CeMMEC1 HCl

Catalog No.C13348 Batch:C1334803

Product Datasheet

Technical Data

Formula	$C_{19}H_{17}ClN_2O_4$					
Molecular Weight	372.8	**CAS No.**	2095432-53-2			
Solubility (25°C)*	In vitro	DMSO	23 mg/mL (61.69 mM)			
		Ethanol	1 mg/mL (2.68 mM)			
		Water	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.

* <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	2.6824 mL	13.4120 mL	26.8240 mL
5 mM	0.5365 mL	2.6824 mL	5.3648 mL
10 mM	0.2682 mL	1.3412 mL	2.6824 mL
50 mM	0.0536 mL	0.2682 mL	0.5365 mL

Biological Activity

Description	CeMMEC1 is an N-methylisoquinolinone derivative that inhibits the second bromodomain of **TAF1** (IC50=0.9 μM).
Targets	TAF1 [1] (Cell-based assay) 1.8 μM(Kd)
In vitro	CeMMEC1 only bound BRD4 very weakly but it shows high affinity for the bromodomains of CREBBP, EP300, BRD9 and the second bromodomain of TAF1[1].

Protocol (from reference)

Cell Assay:[1]

- **Cell lines**
  REDS3 cells
- **Concentrations**
  10 μM
- **Incubation Time**
  24 h
- **Method**
  REDS3 cells were treated with 10 μM of every compound, and live-cell imaging pictures were taken to assess their ability to induce RFP expression 24 h later. From this primary screening 1,286 small molecules were selected as hits and rescreened in the follow-up part, in which REDS3 and WT KBM7 cells were treated in three-point dose response in order to exclude autofluorescent or toxic compounds. 80 small molecules were selected as hits and used to treat WT KBM7 cells and REDS3 cells in eight-point dose (twofold dilution, starting from 100 μM) response and three-point time course (24 h, 48 h and 72 h) to carefully select the best true hits (time- and dose-dependent RFP expression/no autofluorescence). UPLC-MS analysis was done to confirm purity and the correct mass of the small molecules selected; finally, 22 small molecules fulfilled the criteria as screening hits.

References

https://pubmed.ncbi.nlm.nih.gov/27159579/

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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.

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