

Certificate of Analysis

Print Date: Mar 8th 2023

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Product Name: OR-486 Catalog No.: 0483 Batch No.: 8

CAS Number: 7659-29-2

IUPAC Name: 3,5-Dinitrocatechol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_6H_4N_2O_6$ Batch Molecular Weight:200.11Physical Appearance:Yellow solid

Solubility: ethanol to 100 mM

DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

O₂N OH OH NO₂

2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 36.01 2.01 14
Found 36.36 2.01 13.88



Product Information

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CAS Number: 7659-29-2

IUPAC Name: 3,5-Dinitrocatechol

Description:

OR-486 is a potent and selective inhibitor of catechol-O-methyl-transferase.

Physical and Chemical Properties:

Batch Molecular Formula: $C_6H_4N_2O_6$ Batch Molecular Weight: 200.11 Physical Appearance: Yellow solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Store at RT

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:

Mannisto and Kaakola (1990) Rationale for selective COMT inhibitors as adjuncts in the drug treatment of Parkinson's disease. Pharmacol.Toxicol. 66 317. PMID: 2196554.

Borgulya *et al* (1989) Catechol-O-methyltransferase-inhibiting pyrocatechol derivatives: synthesis and structure-activity studies. Helv.Chim.Acta **72** 952.