

# • SAFETY DATA SHEET

Version 8.8  
Revision Date 11/06/2025  
Print Date 11/07/2025

## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : Acetic anhydride-1,1'-<sup>13</sup>C<sub>2</sub>  
Product Number : 487813  
Brand : Aldrich  
CAS-No. : 90980-78-2

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances  
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES  
Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

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## SECTION 2. HAZARDS IDENTIFICATION

**GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)**

**Hazards for the product as supplied**

Flammable liquids : Category 3

Acute toxicity (Oral) : Category 4  
Acute toxicity (Inhalation) : Category 2  
Skin corrosion : Category 1B  
Serious eye damage : Category 1

### Other hazards

None known.

### GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H226 Flammable liquid and vapour.  
H302 Harmful if swallowed.  
H314 Causes severe skin burns and eye damage.  
H330 Fatal if inhaled.

Precautionary statements : **Prevention:**  
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.  
P233 Keep container tightly closed.  
P240 Ground/bond container and receiving equipment.  
P241 Use explosion-proof electrical/ ventilating/ lighting equipment.  
P242 Use only non-sparking tools.  
P243 Take precautionary measures against static discharge.  
P260 Do not breathe mist or vapours.  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P271 Use only outdoors or in a well-ventilated area.  
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.  
P284 Wear respiratory protection.

### Response:

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.  
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with

water/ shower.

P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

Immediately call a POISON CENTER/ doctor.

P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P363 Wash contaminated clothing before reuse.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

**Storage:**

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

P403 + P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

**Disposal:**

P501 Dispose of contents/ container to an approved waste disposal plant.

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### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 90980-78-2

**Components**

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Acetic anhydride-1,1'-13C2	90980-78-2*	>= 90 - <= 100	-

\* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

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### SECTION 4. FIRST AID MEASURES

General advice : First aiders need to protect themselves. Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Immediately call in physician.  
If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

Call a physician immediately.

- In case of eye contact : After eye contact: rinse out with plenty of water.  
Immediately call in ophthalmologist.  
Remove contact lenses.
- If swallowed : After swallowing: make victim drink water (two  
glasses at most), avoid vomiting (risk of perforation).  
Call a physician immediately.  
Do not attempt to neutralise.
- Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
- Protection of first-aiders : For personal protection see section 8.
- Notes to physician : No data available

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## SECTION 5. FIREFIGHTING MEASURES

- Suitable extinguishing media : Water  
Foam  
Carbon dioxide (CO<sub>2</sub>)  
Dry powder
- Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.
- Specific hazards during fire fighting : Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

- Hazardous combustion products : Carbon oxides
- Specific extinguishing : No data available

methods

Further information : Remove container from danger zone and cool with water.  
Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:  
Do not breathe vapours, aerosols.  
Avoid substance contact.  
Ensure adequate ventilation.  
Keep away from heat and sources of ignition.  
Evacuate the danger area, observe emergency procedures, consult an expert.  
Advice for emergency responders:  
For personal protection see section 8.

Environmental precautions : Do not let product enter drains.  
Risk of explosion.

Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills.  
Observe possible material restrictions (see sections 7 and 10).  
Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.  
Take precautionary measures against static discharge.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.  
Avoid generation of vapours/aerosols.

Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place.  
Keep away from heat and sources of ignition.

Keep locked up or in an area accessible only to qualified or authorised persons.

Storage class : 3, Flammable liquids

Recommended storage temperature : Recommended storage temperature see product label.

## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
Acetic anhydride-1,1'-13C2	90980-78-2	TWA	1 ppm	ACGIH
		STEL	3 ppm	ACGIH
		C	5 ppm 20 mg/m3	NIOSH REL
		TWA	5 ppm 20 mg/m3	OSHA Z-1
		TWA	2 ppm	US WEEL
		STEL	5 ppm	US WEEL

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

### Hand protection

Material : butyl-rubber  
Break through time : 480 min  
Glove thickness : 0.7 mm  
Protective index : Full contact

Manufacturer	: Butoject® (KCL 898)
Material	: Latex gloves
Break through time	: 60 min
Glove thickness	: 0.6 mm
Protective index	: Splash contact
Manufacturer	: Lapren® (KCL 706 / Aldrich Z677558, Size M)
Remarks	: This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: <a href="http://www.kcl.de">www.kcl.de</a> ).
Eye protection	: Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles
Skin and body protection	: Flame retardant antistatic protective clothing.
Hygiene measures	: Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: liquid
Color	: colourless
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: -99 °F / -73 °C Method: lit.
Boiling point/boiling range	: 280 - 284 °F / 138 - 140 °C Method: lit.
Flash point	: 120 °F / 49 °C  Method: closed cup

Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: 1.101 g/cm <sup>3</sup> (77 °F / 25 °C)
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Molecular weight	: 104.07 g/mol
Particle characteristics Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity : Can violently decompose at elevated temperatures

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Vapour/air-mixtures are explosive at intense warming.

Chemical stability : Decomposes when moist.

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions : Risk of explosion with:  
ethanol  
potassium permanganate  
Strong oxidizing agents  
perchloric acid  
Nitric acid  
hydrogen peroxide  
chromium(VI) oxide  
barium peroxide  
peroxi compounds  
ammonium nitrate  
with  
Nitric acid  
Exothermic reaction with:  
Ammonia  
Potassium hydroxide  
nitrates  
Sodium hydroxide  
Acetic acid, diluted  
Violent reactions possible with:  
Water  
Possible formation of:  
acetic acid

Conditions to avoid : Heating.

