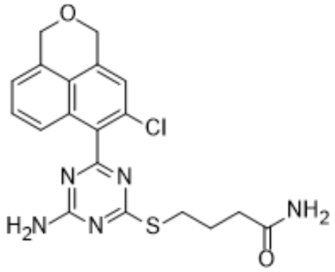
CH5138303

Cat. No.:	HY-100555
CAS No.:	959763-06-5
Molecular Formula:	$C_{19}H_{18}ClN_5O_2S$
Molecular Weight:	415.9
Target:	HSP
Pathway:	Cell Cycle/DNA Damage; Metabolic Enzyme/Protease
Storage:	4°C, protect from light * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



BIOLOGICAL ACTIVITY

Description	CH5138303 is a potent and orally active Hsp90 inhibitor. CH5138303 shows high binding affinity for N-terminal Hsp90α, with K_d of 0.52 nM. CH5138303 shows potent anti-proliferative activity against human cancer cell lines (HCT116 and NCI-N87), with IC_{50} values of 0.098 and 0.066 μM, respectively. CH5138303 shows high oral bioavailability in mice (F=44.0%). CH5138303 shows potent antitumor efficacy in a human NCI-N87 gastric cancer xenograft model[1][2].
IC_{50} & Target	HSP90α 0.52 nM (Kd)
In Vitro	When used in combination with FLC, CH5138303 shows antifungal activitiy against azole-resistant C. albicans, with a FICI (fractional inhibitory concentration index) of 0.500[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	CH5138303 (SCID mice bearing NCI-N87 cells, 0-50 mg/kg, Orally, once daily for 11 days) shows potent antitumor efficacy with TGI (tumor growth inhibition) of 136% and a median effective dose (ED_{50}) of 3.9 mg/kg without significant loss of body weight[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Atsushi Suda, et al. Design and synthesis of 2-amino-6-(1H,3H-benzo[de]isochromen-6-yl)-1,3,5-triazines as novel Hsp90 inhibitors. Bioorganic & Medicinal Chemistry. 15 January 2014;22(2):892-905.

[2]. Yuan R, et al. Effects of Hsp90 Inhibitor Ganetespib on Inhibition of Azole-Resistant Candida albicans. Front Microbiol. 2021 May 20;12:680382.

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