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SZABO-SCANDIC Handels GmbH

Quellenstraße 110, A-1100 Wien

T. +43(0)1 489 3961-0

F. +43(0)1 489 3961-7

mail@szabo-scandic.com

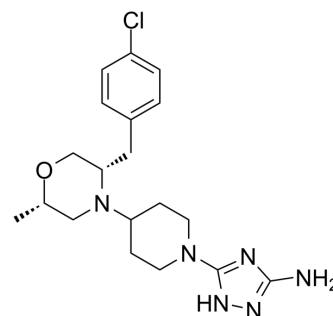
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OATD-01

Cat. No.:	HY-137464A
CAS No.:	2088453-21-6
Molecular Formula:	C ₁₉ H ₂₇ ClN ₆ O
Molecular Weight:	390.91
Target:	Others
Pathway:	Others
Storage:	-20°C, protect from light, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light, stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro	DMSO : 100 mg/mL (255.81 mM; Need ultrasonic)				
	Preparing Stock Solutions	Solvent Concentration Mass	1 mg	5 mg	10 mg
		1 mM	2.5581 mL	12.7907 mL	25.5813 mL
		5 mM	0.5116 mL	2.5581 mL	5.1163 mL
		10 mM	0.2558 mL	1.2791 mL	2.5581 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 (6.40 mM); Clear solution				
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (6.40 mM); Clear solution				
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (6.40 mM); Clear solution				

BIOLOGICAL ACTIVITY

Description	OATD-01 is a highly potent, first-in-class, orally active and selective chitinase inhibitor with low nanomolar activity toward CHIT1 (hCHIT1, IC ₅₀ =23 nM). OATD-01 shows excellent PK profile in multiple species and is selective against a panel of other off-targets. OATD-01 exhibits significant antifibrotic efficacy in vivo and can be used for pulmonary fibrosis (IPF) research ^[1] .
In Vitro	OATD-01 exhibits high affinity toward h/mCHIT1 and h/mAMCase, and the inhibitory constants (K _i) for all four enzymes are 17.3 nM, 26.05 nM, 4.8 nM and 5.7 nM, respectively ^[1] . These K _i values reveals good correlation with earlier established IC ₅₀ data, the IC ₅₀ values are 23 nM, 28 nM, 9 nM and 7.8 nM for hCHIT1, mCHIT1, hAMCase and mAMCase, respectively ^[1] . Off-target in vitro effects of compound OATD-01 have been evaluated at 10 μM in the Eurofins Panlabs panel of 98 in vitro

binding and enzymatic assays, involving diverse molecular classes of proteins^[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

OATD-01 (oral gavage; 30 mg/kg, 100 mg/kg; once daily; 21 days) shows significant antifibrotic efficacy in an animal model of bleomycin-induced pulmonary fibrosis. It reduces the degree of lung fibrosis in a dose-dependent manner, ultimately achieving comparable therapeutic efficacy to reference treatment with Nintedanib in this animal model^[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Female BALB/c mice ^[1]
Dosage:	30 mg/kg, 100 mg/kg
Administration:	Oral gavage; 30 mg/kg, 100 mg/kg; once daily; 21 days
Result:	Reduced the degree of lung fibrosis in vivo ^[1]

CUSTOMER VALIDATION

- Neurosci Res. 2021 Jun 7;S0168-0102(21)00121-8.

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REFERENCES

[1]. Robert Koralewski, et al. Discovery of OATD-01, a First-in-Class Chitinase Inhibitor as Potential New Therapeutics for Idiopathic Pulmonary Fibrosis. J Med Chem. 2020 Dec 24;63(24):15527-15540.

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

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA