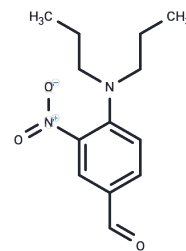


## ALDH3A1-IN-1

## Chemical Properties

|                   |                                                                                                                                                        |
|-------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| CAS No. :         | 1039855-56-5                                                                                                                                           |
| Formula:          | C13H18N2O3                                                                                                                                             |
| Molecular Weight: | 250.29                                                                                                                                                 |
| Storage:          | Store at low temperature<br>Powder: -20°C for 3 years   In solvent: -80°C for 1 year<br><i>Actual storage temperature shall be subject to the COA.</i> |



## Biological Description

|               |                                                                                                                                                                                                                                                             |
|---------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Description   | ALDH3A1-IN-1 (Compound 18) is a potent ALDH3A1 inhibitor with an IC <sub>50</sub> of 1.61 μM. It is more effective than DEAB against patient-derived primary prostate tumor epithelial cells, both as a single agent and in combination with docetaxel [1]. |
| Targets(IC50) | NMDAR, Dehydrogenase                                                                                                                                                                                                                                        |

## Solubility Information

|                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|---------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Solubility          | DMSO: 80 mg/mL (319.63 mM), Sonication is recommended.<br>(< 1 mg/ml refers to the product slightly soluble or insoluble)                                                                                                                                                                                                                                                                                                                                                                                    |
| In vivo Formulation | 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 3.3 mg/mL (13.18 mM), Sonication is recommended.<br><i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i> |

## Preparing Stock Solutions

|       | 1mg       | 5mg        | 10mg       |
|-------|-----------|------------|------------|
| 1 mM  | 3.9954 mL | 19.9768 mL | 39.9537 mL |
| 5 mM  | 0.7991 mL | 3.9954 mL  | 7.9907 mL  |
| 10 mM | 0.3995 mL | 1.9977 mL  | 3.9954 mL  |
| 50 mM | 0.0799 mL | 0.3995 mL  | 0.7991 mL  |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Ibrahim AIM, et al. Expansion of the 4-(Diethylamino)benzaldehyde Scaffold to Explore the Impact on Aldehyde Dehydrogenase Activity and Antiproliferative Activity in Prostate Cancer. J Med Chem. 2022 Mar 10;65(5):3833-3848.

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