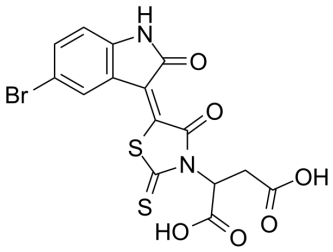
CID5721353

Cat. No.:	HY-100502
CAS No.:	301356-95-6
Molecular Formula:	$C_{15}H_9BrN_2O_6S_2$
Molecular Weight:	457.28
Target:	Apoptosis; Bcl-2 Family
Pathway:	Apoptosis
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (109.34 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1868 mL	10.9342 mL	21.8684 mL
	5 mM	0.4374 mL	2.1868 mL	4.3737 mL
	10 mM	0.2187 mL	1.0934 mL	2.1868 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 (5.47 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.47 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CID5721353 is an inhibitor of BCL6 with an IC_{50} value of 212 μM, which corresponds to a K_i of 147 μM.

IC_{50} & Target

IC50: 212 μM (BCL6)[1]
Ki: 147 μM(BCL6)[1]

In Vitro

BCL6 is a member of the BTB/POZ family of transcription factors. CID5721353 (Compound 79-6) specifically inhibits BCL6 repressor activity. CID5721353 disrupts BCL6 transcriptional complexes and reactivates BCL6 target genes. CID5721353 can specifically kill primary human DLBCL cells. Fifteen of 19 BCL6-positive cases (79%) display greater than 25% loss of viability in response to CID5721353 at 125 or 250 μM[1].

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

In Vivo	In order to test whether CID5721353 (Compound 79-6) can perform as an anti-lymphoma therapeutic agent in vivo, whether it can penetrate tumors after parenteral administration through a distal site is determined. For this purpose 107OCI-Ly7 cells are injected into the right flank of 10 SCID mice and allowed to form tumors. Once tumors reach ~1.5 grams, animals are injected IP with a single dose of 50 mg/kg of CID5721353 in 10% DMSO or vehicle (10% DMSO) and sacrificed at 0.5, 1, 1.5, 3, 6, 12 and 24 hours after CID5721353 administration. Blood and tumors are harvested. Quantitative HPLC/MS analysis of the serum shows that CID5721353 levels peak (to 55 μg/mL, which is equivalent to a 122 μM concentration) one hour after the IP injection. CID5721353 also reaches its highest peak (24.5 ng/mg) at the 1-hour time point in the tumors, and after a sharp decline in levels, decreases gradually over 24 hours[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [1]	Cell number and viability are determined by an EB/AO-based method and cells are cultivated in medium containing 80% RPMI and 20% human serum supplemented with antibiotics, L-glutamine and HEPES for 48 h. Pimary human diffuse large B cell lymphoma (DLBCL) cells are exposed to 125 and 250 μM of CID5721353 or control (DMSO) in triplicates. After 48 h of exposure viability is determined by using an ATP-based luminescent method and EB/AO. Specimens with 20% or higher loss of viability in the controls are discarded[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [1]	Mice[1] Six to eight-week old male SCID mice are subcutaneously injected in the left flank with low-passage 107 human OCI-Ly7 cells. When tumors reach 1500 mm^3 the mice are IP injected with 50 mg/kg of CID5721353 in DMSO (n=8) or DMSO (control, n=2). Blood and tumors are harvested at different time points after injection (30 min, 1 h, 1.5 h, 3 h, 6 h, 12 h and 24 h)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Cerchietti LC, et al. A small-molecule inhibitor of BCL6 kills DLBCL cells in vitro and in vivo. Cancer Cell. 2010 Apr 13;17(4):400-11.

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