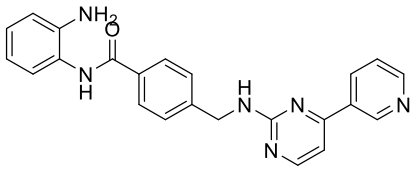
Product data sheet

MedKoo Cat#: 201933 Name: Mocetinostat (MGCD-0103) CAS#: 726169-73-9 (free base) Chemical Formula: $C_{23}H_{20}N_6O$ Exact Mass: 396.16986 Molecular Weight: 396.44	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

Mocetinostat, also known as MGCD-0103, is a rationally designed, orally available, Class 1-selective, small molecule, 2-aminobenzamide HDAC inhibitor with potential antineoplastic activity. Mocetinostat binds to and inhibits Class 1 isoforms of HDAC, specifically HDAC 1, 2 and 3, which may result in epigenetic changes in tumor cells and so tumor cell death; although the exact mechanism has yet to be defined, tumor cell death may occur through the induction of apoptosis, differentiation, cell cycle arrest, inhibition of DNA repair, upregulation of tumor suppressors, down regulation of growth factors, oxidative stress, and autophagy, among others.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	49.67	125.29
DMF	25.0	63.06
DMF:PBS (pH 7.2) (1:1)	0.5	1.26

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.52 mL	12.61 mL	25.22 mL
5 mM	0.50 mL	2.52 mL	5.04 mL
10 mM	0.25 mL	1.26 mL	2.52 mL
50 mM	0.05 mL	0.25 mL	0.50 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Shan W, Jiang Y, Yu H, Huang Q, Liu L, Guo X, Li L, Mi Q, Zhang K, Yang Z. HDAC2 overexpression correlates with aggressive clinicopathological features and DNA-damage response pathway of breast cancer. Am J Cancer Res. 2017 May 1;7(5):1213-1226. PMID: 28560068; PMCID: PMC5446485.
2. Zhang Q, Sun M, Zhou S, Guo B. Class I HDAC inhibitor mocetinostat induces apoptosis by activation of miR-31 expression and suppression of E2F6. Cell Death Discov. 2016 Jun 6;2:16036. doi: 10.1038/cddiscovery.2016.36. PMID: 27551526; PMCID: PMC4979414.

In vivo study

Product data sheet

1. Lee HA, Lee E, Do GY, Moon EK, Quan FS, Kim I. Histone deacetylase inhibitor MGCD0103 protects the pancreas from streptozotocin-induced oxidative stress and β-cell death. Biomed Pharmacother. 2019 Jan;109:921-929. doi: 10.1016/j.biopha.2018.10.163. Epub 2018 Nov 5. PMID: 30551546.
2. Huang HJ, Huang HY, Hsieh-Li HM. MGCD0103, a selective histone deacetylase inhibitor, coameliorates oligomeric Aβ25-35 -induced anxiety and cognitive deficits in a mouse model. CNS Neurosci Ther. 2019 Feb;25(2):175-186. doi: 10.1111/cns.13029. Epub 2018 Jul 5. PMID: 29978554; PMCID: PMC6488906.

7. Bioactivity

Biological target:

Mocetinostat (MGCD0103) is an isotype-selective HDAC (Class I/IV) inhibitor with IC50s of 0.15, 0.29, 1.66 and 0.59 μM for HDAC1, HDAC2, HDAC3 and HDAC11, respectively.

In vitro activity

Treatment of SUM149 and HCC1937 cells with mocetinostat increased the acetylation of H3 lysine 9 (H3K9) and H3K27 in a dose-dependent manner (Figure 4A). Mocetinostat suppressed the proliferation of SUM149 and HCC1937 in MTT assays, with an IC50 value of 0.6 and 2.6 μM, respectively. In the presence of 0.5 μM mocetinostat, the colony formation was reduced by approximately 80% ($P < 0.001$) compared with the control cells (Figure 4B). To examine the effect of mocetinostat on cell cycle progression and apoptosis, this study performed flow cytometry of DNA content in SUM149 and HCC1937 cells. As shown in Figure 4C and 4D, mocetinostat treatment led to a substantial increase in G2/M phase and decreases in G1 and S phase cells, suggesting that it hinders cell-cycle progression, particularly in SUM149 cells. Mocetinostat also potently induced apoptosis in SUM149 and HCC1937 cells, as shown by Annexin V assay and western blot analysis of cleaved caspase-3 (Figure 4A and Supplementary Figure 5).

Reference: Am J Cancer Res. 2017; 7(5): 1213–1226. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5446485/

In vivo activity

MGCD (MGCD0103) treatment significantly inhibited the increase in blood glucose level (Fig. 1A), deformation of pancreatic islets, and infiltration of macrophages (Fig. 1C) in rats injected with a low dose (40 mg/kg) of STZ. In addition, MGCD infusion elevated the expression of SODs in the pancreas, and TEMPOL, an SOD mimetic, restored STZ-induced cell death (Fig. 5G) and activation of caspase-3 (Fig. 5H). These results indicate that MGCD protects the pancreas from the oxidative stress induced by the low dose of STZ through the expression of SODs.

Reference: Biomed Pharmacother. 2019 Jan;109:921-929. https://pubmed.ncbi.nlm.nih.gov/30551546/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.