

Product Data Sheet

Product Name: Entacapone-d10

Cat. No.: GC47294

Chemical Properties

Cas. No. 1185241-19-3

SMILES N#C/C(=C/c1cc(O)c(O)c(c1)[N+](=O)[O-])/C(=O)N(C([2H])([2H])C([2H])([2H])[2H])C([2H])([2H])C([2H])([2H])[2H]

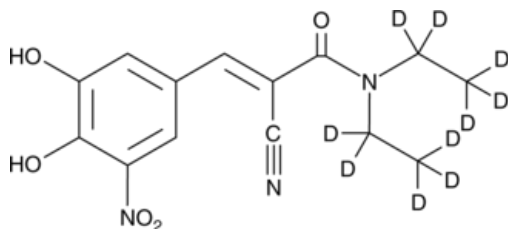
Formula C₁₄H₅D₁₀N₃O₅ M.Wt 315.4

Solubility DMSO : 33.33 mg/mL (105.69 mM; Storage Store at -20°C
Need ultrasonic); H₂O : 2 mg/mL
(6.34 mM; ultrasonic and adjust pH
to 10 with NaOH)

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure



Background

Entacapone-d₁₀ is intended for use as an internal standard for the quantification of entacapone by GC- or LC-MS. Entacapone is a reversible catechol O-methyltransferase (COMT) inhibitor (IC₅₀s = 10, 10, 20, and 160 nM for rat duodenum, brain, erythrocyte, and liver COMT, respectively).¹ It is selective for COMT over monoamine oxidase A (MAO-A) and MAO-B and phenolsulphotransferase M (PST-M) and PST-P (IC₅₀s = >50 μM). Entacapone (10 mg/kg), in combination with L-DOPA and carbidopa , reduces 3-O-methyldopa (3-OMD) levels in the rat striatum and hypothalamus to 52 and 27%, respectively, of the levels in control animals receiving only L-DOPA and carbidopa.² In a 6-

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OHDA rat model of Parkinson's disease, entacapone (10 mg/kg), in combination with L-DOPA and benserazide, increases contralateral turning behavior and striatal extracellular dopamine levels.³ Entacapone also inhibits contraction of colon longitudinal muscle explants from a 6-OHDA rat model of Parkinson's disease ($EC_{50} = 200 \mu M$).⁴ Formulations containing entacapone have been used in the treatment of Parkinson's disease.

1. Nissinen, E., Lindén, I.B., Schultz, E., et al. Biochemical and pharmacological properties of a peripherally acting catechol-O-methyltransferase inhibitor entacapone. *Naunyn-Schmiedeberg's Arch. Pharmacol.* 346(3):262-266(1992)
2. Männistö, P.T., Tuomainen, P., and Tuominen, R.K. Different in vivo properties of three new inhibitors of catechol O-methyltransferase in the rat. *Br. J. Pharmacol.* 105(3):569-574(1992)
3. Gerlach, M., van den Buuse, M., Blaha, C., et al. Entacapone increases and prolongs the central effects of L-DOPA in the 6-hydroxydopamine-lesioned rat. *Naunyn-Schmiedeberg's Arch. Pharmacol.* 370(5):388-394(2004)
4. Li, L.-S., Liu, C.-Z., Xu, J.-D., et al. Effect of entacapone on colon motility and ion transport in a rat model of Parkinson's disease. *World J. Gastroenterol.* 21(12):3509-3518(2015)

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