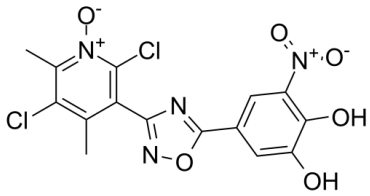
Data Sheet

Product Name:	Opicapone
Cat. No.:	CS-3109
CAS No.:	923287-50-7
Molecular Formula:	$C_{15}H_{10}Cl_2N_4O_6$
Molecular Weight:	413.17
Target:	COMT
Pathway:	Metabolic Enzyme/Protease; Neuronal Signaling
Solubility:	DMSO : 100 mg/mL (242.03 mM; Need ultrasonic); H2O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

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]. IC50 & 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 λ_{ex} 544 λ_{em} 590 over λ_{ex} 485 λ_{em} 538). Opicapone decreases the mitochondrial membrane potential of the cells with IC_{50} of 181 μM[1].
In Vivo: Opicapone inhibits rat peripheral COMT with 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].

PROTOCOL (Extracted from published papers and Only for reference)

Animal Administration: Opicapone is prepared in 0.5% carboxymethylcellulose[1].[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).

References:

[1]. Bonifácio MJ, et al. Pharmacological profile of Opicapone, a third-generation nitrocatechol catechol-O-methyl transferase inhibitor, in the rat. Br J Pharmacol. 2015 Apr;172(7):1739-52.

[2]. Ferreira JJ, et al. Opicapone as an adjunct to L-DOPA in patients with Parkinson's disease and end-of-dose motor fluctuations: a randomised, double-blind, controlled trial. Lancet Neurol. 2016 Feb;15(2):154-165.

CAIndexNames:

1,2-Benzenediol, 5-[3-(2,5-dichloro-4,6-dimethyl-1-oxido-3-pyridinyl)-1,2,4-oxadiazol-5-yl]-3-nitro-

SMILES:

CC1=[N+]([O-])C(Cl)=C(C2=NOC(C3=CC([N+]([O-])=O)=C(O)C(O)=C3)=N2)C(C)=C1Cl

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA