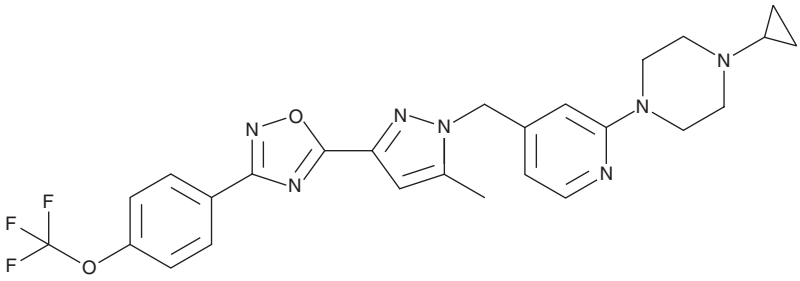
PRODUCT INFORMATION

BAY 87-2243

Item No. 28626

CAS Registry No.:	1227158-85-1
Formal Name:	1-cyclopropyl-4-[4-[[5-methyl-3-[3-[4-(trifluoromethoxy)phenyl]-1,2,4-oxadiazol-5-yl]-1H-pyrazol-1-yl]methyl]-2-pyridinyl]-piperazine
MF:	$C_{26}H_{26}F_3N_7O_2$
FW:	525.5
Purity:	≥98%
UV/Vis.:	λ_{max}: 250 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

BAY 87-2243 is supplied as a crystalline solid. A stock solution may be made by dissolving the BAY 87-2243 in the solvent of choice, which should be purged with an inert gas. BAY 87-2243 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of BAY 87-2243 ethanol and DMSO is approximately 5 mg/ml and approximately 10 mg/ml in DMF.

BAY 87-2243 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, BAY 87-2243 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. BAY 87-2243 has a solubility of approximately 0.3 mg/ml in a 1:2 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

BAY 87-2243 is an inhibitor of mitochondrial complex I, also known as NADH:ubiquinone oxidoreductase, and an inducer of ferroptosis.[1,2] It decreases ATP-dependent luciferase reporter activity and ATP levels in H1299luc cells, effects that can be reversed by addition of the mitochondrial complex II substrate succinate or expression of the *S. cerevisiae* complex I ortholog Ndi1 NADH dehydrogenase.[1] BAY 87-2243 induces production of reactive oxygen species (ROS), increases α-tocopherol-sensitive lipid peroxidation, and decreases glutathione (GSH) levels in SK-MEL-28 and G361 melanoma cells, effects that can be partially reversed by the ferroptosis inhibitor ferrostatin-1 (Item No. 17729) and overexpression of GPX4 or potentiated by GPX4 knockdown.[2] *In vivo*, BAY 87-2243 (0.5-4 mg/kg) reduces tumor weight, hypoxia-inducible factor-1α (HIF-1α) levels, and HIF-1α target gene expression in an H460 mouse xenograft model.[1] It also reduces tumor growth in the MEXF 276 and MEXF 1732 melanoma patient-derived xenograft (PDX) mouse models.[3]

References

1. Ellinghaus, P., Heisler, I., Unterschemmann, K., *et al.* 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(5)**, 611-624 (2013).
2. Basit, F., van Oppen, L.M., Schöckel, L., *et al.* Mitochondrial complex I inhibition triggers a mitophagy-dependent ROS increase leading to necroptosis and ferroptosis in melanoma cells. *Cell Death Dis.* **8(3)**, e2716 (2017).
3. Schöckel, L., Glasauer, A., Basit, F., *et al.* Targeting mitochondrial complex I using BAY 87-2243 reduces melanoma tumor growth. *Cancer Metab.* **3:11** (2015).

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