

## Certificate of Analysis

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**Product Name:** JNJ 63533054

**Catalog No.:** 5666

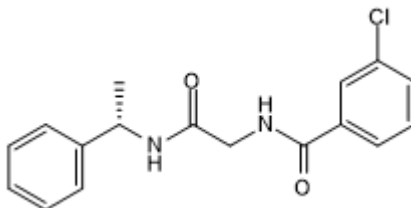
**Batch No.:** 1

CAS Number: 1802326-66-4

IUPAC Name: 3-Chloro-N-[2-oxo-2-[[[(1S)-1-phenylethyl]amino]ethyl]benzamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>17</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>2</sub>  
**Batch Molecular Weight:** 316.78  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 20 mM  
**Storage:** Store at RT  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**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> = -91 (Concentration = 1.04, Solvent = Ethanol)  
 Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.46	5.41	8.84
Found	64.28	5.34	8.76

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

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**Description:**

Potent and selective GPR139 agonist (EC<sub>50</sub> = 16 nM). Selective for GPR139 over a panel of GPCRs, ion channels and transporters, including GPR142. Brain and cell penetrant. Orally bioavailable.

**Physical and Chemical Properties:**

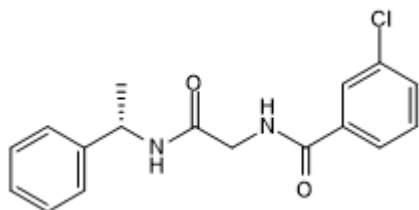
Batch Molecular Formula: C<sub>17</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>2</sub>

Batch Molecular Weight: 316.78

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at RT

**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:**

**Dvorak et al** (2015) Identification and SAR of glycine benzamides as potent agonists for the GPR139 receptor. ACS Med.Chem.Lett. **6** 1015. PMID: 26396690.

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