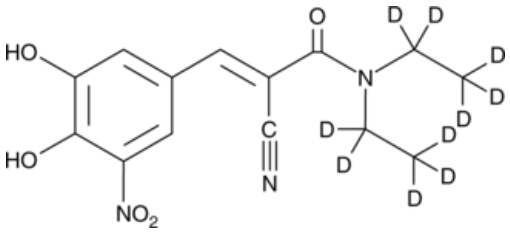
Product Data Sheet

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; Need ultrasonic); H_2O : 2 mg/mL (6.34 mM; ultrasonic and adjust pH to 10 with NaOH)	Storage	Store at -20°C
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-d_{10} 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 (IC_{50}s = 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 (IC_{50}s = >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 μM).[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 entacaponeNaunyn Schmiedebergs 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 ratBr. 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 ratNaunyn Schmiedebergs 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 diseaseWorld J. Gastroenterol.21(12)3509-3518(2015)

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