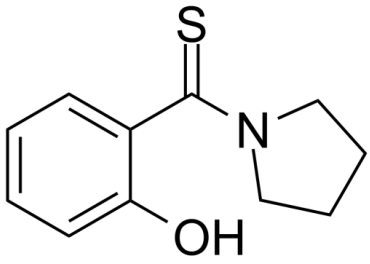
Data Sheet

Product Name:	K-Ras-IN-1
Cat. No.:	CS-4934
CAS No.:	84783-01-7
Molecular Formula:	C11H13NOS
Molecular Weight:	207.29
Target:	Ras
Pathway:	GPCR/G Protein
Solubility:	DMSO : ≥ 28 mg/mL (135.08 mM)



BIOLOGICAL ACTIVITY:

K-Ras-IN-1 is a K-Ras inhibitor, by binding to K-Ras in a hydrophobic pocket that is occupied by Tyr-71 in the apo-Ras crystal structure.(the detailed information refer to the reference)

References:

[1]. Hocker HJ, et al. LIBSA--a method for the determination of ligand-binding preference to allosteric sites on receptor ensembles. J Chem Inf Model. 2014 Feb 24;54(2):530-538.

[2]. Sun Q, et al. Discovery of small molecules that bind to K-Ras and inhibit Sos-mediated activation. Angew Chem Int Ed Engl. 2012 Jun 18;51(25):6140-6143

CAIndexNames:

Methanethione, (2-hydroxyphenyl)-1-pyrrolidinyl-

SMILES:

S=C(C1=CC=CC=C1O)N2CCCC2

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