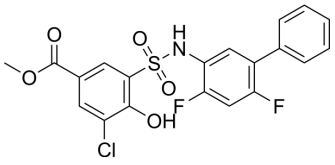
NDI-091143

Cat. No.:	HY-127111
CAS No.:	2375840-87-0
Molecular Formula:	$C_{20}H_{14}ClF_2NO_5S$
Molecular Weight:	453.84
Target:	ATP Citrate Lyase
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 1 year -20°C 6 months



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (220.34 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2034 mL	11.0171 mL	22.0342 mL
	5 mM	0.4407 mL	2.2034 mL	4.4068 mL
	10 mM	0.2203 mL	1.1017 mL	2.2034 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (4.58 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.58 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.58 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NDI-091143 is a potent and high-affinity human ATP-citrate lyase (ACLY) inhibitor with an IC_{50} of 2.1 nM (ADP-Glo assay), a K_i of 7.0 nM and a K_d of 2.2 nM. NDI-091143 inhibits ACLY catalysis allosterically, by stabilizing large conformational changes in the citrate domain that indirectly block the binding and recognition of citrate[1].

IC_{50} & Target

IC50: 2.1 nM (human ATP-citrate lyase); Ki: 7.0 nM (human ATP-citrate lyase); Kd: 2.2 nM (human ATP-citrate lyase)[1]

In Vitro

Thermal shift assays shows that NDI-091143 gives rise to considerable stabilization of both full-length ACLY and the N-

terminal segment. The thermal shift data are consistent with limited proteolysis experiments using full-length ACLY, in which NDI-091143 together with Mg-ATP provided the greatest protection against digestion by chymotrypsin[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Chem Biol Interact. 2022 Sep 26;367:110199.

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REFERENCES

[1]. Wei J, et al. An allosteric mechanism for potent inhibition of human ATP-citrate lyase. Nature. 2019 Apr;568(7753):566-570.

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