

# Aldehyde Dehydrogenase (ALDH)

Aldehyde Dehydrogenases (ALDHs) are a superfamily of NADP\*-dependent enzymes that metabolize endogenous and exogenous aldehydes to corresponding carboxylic acids. This superfamily of proteins is comprised of 19 isozymes, with constitutive activity of at least one isozyme observed in a majority of mammalian tissues. The ALDHs play important roles, among other things, in cellular detoxification, the protection against ultraviolet radiation-induced damage, and amino acid metabolism.

The ALDH1A subfamily plays a pivotal role in embryogenesis and development by mediating retinoic acid signaling. ALDH2, as a key enzyme that oxidizes acetaldehyde, is crucial for alcohol metabolism. ALDH1A1 and ALDH3A1 are lens and corneal crystallins, which are essential elements of the cellular defense mechanism against ultraviolet radiation-induced damage in ocular tissues. Many ALDH isozymes are important in oxidizing reactive aldehydes derived from lipid peroxidation and thereby help maintain cellular homeostasis. Increased expression and activity of ALDH isozymes have been reported in various human cancers and are associated with cancer relapse. As a direct consequence of their significant physiological and toxicological roles, inhibitors of the ALDH enzymes have been developed to treat human diseases.

# Aldehyde Dehydrogenase (ALDH) Inhibitors, Agonists & Antagonists

# 3-Hydroxybenzaldehyde

Cat. No.: HY-76006

3-Hydroxybenzaldehyde is a **precursor** compound for phenolic compounds, such as Protocatechualdehyde (HY-N0295).
3-Hydroxybenzaldehyde is a **substrate** of **aldehyde dehydrogenase** (ALDH) in rats and humans (ALDH2).

**Purity:** ≥98.0%

Clinical Data: No Development Reported Size: 10 mM × 1 mL, 100 mg

# 4-Diethylaminobenzaldehyde

4-Diethylaminobenzaldehyde is a reversible **aldehyde dehydrogenases (ALDHs)** inhibitor, with a  $K_i$  of 4 nM for ALDH1. 4-Diethylaminobenzaldehyde displays potent anti-androgenic effect (IC $_{sn}$ = 1.71 $\mu$ M).

Cat. No.: HY-W016645

Purity: 98.82%

Clinical Data: No Development Reported Size: 10 mM × 1 mL, 100 mg

# 4-Hydroxynonenal

(4-HNE) Cat. No.: HY-113466

4-Hydroxynonenal (4-HNE) is an  $\alpha,\beta$  unsaturated hydroxyalkenal and an oxidative/nitrosative stress biomarker. 4-Hydroxynonenal is a substrate and an inhibitor of acetaldehyde dehydrogenase 2 (ALDH2).

**Purity:** ≥99.0%

Clinical Data: No Development Reported Size: 5 mg, 10 mg, 25 mg, 50 mg

# 4-Hydroxynonenal-d3

(4-HNE-d3) Cat. No.: HY-113466S

4-Hydroxynonenal-d3 (4-HNE-d3) is the deuterium labeled 4-Hydroxynonenal. 4-Hydroxynonenal (4-HNE) is an  $\alpha,\beta$  unsaturated hydroxyalkenal and an oxidative/nitrosative stress biomarker.



Purity: >98% Clinical Data:

Size: 1 mg, 5 mg

### Alda-1

Cat. No.: HY-18936

Alda-1 is a potent and selective ALDH2 agonist, which activates wild-type ALDH2 and restores near wild-type activity to ALDH2\*2.

**Purity:** 99.99%

Clinical Data: No Development Reported

Size:  $10 \text{ mM} \times 1 \text{ mL}$ , 10 mg, 50 mg, 100 mg, 500 mg

## ALDH1A1-IN-2

ALDH1A1-IN-2 is a potent inhibitor of aldehyde dehydrogenase 1a1 (aldh1a1). Aldehyde dehydrogenases (ALDH) constitute a family of enzymes that play a critical role in oxidizing various cytotoxic xenogenic and biogenic aldehydes.

**Purity:** >98%

Clinical Data: No Development Reported

Size: 5 mg, 10 mg, 25 mg, 50 mg, 100 mg

Cat. No.: HY-126003

# ALDH1A2-IN-1

Cat. No.: HY-139031

ALDH1A2-IN-1 is an active site-directed reversible ALDH1A2 inhibitor (IC $_{so}$ =0.91  $\mu$ M; Kd=0.26  $\mu$ M) with several hydrophobic interactions.

