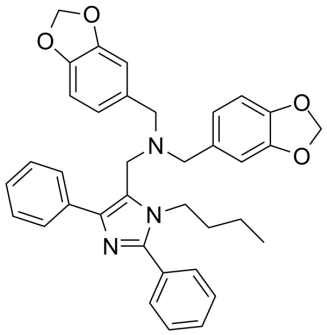
NDT 9513727

Cat. No.:	HY-110060
CAS No.:	439571-48-9
Molecular Formula:	$C_{36}H_{35}N_3O_4$
Molecular Weight:	573.68
Target:	Complement System
Pathway:	Immunology/Inflammation
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (174.31 mM; Need ultrasonic)

Ethanol : 57 mg/mL (99.36 mM; Need ultrasonic and warming)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.7431 mL	8.7157 mL	17.4313 mL
	5 mM	0.3486 mL	1.7431 mL	3.4863 mL
	10 mM	0.1743 mL	0.8716 mL	1.7431 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 (4.36 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (4.36 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.36 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NDT 9513727 is a potent, selective, orally active and competitive inverse agonist of the human C5aR (C5a receptor), with an IC_{50} of 11.6 nM. NDT 9513727 can be used for the research of human inflammatory diseases[1].

IC_{50} & Target

IC50: 11.6 nM (human C5aR)[1]

In Vitro

NDT 9513727 inhibits C5a-stimulated responses, including guanosine 5'-3-O-(thio)triphosphate binding, Ca^{2+} mobilization, oxidative burst, degranulation, cell surface CD11b expression and chemotaxis in various cell types with IC_{50}s from 1.1 to 9.2

nM, respectively[1].

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

In Vivo

NDT 9513727 (3-30 mg/kg; p.o.) exhibits a dose-dependent inhibition of hC5a-induced neutropenia[1].

NDT 9513727 exhibits moderate oral bioavailability (rat 73%, monkey 26%) and C_{max} (rat 5.98 μM, monkey 830 nM) following oral administration (rat 50, monkey 25.2 mg/kg)[1].

NDT 9513727 exhibits moderate plasma elimination half-lives (rat 4.8, monkey 7.9 h) due to low plasma clearance (1.4 L/h/kg and 3.8 L/h/kg respectively) following oral administration (rat 50, monkey 25.2 mg/kg)[1].

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

Animal Model:	Six-week-old Mongolian gerbils[1]
Dosage:	1 mg/kg, 3 mg/kg, 10 mg/kg, 30 mg/kg
Administration:	Oral administration
Result:	Significantly inhibited hC5a-induced neutropenia at 3 mg/kg, 10 mg/kg, 30 mg/kg.

Animal Model:	Rat[1]
Dosage:	50 mg/kg (Pharmacokinetic Analysis)
Administration:	Oral administration
Result:	Oral bioavailability (73%), C_{max} (5.98 μM), $T_{1/2}$ (4.8 h).

Animal Model:	Monkey[1]
Dosage:	25.2 mg/kg (Pharmacokinetic Analysis)
Administration:	Oral administration
Result:	Oral bioavailability (26%), C_{max} (830 nM), $T_{1/2}$ (7.9 h).

REFERENCES

[1]. Robbin M Brodbeck, et al. Identification and characterization of NDT 9513727 [N,N-bis(1,3-benzodioxol-5-ylmethyl)-1-butyl-2,4-diphenyl-1H-imidazole-5-methanamine], a novel, orally bioavailable C5a receptor inverse agonist. J Pharmacol Exp Ther. 2008 Dec;3

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