Tolcapone

Cat. No.: HY-17406

CAS No.: 134308-13-7

Molecular Formula: $C_{14}H_{11}NO_5$

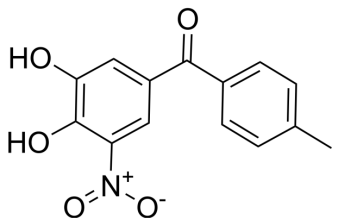
Molecular Weight: 273.24

Target: COMT; Amyloid-β; Apoptosis

Pathway: Metabolic Enzyme/Protease; Neuronal Signaling; Apoptosis

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	1 year
	-20°C	6 months



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (365.98 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.6598 mL	18.2989 mL	36.5979 mL
	5 mM	0.7320 mL	3.6598 mL	7.3196 mL
	10 mM	0.3660 mL	1.8299 mL	3.6598 mL

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 (9.15 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (9.15 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Tolcapone (Ro 40-7592) is a selective, orally active and powerful mixed (peripheral and central) COMT inhibitor with an IC_{50} of 773 nM in the liver[1]. Tolcapone is also a potent inhibitor of α-syn and Aβ42 oligomerization and fibrillogenesis[2]. Tolcapone induces oxidative stress leading to apoptosis and inhibition of tumor growth in neuroblastoma[3].

IC_{50} & Target

COMT[1]

α-syn and Aβ42 oligomerization, fibrillogenesis[2]

In Vitro

Tolcapone is cytotoxic to neuroblastoma (NB) cells with IC_{50} values ranging from 32.27 μM for SMS-KCNR cells to 219.8 μM for MGT9-102-08 primary cells[3].

?Tolcapone (25, 50,75, 100 μM) treatment activates downstream apoptotic events in NB cells. Tolcapone induces caspase-

mediated apoptosis in neuroblastoma[3].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[3]

Cell Line:	BE(2)-C, SMS-KCNR, CHLA-90, SH-SY5Y, MGT-015-08 and MGT9-102-08
Concentration:	1.5625~400 μM
Incubation Time:	48 hours
Result:	IC_{50}s of 32.27, 72.31, 80.29, 109.4, 174.6, 219.8 μM for SMS-KCNR, SH-SY5Y, BE(2)-C, CHLA-90, MGT-015-08 and MGT9-102-08, respectively.

Cell Viability Assay[3]

Cell Line:	NB cell lines: BE(2)-C, SMS-KCNR, CHLA-90, SH-SY5Y, MGT-015-08 and MGT9-102-08
Concentration:	25, 50, 75, 100 μM
Incubation Time:	
Result:	A dose-dependent increase in cleaved caspase-3 and cleaved PARP protein in all six NB cell lines and a subsequent decrease in whole caspase-3 and whole PARP protein.

In Vivo

Tolcapone (125 mg/kg; orally) inhibits tumor growth and prolongs survival in vivo. There are no adverse events or differences in weight or behavior noted in the mice[3].

Animal Model:	4-week-old female nude mice (nu/nu) bearing SMS-KCNR xenograft models [3]
Dosage:	125 mg/kg
Administration:	Treated orally every 24 h for 35 days
Result:	Decreased tumor volume compared to control. Resulted in a smaller average tumor of 490±310 mm^3 compared to control tumors of 1100±450 mm^3.

CUSTOMER VALIDATION

- Biotechnol Bioeng. 2021 Sep 3.

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REFERENCES

[1]. Catechol-O-methyltransferase: variation in enzyme activity and inhibition by entacapone and tolcapone. C De Santi, et al. Eur J Clin Pharmacol. 1998 May;54(3):215-9.

[2]. Saviana Di Giovanni, et al. 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. 2010 May 14;285(20):14941-14954.

[3]. Tyler Maser,et al. Tolcapone induces oxidative stress leading to apoptosis and inhibition of tumor growth in Neuroblastoma.Cancer Med. 2017 Jun;6(6):1341-1352.