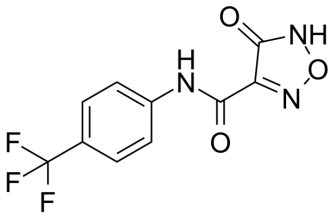
DHODH-IN-13

Cat. No.:	HY-135677
CAS No.:	1364791-86-5
Molecular Formula:	$C_{10}H_6F_3N_3O_3$
Molecular Weight:	273.17
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.



BIOLOGICAL ACTIVITY

Description	DHODH-IN-13 (Compound 7a) is a hydroxyfurazan analog of A771726. DHODH-IN-13 is a dihydroorotate dehydrogenase (DHODH) inhibitor with an IC_{50} of 4.3 μM for rat liver DHODH. DHODH-IN-13 can be used for rheumatoid arthritis[1].
IC_{50} & Target	IC50: 4.3 μM for (Rat liver DHODH)[1]
In Vitro	DHODH-IN-13 (Compound 7a) is a hydroxyfurazan analog of A771726 and is stable under physiological conditions. When DHODH-IN-13 is docked in silico at the DHODH active site, a BQN-like pose is obtained with the deprotonated furazan hydroxyl facing Arg136 instead of Tyr356, thus effectively mimicking the carboxyl group of BQN and related compounds[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Lolli ML, et al. New inhibitors of dihydroorotate dehydrogenase (DHODH) based on the 4-hydroxy-1,2,5-oxadiazol-3-yl (hydroxyfurazanyl) scaffold. Eur J Med Chem. 2012 Mar;49:102-9.

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