# AU1235

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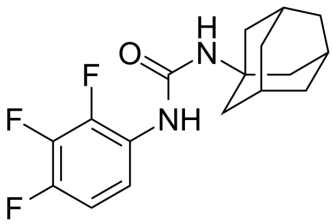
|---|---|
| **Cat. No.:** | HY-101867 |
| **CAS No.:** | 1338780-86-1 |
| **Molecular Formula:** | $C_{17}H_{19}F_3N_2O$ |
| **Molecular Weight:** | 324.34 |
| **Target:** | Bacterial |
| **Pathway:** | Anti-infection |

**Storage:**

| | | |
|---|---|---|
| Powder | -20°C | 3 years |
| | 4°C | 2 years |
| In solvent | -80°C | 2 years |
| | -20°C | 1 year |



## SOLVENT & SOLUBILITY

**In Vitro**

DMSO : 25 mg/mL (77.08 mM; Need ultrasonic)

| Preparing Stock Solutions | Solvent / Mass / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|---|
| | 1 mM | 3.0832 mL | 15.4159 mL | 30.8318 mL |
| | 5 mM | 0.6166 mL | 3.0832 mL | 6.1664 mL |
| | 10 mM | 0.3083 mL | 1.5416 mL | 3.0832 mL |

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

**In Vivo**

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.71 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.71 mM); Clear solution

## BIOLOGICAL ACTIVITY

**Description**

AU1235, an adamantyl urea, is a potent MmpL3 inhibitor. The Mycobacterium tuberculosis protein MmpL3 performs an essential role in cell wall synthesis, since it effects the transport of trehalose monomycolates across the inner membrane[1] [2].

**In Vitro**

AU1235 is similarly active against MDR isolates of M. tb displaying resistance to isoniazid, rifampicin, and pyrazinamide in addition to streptomycin, fluoroquinolones and/or ethambutol. AU1235 also inhibits Mycobacterium smegmatis and Mycobacterium fortuitum although the MICs (3.2 to 6.4 μg/ml) are significantly higher than against M. tb and M. bovis BCG[2].

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

## CUSTOMER VALIDATION

- ACS Infect Dis. 2020 Feb 14;6(2):324-337.
- J Biol Chem. 2019 Nov 15;294(46):17512-17523.

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## REFERENCES

[1]. McNeil MB, et al. Multiple Mutations in Mycobacterium tuberculosis MmpL3 Increase Resistance to MmpL3 Inhibitors. mSphere. 2020;5(5):e00985-20. Published 2020 Oct 14.

[2]. Grzegorzewicz AE, et al. Inhibition of mycolic acid transport across the Mycobacterium tuberculosis plasma membrane. Nat Chem Biol. 2012;8(4):334-341. Published 2012 Feb 19.

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

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