

**Product Name:** AF 64394

**Catalog No.:** 6931

**Batch No.:** 1

CAS Number: 1637300-25-4

IUPAC Name: *N*-[[4-Chloro-2-(1-methylethoxy)phenyl]methyl]-5-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>21</sub>H<sub>20</sub>ClN<sub>5</sub>O.<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O

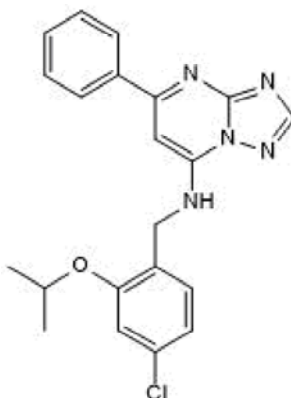
**Batch Molecular Weight:** 407.38

**Physical Appearance:** Off White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.3% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	61.91	5.32	17.19
Found	61.64	4.91	16.86

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

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**Description:**

Potent and selective GPR3 inverse agonist ( $pIC_{50} = 7.3$ ). Selective for GPR3 over GPR6 and GPR12 ( $pIC_{50}$  values are 5.1 and 4.9, respectively).

**Physical and Chemical Properties:**

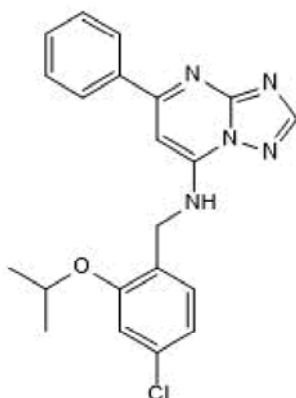
Batch Molecular Formula:  $C_{21}H_{20}ClN_5O \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 407.38

Physical Appearance: Off White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**Storage:** Store at  $-20^{\circ}C$

**Solubility & Usage Info:**

DMSO to 100 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  $45-60^{\circ}C$  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  $-20^{\circ}C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Godlewski et al (2015)** Mice lacking GPR3 receptors display late-onset obese phenotype due to impaired thermogenic function in brown adipose tissue. *Sci.Rep.* **5** 14953. PMID: 26455425.

**Jensen et al (2014)** The identification of GPR3 inverse agonist AF64394; the first small molecule inhibitor of GPR3 receptor function. *Bioorg.Med.Chem.Lett.* **24** 5195. PMID: 25442311 .

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