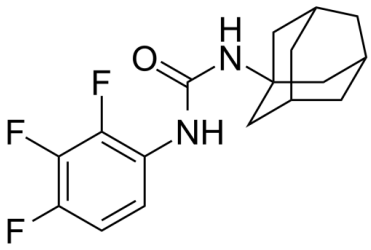
Data Sheet

Product Name:	AU1235
Cat. No.:	CS-6863
CAS No.:	1338780-86-1
Molecular Formula:	C17H19F3N2O
Molecular Weight:	324.34
Target:	Bacterial
Pathway:	Anti-infection
Solubility:	DMSO : 6 mg/mL (18.50 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

AU1235 is an **adamantyl urea** inhibitor of **Mycobacterium tuberculosis**. **In Vitro:** AU1235 has a minimum inhibitory concentration (MIC) of 0.1 μg/mL (0.3 μM) (minimum bactericidal concentration of 0.1 μg/mL. AU1235 is similarly active against MDR clinical 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 (MICs=3.2 to 6.4 μg/mL). AU1235 (10 times MIC) does not increase the killing effect within the first 7 days indicating that the killing is time-dependent rather than concentration-dependent. In an anaerobic model involving non-replicating M. tb H37Rv bacilli, AU1235 at 10 μg/mL shows no detectable activity suggesting that it acts on a biosynthetic pathway required for active bacterial multiplication. AU1235 does not inhibit the biosynthesis of mycolic acids per se but specifically their ability to be transferred onto their cell wall and outer membrane acceptors, possibly as a result of altered TMM translocation across the plasma membrane[1].

References:

[1]. Grzegorzewicz AE, et al. Inhibition of mycolic acid transport across the Mycobacterium tuberculosis plasma membrane. Nat Chem Biol. 2012 Feb 19;8(4):334-41.

CAIndexNames:

Urea, N-tricyclo[3.3.1.13,7]dec-1-yl-N'-(2,3,4-trifluorophenyl)-

SMILES:

O=C(NC(C=CC(F)=C1F)=C1F)NC2(C[C@H](C3)C4)C[C@H]4C[C@H]3C2

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

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