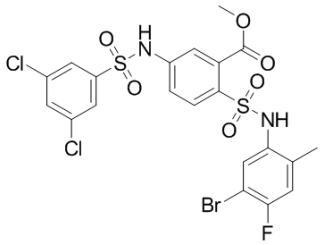
MDL-800

Cat. No.:	HY-119376
CAS No.:	2275619-53-7
Molecular Formula:	$C_{21}H_{16}BrCl_2FN_2O_6S_2$
Molecular Weight:	626.3
Target:	Sirtuin
Pathway:	Cell Cycle/DNA Damage; Epigenetics
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 : 125 mg/mL (**199.58 mM;** Need ultrasonic)
H_2O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.5967 mL	7.9834 mL	15.9668 mL
	5 mM	0.3193 mL	1.5967 mL	3.1934 mL
	10 mM	0.1597 mL	0.7983 mL	1.5967 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: ≥ 2.08 mg/mL (3.32 mM); Clear solution
2. Add each solvent one by one: **10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline**
   Solubility: ≥ 2.08 mg/mL (3.32 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

MDL-800 is an allosteric and selective **SIRT6** activator. MDL-800 increases SIRT6 deacetylation activity with an **EC_{50}** of 10.3 μM[1].

IC_{50} & Target

SIRT6
10.3 μM (EC50)

In Vitro

MDL-800 potently activates SIRT6 at ~10 μM but shows no activity toward SIRT1, SIRT3, SIRT4, and HDAC1-11 at concentrations up to 50 or 100 μM. Although MDL-800 exhibits weak activity toward SIRT2, SIRT5, and SIRT7, the EC

$_{50}$ or IC_{50} values are greater than 100 μM, tenfold less than that against SIRT6[1].
MDL-800 directly activates SIRT6 deacetylation by increasing the binding affinities of acetylated substrates and cofactor as well as increasing the catalytic efficiency of SIRT6[1].
MDL-800 (1-1000 μM; 48 hours) decreases the proliferation of Bel7405, PLC/PRF/5, and Bel7402 cells with IC_{50}s for cell growth (IC_{50}-growth) of 23.3 μM, 18.6 μM, and 24.0 μM, respectively, and EC_{50}s for cell death (EC_{50}-death) of 90.4 μM, 87.0 μM, and 106.5 μM, respectively[1].
MDL-800 (0-50 μM; 24 and 48 hours) decreases both H3K9ac and H3K56ac at a concentration of 10 μM and shows a dose-dependent effect in Bel7405, PLC/PRF/5, and Bel7402 cells at 24 and 48 h[1].

Cell Proliferation Assay[1]

Cell Line:	Bel7405, PLC/PRF/5, and Bel7402 cells
Concentration:	1, 10, 100 , 1000 μM
Incubation Time:	48 hours
Result:	Decreased the proliferation of Bel7405, PLC/PRF/5, and Bel7402 cells with IC_{50}s of 23.3 μM, 18.6 μM, and 24.0 μM, respectively.

Western Blot Analysis[1]

Cell Line:	Bel7405, PLC/PRF/5, and Bel7402 cells
Concentration:	0, 5, 10, 25, and 50 μM
Incubation Time:	24 and 48 hours
Result:	Decreased both H3K9ac and H3K56ac at a concentration of 10 μM and showed a dose-dependent effect in all three cell lines at 24 h and 48 h.

In Vivo

MDL800 shows effective antitumor efficacy in female BALB/c nude mice with Bel7405 xenograft tumor mode.
MDL800 (50-150 mg/kg; intraperitoneal injection; over 2 weeks) suppresses the growth of Bel7405 xenografts in a dose-dependent manner compared with vehicle alone[1].

Animal Model:	Six-week-old female BALB/c nude mice with Bel7405 xenograft tumor mode[1]
Dosage:	50, 100, and 150 mg/kg
Administration:	Intraperitoneal injection; over 2 weeks.
Result:	Suppressed the growth of Bel7405 xenografts in a dose-dependent manner. Decreased tumor weight and size.

REFERENCES

[1]. Huang Z, et al. Identification of a cellularly active SIRT6 allosteric activator. Nat Chem Biol. 2018 Dec;14(12):1118-1126.

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