



# **Data Sheet**

 Product Name:
 D-Lin-MC3-DMA

 Cat. No.:
 CS-0044321

 CAS No.:
 1224606-06-7

 Molecular Formula:
 C<sub>43</sub>H<sub>79</sub>NO<sub>2</sub>

 Molecular Weight:
 642.09

Target: Others
Pathway: Others

Solubility: DMSO: 250 mg/mL (389.35 mM; Need ultrasonic); Ethanol:

16.67 mg/mL (25.96 mM; Need ultrasonic)

#### **BIOLOGICAL ACTIVITY:**

D-Lin-MC3-DMA, an ionizable amino lipid, is a potent siRNA delivery vehicle. **In Vivo**: Lipid nanoparticles (LNPs) containing distearoylphosphatidlycholine (DSPC), and ionizableamino-lipids such as dilinoleylmethyl-4-dimethylaminobutyrate (DLin-MC3-DMA) are potent siRNA delivery vehicles in vivo. LNP-siRNA systems optimize to achieve maximum gene silencing potency in hepatocytesfollowing IV administration in mice contain DLin-MC3-DMA (MC3), DSPC, cholesterol and a polyethyleneglycol (PEG)-lipid at mole ratios of 50/10/38.5/1.5. DLin-MC3-DMA exhibits an optimized pK<sub>a</sub> value that leads to dramatically enhanced potency<sup>[1]</sup>.

### References:

[1]. Kulkarni JA, et al. Design of lipid nanoparticles for in vitro and in vivo delivery of plasmid DNA. Nanomedicine. 2017 May;13(4):1377-1387.

#### **CAIndexNames**:

Butanoic acid, 4-(dimethylamino)-, (10Z,13Z)-1-(9Z,12Z)-9,12-octadecadien-1-yl-10,13-nonadecadien-1-yl ester

### **SMILES:**

O=C(OC(CCCCCCC/C=C\C/C=C\CCCCC)CCCCCC/C=C\C/C=C\CCCCC)CCCN(C)C

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

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# **Certificate of Analysis**

 Product Name:
 D-Lin-MC3-DMA

 Cat. No.:
 CS-0044321

 CAS No.:
 1224606-06-7

**Batch No.:** 64686

Chemical Name: Butanoic acid, 4-(dimethylamino)-, (10Z,13Z)-1-(9Z,12Z)-9,12-octadecadien-1-yl-10,13-

nonadecadien-1-yl ester

# PHYSICAL AND CHEMICAL PROPERTIES

Molecular Formula:  $C_{43}H_{79}NO_2$ Molecular Weight: 642.09

Storage: Pure form, Storage temp. 2-8°C

**Chemical Structure:** 

.....

# **ANALYTICAL DATA**

Appearance: Colorless to light yellow (Liquid)

<sup>1</sup> H NMR Spectrum: Consistent with structure

MS: Consistent with structure

Purity (NMR): >98.0%

**Conclusion:** The product has been tested and complies with the given specifications.

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# **Safety Data Sheet**

Revision Date: Jun-2-2020 Print Date: Jun-2-2020

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifier

 Product name :
 D-Lin-MC3-DMA

 Catalog No. :
 CS-0044321

 CAS No. :
 1224606-06-7

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

Identified uses: Laboratory chemicals, manufacture of substances.

# 1.3 Details of the supplier of the safety data sheet

 Company:
 ChemScene LLC

 Tel:
 732-484-9848

 Fax:
 888-484-5008

E-mail: sales@chemscene.com

### 1.4 Emergency telephone number

Emergency Phone #: 732-484-9848

# 2. HAZARDS IDENTIFICATION

### 2.1 Classification of the substance or mixture

Not a hazardous substance or mixture.

### 2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

#### 2.3 Other hazards

None

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

# 3.1 Substances

Formula:  $C_{43}H_{79}NO_2$  Molecular Weight: 642.09

CAS No.: 1224606-06-7

# 4. FIRST AID MEASURES

# 4.1 Description of first aid measures

### Eye contact

Remove any contact lenses, locate eye-wash station, and flush eyes immediately with large amounts of water. Separate eyelids with fingers to ensure adequate flushing. Promptly call a physician.

# Skin contact

Rinse skin thoroughly with large amounts of water. Remove contaminated clothing and shoes and call a physician.

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#### Inhalation

Immediately relocate self or casualty to fresh air. If breathing is difficult, give cardiopulmonary resuscitation (CPR). Avoid mouth-to-mouth resuscitation.

### Ingestion

Wash out mouth with water; Do NOT induce vomiting; call a physician.

# 4.2 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).

### 4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

### 5. FIRE FIGHTING MEASURES

#### 5.1 Extinguishing media

# Suitable extinguishing media

Use water spray, dry chemical, foam, and carbon dioxide fire extinguisher.

# 5.2 Special hazards arising from the substance or mixture

During combustion, may emit irritant fumes.

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus and protective clothing.

### **6. ACCIDENTAL RELEASE MEASURES**

### 6.1 Personal precautions, protective equipment and emergency procedures

Use full personal protective equipment. Avoid breathing vapors, mist, dust or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

Refer to protective measures listed in sections 8.

