

## Certificate of Analysis

**Product Name:** ABP 688

**Catalog No.:** 5229

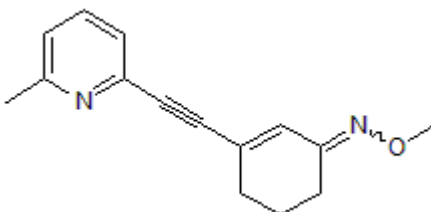
**Batch No.:** 1

CAS Number: 924298-51-1

IUPAC Name: 3-[2-(6-Methyl-2-pyridinyl)ethynyl]-2-cyclohexene-1-one O-methylxime

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>15</sub>H<sub>16</sub>N<sub>2</sub>O  
**Batch Molecular Weight:** 240.3  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 100 mM  
 1eq. HCl to 50 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.47 (Ethyl acetate:Petroleum ether [3:7])  
**HPLC:** Shows 99.6% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	74.97	6.71	11.66
Found	74.92	6.71	11.61

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

## Product Information

[www.tocris.com](http://www.tocris.com)

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### Description:

High affinity human mGlu<sub>5</sub> receptor antagonist ( $K_i = 1.7$  nM). Inhibits glutamate-induced calcium release from L(tk-) cells expressing human mGlu<sub>5</sub> receptors ( $IC_{50} = 2.3$  nM).

### Physical and Chemical Properties:

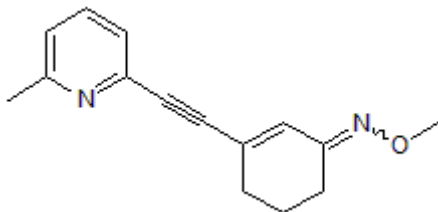
Batch Molecular Formula: C<sub>15</sub>H<sub>16</sub>N<sub>2</sub>O

Batch Molecular Weight: 240.3

Physical Appearance: Yellow solid

**Minimum Purity:** >98%

### Batch Molecular Structure:



**Storage:** Store at -20°C

**CAUTION** - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

### Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl 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:

**Hintermann et al** (2007) ABP688, a novel selective and high affinity ligand for the labeling of mGlu<sub>5</sub> receptors: identification, *in vitro* pharmacology, pharmacokinetic and biodistribution studies. *Bioorg.Med.Chem.* **15** 903. PMID: 17110115.

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