ML318

Cat. No.: HY-129123

CAS No.: 1610516-67-0

Molecular Formula: $C_{14}H_8F_4N_2$

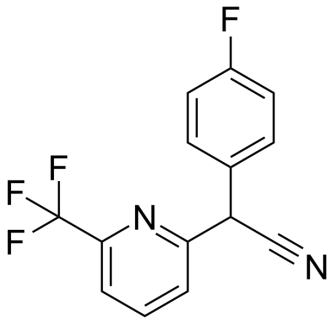
Molecular Weight: 280.22

Target: Antibiotic

Pathway: Anti-infection

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (356.86 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.5686 mL	17.8431 mL	35.6862 mL
	5 mM	0.7137 mL	3.5686 mL	7.1372 mL
	10 mM	0.3569 mL	1.7843 mL	3.5686 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: 2.5 mg/mL (8.92 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (8.92 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

ML318 is a biaryl nitrile inhibitor of PvdQ acylase with an IC_{50} of 20 nM by binding in the acyl-binding site. ML318 inhibits P. aeruginosa (PAO1) with an IC_{50} of 19 μM. ML318 prevents pyoverdine production and limits the growth of P. aeruginosa under iron-limiting conditions[1].

IC_{50} & Target

IC50: 20 nM (PvdQ acylase)[1]

REFERENCES

[1]. Jacqueline M Wurst, et al. Identification of inhibitors of PvdQ, an enzyme involved in the synthesis of the siderophore pyoverdine. ACS Chem Biol. 2014 Jul 18;9(7):1536-

44.

Caution: Product has not been fully validated for medical applications. For research use only.

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