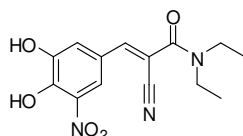




## Certificate of Analysis

**Axon Catalogue ID:** 3389 **Batch Number:** 1  
**Product Name:** Entacapone  
**Alternative Name(s):** OR-611; (E)-Entacapone  
**IUPAC Name:** (E)-2-Cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-diethylacrylamide

**Structure:**



**Amount:**

**CAS number(s):** 130929-57-6  
**Molecular Formula:** C<sub>14</sub>H<sub>15</sub>N<sub>3</sub>O<sub>5</sub> **Molecular Weight:** 305.29  
**Batch Molecular Formula:** C<sub>14</sub>H<sub>15</sub>N<sub>3</sub>O<sub>5</sub> **Batch Molecular Weight:** 305.29  
**Appearance:** Dark-yellow solid **Observed mp:** 163 °C  
**TLC (R<sub>f</sub>):** 0.6 DCM/DMSO (4:1)  
**Chemical Purity:** 98.1%  
**Optical Purity (ee):** N.A.  
**<sup>1</sup>H-NMR (300 MHz):** Analytical data confirm chemical structure  
**Mass Spec:** Analytical data confirm chemical structure  
**Microanalysis:** Calculated: C 55.08, H 4.95, N 13.76; Found: C 55.19, H 4.85, N 13.85  
**Storage Conditions:** Desiccate at -20 °C

Solubility Data:	Solvent	Solubility		Remarks
		(mg/ml)	(mM)	
	Water	0.0	0.0	Insoluble
	0.1N NaOH (aq)	2.0	6.6	
	0.1N HCl (aq)			Not Tested
	DMSO	30.0	98.3	* Sonication
	EtOH			Not Tested

**Remarks:** \* Sonication enhanced solubility.

**QC Date:** 06-05-2021

The purity of Axon Ligands is confirmed by HPLC, MS, NMR and/or microanalysis. Analytical data are available upon request. Request can be submitted by e-mail to [info@axonmedchem.com](mailto:info@axonmedchem.com) indicating Catalogue ID and Batch number.

**Caution: Not fully tested. For research purposes only**