Print Date: Mar 6th 2014

# Certificate of Analysis

www.tocris.com

**Product Name: ML 190** **Catalog No.: 4866** **Batch No.: 1**

CAS Number: 1355244-02-8

IUPAC Name: *N*-[3-[4-(4-Methoxyphenyl)-1-piperazinyl]propyl]-1-methyl-6-oxopyrido[2,3-*e*]pyrrolo[1,2-*a*]pyrazine-5(6*H*)-acetamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{27}H_{32}N_6O_3.¼H_2O$

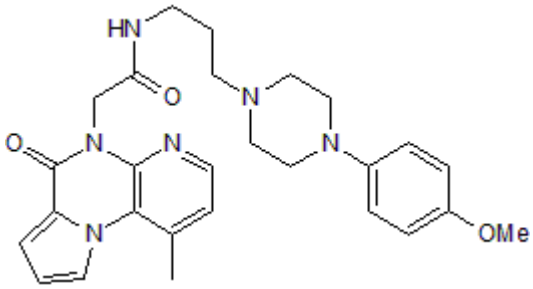
**Batch Molecular Weight:** 493.08

**Physical Appearance:** White solid

**Solubility:** DMSO to 20 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.38 (Chloroform:Methanol [9:1])

**HPLC:** Shows 98.2% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 65.77 | 6.64 | 17.04 |
| Found | 65.86 | 6.63 | 17.07 |

**Product Name: ML 190** **Catalog No.: 4866** **Batch No.: 1**

CAS Number: 1355244-02-8

IUPAC Name: *N*-[3-[4-(4-Methoxyphenyl)-1-piperazinyl]propyl]-1-methyl-6-oxopyrido[2,3-*e*]pyrrolo[1,2-*a*]pyrazine-5(6*H*)-acetamide

**Description:**

Selective κ opioid receptor (KOP) antagonist ($IC_{50}$ = 120 nM in a β-arrestin assay); displays >267-fold selectivity over μ and δ opioid receptors.

**Physical and Chemical Properties:**

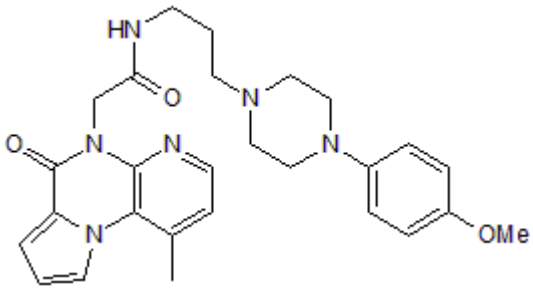
Batch Molecular Formula: $C_{27}H_{32}N_6O_3.¼H_2O$

Batch Molecular Weight: 493.08

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 20 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:**

**Hedrick** *et al* (2011) Antagonist for the kappa opioid receptor. Probe Reports from the NIH Molecular Libraries Pro. PMID: 22091479.

**Frankowski** *et al* (2012) Discovery of small molecule kappa opioid receptor agonist and antagonist chemotypes through a HTS and hit refinement strategy. ACS Chem.Neurosci. ***3*** (3) 221. PMID: 22737280.