**Purity:** >98%

Clinical Data: No Development Reported

Size: 1 mg, 5 mg

# ALDH1A3-IN-1

ALDH1A3-IN-1 (Compound 14) is a potent **ALDH1A3** inhibitor, with an IC $_{50}$  of 0.63  $\mu$ M and a K $_{i}$  of 0.46  $\mu$ M. ALDH1A3-IN-1 can be studied in **prostate** cancer

Purity: >98%

Clinical Data: No Development Reported

Size: 1 mg, 5 mg



Cat. No.: HY-144667

## ALDH1A3-IN-3

Cat. No.: HY-W017186

ALDH1A3-IN-3 (compound 16) is a potent inhibitor of ALDH1A3, with an IC $_{\rm 50}$  of 0.26  $\mu M.$  ALDH1A3-IN-3 is also a good ALDH3A1 substrate. ALDH1A3-IN-3 can be used for the research of prostate cancer.

**Purity:** 98.87%

Clinical Data: No Development Reported

Size: 1 g

# BODIPY aminoacetaldehyde

(BAAA) Cat. No.: HY-136594

BODIPY aminoacetaldehyde (BAAA) is a fluorescent substrate for both murine and human aldehyde dehydrogenase (ALDH). BODIPY aminoacetaldehyde consists of an aminoacetaldehyde moiety bonded to the BODIPY fluorochrome and can be used to label stem cells.

taldehyde moiety bonded to ne and can be used to label

**Purity:** >98%

Clinical Data: No Development Reported

Size: 5 mg, 10 mg

Tel: 609-228-6898 Fax: 609-228-5909 Email: sales@MedChemExpress.com

#### CM037

(A37) Cat. No.: HY-110294

CM037 is a selective inhibitor of ALDH1A1 (aldehyde dehydrogenase 1A1) with an  $IC_{s0}$  of 4.6  $\mu M_{\odot}$ 

**Purity:** >98%

Clinical Data: No Development Reported

Size: 1 mg, 5 mg

# CM10

CM10 is a potent and selective aldehyde dehydrogenase 1A (ALDH1A) family inhibitor, with IC $_{50}$ S of 1700, 740, and 640 nM for ALDH1A1, ALDH1A2, and ALDH1A3, respectively. CM10 does not inhibit any of the other ALDH family members.



Cat. No.: HY-135841

**Purity:** 99.53%

Clinical Data: No Development Reported

Size: 10 mM × 1 mL, 5 mg, 10 mg, 25 mg, 50 mg, 100 mg

# CM121

Cat. No.: HY-139032

CM121 is an active site-directed reversible ALDH1A2 inhibitor (IC $_{50}$ =0.54  $\mu$ MKd=1.1  $\mu$ M) with a variety of hydrophobic interactions.

**Purity:** >98%

Clinical Data: No Development Reported

Size: 1 mg, 5 mg

#### CVT-10216

Cat. No.: HY-19801

CVT-10216 is a highly selective, reversible aldehyde dehydrogenase-2 (ALDH-2) inhibitor with an IC $_{50}$  of 29 nM. CVT-10216 also has inhibitory effect of ALDH-1 with an IC $_{50}$  of 1.3  $\mu$ M.

**Purity:** ≥99.0%

Clinical Data: No Development Reported

Size: 10 mM × 1 mL, 5 mg, 10 mg, 25 mg, 50 mg

#### Disulfiram

(Tetraethylthiuram disulfide; TETD) Cat. No.: HY-B0240

Disulfiram (Tetraethylthiuram disulfide) is a specific inhibitor of aldehyde-dehydrogenase (ALDH1), used for the treatment of chronic alcoholism by producing an acute sensitivity to alcohol.

Purity: 99.77% Clinical Data: Launched

Size: 10 mM × 1 mL, 500 mg, 1 g, 5 g

# **EN40**

Cat. No.: HY-122577

EN40 is a potent, selective aldehyde dehydrogenase 3A1 (ALDH3A1) inhibitor as a covalent ligand, exhibits an  $IC_{50}$  value of 2 uM.



**Purity:** 95.15%

Clinical Data: No Development Reported
Size: 5 mg, 10 mg, 25 mg, 50 mg, 100 mg

## KS106

Cat. No.: HY-146683

KS106 is a potent **ALDH** inhibitor with  $\rm IC_{50}S$  of 334, 2137, 360 nM for ALDH1A1, ALDH2, and ALDH3A1, respectively. KS106 shows antiproliferative and anticancer effects with low low toxic.

**Purity:** > 98%

Clinical Data: No Development Reported

Size: 1 mg, 5 mg

## MeDTC

(S-Methyl-N,N-diethylthiocarbamate Sulfone) Cat. No.: HY-115757

MeDTC (S-Methyl-N,N-diethylthiocarbamate Sulfone), a Disulfiram metabolite, is a potent, irreversible aldehyde dehydrogenase (ALDH) inhibitor.



