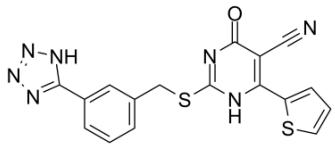
TES-991

Cat. No.:	HY-112619		
CAS No.:	1883602-20-7		
Molecular Formula:	$C_{17}H_{11}N_7OS_2$		
Molecular Weight:	393.45		
Target:	Others		
Pathway:	Others		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 62.5 mg/mL (158.85 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	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

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (5.29 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.29 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

TES-991 is a potent and selective human α-Amino-β-carboxymuconate-ε-semialdehyde Decarboxylase (ACMSD) inhibitor, with an IC_{50} of 3 nM.

IC_{50} & Target

IC50: 3 nM (hACMSD)[1].

In Vitro

TES-991 (compounds 21) is able to significantly increase intracellular NAD^+ levels, providing further proof of their mechanism of action. TES-991 shows an inhibition of cytochrome P450 2C19, suggesting a possible involvement of the 2H-tetrazole motif in this interaction[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo	After the intravenous administration of 0.5 mg/kg, TES-991 (compound 21) shows low blood clearance, with low volumes of distribution and halflives ($t_{1/2}$) 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[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[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.

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