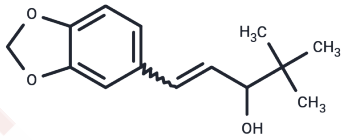
Data Sheet (Cat.No.T4498)

TargetMol

Stiripentol

Chemical Properties



CAS No. : 49763-96-4

Formula: C14H18O3

Molecular Weight: 234.29

Storage: Store at low temperature
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Stiripentol (BCX2600) (STP) is an anticonvulsant agent, which can inhibit N-demethylation of CLB to NCLB mediated by CYP3A4 (noncompetitively) and CYP2C19 (competitively) with Ki of 1.59/0.516 μM and IC50 of 1.58/3.29 μM, respectively.
Targets(IC50)	Cytochromes P450
In vitro	The inhibition of CLB demethylation by Stiripentol (STP) is best described by a noncompetitive inhibition model with apparent Ki (1.6 μM) for the cDNA-expressing CYP3A4 and by a competitive inhibition model with Ki (0.52 μM) for the cDNA-expressing CYP2C19. Formation of OH-NCLB from NCLB by cDNA-expressing CYP2C19 is competitively inhibited by Stiripentol (STP) with a Ki: 0.14 μM [1].
In vivo	In mice treated with Stiripentol (STP) monotherapy, the difference between BT1 (39.67 ±1.09°C) and BT2 (41.32±1.05°C) is statistically significant (t=3.097, p<0.05). The difference in BT2 between Stiripentol (STP) monotherapy and CLB monotherapy is also statistically significant (t=2.615, p<0.05). In mice treated with Stiripentol (STP)+CLB combination therapy, the difference between BT1 (40.18±0.58°C) and BT2 (43.03±0.49°C) is statistically significant (t=10.44, p<0.01) [2].
Cell Research	The inhibition constants (apparent Ki) of Stiripentol (STP) for CLB demethylation by CYP3A4 and CYP2C19 are determined using various concentrations of CLB (2, 10, 20, 40, 60, and 100 μM) with increasing concentrations of Stiripentol (STP) (0, 0.5, 1, 2, and 5 μM). Concerning NCLB hydroxylation by CYP2C19, the apparent Ki is similarly determined with different concentrations of NCLB (1.5, 4, 6, 8, 12, and 14 μM) and STP (0, 0.1, 0.5, 1, and 2 μM). IC50 values are determined by coincubation of the substrate at the concentration in the range of the therapeutic plasma concentrations (2 μM CLB or 14 μM NCLB) with increasing concentrations of Stiripentol (STP) (0.001-10 μM) [1].
Animal Research	Two age groups, p1M (n=18, age 4 weeks) and p5M (n=18, age 5-10 months), of Scn1aRX/+ mice are assigned in this experiment. Both groups are divided randomly into three subgroups (n=6), and each subgroup is administered Stiripentol (STP) (300 mg/kg) alone, CLB (6.62 mg/kg) alone, or a combination of Stiripentol (STP) (p1M; 150 mg/kg, p5M; 300 mg/kg) and CLB (6.62 mg/kg). All drugs are administered by intraperitoneal injection (i.p.) after a 48-h recovery from baseline seizure study. Blood samples are collected at 1 h and 20 min after administration of CLB or STP+CLB for measurement of plasma concentrations of CLB and N-desmethylclobazam, respectively [2].

Solubility Information

Solubility	DMSO: 250 mg/mL (1067.05 mM),Sonication is recommended. Ethanol: 30 mg/mL (128.05 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (21.34 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	4.2682 mL	21.3411 mL	42.6821 mL
5 mM	0.8536 mL	4.2682 mL	8.5364 mL
10 mM	0.4268 mL	2.1341 mL	4.2682 mL
50 mM	0.0854 mL	0.4268 mL	0.8536 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.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Giraud C, et al. In vitro and in vivo inhibitory effect of stiripentol on clobazam metabolism.Drug Metab Dispos. 2006 Apr;34(4):608-11. Epub 2006 Jan 13.

Avdeef A, Kansy M. Predicting Solubility of Newly-Approved Drugs (2016–2020) with a Simple ABSOLV and GSE (Flexible-Acceptor) Consensus Model Outperforming Random Forest Regression. Journal of Solution Chemistry. 2022: 1-36.

Cao D, et al. Efficacy of stiripentol in hyperthermia-induced seizures in a mouse model of Dravet syndrome. Epilepsia. 2012 Jul;53(7):1140-5.

Tel:781-999-4286 E_mail:info@targetmol.com Address:34 Washington Street,Wellesley Hills,MA 02481