

CAY10603

## Chemical Properties

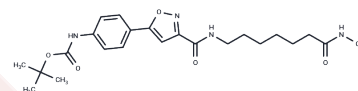
CAS No. : 1045792-66-2

Formula: C<sub>22</sub>H<sub>30</sub>N<sub>4</sub>O<sub>6</sub>

Molecular Weight: 446.5

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



## Biological Description

Description	CAY10603 (BML-281) is a potent and selective HDAC6 inhibitor.
Targets(IC50)	HDAC
In vivo	CAY10603 exhibits effective anti-proliferative activity against pancreatic cancer cell lines by inhibiting HDAC6, with an IC <sub>50</sub> of less than 1 μM.
Kinase Assay	HDAC Inhibition Assays: Purified HDACs are incubated with 1 mM carboxyfluorescein (FAM)-labeled acetylated peptide substrate and test compound for 17 h at 25 °C in HDAC assay buffer containing 100 mM HEPES (pH 7.5), 25 mM KCl, 0.1% BSA, and 0.01% Triton X-100. Reactions are terminated by the addition of buffer containing 0.078% SDS for a final SDS concentration of 0.05%. Substrate and product are separated electrophoretically using a Caliper LabChip 3000 system with blue laser excitation and green fluorescence detection (CCD2). The fluorescence intensity in the substrate and product peaks is determined using the Well Analyzer software on the Caliper system. The reactions are performed in duplicate for each sample. IC <sub>50</sub> values are automatically calculated using the IDBS XLFit version 4.2.1 plug-in for Microsoft Excel and the XLFit 4-Parameter Logistic Model: $((A+((B-A)/(1+((C/x)^D)))))$ , in which x is compound concentration, A and B are respectively the estimated minimum and maximum of percent inhibition, C is the inflection point, and D is the Hill slope of the sigmoidal curve. The standard errors of the IC <sub>50</sub> values are automatically calculated using the IDBS XLFit version 4.2.1 plug-in for Microsoft Excel and the formula $xf4\_FitResultStdError$ .
Cell Research	The pancreatic cancer cell lines BxPc-3, HupT3, Mia Paca-2, Panc 04.03, and SU 86.86 are grown in medium (DMEM or RPMI) containing 10% fetal calf serum and l-glutamine. Pancreatic cancer cells are plated out in duplicate into 6 wells of a 96-well microtiter plate. Four hours post plating, individual wells are treated with diluent (DMSO) or varying concentrations of SAHA or the indicated HDACIs from a concentration of 1 nM to 50 mM. Cytotoxicity is measured at time "0", and 72 h post treatment using the colorimetric MTT assay according to the manufacturer's suggestions. The IC <sub>50</sub> values are calculated using XLfit.(Only for Reference)

## Solubility Information

## A DRUG SCREENING EXPERT

Solubility	H2O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: 5 mg/mL (11.2 mM), Heating is recommended. DMSO: 145 mg/mL (324.75 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: < 10 mg/mL (22.4 mM), Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 10 mg/mL (22.4 mM), Solution. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

### Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.2396 mL	11.1982 mL	22.3964 mL
5 mM	0.4479 mL	2.2396 mL	4.4793 mL
10 mM	0.224 mL	1.1198 mL	2.2396 mL
50 mM	0.0448 mL	0.224 mL	0.4479 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

### Reference

Kozikowski AP, et al. J Med Chem. 2008, 51(15), 4370-4373.

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