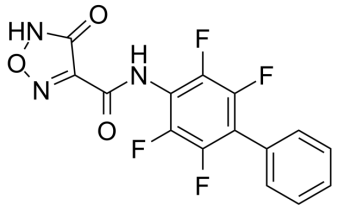
DHODH-IN-14

Cat. No.:	HY-135678
CAS No.:	1364791-93-4
Molecular Formula:	$C_{15}H_7F_4N_3O_3$
Molecular Weight:	353.23
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-14 (Compound 7l) is a hydroxyfurazan analog of A771726. DHODH-IN-14 is a dihydroorotate dehydrogenase (DHODH) inhibitor with an IC_{50} of 0.49 μM for rat liver DHODH. DHODH-IN-14 can be used for rheumatoid arthritis[1].
IC_{50} & Target	IC50: 0.49 μM (Rat liver DHODH)[1]
In Vitro	DHODH-IN-14 (Compound 7l) is a hydroxyfurazan analog of A771726, in which the biphenyl scaffold with fluoro substituents. Moving to derivatives DHODH-IN-14, no major differences were observed among the poses obtained on 1UUO and 1D3G; in both cases DHODH-IN-14 is found to bind in a BQN-like fashion, namely with the deprotonated hydroxyfurazan moiety facing Arg136, thus effectively mimicking the carboxyl group of BQN and related compounds. While on 1D3G and 1UUO the hydroxyfurazan is in no case found to interact with Tyr356 in a Leflunomide-like fashion, a significant fraction of such poses is found when 2BXV is used as the docking target[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.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA