

## Certificate of Analysis

**Product Name:** AP 18

**Catalog No.:** 3296

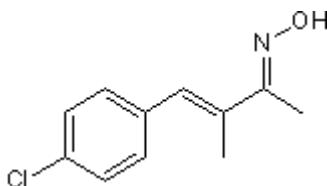
**Batch No.:** 2

CAS Number: 55224-94-7

IUPAC Name: 4-(4-Chlorophenyl)-3-methyl-3-buten-2-one oxime

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>11</sub>H<sub>12</sub>ClNO  
**Batch Molecular Weight:** 209.67  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.19 (Ethyl acetate:Petroleum ether [95:5])  
**HPLC:** Shows 99.8% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	63.01	5.77	6.68
Found	62.97	5.76	6.67

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

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**Description:**

Reversible TRPA1 channel blocker (IC<sub>50</sub> values are 3.1 and 4.5 μM at human and mouse TRPA1 respectively). Blocks cinnamyldehydro-induced but not capsaicin-induced nociception and reverses mechanical hyperalgesia in vivo. Also blocks TRPA1 pore dilation (IC<sub>50</sub> = 10.3 μM for the inhibition of Yo-Pro uptake).

**Physical and Chemical Properties:**

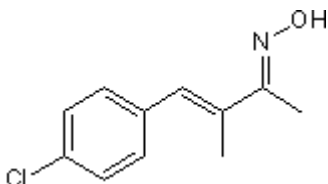
Batch Molecular Formula: C<sub>11</sub>H<sub>12</sub>ClNO

Batch Molecular Weight: 209.67

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Petrus et al** (2007) A role of TRPA1 in mechanical hyperalgesia is revealed by pharmacological inhibition. *Mol.Pain* **3** 40. PMID: 18086313.

**Chen et al** (2009) Pore dilation occurs in TRPA1 but not in TRPM8 channels. *Mol.Pain* **5** 3. PMID: 19159452.

**Taylor-Clark et al** (2009) Nitrooleic acid, an endogenous product of nitrative stress, activates nociceptive sensory nerves via the direct activation of TRPA1. *Mol.Pharmacol.* **75** 820. PMID: 19171673.

**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol 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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