

## Certificate of Analysis

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**Product Name:** YM 298198 hydrochloride

**Catalog No.:** 2448

**Batch No.:** 1

CAS Number: 1216398-09-2

IUPAC Name: 6-Amino-*N*-cyclohexyl-*N*,3-dimethylthiazolo[3,2-*a*]benzimidazole-2-carboxamide hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>OS.HCl.H<sub>2</sub>O

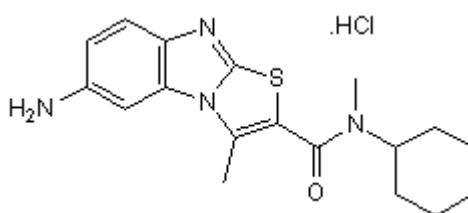
**Batch Molecular Weight:** 396.93

**Physical Appearance:** Cream solid

**Solubility:** water to 100 mM

**Storage:** Desiccate at +4°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.4 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows >99.1% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	54.47	6.35	14.11
Found	54.15	6.01	13.83

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**Description:**

Non-competitive antagonist with high affinity and selectivity for mGlu<sub>1</sub> receptors ( $K_i = 19$  nM); inactive at other mGlu receptor subtypes (mGlu<sub>2-7</sub>), ionotropic receptors and glutamate transporters ( $IC_{50} > 10$  μM). Inhibits glutamate-induced IP production more potently than CPCCOEt ( $IC_{50}$  values are 16 nM and 6.3 μM respectively), and is orally active in vivo, demonstrating an antinociceptive effect in hyperalgesic mice. Desmethyl derivative (Cat. No. 2447) also available.

**Physical and Chemical Properties:**

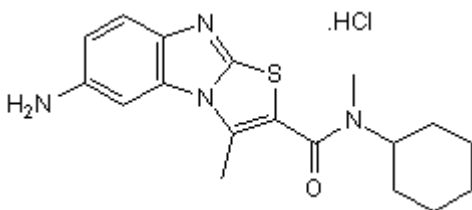
Batch Molecular Formula: C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>OS.HCl.H<sub>2</sub>O

Batch Molecular Weight: 396.93

Physical Appearance: Cream solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**Kohara et al** (2005) Radioligand binding properties and pharmacological characterization of 6-Amino-*N*-cyclohexyl-*N*,3-dimethyl-thiazolo [3,2-*a*]benzimidazole-2-carboxamide (YM-298198), a high-affinity, selective and noncompetitive antagonist of metabotropic glutamate receptor type 1. *J.Pharmacol.Exp.Ther.* **315** 163. PMID: 15976016.

**Emery et al** (2010) The protective signaling of metabotropic glutamate receptor 1 is mediated by sustained, β-arrestin-1-dependent ERK phosphorylation. *J.Biol.Chem.* **285** 26041. PMID: 20566651.

**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**

water 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°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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