TOCRIS
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Print Date: Jan 13th 2016

Certificate of Analysis

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Product Name: **ML 239** **Catalog No.: 4829** **Batch No.: 2**

CAS Number: 1378872-36-6

IUPAC Name: 2-(2,4,6-Trichlorophenoxy)acetic acid (2*E*)-2-(1*H*-pyrrol-2-ylmethylene)hydrazide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_{10}Cl_3N_3O_2$

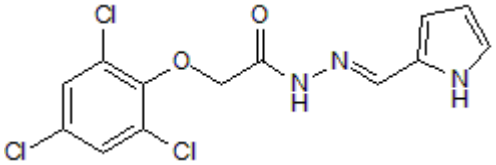
Batch Molecular Weight: 346.6

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Dichloromethane)

HPLC: Shows 98.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	45.05	2.91	12.12
Found	45.26	2.87	11.87

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Description:

Breast cancer stem cell inhibitor (IC_{50} = 1.16 µM). Exhibits 24-fold selectivity for breast cancer stem cells over normal mammary epithelial cells. Also cytotoxic towards MDA-MB-231 breast cancer cells in vitro.

Physical and Chemical Properties:

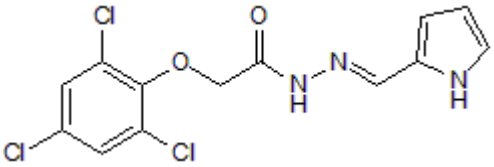
Batch Molecular Formula: $C_{13}H_{10}Cl_3N_3O_2$

Batch Molecular Weight: 346.6

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

References:

Carmody *et al* (2012) Phenotypic high-throughput screening elucidates target pathway in breast cancer stem cell-like cells. J.Biol.Chem. ***17*** 1204. PMID: 22941295.

Germain *et al* (2012) Identification of a selective small molecule inhibitor of breast cancer stem cells. Bioorg.Med.Chem.Lett. ***22*** 3571. PMID: 22503247.

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