

## Certificate of Analysis

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**Product Name:** Entacapone

**Catalog No.:** 4720

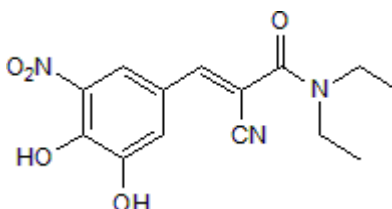
**Batch No.:** 1

CAS Number: 130929-57-6

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

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>14</sub>H<sub>15</sub>N<sub>3</sub>O<sub>5</sub>  
**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  
**<sup>1</sup>H 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 (IC<sub>50</sub> 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:**

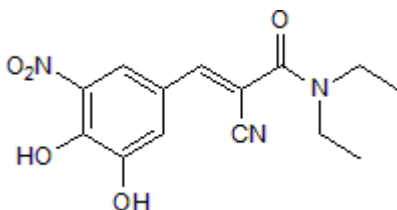
Batch Molecular Formula: C<sub>14</sub>H<sub>15</sub>N<sub>3</sub>O<sub>5</sub>

Batch Molecular Weight: 305.29

Physical Appearance: Yellow solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**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.

**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.

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