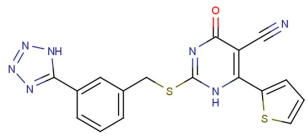
Data Sheet (Cat.No.T13132)

TargetMol
A DRUG SCREENING EXPERT

TES-991

Chemical Properties



CAS No.:	1883602-20-7
Formula:	C17H11N7OS2
Molecular Weight:	393.45
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Targets(IC_{50})	hACMSD: 3 nM
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) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.542 mL	12.708 mL	25.416 mL
5 mM	0.508 mL	2.542 mL	5.083 mL
10 mM	0.254 mL	1.271 mL	2.542 mL
50 mM	0.051 mL	0.254 mL	0.508 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. 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.

Inhibitors · Natural Compounds · Compound Libraries

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