



Certificate of Analysis

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Product Name: VU 1545 Catalog No.: 3325 Batch No.: 1

CAS Number: 890764-63-3

IUPAC Name: N-[1-(2-Fluorophenyl)-3-phenyl-1*H*-pyrazol-5-yl]-4-nitrobenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₁₅FN₄O₃

Batch Molecular Weight: 402.38

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.3$ (Dichloromethane)

HPLC: Shows 98.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 65.67 3.76 13.92 Found 65.29 3.77 13.9



Product Information

Print Date: Feb 11th 2020

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CAS Number: 890764-63-3

IUPAC Name: N-[1-(2-Fluorophenyl)-3-phenyl-1*H*-pyrazol-5-yl]-4-nitrobenzamide

Description:

Metabotropic glutamate receptor 5 (mGlu₅) positive allosteric modulator (EC₅₀ = 9.6 nM, K_i = 156 nM at rat mGlu₅).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{22}H_{15}FN_4O_3$

Batch Molecular Weight: 402.38 Physical Appearance: 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).

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:

de Paulis *et al* (2006) Substituent effects of *N*-(1,3-diphenyl-1*H*-pyrazol-5-yl)benzamides on positive allosteric modulation of the metabotropic glutamate-5 receptor in rat cortical astrocytes. J.Med.Chem. **49** 3332. PMID: 16722652.

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