# 6.2 Environmental precautions

Try to prevent further leakage or spillage. Keep the product away from drains or water courses.

### 6.3 Methods and materials for containment and cleaning up

Absorb solutions with finely-powdered liquid-binding material (diatomite, universal binders); Decontaminate surfaces and equipment by scrubbing with alcohol; Dispose of contaminated material according to Section 13.

# 7. HANDLING AND STORAGE

# 7.1 Precautions for safe handling

Avoid inhalation, contact with eyes and skin. Avoid dust and aerosol formation. Use only in areas with appropriate exhaust ventilation.

# 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly sealed in cool, well-ventilated area. Keep away from direct sunlight and sources of ignition.

Recommended storage temperature: Pure form, Storage temp. 2-8°C

Shipping at room temperature if less than 2 weeks.

### 7.3 Specific end use(s)

No data available.

# 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

# 8.1 Control parameters

# Components with workplace control parameters

This product contains no substances with occupational exposure limit values.

# 8.2 Exposure controls

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# **Engineering controls**

Ensure adequate ventilation. Provide accessible safety shower and eye wash station.

# Personal protective equipment

**Eye protection** Safety goggles with side-shields.

Hand protectionProtective gloves.Skin and body protectionImpervious clothing.Respiratory protectionSuitable respirator.

**Environmental exposure controls**Keep the product away from drains, water courses or the soil. Clean

spillages in a safe way as soon as possible.

### 9. PHYSICAL AND CHEMICAL PROPERTIES

# 9.1 Information on basic physical and chemical properties

Appearance Liquid

Odor No data available Odor threshold No data available рΗ No data available No data available Melting/freezing point Boiling point/range No data available Flash point No data available No data available **Evaporation rate** Flammability (solid, gas) No data available Upper/lower flammability or explosive limits No data available Vapor pressure No data available Vapor density No data available Relative density No data available Water Solubility No data available Partition coefficient No data available

Auto-ignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableExplosive propertiesNo data availableOxidizing propertiesNo data available

# 9.2 Other safety information

No data available.

# 10. STABILITY AND REACTIVITY

# 10.1 Reactivity

No data available.

### 10.2 Chemical stability

Stable under recommended storage conditions.

# 10.3 Possibility of hazardous reactions

No data available.

# 10.4 Conditions to avoid

No data available.

# 10.5 Incompatible materials

Strong acids/alkalis, strong oxidising/reducing agents.

# 10.6 Hazardous decomposition products

Under fire conditions, may decompose and emit toxic fumes.

Other decomposition products - no data available.

# 11.TOXICOLOGICAL INFORMATION

# 11.1 Information on toxicological effects

### Acute toxicity

Classified based on available data. For more details, see section 2

# Skin corrosion/irritation

Classified based on available data. For more details, see section 2

### Serious eye damage/irritation

Classified based on available data. For more details, see section 2

### Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

# Germ cell mutagenicity

Classified based on available data. For more details, see section 2

# Carcinogenicity

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

ACGIH: No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by ACGIH.

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

OSHA: No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by OSHA.

# Reproductive toxicity

Classified based on available data. For more details, see section 2

# Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

# Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

# Aspiration hazard

Classified based on available data. For more details, see section 2

### Additional information

This information is based on our current knowledge. However the chemical, physical, and toxicological properties have not been completely investigated.

# 12. ECOLOGICAL INFORMATION

# 12.1 Toxicity

No data available.

### 12.2 Persistence and degradability

No data available.

### 12.3 Bioaccumlative potential

No data available.

### 12.4 Mobility in soil

No data available.

#### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment unavailable as chemical safety assessment not required or not conducted.

#### 12.6 Other adverse effects

No data available.

### 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

#### **Product**

Dispose substance in accordance with prevailing country, federal, state and local regulations.

### Contaminated packaging

Conduct recycling or disposal in accordance with prevailing country, federal, state and local regulations.

# 14. TRANSPORT INFORMATION

# DOT (US)

This substance is considered to be non-hazardous for transport.

#### **IMDG**

This substance is considered to be non-hazardous for transport.

#### IATA

This substance is considered to be non-hazardous for transport.

### 15. REGULATORY INFORMATION

### SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

# SARA 313 Components:

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.

### SARA 311/312 Hazards:

No SARA Hazards.

# Massachusetts Right To Know Components:

No components are subject to the Massachusetts Right to Know Act.

### Pennsylvania Right To Know Components:

No components are subject to the Massachusetts Right to Know Act.

# New Jersey Right To Know Components:

No components are subject to the Massachusetts Right to Know Act.

# California Prop. 65 Components:

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or anyother reproductive harm.

# **16. OTHER INFORMATION**

Copyright 2020 ChemScene. The above information is correct to the best of our present knowledge but does not purport to be all inclusive and should be used only as a guide. The product is for research use only and for experienced personnel. It must only be handled by suitably qualified experienced scientists in appropriately equipped and authorized facilities. The burden of safe use of this material rests entirely with the user. ChemScene disclaims all liability for any damage resulting from handling or from contact with this product.

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MS Report from Instrument: LCMS-02

Catalog No: CS-0044321





