

Certificate of Analysis

Print Date: May 1st 2020

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Product Name: trans-Ned 19 Catalog No.: 3954 Batch No.: 3

CAS Number: 1354235-96-3

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

3-carboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

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

Batch Molecular Weight: 523.6

Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 68.82 6.16 10.7 Found 68.78 6.21 10.71

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



Product Information

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IUPAC Name: (1R,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

Description:

Nicotinic acid adenine dinucleotide phosphate (NAADP) antagonist. Inhibits NAADP-mediated Ca^{2+} release (IC_{50} = 6 nM); also inhibits [32 P]NAADP binding (IC_{50} = 0.4 nM). Fluorescently labels NAADP receptors in intact cells. Stereosiomer of cis-Ned 19 (Cat. No. 3953).

Physical and Chemical Properties:

Batch Molecular Formula: C₃₀H₃₁FN₄O₃.½H₂O

Batch Molecular Weight: 523.6 Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

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.

Rosen et al (2009) Analogues of the nicotinic acid adenine dinucleotide phosphate (NAADP) antagonist Ned-19 indicate two binding sites on the NAADP receptor. J.Biol.Chem. **284** 34930. PMID: 19826006.

Thai et al (2009) NAADP receptors mediate calcium signaling stimulated by endothelin-1 and NE in renal afferent arterioles. Am.J.Physiol.Renal Physiol. **297** F510. PMID: 19439521.

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