Incompatible materials : No data available

Hazardous decomposition products : In the event of fire: see section 5

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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - 630 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: Acetic anhydride

LC50 Inhalation - Rat - 4 h - > 0.5 - < 2 mg/l - vapour

(OECD Test Guideline 412)

Remarks: (ECHA)

The value is given in analogy to the following substances: Acetic anhydride

Dermal: No data available

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**Skin corrosion/irritation**

Skin - in vitro assay

Result: Causes burns. - 4 h

Remarks: (ECHA)

The value is given in analogy to the following substances: Acetic anhydride

**Serious eye damage/eye irritation**

Eyes - Rat

Result: Corrosive - 24 h

Remarks: (ECHA)

The value is given in analogy to the following substances: Acetic anhydride

Remarks: Causes serious eye damage.

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances: Acetic anhydride

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: Acetic anhydride

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Remarks: The value is given in analogy to the following substances: Acetic anhydride

Test Type: Micronucleus test

Species: Rat

Cell type: Bone marrow

Application Route: inhalation (vapour)

Method: OECD Test Guideline 474

Result: negative

Remarks: The value is given in analogy to the following substances: Acetic anhydride

**Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

No data available

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**SECTION 12. ECOLOGICAL INFORMATION****Ecotoxicity****Components:****Acetic anhydride-1,1'-13C2:**

Toxicity to fish	: LC50 (Oncorhynchus mykiss (rainbow trout)): > 300.82 mg/l End point: mortality Exposure time: 96 h Test Type: semi-static test Method: OECD Test Guideline 203 GLP: yes Remarks: (in analogy to similar products)
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): > 1,000 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: Acetic anhydride
Toxicity to algae/aquatic plants	: ErC50 (Skeletonema costatum): > 300.82 mg/l Exposure time: 72 h Test Type: static test Method: ISO 10253 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: Acetic anhydride
Toxicity to microorganisms	: NOEC (Pseudomonas putida): 1,150 mg/l Exposure time: 16 h

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Test Type: static test  
Remarks: (ECHA)  
The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: Acetic anhydride

## **Persistence and degradability**

### **Components:**

#### **Acetic anhydride-1,1'-13C2:**

Biodegradability : Zahn-Wellens Test  
Result: Readily biodegradable.  
Biodegradation: > 95 %  
Exposure time: 5 d  
Method: OECD Test Guideline 302B  
Remarks: The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: Acetic anhydride

## **Bioaccumulative potential**

### **Components:**

#### **Acetic anhydride-1,1'-13C2:**

Bioaccumulation : Remarks: No bioaccumulation is to be expected (log Pow <= 4).

## **Mobility in soil**

No data available

## **Other adverse effects**

No data available

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## **SECTION 13. DISPOSAL CONSIDERATIONS**

### **Disposal methods**

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## **SECTION 14. TRANSPORT INFORMATION**

### **International Regulations**

#### **IATA-DGR**

UN/ID No. : UN 1715

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Proper shipping name : Acetic anhydride  
 Class : 8  
 Subsidiary risk : 3  
 Packing group : II  
 Labels : Class 8 - Corrosive substances, Class 3 - Flammable liquids  
 Packing instruction (cargo aircraft) : 855  
 Packing instruction (passenger aircraft) : 851

#### IMDG-Code

UN number : UN 1715  
 Proper shipping name : ACETIC ANHYDRIDE

Class : 8  
 Subsidiary risk : 3  
 Packing group : II  
 Labels : 8 (3)  
 EmS Code : F-E, S-C  
 Marine pollutant : no

#### Transport in bulk according to IMO instruments

Not applicable for product as supplied.

#### National Regulations

##### 49 CFR Road

UN/ID/NA number : UN 1715  
 Proper shipping name : Acetic anhydride

Class : 8  
 Subsidiary risk : 3  
 Packing group : II  
 Labels : Class 8 - Corrosive substances, Class 3 - Flammable liquids  
 ERG Code : 137  
 Marine pollutant : no

Poison Inhalation Hazard : No

#### Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

## SECTION 15. REGULATORY INFORMATION

#### CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
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Acetic anhydride-1,1'-13C2	90980-78-2	5000	5000
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#### **SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

#### **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Fire Hazard  
Acute Health Hazard

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

#### **US State Regulations**

##### **Massachusetts Right To Know**

Acetic anhydride-1,1'-13C2 90980-78-2

##### **Pennsylvania Right To Know**

Acetic anhydride-1,1'-13C2 90980-78-2

##### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

##### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

##### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

#### **The components of this product are reported in the following inventories:**

TSCA : Product contains substance(s) not listed on TSCA inventory.

#### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

#### **Full text of other abbreviations**

ACGIH : USA. ACGIH Threshold Limit Values (TLV)  
NIOSH REL : USA. NIOSH Recommended Exposure Limits  
OSHA Z-1 : USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants  
US WEEL : USA. Workplace Environmental Exposure Levels (WEEL)

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ACGIH / TWA	: 8-hour, time-weighted average
ACGIH / STEL	: Short-term exposure limit
NIOSH REL / C	: Ceiling value not be exceeded at any time.
OSHA Z-1 / TWA	: 8-hour time weighted average
US WEEL / TWA	: 8-hr TWA
US WEEL / STEL	: Short-Term TWA

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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Revision Date : 11/06/2025

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