Entacapone

Cat. No.: HY-14280

CAS No.: 130929-57-6

Molecular Formula: $C_{14}H_{15}N_3O_5$

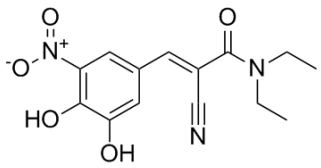
Molecular Weight: 305.29

Target: COMT

Pathway: Metabolic Enzyme/Protease; Neuronal Signaling

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 : 33.33 mg/mL (109.17 mM; Need ultrasonic)

H_2O : 2 mg/mL (6.55 mM; ultrasonic and adjust pH to 10 with NaOH)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.2756 mL	16.3779 mL	32.7557 mL
5 mM	0.6551 mL	3.2756 mL	6.5511 mL
10 mM	0.3276 mL	1.6378 mL	3.2756 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: ≥ 2.5 mg/mL (8.19 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (6.81 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (8.19 mM); Clear solution; Need warming

BIOLOGICAL ACTIVITY

Description

Entacapone is a potent, reversible, peripherally acting and orally active catechol-O-methyltransferase (COMT) inhibitor. Entacapone inhibits COMT from rat brain, erythrocytes and liver with IC_{50} values of 10 nM, 20 nM, and 160 nM, respectively. Entacapone is selective for COMT over other catecholamine metabolizing enzymes, including MAO-A, MAO-B, phenolsulphotransferase M (PST-M) and PST-P (IC_{50}s>50 μM). Entacapone can be used for the research of Parkinson's disease[1]. Entacapone serves as a inhibitor of FTO demethylation with an IC_{50} of 3.5 μM, can be used for the research of metabolic disorders[2].

IC_{50} & Target	IC50: 10 nM (rat brain COMT); 20 nM (rat erythrocyte COMT); 160 nM (rat liver COMT)[1]
In Vitro	Entacapone (50 μM, 48 hours) enhances the amount of m6A on mRNA in Hep-G2 cells. It does not show any inhibitory effect on the enzymatic activity of the RNA m6A demethylase AlkB homolog 5 (ALKBH5) or the ten-eleven translocation methylcytosine dioxygenase 1 (TET1), nor does it alter the DNA methylation or histone methylation patterns in entacapone-treated Hep-G2 cells[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Entacapone (oral administration; 600 mg/kg per day; 3-9 weeks) results in a dose-response effect dose-response effect. After 3 weeks, mouse body weight are decreased by 10.1% compared to controls, and shows similar food intake fat mass and fat mass ratio reduced after entacapone treatment. Entacapone also increases the energy expenditure of mice: reductions in total cholesterol (17.6%), low-density lipoprotein cholesterol (31.0%), and triglycerides (10.2%) in mice[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	High-fat diet-induced obese (DIO) mouse model[2]
Dosage:	600 mg/kg
Administration:	Oral administration; 600 mg/kg per day; 3-9 weeks
Result:	Regulated the metabolic disorders in DIO mouse.

CUSTOMER VALIDATION

- Sensor Actuat B-Chem. 2021, 129983.

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REFERENCES

[1]. E Nissinen, et al. Biochemical and pharmacological properties of a peripherally acting catechol-O-methyltransferase inhibitor entacapone. Naunyn Schmiedebergs Arch Pharmacol. 1992 Sep;346(3):262-6.

[2]. Shiming Peng, et al. Identification of entacapone as a chemical inhibitor of FTO mediating metabolic regulation through FOXO1. Sci Transl Med

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