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Certificate of Analysis

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Print Date: Jul 1st 2019

Product Name: BRL 50481

CAS Number:433695-36-4IUPAC Name:N,N,2-Trimethyl-5-nitro-benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C₉H₁₂N₂O₄S 244.26 Cream solid ethanol to 100 mM DMSO to 100 mM Store at +4°C

Meoo

NO₂

Storage: Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: Melting Point: HPLC: ¹H NMR: Mass Spectrum: Microanalysis: R_f = 0.2 (Ethyl acetate:Hexane [3:7]) Between 70 - 71°C Shows 99.0% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen

NMe₂

		J	
Theoretical	44.25	4.95	11.46
Found	43.92	4.89	11.29

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

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Catalog No.: 2237

Batch No.: 1

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Product Name: BRL 50481

CAS Number: 433695-36-4

IUPAC Name: *N*,*N*,2-Trimethyl-5-nitro-benzenesulfonamide

Description:

Selective, substrate-competitive inhibitor of phosphodiesterase (PDE) 7 (K_i = 180 nM). Displays > 200-fold selectivity over PDE1B, PDE1C, PDE2, PDE3, PDE4A4 and PDE5.

Physical and Chemical Properties:

Batch Molecular Formula: C₉H₁₂N₂O₄S Batch Molecular Weight: 244.26 Physical Appearance: Cream solid

Minimum Purity: >99%

Batch Molecular Structure:

Me 0 0 NMe2 NO2

Storage: Store at +4°C

Solubility & Usage Info: ethanol to 100 mM

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 $45-60^{\circ}C$ water bath).

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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.

Licensing Information:

Sold with the permission of GlaxoSmithKline

References:

Smith *et al* (2004) Discovery of BRL 50481 [3-(*N*,*N*-dimethylsulfonamido)-4-methyl-nitrobenzene], a selective inhibitor of phosphodiesterase 7: in vitro studies in human monocytes, lung macrophages, and CD8⁺ T-lymphocytes. Mol.Pharmacol. **66** 1679. PMID: 15371556.

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