

Certificate of Analysis

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Product Name: VU 0409551

Catalog No.: 5693

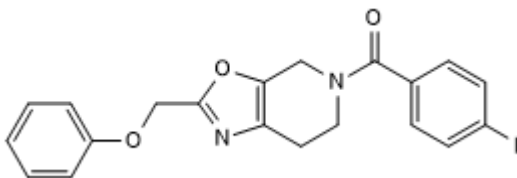
Batch No.: 1

CAS Number: 1363281-27-9

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₇FN₂O₃
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 99.5% purity
¹H 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

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

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

Description:

Selective mGlu₅ positive allosteric modulator (EC₅₀ = 260 nM). Selective for mGlu₅ over other mGluR subtypes, as well as 66 other receptors and ion channels. Selectively potentiates mGlu₅ signaling via G_{αq}. Exhibits wake-promoting, antipsychotic-like and cognition-enhancing effects in animal models. Brain penetrant and orally available.

Physical and Chemical Properties:

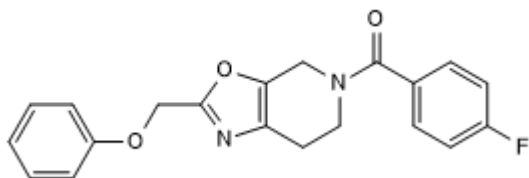
Batch Molecular Formula: C₂₀H₁₇FN₂O₃

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:

Conde-Ceide et al (2015) Discovery of VU0409551/JNJ-46778212: An mGlu₅ positive allosteric modulator clinical candidate targeting schizophrenia. *ACS Med.Chem.Lett.* **6** 716. PMID: 26157544.

Rook et al (2015) Biased mGlu₅-positive allosteric modulators provide *in vivo* efficacy without potentiating mGlu₅ modulation of NMDAR currents. *Neuron* **86** 1029. PMID: 25937172.

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