

**Product Name:** MRS 3777 hemioxalate

**Catalog No.:** 2403

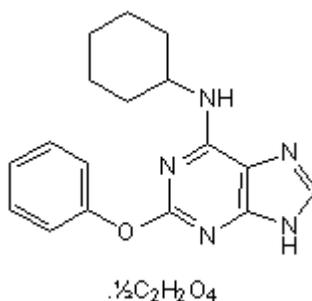
**Batch No.:** 1

CAS Number: 1186195-57-2

IUPAC Name: 2-Phenoxy-6-(cyclohexylamino)purine hemioxalate

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:**  $C_{17}H_{19}N_5O \cdot \frac{1}{2}C_4H_4O_4 \cdot \frac{1}{4}H_2O$   
**Batch Molecular Weight:** 358.89  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 50 mM  
**Storage:** Desiccate at RT  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:**  $R_f = 0.15$  (Chloroform:Methanol [95:5])  
**HPLC:** Shows 100% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	60.24	5.76	19.51
Found	60.37	5.63	19.61

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

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**Description:**

High affinity adenosine A<sub>3</sub> receptor antagonist (K<sub>i</sub> = 47 nM) that displays > 200-fold selectivity versus A<sub>1</sub>, A<sub>2A</sub> and A<sub>2B</sub> receptors.

**Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>17</sub>H<sub>19</sub>N<sub>5</sub>O.½C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>.¼H<sub>2</sub>O

Batch Molecular Weight: 358.89

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Perreira et al** (2005) "Reversine" and its 2-substituted adenine derivatives as potent and selective A<sub>3</sub> adenosine receptor antagonists. *J.Med.Chem.* **48** 4910. PMID: 16033270.

**Jacobson and Gao** (2006) Adenosine receptors as therapeutic targets. *Nat.Rev.Drug Discov.* **5** 247. PMID: 16518376.

**Moro et al** (2006) Progress in the pursuit of therapeutic adenosine receptor antagonists. *Med.Res.Rev.* **26** 131. PMID: 16380972.

**Storage:** Desiccate at RT

**Solubility & Usage Info:**

DMSO to 50 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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