved in DNA methylation and histone modification, and it is well-established that alteration of the epigenetic landscape is a feature of myeloid leukemias. Decitabine is considered a prodrug, as it requires transport into cells and subsequent phosphorylation by distinct kinases to generate the active molecule 5-aza-2'-deoxycytidine-triphosphate, which is incorporated by DNA polymerase during DNA replication. Once incorporated into DNA, decitabine is recognized as a substrate by DNA methyltransferase enzymes (DNMTs), specifically DNMT1, but due to the presence of an N5 rather than C5 atom, traps the DNMT through the irreversible formation of a covalent bond. At low concentrations, this mode of action depletes DNMTs and results in global DNA hypomethylation while at high concentrations, it additionally results in double-strand breaks and cell death. The general hypothesis regarding decitabine's therapeutic efficacy is that the global hypomethylation it induces results in the expression of previously silent tumour suppressor genes. However, there are other putative mechanisms also related to this change in DNA methylation, including indirect alteration of transcription through effects on transcription factors, indirectly altering

histone modifications and chromatin structure, and activating pathways involved in DNA damage response. The overall effect of decitabine is a decrease in neoplastic cell proliferation and an increase in the expression of tumour suppressor genes.

- DrugBank

9.9 Human Metabolite Information

9.9.1 Cellular Locations

Cytoplasm

- Human Metabolome Database (HMDB)

9.10 Biochemical Reactions

- PubChem

10 Use and Manufacturing

10.1 Uses

10.1.1 Use Classification

Human drugs -> Orphan -> Dacogen -> EMA Drug Category

- European Medicines Agency (EMA)

Antineoplastic agents -> Human pharmacotherapeutic group

- European Medicines Agency (EMA)

Human Drugs -> FDA Approved Drug Products with Therapeutic Equivalence Evaluations (Orange Book) -> Active Ingredients

- FDA Orange Book

11 Safety and Hazards

11.1 Hazards Identification

11.1.1 GHS Classification

Showing 1 of 2 View More

Pictogram(s)	 Irritant Health Hazard
Signal	Danger
GHS Hazard Statements	H302 (93.33%): Harmful if swallowed [**Warning** Acute toxicity, oral] H315 (93.33%): Causes skin irritation [**Warning** Skin corrosion/irritation] H319 (93.33%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H335 (93.33%): May cause respiratory irritation [**Warning** Specific target organ toxicity, single exposure; Respiratory tract irritation] H341 (93.33%): Suspected of causing genetic defects [**Warning** Germ cell mutagenicity] H360 (93.33%): May damage fertility or the unborn child [**Danger** Reproductive toxicity]
Precautionary Statement Codes	P203, P261, P264, P264+P265, P270, P271, P280, P281, P301+P317, P302+P352, P304+P340, P305+P351+P338, P318, P319, P321, P330, P332+P317, P337+P317, P362+P364, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 45 companies from 6 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)

11.1.2 Hazard Classes and Categories

Acute Tox. 4 (93.33%)

Skin Irrit. 2 (93.33%)

Eye Irrit. 2 (93.33%)

STOT SE 3 (93.33%)

Muta. 2 (93.33%)

Repr. 1B (93.33%)

▸ European Chemicals Agency (ECHA)

Acute Tox. 4 (100%)

Carc. 1B (100%)

▸ European Chemicals Agency (ECHA)

11.1.3 Fire Hazards

Flash point data for this chemical are not available. It is probably combustible. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

11.2 First Aid Measures

11.2.1 First Aid

EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with **water** or **normal saline** solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop. SKIN: IMMEDIATELY flood affected skin with **water** while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and **water**. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment. INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. IMMEDIATELY call a physician and be prepared to transport the victim to a hospital even if no symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing. INGESTION: If the victim is conscious and not convulsing, give 1 or 2 glasses of **water** to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Generally, the induction of vomiting is NOT recommended outside of a physician's care due to the risk of aspirating the chemical into the victim's lungs. However, if the victim is conscious and not convulsing and if medical help is not readily available, consider the risk of inducing vomiting because of the high toxicity of the chemical ingested. Ipecac syrup or salt **water** may be used in such an emergency. IMMEDIATELY transport the victim to a hospital. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

11.3 Fire Fighting

Fires involving this material can be controlled with a dry chemical, **carbon dioxide** or **Halon** extinguisher. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

11.4 Handling and Storage

11.4.1 Nonfire Spill Response

SMALL SPILLS AND LEAKAGE: If you spill this chemical, you should dampen the solid spill material with **water**, then transfer the dampened material to a suitable container. Use absorbent paper dampened with **water** to pick up any remaining material. Seal your contaminated clothing and the absorbent paper in a vapor-tight plastic bag for eventual disposal. Wash all contaminated surfaces with a soap and **water** solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned. STORAGE PRECAUTIONS: You should protect this chemical from exposure to light. Keep the container tightly closed under an inert atmosphere, and store it in a freezer. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

11.5 Exposure Control and Personal Protection

11.5.1 Personal Protective Equipment (PPE)

RECOMMENDED RESPIRATOR: Where the neat test chemical is weighed and diluted, wear a NIOSH-approved half face respirator equipped with a combination filter cartridge, i.e. organic vapor/acid gas/HEPA (specific for organic vapors, HCl, acid gas, SO2 and a high efficiency particulate filter). (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

11.6 Stability and Reactivity

11.6.1 Air and Water Reactions

Probably light and air sensitive. Water soluble. Decomposes in aqueous solution at a rate that depends on pH: at pH 7 the drug is more stable than at pH 9, but is less stable than at pH 6. At pH 7 and 99°F, approximately 7% conversion occurs in 1 hour (NTP, 1992).

