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Print Date: Jan 13th 2022

# Certificate of Analysis

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**Product Name:** **VU 0409551** **Catalog No.: 5693** **Batch No.: 1**

CAS Number: 1363281-27-9

IUPAC Name: [6,7-Dihydro-2-(phenoxymethyl)oxazolo[5,4-*c*]pyridin-5(4*H*)-yl](fluorophenyl)methanone

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{20}H_{17}FN_2O_3$

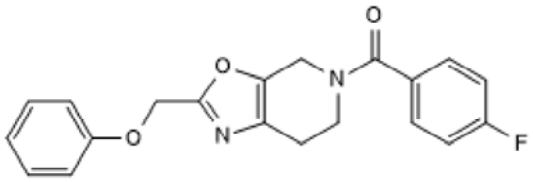
**Batch Molecular Weight:** 352.36

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM
ethanol to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.56 (Ethyl acetate)

**HPLC:** Shows 99.1% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 68.17 | 4.86 | 7.95 |
| Found | 68.2 | 4.54 | 7.99 |



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**Description:**

VU 0409551 is a selective $mGlu_5$ positive allosteric modulator ($EC_{50}$ = 260 nM). Selective for $mGlu_5$ over other mGluR subtypes, as well as 66 other receptors and ion channels. Selectively potentiates $mGlu_5$ signaling via $G_{\alpha q}$. Exhibits wake-promoting, antipsychotic-like and cognition-enhancing effects in animal models. Brain penetrant and orally available.

**Physical and Chemical Properties:**

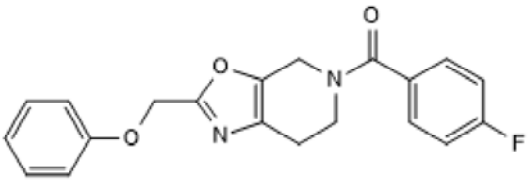
Batch Molecular Formula: $C_{20}H_{17}FN_2O_3$

Batch Molecular Weight: 352.36

Physical Appearance: White solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**




**Storage:** Store at +4°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:**

**Ghoshal** *et al* (2017) Role of mGlu5 receptors and inhibitory neurotransmission in M1 dependent muscarinic LTD in the prefrontal cortex: implications in Schizophrenia. ACS Chem.Neurosci. ***8*** 2254. PMID: 28679049.

**Conde-Ceide** *et al* (2015) Discovery of VU0409551/JNJ-46778212: An $mGlu_5$ positive allosteric modulator clinical candidate targeting schizophrenia. ACS Med.Chem.Lett. ***6*** 716. PMID: 26157544.

**Rook** *et al* (2015) Biased $mGlu_5$-positive allosteric modulators provide *in vivo* efficacy without potentiating $mGlu_5$ modulation of NMDAR currents. Neuron ***86*** 1029. PMID: 25937172.



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