**Opicapone**

**Cat. No.:** HY-14896  
**CAS No.:** 923287-50-7  
**Molecular Formula:** $\text{C}_{12}\text{H}_{10}\text{Cl}_{2}\text{N}_{4}\text{O}_{6}$  
**Molecular Weight:** 413.17  
**Target:** COMT  
**Pathway:** Metabolic Enzyme/Protease; Neuronal Signaling  
**Storage:**  
- Powder: -20°C 3 years, 4°C 2 years  
- In solvent: -80°C 6 months, -20°C 1 month

**SOLVENT & SOLUBILITY**

**In Vitro**  
DMSO: 100 mg/mL (242.03 mM; Need ultrasonic)  
H$_2$O: < 0.1 mg/mL (insoluble)

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent</th>
<th>Mass</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 mM</td>
<td></td>
<td>2.4203 mL</td>
<td>12.1016 mL</td>
<td>24.2031 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td></td>
<td>0.4841 mL</td>
<td>2.4203 mL</td>
<td>4.8406 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td></td>
<td>0.2420 mL</td>
<td>1.2102 mL</td>
<td>2.4203 mL</td>
</tr>
</tbody>
</table>

Please refer to the solubility information to select the appropriate solvent.

**In Vivo**  
1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
   Solubility: ≥ 2.5 mg/mL (6.05 mM); Clear solution  
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)  
   Solubility: 2.5 mg/mL (6.05 mM); Suspended solution; Need ultrasonic

**BIOLOGICAL ACTIVITY**

**Description**  
Opicapone (BIA 9-1067) is a potent third-generation catechol-O-methyltransferase (COMT) inhibitor for the research of Parkinson’s disease and motor fluctuations. Opicapone decreases the ATP content of the cells with an IC$_{50}$ of 98 μM$^{[1]}$.

**IC$_{50}$ & Target**  
COMT$^{[1]}$

**In Vitro**  
Opicapone has a prolonged inhibitory effect on peripheral COMT, which extends the bioavailability of L-DOPA, without inducing toxicity. Opicapone decreases the ATP content of the cells with IC$_{50}$ values of 98 μM. Incubation of human primary hepatocytes for 24 h with increasing concentrations of Ro 40-7592, OR-611 or Opicapone resulted in a concentration-dependent decrease in the mitochondrial membrane potential of the cells, evaluated by the ratio JC-1 aggregates over JC-1...
monomer (ratio $\lambda_{\text{ex}}$ 544 $\lambda_{\text{em}}$ 590 over $\lambda_{\text{ex}}$ 485 $\lambda_{\text{em}}$ 538). Opicapone decreases the mitochondrial membrane potential of the cells with $\text{IC}_{50}$ of 181 $\mu$M$^1$. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

### In Vivo

Opicapone inhibits rat peripheral COMT with $\text{ED}_{50}$ values below 1.4 mg/kg up to 6 h post-administration. The effect is sustained over the first 8 h and by 24 h COMT had not returned to control values. A single administration of Opicapone resulted in increased and sustained plasma L-DOPA levels with a concomitant reduction in 3-OMD from 2 h up to 24 h post-administration, while Ro 40-7592 produces significant effects only at 2 h post-administration. The effects of Opicapone on brain catecholamines after L-DOPA administration are sustained up to 24 h post-administration. Opicapone is also the least potent compound in decreasing both the mitochondrial membrane potential and the ATP content in human primary hepatocytes after a 24 h incubation period$^1$. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

### PROTOCOL

#### Animal Administration $^1$

Rats$^1$

Male Wistar rats (240) are used. In experiments designed to evaluate the efficacy of the compound at inhibiting COMT, animals are administered Opicapone (0.03, 0.1, 0.3, 0.6, 1, 3 and 10 mg/kg) and are killed at 2 and 6 h post-administration. In experiments designed to evaluate COMT time-activity profile, animals are given Opicapone (3 mg/kg) and are killed at different post-administration periods (15 and 30 min, and 1, 2, 4, 8, 18, 24, and 48 h). In experiments designed to evaluate the effects of the compounds on central catecholamines, animals are given 3 mg/kg Opicapone or Ro 40-7592 and 1 h before being killed, animals are administered L-DOPA/benserazide (L-DOPA 12 mg/kg and benserazide 3 mg/kg). MCE has not independently confirmed the accuracy of these methods. They are for reference only.

### CUSTOMER VALIDATION

- Ecotoxicol Environ Saf. 2022 Dec 9;249:114340.
- Toxicol Lett. 2022 Jul 7;S0378-4274(22)00147-3.

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### REFERENCES


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

Tel: 609-228-6898
Fax: 609-228-5909
E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA