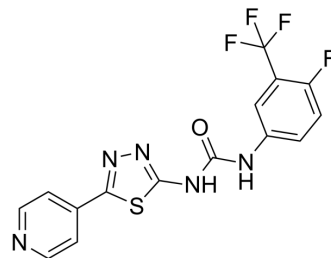


## ML216

<b>Cat. No.:</b>	HY-12342		
<b>CAS No.:</b>	1430213-30-1		
<b>Molecular Formula:</b>	C <sub>15</sub> H <sub>9</sub> F <sub>4</sub> N <sub>3</sub> OS		
<b>Molecular Weight:</b>	383		
<b>Target:</b>	DNA/RNA Synthesis		
<b>Pathway:</b>	Cell Cycle/DNA Damage		
<b>Storage:</b>	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



## SOLVENT & SOLUBILITY

<b>In Vitro</b>	DMSO : 20 mg/mL (52.22 mM; Need ultrasonic)			
		Solvent Concentration	Mass	
			1 mg	5 mg
			10 mg	
<b>Preparing Stock Solutions</b>	<b>1 mM</b>	2.6110 mL	13.0548 mL	26.1097 mL
	<b>5 mM</b>	0.5222 mL	2.6110 mL	5.2219 mL
	<b>10 mM</b>	0.2611 mL	1.3055 mL	2.6110 mL
Please refer to the solubility information to select the appropriate solvent.				
<b>In Vivo</b>	1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: 2 mg/mL (5.22 mM); Suspended solution; Need ultrasonic			

## BIOLOGICAL ACTIVITY

<b>Description</b>	ML216 (CID-49852229) is a potent, selective and cell permeable inhibitor of the DNA unwinding activity of BLM helicase with IC <sub>50</sub> s of 2.98 μM and 0.97 μM for BLM <sup>full-length</sup> and BLM <sup>636-1298</sup> , respectively. ML216 inhibits ssDNA-dependent ATPase activity of BLM with a K <sub>i</sub> of 1.76 μM. Antitumor activity <sup>[1][2]</sup> .
<b>IC<sub>50</sub> &amp; Target</b>	IC <sub>50</sub> : 2.98 μM (BLM <sup>full-length</sup> ) and 0.97 μM (BLM <sup>636-1298</sup> ) <sup>[1]</sup>
<b>In Vitro</b>	ML216 (12.5-50 μM; 24-72 hours; PSNG5 and PSNG13cells) treatment inhibits the proliferation of PSNF5 cells in a concentration-dependent manner, but not of PSNG13 cells <sup>[1]</sup> . ?ML216 treatment leads to a statistically significant increase in the frequency of sister chromatid exchanges (SCEs) in PSNF5 cells, but not in PSNG13 cells <sup>[1]</sup> . ?ML216 increases the sensitivity of PSNF5 cells to aphidicolin but has no sensitizing effect on isogenic PSNG13 cells devoid of BLM <sup>[1]</sup> .

?ML216 inhibits both the full length WRN (IC<sub>50</sub> of 5 μM) and a truncated WRN<sup>500-946</sup> (IC<sub>50</sub> of 12.6 μM), with the former being 2.5-fold more sensitive to inhibition. BLM is a little more sensitive than WRN to inhibition by ML216 (1.7-fold based on IC<sub>50</sub> values). Despite the detectable inhibition of WRN by ML216, this compound appears selective for BLM in human cells. ML216 inhibits proliferation of WRN<sup>+</sup> and WRN<sup>?</sup> cells equally well, and similarly sensitized both cell types to aphidicolin<sup>[1]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

#### Cell Proliferation Assay<sup>[1]</sup>

Cell Line:	PSNG5 and PSNG13cells
Concentration:	12.5 μM or 50 μM
Incubation Time:	24 hours, 48 hours, 72 hours
Result:	Inhibited the proliferation of PSNF5 cells, but not of PSNG13 cells, and did so in a concentration-dependent manner.

#### In Vivo

Although ML216 inhibits unwinding by the sequence-related BLM and WRN helicases similarly in vitro, the apparent dependence on BLM for ML216 to exert its biological effects in human cells suggests BLM specificity for the drug's mechanism of action in vivo. A co-crystal structure of BLM in complex with inhibitor would be informative. Cellular cues in vivo may induce a specific conformation of WRN that makes it resistant to ML216<sup>[2]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## CUSTOMER VALIDATION

- J Transl Med. 2023 Jul 6;21(1):445.
- Cells. 2022 Dec 29;12(1):145.
- Cells. 2023, 12(1), 145.
- Am J Cancer Res. 2021 Apr 15;11(4):1347-1368.

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## REFERENCES

[1]. Nguyen GH, et al. A small molecule inhibitor of the BLM helicase modulates chromosome stability in human cells. Chem Biol. 2013 Jan 24;20(1):55-62.

[2]. Banerjee T, et al. A new development in DNA repair modulation: discovery of a BLM helicase inhibitor. Cell Cycle. 2013 Mar 1;12(5):713-4.

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

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