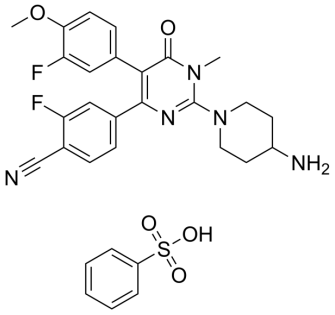
Pulrodemstat benzenesulfonate

Cat. No.:	HY-129388B
CAS No.:	2097523-60-7
Molecular Formula:	$C_{30}H_{29}F_2N_5O_5S$
Molecular Weight:	609.64
Target:	Histone Demethylase
Pathway:	Epigenetics
Storage:	4°C, sealed storage, away from moisture * In solvent : -80°C, 2 years; -20°C, 1 year (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (82.02 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.6403 mL	8.2016 mL	16.4031 mL
	5 mM	0.3281 mL	1.6403 mL	3.2806 mL
	10 mM	0.1640 mL	0.8202 mL	1.6403 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: ≥ 2.08 mg/mL (3.41 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (3.41 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CC-90011 benzenesulfonate is a potent, selective, reversible and orally active inhibitor of lysine specific demethylase-1 (LSD1) with an IC_{50} of 0.25 nM. CC-90011 benzenesulfonate is less enzymatic inhibition against LSD2, MOA-A, and MAO-B. CC-90011 benzenesulfonate induces acute myeloid leukemia (AML) and small cell lung cancer (SCLC) cells differentiation and has potent anticancer activity[1].

IC_{50} & Target

KDM1/LSD1

In Vitro

CC-90011 (Compound 11) shows potent induction of on-target cellular differentiation marker CD11b in THP-1 cell line with an EC_{50} of 7 nM, antiproliferative activity in AML kasumi-1 cells with an EC_{50} of 2 nM[1].
Suppression of GRP is observed with treatment of CC-90011 (4 days) in a dose-dependent manner and at pharmacologically useful concentrations (EC_{50}=3 nM, H209 and 4 nM, H1417). CC-90011 (12 days) treatment of SCLC cells results in potent

	antiproliferative activity (EC_{50}=6 nM, H1417) that correlated with GRP suppression[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	CC-90011 (5 mg/kg; oral administration; daily; for 30 days) treatment inhibits tumor growth in patient-derived xenograft SCLC models[1]. CC-90011 (once a day; for 4 days) treatment results in robust downregulation of GRP mRNA levels at 2.5 mg/kg and maximum suppression of GRP at 5 mg/kg in a SCLC human tumor xenograft (H1417) mice[1]. After i.v. administration, CC-90011 (Compound 11; 5 mg/kg) has systemic clearance of 32.4 mL/min/kg, elimination half-life of 2 h, and a high volume of distribution of 7.5 L/kg. CC-90011 (Compound 11; 5 mg/kg) is readily absorbed after oral administration with an $AUC_{0\text{-}24h}$ of 1.8 μM·h, C/sub>max of 0.36 μM, and oral bioavailability of 32%[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	BALB/c nude mice bearing small cell lung carcinoma (SCLC)[1]
Dosage:	5 mg/kg
Administration:	Oral administration; daily; for 30 days
Result:	Showed a tumor growth inhibition (TGI) of 78% at 5 mg/kg with no body weight loss.

CUSTOMER VALIDATION

- Eur J Med Chem. 2023 Nov 5;259:115684.
- ACS Pharmacol Transl Sci. November 12, 2021.

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REFERENCES

[1]. Toufike Kanouni, et al. Discovery of CC-90011: A Potent and Selective Reversible Inhibitor of Lysine Specific Demethylase 1 (LSD1). J Med Chem. 2020 Dec 10;63(23):14522-14529.

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