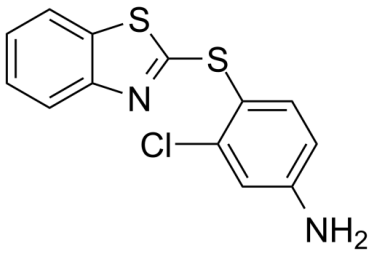
Data Sheet

Product Name:	KRAS inhibitor-9
Cat. No.:	CS-0139330
CAS No.:	300809-71-6
Molecular Formula:	$C_{13}H_9ClN_2S_2$
Molecular Weight:	292.81
Target:	Apoptosis; Ras
Pathway:	Apoptosis; GPCR/G Protein
Solubility:	DMSO : 250 mg/mL (853.80 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

KRAS inhibitor-9, a potent **KRAS** inhibitor ($\mathbf{K_d}$=92 μM), blocks the formation of GTP-KRAS and downstream activation of KRAS. KRAS inhibitor-9 binds to KRAS G12D, KRAS G12C and KRAS Q61H protein with a moderate binding affinity. KRAS inhibitor-9 causes G2/M cell cycle arrest and induces **apoptosis**. KRAS inhibitor-9 selectively inhibits the proliferation of NSCLC cells with KRAS mutation but not normal lung cells[1]. **In Vitro:** KRAS inhibitor-9 bound to KRASG12D, KRAS G12C and KRAS Q61H protein with a moderate binding affinity of -5.38, -5.41, and -3.97 kcal/mol, respectively[1].

KRAS inhibitor-9 (0-100 μM) shows strong inhibition selectivity in NSCLC cells with IC_{50}s ranging from 39.56 to 66.02 μM for H2122, H358 and H460 cells (at 72 hours)[1].

KRAS inhibitor-9 (0-100 μM; 24 hours) blocks GTP-KRAS formation in H2122, H358 and H460 cells[1].

KRAS inhibitor-9 (25-100 μM; 48 hours) inhibits the activation of KRAS downstream signaling pathway[1].

KRAS inhibitor-9 (0-100 μM; 24-72 hours) induces cell cycle arrest and apoptosis in NSCLC[1].

References:

[1]. Xie C, et al. Identification of a New Potent Inhibitor Targeting KRAS in Non-small Cell Lung Cancer Cells. Front Pharmacol. 2017;8:823. Published 2017 Nov 14.

CAIndexNames:

Benzenamine, 4-(2-benzothiazolylthio)-3-chloro-

SMILES:

NC1=CC=C(SC2=NC3=CC=CC=C3S2)C(Cl)=C1

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA