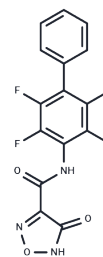


DHODH-IN-14

Chemical Properties

CAS No. :	1364791-93-4
Formula:	C ₁₅ H ₇ F ₄ N ₃ O ₃
Molecular Weight:	353.23
Appearance:	no data available
Storage:	Powder: -20°C for 3 years In solvent: -80°C for 1 year



Biological Description

Description	DHODH-IN-14 is an analog of hydroxyfuran pyrimidine A771726. DHODH-IN-14 is a dihydroorotate dehydrogenase (DHODH) inhibitor IC ₅₀ 0.49 μM mouse liver DHODH. DHODH-IN-14 can be used for rheumatoid arthritis.
Targets(IC ₅₀)	Dehydrogenase
In vitro	DHODH-IN-14 is a hydroxyfuran analog of A771726, which contains a biphenyl scaffold with a fluorine substituent. Turning to the derivative DHODH-IN-14, no major differences were observed between the poses obtained on 1UUO and 1D3G. In both cases, it was found that DHODH-IN-14 was bound in a BQN-like manner, that is, the deprotonated hydroxyfuran part faced Arg136, thus effectively mimicking the carboxyl groups of BQN and related compounds. Although it was not found on 1D3G and 1UUO that hydroxyfuran interacted with Tyr356 in a similar way to leflunomide, when 2BXV was used as a docking target, a large portion of such postures were found[1].

Solubility Information

Solubility	DMSO: 50 mg/mL (141.55 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.831 mL	14.1551 mL	28.3102 mL
5 mM	0.5662 mL	2.831 mL	5.662 mL
10 mM	0.2831 mL	1.4155 mL	2.831 mL
50 mM	0.0566 mL	0.2831 mL	0.5662 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Reference

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.