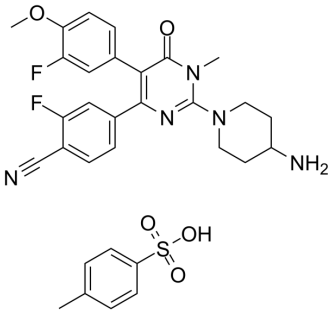
Pulrodemstat Methylbenzenesulfonate

Cat. No.:	HY-129388
CAS No.:	2097523-57-2
Molecular Formula:	$C_{31}H_{31}F_2N_5O_5S$
Molecular Weight:	623.67
Target:	Histone Demethylase
Pathway:	Epigenetics
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	CC-90011 Methylbenzenesulfonate 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 Methylbenzenesulfonate is less enzymatic inhibition against LSD2, MOA-A, and MAO-B. CC-90011 Methylbenzenesulfonate induces acute myeloid leukemia (AML) and small cell lung cancer (SCLC) cells differentiation and has potent anticancer activity[1].
IC_{50} & Target	IC50: 0.25 nM (LSD1)[1]
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; 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

- 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.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA