# **Certificate of Analysis**

## www.tocris.com

Print Date: Feb 27th 2023

### Product Name: ML 162

OCR ]

Catalog No.: 7821 Batch No.: 1

CAS Number: IUPAC Name:

a biotechne

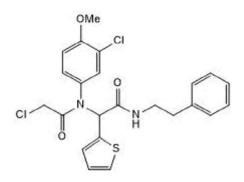
1035072-16-2

2-[(Chloroacetyl)(3-chloro-4-methoxyphenyl)amino]-N-(2-phenylethyl)-2-thien-2-ylacetamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C<sub>23</sub>H<sub>22</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub>S 477.41 Off-white solid DMSO to 100 mM ethanol to 20 mM Store at -20°C

Storage: Batch Molecular Structure:



### 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: Shows 99.4% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 57.86 4.65 5.87 Found 57.74 4.55 5.7

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

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# TOCRIS a biotechne brand

## **Product Information**

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#### Product Name: ML 162

CAS Number: 1035072-16-2

2-[(Chloroacetyl)(3-chloro-4-methoxyphenyl)amino]-N-(2-phenylethyl)-2-thien-2-ylacetamide

#### **Description:**

**IUPAC Name:** 

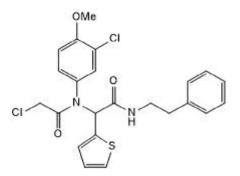
ML 162 is a covalent glutathione peroxidase 4 (GPX4) inhibitor. It induces ferroptosis in vivo. It is selectively lethal to mutant RAS oncogene-expressing cell lines ( $IC_{50}$  = 25 and 578 nM for HRAS<sup>G12V</sup>-expressing and wild-type BJ fibroblasts, respectively).

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>23</sub>H<sub>22</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub>S Batch Molecular Weight: 477.41 Physical Appearance: Off-white solid

#### Minimum Purity: ≥98%

#### **Batch Molecular Structure:**



#### **Storage:** Store at -20°C

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  $45-60^{\circ}C$  water bath).

Catalog No.: 7821

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:**

Karaj et al (2022) Tunable cysteine-targeting electrophilic heteroaromatic warheads induce ferroptosis. J.Med.Chem. 65 11788. PMID: 35984756.

Luo et al (2022) Intracellular delivery of glutathione peroxidase degrader induces ferroptosis in vivo. Angew.Chem.Int.Ed.Engl. 39 e202206277. PMID: 35924720.

Weïwer et al (2012) Development of small-molecule probes that selectively kill cells induced to express mutant RAS. Bioorg.Med.Chem.Lett. 22 1822. PMID: 22297109.

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