

Certificate of Analysis

Product Name: ML 221

Catalog No.: 4748

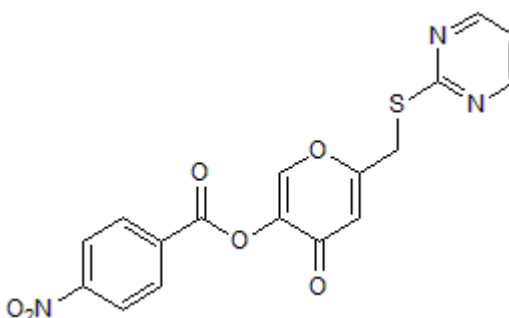
Batch No.: 1

CAS Number: 877636-42-5

IUPAC Name: 5-[(4-Nitrobenzoyl)oxy]-2-[(2-pyrimidinylthio)methyl]-4H-pyran-4-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₁N₃O₆S
Batch Molecular Weight: 385.35
Physical Appearance: Brown solid
Solubility: DMSO to 10 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.99	2.88	10.9
Found	52.67	3.02	10.9

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

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Description:

Apelin receptor (APJ) antagonist (IC₅₀ values are 0.70 and 1.75 μM in a cAMP assay and β-arrestin assay, respectively). Displays >37-fold selectivity over the closely related angiotensin II type 1 (AT₁) receptor. Exhibits no toxicity towards human hepatocytes at concentrations >50 μM.

Physical and Chemical Properties:

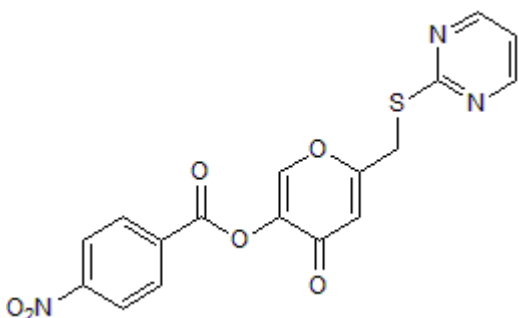
Batch Molecular Formula: C₁₇H₁₁N₃O₆S

Batch Molecular Weight: 385.35

Physical Appearance: Brown solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Maloney et al (2012) Discovery of 4-oxo-6-((pyrimidin-2-ylthio)methyl)-4H-pyran-3-yl 4-nitrobenzoate (ML221) as a functional antagonist of the apelin (APJ) receptor. *Bioorg.Med.Chem.Lett.* **22** 6656. PMID: 23010269.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 10 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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