

Product Name: Opicapone

Catalog No.: 7668

Batch No.: 1

CAS Number: 923287-50-7

IUPAC Name: 5-[3-(2,5-Dichloro-4,6-dimethyl-1-oxido-3-pyridinyl)-1,2,4-oxadiazol-5-yl]-3-nitro-1,2-benzenediol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₀Cl₂N₄O₆·¼H₂O

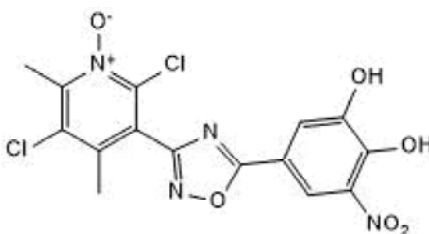
Batch Molecular Weight: 417.67

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	43.14	2.53	13.41
Found	43.02	2.47	13.3

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

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Description:

Opicapone is a reversible catechol O-methyltransferase inhibitor (COMT) inhibitor (IC₅₀ = 224 nM). Decreases the ATP content and mitochondrial membrane potential in cells (IC₅₀ values are 98 μM and 181 μM respectively). When administered with L-DOPA (Cat. No. 3788) it attenuates Parkinson's-like symptoms in an MPTP-induced animal model.

Physical and Chemical Properties:

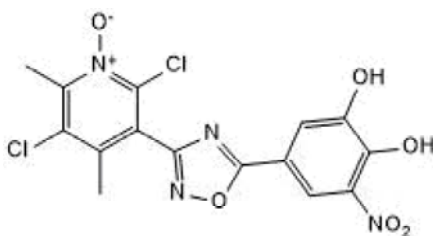
Batch Molecular Formula: C₁₅H₁₀Cl₂N₄O₆·¼H₂O

Batch Molecular Weight: 417.67

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Bonifácio et al (2021) Opicapone enhances the reversal of MPTP-induced Parkinson-like syndrome by levodopa in cynomolgus monkeys. *Eur.J.Pharmacol.* **892** 173742. PMID: 33220276.

Ettcheto et al (2020) The preclinical discovery and development of opicapone for the treatment of Parkinson's disease. *Expert Opin.Drug Discov.* **15** 993. PMID: 32450711.

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 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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