

Product Name: ML 337

Catalog No.: 4982

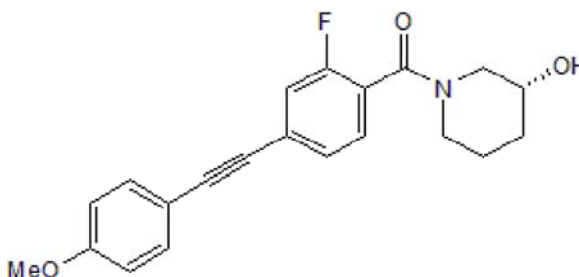
Batch No.: 1

CAS Number: 1443118-44-2

IUPAC Name: [2-Fluoro-4-[2-(4-methoxyphenyl)ethynyl]phenyl][(3R)-3-hydroxy-1-piperidiny]methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₀FNO₃
Batch Molecular Weight: 353.39
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
ethanol to 20 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.42 (Chloroform:Methanol [95:5])
HPLC: Shows 99.6% purity
Chiral HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = -28.8 (Concentration = 1, Solvent = Methanol)
Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	71.37	5.7	3.96
Found	71.33	5.65	4.01

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

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IUPAC Name: [2-Fluoro-4-[2-(4-methoxyphenyl)ethynyl]phenyl][(3*R*)-3-hydroxy-1-piperidinyl]methanone

Description:

Selective negative allosteric modulator of mGlu₃ (IC₅₀ = 593 nM). Displays no activity at mGlu₁, mGlu₂ or mGlu₄₋₈ at concentrations up to 30 μM. Brain penetrant.

Physical and Chemical Properties:

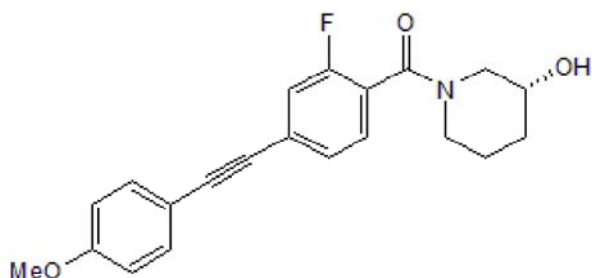
Batch Molecular Formula: C₂₁H₂₀FNO₃

Batch Molecular Weight: 353.39

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Wenthur *et al* (2013) Discovery of (*R*)-(2-fluoro-4-((4-methoxyphenyl)ethynyl)phenyl) (3-hydroxypiperidin-1-yl)methanone (ML337), an mGlu₃ selective and CNS penetrant negative allosteric modulator (NAM). *J.Med.Chem.* **56** 5208. PMID: 23718281.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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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