Bempedoic acid

Cat. No.: HY-12357

CAS No.: 738606-46-7

Molecular Formula: $C_{19}H_{36}O_5$

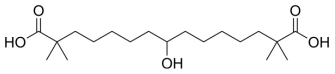
Molecular Weight: 344.49

Target: ATP Citrate Lyase; AMPK

Pathway: Metabolic Enzyme/Protease; Epigenetics; PI3K/Akt/mTOR

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (290.28 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.9028 mL	14.5142 mL	29.0284 mL
5 mM	0.5806 mL	2.9028 mL	5.8057 mL
10 mM	0.2903 mL	1.4514 mL	2.9028 mL

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

In Vivo

1. Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline
   Solubility: ≥ 2.87 mg/mL (8.33 mM); Clear solution
2. Add each solvent one by one: 5% DMSO >> 95% (20% SBE-β-CD in saline)
   Solubility: 2.87 mg/mL (8.33 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (7.26 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.26 mM); Clear solution
5. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.26 mM); Clear solution
6. Add each solvent one by one: 1% DMSO >> 99% saline
   Solubility: 0.57 mg/mL (1.65 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description Bempedoic acid (ETC-1002) is an ATP-citrate lyase (ACL) inhibitor[1]. Bempedoic acid (ETC-1002) activates AMPK[2].

IC_{50} & Target	AMPK
In Vitro	Bempedoic acid (ETC-1002) activates AMP-activated protein kinase in a Ca^{2+}/calmodulin-dependent kinase β-independent and liver kinase β 1-dependent manner, without detectable changes in adenylate energy charge. Bempedoic acid is shown to rapidly form a CoA thioester in liver, which directly inhibits ATP-citrate lyase[1]. In cells treated with Bempedoic acid (ETC-1002), increased levels of AMP-activated protein kinase (AMPK) phosphorylation coincide with reduced activity of MAP kinases and decreased production of proinflammatory cytokines and chemokines[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	A marked and sustained increase in AMPK and ACC phosphorylation is found in rat livers following two weeks of treatment with Bempedoic acid (ETC-1002). Bempedoic acid is >100-fold more prevalent than the CoA thioester in rat liver and is associated with AMPK activation[1]. Bempedoic acid (ETC-1002) suppresses thioglycollate-induced homing of leukocytes into mouse peritoneal cavity. In a mouse model of diet-induced obesity, Bempedoic acid restores adipose AMPK activity, reduces JNK phosphorylation, and diminishes expression of macrophage-specific marker 4F/80[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [1]	Glucose production is measured in primary rat hepatocyte cultures. Cells are cultured in glucose- and phenol red-free DMEM, containing 10 mM lactate, 1 mM pyruvate, and nonessential amino acids. Cells are incubated with various concentrations of Bempedoic acid (0.1 to 100 μM)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [1]	Rats: Prior to single-dose Bempedoic acid administration, Male Wistar Han rats are fasted for 48 h and refed a high-carbohydrate diet for an additional 48 h. For two-week assessment, rats are maintained on standard chow diet and dosed by oral gavage with Bempedoic acid at 30 mg/kg/day for two weeks in the morning. Following nutritional staging and/or dosing, food is withdrawn 2 h prior to last the oral dose of ehicle control or Bempedoic acid[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Acta Pharm Sin B. 18 June 2022.
- Hepatology. 2021 Jan;73(1):160-174.
- Cell Death Dis. 2023 Nov 7;14(11):722.
- Cell Death Dis. 2021 Nov 27;12(12):1113.
- Cell Death Dis. 2021 Jun 1;12(6):564.

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REFERENCES

[1]. Pinkosky SL, et al. AMP-activated protein kinase and ATP-citrate lyase are two distinct molecular targets for ETC-1002, a novel small molecule regulator of lipid and carbohydrate metabolism. J Lipid Res. 2013 Jan;54(1):134-51.

[2]. Filippov S, et al. ETC-1002 regulates immune response, leukocyte homing, and adipose tissue inflammation via LKB1-dependent activation of macrophage AMPK. J Lipid Res. 2013 Aug;54(8):2095-108.

Caution: Product has not been fully validated for medical applications. For research use only.

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