**Purity:** >98%

Clinical Data: No Development Reported

Size: 5 mg

## NCT-501

Cat. No.: HY-18768

NCT-501 is a potent and selective theophylline-based inhibitor of aldehyde dehydrogenase 1A1 (ALDH1A1), inhibits hALDH1A1 with  $IC_{so}$  of 40 nM, typically shows better selectivity over other ALDH isozymes and other dehydrogenases (hALDH1B1, hALDH3A1, and...



Clinical Data: No Development Reported

Size: 10 mM × 1 mL, 5 mg, 10 mg, 50 mg, 100 mg

# NCT-501 hydrochloride

Cat. No.: HY-18768A

NCT-501 hydrochloride is a potent and selective theophylline-based inhibitor of aldehyde dehydrogenase 1A1 (ALDH1A1), inhibits hALDH1A1 with IC $_{50}$  of 40 nM, typically shows better selectivity over other ALDH isozymes and other dehydrogenases (hALDH1B1, hALDH3A1, and...

**Purity:** >98%

Clinical Data: No Development Reported

Size: 1 mg, 5 mg



#### NCT-505

NCT-505 is a potent and selective aldehyde dehydrogenase (ALDH1A1) inhibitor, with an IC. of 7 nM, and weakly inhibits hALDH1A2, hALDH1A3, hALDH2, hALDH3A1 (IC<sub>so</sub>s, >57, 22.8, 20.1,  $>57 \mu M)$ .

Purity: 98 41%

Clinical Data: No Development Reported Size: 5 mg, 10 mg, 25 mg



Cat. No.: HY-112277

# NCT-506

NCT-506 is an orally bioavailable aldehyde dehydrogenase 1A1 (ALDH1A1) inhibitors with an IC<sub>50</sub> of 7 nM.

Cat. No.: HY-112278

Purity: >98%

Clinical Data: No Development Reported Size: 5 mg, 10 mg, 25 mg, 50 mg, 100 mg

## Nitrefazole

(EMD-15700) Cat. No.: HY-107030

Nitrefazole is a 4-nitroimidazole derivative with strong and long lasting inhibition of aldehyde dehydrogenase (ALDH), an enzyme involved in the metabolism of alcohol.

Purity: >98%

Clinical Data: No Development Reported

1 mg, 5 mg

## Prunetin

Prunetin, an O-methylated isoflavone, possesses anti-inflammatory activity. Prunetin is a potent human aldehyde dehydrogenases inhibitor.



Cat. No.: HY-N2597

Purity: 99.01%

Clinical Data: No Development Reported 1 mg, 5 mg, 10 mg

#### RV01

Cat. No.: HY-126241

НО

RV01 is an analogue of resveratrol, inhibits DNA damage, reduces acetaldehyde dehydrogenase 2 (ALDH2) mRNA expression induced by ethanol, and exhibits hydroxyl radical scavenging activity. RV01 decreases iNOS expression, with anti-neuroinflammatory activity.

Purity: 98.0%

Clinical Data: No Development Reported

Size: 10 mM × 1 mL, 5 mg, 10 mg, 50 mg, 100 mg

#### **Taraxerone**

Taraxerone is isolated from Sedum sarmentosum. Taraxerone enhances effects on alcohol dehydrogenase (ADH) and acetaldehyde dehydrogenase (ALDH) activities with EC50 values of 512.42 and 500.16 μM, respectively.

≥98.0%

Clinical Data: No Development Reported

Size: 1 mg, 5 mg



Cat. No.: HY-N1177

# Win 18446

Cat. No.: HY-W011094

Win 18446 is an orally active testes-specific enzyme ALDH1a2 inhibitor, with an  $IC_{so}$  of 0.3  $\mu M$ . Win 18446 reversibly inhibits spermatogenesis in many species and inhibits Retinoic acid (HY-14649) biosynthesis from Retinol (HY-B1342) within the

Clinical Data: No Development Reported 10 mM × 1 mL, 50 mg Size:

# α-NETA

Purity:

 $\alpha\textsc{-NETA}$  is a potent and noncompetitive cholineacetyltransferase (ChA) inhibitor with an  $IC_{50}$  of 9  $\mu$ M.  $\alpha$ -NETA is a potent ALDH1A1 (IC<sub>50</sub>=0.04  $\mu$ M) and chemokine-like receptor-1 (CMKLR1) antagonist.

Purity: ≥98.0%

Clinical Data: No Development Reported 5 mg, 10 mg, 25 mg, 50 mg, 100 mg Size:



Cat. No.: HY-138097