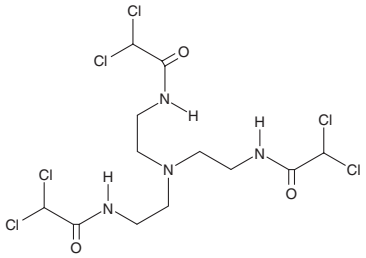
PRODUCT INFORMATION

CAY10703

Item No. 18911

CAS Registry No.:	1841421-67-7
Formal Name:	N,N',N''-(nitrilotris(ethane-2,1-diyl))*tris*(2,2-dichloroacetamide)
MF:	$C_{12}H_{18}Cl_6N_4O_3$
FW:	479.0
Purity:	≥95%
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

CAY10703 is supplied as a crystalline solid. A stock solution may be made by dissolving the CAY10703 in the solvent of choice, which should be purged with an inert gas. CAY10703 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of CAY10703 in ethanol is approximately 20 mg/ml and approximately 30 mg/ml in DMSO and DMF.

CAY10703 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, CAY10703 should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. CAY10703 has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Dichloroacetate (DCA) is an inhibitor of all pyruvate dehydrogenase kinase (PDHK) isoforms, which are enzymes that phosphorylate and inhibit PDH in mitochondria.[1,2] Inhibition of PDHK shifts cell metabolism from glycolysis to mitochondrial glucose oxidation, an effect that has relevance to cancer, type 2 diabetes, and other diseases.[2,3] CAY10703 is a DCA trimer that is at least 10-fold more cytotoxic against leukemia cell lines than DCA.[4] It is approximately 3-fold less cytotoxic than DCA against peripheral blood mononuclear cells from healthy blood donors. CAY10703 significantly reduces both basal and maximal respiration in leukemia cells.[4] It is stable *in vivo* after subcutaneous inoculation, remaining in circulation for more than five hours after injection.[4]

References

1. Whitehouse, S., Cooper, R.H., and Randle, P.J. Mechanism of activation of pyruvate dehydrogenase by dichloroacetate and other halogenated carboxylic acids. *Biochem. J.* **141(3)**, 761-774 (1974).
2. Rodrigues, A.S., Correia, M., Gomes, A., *et al*. Dichloroacetate, the pyruvate dehydrogenase complex and the modulation of mESC pluripotency. *PLoS One* **10(7)**, July 2015 (2015).
3. Ruggieri, V., Agriesti, F., Scrima, R., *et al*. Dichloroacetate, a selective mitochondria-targeting drug for oral squamous cell carcinoma: A metabolic perspective of treatment. *Oncotarget* **6(2)**, 1217-1230 (2015).
4. Trapella, C., Voltan, R., Melloni, E., *et al*. Design, synthesis, and biological characterization of novel mitochondria targeted dichloroacetate-loaded compounds with antileukemic activity. *J. Med. Chem.* **59(1)**, 147-156 (2016).

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