

Certificate of Analysis

Print Date: Jan 14th 2016

Batch No.: 1

www.tocris.com

Catalog No.: 5046

Product Name: LM11A 31 dihydrochloride

CAS Number: 1243259-19-9

IUPAC Name: (2S,3S)-2-Amino-3-methyl-N-[2-(4-morpholinyl)ethyl]pentanamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_{25}N_3O_2.2HCI.4H_2O$

Batch Molecular Weight: 320.77

Physical Appearance: Pale yellow solid

Solubility: water to 100 mM

DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: R_f = 0.22 (12% MeOH and 0.2% aq. NH4OH (35% wt/wt/) in DCM)

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = +44.6$ (Concentration = 1, Solvent = Water)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 44.93 8.64 13.1 Found 45.11 8.61 12.77



Product Information

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CAS Number: 1243259-19-9

IUPAC Name: (2S,3S)-2-Amino-3-methyl-*N*-[2-(4-morpholinyl)ethyl]pentanamide dihydrochloride

Description:

Nonpeptide p75NTR ligand; blocks p75-mediated cell death and also increases proliferation and survival of hippocampal neural progenitors. Exhibits no effect on nerve growth factor (NGF) binding to TrkA. Prevents and reverses atrophy of cholinergic neurites, as well as reversing Alzheimer's Disease (AD) pathologies in mid- to late-stage AD mice models. Shown to promote functional recovery in a mouse model of spinal cord injury. Orally available and brain penetrant.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₂H₂₅N₃O₂.2HCl.1/4H₂O

Batch Molecular Weight: 320.77

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Desiccate at RT. This product is packaged under an inert atmosphere.

Solubility & Usage Info:

water to 100 mM DMSO to 100 mM

CAUTION - This product is extremely hygroscopic and we recommend that it is desiccated upon arrival. It has been packed under inert atmosphere, and should be kept under inert atmosphere during and after weighing.

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:

Massa et al (2006) Small, nonpeptide p75NTR ligands induce survival signaling and inhibit proNGF-induced death. J.Neurosci. 26 5288. PMID: 6707781.

Tep *et al* (2013) Oral administration of a small molecule targeted to block proNGF binding to p75 promotes myelin sparing and functional recovery after spinal cord injury. J.Neurosci. **33** 397. PMID: 23303920.

Shi et al (2013) A small molecule P75NTR ligand protects neurogenesis after traumatic brain injury. Stem Cells [Epub ahead of print]. PMID: 23940017.

Simmons *et al* (2014) A small molecule p75^{NTR} ligand, LM11A-31, reverses cholinergic neurite dystrophy in Alzheimer's disease mouse models with mid- to late-stage disease progression. PLoS One **9** e102136. PMID: 25153701.