

Certificate of Analysis

Print Date: Dec 10th 2020

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Product Name: Disulfiram Catalog No.: 3807 Batch No.: 2

CAS Number: 97-77-8 EC Number: 202-607-8

IUPAC Name: Bis(diethylthiocarbamyoyl)disulfide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{10}H_{20}N_2S_4$ Batch Molecular Weight: 296.54

Physical Appearance: Off-white solid

Solubility: DMSO to 20 mM ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

¹H NMR: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 40.51 6.8 9.45 Found 40.4 6.85 9.39



Product Information

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Description:

Inhibitor of aldehyde dehydrogenase that displays antialcoholism activity. Shown to reversibly stimulate $Ca^{2+}\text{-}ATP$ ase activity and inhibit V-ATPase (EC $_{50}$ = 26 $\mu\text{M}).$ Also inhibits expression of MMP-2 and MMP-9 and displays anti-invasive activity. Pyroptosis inhibitor; binds gasdermin D (GSDMD) and inhibits pore formation. Also inhibits SARS-CoV-2 main protease (Mpro; IC $_{50}$ = 9.35 μM) and inhibits viral replication in Vero cells in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{10}H_{20}N_2S_4$ Batch Molecular Weight: 296.54 Physical Appearance: Off-white solid

Batch Molecular Structure:

$$Et_2N$$
 S
 S
 S
 NEt_2

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 20 mM ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Jin et al (2020) Structure of Mpro from SARS-CoV-2 and discovery of its inhibitors. Nature 582 289. PMID: 32272481.

Pandeya et al (2019) Gasdermin D (GSDMD) as a new target for the treatment of infection. Medchemcomm 10 660. PMID: 31191857.

Fisher *et al* (2010) The ethanol metabolite acetaldehyde increases paracellular drug permeability *in vitro* and oral bioavailability *in vivo*. J.Pharmacol.Exp.Ther. **332** 326. PMID: 19820208.