

Certificate of Analysis

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Product Name: Entacapone

Catalog No.: 4720

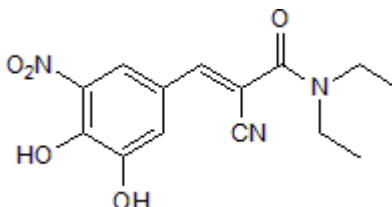
Batch No.: 1

CAS Number: 130929-57-6

IUPAC Name: (2*E*)-2-Cyano-3-(3,4-dihydroxy-5-nitrophenyl)-*N,N*-diethyl-2-propenamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₁₅N₃O₅
Batch Molecular Weight: 305.29
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
 ethanol to 10 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

Melting Point: Between 161 - 162°C
HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.08	4.95	13.76
Found	55.12	5.01	13.75

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Potent catechol O-methyltransferase (COMT) inhibitor (IC₅₀ values are 14.3, 20.1 and 73.3 nM for rat liver soluble COMT, total COMT and membrane-bound COMT respectively). Increases bioavailability of levodopa when given as an adjunct therapy for Parkinson's disease. Inhibits α-synuclein aggregation in an in vitro assay; blocks α-synuclein-induced cell death in PC-12 cells.

Physical and Chemical Properties:

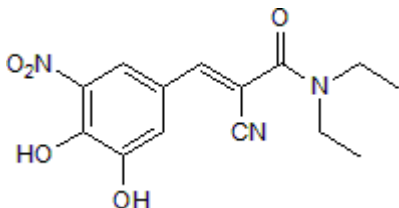
Batch Molecular Formula: C₁₄H₁₅N₃O₅

Batch Molecular Weight: 305.29

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 10 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Merello *et al* (1994) Effect of entacapone, a peripherally acting catechol-O-methyltransferase inhibitor, on the motor response to acute treatment with levodopa in patients with Parkinson's disease. *J.Neurol.Neurosurg.Psychiatry* **57** 186. PMID: 8126502.

Forsberg *et al* (2003) Pharmacokinetics and pharmacodynamics of entacapone and tolcapone after acute and repeated administration: a comparative study in the rat. *J.Pharmacol.Exp.Ther.* **304** 498. PMID: 12538800.

Di Giovanni *et al* (2010) Entacapone and tolcapone, two catechol O-methyltransferase inhibitors, block fibril formation of alpha-synuclein and beta-amyloid and protect against amyloid-induced toxicity. *J.Biol.Chem.* **285** 14941. PMID: 20150427.

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