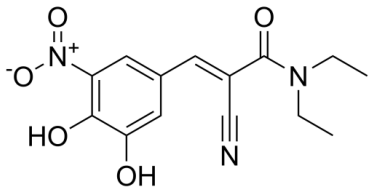
Data Sheet

Product Name:	Entacapone
Cat. No.:	CS-1266
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
Solubility:	H_2O : 2 mg/mL (ultrasonic;adjust pH to 10 with NaOH);DMSO : 33.33 mg/mL (ultrasonic)



BIOLOGICAL ACTIVITY:

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]. IC50 & 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].
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].

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

CAIndexNames:

2-Propenamide, 2-cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-diethyl-, (2E)-

SMILES:

O=C(N(CC)CC)/C(C#N)=C/C1=CC([N+]([O-])=O)=C(O)C(O)=C1

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

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