# **Product** Data Sheet

# **Plevitrexed**

Cat. No.: HY-13728

CAS No.: 153537-73-6

Molecular Formula:  $C_{26}H_{25}FN_8O_4$ Molecular Weight: 532.53

Target: Thymidylate Synthase

Pathway: Apoptosis

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: 100 mg/mL (187.78 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	1.8778 mL	9.3891 mL	18.7783 mL
	5 mM	0.3756 mL	1.8778 mL	3.7557 mL
	10 mM	0.1878 mL	0.9389 mL	1.8778 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: 2.5 mg/mL (4.69 mM); Clear solution; Need ultrasonic
- Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (4.69 mM); Clear solution; Need ultrasonic

### **BIOLOGICAL ACTIVITY**

Description

Plevitrexed (ZD 9331; BGC 9331) is an orally active and potent thymidylate synthase (TS) inhibitor with a  $K_i$  of 0.44 nM. Plevitrexed is taken up via the  $\alpha$ -folate receptor as well as the reduced folate carrier. Plevitrexed is used for gastric cancer in clinical<sup>[1][2][3]</sup>. Plevitrexed is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

In Vitro

ZD9331 inhibits the transport of [ $^3$ H]-methotrexate into L1210 and W1L2 cells with a K<sub>i</sub> of-1  $\mu$ M $^{[3]}$ . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

### **REFERENCES**

- [1]. Tochowicz A, et al. Development and binding mode assessment of N-[4-[2-propyn-1-yl[(6S)-4,6,7,8-tetrahydro-2-(hydroxymethyl)-4-oxo-3H-cyclopenta[g]quinazolin-6-yl]amino]benzoyl]-l-y-glutamyl-D-glutamic acid (BGC 945), a novel thymidylate synthase inhibitor that targets tumor cells. J Med Chem. 2013 Jul 11;56(13):5446-55.
- [2]. A. Thomas, et al. A phase I/II study of plevitrexed with nutritional vitamin supplementation in gastric cancer.
- [3]. Marsham PR, et al. Design and synthesis of potent non-polyglutamatable quinazoline antifolate thymidylate synthase inhibitors. J Med Chem. 1999 Sep 23;42(19):3809-20.

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

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