DFBTA

Cat. No.: HY-146334

CAS No.: 2966044-07-3

Molecular Formula: $C_{18}H_{10}ClF_2NO_3S$

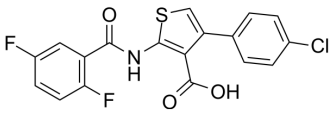
Molecular Weight: 393.79

Target: Chloride Channel

Pathway: Membrane Transporter/Ion Channel

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 (253.94 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5394 mL	12.6971 mL	25.3942 mL
	5 mM	0.5079 mL	2.5394 mL	5.0788 mL
	10 mM	0.2539 mL	1.2697 mL	2.5394 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (6.35 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

DFBTA is an orally active, potent and little brain penetrated ANO1 (Calcium-activated chloride channel anoctamin-1) inhibitor, with an IC_{50} of 24 nM. DFBTA shows analgesic efficacy for inflammatory pain[1].

IC_{50} & Target

IC_{50}: 0.024 ± 0.012 μM (ANO1), 8.7 ± 1.0 μM (ANO2)[1]

In Vitro

DFBTA shows very weak cytotoxicity and cardiotoxicity (HEK293 proliferation IC50 > 30 μM, hERG IC50 > 30 μM)[1]

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

In Vivo

DFBTA (C57BL/6 mice; 40-80 mg/kg, IG; 40 mg/kg, IV; once) shows weak acute toxicity, with mouse minimum lethal dosage (MLD) > 1000 mg/kg[1].

DFBTA (C57BL/6 mice, 1000 mg/kg, Orally, once) shows excellent pharmacokinetics properties with oral bioavailability > 75% and little brain penetration (<1.5% brain/plasma)[1].

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

REFERENCES

[1]. Wang Y, et al. Optimization of 4-arylthiophene-3-carboxylic acid derivatives as inhibitors of ANO1: Lead optimization studies toward their analgesic efficacy for inflammatory pain. Eur J Med Chem. 2022 Jul 5;237:114413.

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