

Product Name: TH 588

Catalog No.: 5334

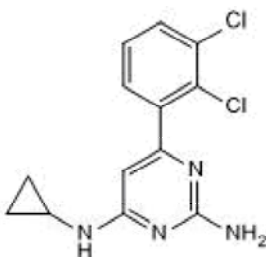
Batch No.: 1

CAS Number: 1609960-31-7

IUPAC Name: *N*⁴-Cyclopropyl-6-(2,3-dichlorophenyl)-2,4-pyrimidinediamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₁₂Cl₂N₄
Batch Molecular Weight: 295.17
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.9	4.1	18.98
Found	52.91	4.03	18.82

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

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IUPAC Name: *N*⁴-Cyclopropyl-6-(2,3-dichlorophenyl)-2,4-pyrimidinediamine

Description:

Potent MTH1 inhibitor (IC₅₀ = 5 nM). Induces oxidative DNA damage and reduces survival in cancer cells. Inhibits growth of breast and colorectal cancer xenografts in mice.

Physical and Chemical Properties:

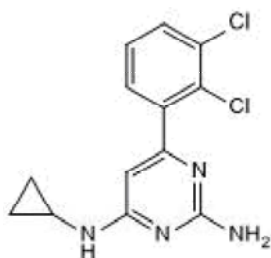
Batch Molecular Formula: C₁₃H₁₂Cl₂N₄

Batch Molecular Weight: 295.17

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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.

Licensing Information:

Sold under license from Thomas Helleday's Foundation for Medical Research and Oxcia AB.

References:

Gad *et al* (2014) MTH1 inhibition eradicates cancer by preventing sanitation of the dNTP pool. *Nature* **508** 215. PMID: 24695224.

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