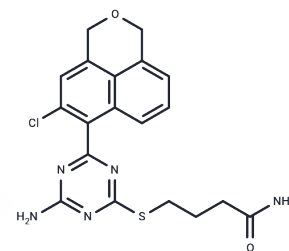


CH5138303

## Chemical Properties

CAS No. : 959763-06-5  
 Formula: C<sub>19</sub>H<sub>18</sub>ClN<sub>5</sub>O<sub>2</sub>S  
 Molecular Weight: 415.9  
 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	CH5138303 is an orally available Hsp90 inhibitor with Kd of 0.48 nM.
Targets(IC50)	HSP
In vitro	CH5138303 shows high affinity to Hsp90 $\alpha$ and potent cell growth inhibitory activity against an HCT116 colorectal cancer cell line and an NCI-N87 gastric cancer cell line with IC <sub>50</sub> of 98 nM and 66 nM, respectively. [1] Besides, CH5138303 also demonstrates liver microsomal stability. [1]
In vivo	CH5138303 (50 mg/kg p.o.) displays high oral bioavailability in mice and produces potent antitumor efficacy in a human NCI-N87 gastric cancer xenograft model.[1]
Kinase Assay	Surface plasmon resonance direct binding assay for Hsp90 $\alpha$ : Measurements are performed on a Biacore2000 at a flow rate of 30 $\mu$ L/min, 25 °C in 50 mM Tris-based saline, pH 7.6, 0.005% Tween20 and 1% DMSO. Biotinylated N-terminal Hsp90 $\alpha$ (9-236) is coupled on a streptavidin-coated surface of a sensorchip to a density of ca. 2000 RU.
Cell Research	HCT116 cell line and NCI-N87 cell line are cultured according to the supplier's instructions. Cells suspended in a medium are added to solutions containing various concentrations of the test substance, and the cells are cultured at 37 °C in 5% CO <sub>2</sub> . Four days later, Cell Counting Kit-8 solution is added and absorbance at 450 nm is measured with Microplate-Reader iMark. Antiproliferative activity is calculated by the formula $(1 - T/C) \times 100$ (%), where T represents the absorbance of drug-treated cells and C that of untreated control cells at 450 nm. The 50% inhibition concentration (IC <sub>50</sub> ) values are calculated using Microsoft Excel 2007.(Only for Reference)

## Solubility Information

Solubility	Ethanol: <1 mg/mL, H <sub>2</sub> O: <1 mg/mL, DMSO: 77 mg/mL (185.14 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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### Preparing Stock Solutions

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	1mg	5mg	10mg
1 mM	2.4044 mL	12.0221 mL	24.0442 mL
5 mM	0.4809 mL	2.4044 mL	4.8088 mL
10 mM	0.2404 mL	1.2022 mL	2.4044 mL
50 mM	0.0481 mL	0.2404 mL	0.4809 mL

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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

Suda A, et al. Bioorg Med Chem. 2014, 22(2), 892-905.

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