bio-techne
TOCRIS

Print Date: May 17th 2024

Certificate of Analysis

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Product Name: **VU 0469650 hydrochloride** **Catalog No.: 5379** **Batch No.: 1**

CAS Number: 1443748-47-7

IUPAC Name: 3-[(3*R*)-3-Methyl-4-(tricyclo[3.3.1.1^{3,7}]dec-1-ylcarbonyl)-1-piperazinyl]-2-pyridinecarbonitrile hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{28}N_4O.HCl$

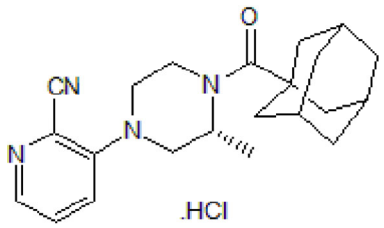
Batch Molecular Weight: 400.94

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.32 (Ethyl acetate:Petroleum ether [5:5])

HPLC: Shows 99.8% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -50 (Concentration = 4, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.9	7.29	13.97
Found	66.15	7.28	14.03

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Description:

VU 0469650 hydrochloride is a potent and selective negative allosteric modulator of $mGlu_1$ (IC_{50} = 99 nM). Exhibits >100-fold selectivity for $mGlu_1$ over $mGlu_{2-8}$ and 68 other GPCRs, ion channels, kinases and transporters. Brain penetrant.

Physical and Chemical Properties:

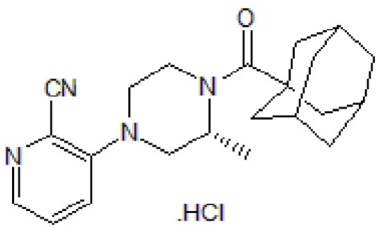
Batch Molecular Formula: $C_{22}H_{28}N_4O.HCl$

Batch Molecular Weight: 400.94

Physical Appearance: Yellow 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Lovell *et al* (2013) *N*-Acyl-*N'*-arylpiperazines as negative allosteric modulators of $mGlu_1$: Identification of VU0469650, a potent and selective tool compound with CNS exposure in rats. Bioorg.Med.Chem.Lett. ***23*** 3713. PMID: 23727046 .