

# **Data Sheet**

Product Name: Delamanid

Cat. No.: CS-5866

CAS No.: 681492-22-8

Molecular Formula: C25H25F3N4O6

Molecular Weight: 534.48

Target: Bacterial

Pathway: Anti-infection

**Solubility:** H2O: < 0.1 mg/mL (insoluble); DMSO:  $\geq 50 \text{ mg/mL}$  (93.55 mM)

#### **BIOLOGICAL ACTIVITY:**

Delamanid, a newer **mycobacterial cell wall synthesis** inhibitor, inhibits the synthesis of mucolic acids<sup>[1]</sup>. **In Vitro**: Delamanid inhibits the synthesis of mucolic acids, cruciala component of the cell wall of the Mycobacterium tuberculosis complex<sup>[1]</sup>.

Delamanid shows more potent antibacterial activity against drug-susceptible and drug-resistant strains of M. tuberculosis<sup>[2]</sup>.

Delamanid do not affect rifampin, pyrazinamide, and isoniazid exposure; the ethambutol AUC $\tau$  and Cmax values are about 25% higher with delamanid coadministration<sup>[3]</sup>.

In Vivo: Delamanid (orally administration; 30 mg/kg; 5 days) results in sterile cures in a mouse model of VL<sup>[4]</sup>.

### References:

- [1]. Sotgiu G et al. Delamanid (OPC-67683) for treatment of multi-drug-resistant tuberculosis. Expert Rev Anti Infect Ther. 2015 Mar;13(3):305-15.
- [2]. Xavier AS et al. Delamanid: A new armor in combating drug-resistant tuberculosis. J Pharmacol Pharmacother. 2014 Jul;5(3):222-4
- [3]. Mallikaarjun S et al. Delamanid Coadministered with Antiretroviral Drugs or Antituberculosis Drugs Shows No Clinically Relevant Drug-Drug Interactions in Healthy Subjects. Antimicrob Agents Chemother. 2016 Sep 23;60(10):5976-85.
- [4]. Patterson S et al.The anti-tubercular drug delamanid as a potential oral treatment for visceral leishmaniasis. Elife. 2016 May 24;5.

# CAIndexNames:

Imidazo[2,1-b]oxazole, 2,3-dihydro-2-methyl-6-nitro-2-[[4-[4-[4-(trifluoromethoxy)phenoxy]-1-piperidinyl]phenoxy]methyl]-, (2R)-

# **SMILES:**

FC(F)(F)OC1 = CC = C(OC2CCN(C3 = CC = C(OC[C@@]4(C)CN5C(O4) = NC([N+]([O-]) = O) = C5)C = C3)CC2)C = C1

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

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