

## SAFETY DATA SHEET

Version 8.11  
Revision Date 03/02/2024  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : DCA Deblock (0.36M dichloroacetic acid in toluene)

Product Number : 707066  
Brand : Aldrich

**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**

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

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225  
Skin irritation (Category 2), H315  
Serious eye damage (Category 1), H318  
Carcinogenicity (Category 2), H351

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Reproductive toxicity (Category 1B), H360  
 Effects on or via lactation, H362  
 Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336  
 Specific target organ toxicity - repeated exposure (Category 2), Central nervous system, H373  
 Specific target organ toxicity - repeated exposure, Oral (Category 2), Brain, Liver, Testes, H373  
 Aspiration hazard (Category 1), H304  
 Short-term (acute) aquatic hazard (Category 2), H401  
 Long-term (chronic) aquatic hazard (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H336	May cause drowsiness or dizziness.
H351	Suspected of causing cancer.
H360	May damage fertility or the unborn child.
H362	May cause harm to breast-fed children.
H373	May cause damage to organs (Central nervous system) through prolonged or repeated exposure.
H373	May cause damage to organs (Brain, Liver, Testes) through prolonged or repeated exposure if swallowed.
H401	Toxic to aquatic life.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
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 vapors.
P263	Avoid contact during pregnancy/ while nursing.
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.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face

P301 + P310	protection.
P303 + P361 + P353	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P304 + P340 + P312	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P305 + P351 + P338 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P308 + P313	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.
P331	IF exposed or concerned: Get medical advice/ attention.
P332 + P313	Do NOT induce vomiting.
P362	If skin irritation occurs: Get medical advice/ attention.
P370 + P378	Take off contaminated clothing and wash before reuse.
P403 + P233	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep container tightly closed.
P405	Store in a well-ventilated place. Keep cool.
P501	Store locked up.
	Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## SECTION 3: Composition/information on ingredients

### 3.2 Mixtures

Synonyms : DEBLOCK (0.36M dichloroacetic acid in toluene)

Formula :  $C_2H_2Cl_2O_2$

Molecular weight : 128.94 g/mol

Component		Classification	Concentration
<b>Toluene</b>			
CAS-No.	108-88-3	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 3; H225, H315, H361, H336, H373, H304, H401, H412 Concentration limits: 20 %: STOT SE 3, H336;	>= 90 - <= 100 %
EC-No.	203-625-9		
Index-No.	601-021-00-3		
Registration number	01-2119471310-51-XXXX		
<b>Dichloroacetic Acid</b>			
CAS-No.	79-43-6	Met. Corr. 1; Acute Tox. 3; Skin Corr. 1A; Eye Dam. 1; Carc. 2; Repr. 1B; Lact. ; STOT RE 2; Aquatic Acute 1; H290, H311, H314, H318, H351, H360, H362, H373, H400	>= 1 - < 5 %
EC-No.	201-207-0		
Index-No.	607-066-00-5		
Registration number	01-2120767065-52-XXXX		

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### **General advice**

Show this material safety data sheet to the doctor in attendance.

#### **If inhaled**

After inhalation: fresh air. Call in physician.

#### **In case of skin contact**

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

#### **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: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

### 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) and/or in section 11

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

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### **Suitable extinguishing media**

Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### **Unsuitable extinguishing media**

For this substance/mixture no limitations of extinguishing agents are given.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Hydrogen chloride gas

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

### 5.3 Advice for firefighters

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

#### 5.4 Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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### SECTION 6: Accidental release measures

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

Advice for non-emergency personnel: Do not breathe vapors, 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. For personal protection see section 8.

#### 6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

#### 6.3 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.

#### 6.4 Reference to other sections

For disposal see section 13.

