Proteins

Product Data Sheet



Cat. No.: HY-W587663 CAS No.: 21253-58-7 Molecular Formula: $C_{13}H_{16}N_{4}O_{3}$ Molecular Weight: 276.29

Dihydrofolate reductase (DHFR) Target: Pathway: Metabolic Enzyme/Protease

Storage: Powder -20°C 3 years

> 4°C 2 years -80°C 6 months In solvent

-20°C 1 month

SOLVENT & SOLUBILITY

In Vitro

DMSO: 50 mg/mL (180.97 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	3.6194 mL	18.0969 mL	36.1939 mL
	5 mM	0.7239 mL	3.6194 mL	7.2388 mL
	10 mM	0.3619 mL	1.8097 mL	3.6194 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

4 '-DTMP is a DHFR inhibitor with Ki of 5.1 nM (DHFRWT) and 34.3 nM (DHFRL28R), respectively. 4 '-DTMP carries a polar Description

modification that induces additional local interactions with the enzyme. In particular, the hairpin structure on the M20 ring

is related to the internal communication of the DHFR. 4 '-DTMP has potential inhibition of E.coli^[1].

Ki: 5.1 nM (WT), 34.3 nM (L28R)^[1] IC₅₀ & Target

REFERENCES

[1]. Cetin E, et al. Kinetic Barrier to Enzyme Inhibition Is Manipulated by Dynamical Local Interactions in E. coli DHFR. J Chem Inf Model. 2023 Aug 14;63(15):4839-4849.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

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