

## **Product** Data Sheet

# (-)-PX20606 (trans isomer)

 Cat. No.:
 HY-100443B

 CAS No.:
 1268244-88-7

 Molecular Formula:
 C<sub>29</sub>H<sub>22</sub>Cl<sub>3</sub>NO<sub>4</sub>

Molecular Weight: 554.85

Target: FXR; Autophagy

Pathway: Metabolic Enzyme/Protease; Autophagy

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

#### **SOLVENT & SOLUBILITY**

In Vitro Ethanol : ≥ 50 mg/mL (90.11 mM)

\* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	1.8023 mL	9.0114 mL	18.0229 mL
	5 mM	0.3605 mL	1.8023 mL	3.6046 mL
	10 mM	0.1802 mL	0.9011 mL	1.8023 mL

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

In Vivo

- 1. Add each solvent one by one: 10% EtOH >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (4.51 mM); Clear solution
- 2. Add each solvent one by one: 10% EtOH >> 90% corn oil Solubility: ≥ 2.5 mg/mL (4.51 mM); Clear solution

### **BIOLOGICAL ACTIVITY**

Description	(-)-PX20606 trans isomer is a FXR agonist with EC <sub>50</sub> s of 18 and 29 nM for FXR in FRET and M1H assay, respectively.
IC <sub>50</sub> & Target	EC50: 18 nM (FXR in FRET assay), 29 nM (FXR in M1H assay) <sup>[1]</sup>

#### **REFERENCES**

[1]. Kinzel O, et al. Novel substituted isoxazole FXR agonists with cyclopropyl, hydroxycyclobutyl and hydroxyazetidinyl linkers: Understanding and improving key determinants of pharmacological properties. Bioorg Med Chem Lett. 2016 Aug 1;26(15):3746-53.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$ 

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