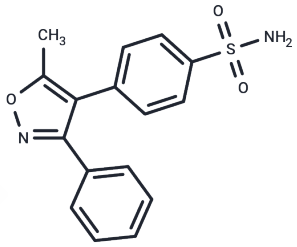
Data Sheet (Cat.No.T0219)

TargetMol

Valdecoxib

Chemical Properties



CAS No. : 181695-72-7

Formula: C16H14N2O3S

Molecular Weight: 314.36

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	Valdecoxib (SC 65872) is a prescription drug used in the treatment of osteoarthritis, rheumatoid arthritis, and painful menstruation and menstrual symptoms. It is classified as a nonsteroidal anti-inflammatory drug, or NSAID, and should not be taken by anyone allergic to these types of medications.
Targets(IC50)	COX
In vitro	Valdecoxib demonstrates significant efficacy in acute and chronic inflammation models in rats, with ED50 values of 0.06 mg/kg for carrageenan air-pouch inflammation, 5.9 mg/kg for paw edema, and 0.03 mg/kg for nonspecific arthritis. When administered alone, valdecoxib shows slow absorption in vivo, achieving a maximum inhibition of 16% in edema at 3 hours post-administration. In contrast, the valdecoxib complexes VALD-βCd and VALD-SBE7βCd exhibit high absorption rates, suppressing over 50% of edema within 1 hour, and achieving a maximum inhibition of 66% at 3 hours. Orally administered valdecoxib inhibits carrageenan-induced rat paw edema with an ED50 value of 10.2 mg/kg. In a rat model of nonspecific arthritis, oral valdecoxib shows chronic anti-inflammatory activity, with an ED50 of 0.032 mg/kg/day. Valdecoxib also inhibits prostaglandin production at the inflammation site in rats with carrageenan air-pouch inflammation when administered orally, with an ED50 value of 0.02 mg/kg.
In vivo	Valdecoxib inhibits the production of PGE2 in plasma induced by lipopolysaccharides (IC50: 0.89 μM) and suppresses the generation of TxB2 in plasma (IC50: 25.4 μM). It binds to COX-2 with a Ka of 1.1×10^5 M/s and exhibits a strong overall saturable binding affinity to COX-2 of 2.6 nM. After 15 minutes (DP15), valdecoxib has a solubility percentage of 10.5%, while its hydrophilic derivatives (VALD-βCd, VALD-HPβCd, and VALD-SBE7βCd complexes) display significantly increased solubility percentages of 50%, 91%, and 93%, respectively.

Solubility Information

Solubility	DMSO: 60 mg/mL (190.86 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.1811 mL	15.9053 mL	31.8107 mL
5 mM	0.6362 mL	3.1811 mL	6.3621 mL
10 mM	0.3181 mL	1.5905 mL	3.1811 mL
50 mM	0.0636 mL	0.3181 mL	0.6362 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Reference

Talley JJ, et al. J Med Chem, 2000, 43(5), 775-777.
Gierse JK, et al. J Pharmacol Exp Ther, 2005, 312(3), 1206-12012.
Hood WF, et al. Mol Pharmacol, 2003, 63(4), 870-877.
Rajendrakumar K, et al. Eur J Pharm Biopharm, 2005, 60(1), 39-46.
Zhang JY, et al. Drug Metab Dispos, 2003, 31(4), 491-501.