AZD-5672

Cat. No.: HY-119101

CAS No.: 780750-65-4

Molecular Formula: $C_{32}H_{38}F_2N_2O_5S_2$

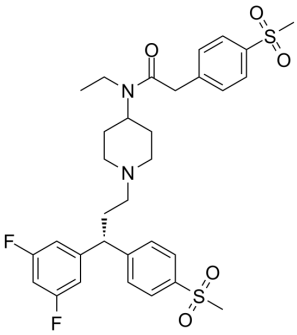
Molecular Weight: 632.78

Target: Potassium Channel; CCR; P-glycoprotein

Pathway: Membrane Transporter/Ion Channel; GPCR/G Protein; Immunology/Inflammation

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 : 33.33 mg/mL (52.67 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.5803 mL	7.9016 mL	15.8033 mL
	5 mM	0.3161 mL	1.5803 mL	3.1607 mL
	10 mM	0.1580 mL	0.7902 mL	1.5803 mL

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

BIOLOGICAL ACTIVITY

Description

AZD-5672 is an orally active, potent, and selective CCR5 antagonist (IC_{50}=0.32 nM). AZD-5672 shows moderate activity against the hERG ion channel (binding IC_{50}=7.3 μM). AZD5672 is a substrate of human P-gp, and inhibits P-gp-mediated digoxin transport (IC_{50}=32 μM). AZD-5672 can be used for the research of rheumatoid arthritis[1][2][3].

IC_{50} & Target

CCR5	hERG	hP-gp
0.32 nM (IC_{50})	7.3 μM (IC_{50})	32 μM (IC_{50})

In Vitro

AZD-5672 (0, 0.1, 0.3, 1, 3, 10, 30, and 100 μM) inhibits P-gp-mediated digoxin transport in a concentration-dependent manner (mean apparent IC_{50}: 32 μM) in Caco-2 cells[2].

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

In Vivo

In vivo pharmaeokineties data for AZD-5672 (compound 1)[1]

Species	CI[a]	V_{ss}[a] (L/kg)	$t_{1/2}$[a] (h)

	(mL/min/kg)		
Rat	28	5.3	2.6
Dog	18	5.7	3.9

[a] AZD-5672 dosed 1-2 mg/kg i.v.

[b] AZD-5672 dosed 2-5 mg/kg p.o.

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

REFERENCES

[1]. Cumming JG, et al. Balancing hERG affinity and absorption in the discovery of AZD5672, an orally active CCR5 antagonist for the treatment of rheumatoid arthritis. Bioorg Med Chem Lett. 2012 Feb 15;22(4):1655-9.

[2]. Elsby R, et al. The utility of in vitro data in making accurate predictions of human P-glycoprotein-mediated drug-drug interactions: a case study for AZD5672. Drug Metab Dispos. 2011 Feb;39(2):275-82.

[3]. Gerlag DM, et al. Preclinical and clinical investigation of a CCR5 antagonist, AZD5672, in patients with rheumatoid arthritis receiving methotrexate. Arthritis Rheum. 2010 Nov;62(11):3154-60.

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