



Certificate of Analysis

www.tocris.com

Product Name: M 25 Catalog No.: 4917 Batch No.: 1

IUPAC Name: N-[[1-(2-Methoxyphenyl)-1*H*-indazol-5-yl]methyl]-2-propylpentanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{29}N_3O_2$

Batch Molecular Weight: 379.5

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.29$ (Ethyl acetate:Petroleum ether [1:2])

HPLC: Shows >99.6% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 72.79 7.7 11.07 Found 72.78 7.82 11.02

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



Print Date: Jan 25th 2014

www.tocris.com



Product Name: M 25 Catalog No.: 4917 Batch No.: 1

IUPAC Name: N-[[1-(2-Methoxyphenyl)-1*H*-indazol-5-yl]methyl]-2-propylpentanamide

Description:

Potent Smoothened (Smo) receptor antagonist ($IC_{50} = 5$ nM). Inhibits the Hedgehog signaling pathway. Inhibits Shh induced Gli luciferase reporter activity in Shh-light 2 cells ($IC_{50} = 5$ nM). Antagonizes GSA-10 and SAG-mediated differentiation of the C3H10T1/2 cell line (IC_{50} values are 69 and 115 nM, respectively).

Physical and Chemical Properties:

Batch Molecular Formula: C₂₃H₂₉N₃O₂ Batch Molecular Weight: 379.5 Physical Appearance: Orange solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Dessole *et al* (2009) Discovery of *N*-[(1-aryl-1*H*-indazol-5-yl)methyl]amides derivatives as smoothened antagonists for inhibition of the hedgehog pathway. Bioorg.Med.Chem.Lett. **19** (15) 4191. PMID: 19540115.

Gorojankina *et al* (2013) Discovery, molecular and pharmacological characterization of GSA-10, a novel small-molecule positive modulator of Smoothened. Mol.Pharmacol. *83* 1020. PMID: 23448715.

