Product Datasheet

Technical Data

Formula	$C_{31}H_{29}N_5O_3S_2$					
Molecular Weight	583.73	**CAS No.**	1431866-33-9			
Solubility (25°C)*	In vitro	DMSO	100 mg/mL (171.31 mM)			
		Water	Insoluble			
		Ethanol	Insoluble			
	In vivo (Add solvents to the product individually and in order)	Oral Administration	Homogeneous suspension	CMC-NA	≥5mg/ml	Taking the 1 mL working solution as an example, add 5 mg of this product to 1 ml of CMC-Na solution, mix evenly to obtain a homogeneous suspension with a final concentration of 5 mg/ml.
		Injection	Clear solution	5%DMSO [1]→ 40%PEG300 [2]→ 5%Tween80 [3]→ 50%ddH2O Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	2.500mg/ml (4.28mM)	Taking the 1 mL working solution as an example, add 50 μL of 50 mg/ml clarified DMSO stock solution to 400 μL PEG300, mix evenly to clarify it; add 50 μL Tween80 to the above system, mix evenly to clarify it; then continue to add 500 μL ddH2O to adjust the volume to 1 mL. The mixed solution should be used immediately for optimal results.
			Clear solution	5% DMSO [1]→ 95% corn oil Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	0.800mg/ml (1.37mM)	Taking the 1 mL working solution as an example, add 50 μL of 16 mg/ml clear DMSO stock solution to 950 μL of corn oil and mix evenly. The mixed solution should be used immediately for optimal results.

* <1 mg/ml means slightly soluble or insoluble.
* Please note that Capsid Bio tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.
* Room temperature shipping (Stability testing shows this product can be shipped at 2-8°C for storage purposes.)

Preparing Stock Solutions

Concentration \ Volume \ Mass	1 mg	5 mg	10 mg
1 mM	1.7131 mL	8.5656 mL	17.1312 mL
5 mM	0.3426 mL	1.7131 mL	3.4262 mL
10 mM	0.1713 mL	0.8566 mL	1.7131 mL
50 mM	0.0343 mL	0.1713 mL	0.3426 mL

Biological Activity

Description	WEHI-539 has high affinity (IC50=1.1 nM) and selectivity for **BCL-XL** and potently kills cells by selectively antagonizing its prosurvival activity. This compound has more than a 400-fold higher affinity for BCL-XL versus other prosurvival BCL-2 family members.
Targets	Bcl-xL [1] (Cell-free assay) 1.1 nM
In vitro	WEHI-539 shows good selectivity for BCL-XL. The tight ligand of this compound retains this selectivity (500-fold over BCL-2 and 400-fold over BCL-W, MCL-1 and A1). It kills fibroblasts that lack MCL-1. Thus, this compound not only binds very tightly to BCL-XL, with IC50 and KD values close to or below 1 nM as well as a slow dissociation rate, but also invokes apoptotic responses that depend on BAX, BAK or both; furthermore, its biological activity is related to its binding profile, as elevated amounts of MCL-1, BCL-2 and BCL-W confer marked resistance, and its ability to destroy platelets is a well-validated marker of on-target BCL-XL inhibition. In addition, this chemical induces a preferentially BAK-dependent apoptotic response in MEFs by selectively inhibiting BCL-XL[1].

Protocol (from reference)

Kinase Assay:[1]

- **AlphaScreen assay**
  The assay buffer (stock 50 mM HEPES and 100 mM NaCl, pH 7.5) is prepared fresh daily and adjusted to 5 mM DTT, casein (0.1 mg/mL sodium salt; aliquots stored at -20 °C) and Tween 20 such that the

Cell Assay:[1]

- **Cell lines**
  MEFs
- **Concentrations**
  10 μM
- **Incubation Time**
  1 h
- **Method**

Wild-type (WT), mcl-1$^{-/-}$, bcl-2$^{-/-}$ or bcl-x$^{-/-}$ MEFs were treated with 10 μM WEHI-539 or ABT-737 for 1 h and fractionated into mitochondrial-enriched (pellet) and cytosolic (soluble) fractions, which were subjected to SDS-PAGE and immunoblotted with antibody against cytochrome c (anti-cyt c); HSP70 was used as a loading control.

References

https://pubmed.ncbi.nlm.nih.gov/23603658/

RETURN POLICY

Capsid Bio's Unconditional Return Policy ensures a smooth online shopping experience for our customers. If you are in any way unsatisfied with your purchase, you may return any item(s) within 7 days of receiving it. In the event of product quality issues, either protocol related or product related problems, you may return any item(s) within 365 days from the original purchase date. Please follow the instructions below when returning products.

SHIPPING & STORAGE

Capsid Bio products are transported at room temperature. If you receive the product at room temperature, please rest assured, the Capsid Bio Quality Inspection Department has conducted experiments to verify that the normal temperature placement of one month will not affect the biological activity of powder products. After collecting, please store the product according to the requirements described in the datasheet. Most Capsid Bio products are stable under the recommended conditions.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

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