DHODH-IN-12

Molecular Weight:

Cat. No.: HY-135676 CAS No.: 1263303-93-0 Molecular Formula: $C_{10}H_9N_3O_2$

Target: Dihydroorotate Dehydrogenase; DNA/RNA Synthesis Pathway: Metabolic Enzyme/Protease; Cell Cycle/DNA Damage

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

203.2

Product Data Sheet

BIOLOGICAL ACTIVITY

Description	DHODH-IN-12 (Compound 12b) is a Leflunomide derivative and a weak dihydroorotate dehydrogenase (DHODH) inhibitor with a pK $_{\rm a}$ of 5.07 $^{[1]}$.
IC ₅₀ & Target	pKa: 5.07 (DHODH) ^[1]
In Vitro	Designed a compound structurally related to Leflunomide, containing the furazan ring (Compound 12a), is designed. Compound 12a undergo ring 4 scission under physiological pH conditions to afford the corresponding cyano-oximes DHODH-IN-12 (Compound 12b). DHODH-IN-12 has been assayed as a DHODH inhibitor; its low potency is probably due to the unfavourable stereochemistry of the oxime substructure ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Giorgis M, et al. 1,2,5-Oxadiazole analogues of leflunomide and related compounds. Eur J Med Chem. 2011 Jan;46(1):383-92.

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

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