

Certificate of Analysis

Print Date: Sep 4th 2019

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Product Name: VU 6005649 Catalog No.: 6893 Batch No.: 1

CAS Number: 2137047-43-7

IUPAC Name: 3-(2,3-Difluoro-4-methoxyphenyl)-2,5-dimethyl-7-(trifluoromethyl)pyrazolo[1,5-a]pyrimidine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{12}F_5N_3O$

Batch Molecular Weight: 357.28

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 53.79 3.39 11.76 Found 53.82 3.36 11.67

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



Product Information

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Description:

Positive allosteric modulator of mGlu $_7$ and mGlu $_8$ receptors (EC $_{50}$ = 0.65 μ M and 2.6 μ M for mGlu $_7$ and mGlu $_8$, respectively). Displays >3.8 fold selectivity for mGlu $_7$ and mGlu $_8$ over other mGlu receptors (EC $_{50}$ >10 μ M for mGlu $_{1,2,3,4,5,6}$). Also NK $_1$ receptor antagonist (K $_1$ = 650 nM, IC $_{50}$ = 3.4 μ M). Brain penetrant.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{16}H_{12}F_5N_3O$

Batch Molecular Weight: 357.28 Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM ethanol to 50 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:

Abe et al (2017) Discovery of VU6005649, a CNS penetrant mGlu_{7/8} receptor PAM derived from a series of pyrazolo[1,5-a]pyrimidines. ACS.Med.Chem.Lett. **8** 1110. PMID: 29057060.