

Certificate of Analysis

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Print Date: Jan 14th 2016

Product Name: VU 0357121 Catalog No.: 4437 Batch No.: 1

CAS Number: 433967-28-3

IUPAC Name: 4-Butoxy-*N*-(2,4-difluorophenyl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{17}F_2NO_2$

Batch Molecular Weight: 305.32
Physical Appearance: White solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 66.88 5.61 4.59 Found 66.68 5.62 4.66



Product Information

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CAS Number: 433967-28-3

IUPAC Name: 4-Butoxy-N-(2,4-difluorophenyl)benzamide

Description:

Positive allosteric modulator of $mGlu_5$ receptors (EC₅₀ = 33 nM). Binds to a site distinct from that bound by MPEP (Cat. No. 1212).

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₁₇F₂NO₂ Batch Molecular Weight: 305.32 Physical Appearance: White solid

Minimum Purity: >99%

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:

Hammond *et al* (2010) Discovery of a novel chemical class of mGlu₅ allosteric ligands with distinct modes of pharmacology. ACS Chem.Neurosci. **1** 702. PMID: 20981342.