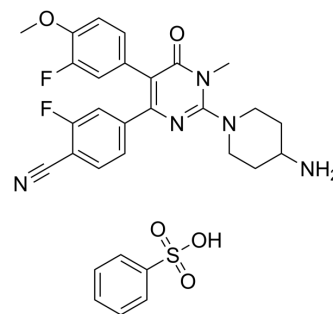


Pulrodemstat benzenesulfonate

Cat. No.:	HY-129388B
CAS No.:	2097523-60-7
Molecular Formula:	C ₃₀ H ₂₉ F ₂ N ₅ O ₅ S
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 Concentration	Mass	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_{0-24h} of 1.8 $\mu\text{M}\cdot\text{h}$, $C_{sub>max}$ 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.

Caution: Product has not been fully validated for medical applications. For research use only.

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