

Certificate of Analysis

Product Name: Tolcapone

Catalog No.: 5864

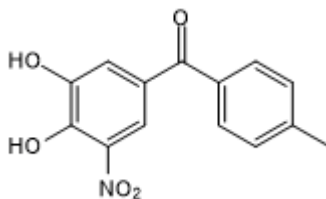
Batch No.: 1

CAS Number: 134308-13-7

IUPAC Name: (3,4-Dihydroxy-5-nitrophenyl)(4-methylphenyl)methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₁₁NO₅
Batch Molecular Weight: 273.24
Physical Appearance: Yellow solid
Solubility: ethanol to 100 mM
 DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.54	4.06	5.13
Found	61.77	4.07	5.08

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

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Description:

COMT inhibitor. Inhibits both brain and peripheral COMT. Also binds transthyretin (TTR) with high affinity (K_{d1} and K_{d2} values are 21 and 58 nM, respectively). Inhibits TTR aggregation in human plasma and prevents TTR-induced cytotoxicity in vitro. Stabilizes TTR in mice and humans in vivo. Orally bioavailable.

Physical and Chemical Properties:

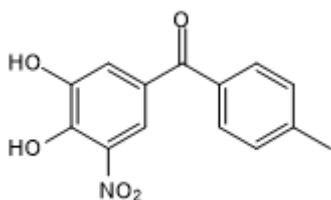
Batch Molecular Formula: C₁₄H₁₁NO₅

Batch Molecular Weight: 273.24

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°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:

ethanol to 100 mM

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.

References:

Sant'Anna et al (2016) Repositioning tolcapone as a potent inhibitor of transthyretin amyloidogenesis and associated cellular toxicity. *Nat. Commun.* **7** 10787. PMID: 26902880.

Männistö et al (1992) Different *in vivo* properties of three new inhibitors of catechol O-methyltransferase in the rat. *Br.J.Pharmacol.* **105** 569. PMID: 1628144.

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