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

11.6.2 Reactive Group

Alcohols and Polyols

Amides and Imides

Amines, Phosphines, and Pyridines

CAMEO Chemicals

11.6.3 Reactivity Profile

5-AZA-2'-DEOXYCYTIDINE is an organic compound with both amine and alcohol substituents. Amines are chemical bases. They neutralize acids to form salts plus water. These acid-base reactions are exothermic. The amount of heat that is evolved per mole of amine in a neutralization is largely independent of the strength of the amine as a base. Amines may be incompatible with isocyanates, halogenated organics, peroxides, phenols (acidic), epoxides, anhydrides, and acid halides. Flammable gaseous hydrogen is generated by amines in combination with strong reducing agents, such as hydrides.

CAMEO Chemicals

12 Toxicity

12.1 Toxicological Information

12.1.1 Toxicity Summary

Decitabine has demonstrated mutagenic potential in L5178Y mouse lymphoma cells and an _Escherichia coil lac-I_ transgene within the colonic DNA of mice. Decitabine treatment increased chromosomal rearrangements in fruit fly larvae. In mouse models, decitabine exposure _in utero_ (approximately 7% of the recommended daily dose) resulted in decreased weight and decreased male fertility. Adult male mice administered with between 0.3 and 1% of the recommended daily dose of decitabine three times a week for seven weeks had smaller testes with abnormal histology, decreased sperm count, and decreased fertility. There is no known antidote for decitabine overdose. Patients experiencing an overdose are at an increased risk of severe adverse effects such as myelosuppression, including prolonged and severe neutropenia and thrombocytopenia. Symptomatic and supportive measures are recommended.

▶ DrugBank

12.1.2 Hepatotoxicity

In early clinical trials using high doses of decitabine, serum enzyme elevations occurred in up to 16% of patients with underlying liver disease or liver metastases, but rarely in persons without hepatic illness. In subsequent studies, serum ALT elevations were reported in 5% to 15% of treated patients, but all were self-limited and no clinically apparent liver injury was reported. Recent studies have reported elevations in serum **bilirubin** levels in 7% to 12% of treated patients, but the elevations resolved rapidly and were not associated with other clinical or laboratory evidence of liver injury. Monitoring of serum enzyme levels during treatment is recommended only in patients with concurrent liver disease.

Likelihood score: E* (unproven but suspected, rare cause of clinically apparent liver injury).

▶ LiverTox

12.1.3 Drug Induced Liver Injury

Compound	decitabine
DILI Annotation	Ambiguous DILI-concern
Severity Grade	4
Label Section	Adverse reactions
References	M Chen, V Vijay, Q Shi, Z Liu, H Fang, W Tong. FDA-Approved Drug Labeling for the Study of Drug-Induced Liver Injury, Drug Discovery Today, 16(15-16):697-703, 2011. PMID:21624500 DOI:10.1016/j.drudis.2011.05.007 M Chen, A Suzuki, S Thakkar, K Yu, C Hu, W Tong. DILIrank: the largest reference drug list ranked by the risk for developing drug-induced liver injury in humans. Drug Discov Today 2016, 21(4): 648-653. PMID:26948801 DOI:10.1016/j.drudis.2016.02.015

▶ Drug Induced Liver Injury Rank (DILIrank) Dataset

12.1.4 Acute Effects

ChemIDplus

12.1.5 Protein Binding

Decitabine exhibits negligible (< 1%) plasma protein binding.

DrugBank

13 Associated Disorders and Diseases

- Comparative Toxicogenomics Database (CTD)

14 Literature

14.1 Coronavirus Studies

PubChem

14.2 NLM Curated PubMed Citations

PubChem

14.3 Springer Nature References

Springer Nature

14.4 Thieme References

Thieme Chemistry

14.5 Depositor Provided PubMed Citations

PubChem

14.6 Synthesis References

Julian Paul Henschke, Xiaoheng Zhang, Jianbo Yu, Kun Hu, Lijun Mei, "Synthesis of Decitabine." U.S. Patent US20100087637, issued April 08, 2010.

