

**Product Name:** ML 337

**Catalog No.:** 4982

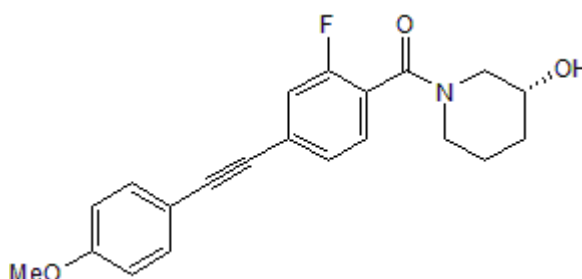
**Batch No.:** 1

**CAS Number:** 1443118-44-2

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>21</sub>H<sub>20</sub>FNO<sub>3</sub>  
**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<sub>f</sub> = 0.42 (Chloroform:Methanol [95:5])  
**HPLC:** Shows >99.6% purity  
**Chiral HPLC:** Shows >99.8% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -28.8 (Concentration = 1, Solvent = Methanol)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	71.37	5.7	3.96
Found	71.33	5.65	4.01

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**Description:**

Selective negative allosteric modulator of mGlu<sub>3</sub> (IC<sub>50</sub> = 593 nM). Displays no activity at mGlu<sub>1</sub>, mGlu<sub>2</sub> or mGlu<sub>4-8</sub> at concentrations up to 30 μM. Brain penetrant.

**Physical and Chemical Properties:**

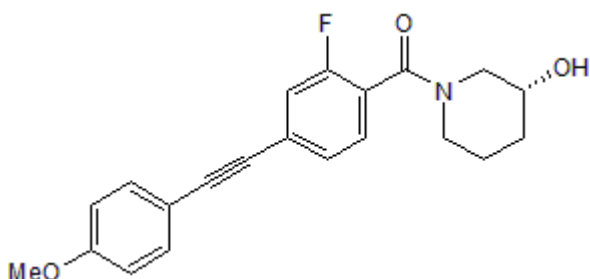
Batch Molecular Formula: C<sub>21</sub>H<sub>20</sub>FNO<sub>3</sub>

Batch Molecular Weight: 353.39

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**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.

**References:**

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

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