TOCRIS
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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **ML 289** **Catalog No.: 4976** **Batch No.: 1**

CAS Number: 1382481-79-9

IUPAC Name: [(3*R*)-3-(Hydroxymethyl)-1-pipridinyl][4-[2-(4-methoxyphenyl)ethynyl]phenyl]methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{23}NO_3$

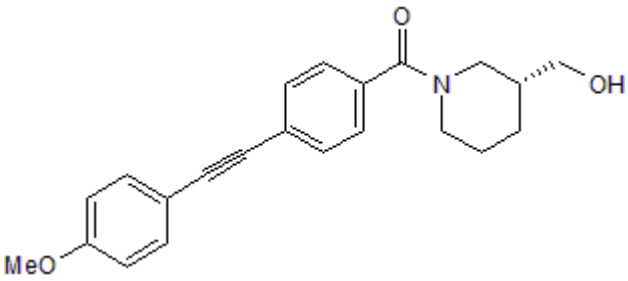
Batch Molecular Weight: 349.42

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 = 0.3 (Ethyl acetate:Petroleum ether [1:3])

HPLC: Shows >99.3% purity

Chiral HPLC: Shows >99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	75.62	6.63	4.01
Found	75.51	6.65	3.98

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Description:

Selective negative allosteric modulator at $mGlu_3$ receptors (IC_{50} = 660 nM). Exhibits 15-fold selectivity for $mGlu_3$ over $mGlu_2$. Centrally penetrant.

Physical and Chemical Properties:

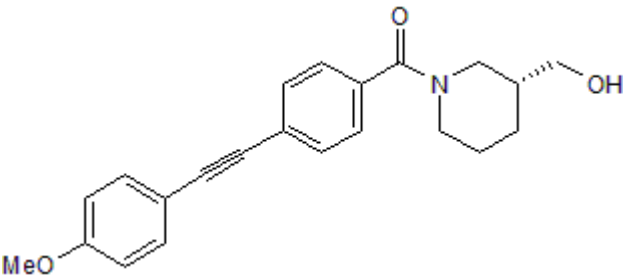
Batch Molecular Formula: $C_{22}H_{23}NO_3$

Batch Molecular Weight: 349.42

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:

Sheffler *et al* (2012) Development of a novel, CNS-penetrant, metabotropic glutamate receptor 3 (mGlu3) NAM probe (ML289) derived from a closely related mGlu5 PAM. Bioorg.Med.Chem.Lett. ***22*** 3921. PMID: 22607673.