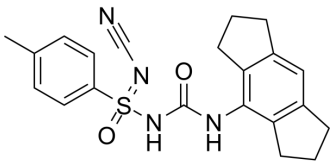
NLRP3-IN-17

Cat. No.:	HY-153261
CAS No.:	2254432-75-0
Molecular Formula:	$C_{21}H_{22}N_4O_2S$
Molecular Weight:	394.49
Target:	NOD-like Receptor (NLR)
Pathway:	Immunology/Inflammation
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 : 33.33 mg/mL (84.49 mM; ultrasonic and warming and heat to 80°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5349 mL	12.6746 mL	25.3492 mL
	5 mM	0.5070 mL	2.5349 mL	5.0698 mL
	10 mM	0.2535 mL	1.2675 mL	2.5349 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 (6.34 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (6.34 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (6.34 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

NLRP3-IN-17 is a potent, selective and orally active NLRP3 inflammasome inhibitor with an IC_{50} value of 7 nM. NLRP3-IN-17 significantly inhibits NLRP3 dependent IL-1β secretion in mice and can be used for chronic inflammatory diseases research [1].

IC_{50} & Target

NLRP3 inflammasome
7 nM (IC_{50})

In Vivo

NLRP3-IN-17 (compound 15) (3 mg/kg; po) displays desired PK profile, the AUC, t and F% values are 4.2 μg.h/mL, 2.91 h, and 56%, respectively[1].

NLRP3-IN-17 (10 mg/kg; po; single dosage) significantly inhibit NLRP3 dependent IL-1β secretion in acute in vivo LPS+ATP challenged model in female C57BL/6 mice, it decreases the IL-1β levels by 44%[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Sameer Agarwal, et al. Discovery of N-Cyano-sulfoximineurea Derivatives as Potent and Orally Bioavailable NLRP3 Inflammasome Inhibitors. ACS Med Chem Lett. 2020 Feb 27;11(4):414-418.

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