DrugBank

14.7 Metabolite References

Human Metabolome Database (HMDB)

14.8 General References

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3. Daskalakis M, Blagitko-Dorfs N, Hackanson B: Decitabine. Recent Results Cancer Res. 2010;184:131-57. doi: 10.1007/978-3-642-01222-8_10. [PMID:20072836]
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11. FDA Approved Drug Products: decitabine for injection
12. Cayman Chemical: decitabine MSDS
13. SignalChem decitabine product sheet

DrugBank

14.9 Chemical Co-Occurrences in Literature

PubChem

14.10 Chemical-Gene Co-Occurrences in Literature

PubChem

14.11 Chemical-Disease Co-Occurrences in Literature

PubChem

15 Patents

US8618075
US8268800
US9567363

DrugBank

15.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

15.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=XAUDJQYHKZQPEU-KVQBGUIXSA-N

PATENTSCOPE (WIPO)

15.3 FDA Orange Book Patents

Patent	8268800
Expiration	Aug 22, 2030
Applicant	OTSUKA
Drug Application	N212576 (Prescription Drug: INQOVI. Ingredients: CEDAZURIDINE | DECITABINE)

FDA Orange Book

Patent	8618075
Expiration	Oct 16, 2028
Applicant	OTSUKA
Drug Application	N212576 (Prescription Drug: INQOVI. Ingredients: CEDAZURIDINE | DECITABINE)

FDA Orange Book

Patent	9567363
Expiration	Oct 16, 2028
Applicant	OTSUKA
Drug Application	N212576 (Prescription Drug: INQOVI. Ingredients: CEDAZURIDINE | DECITABINE)

FDA Orange Book

16 Biomolecular Interactions and Pathways

16.1 Drug-Gene Interactions

Drug Gene Interaction database (DGIdb)

16.2 Chemical-Gene Interactions

16.2.1 CTD Chemical-Gene Interactions

Comparative Toxicogenomics Database (CTD)

16.3 DrugBank Interactions

DrugBank

16.4 Drug-Drug Interactions

DrugBank

16.5 Pathways

PubChem

17 Biological Test Results

17.1 BioAssay Results

PubChem

18 Classification

18.1 MeSH Tree

- Medical Subject Headings (MeSH)

18.2 NCI Thesaurus Tree

- NCI Thesaurus (NCIt)

18.3 ChEBI Ontology

ChEBI

18.4 KEGG: USP

KEGG

18.5 KEGG: ATC

KEGG

18.6 KEGG: Target-based Classification of Drugs

KEGG

18.7 KEGG: Drug Groups

KEGG

18.8 KEGG: Drug Classes

KEGG

18.9 WHO ATC Classification System

▶ WHO Anatomical Therapeutic Chemical (ATC) Classification

18.10 FDA Pharm Classes

▶ FDA Pharm Classes

18.11 ChemIDplus

ChemIDplus

18.12 CAMEO Chemicals

CAMEO Chemicals

18.13 ChEMBL Target Tree

ChEMBL

18.14 UN GHS Classification

UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

18.15 NORMAN Suspect List Exchange Classification

NORMAN Suspect List Exchange

18.16 EPA DSSTox Classification

EPA DSSTox

18.17 FDA Drug Type and Pharmacologic Classification

- National Drug Code (NDC) Directory

19 Information Sources

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5-AZA-2'-DEOXYCYTIDINE
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CAMEO Chemical Reactivity Classification
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Decitabine [USAN:INN:BAN]
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ChemIDplus Chemical Information Classification
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Decitabine
https://www.drugbank.ca/drugs/DB01262

5. ## EPA DSSTox

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Decitabine
https://comptox.epa.gov/dashboard/DTXSID7030432

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https://echa.europa.eu/substance-information/-/substanceinfo/100.017.355

1-(2-Deoxy-a-D-ribofuranosyl)-5-azacytosine
https://echa.europa.eu/information-on-chemicals

4-amino-1-(2-deoxy-β-D-erythro-pentofuranosyl)-1,3,5-triazin-2(1H)-one
https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/12514

1-(2-Deoxy-a-D-ribofuranosyl)-5-azacytosine
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8. ## ChEBI

5-aza-2'-deoxycytidine
http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:50131

ChEBI Ontology
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FDA Pharmacological Classification
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24. ## FDA/SPL Indexing Data

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https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

25. ## NIPH Clinical Trials Search of Japan
https://rctportal.niph.go.jp/en/

26. ## NLM RxNorm Terminology

https://rxnav.nlm.nih.gov/id/rxnorm/15657

27. ## PubChem
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28. ## SpectraBase
5-Aza-2'-deoxycytidine
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5-Aza-2'-Deoxycytidine
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29. ## Springer Nature
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30. ## Thieme Chemistry

31. ## Wikidata

Decitabine
https://www.wikidata.org/wiki/Q1181878

32. ## Medical Subject Headings (MeSH)

Decitabine
https://www.ncbi.nlm.nih.gov/mesh/2027933
MeSH Tree
http://www.nlm.nih.gov/mesh/meshhome.html
Enzyme Inhibitors
https://www.ncbi.nlm.nih.gov/mesh/68004791
Antimetabolites, Antineoplastic
https://www.ncbi.nlm.nih.gov/mesh/68000964

33. ## KEGG

USP drug classification
http://www.genome.jp/kegg-bin/get_htext?br08302.keg
Anatomical Therapeutic Chemical (ATC) classification

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Target-based classification of drugs
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Drug Groups
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Drug Classes
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34. ## UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

GHS Classification Tree
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36. ## PATENTSCOPE (WIPO)

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37. ## NCBI

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