

Certificate of Analysis

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: C₂₇H₃₂N₆O₃·¼H₂O

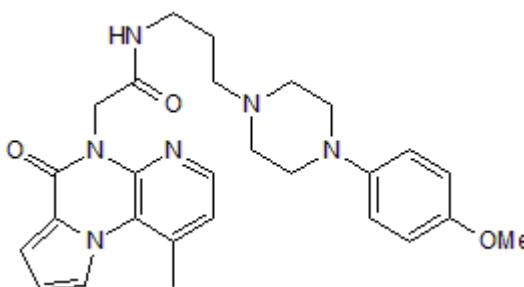
Batch Molecular Weight: 493.08

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

¹H 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

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

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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:

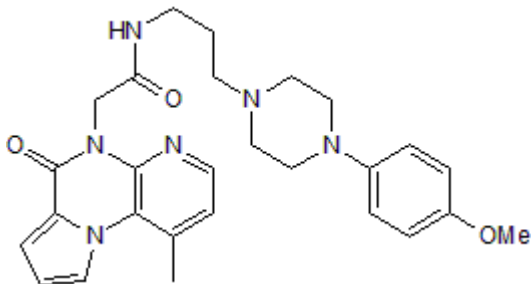
Batch Molecular Formula: $C_{27}H_{32}N_6O_3 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 493.08

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



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** 221. PMID: 22737280.

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.

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