

Certificate of Analysis

Print Date: Jan 15th 2016

www.tocris.com

Product Name: IBC 293 Catalog No.: 2469 Batch No.: 1

CAS Number: 306935-41-1

IUPAC Name: 1-(1-Methylethyl)-1*H*-benzotriazole-5-carboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C10H11N3O2·O.1H₂O

Batch Molecular Weight: 207.02

Physical Appearance: Beige solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:

HO₂C N N

2. ANALYTICAL DATA

HPLC: Shows >98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Theoretical 58.02 5.45 20.3 Found 57.91 5.49 20.02

Carbon Hydrogen Nitrogen



Product Information

Print Date: Jan 15th 2016

www.tocris.com

Product Name: IBC 293 Catalog No.: 2469 Batch No.: 1

CAS Number: 306935-41-1

IUPAC Name: 1-(1-Methylethyl)-1*H*-benzotriazole-5-carboxylic acid

Description:

Highly selective agonist for GPR109B (HM74), human orphan G-protein-coupled receptor expressed in adipocytes. Selective for GPR109B over niacin receptor GPR109A (HM74A); EC $_{50}$ values are 400 nM and > 1 μ M respectively. Inhibits isoproterenol-stimulated lipolysis in vitro in isolated human adipocytes.

Physical and Chemical Properties:

Batch Molecular Formula: C10H11N3O2.O.1H2O

Batch Molecular Weight: 207.02 Physical Appearance: Beige solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

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:

Semple et al (2006) 1-Alkyl-benzotriazole-5-carboxylic acids are highly selective agonists of the human orphan G-protein-coupled receptor GPR109b. J.Med.Chem. 49 1227. PMID: 16480258.