

Certificate of Analysis

Print Date: Dec 13th 2017

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Product Name: cis-Ned 19 Catalog No.: 3953 Batch No.: 1

CAS Number: 1137264-00-6

IUPAC Name: (1S,3S)-1-[3-[[4-(2-Fluorophenyl)piperazin-1-yl]methyl]-4-methoxyphenyl]-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-

3-carboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{30}H_{31}FN_4O_3.1\frac{1}{2}H_2O$

Batch Molecular Weight: 541.61

Physical Appearance: Cream solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

Microanalysis:

TLC: $R_f = 0.27$ (Chloroform:Methanol [4:1])

HPLC: Shows 97.7% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical 66.53 6.33 10.34 Found 66.87 6.07 10.17

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Product Information

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Description:

Irreversible nicotinic acid adenine dinucleotide phosphate (NAADP) antagonist; inhibits Ca²+ release (IC $_{50}$ = 800 nM) and [³²P]NAADP binding (IC $_{50}$ = 15 μ M). Stereoisomer of trans-Ned 19. Fluorescently labels NAADP receptors in intact cells (excitation 351 and 365 nm using an ultraviolet Argon laser). Isomer of trans-Ned 19.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₀H₃₁FN₄O₃.1½H₂O

Batch Molecular Weight: 541.61 Physical Appearance: Cream solid

Minimum Purity: >97%

Batch Molecular Structure:

Storage: Store at -20°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:

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:

Naylor et al (2009) Identification of a chemical probe for NAADP by virtual screening. Nat.Chem.Biol. 5 220. PMID: 19234453.