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### SECTION 7: Handling and storage

#### 7.1 Precautions for safe handling

##### Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

##### Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

##### Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

#### 7.2 Conditions for safe storage, including any incompatibilities

##### 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 authorized persons.

##### Storage class

Storage class (TRGS 510): 3: Flammable liquids

#### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Toluene	108-88-3	TWA	100 ppm 375 mg/m3	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)
		STEL	150 ppm 560 mg/m3	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)
		TWA	200 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
	Remarks	Z37.12-1967		
		CEIL	300 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.12-1967		
		Peak	500 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.12-1967		
		TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Visual impairment Female reproductive Pregnancy loss 2023 Adoption Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen		
		TWA	100 ppm 375 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	150 ppm 560 mg/m3	USA. NIOSH Recommended Exposure Limits
Dichloroacetic Acid	79-43-6	TWA	0.5 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Toluene	108-88-3	Toluene	0.02 mg/l	In blood	ACGIH - Biological Exposure Indices (BEI)

	Remarks	Prior to last shift of workweek			
		Toluene	0.03 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			
		o-Cresol	0.3mg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

## 8.2 Exposure controls

### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

### Personal protective equipment

#### Eye/face 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 protection

required

#### Body Protection

Flame retardant antistatic protective clothing.

#### Respiratory protection

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.

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.

#### Control of environmental exposure

Do not let product enter drains. Risk of explosion.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                   |   |
|-------------------|---|
| a) Appearance     | Form: clear, liquid<br>Color: colorless |
| b) Odor           | No data available                       |
| c) Odor Threshold | No data available                       |

d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	110 - 111 °C 230 - 232 °F at 1,013 hPa
g) Flash point	5 °C (41 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 8 %(V) Lower explosion limit: 1.2 %(V)
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	0.884 g/cm <sup>3</sup>
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapors may form explosive mixture with air.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Warming.

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### 10.5 Incompatible materials

Strong bases, Strong oxidizing agents, Strong reducing agents

### 10.6 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

#### Mixture

##### Acute toxicity

Oral: No data available

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute toxicity estimate Oral - > 5,000 mg/kg  
(Calculation method)

Inhalation: No data available

Symptoms: Possible symptoms:, mucosal irritations

Acute toxicity estimate Inhalation - 4 h - 26.47 mg/l - vapor(Calculation method)

Dermal: No data available

Acute toxicity estimate Dermal - > 5,000 mg/kg  
(Calculation method)

##### Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

##### Serious eye damage/eye irritation

Remarks: Mixture causes serious eye damage.

##### Respiratory or skin sensitization

No data available

##### Germ cell mutagenicity

No data available

##### Carcinogenicity

Evidence of a carcinogenic effect.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Dichloroacetic Acid)

NTP: RAHC - Reasonably anticipated to be a human carcinogen (Dichloroacetic Acid)

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

May harm the unborn child.

May impair fertility.

##### Specific target organ toxicity - single exposure

Mixture may cause drowsiness or dizziness.

**Specific target organ toxicity - repeated exposure**

Mixture may cause damage to organs through prolonged or repeated exposure.

- Central nervous system

Mixture may cause damage to organs through prolonged or repeated exposure.

- Brain, Liver, Testes

**Aspiration hazard**

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

**11.2 Additional Information**

Lung irritation, chest pain, pulmonary edema, Inhalation studies on toluene have demonstrated the development of inflammatory and ulcerous lesions of the penis, prepuce, and scrotum in animals.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

**Components****Toluene****Acute toxicity**

LD50 Oral - Rat - male - 5,580 mg/kg

(Directive 67/548/EEC, Annex V, B.1.)

LC50 Inhalation - Rat - male - 4 h - 25.7 mg/l - vapor

(OECD Test Guideline 403)

LD50 Dermal - Rabbit - male - > 5,000 mg/kg

Remarks: (ECHA)

**Skin corrosion/irritation**

Skin - Rabbit

Result: irritating - 4 h

(Regulation (EC) No. 440/2008, Annex, B.4)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

**Respiratory or skin sensitization**

Maximization Test - Guinea pig

Result: negative  
(Regulation (EC) No. 440/2008, Annex, B.6)

**Germ cell mutagenicity**

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Result: negative

Test Type: Ames test

Test system: S. typhimurium

Result: negative

Species: Rat - Bone marrow

Result: negative

Remarks: (ECHA)

**Carcinogenicity**

No data available

**Reproductive toxicity**

Suspected of damaging the unborn child.

