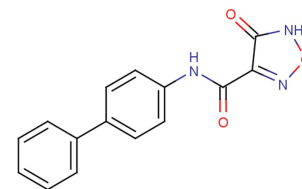


## DHODH-IN-15

## Chemical Properties

CAS No.:	1364791-88-7
Formula:	C <sub>15</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>
Molecular Weight:	281.27
Appearance:	N/A
Storage:	0-4°C for short term (days to weeks), or -20°C for long term (months).



## Biological Description

Description	DHODH-IN-15 is the hydroxyfuran analogue of A771726. DHODH-IN-15 is a dihydroorotate dehydrogenase (DHODH) inhibitor with an IC <sub>50</sub> of 11 μM for rat liver DHODH. DHODH-IN-15 can be used for rheumatoid arthritis.
Targets(IC <sub>50</sub> )	Rat liver DHODH: 11 μM
In vitro	DHODH-IN-15 is a hydroxyfuran analogue of A771726, in which the biphenyl skeleton does not carry any substituents. Turning to the derivative DHODH-IN-15, no major differences were observed between the poses obtained on 1UUO and 1D3G. In both cases, DHODH-IN-15 was found to bind in a BQN-like manner, ie, the deprotonated hydroxyfuran part faced Arg136, thus effectively mimicking the carboxyl groups of BQN and related compounds. On 1D3G and 1UUO, in any case, no interaction of Tyr356 with Leflunomide was found, but when 2BXV was used as a docking target, a large part of this posture was found.

## Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble
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## Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.555 mL	17.777 mL	35.553 mL
5 mM	0.711 mL	3.555 mL	7.111 mL
10 mM	0.356 mL	1.778 mL	3.555 mL
50 mM	0.071 mL	0.356 mL	0.711 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 °C for 6 months; - 20 °C for 1 month. Please use it as soon as possible.

## Reference

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

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