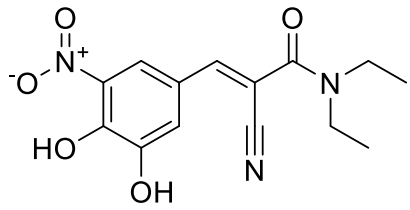
Product data sheet

MedKoo Cat#: 540117 Name: Entacapone CAS#: 130929-57-6 Chemical Formula: $C_{14}H_{15}N_3O_5$ Exact Mass: 305.1012 Molecular Weight: 305.29	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
Entacapone is a COMT inhibitor used to treat Parkinson's Disease. It reduces clearance of L-DOPA, improves motor function, and prevents α-synuclein and amyloid-β oligomerization and fibril formation.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	38.72	126.83
DMSO:PBS (pH 7.2) (1:1)	0.5	1.64
DMF	30.0	98.27
Ethanol	3.35	10.97
Water	2.0	6.55

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.28 mL	16.38 mL	32.76 mL
5 mM	0.66 mL	3.28 mL	6.55 mL
10 mM	0.33 mL	1.64 mL	3.28 mL
50 mM	0.07 mL	0.33 mL	0.66 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Jin L, Gao W, Liu C, Zhang N, Mukherjee S, Zhang R, Dong H, Bhunia A, Bednarikova Z, Gazova Z, Liu M, Han J, Siebert HC. Investigating the inhibitory effects of entacapone on amyloid fibril formation of human lysozyme. Int J Biol Macromol. 2020 Oct 15;161:1393-1404. doi: 10.1016/j.ijbiomac.2020.07.296. Epub 2020 Aug 1. PMID: 32750483.
2. Peng S, Xiao W, Ju D, Sun B, Hou N, Liu Q, Wang Y, Zhao H, Gao C, Zhang S, Cao R, Li P, Huang H, Ma Y, Wang Y, Lai W, Ma Z, Zhang W, Huang S, Wang H, Zhang Z, Zhao L, Cai T, Zhao YL, Wang F, Nie Y, Zhi G, Yang YG, Zhang EE, Huang N. Identification of entacapone as a chemical inhibitor of FTO mediating metabolic regulation through FOXO1. Sci Transl Med. 2019 Apr 17;11(488):eaau7116. doi: 10.1126/scitranslmed.aau7116. PMID: 30996080.

In vivo study

1. Soliman E, Shewaikh SM, Fahmy A, Elshazly S. Entacapone scavenges peroxynitrite and protects against kidney and liver injuries induced by renal ischemia/reperfusion in rats. Int Urol Nephrol. 2021 Aug;53(8):1713-1721. doi: 10.1007/s11255-021-02827-5. Epub 2021 Mar 6. PMID: 33675481.

2. Yoo DY, Jung HY, Kim W, Hahn KR, Kwon HJ, Nam SM, Chung JY, Yoon YS, Kim DW, Hwang IK. Entacapone promotes hippocampal neurogenesis in mice. Neural Regen Res. 2021 Jun;16(6):1005-1110. doi: 10.4103/1673-5374.300447. PMID: 33269743; PMCID: PMC8224137.

7. Bioactivity

Biological target:

Entacapone is a potent, reversible, peripherally acting and orally active catechol-O-methyltransferase (COMT) inhibitor.

In vitro activity

After incubation at pH 2.2, 60 °C for 192 h, HL formed aggregates. However, under the same conditions, when HL (70 μM) was incubated together with Ent (Entacapone) at a concentration ranging from 70 μM to 700 μM, a noticeable decrease in RLS scattering was observed (Fig. 1). This result allowed us to infer that Ent might be the reason for reducing the aggregation of HL amyloid fibrillation. The inhibition constant (Λ) of Ent against HL aggregation was further obtained by Eq. (1), and the fitted curve is shown in Fig. 1. The Λ value of Ent was determined to be $(3.0 \pm 0.5) \times 10^3\ M^{-1}$. Hence, scattering results indicated that Ent inhibits HL aggregation.

Reference: Int J Biol Macromol. 2020 Oct 15;161:1393-1404. https://pubmed.ncbi.nlm.nih.gov/32750483/

In vivo activity

Pre-treatment with either entacapone or FeTPPS improved renal function as indicated by a significant reduction in serum creatinine and urea when compared to I/R group ($P < 0.05$). I/R injury increased renal levels of NO (4-folds, $P < 0.05$), iNOS (4-folds, $P < 0.05$), and 3-nitrotyrosine (5-folds, $P < 0.05$) compared to sham control. These effects were abrogated in animals pre-treated with entacapone or FeTPPS before being subjected to I/R ($P < 0.05$). In addition, entacapone or FeTPPS significantly inhibited I/R-induced elevation in renal TNF-α levels (78% and 58%, respectively) and caspase-3 activity (72% and 56%, respectively) indicating the reduction of both inflammation and apoptosis in the kidney ($P < 0.05$). The two drugs also improved kidney and liver functions in rats with renal I/R injury.

Reference: Int Urol Nephrol. 2021 Aug;53(8):1713-1721. https://pubmed.ncbi.nlm.nih.gov/33675481/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.