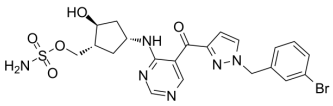
ML-792

Cat. No.:	HY-108702
CAS No.:	1644342-14-2
Molecular Formula:	$C_{21}H_{23}BrN_6O_5S$
Molecular Weight:	551.41
Target:	E1/E2/E3 Enzyme
Pathway:	Metabolic Enzyme/Protease
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 : 100 mg/mL (181.35 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8135 mL	9.0677 mL	18.1353 mL
	5 mM	0.3627 mL	1.8135 mL	3.6271 mL
	10 mM	0.1814 mL	0.9068 mL	1.8135 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 (3.77 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (3.77 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.77 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ML-792 is a potent and selective inhibitor of SAE/SUMO1 and SAE/SUMO2 in enzymatic assays (IC_{50} values of 3 and 11 nM, respectively) compared with NAE/NEDD8 and UAE/ubiquitin (IC_{50}> values of 32 μM and >100 μM, respectively)[1].

IC_{50} & Target

IC50: 3 nM (SAE/SUMO1), 11 nM (SAE/SUMO2)[1]

In Vitro

ML-792 (0.0007-5 μM; 4 hours) inhibits SAE and SUMO-pathway activities in HCT116 cells[1].
ML-792 (0.001-10 μM; 72 hours) inhibits cell proliferation and decreases cancer cell viability in MDA-MB-468, MDA-MB-231,

HCT116, Colo-205, and A375[1].

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

Cell Viability Assay[1]

Cell Line:	Human breast cancer cells MDA-MB-468 and MDA-MB-231; human colon carcinoma cells HCT116 and Colo-205; human melanoma cell line A375
Concentration:	0.001, 0.01, 0.1, 1, 10 μM
Incubation Time:	72 hours
Result:	Demonstrated a dose-dependent viability effect with EC_{50} values of 0.06 μM in MDA-MB-468 cells to 0.45 μM in A375 cells.

Western Blot Analysis[1]

Cell Line:	HCT116 cells
Concentration:	0, 0.0007, 0.002, 0.007, 0.02, 0.06, 0.19, 0.56, 1.7, 5 μM
Incubation Time:	4 hours
Result:	Revealed a dose-dependent decrease in the SAE and UBC9 thioester levels.

CUSTOMER VALIDATION

- Nat Commun. 2022 Nov 11;13(1):6840.
- Nat Commun. 2022 Sep 29;13(1):5726.
- Nat Commun. 2022 Sep 3;13(1):5204.
- Mol Cell. 2023 Jan 14;S1097-2765(23)00003-5.
- Mol Cell. 2020 Jul 2;79(1):54-67.e7.

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REFERENCES

[1]. He X, et al. Probing the roles of SUMOylation in cancer cell biology by using a selective SAE inhibitor. Nat Chem Biol. 2017 Nov;13(11):1164-1171.

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