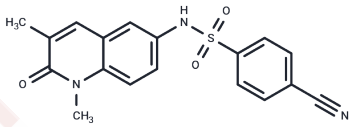
# Data Sheet (Cat.No.T16321)

TargetMol

NI-42

## Chemical Properties



CAS No. : 1884640-99-6

Formula: C18H15N3O3S

Molecular Weight: 353.39

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

## Biological Description

| | |
|---|---|
| Description | NI-42 is a structurally orthogonal chemical probe for the BRPFs and is biased. It effective inhibitor of the BRD of the BRPFs (IC50s of BRPF1/2/3=7.9/48/260 nM; Kds of BRPF1/2/3=40/210/940 nM). It also has excellent selectivity over nonclass IV BRD proteins. |
| Targets(IC50) | Epigenetic Reader Domain |
| In vitro | NI-42 displays IC50s of 82, 310, and 4500 nM for BRD7, BRD9, and BRD4 (BD1), respectively. It has a Kd of 1130 nM for BRD9. |

## Solubility Information

| | |
|---|---|
| Solubility | DMSO: 95 mg/mL (268.82 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 (9.34 mM),Sonication is recommended.<br>*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.* |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|---|---|---|---|
| 1 mM | 2.8297 mL | 14.1487 mL | 28.2973 mL |
| 5 mM | 0.5659 mL | 2.8297 mL | 5.6595 mL |
| 10 mM | 0.283 mL | 1.4149 mL | 2.8297 mL |
| 50 mM | 0.0566 mL | 0.283 mL | 0.5659 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

Igoe N, et al. Design of a Biased Potent Small Molecule Inhibitor of the Bromodomain and PHD Finger-Containing (BRPF) Proteins Suitable for Cellular and in Vivo Studies. J Med Chem. 2017 Jan 26;60(2):668-680.