

**Product Name:** TH 5487

**Catalog No.:** 6749

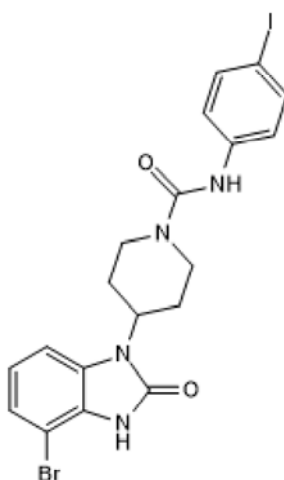
**Batch No.:** 1

CAS Number: 2304947-71-3

IUPAC Name: 4-(4-Bromo-2,3-dihydro-2-oxo-1*H*-benzimidazol-1-yl)-*N*-(4-iodophenyl)-1-piperidinecarboxamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>19</sub>H<sub>18</sub>BrIN<sub>4</sub>O<sub>2</sub>  
**Batch Molecular Weight:** 541.18  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.6 (Ethyl acetate)  
**HPLC:** Shows 98.9% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	42.17	3.35	10.35
Found	42.22	3.31	10.34

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

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**Description:**

Selective 8-oxoguanine DNA glycosylase 1 (OGG1) inhibitor (IC<sub>50</sub> = 342 nM). Selective for OGG1 over other base excision repair enzymes. Inhibits OGG1 binding to 8-oxoG in DNA and suppresses proinflammatory gene expression in TNF- $\alpha$  stimulated lung epithelial cells in vitro. Also inhibits proinflammatory gene expression and neutrophil recruitment in TNF- $\alpha$ -challenged mouse lungs in vivo.

**Physical and Chemical Properties:**

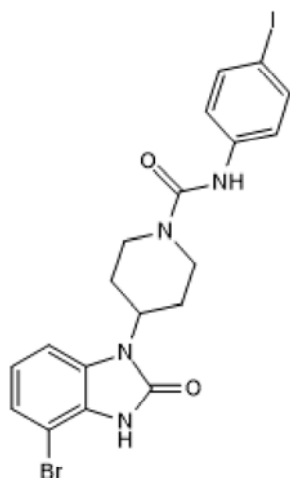
Batch Molecular Formula: C<sub>19</sub>H<sub>18</sub>BrIN<sub>4</sub>O<sub>2</sub>

Batch Molecular Weight: 541.18

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°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

**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:**

**Visnes *et al*** (2018) Small-molecule inhibitor of OGG1 suppresses proinflammatory gene expression and inflammation. *Science* **362** 834. PMID: 30442810.

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