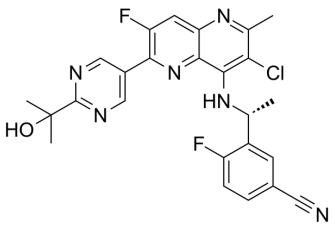
TNF-α-IN-2

Cat. No.:	HY-134471
CAS No.:	2074702-04-6
Molecular Formula:	$C_{25}H_{21}ClF_2N_6O$
Molecular Weight:	494.92
Target:	TNF Receptor
Pathway:	Apoptosis
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (202.05 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0205 mL	10.1026 mL	20.2053 mL
	5 mM	0.4041 mL	2.0205 mL	4.0411 mL
	10 mM	0.2021 mL	1.0103 mL	2.0205 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.05 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.05 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

TNF-α-IN-2 is a potent and orally active inhibitor of tumor necrosis factor alpha (TNFα), with an IC_{50} of 25 nM in the HTRF assay. TNF-α-IN-2 distorts the TNFα trimer upon binding, leading to aberrant signaling when the trimer binds to TNFR1. TNF-α-IN-2 can be used for the research of rheumatoid arthritis[1].

IC_{50} & Target

CD40
25 nM (IC_{50})

In Vitro

TNF-α-IN-2 (compound 42) (30 min) inhibits the E-selectin expression induced by soluble TNFα in HUVECs, with an IC_{50} of 30 nM[1].

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

In Vivo

TNF-α-IN-2 (5-25 mg/kg; p.o. 1 h before TNF stimulation) inhibits TNF-induced IL-6 in mice[1].

TNF-α-IN-2 (2-10 mg/kg; p.o. twice daily for 10 d) dose dependently reduces both the clinical score as well as the levels of inflammatory cytokines and leukocyte cell surface receptors in mice[1].

TNF-α-IN-2 (0.5 mg/kg; i.v.) exhibits long $t_{1/2}$ (6.2 h), low CL (6.6 mL/min•kg), and V_{ss} (3.2 L/kg) in mice[1].

TNF-α-IN-2 (2 mg/kg; p.o.) exhibits good oral bioavailability (58%), C_{max} (0.47 μM), and AUC_{tot} (5.9 μM•h) in mice[1].

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

Animal Model:	Female C57Bl/6 mice[1]
Dosage:	5, 25 mg/kg
Administration:	P.o. 1 h prior to TNF stimulation
Result:	Inhibited IL-6 moderately at 5 mg/kg while the inhibition at 25 mg/kg was similar to mouse Enbrel, which served as the positive control in the study.

REFERENCES

[1]. Xiao HY, et, al. Biologic-like In Vivo Efficacy with Small Molecule Inhibitors of TNFα Identified Using Scaffold Hopping and Structure-Based Drug Design Approaches. J Med Chem. 2020 Dec 1.

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