

Certificate of Analysis

Print Date: Aug 24th 2017

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Product Name: TCS PrP Inhibitor 13 Catalog No.: 3238 Batch No.: 1

CAS Number: 34320-83-7

IUPAC Name: 2,4-Dihydro-5-(4-nitrophenyl)-2-phenyl-3*H*-pyrazol-3-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{11}N_3O_3$ Batch Molecular Weight:281.27

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:

ON-N NO₂

C₁₅H₁₁N₃O₃ Mol. Wt.: 281.27

2. ANALYTICAL DATA

Melting Point: At 191°C

HPLC: Shows >98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 64.05 3.94 14.94 Found 64.17 3.84 15.06

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Product Information

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IUPAC Name: 2,4-Dihydro-5-(4-nitrophenyl)-2-phenyl-3*H*-pyrazol-3-one

Description:

Antiprion agent. Potently inhibits protease-resistant prion protein (PrP-res) accumulation in two types of prion-infected mouse neuroblastoma (N2a) cell lines (IC $_{50}$ = 3 nM). Also reduces PrP expression and decreases proliferation and survival in schwannoma cell lines.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₅H₁₁N₃O₃ Batch Molecular Weight: 281.27 Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

C₁₅H₁₁N₃O₃ Mol. Wt.: 281.27 Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol to 25 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:

Provenzano *et al* (2017) Cellular prion protein (PrPC) in the development of Merlin-deficient tumours. Oncogene.. PMID: 28692055. **Kimata** *et al* (2007) New series of antiprion compounds: pyrazolone derivatives have potent activity of inhibiting protease-resistant prion protein accumulation. J.Med.Chem. *50* 5053. PMID: 17850126.

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