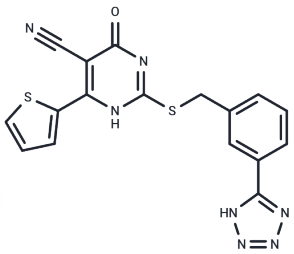
Data Sheet (Cat.No.T13132)

TES-991

Chemical Properties



CAS No. : 1883602-20-7

Formula: C17H11N7OS2

Molecular Weight: 393.45

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	TES-991 is a potent and selective inhibitor of human α-Amino-β-carboxymuconate-ε-semialdehyde Decarboxylase (ACMSD), with an IC50 of 3 nM.
Targets(IC50)	Others,Cytochromes P450
In vitro	TES-991 significantly increase intracellular NAD+ levels, providing further proof of their mechanism of action. TES-991 exhibits an inhibition of cytochrome P450 2C19, suggesting a possible involvement of the 2H-tetrazole motif.
In vivo	TES-991(intravenous,0.5 mg/kg) shows low blood clearance, with low volumes of distribution and halflives (t1/2) of about 4.0 and 5.0 h, respectively, although after oral administration at 5 mg/kg, the blood concentrations of TES-991 is quantifiable for up to 8 h. A moderate systemic exposure is observed for the 2H-tetrazole analogue, TES-991, a good systemic exposure is recorded for the free acid.

Solubility Information

Solubility	DMSO: 62.5 mg/mL (158.85 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 2.5 mg/mL (6.35 mM),Sonication is recommended. *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	2.5416 mL	12.7081 mL	25.4162 mL
5 mM	0.5083 mL	2.5416 mL	5.0832 mL
10 mM	0.2542 mL	1.2708 mL	2.5416 mL
50 mM	0.0508 mL	0.2542 mL	0.5083 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

Pellicciari R, et al. α-Amino-β-carboxymuconate-ε-semialdehyde Decarboxylase (ACMSD) Inhibitors as Novel Modulators of De Novo Nicotinamide Adenine Dinucleotide (NAD+) Biosynthesis. J Med Chem. 2018 Feb 8;61(3): 745-759.