Certificate of Analysis

Print Date: Jan 14th 2016

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Product Name: trans-Ned 19

TOCRIS

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Catalog No.: 3954 Batch No.: 2

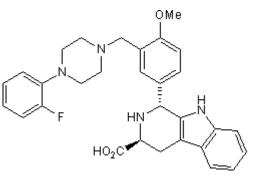
CAS Number: IUPAC Name:

(1*R*,3*S*)-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

1354235-96-3

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: $C_{30}H_{31}FN_4O_3$.³/₄H₂O 528.1 White solid DMSO to 100 mM Store at -20°C



2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Microanalysis: $R_f = 0.16$ (Chloroform:Methanol [4:1]) Shows 99.1% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 68.23 6.2 10.61

Theoretical	68.23	6.2	10.61
Found	67.83	5.79	10.59

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

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Description:

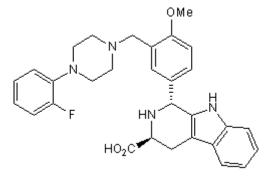
Nicotinic acid adenine dinucleotide phosphate (NAADP) antagonist. Inhibits NAADP-mediated Ca²⁺ release (IC₅₀ = 6 nM); also inhibits [³²P]NAADP binding (IC₅₀ = 0.4 nM). Fluorescently labels NAADP receptors in intact cells. Stereosiomer of cis-Ned 19 (Cat. No. 3953).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{30}H_{31}FN_4O_3$. $^{3}_{4}H_2O$ Batch Molecular Weight: 528.1 Physical Appearance: 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 norepinephrine in renal afferent arterioles. Am.J.Physiol.Renal Physiol. **297** F510. PMID: 19439521.

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