**Proteins** 

# Inhibitors



## **Product** Data Sheet

## MRT-83 hydrochloride

Cat. No.: HY-18287A CAS No.: 1359944-60-7 Molecular Formula:  $\mathsf{C}_{31}\mathsf{H}_{31}\mathsf{ClN}_4\mathsf{O}_5$ 

Molecular Weight: 575.05 Target: Smo

Pathway: Stem Cell/Wnt

Storage: 4°C, sealed storage, away from moisture

\* In solvent: -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)

### **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 250 mg/mL (434.74 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	1.7390 mL	8.6949 mL	17.3898 mL
	5 mM	0.3478 mL	1.7390 mL	3.4780 mL
	10 mM	0.1739 mL	0.8695 mL	1.7390 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: ≥ 2.08 mg/mL (3.62 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.08 mg/mL (3.62 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (3.62 mM); Clear solution

#### **BIOLOGICAL ACTIVITY**

Description	MRT-83 (hydrochloride) is the potent antagonist of Smoothened (Smo) receptor. MRT-83 (hydrochloride) inhibits the Hedgehog (Hh) signaling pathway and BODIPY-cyclopamine binding to human Smo. MRT-83 (hydrochloride) has the potential for researching cancer disease <sup>[1]</sup> .
IC <sub>50</sub> & Target	$Smo^{[1]}$
In Vitro	MRT-83 (hydrochloride) (compound 86) has $IC_{50}$ s of 15 and 11 nM respectively in Shh-light2 and C3H10T1/2 cells in the biological activity assay <sup>[1]</sup> .  MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES							
[1]. Solinas A, et al. Acylthiourea, acylurea, and acylguanidine derivatives with potent hedgehog inhibiting activity. J Med Chem. 2012;55(4):1559-1571.							
		t been fully validated for m Fax: 609-228-5909					
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