**Specific target organ toxicity - single exposure**

Inhalation - May cause drowsiness or dizziness. - Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Specific target organ toxicity - repeated exposure**

Inhalation - May cause damage to organs through prolonged or repeated exposure.

- Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Aspiration hazard**

Aspiration may cause pulmonary edema and pneumonitis.

**Dichloroacetic Acid**

**Acute toxicity**

LD50 Oral - Rat - 2,820 mg/kg

(OECD Test Guideline 401)

Inhalation: Corrosive to respiratory system.

LD50 Dermal - Rabbit - 797 mg/kg

Remarks: (ECHA)

**Skin corrosion/irritation**

Skin - Rabbit

Result: Causes severe burns.

Remarks: (RTECS)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Causes serious eye damage.

Remarks: (RTECS)

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

Result: negative

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Result: negative

Species: Mouse - male - Liver cells

Result: negative

Remarks: (ECHA)

Method: OECD Test Guideline 475

Species: Rat - male and female - Bone marrow

Result: negative

**Carcinogenicity**

Suspected of causing cancer.

**Reproductive toxicity**

May damage the unborn child.

May damage fertility. Studies indicating a hazard to babies during the lactation period

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

Oral - May cause damage to organs through prolonged or repeated exposure.

- Brain, Liver, Testes

**Aspiration hazard**

No data available

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**SECTION 12: Ecological information****12.1 Toxicity****Mixture**

No data available

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

## 12.6 Endocrine disrupting properties

No data available

## 12.7 Other adverse effects

No data available

### Components

#### Toluene

Toxicity to fish	flow-through test LC50 - Oncorhynchus kisutch (coho salmon) - 5.5 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Ceriodaphnia dubia (water flea) - 3.78 mg/l - 48 h (US-EPA)
Toxicity to bacteria	static test EC50 - Bacteria - 84 mg/l - 24 h Remarks: (ECHA)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Oncorhynchus kisutch (coho salmon) - 1.39 mg/l - 40 d Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	NOEC - Ceriodaphnia dubia (water flea) - 0.74 mg/l - 7 d (US-EPA)

#### Dichloroacetic Acid

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

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. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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**SECTION 14: Transport information****DOT (US)**

UN number: 1993    Class: 3    Packing group: II  
Proper shipping name: Flammable liquids, n.o.s. (Toluene, Dichloroacetic Acid) (Toluene, Dichloroacetic Acid)  
Reportable Quantity (RQ): 1029 lbs  
Poison Inhalation Hazard: No

**IMDG**

UN number: 1993    Class: 3    Packing group: II EMS-No: F-E, S-E  
Proper shipping name: FLAMMABLE LIQUID, N.O.S. (Toluene, Dichloroacetic Acid) (Toluene, Dichloroacetic Acid)  
Marine pollutant : yes

**IATA**

UN number: 1993    Class: 3    Packing group: II  
Proper shipping name: Flammable liquid, n.o.s. (Toluene, Dichloroacetic Acid) (Toluene, Dichloroacetic Acid)

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**SECTION 15: Regulatory information****SARA 302 Components**

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

**SARA 313 Components**

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

**SARA 311/312 Hazards**

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

**California Prop. 65 Components**

	CAS-No.	Revision Date
, which is/are known to the State of California to cause cancer, and Dichloroacetic Acid	79-43-6	2015-08-25

	CAS-No.	Revision Date
, which is/are known to the State of California to Aldrich - 707066		

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## SECTION 16: Other information

### Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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