

Product Name: BAY 87-2243

Catalog No.: 6980

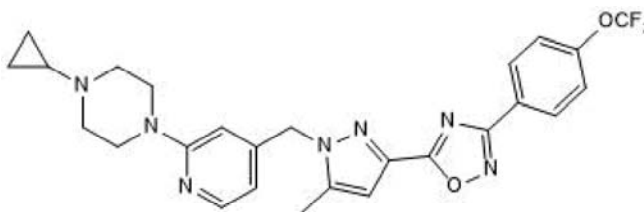
Batch No.: 1

CAS Number: 1227158-85-1

IUPAC Name: 1-Cyclopropyl-4-[[4-[[5-methyl-3-[3-[4-(trifluoromethoxy)phenyl]-1,2,4-oxadiazol-5-yl]-1*H*-pyrazol-1-yl]methyl]-2-pyridinyl]piperazine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₂₆F₃N₇O₂
Batch Molecular Weight: 525.54
Physical Appearance: White solid
Solubility: DMSO to 50 mM
 ethanol to 20 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.42	4.99	18.66
Found	59.63	5.05	18.4

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Description:

Mitochondrial complex I inhibitor. Exhibits no effect on mitochondrial complex III. Induces mitochondrial permeability transition pore (mPTP) opening, stimulates autophagosome formation and mitophagy, and increases ROS levels. Activates necroptotic and ferroptotic cell death. Also inhibits hypoxia-induced gene activation. Induces cell death in melanoma cell lines in vitro and exhibits antitumor activity in a mouse NSCLC xenograft model in vivo.

Physical and Chemical Properties:

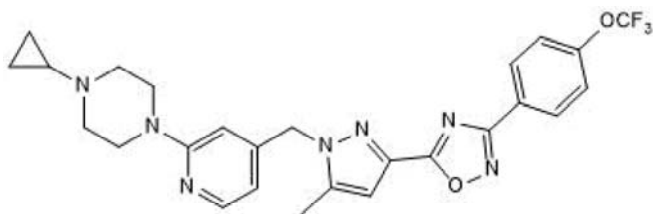
Batch Molecular Formula: C₂₆H₂₆F₃N₇O₂

Batch Molecular Weight: 525.54

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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°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:

Basit et al (2017) Mitochondrial complex I inhibition triggers a mitophagy-dependent ROS increase leading to necroptosis and ferroptosis in melanoma cells. *Cell Death Dis.* **8** e2716. PMID: 28358377.

Ellinghaus et al (2013) BAY 87-2243, a highly potent and selective inhibitor of hypoxia-induced gene activation has antitumor activities by inhibition of mitochondrial complex I. *Cancer Med.* **2** 611. PMID: 24403227.

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