TOCRIS a biotechne brand

Certificate of Analysis

www.tocris.com

Product Name: PD 176252

Catalog No.: 2602 Batch No.: 5

CAS Number: IUPAC Name:

 $(S)-N-[[1-(5-Methoxy-2-pyridinyl)cyclohexyl]methyl]-\alpha-methyl-\alpha-[[[-(4-nitrophenyl)amino]carbonyl]amino-1H-indole-3-propanamide$

1. PHYSICAL AND CHEMICAL PROPERTIES

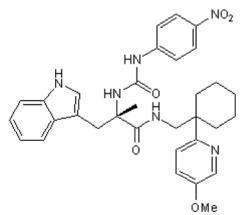
204067-01-6

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

Solubility: Storage:

Batch Molecular Structure:

 $C_{32}H_{36}N_6O_5$ 584.67 Light yellow solid DMSO to 100 mM Store at +4°C



2. ANALYTICAL DATA

HPLC: Chiral HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 98.9% purity Shows 99.8% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 65.74 6.21 14.37 Found 65.61 6.26 14.52

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

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 $(S)-N-[[1-(5-Methoxy-2-pyridinyl)cyclohexyl]methyl]-\alpha-methyl-\alpha-[[[-(4-nitrophenyl)amino]carbonyl]amino-1H-indole-3-propanamide$

Description:

IUPAC Name:

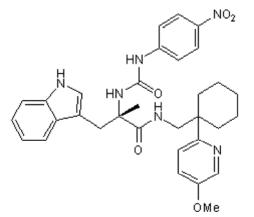
Non-peptide gastrin-releasing peptide receptor (GRP-R, BB₂) and neuromedin B receptor (NMB-R, BB₁) antagonist (K_i values are 0.17 and 1.0 nM for BB₁ and BB₂ respectively). Inhibits proliferation of rat C6 glioma cells ($IC_{50} = 2 \mu M$) and inhibits NCI-H1299 xenograft proliferation in nude mice ($IC_{50} = 5 \mu M$).

Physical and Chemical Properties:

Batch Molecular Formula: C₃₂H₃₆N₆O₅ Batch Molecular Weight: 584.67 Physical Appearance: Light yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°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).

Catalog No.: 2602

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:

Schepetkin *et al* (2011) Gastrin-releasing peptide/neuromedin B receptor antagonists pD176252, PD168368, and related analogs are potent agonists of human formyl-peptide receptors. Mol.Pharmacol. **79** 77. PMID: 20943772.

Moody *et al* (2003) Nonpeptide gastrin releasing peptide receptor antagonists inhibit the proliferation of lung cancer cells Eur.J.Pharmacol. **474** 21. PMID: 12909192.

Moody *et al* (2000) Nonpeptide neuromedin B receptor antagonists inhibit the proliferation of C6 cells Eur.J.Pharmacol. **409** 133. PMID: 11104826.

Ashwood et al (1998) PD 176252 - the first high affinity non-peptide gastrin-releasing peptide (BB2) receptor antagonist Bioorg.Med.Chem.Lett. 8 2589. PMID: 9873586.

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